FURTHER DEVELOPMENTS OF A FINITE VOLUME BASED ALE INTERFACE TRACKING METHOD

HEBA ALKAFRI[1] and HOLGER MARSCHALL[1]

[1]Department of Mathematics, Computational Multiphase Flow, Technical University of Darmstadt, Germany; heba.alkafri@tu-darmstadt.de & holger.marschall@tu-darmstadt.de

Keywords: *Multiphase flow, Finite volume method, ALE Interface tracking, Dirichlet-Neumann coupling, FOAM-extend C++.*

Various enhancements for an Arbitrary Lagrangian-Eulerian (ALE) Interface-Tracking method are presented for the simulation of two-phase flow of Newtonian incompressible fluids separated by sharp capillary interfaces. The methodology is based on the work of Tuković and Jasak [1]. The two-phase Navier-Stokes equations in two-field formulation are solved in coupled manner using collocated finite volume method (FVM) on two unstructured moving meshes of general topology. To this end, in order to consistently enforce the jump and transmission conditions at the fluid interface, we have developed a partitioned coupling approach through an iterative Dirichlet-Neumann algorithm. For a stable and convergent procedure, coupled boundary conditions are devised deploying the finite area method (FAM) provided in FOAM-extend. Mesh-skewness errors resulting from significant interface deformation are corrected for in a second-order fashion. Interpolation between interfacial boundary patches is accomplished by means of General-Grid-Interface (GGI) interpolation [2].

This contribution will further detail on the concept of a unified framework for both partitioned and monolithic coupling using the FOAM-extend C++ library. Validation is accomplished for a selection of test cases for capillarity-dominated two-phase flow.

References

[1] Ž. Tuković and H. Jasak. "A moving mesh finite volume interface tracking method for surface tension dominated interfacial fluid flow". In: *Computers & Fluids* 55 (Feb. 2012), pp. 70–84. DOI: 10.1016/j.compfluid.2011.11.003.

[2] I. D. Dominicis, G. Cvijetić, M. Willetts, and H. Jasak. "Enhanced Turbomachinery Capabilities for Foam-Extend: Development and Validation". In: *OpenFOAM®*. Springer International Publishing, 2019, pp. 145–155. DOI: 10.1007/978-3-319-60846-4_11.

LIKE OPENFOAM, BUT IN PYTHON

ROBERT ANDERLUH[1], HRVOJE JASAK[2],
[1]*University of Cambridge, ra598@cam.ac.uk*
[2]*University of Cambridge, hj348@cam.ac.uk, Wikki LTD, h.jasak@wikki.co.uk*

Keywords: *OpenFOAM, Python, finite volume method*

C++ is the workhorse programming language of today's scientific computing community. That is so due to its intrinsic properties of supporting an object-oriented approach, as well as an abundance of other modern programming paradigms. Also, its efficiency in computationally-intense applications is well recognized and appreciated in the scientific and engineering communities. This is because of the fact that it is a statically typed, compiled and well optimized language. Also, it offers the programmer access to memory management at a relatively low level. However, using C++ for code construction is considered to be laborious compared to some other languages.

OpenFOAM [1] is an example of that. It is written in C++, utilizing many of its advanced features. It is written in a highly object-oriented fashion. Essentially, everything present in OpenFOAM is a custom-tailored object of sorts. This approach is advantageous for managing complexity of OpenFOAM, which is a matter of utmost importance due to the fact that it offers the users the ability to use a broad and ever-expanding array of continuum models, most of which is implemented in a finite volume method framework with support for unstructured polyhedral meshes. Also, the way the finite volume method is implemented into OpenFOAM's class structure makes the top level code easily readable, due to visual mimicking of differential equations. The highly-object-oriented approach that enables the maintainers of OpenFOAM to manage complexity of the code also makes it harder for newcomers to read through the code at a somewhat deeper level, as the code structure is written in a way that makes the top-level code very readable, but can be complex at the medium and low levels.

Python as a programming language seems like a complete opposite to C++: it is considered easy to read and learn, but is less efficient with computationally-intense applications. As opposed to C++, which is statically typed and compiled, it is dynamically typed and interpreted. Memory management in Python is more user-friendly then the equivalent in C++, as it is handled in a way that the programmer can afford to be more distanced from it during code construction. Also, it is very easy to import open-source modules, which makes it easier for the programmer to include external functionalities in his code and reduce the code construction time. Some of Python's modules and functionalities (e.g. NumPy [2]) are written in C, which enables them to remove the usual Python overhead and be more efficient. Python also offers some other potential efficiency improvements: Just-In-Time compilers, static compilers, etc.

The above stated points make Python a programming language which can be well suited as a choice for a rapid-prototyping use. New scientific computing functionalities can first be implemented using Python as an alternative to computationally more efficient languages, such as C++. A novel scientific idea or method can be explored and implemented in a Python-based code, which, after optimisation and debugging of algorithms, could then more easily be implemented in a more computationally efficient framework, e.g. OpenFOAM.

In this work, a Python-based implementation of OpenFOAM's basic classes is presented. Mainly, the fvMatrix, fvMesh and GeometricField class hierarchy, with some of the functionality which is present in their base classes in the original OpenFOAM C++ code. The main logic present in OpenFOAM's classes is preserved, mostly in terms of the most necessary member functions (methods in Python) and member data (attributes in Python). The input and output formats are similar to the OpenFOAM format. This enables the user to use any existing OpenFOAM mesh as an input to the code, as well as use OpenFOAM's existing post-processing tools. The code structure is presented and verified by assembling a top-level solver equivalent to OpenFOAM's laplacianFoam solver and comparing the results. The differences between the Python and C++ implementations are discussed.

A visualization of the results achieved by the Python implementation is shown in a set of figures. The first simulation in question is the standard flange case which can be found in OpenFOAM's tutorials and is shown in Figure 1. The simulations were ran without non-orthogonal correction and using the Gauss-Seidel iterative solver with an absolute residual tolerance of 1e-6 for every time step.

The second simulation is a modification of the lid-driven cavity case geometry, usually used for verifying fluid flow solvers. The equivalent OpenFOAM and Python code results are shown in Figures 2 and 3.

AN OPENFOAM SET-UP FOR SIMULATING THERMAL WINDS IN MOUNTAIN/VALLEY CONFIGURATIONS

RATHAN B. ATHOTA[1*], JOSE I. ROJAS [1], SANTIAGO ARIAS [1] AND ADELINE MONTLAUR [1],
[1*,1]*Department of Physics − Division of Aerospace Engineering, Universitat Politcnica de Catalunya, c/ Esteve Terradas, 7, 08860 Castelldefels, Spain*
rathan.babu.athota@upc.edu, josep.ignasi.rojas@upc.edu, santiago.arias@upc.edu, adeline.de.montlaur@upc.edu

Keywords: *thermal wind, slope, mountain, valley, anabatic, katabatic, CFD, OpenFOAM*

Exploring novel renewable energy resources such as thermal winds in mountainous areas and valleys is critical to reduce the energy production from fossil fuels and thus mitigating climate change. These winds occur due to thermal gradients and related buoyancy effects. Basically, the latter are mainly associated with the diurnal heating-cooling cycles of the lower layers of the atmosphere. Thermal winds usually develop by convection over complex terrains of different scales, and they invert their direction twice a day, driven by the emergence and dissipation of temperature inversions. Namely, these winds will blow up-valley (anabatic winds), or from the plain to the mountain massif during day-time. Contrary, during night-time, these winds will blow down-valley (katabatic winds), or from the mountain massif to the plain. Former investigations have shown that thermal winds can reach comparably high speeds [1], which could be interesting for wind energy applications. Moreover, in comparison with synoptic winds, thermal winds exhibit higher periodicity and regularity, resulting in better predictability of wind energy production, which is key to the energy market and matching the demand, given that wind and solar energy cannot be controlled at will.

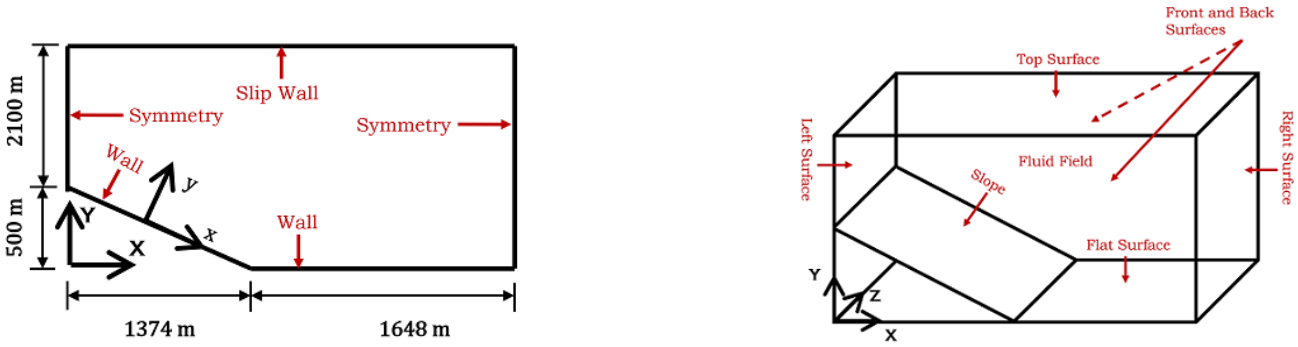


Figure 1: Domain with boundary conditions: 2D view (left) and 3D view (right)

The present work analyses the generation of thermal winds in mountainous areas and valleys using OpenFOAM, which is an open source C++ code used for computational fluid dynamic (CFD) simulations. For our simulations, an idealized mountain-valley model with a mountain slope angle of 20^o was used (see Fig. 1), and the domain was discretized using $blockMeshDict$ file. The $buoyantBoussinesqPimpleFoam$ solver was first validated along with boundary conditions by reproducing the results of Schumann [2] and Axelsen and van Dop [3]. In addition, the effect of different turbulence models and boundary conditions on the top surface was evaluated (see Fig.1) and compared with those previous investigations. Results have shown that a K-epsilon turbulence model with a slip wall boundary condition on the top surface was able to simulate accurate data, when compared with RNG-K-epsilon model. Altitude dependent and altitude independent types of initial conditions were implemented in the fluid field to investigate the stability of the flow. Results proved to be very sensitive to the choice of field temperature initial conditions, and it was found that the evolution of up-slope and down-slope winds was satisfactory simulated by applying constant temperature as initial condition of the domain field (see Fig. 2). Effect of pressure initial conditions was also studied by comparing altitude-dependent and constant pressure conditions. Results showed that the error between these two initial conditions was less than 1%, so for consistency reason with the chosen temperature initial conditions, an altitude-independent pressure initial condition was selected.

DEVELOPMENT AND VALIDATION OF A PHASE-FIELD METHOD FOR AN ARBITRARY NUMBER OF IMMISCIBLE INCOMPRESSIBLE FLUIDS

MILAD BAGHERI[1], MARTIN WÖRNER[2], and HOLGER MARSCHALL[1]

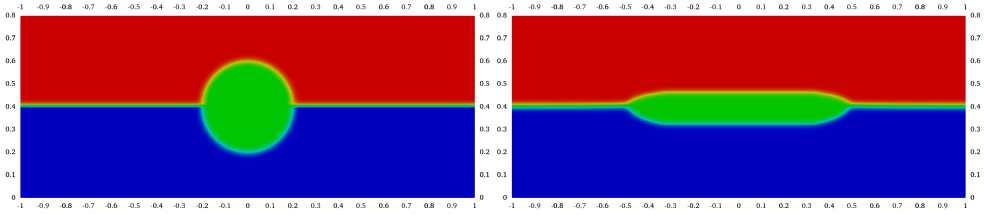
[1]Department of Mathematics, Computational Multiphase Flow, Technical University of Darmstadt, Germany, milad.bagheri@tu-darmstadt.de & holger.marschall@tu-darmstadt.de
[2]Institute of Catalysis Research and Technology, Karlsruhe Institute of Technology (KIT), Germany, martin.woerner@kit.edu

Keywords: *Phase-Field; Cahn-Hilliard Navier-Stokes; Immiscible mutliphase flows; Consistency conditions*

We present the most recent work concerning method development, implementation and validation of N ($N > 2$) immiscible, incompressible and isothermal fluids enhancing further our library for the diffuse interface phase-field interface capturing method in FOAM-extend 4.0/4.1. The phase-field method is an energic variational formulation based on the work of Cahn and Hilliard [1] where the interface is composed of a physical diffuse layer resembling realistic interfaces.

The extension from a two-phase ($N = 2$) to the generic multiphase ($N > 2$) flow framework requires obeying to consistency conditions. The model is fully reduction consistent [2, 3, 4], i.e. the N-phase model reduces to the traditional two-phase model upon existence of only two phases in the system. This principle is vital to eliminate generation of fictitious phases [4]. Furthermore, the model preserves phase volumes and ensures momentum conservation according to Huang et al. [4], which we follow in this study.

To validate the implemented model the floating liquid lens problem depicted in Figure 1 (a) is simulated. In this problem a liquid oil drop is initially floating on the air-water interface and will spread depending on the magnitude of the gravitational acceleration and surface tension coefficients. The final thickness of the drop will be compared to an equilibrium solution and an asymptotic analysis available in literature. Figure 1 (b) illustrates the final shape of the oil drop when $|g| = 9.8\,m^2/s$.



(a) Initial configuration (b) Final configuration $|g| = 9.8\,m^2/s$

Figure 1: Preliminary results for the floating liquid lens problem. Blue: Water, Red: Air, Green: Oil.

Moreover, the three-phase dam break problem depicted in Figure 2 is also considered as a validation case where both water and oil columns are initially held at rest by artificial walls. At $t = 0$ these walls are removed and both columns collapse. The results of this validation case will be compared with the experimental and numerical data available in the literature. Evolution of the phases at two different time instances are shown in Figure 2 (b) and (c), respectively.

ANALYSIS OF LUBRICATED POINT CONTACTS USING THE FINITE AREA METHOD

VANJA ŠKURIĆ[1], LUKA BALATINEC[2] and HRVOJE JASAK[3]

[1]*Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, vanja.skuric@fsb.hr*

[2]*Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, luka.balatinec@fsb.hr*

[3]*Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, hrvoje.jasak@fsb.hr*

Keywords: *Lubricated Point Contact, Finite Area Method, FVM, OpenFOAM*

Numerical modelling has emerged as a valid alternative to costly experimental methods used for contact analysis in various applications (metal forming, bearing design, etc.). The existing design tools rarely focus on calculating the effects of microscopic contact and friction. Numerical methods can be a useful add-on for calculating such effects and also lubrication effects for rough surfaces in contact.

A numerical framework based on the Finite Area Method (FAM) [1] is presented as a viable tool for simulations of lubricated contact of rough surfaces [2]. A FAM contact boundary condition was implemented for the hyperelastoplastic finite volume deformation solver [3], as a part of the `foam-extend` library. The framework combines lubricant flow, thermal and asperity contact model, which enables the calculation of contact pressure and traction for all lubrication regimes. Moreover, the framework provides additional data, such as film thickness, temperature, contact area, etc., which is invaluable for analysing the properties of lubricants. It was used for numerical simulations of a ball-on-disc tribometer and the results were validated against numerical and experimental data [4, 5]. Two sets of simulations were performed with varying entrainment speeds and contact loads: for a hydrodynamic lubrication regime (Turbo T9 oil) and a mixed lubrication regime (Turbo T68 oil). The results are presented showing friction thickness, contact and hydrodynamic pressure, contact area, film temperature, etc.

In conclusion, the numerical framework showed that acceptable accuracy can be achieved for numerical simulations of lubricated point contacts, if there is complete information regarding the lubricant transport properties and a measured surface roughness.

References

[1] Ž. Tuković, "The finite volume method on domains of changeable shape," Ph.D. dissertation, 2005.

[2] V. Škurić, "Numerical simulation of lubricated wire rolling and drawing," Ph.D. dissertation, 2019.

[3] P. Cardiff, Ž. Tuković, P. D. Jaeger, M. Clancy, and A. Ivanković, "A lagrangian cell-centred finite volume method for metal forming simulation," *International Journal for Numerical Methods in Engineering*, vol. 109, no. 13, pp. 1777–1803, Sep. 2016. [Online]. Available: https://doi.org/10.1002/nme.5345

[4] W. Habchi, P. Vergne, S. Bair, O. Andersson, D. Eyheramendy, and G. Morales-Espejel, "Influence of pressure and temperature dependence of thermal properties of a lubricant on the behaviour of circular TEHD contacts," *Tribology International*, vol. 43, no. 10, pp. 1842–1850, Oct. 2010. [Online]. Available: https://doi.org/10.1016/j.triboint.2009.10.002

[5] J. Guegan, A. Kadiric, A. Gabelli, and H. Spikes, "The relationship between friction and film thickness in EHD point contacts in the presence of longitudinal roughness," *Tribology Letters*, vol. 64, no. 3, Oct. 2016. [Online]. Available: https://doi.org/10.1007/s11249-016-0768-6

TAILORING THE GEOMETRICALLY-EXACT FINITE VOLUME BEAM SOLVER TO MODEL POLYGONAL WIRE CROSS-SECTION GEOMETRIES

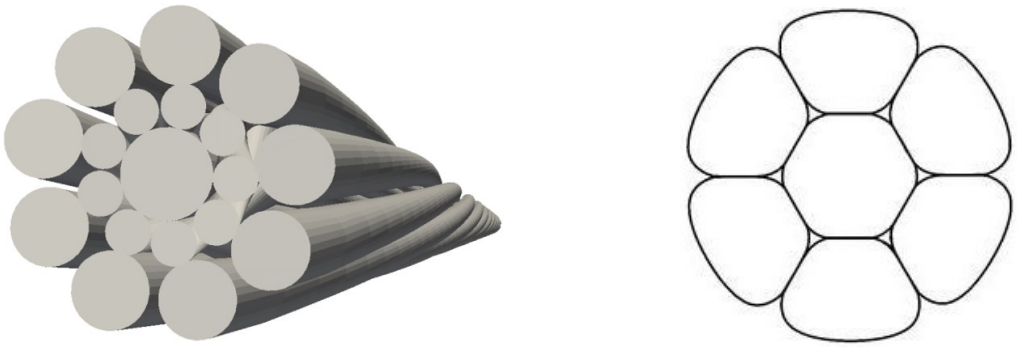
SEEVANI BALI[1,2,4,6,a], ŽELJKO TUKOVIĆ[3,b], PHILIP CARDIFF[1,4,5,c], MERT CELIKIN[1,4,5,d], VIKRAM PAKRASHI[1,2,4,6,e]

[1]*School of Mechanical and Materials Engineering, University College Dublin, Ireland*
[2]*SFI MaREI Centre, University College Dublin, Ireland*
[3]*Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Croatia*
[4]*Bekaert University Technology Centre, School of Mechanical and Materials Engineering, University College Dublin, Ireland*
[5]*SFI I-Form Centre, University College Dublin, Ireland*
[6]*Dynamical Systems and Risk Laboratory, School of Mechanical and Materials Engineering, University College Dublin, Ireland*

[a]*seevani.bali@ucdconnect.ie* [b]*Zeljko.Tukovic@fsb.hr* [c]*philip.cardiff@ucd.ie*
[d]*mert.celikin@ucd.ie* [e]*vikram.pakrashi@ucd.ie*

Keywords: *geometrically exact beam, finite volume method, polygonal cross-sections, finite rotations, large displacements*

In this work, extension of finite volume solver for geometrically exact Simo-Reissner beam to model polygonal cross sectional wire geometries is presented. Structural components like wire ropes and cables are used in various sectors of engineering; the geometric configuration and wire arrangement in a particular rope is tailored to the field of application [1] and hence, creating specific configuration of wire geometries is essential to simulate the forces and/or moments acting in the rope strands. Being slender in geometry, the individual wires in the rope assembly can be modelled as beams. Several beam theories, including the most general geometrically exact beam theory [2] have been developed and their implementation using finite element method has been investigated in-detail in literature. Recent developments of Tuković et al. [3] have focused on the implementation of geometrically exact Simo-Reissner's beam theory using finite volume discretisation in OpenFOAM to model shear-deformable circular cross-sectional beams. The current work presents an extension to the solver for modelling beams with polygonal cross sections. The present task is a part of the authors' overall objective to create a novel computation suite for modelling wire ropes for large spatial displacements and finite rotations [4] subjected to tension and torsional loads. An instance of rope strand geometric models which would be used in the numerical simulations is shown in the Figure 1. For these models, the nonlinear stress resultant equations of spatial forces and moments are linearised and iteratively solved for incremental displacements and rotations using Newton-Raphson procedure [3].



(a) (1+9+9) Seale wire strand **(b) (1+6) compacted strand**

Figure 1: Geometric models of rope strands with different wire cross sections: circular and polygonal

Modeling Convective Heat Transfer of Air in a Data Center using OpenFOAM - Evaluation of the Boussinesq Buoyancy Approximation

H.A. Barestrand[1], A-L. Ljung[2], J. Summers[3], T.S. Lundström[4]
[1]*H.A. Barestrand, Luleå University of Technology, henrik.barestrand@ltu.se*
[2]*A-L. Ljung, Luleå University of Technology, anna-lena.ljung@ltu.se*
[3]*J. Summers, ICE Data center, RISE, jon.summers@ri.se*
[4]*T.S. Lundström, Luleå University of Technology, staffan.lundstrom@ltu.se*

Keywords: *Data Center, Boussinesq, Buoyancy, Richardson number, Hot air convection*

The data center industry faces numerous challenges when it comes to cooling the equipment and distributing IT workload efficiently. Different advanced tools have therefore been used to study the heat transfer within data centers. To exemplify, numerous use of Computational Fluid Dynamics (CFD) in simulating scenarios of the air convection beforehand yield information on cooling performance. This includes information on whether the air in the data center is effectively delivered [1]. This work builds upon previously demonstrated capability of OpenFOAM to simulate data center convection heat transfer by Summers et al. [2]. It is also to be a sound base for further turbulence studies in data center open airflow situations based on the work by Wibron et al. [3].
When doing CFD on data centres a number of aproximations are introduced on the geometry and boundary conditions. Here focus in emphasized on the extent to which the Boussinesq approximation of buoyancy can be used when simulating this sort of convective heat transfer. The approximation is based on a linear expansion of the buoyant density in terms of teperature and may reduce the computational load for scenarios where there are limited temperature differences in the hot air.
In OpenFOAM terms, the solvers compared are *BuoyantBoussinesqPimpleFoam* and *BuoyantPimpleFoam*. The latter uses a compressible formulation for the pressure and implements a different form of the energy equation. The difference of interest in the energy equation stem from the buoyant term at higher Richardson number (Equation (1)).

$$\mathrm{Ri} = \frac{g\nabla_z(\rho)}{\rho(\nabla_z(u))^2} = \frac{\text{buoyancy term}}{\text{flow shear term}} = \frac{Gr}{Re^2} \tag{1}$$

The solvers are run and numerically verified on two different flow configurations. One where the global Richardson number is estimated below 0.5 and one situation where buoyant forces play a bigger role. For the second scenario, forced convection is reduced by lowering the mass flow through modeled racks and cooling units while retaining the heat generation. In this way it is possile to observe the effects of how the buoyancy is modeled by the heat distribution on the return side of different cooling units. In addition to the Boussinesq approximation, the effects of uniform static outlet pressure as a boundary condition on cooling units is investigated.

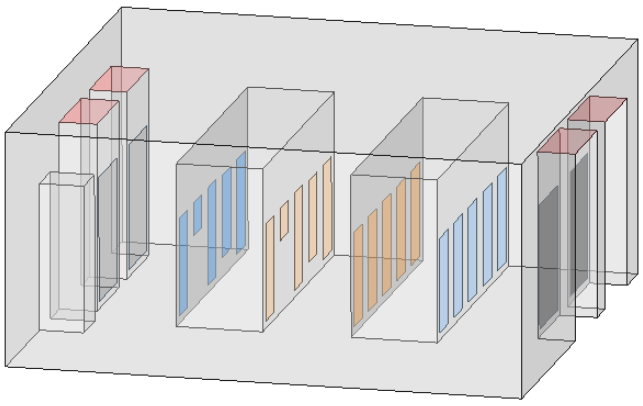


Figure 1: The hard floor configuration data center hall studied.

VOF-LES SIMULATION OF THE JET WIPING PROCESS: VALIDATION AND MULTISCALE MODAL ANALYSIS

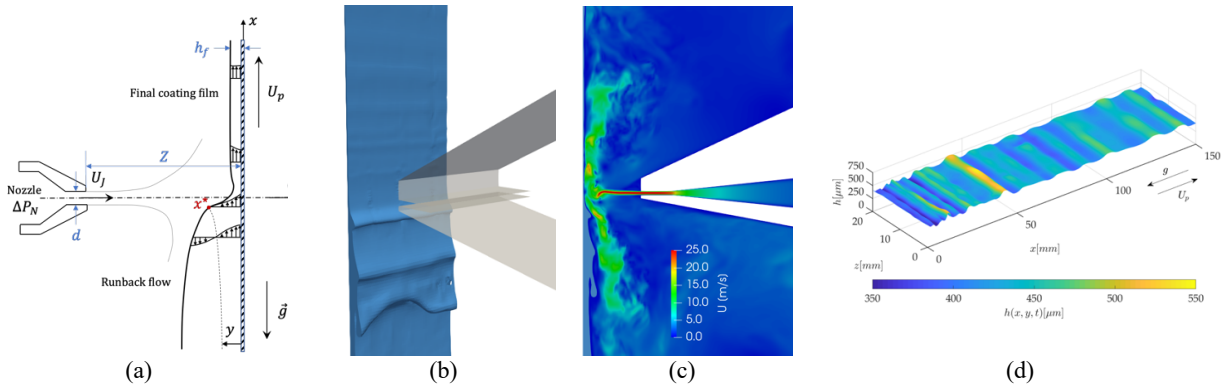
DAVID BARREIRO-VILLAVERDE[1], ANNE GOSSET[2], MIGUEL ALFONSO MENDEZ[3]
[1]*CITIC Research, Universidade da Coruña, david.barreiro1@udc.es*
[2]*Technological Research Center (CIT), Universidade da Coruña, anne.gosset@udc.es*
[3]*Environmental and Applied Fluid Dynamics, von Karman Institute, miguel.alfonso.mendez@vki.ac.be*

Keywords: *two-phase flow, Large Eddy Simulation, Volume Of Fluid, modal analysis, jet wiping*

Jet wiping is a coating process in which a liquid is dragged by a flat substrate moving upwards after dipping in a coating bath. In order to control accurately the thickness of the liquid film deposited on the surface, two slot gas jets impinge on both sides of the film, acting literarily as "air-knives": the final coating thickness is reduced and the excess liquid flows back to the bath as a *runback,* as shown in Fig.1(a). In spite of its undeniable advantage to be contactless, the process is limited by the appearance of large amplitude waves on the final product after solidification, known as *undulations*, of main concern for quality standards. The experimental investigations conducted by Gosset et al. [1] and Mendez et al. [2] suggest that their origin is a hydrodynamic feedback mechanism between the gas jet and the liquid film. The objective of this work is twofold: first, it aims at resolving numerically the liquid-gas coupling with the Volume Of Fluid (VOF) method and Large Eddy Simulation (LES) for turbulence modelling, and validate the results with experiments. Second, it seeks to identify the basic mechanism of wave formation using a novel modal analysis decomposition technique [3,4], and link it with the jet behaviour.

Three wiping test cases experimentally characterized in Mendez et al. [2] are simulated with the VOF formulation implemented in the *interFoam* solver, while a Smagorinsky LES model is used to accurately predict the gas jet behaviour. The Multiscale Proper Orthogonal Decomposition (mPOD) [3] is used to identify the coherent patterns in the liquid and gas dynamics, characterized by a wide range of spatial and time scales. mPOD is a data-driven decomposition that combines the advantages of energy (Proper Orthogonal Decomposition) and frequency (Dynamic Mode Decomposition) based methods: the spectral content of the modes is restricted to a certain frequency range by using Multi Resolution Analysis (MRA). The decomposition is performed using the open-source package MODULO [4].

An overview of the results for one test case is shown in Fig.1, with the 3D reconstruction of the liquid film interface (b), the contour map of the gas velocity field in the midplane (c), and the final film thickness distribution after post-processing of the volume fraction fields (d). In this wiping condition, the liquid film features two-dimensional wave patterns in both the final film and runback flow. It can be seen how the gas jet, after impingement, divides into two side jets, the bottom one being substantially deflected by the large waves on the runback.



(a) (b) (c) (d)

Figure 1: Sketch of the jet wiping process (a), 3D film reconstruction (b), contour map of the velocity field in a midplane (c), and the final film thickness distribution (d).

The numerical model is successfully validated in terms of final film mean thickness and liquid/gas frequency content. The spectra in Fig.2(a) are computed from the leading mode obtained in the multiscale analysis of the final film $\widehat{\mathcal{H}}_{ff}$, the runback flow $\widehat{\mathcal{H}}_{rb}$ and the gas jet $\widehat{\mathcal{Y}}$. The agreement between the experimental and numerical data is remarkable, as is the fact that the same frequency peak is detected in the three quantities. This is clearly the proof that the undulations are produced by a coupling mechanism in which the film and the gas jet are locked onto a certain frequency, as suggested in the hydrodynamic feedback hypothesis. In the other two test cases, characterized by more three-dimensional wave patterns, the gas jet and runback wave frequencies are also in good agreement. In spite of a slower convergence of the mPOD decomposition, i.e. more modes are needed to describe the film dynamics, the same basic 2D mechanism is detected, in which the jet motion is coupled with the large runback waves: the *2D coupled mode*.

TOWARDS IMPLICIT IMPLEMENTATION OF PENALTY BASED CONTACT BOUNDARY CONDITION

IVAN BATISTIĆ[1], ŽELJKO TUKOVIĆ[2], PHILIP CARDIFF[3]
[1]*University of Zagreb, Faculty of Mechanical Engineering and Naval Architecture, zeljko.tukovic@fsb.hr*
[2]*University of Zagreb, Faculty of Mechanical Engineering and Naval Architecture, ivan.batistic@fsb.hr*
[3]*University College Dublin, School of Mechanical and Materials Engineering, philip.cardiff@ucd.ie*

Keywords: *computational contact mechanics, finite volume method, implicit coupling, penalty method*

The current implementation of the contact model in the *solids4Foam* toolbox [1] is based on explicit coupling between bodies in contact. At contact boundaries, the Neumann boundary condition is used and specified contact force is calculated explicitly using the penalty law [2]. Such an implementation is robust and can be successfully applied to a large spectrum of contact problems. To ensure convergence of explicit coupling it is necessary to apply appropriate under-relaxation factor on the contact force. The under–relaxation factor, as well as penalty factor are user–specified and their value must be carefully set to obtain acceptable accuracy and to ensure acceptable convergence rate. The acceptable range value of the under–relaxation factor is inversely proportional to the specified penalty factor and tuning these factors can be a troublesome task, especially for an inexperienced user.

This work presents the penalty based implicit coupling between the deformable body and rigid analytical surface. With implicit coupling, it is expected that calculated contact force can be prescribed at contact boundary without under–relaxation which means that optimal convergence rate can be achieved for any user-defined penalty factor. The presented approach can be seen as a first step towards the implementation of the implicit coupling between two deformable bodies in contact. The deformable body is modelled as a linear-elastic with total displacement $\boldsymbol{u}$ as a dependent variable. After discretisation procedure, obtained system of linear algebraic equations is solved in a segregated manner.

At contact boundary (denoted with subscript c) contact traction (contact force) can be decomposed into normal and tangential component [3, 4]:

$$(\boldsymbol{t})_c = (\boldsymbol{t}_n)_c + (\boldsymbol{t}_t)_c = \underbrace{(2\mu_c + \lambda_c)\boldsymbol{n}_c \cdot \boldsymbol{\nabla}\boldsymbol{u}_n + \lambda_c \boldsymbol{n}_c \mathrm{tr}(\boldsymbol{\nabla}_t \boldsymbol{u}_t)}_{(\boldsymbol{t}_n)_c} + \underbrace{\mu_c \boldsymbol{n}_c \cdot \boldsymbol{\nabla}\boldsymbol{u}_t + \mu_c \boldsymbol{\nabla}_t u_n}_{(\boldsymbol{t}_t)_c}, \tag{1}$$

where subscripts n and t represent the normal and tangential components of vector, respectively. λ_c and μ_c are first and second Lamé parameter, $\boldsymbol{\nabla}_t$ is tangential gradient operator, calculated using extrapolated method [3]. Normal component of the traction vector is defined using the penalty law:

$$(\boldsymbol{t}_n)_c = -\varepsilon_n g_n^* \boldsymbol{n}_c - \varepsilon_n((\boldsymbol{u}_n)_c - (\boldsymbol{u}_n)_c^*), \qquad g_n \geqslant 0, \tag{2}$$

where g_n is normal penetration and ε_n is normal penalty factor. The superscript $*$ denotes the calculated quantities from the previous outer iteration. The first term on the right–hand side represents explicitly calculated contact traction whereas the second term represents implicit correction which tends to zero during convergence. Combining Eq. (1) with Eq. (2) normal component of the boundary displacement is obtained:

$$(\boldsymbol{u}_n)_c = \frac{\varepsilon_n C}{(1 + C\varepsilon_n)}((\boldsymbol{u}_n)_c^* - \boldsymbol{n}_c g_n^*) - \frac{C}{(1 + C\varepsilon_n)}\lambda \boldsymbol{n}_c \mathrm{tr}(\boldsymbol{\nabla}_t \boldsymbol{u}_t) + \frac{1}{(1 + C\varepsilon_n)}(\boldsymbol{n}_c \boldsymbol{n}_c) \cdot \boldsymbol{u}_P, \tag{3}$$

where $C = \delta_n/(2\mu_c + \lambda_c)$. Using Eq. (3) the normal component of the contact boundary gradient $(\boldsymbol{g_n})_c = ((\boldsymbol{u}_n)_c - (\boldsymbol{u}_n)_P)\delta_n^{-1}$ can be written as:

$$(\boldsymbol{g}_n)_c = \underbrace{\frac{\varepsilon_n C}{\delta_n(1 + C\varepsilon_n)}((\boldsymbol{u}_n)_c^* - g_n^*) - \frac{C}{\delta_n(1 + C\varepsilon_n)}\lambda \boldsymbol{n}_c \mathrm{tr}(\boldsymbol{\nabla}_t \boldsymbol{u}_t)}_{\text{I.}} + \underbrace{\frac{1}{\delta_n(1 + C\varepsilon_n)}(\boldsymbol{n}_c \boldsymbol{n}_c)}_{\text{II.}} \cdot \boldsymbol{u}_P - \underbrace{\frac{1}{\delta_n}}_{\text{III.}} \boldsymbol{u}_P. \tag{4}$$

Do Liquid Drops Roll or Slide on Inclined Surfaces? – Detailed Analysis using a Diffuse-Interface Phase-Field Method

Bodziony, F.[1], Li, X.[2], Berger, R.[2], Butt, H.J.[2] and Marschall, H.[1]
[1]*Department of Mathematics, Computational Multiphase Flow, Technical University of Darmstadt, Germany*
[2]*Physics of Interfaces, Max Planck Institute for Polymer Research, Mainz, Germany*

Keywords: *Direct Numerical Simulation, Phase-Field Method, Sliding Droplet*

We consider numerical simulations of the motion of a three-dimensional droplet on an inclined solid substrate. The simulations are performed using our diffuse interface phase-field solver – phaseFieldFoam (FOAM-extend 4.0 and 4.1). The solver has been enhanced to use a moving reference-frame technique, to follow the droplet's center-of-mass, effectively reducing the computational effort (domain size, cp. Fig. 1). We study the effects that inclination angle, Eotvos number and contact angle have on forces acting on droplets, as well as their influence on the droplet's kinetic, interfacial and dissipative energy. The sliding velocity (and droplet shape) is also discussed for various inclination angles and compared with experiments. For all these cases, contact line hysteresis is observed, and its effect on droplet motion is described.

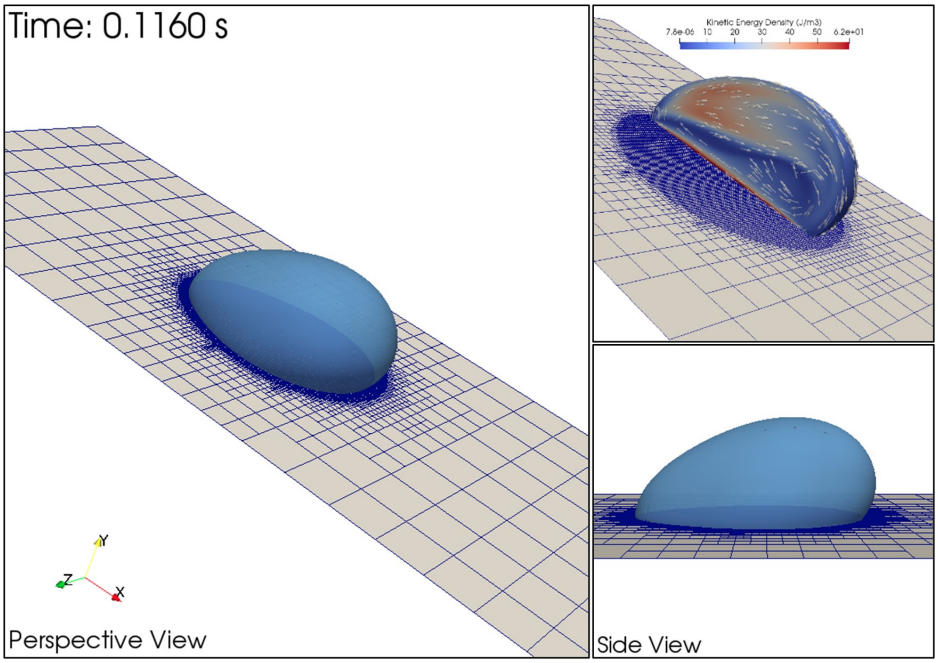


Figure 1: Direct Numerical Simulation of a droplet moving down an inclined wall using a moving frame-of-reference technique (air-water system at 25°C, equilibrium contact angle 105° and inclination angle 40°)

Acknowledgments

This work is funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 265191195 – SFB 1194.

CFD STUDY ON IRWIN PROBE FLOWS USING OPENFOAM

PEDRO M. BRITO[1], ALMERINDO D. FERREIRA[2], ANTONIO C. M. SOUSA[3]
[1] *ADAI-LAETA, Dep. Mechanical Engineering, University of Coimbra, Coimbra, Portugal*
pedro.brito@dem.uc.pt
[2] *ADAI-LAETA, Dep. Mechanical Engineering, University of Coimbra, Coimbra, Portugal*
almerindo.ferreira@dem.uc.pt
[3] *Dep. Mechanical Engineering, University of New Brunswick, New Brunswick, Canada*
asousa@unb.ca

Keywords: *Irwin sensor, CFD, Tip vortex, Interference*

Abstract

In this preliminary work, three-dimensional Computational Fluid Dynamics (CFD) simulations are performed to characterize the complex flow field and pressure distribution developed around and within an Irwin probe, at distinct low-Reynolds regimes. The emergence of robust flow structures past the sensor is categorised and preventive spacing intervals, necessary to mitigate mutual interference, is numerically evaluated. The computations corroborate the original spacing recommendations by Irwin. For typical operation conditions, long streamwise tip vortices are observed in the wake of a single sensor. In addition, the predictions suggest the existence of a low-Reynolds number threshold, below which such structures are supressed, resulting in diminished interference effects. Numerical results also suggest a nearly uniform axial pressure distribution and place in evidence very interesting flow field characteristics.

Introduction

Irwin probes are surface-mountable sensors capable of relating pressure differences (Δp) to the wind speed. This device was developed to measure pedestrian-level wind conditions in wind tunnels, at heights of a few millimetres above model street surfaces, and first described by Irwin [1] as a compact, omnidirectional and nearly non-intrusive wind sensor, opposing traditional alternatives, such as thermal anemometers and Pitot tubes.

Irwin sensors feature simple axisymmetric geometries, are inexpensive and well suited for synchronous multi-sensor operation. As depicted in **Figure 1**.a), the architecture of the Irwin probe resembles the assembly of a circular cavity (depth H and diameter D) with a deep-seated, concentric tube (external diameter d and length $H + h$), with $D/d > 1$ and h the selected protruding height above surface-level. Two pressure readings are collected during operation, one from within the cavity and the other from inside the tube, establishing a pressure difference output (Δp). Unsteady simulations were performed for three distinct low-Reynolds numbers (Re_d = 100, 200 and 500), reproducing a full-scale Irwin probe installed in a flat plate, fully immersed in a developing boundary layer airflow.

The present CFD study aims to explain the complexity of the flow field developed around and inside an Irwin probe. The key objectives are to identify robust flow features responsible for the occurrence of streamwise interference and to review preventive spacing intervals under laminar flow conditions. In addition, the present work aims to describe the static pressure field distribution inside the probe, and how it translates into a measurable pressure difference.

Numerical method

The numerical simulations were performed using OpenFOAM® v7 [2]. To solve the coupled Navier-Stokes equations, the computations were based on the PISO algorithm, for transient incompressible flows [3]. The PISO algorithm was operated in laminar mode (*i.e.* with turbulence switched off) for all Reynolds number tested ($100 \leq Re_d \leq 500$) and the mesh was created using the `blockMesh` utility, comprising about 12 million hexagonal cells, as illustrated in Figure 2).

Results and Conclusions

The numerical method was used to predict the occurrence of streamwise interference, evaluating the velocity field recovery in the wake of the protruding sensor. It was found that streamwise spacing between sensors should be at least $10d$, close to the initially-proposed $12d$-requirement by Irwin [1], even at laminar operation regimes of $Re_h \sim O(10^2)$. Further examination of the wake, at Re_d = 500, revealed the appearance of a pair of robust tip vortices, spanning far downstream the sensor (see Figure 2.a). These coherent vortical structures are thought to strengthen interference effects. Interestingly, the inner-sensor static pressure distribution estimates indicate that the sensor output (Δp) is independent of the depth of the sensor, provided that the cavity is deeper than the height of the tubular protrusion ($H/h > 1$), since the pressure field inside the cavity is found to be nearly uniform, radially and height-wise (Figure 2.b).

NUMERICAL STUDY OF THE FLOW INTO A POOL INDUCED BY A VERTICAL JET

RITA F. CARVALHO[1], PEDRO M. LOPES[2], MD NAZMUL AZIM BEG[3]
[1]*University of Coimbra, MARE, Dept. of Civil Engineering, Coimbra, Portugal, ritalmfc@dec.uc.pt*
[2]*University of Coimbra, MARE, Dept. of Civil Engineering & MATEREO, Coimbra, Portugal*
[3]*Department of River Coastal Science and Engineering, Tulane University, Louisiana, USA, mbeg@tulane.edu*

Keywords: *Jet, Plunge pool free-surface flow, Air-entrainment, Turbulence, Energy dissipation .*

This research aims to investigate the flow of a jet into a plunge pool by OpenFOAM® simulations, considering different solvers (interFoam, airInterFoam and EulerFoam), which consider the description air-entrainment in different ways. Velocity, pressure and air concentration profiles will be compared.

Following the work of numerical simulation of jet into pools at the University of Coimbra, Portugal [1,2] where no detailed data was possible, and the work of [3], where simulations with a 3D SPH model were for a vertical high-speed jet, we now look for an experimental work realized in 2007 at the Laboratory of Hydraulic Constructions (LCH) of the École Polytecthnique Fédérale de Lausanne (EPFL), Switzerland, which detailed data are available (Figure 1 [3,4]). The installation is fed by a closed-circuit and was tested under different conditions of flow Q between 30 and 120 l/s, feeding a circular jet with a nozzle exit diameter D = 0.072 m, distancing from 0.7 from the 3 meteres diameter pool bottom. Water pool depth also varied according different conditions from 0.072 to 0.87 m. According to [4], pressure measurements at the jet outlet were made with a 3 mm diameter piezo-resistive micro-transducer of type Kulite XTL-190-17BAR-A (flush mounted on the pool bottom) with a sampling frequency of 2 kHz for 32.5 s, which estimate accuracy is 0.1% and discharge measurements were performed with an electromagnetic flowmeter of 1% accuracy (see [4] for details).

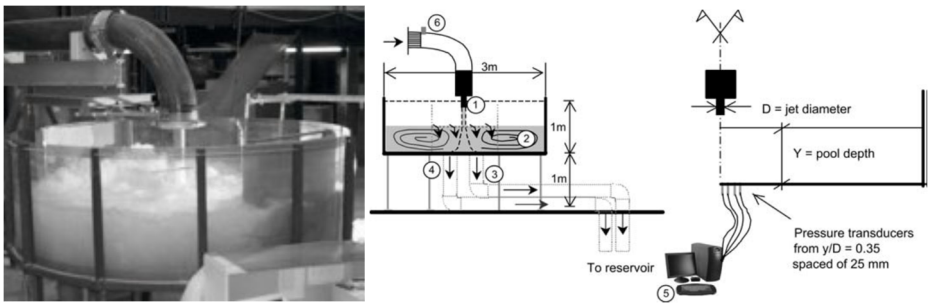


Figure 1: Photo, Sketch and Geometry of the experimental installation at the EPFL: a) photo from [4]; b) schema from [4] and geometry with mesh

Numerical model used within OpenFOAM® is based on the Reynolds-Averaged Navier–Stokes equations (RANS), governing the motion of the 3D incompressible and isothermal flows, considering the free surface described by a standard Volume-Of-Fluid method (VOF) – interFoam, other code based on interFoam in which some issues related to the air-entrainment were implemented – airInterFoam [1] and a multiphase flow Euler/EulerFoam. Turbulence is described by a SST k-ω turbulence model. Water and air were considered Newtonian fluids with kinematic viscosity equal to 1e-06 and 1.48e-05 and density equal to 1000 and 1, respectively. Computational mesh was constructed using (Figure 1 in red and Figure 2). Boundary Conditions comprise inlet, outlet, walls (pipe, nozzle and pool) and atmosphere (at all around, upper part). Initial conditions considered a water volume with constant depth and the pool, and inside the pipe with velocity calculated according discharge flow measured in the experimental installation.

NUMERICAL STUDY OF THE FLOW TRANSITION IN A SEWER BETWEEN MANHOLES

RITA F. CARVALHO[1], MD NAZMUL AZIM BEG[2], PEDRO M. LOPES[3]
[1]*University of Coimbra, MARE, Dept. of Civil Engineering, Coimbra, Portugal, ritalmfc@dec.uc.pt*
[2]*Department of River Coastal Science and Engineering, Tulane University, Louisiana, USA, mbeg@tulane.edu*
[3]*University of Coimbra, MARE, Dept. of Civil Engineering & MATEREO, Coimbra, Portugal*

Keywords: *Flow Transition, free-surface/pressurize flow, Sewer/Urban drainage system, Steady/Unsteady flow.*

This research aims to investigate the accuracy of OpenFOAM® simulations on a free-surface/pressurize flow transition occurring in a sewer drainage between two manholes and analyse what are the acceptable simplifications in the domain and what are the implications of that simplifications.

Experiments were done in the Dual Drainage and Multi Link Element installation at the University of Coimbra, Portugal (DD-MLE) which is a real-scale system comprising among others a short 8 m pipe between two 1 m diameter manholes, other pipes connecting the different elements and equipment such as several electric valves, pressure transducers and flow-meters which can be controlled by a computer (Figure 1 [1]). The installation is fed by the main closed-circuit of the laboratory and was tested under different conditions as steady and unsteady state namely the sudden increase of the upstream flow (operating Valve 1) and constrain of downstream flow (operating Valve 2), during which measuring flow rate, pressure and water depth in different parts of the pipe were recorded.

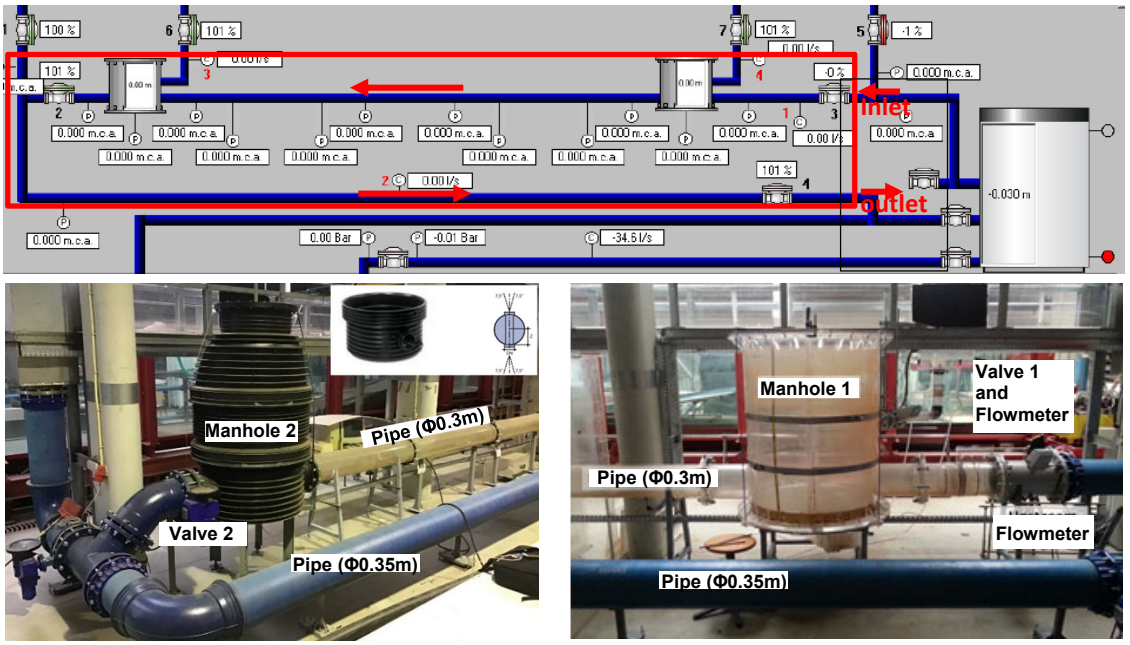


Figure 1: Sketch and photos of Dual Drainage and Multi Link Element installation at the University of Coimbra, Portugal

Numerical model used within OpenFOAM® is based on the Reynolds-Averaged Navier–Stokes equations (RANS), governing the motion of the 3D incompressible and isothermal flows, considering the free surface described by a Volume-Of-Fluid method (VOF) – interFoam, in which some issues related to the air-entrapment were implemented – airInterFoam [2] and were the turbulence is described by a SST k-ω turbulence model. Water and air were considered Newtonian fluids with kinematic viscosity equal to 1e-06 and 1.48e-05 and density equal to 1000 and 1, respectively. Computational mesh was constructed for the geometry of the manholes, the pipe between them as well as upstream and downstream pipes (Figure 1 in red and Figure 2). Boundary Conditions comprise inlet, outlet, walls (every pipes and manholes bottom and walls) and atmosphere (at the manholes upper part). Initial conditions considered a water volume, which fills the inlet and outlet pipe and a fill half pipe with constant depth, with velocity calculated according discharge flow measured in the experimental installation [3] and [4].

Investigating the Scalability of OpenFOAM and decomposition strategies

Maria E. F. Chame [1], Pedro C. de Mello [1],Eduardo A. Tannuri [1]
[1]*Numerical Offshore Tank, University of São Paulo, Brazil*

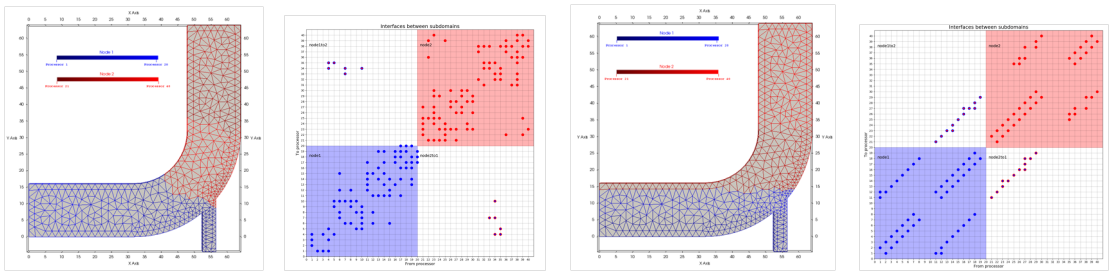
Keywords: decomposition, scalability, parallel simulation

Introduction

Calculations were carried out using the research cluster SGI facility, which has a total of 48 nodes and 960 cores. Each node consists of an Intel Xeon E5-2680 v2 processor, with 20 cores per node, having a 2.8 GHz frequency and 25.6MB cache per chip (a common shared L3 cache). The facility is provided with 128 GB RAM and 148 TB central storage. The operating system is CentOS release Linux 6.3. OpenFoam 6 was compiled with the INTEL COMPILER and MPI-library (2.1.1). Scaling is how the performance of a parallel application changes as the number of processors is increased, for further related work on parallel calculation in OpenFOAM see [1] and [2]. In this paper, some aspects of OpenFOAM parallel features were investigated, as well as, strong and weak scaling.

2D incompressible flow through an elbow - OpenFOAM tutorial case

Based on the elbow tutorial case that comes with OpenFOAM-v6 three different decomposition methods were tested. This is depicted in Figure 1, due to space limitations, only two methods are shown.



(a) Scotch **(b) Simple**

Figure 1: Decompose - tutorial case 2D

3D incompressible flow around the KVLCC2 Model Hull

Steady calculations of KVLCC2 were performed in calm water at a scale of 1:46. In Table 1 all the numerical setup was kept constant and different decomposition choices in X, Y and Z were tested. The 6.4 million-cell mesh was divided into up to 120 subdomains for the scalability study, and the execution time was stored, as shown in Figure 2. An overview of the execution time spent in each step can be seen in Figure 3. Strong scalability study offers an understanding of application scaling, where the mesh size is keep fixed and spread over an increasing number of cores. In the case of weak scaling, both the number of cores and cells are increased. Figure 4 shows weak and strong scaling results and Figure 5 how the nodes exchange information during computations for each decomposition method.

References

[1] O. Rivera, K. Fürlinger, and D. Kranzlmüller, "Investigating the scalability of openfoam for the solution of transport equations and large eddy simulations," in *International Conference on Algorithms and Architectures for Parallel Processing*. Springer, 2011, pp. 121–130.

[2] O. Rivera and K. Furlinger, "Parallel aspects of openfoam with large eddy simulations," in *2011 IEEE International Conference on High Performance Computing and Communications*. IEEE, 2011, pp. 389–396.

DEMOCRATISATION OF OPENFOAM SIMULATIONS FOR THE METAL FORMING INDUSTRY

MICHAEL CLANCY[1,2,3], ALOJZ IVANKOVIC[1,2,3], PHILIP CARDIFF[1,2,3]
[1]*School of Mechanical and Materials Engineering, University College Dublin, Belfield, D4, Dublin, Ireland*
[2]*Bekaert UTC, School of Mechanical and Materials Engineering, University College Dublin, Ireland*
[3]*SFI I-Form Centre, University College Dublin, Ireland*
michael.clancy@ucdconnect.ie, philip.cardiff@ucd.ie

Deployment, simulation tools, open source software

The increasing adoption of open source simulation packages such as OPENFOAM within industry has widened the potential user base of these tools. A main attraction to companies using such software is freedom from restrictive and cost-prohibitive software licencing as well as customisation flexibility. Currently industry use of software such as OPENFOAM is either handled by a few expert users within a company where simulation throughput is limited, or relies on third party support where the companies specific expert knowledge may not be fully utilised. A challenge is therefore seen in how to disseminate domain specific simulation experience by experts within industry. A successful example of this being the availability of simple FEM analysis procedures directly within CAD packages.

A case study is presented showcasing the potential of single-web-page application frameworks [1], containerisation and deployment software [2, 3] and other Free-Open-Source-Software resources to quickly build a user friendly simulation workflow. This case study specifically deals with delivering a solution procedure for metal forming applications using OpenFOAM. The aim of this work is to illustrate how the transition of developed solvers from single user research interests, to industry tools can be made.

The tool enables Bekaert engineers to quickly determine the tool forces and geometry outputs for a variety of metal forming operations. A streamlined web application accepts input describing the main features of the simulation. Communication with the backend server leads to containerised metal forming simulations being setup to run either locally or through the use of cloud computing services. Continuous integration and development software allows simulations to be run using the latest stable release of finite volume metal forming solvers based on the work of [4].

Acknowledgments

Additionally, the authors want to acknowledge project affiliates, Bekaert, through the Bekaert University Technology Centre (UTC) at University College Dublin (www.ucd.ie/bekaert), and I-Form, funded by Science Foundation Ireland (SFI) Grant Number 16/RC/3872, co-funded under European Regional Development Fund and by I-Form industry partners. Provision of computational facilities and support from the DJEI/DES/SFI/HEA Irish Centre for High-End Computing (ICHEC, www.ichec.ie) and ResearchIT Sonic cluster, funded by UCD IT Services and the Research Office is gratefully acknowledged. The authors thank all those involved in the organisation of OFW16 and to all the contributors that will enrich this event.

References

[1] "Angular framework," https://www.angular.io/.

[2] "Docker virtualization software," https://www.docker.com/.

[3] "Kubernetes container-orchestration," https://www.kubernetes.io/.

[4] P. Cardiff, Ž. Tuković, P. D. Jaeger, M. Clancy, and A. Ivanković, "A lagrangian cell-centred finite volume method for metal forming simulation," *International journal for numerical methods in engineering*, vol. 109, no. 13, pp. 1777–1803, 2017.

COUPLED 3D CALCULATION OF FLUID FLOW, HEAT AND MASS TRANSPORT, AND PHASE BOUNDARY SHAPE FOR CRYSTAL GROWTH PROCESSES

KASPARS DADZIS, ARVED ENDERS-SEIDLITZ
Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489, Berlin, Germany
kaspars.dadzis@ikz-berlin.de, arved.enders-seidlitz@ikz-berlin.de

Keywords: *fluid flow; heat and mass transport; phase change; dynamic mesh*

Crystalline materials are essential elements of many modern technologies, with silicon being one of the most prominent examples reaching a global production volume of 10^6 tons per year. Crystalline silicon can be obtained using a variety of growth methods from the melt (see Fig. 1), which are selected considering the balance between material quality and process costs. For example, the material perfection in the FZ method allowed to re-define the international kilogram standard with a silicon sphere in 2019, but the FZ method requires complex growth setup and process control as well as expensive raw material. Despite the differences in technology and process geometry, all these methods share the same basic physical picture with a molten zone, the growing crystal, and the crystallization front in between. In all cases various forces generate a flow in the melt influencing the heat and mass transport and thus playing a key role for material quality, see, e.g., [1]. These flows have been investigated in the literature by several research groups, often employing OpenFOAM for 3D simulation (e.g., [2, 3] for FZ; [4, 5] for CZ; [6, 7] for DS). However, the interaction between the melt flow and the crystallization front and consequently the mass transport across the interface (dopants or impurities) have been neglected or simplified in most of the models.

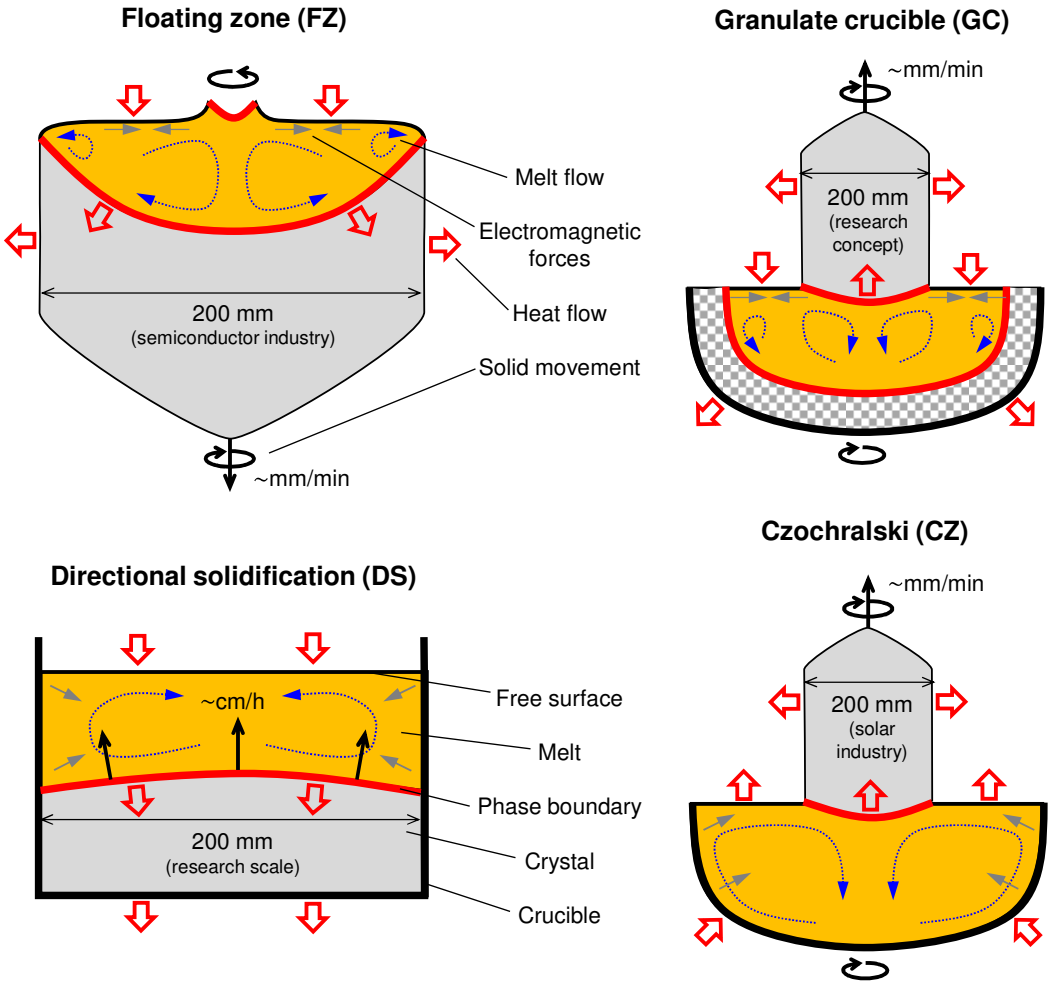


Figure 1: Growth methods for 8 inch silicon crystals (in different stages of development) from the melt. Typical geometries of the melt and the (growing) crystal as well as expected patterns of melt flow and heat transport are shown.

CHARACTERIZATION OF INTERNAL FLOW IN CAVITATING FUEL INJECTOR NOZZLES

SAI DARBHA[1], DANIEL DUKE[2], DAVID SCHMIDT[3]
[1]*Laboratory for Turbulence Research in Aerospace & Combustion (LTRAC), Department of Mechanical and Aerospace Engineering, Monash University, sai.darbha@monash.edu*
[2]*Laboratory for Turbulence Research in Aerospace & Combustion (LTRAC), Department of Mechanical and Aerospace Engineering, Monash University, daniel.duke@monash.edu*
[3]*Department of Mechanical and Industrial Engineering, University of Massachusetts, Amherst, schmidt@acad.umass.edu*

Keywords: *Homogeneous relaxation model, cavitation, multiphase flow, fuel injector nozzle*

The internal flow in fuel injector nozzles governs the spray quality and the combustion characteristics in a direct injection engine. Experimental investigation of the internal flow is limited due to lack of optical access owing to the scattering of light at the liquid-vapor interfaces. In this study, numerical simulations have been carried out within the OpenFOAM framework with a canonical fuel injector nozzle geometry. Unsteady RANS turbulence models have been used. The performance of different solvers based on both the homogeneous flow assumption and the bubble-dynamics based models characterized in this work. Firstly, the simulations are carried out using the OpenFOAM's cavitatingFoam solver which uses the Homogeneous Equilibrium Model (HEM). These simulations have been compared against the bubble-dynamics based Mass Transfer Model using OpenFOAM's 'interFOAM' solver, which incorporates the Schnerr-Sauer cavitation model. Lastly, an in-house solver based on the Homogeneous Relaxation Model (HRM), which incorporates the realistic heat transfer rates between the phases has been incorporated. To validate the simulations, they have also been benchmarked against the X-ray experiments carried out by Duke et al [1]. It has been observed that HRM solver predicts the cavitation cloud shedding and the closure region within the nozzle more accurately than the HEM solver.

Acknowledgements

The authors acknowledge the funding support received from Australian Research Council (ARC Grant ID: DP200102016).

References

[1] D. J. Duke et al., "X-ray radiography of cavitation in a beryllium alloy nozzle," International Journal of Engine Research, vol. 18, no. 1-2, pp. 39-50, 2017, doi: 10.1177/1468087416685965.

A DRIFT-FLUX-BASED METHOD FOR WASTEWATER TREATMENT APPLICATIONS

DANIEL DEISING[1], CHRIS ROBINSON[2], FRANZ JACOBSEN[3], EUGENE DEVILLIERS[4]
[1] *ENGYS GmbH, d.deising@engys.com*
[2] *CER Technologies Ltd., CERTechnologiesLtd@gmail.com*
[3] *ENGYS Austr., f.jacobsen@engys.com*
[4] *ENGYS Ltd., e.devilliers@engys.com*

Keywords: *Drift Flux, VOF, Multiphase, GIB, Wastewater Treatment*

Accurate prediction of solids settling is an important design step for the construction and enhancement of wastewater treatment plants. The most common of such facilities is the activated sludge plant (ASP) which mainly functions on the principle of biological oxidation [2]. ASP's consist of two main process units, a biological reactor and a settling tank.
In the former process, microorganisms degrade, and grow on, the organic compounds present in the wastewater. To degrade the waste, the biomass may be supplied with oxygen by an aeration system. This diffused or mechanical aeration also keeps the microorganisms in suspension. If nitrogen and phosphorus also must be removed, additional units without oxygen supply can be placed in a specific configuration with the aeration tanks. In these tanks separate mixers thoroughly suspend the microorganisms. Hence, the system consists of a sequence of interconnected aerobic, anoxic and anaerobic biological reactors. To complete the activated sludge system, produced biomass has to be separated from the clean water. For this, sedimentation is usually applied and takes place in the settling tank. In order to maintain the desired biomass concentration in the biological reactor a large portion of the settled solids is returned or recycled (the so-called Return Activated Sludge RAS); the part wasted corresponds to the produced biomass.
Suitable Computational Fluid Dynamics (CFD) methods applied to this chain of applications generally cover Lagrangian particle tracking and Euler-Euler methods. However, the most established method for modelling the interaction of the solids and liquid is the specification of a phase drift flux model stemming from experimental results, instead of describing the force interaction between the fluids. Essentially this is a strong methodological simplification compared to standard Euler-Euler approaches but needs closer examination with regard to numerical discretisation.
The resulting method strongly resembles a conventional VOF [1] method, only with an additional advection component due to phase drift. Improvements to the existing driftFluxFoam solver and generalisation to multi-species scenarios (essentially particle size distribution) are shown and alternative implementations based on single phase solvers are discussed. Furthermore, we present different applications of the model specific to wastewater treatment. Here, changes in water level over time are modelled via the generalised internal boundary (GIB) method [3] and other conventional moving mesh approaches [4].

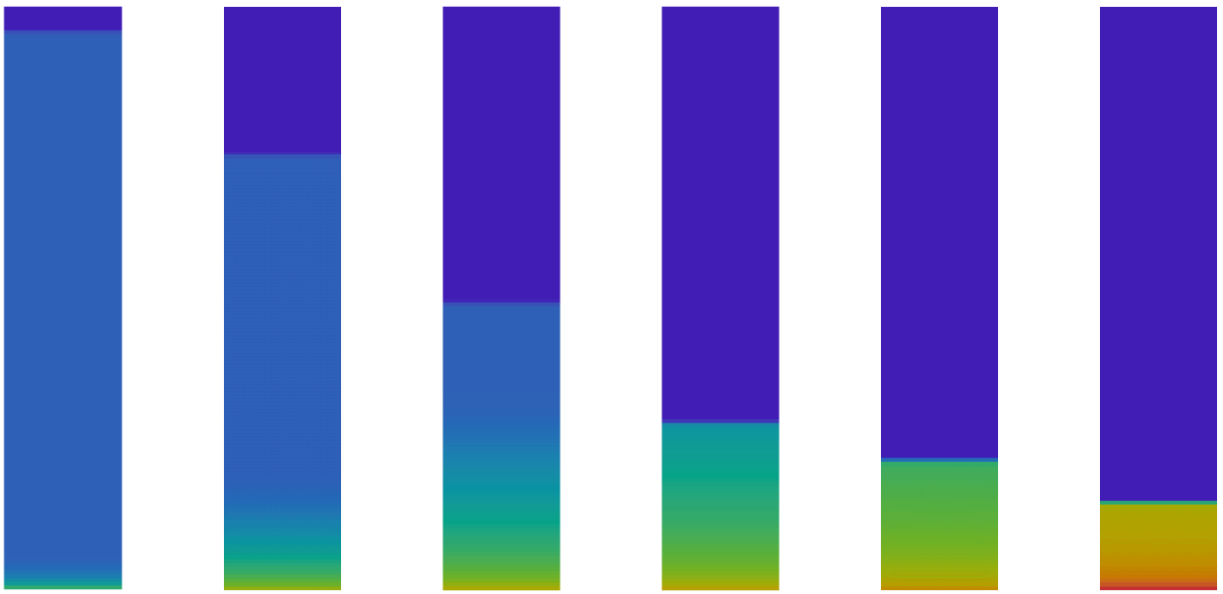


Figure 1: Concentration field (0-37g/l) over time for 1D settling case (left to right t=0.5, 3, 6, 10, 20, 130 min)

Performance of the Schnerr-Sauer Cavitation Model with a Discussion of Conditions Relevant for Lubrication

Fran Delić[1], Hrvoje Jasak[2],
[1]*University of Cambridge, fd381@cam.ac.uk*
[2]*University of Cambridge, hj348@cam.ac.uk, Wikki LTD, h.jasak@wikki.co.uk*

Keywords: *OpenFOAM, cavitation, lubrication, Schnerr-Sauer model*

Cavitation is a physical phenomena in which vapour cavities are generated in the main fluid flow as a consequence of a local drop in fluid pressure. As the pressure increases, the cavities implode, resulting in strong shock-waves which cause noise, vibrations, erosion and the disruption of the main fluid flow. Consequently, limitations on many engineering devices are determined by cavitation, more specifically its onset, type and propagation. While cavitation is known to play a vital role in the design of ship propellers, centrifugal pumps and valves, it also has an impact on the performance of lubricants [1].
Lubricants in lubricated contact are exposed to cavitating flow conditions and the behaviour of cavitation bubbles has an impact on the load-bearing characteristics. Therefore, accurate modelling of cavitation in lubricated contact increases the performance and longevity of the lubricated devices.
In this paper, the three-dimensional form of the Schnerr-Sauer model [2] is presented, along with its intended uses and limitations. Using the interPhaseChangeFoam solver in the two-phase free surface formulation currently available in OpenFOAM [3], the Schnerr-Sauer model is validated against experimental results [4] for the flow around a NACA-0009 hydrofoil.
Simulation results are compared to experimental data and different simulation set-ups are considered, with particular attention to steady-state and transient behaviour. Furthermore, the influence of turbulence on cavitation creation and propagation is explored. The performance of the Schnerr-Sauer model is discussed and the sensitivity of model parameters on the solution is evaluated. Furthermore, the influence of model parameters on the stability of the solution is checked.
In order to predict the performance of the Schnerr-Sauer model for hydrodynamic lubrication simulations, an estimate of the influence of of non-Newtonian rheology, viscosity and cavitation variables is discussed. Using the conclusions from the numerical results, the applicability of the model for simulations with lubricated contact is evaluated and further improvements are suggested.

Acknowledgments

The authors thank all those involved in the organisation of OFW16 and to all the contributors that will enrich this event.

References

[1] D. Gropper, L. Wang, and T. J. Harvey, "Hydrodynamic lubrication of textured surfaces: a review of modeling techniques and key findings," *Tribology International*, vol. 94, pp. 509–529, 2016.

[2] J. Sauer and G. Schnerr, "Development of a new cavitation model based on bubble dynamics," *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, vol. 81, no. S3 S3, pp. 561–562, 2001.

[3] OpenCFD, *OpenFOAM*, Accessed on: 14 Feb 2021 [Online]. Available: https://www.openfoam.com.

[4] P. Dupont, "Etude de la dynamique d'une poche de cavitation partielle en vue de la prédiction de l'érosion dans les turbomachines hydrauliques," EPFL, Tech. Rep., 1993.

CFD coupling methodology for realistic coastal engineering applications

BENEDETTO DI PAOLO[1], JAVIER L. LARA[2], GABRIEL BARAJAS[3], INIGO J. LOSADA[4]
[1]*IHCantabria, Instituto de Hidraulica Ambiental de La Universidad de Cantabria, benedetto.dipaolo@unican.es*
[2]*IHCantabria, Instituto de Hidraulica Ambiental de La Universidad de Cantabria, jav.lopez@unican.es*
[3]*IHCantabria, Instituto de Hidraulica Ambiental de La Universidad de Cantabria, gabriel.barajas@unican.es*
[4]*IHCantabria, Instituto de Hidraulica Ambiental de La Universidad de Cantabria, inigo.losada@unican.es*

Keywords: *coupling, 2D-3D, OpenFOAM, one-way, two-way*

Computational Fluid Dynamics (CFD) modelling of coastal, ocean and offshore engineering applications is widely used as it is essential to properly deal with wave-structure interaction (WSI). However, its high accuracy comes with an extremely high computational time, especially when large 3D domain need to be simulated. Therefore, in the last few decades, the scientific community has focused on the development of coupling methodologies with the aim of reducing the computational cost while preserving a good accuracy in reproducing the hydrodynamics ([1]). In this work, we present several applications of recently published bi-dimensional/three-dimensional (2D-3D) Navier-Stokes (NS) based couplings for studying wave structure interaction ([2]). The couplings are specified via one-way or two-way exchange of flow information, thus providing a complete tool to address one or bi-directional processes in which the three-dimensional flow is expected to be confined around the structures. The implementations are based on the OpenFOAM platform. The implementations have been successfully applied to study several cases, i.e. wave impact on breakwaters and innovative breakwaters for wave energy conversion, wave interaction with monopiles, tsunami impact and inundation on buildings and reservoir, and finally wave loads on submerged intake towers. Figure 1 shows an example of a two-way simulation of wave interaction with an innovative breakwater for wave energy conversion. More results will be shown at the conference.

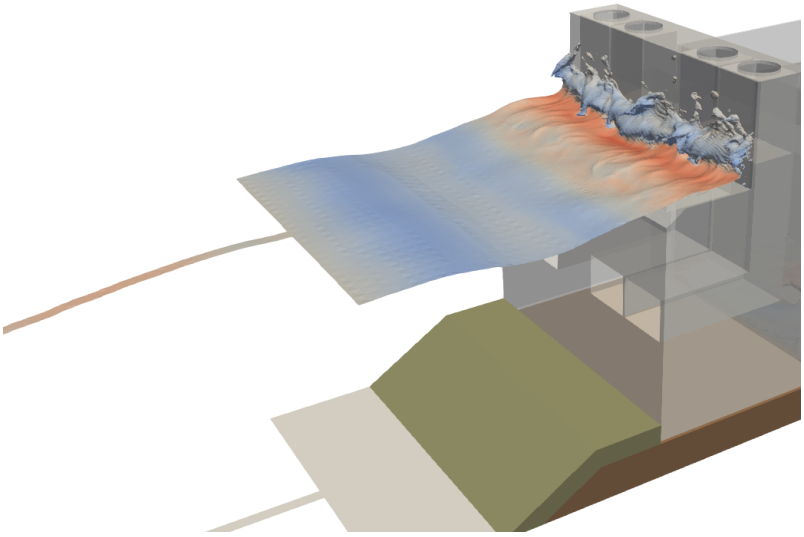


Figure 1: Wave interaction with an innovative breakwater for wave energy conversion.

References

[1] K. Sitanggang and P. J. Lynett, "Multi-scale simulation with a hybrid Boussinesq-RANS hydrodynamic," *Int. J. Numer. Meth. Fluids*, vol. 62, pp. 1013–1046, 2010.

[2] B. Di Paolo, J. L. Lara, G. Barajas, and Í. J. Losada, "Wave and structure interaction using multi-domain couplings for navier-stokes solvers in openfoam®. part i: Implementation and validation," *Coastal Engineering*, vol. 164, p. 103799, 2021.

MODELLING OF LIQUID-LIQUID SEPARATION IN A CENTRIFUGAL DEVICE USING THE EULER-EULER MULTIPHASE SOLVER TWOPHASEEULERFOAM

DRAGANA DIMITRIJEVIĆ[1], MARKUS BÖSENHOFER[1, 2], BAHRAM HADDADI[1] , MICHAEL HARASEK[1]

[1]*Institute of Chemical, Environmental and Bioscience Engineering, TU Wien, Vienna, Austria*
[2]*K1-MET GmbH, Area 4 – Simulation and Analyses, Stahlstraße 14, 4020 Linz, Austria*
dragana.dimitrijevic@tuwien.ac.at

Keywords: *CFD, OpenFOAM, multiphase, separation*

In separation processes and techniques the use of centrifugal force appeared to have a strong impact in separation of phases. Unlike the gravity being constant, centrifugal force strength can be varied either by change in the rotational speed or equipment dimensions. Devices for performing this unit operation are cyclone separators for gas suspension, hydrocyclones for liquid-solid suspensions and centrifuges for liquid-solid, liquid-liquid and gas-gas separation. In such devices the heterogeneous suspension is subjected to the centrifugal force to separate the phases of different density. Here, two group of devices can be distinguished: cyclones and hydrocyclones where centrifugal force is created by rotation of suspension entering the apparatus through a tangential inlet itself with respect to the stationary apparatus and centrifuges where centrifugal force is created with the suspension undergoing rotation with respect to the revolving apparatus boundary [1]. Replacing the gravity with the centrifugal force enables the separation of liquids of low density difference and those with tendency to emulsify [2].
This work will focus on the use of centrifugal force created in revolving devices or by revolving parts of the device. Alignment (horizontal or vertical), geometry, pressure, internals, etc. can be varied for such devices to control the separation process.
The goal of this work is to model the separation of a binary mixture in a centrifugal separator device using Computational Fluid Dynamics (CFD). The simulation results will be compared with experimental data from experiments, e.g. flow behaviour and separation efficiency of the simulated centrifugal device. The separation device is rather small which is one of the challenges of this work because separation of two liquid phases at this scale is not widely known and explored. Moreover, current research suggests that the prediction of liquid-liquid separation in small devices is challenging due to the complex hydrodynamic processes [3].
The CFD simulations are carried out using the Euler-Euler multiphase solver twoPhaseEulerFoam of the CFD toolbox OpenFOAM®. The solver employs the two-fluid concept for a continuous and dispersed phase [4].
The investigated process aims to separate a mixture of water and cyclohexane in a lab-scale centrifugal separator. The separation zone is cylinder of 50 mm diameter and length of 150 mm. The mixture is introduced at a Reynolds number of approx. 120 via the feeding pipe, which is 8 mm in diameter and is located at the separation zone's shaft. The process is operated at ambient pressure (1 atm) and temperature (20 °C) and centrifugal forces are introduced via rotation of the separation zone.

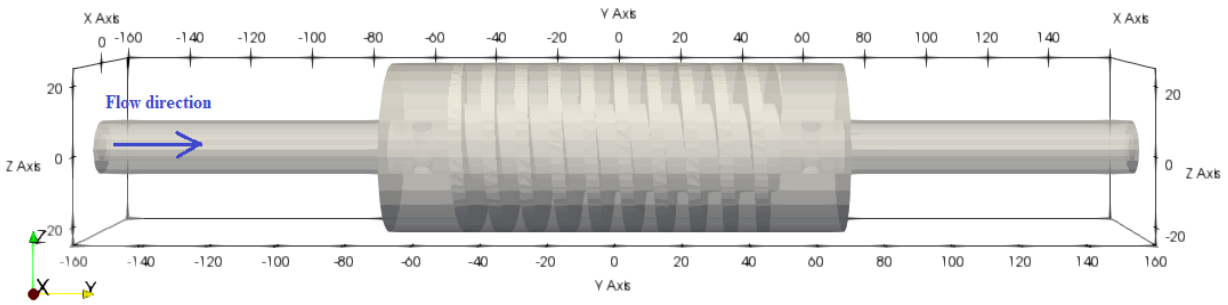


Figure 1: Representation of the geometry to be simulated; exported from ParaView – dimensions in [mm]

MESO-SCALE SOLIDIFCATION MODELS FOR METALLIC ADDITIVE MANUFACTURING PROCESSES

DANIEL DREELAN[1], ALOJZ IVANKOVIC[2], DAVID J. BROWNE[3]
[1]*University College Dublin, Sch. of Mech. & Materials Engineering, daniel.dreelan@ucdconnect.ie*
[2] *University College Dublin, Sch. of Mech. & Materials Engineering, alojz.ivankovic@ucd.ie*
[3] *University College Dublin, Sch. of Mech. & Materials Engineering, david.browne@ucd.ie*

Keywords:
Additive Manufacturing, Crystal Growth, Solidification, Material Science, Microstructure, Thermal Stress, Porosity

The advent of additive manufacturing (AM) in recent decades has presented new challenges to the metallurgical and numerical modelling communities. The effects that processing parameters have on the mechanical performance of AM produced parts have yet to be fully understood, with microstructural modelling proving to be a powerful tool which offers deeper insights than would be possible by experiment alone. AM processes boast several revolutionary advantages compared to traditional manufacturing processes. Near net shape, highly optimised structures can be produced by a single machine and can be tailored to new applications with minimal machine downtime and cost to the manufacturer. However, widespread adoption of AM is still hampered by anisotropic mechanical properties, and poor fatigue performance.

The mechanical performance of a material is not only dependent on its chemical makeup, but also the distribution of phases in its microstructure. The thermal, flow and solute conditions during solidification are critically important in determining grain size, crystallographic texture & orientation, as well as residual stresses and porosity, all of which contribute fundamentally to mechanical performance. During the Powder Bed Fusion (PBF) process, a 3D part is generated layer by layer by melting powder with a high energy heat source such as a laser or electron beam. Due to the extreme thermal gradients and cooling rates resulting from these aggressive heating and cooling cycles, and the fact that partial or full remelting of previous layers occurs at every pass, predominantly columnar microstructures are observed in as-printed parts. This crystallographic texture leads to high anisotropy in final mechanical properties, as well as an elevated risk of hot cracking or tearing at the boundaries between columnar grains during the printing process.

Our ambition is to develop a multi-scale approach to model the powder bed fusion process from melting to solidification: grain nucleation, growth and impingement, residual stresses and porosity. In order to feasibly predict microstructural features at the scale of an entire part, trade-offs need to be made between accuracy and efficiency.

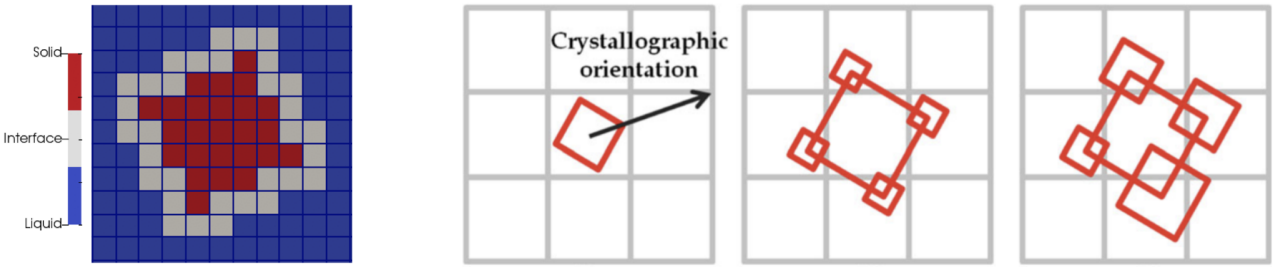


Figure 1: Cellular automata representation of the discrete states of the solidification model (*left*). Schematic representation of the interface propagation algorithm used [1] (*right*).

Cellular automata have proven to be a fast and efficient technique for microstructure modelling of AM processes. Their defining characteristic is that they are semi-discrete, as each cell can exist in only one of a number of discrete states at any given moment. For solidification, these states would naturally be solid and liquid. In order to continuously model the transition between solid and liquid, a single layer of interface cells is used to separate solid and liquid cells as illustrated in fig.1. The advantage of discrete states here is that growth is only calculated for interface cells, which typically make up only a small fraction of the total cells in the domain, meaning that the majority of cells are essentially ignored during the computation. This allows for the nucleation and growth of large numbers of individual grains in domain sizes up to the scale of an entire part. Undercooling, i.e., the temperature difference below the liquidus temperature, is considered to be the driving force for solidification, with growth velocities increasing non-linearly with increasing undercooling.

NUMERICAL SIMULATIONS OF COUNTER-ROTATING PUMP-TURBINE WITH A NEW HEAD-LOSS PRESSURE BOUNDARY CONDITION

JONATHAN FAHLBECK[1,*], HÅKAN NILSSON[1], SAEED SALEHI[1]
[1] *Department of Mechanics and Maritime Sciences, Chalmers University of Technology, Sweden*
*Email for correspondence: fahlbeck@chalmers.se

Keywords: *Pump-turbine, pump-storage, counter-rotating, headLossPressure, head-losses*

With an increasing amount of energy from renewable sources, such as wind and solar, the need of complementary controllable energy sources increases. Hydropower plays a key role to provide a stable and flexible electrical grid. By storing large amount of water when there is excess power in the grid, and later utilise the stored water when there is a lack of power, hydropower is a stabilising unit for the electrical grid [1]. The ALPHEUS EU project has the aim to develop a low-head to ultra low-head seawater based Pumped Hydropower Storage (PHS) solution with a pump-turbine unit [2, 3]. The main goal of the ALPHEUS project is that the pump-turbine unit should have a round-trip efficiency of 70 - 80 % and a switching time of about 120 s. PHS use the potential energy by pumping water to a reservoir. The potential energy is later extracted by reversing the pump to a turbine. Three pump-turbine concepts are to be investigated, a counter-rotating shaft-driven, a counter-rotating rim-driven, and a positive-displacement alternative. A rigorous optimisation process will be applied to maximize the round-trip efficiency for a wide range of operating conditions. In this work an initial design of a counter-rotating shaft-driven alternative is considered. In the ALPHEUS project an optimised counter-rotating shaft-driven pump-turbine will be experimentally evaluated in model scale, in the hydraulic laboratory at TU Braunschweig. The experiments are partly made in order to generate experimental test data. The numerical models are later going to be evaluated with the experimental test data. The experimental test facility consists of a two open reservoir surfaces, upper and lower. In turbine-mode, water flows from the upper to the lower reservoir, and it is pumped from the lower to the upper in pump-mode. The reservoirs are connected with a series of pipes, including bends and other obstacles in the flow path. The machine is going to be tested at different operating conditions and it is thus hard to estimate the flow rate for any given case. This is because head, or pressure, losses scale quadratic to a change in flow rate. An option to overcome this problem in a numerical framework is to include head losses at the boundaries of the computational domain. The flow rate in the simulation is calculated as a balance between the available pressure and the losses in the system. In OpenFOAM there is not any available boundary condition that can include up-/down-stream losses at a patch. This present work demonstrates a new pressure boundary condition, `headLossPressure`, developed by Fahlbeck [4]. The boundary condition is an extension of the available `totalPressure` boundary condition. It uses the volumetric flux to adjust the static pressure on the patch according the Bernoulli equation [5]. The `headLossPressure` is an incompressible pressure boundary condition for in-/outflow patches. If the patch has inflow the losses are subtracted, and for an outflow patch the losses are added.

The basic functionality of the `headLossPressure` boundary condition is evaluated on a simple test case by Fahlbeck [4]. In this work the boundary condition is used together with the initial design of a model scale counter-rotating shaft-driven pump-turbine in the ALPHEUS project. The blade geometries shown in Figure 1a were designed by the Advanced Design Technology Ltd (ADT) company. The diameter of the runners is 27 cm, runner 1 (red) has eight blades, and runner 2 (blue) has seven blades. Runner 1 has a rotational speed of 1453 RPM in pump mode and 832 RPM in turbine mode, runner 2 rotates at 90 % of the speed of the first runner in each mode.

The numerical simulations are made on the computational domain shown in Figure 1b. The numerical simulations are made with unsteady CFD at one operating condition in both pump and turbine modes. The numerical framework includes the two rotating runners, hub, support-struts, and contraction/extraction parts. The simulations utilise the unsteady incompressible `pimpleFoam` solver and the k-ω SST model is used to account for turbulence. The convective terms of the momentum equations are discretised using the LUST scheme, and temporal discretisation with the backward scheme. The `pressureInletOutletVelocity` and `headLossPressure` are used as boundary conditions for velocity and pressure, respectively, at both the inlet and the outlet. The pressure boundary condition is set to operate with a total height difference of 8 m, the full pipe length is roughly 16 m, one 90° bend, and some additional flow obstacles are included.

BUBBLE PLUME APPLICATION IN WATER OXYGENATION USING DEVELOPED MPPICFOAM

FARZAD FARAJIDIZAJI[1], MICHEAL CAIRNS[2], THOMAS Y ABADIE[3], BEN BREEN[4], YAN DELAURE[5]

[1]*School of Mechanical and Manufacturing Engineering, Dublin City University, Ireland, farzad.farajidizaji@dcu.ie*
[2]*School of Mechanical and Manufacturing Engineering, Dublin City University, Ireland, cairns.micheal2@mail.dcu.ie*
[3]*Department of Chemical Engineering, South Kensington Campus, Imperial College London, U.K. t.abadie@imperial.ac.uk*
[4]*Sulzer Pump Solutions Ireland Ltd, Ben.Breen@sulzer.com*
[5]*School of Mechanical and Manufacturing Engineering, Dublin City University, Ireland, yan.delaure@dcu.ie*

Keywords: *Bubble Plume, MPPICFoam, Oxygenation, Bubble Dynamic*

Bubble plumes occur in oceanic waters and lakes naturally [1], and are widely used in industrial mass transfer processes. The MPPICFoam solver has been used in this study to simulate oxygen transfer to water from microbubble plumes. MPPIC (Multiphase particle-in-cell) [2] is a Eulerian-Lagrangian method, which was originally developed to simulate granular flow covering a broad range of solid particle loading. It has been adapted in this study with a modified drag model and the coupling of two scalar transport equations for dissolved oxygen and nitrogen transport. Bubbles dynamics can change dramatically depending on the flow regime going from rigid like spherical bubbles in the sub-millimetric range to deformable spherical cap or ellipsoidal shapes for the larger bubbles. A general drag coefficient which accounts for a wide range of flow regimes in pure water [3] has been incorporated into the MPPIC library;

$$C_D = max\left[min\left[\frac{16}{Re}(1+0.15Re^{0.687}),\frac{48}{Re}\right],\frac{8}{3}\frac{Eo}{Eo+4}\right] \quad (1)$$

where the Eötvös number is defined as $Eo = g\Delta\rho d/\gamma$. γ is the surface tension, d the bubble diameter, $\Delta\rho$ the difference between the carrier liquid density ρ_f and the gas phase density ρ_g. In order to account for dissolve oxygen transfer, it has been assumed, in the current solution, that each bubble is an infinite source of oxygen and it constantly diffusing oxygen to the environment based on Henry's law [4]. The oxygen flux, S_0, across the unit interface area is expressed as [5];

$$S_0 = k(C_s - C_b), \quad (2)$$

where k is the gas transfer coefficient, C_s is the oxygen concentration at the equilibrium state, and C_b is the oxygen concentration in the liquid. The total pressure of each individual bubble has been calculated by adding atmospheric pressure, hydrostatic pressure as well as the effect of surface tension on bubble pressure as below;

$$p_b = p_{atm} + \rho_f g z + \frac{4\gamma}{d}, \quad (3)$$

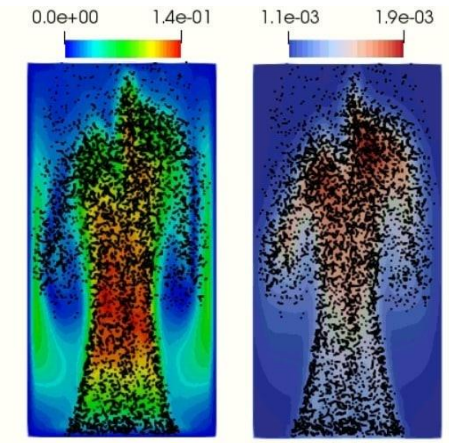


Figure 1: Bubble plume simulation-velocity(m/s) contour (left figure) and dissolved oxygen(gram/litre) contour (right figure) in early time-steps

WAVE INTERACTION WITH A TENSION-LEG OFFSHORE WIND TURBINE PLATFORM WITH A PERFORATED OUTER CYLINDER REPRESENTED BY POROUS MEDIA

ANNA FEICHTNER[1], GAVIN TABOR[2], ED MACKAY[3], PHILIPP R. THIES[3], LARS JOHANNING[3]
[1]*Renewable Energy Group, CEMPS, University of Exeter, af506@exeter.ac.uk*
[2] *Engineering, CEMPS, University of Exeter, g.r.tabor@exeter.ac.uk*
[3]*Renewable Energy Group, CEMPS, University of Exeter*

Keywords: *CFD, wave-structure interaction, dynamic mesh, porous media, moving porous body*

One of the key engineering challenges of floating offshore wind turbines is the stability of the platform, which affects loads on mooring lines and the turbine. Equipping the platforms with porous outer shrouds has the potential to function as a passive motion damping mechanism to attenuate the motion responses, resulting in reduced loads on the mooring and structure and larger ranges of operational conditions.

This work presents CFD modelling of wave interaction with a tension-leg platform (TLP) equipped with an outer perforated cylinder. The perforated cylinder is represented by its macro-scale effects on the fluid flow by means of a porous zone, as shown in Figure 1. The open-source code OpenFOAM is used in combination with the OlaFlow/IHFoam [1] library, solving the Volume-Averaged RANS (VARANS) equations. The flow through the porous barrier is approximated using a model for the pressure drop as a function of flow velocity, rather than explicit modelling of the flow through the openings. This macro-scale approach requires fewer mesh cells than explicit modelling approaches, with a corresponding reduction in computational requirements. The pressure-drop coefficients are defined as a function of porosity based on work by [2, 3] and [4]. The validity of this porosity representation was demonstrated for wave interaction with thin perforated static structures in [5, 6] and is extended here to moving bodies.

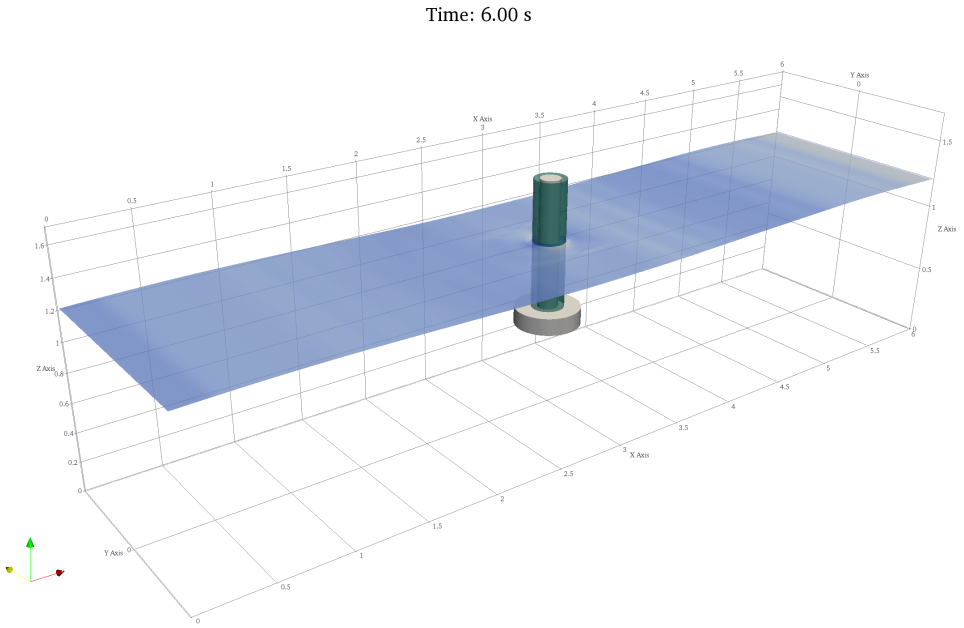


Figure 1: Wave interaction with a simplified TLP (in gray) equipped with a porous cylinder (in green).

Due to the relatively small motions of a TLP, a dynamic/deforming-mesh method is considered to be most appropriate and computationally efficient. OpenFOAM's 6-degree-of-freedom (DOF)-motion solver has been extended to account for the

CFD-DEM MODELING OF PARTICLE-LADEN VISCOELASTIC FLOWS IN HYDRAULIC FRACTURING OPERATIONS

C. FERNANDES[1], S.A. FAROUGHI[2], R. RIBEIRO[1], J. MIGUEL NÓBREGA[1], G.H. MCKINLEY[3]

[1]Institute for Polymers and Composites, University of Minho, Campus de Azurém, 4800-058 Guimarães, Portugal, cbpf@dep.uminho.pt, a58714@alunos.uminho.pt, mnobrega@dep.uminho.pt
[2]Petrolern LLC, 1048 Arbor Trace NE, Atlanta, GA 30319, USA, faroughisalah@gmail.com
[3]Hatsopoulos Microfluids Laboratory, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA, gareth@mit.edu

Keywords: *Random arrays of spheres, Drag coefficient, Viscoelastic fluids, Oldroyd-B model, Eulerian-Lagrangian formulation, Discrete particle method*

The ability to simulate the behavior of dense suspensions, using computationally-efficient Eulerian-Lagrangian techniques, requires accurate particulate-phase drag models that are valid for a wide range of process fluids and material parameters. The currently available closed-form drag models – which enable rapid calculation of the momentum exchange between the continuous and dispersed phases – are only valid for dilute suspensions with inelastic base fluids. The present work aims at developing appropriate drag models for moderately-dense suspensions (particle volume fractions < 20%), in which the continuous phase has viscoelastic characteristics. To this end, we parametrize the suspension properties through the Deborah number and the particle volume fraction, and compute the evolution in the drag coefficient of spheres translating through a viscoelastic fluid that is described by the Oldroyd-B model. To calculate the drag coefficient, we resort to three-dimensional direct numerical simulations (DNS) of unconfined viscoelastic creeping flows ($Re < 0.1$) past random arrays of stationary spheres, over a wide range of Deborah numbers ($De < 5$), volume fractions ($\varphi < 20\%$) and particle configurations. From these calculations we obtain a closure law $F(De, \varphi)$ for the drag force in a fluid described by the quasi-linear Oldroyd-B viscoelastic fluid model (with fixed retardation ratio $\beta=0.5$), which is, on average, within 4.7% of the DNS results. Subsequently, this closure law was incorporated into a CFD-DEM Eulerian-Lagrangian solver to handle particle-laden viscoelastic flow calculations, and two case studies were simulated to assess the accuracy and robustness of our numerical approach. These tests consisted of simulating the settling process in Newtonian and viscoelastic fluids within eccentric annular pipes and rectangular channels; configurations commonly employed in hydraulic fracturing operations. The numerical results obtained were found to be in good agreement with experimental data available for suspensions in Newtonian matrix fluids. For the case of viscoelastic fluids, the resulting particle distribution is presented for different elasticity numbers (i.e., $El = De/Re$) and particle volume fractions, and the results provide additional insights into the pronounced effects of viscoelastic matrix fluids in hydraulic fracturing operations.

Acknowledgements

This work is funded by FEDER funds through the COMPETE 2020 Programme and National Funds through FCT (Portuguese Foundation for Science and Technology) under the projects UID-B/05256/2020, UID-P/05256/2020 and MIT-EXPL/TDI/0038/2019 – APROVA – Aprendizagem PROfunda na modelação de escoamentos com fluidos de matriz Viscoelástica Aditivados com partículas (POCI-01-0145-FEDER-016665). The authors would like to acknowledge the Minho University cluster under the project NORTE-07-0162-FEDER-000086 (URL: http://search6.di.uminho.pt), the Minho Advanced Computing Center (MACC) (URL: https:// macc.fccn.pt), the Texas Advanced Computing Center (TACC) at The University of Texas at Austin (URL:http://www.tacc.utexas.edu), the Gompute HPC Cloud Platform (URL: https://www.gompute.com) for providing HPC resources that have contributed to the research results reported within this work.

GFMFOAM: A VOLUME OF FLUID AND GHOST FLUID METHOD SOLVER FOR INCOMPRESSIBLE FREE SURFACE FLOW

PAULIN FERRO[1], PAUL LANDEL[2], MARC PESCHEUX[3]
[1]*SARL G-MET Technologies, paulin.ferro@g-met.fr*
[2]*SARL G-MET Technologies, paul.landel@g-met.fr*
[3]*SARL G-MET Technologies, marc.pescheux@g-met.fr*

Keywords: *VoF, GFM, free surface flows*

Incompressible two phases flows are widely used for ship and offshore hydrodynamic applications and still remain challenging to simulate properly. In this context two types of problems are generally encountered: transient simulations such as waves loads, seakeeping or any violent free surface flow and steady-state problems such as hydrodynamic resistances of ships/structures. While the first family of problems requires low Courant-Friedrichse-Lewy (CFL) numbers, the second one can accept high CFL numbers (> 100) in order to reduce the simulation time as long as the accuracy is preserved (which is a challenge for CFD codes). In a marine context, authors have traditionally reported the limitations of the standard incompressible two-phase flow solver interFoam. Firstly, Meyer et al. [1] have shown that MULES algorithm (Multidimensional Universal Limiter with Explicit Solution, [2]) needs additional iterations (PISO [3] and SIMPLE [4]) and sub-cycles for sufficient stability in comparison to a commercial solution for large time step simulations. Secondly, the presence of spurious air velocities has been widely reported ([5], [6], [7]). Vukčević et al. [6] have stated that spurious air velocities occur due to the imbalance between pressure and density gradients during the pressure-velocity coupling and propose the use of the Ghost Fluid Method (GFM) [8] to solve this issue. In this context, an incompressible two-phase flow solver (named gfmFoam) based on Volume-of-Fuid [9] and GFM is proposed. Firstly, in gfmFoam, the convection term in the phase fraction equation is discretized using algebraic schemes: CICSAM [10], MCICSAM [11], HRIC [9], MHRIC [13] or BICS [14] unlike the standard approach : MULES. The deferred correction method is retained to increase numerical stability. Secondly, gfmFoam benefits of the GFM for pressure and density discontinuity handling (Figure 1). As indicated above, the use of GFM is motivated by its ability to alleviate light phase acceleration and preserve a continuous velocity field across the free surface. This results in lower CFL number allowing larger time step. The method, implemented following [6] has a different momentum formulation [15]. Finally, gfmFoam is tested on various test cases ranging from dam break transients to ship resistance assessment. Comparisons with interFoam solver are carried out in term of accuracy, robustness and CPU time.

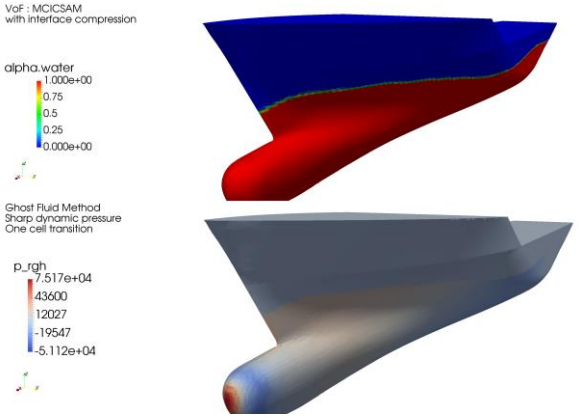


Figure 1: Full Scale Kriso Container Ship (KCS) [16] simulation with gfmFoam

Acknowledgements

The authors thank all those involved in the organisation of OFW16 and to all the contributors that will enrich this event.

References

[1] Meyer, J., Renzsch, H., Graf, K. and Slawig, T., Advanced CFD-Simulations of free-surface flows around modern sailing yachts using a newly developed OpenFOAM solver, The 22nd Chesapeake Sailing Yacht Symposium, Annapolis-Maryland, (2016).

[2] Damián, S.M., Nigro, N.M., 2014. An extended mixture model for the simultaneous treatment of small-scale and large-scale interfaces. Int. J. Numer. Methods Fluid. 75 (8), 547–574.

Magneto-Thermal-Hydrodynamics of Low Temperature Plasmas for Advanced Manufacturing Applications

Tom Flint[1], Mike Smith[2], Pratheek Shanthraj[3]
[1]*The University of Manchester, Thomas.Flint@manchester.ac.uk*
[2]*The University of Manchester, Mike.C.Smith@manchester.ac.uk*
[3]*The University of Manchester, Pratheek.Shanthraj@manchester.ac.uk*

Keywords: *Magnetohydrodynamics; Welding; Mass Transfer; Additive Manufacturing*

Fusion welding is the most common method for assembling large metallic structures, often in safety critical applications such as nuclear power plant reactor pressure vessels, and joints in commercial jet engines. In fusion welding, a concentrated heat source is established through an electrical arc discharge. This heat is generated through Ohmic heating of the low electrical conductivity shielding gas, and generally high conductivity metallic substrate. This causes localised melting that is used to join components. This localised heating leads to the generation of steep temperature gradients and rapid thermal transients, which in turn lead to large variations in micro-structure and mechanical properties, and the generation of substantial levels of residual stress. There is a considerable interest in the mathematical modelling of fusion welding processes, for process optimisation and quality control.

Mathematical modelling of the fusion welding process requires a description of the momentum transfer between the shielding gas and substrate, the heat transport within the system, the conservation of mass of the chemical components present in the domain, and the evolution of the magnetic field evolution in the system. It is possible to capture all the heat and mass transfer physics in these processes by developing a mathematically descriptive framework that addresses all of the above.

In this work we present a magnetohydrodynamic (MHD) formulation that is capable of describing systems with gradients in electrical conductivity, when the magnetic permeability in the domain is constant. The derived MHD induction equation, in terms of the magnetic field, is coupled with the Navier-Stokes equation, a multi-component volume of fluid description, and an energy transport equation. The final set of equations are implemented in OpenFOAM. The framework is first validated against the Hartmann flow problem, where excellent agreement with the analytical flow profile is observed. The framework is then used to simulate electrical arc welding processes involving Aluminium and Stainless steel alloys (chosen to maintain a constant magnetic permeability in the domain).

The thermal-fluid dynamics of a multi-phase mixture is described through the conservation laws for momentum, composition and energy transport. These relations are supplemented with a multi-component magnetic induction equation that describes the evolution of the magnetic field in the domain with gradients in electrical conductivity. Assuming magnetic permeability is constant in the domain($\nabla \mu_M = 0$), a transient magnetic induction equation is formulated from the following Maxwells equations:

$$\frac{\partial \boldsymbol{D}}{\partial t} + \boldsymbol{J} = \nabla \times \frac{\boldsymbol{B}}{\mu_M}, \tag{1a}$$

$$0 = \nabla \cdot \boldsymbol{B}, \tag{1b}$$

$$\frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \boldsymbol{E}, \tag{1c}$$

$$\boldsymbol{J} = \sigma_E \left[\boldsymbol{E} + \boldsymbol{U} \times \boldsymbol{B}\right], \tag{1d}$$

where $\boldsymbol{D}$ is the electric flux density, $\boldsymbol{E}$ is the electric field intensity, $\boldsymbol{J}$ is the electric current density, $\boldsymbol{U}$ the velocity, and $\boldsymbol{B}$ is the magnetic field. Furthermore σ_E is the electrical conductivity of the medium, and μ_M is the magnetic permeability. The temporal induction equation is coupled to the Navier-Stokes equations for multi-phase flow using the one-fluid approach [1, 2, 3].

$$\frac{\partial \left(\rho \boldsymbol{U}\right)}{\partial t} + \nabla \cdot \left(\rho \boldsymbol{U} \otimes \boldsymbol{U}\right) = -\nabla P + \nabla \cdot \boldsymbol{\tau} + \left(\boldsymbol{J} \times \boldsymbol{B}\right) + \boldsymbol{\Phi}. \tag{2}$$

where ρ the mass density, P is the fluid pressure, and $\boldsymbol{\tau}$ is the viscous stress tensor. In Equation 2, the Lorentz force, $\boldsymbol{J} \times \boldsymbol{B}$, is included. The Lorentz force is a body force induced in a fluid carrying a charge density in a magnetic field, $\boldsymbol{B}$. Additional

Numerical Modelling Approaches for Simulating Powder Bed Fusion Processes

Tom Flint[1], Gowthaman Parivendhan[2], Mike Smith[1], Alojz Ivanković[2], Philip Cardiff[2]
[1]*Dalton Nuclear Institute, The University of Manchester, Thomas.Flint@manchester.ac.uk*
[2]*University College Dublin, gowthaman.parivendhan@ucdconnect.ie*

Keywords: *Advanced Manufacturing; State Transition; Powder Bed Fusion*

Powder bed fusion (PBF) processing is a rapidly developing additive manufacturing technique, where layers of metallic substrate are deposited via the application of a concentrated heat source causing localised melting and vaporisation, before the substrate solidifies into its final configuration. During these processes, with sufficient power density, the heat source may cause localised vaporisation. This vaporisation generates a recoil effect due to the large increase in volume of the metallic phase. With even greater power density, the heat source generates a thermo-capillary, or 'keyhole', through the substrate allowing large penetration of the heat source as in electron beam welding. The recoil effect is known to be the dominant force in the thermo-capillary; stabilising the structure against collapse. Predicting substrate evolution during PBF processes is a complex challenge involving the prediction of heat and mass transfer in the fluid state, prediction of the micro-structural evolution, and predictions of the residual stress and distortion that develop in the component. The first step in developing a modelling framework for PBF processes is understanding the complex heat and fluid flow. This is the driving force for the micro-structural and mechanical changes in the substrate.

Modelling the heat and mass transfer in the PBF process relies on a mathematical description of the conservation of momentum, conservation of mass, a description of energy transport in the domain, and finally a description of the evolution of the interface between the metallic substrate and the shielding gaseous and/or vapour phase. The state of the art approaches in the literature assume that both the metallic substrate and gaseous components in the domain are incompressible, with $\nabla \cdot \boldsymbol{U} = 0$, with an additional phenomenological recoil surface force added to describe the momentum induced by the vaporising substrate [1]. However, recently a new approach was proposed, capable of describing the evolution of multi-component substrates experiencing fusion and vaporisation state transitions [2]. In this approach, instead of assuming the material derivative of density is negligible to derive the continuity equation, the change in density due to vaporisation and condensation is explicitly included in the framework, and the resulting recoil force at the interface of the metallic substrate a consequence of this step-change in density through vaporisation transitions. This approach is also capable of predicting the diffusive and advective mixing in the liquid and vapour states through the solution of N advection-diffusion equations for the chemical components present in the domain. This approach has been successfully applied to predict the more fundamental scenarios of binary vapour bubble collapse into a heterogeneous binary mixture, and the evolution of a thermo-capillary in an electron beam weld - showing the effects of preferential element evaporation from the substrate [2].

Frameworks using the $\nabla \cdot \boldsymbol{U} = 0$ continuity constraint, and phenomenological recoil term, have been shown to predict the evolution of the substrate effectively during PBF processes. Therefore the additional fidelity achieved, by explicitly accounting for the density change through the vaporisation state transition, may not be required when modelling PBF processes due to the relatively low rate of vapourisation in these processes. The higher fidelity approach may therefore only be beneficial when the multi-component nature of the substrate, and explicit description of the recoil effect at the interface, is required.

In this work, we compare the two approaches to modelling the PBF process. The melting and solidification along a track of Ti-6Al-4V powder is investigated. In approach 1, where the $\nabla \cdot \boldsymbol{U} = 0$ continuity constraint is used, the domain contains two phases (metallic and gaseous). To make the results comparable, in the second approach instead of decomposing the alloy substrate into chemical components as in [2], only a single metallic flavour is considered; such that the domain in the second approach contains a metallic condensed phase, a metallic vapour phase, and a shielding gas phase. In both approaches the same form of the Navier-Stokes equations are used to describe the flow, using the 'one fluid' approach:

$$\frac{\partial (\rho \boldsymbol{U})}{\partial t} + \nabla \cdot (\rho \boldsymbol{U} \otimes \boldsymbol{U}) = -\nabla P + \nabla \cdot \boldsymbol{\tau} + \boldsymbol{\Phi}. \tag{1}$$

where $\boldsymbol{U}$ is the velocity, ρ the mass density, P is the fluid pressure, and $\boldsymbol{\tau}$ is the viscous stress tensor. In the approach of Flint et al. the full form of the stress tensor is used as the divergence of the velocity field is non-zero. Additional effects, such

MOMENTUM EXTRACTION BY POROUS FORMS FROM BOUNDARY LAYER FLOWS

EDEN FURTAK-COLE[1] and JACK GILLIES[2]
[1]*Desert Research Institute, efurtak@dri.edu*
[2]*Desert Research Institute, jack.gillies@dri.edu*

Keywords: *Porous forms, Spalart-Allmaras IDDES, drag force measurement, wind tunnel validation*

Porous forms are ubiquitous on the Earth's surface, yet their effects on the planetary boundary layer are largely absent from atmospheric models. Boundary-layer flows have important implications for wind erosion, pollutant dispersion, fluxes of moisture, and wind power generation. Computational fluid dynamics simulations can be applied to these problems, though the treatment porous forms remains under-developed. While fully resolving the flow through most vegetative [1] or manufactured porous structures[2] remains computationally intractable, it is often not known what the appropriate momentum extraction term in the Navier-Stokes equations should be for a given porous form. For this reason it is desirable that wind tunnel studies of porous forms be used to validate CFD simulation. In particular, studies of porous forms of complexity that straddles what is possible with both fully-resolved geometries in clear fluid simulation, and simulation using porous media momentum extraction terms.

This study focuses on manufactured porous forms, tested in a recirculating wind tunnel with an 8 m long, 0.76 m (high) x 0.92 m (wide) working section with a smooth plywood floor. Porous cubes were constructed with cylindrical holes. Different permeabilities and porosities were created by varying the number and diameters of the holes, though the frontal area was held constant across all the forms created. Holes were created in three directions normal to the sides of the cubes: front to back (FB), side to side (SS), and top to bottom (TB). The combinations tested were FB, FB-SS, and FB-SS-TB. In each case, the flux through the bottom face was zero. Wind speed was measured using a Pitot-static tube positioned 5 cm (0.5 h, where h = 10 cm, the height of the largest elements) above the wind tunnel floor, 5 cm (0.5 h) in front of the element, and 5 cm (0.5 h) to the side. A second Pitot-static tube was positioned 20 cm (2 h) above the wind tunnel floor directly above the element. Flow velocity in the wind tunnel was prescribed at five levels, and a quadratic relationship between velocity and drag force on the porous forms was observed.

Eddy-resolving simulations were performed on a selection of experiments using pimpleFOAM with a Spalart-Allmaras IDDES turbulence model [3]. A small section of the wind tunnel around the porous forms was modeled. The inlet boundary condition for this section was constructed from measurements taken in the wind tunnel. A log-layer inlet was based on the measured free-stream velocity and known aerodynamic roughness of the wind tunnel. This one dimensional function was applied to the two dimensional inlet as a function of nearest wall distance.

Excellent agreement between the measured and simulated forces on the form were observed at a moderate computational cost. The ratio of wind speeds measured in front and behind the forms was also in good agreement between the simulations and experimental data. Data from the openFOAM simulations offer a view of the internal flow structure, providing insight into the internal Reynolds number, turbulent wake, and fluxes through the faces of the form. The number and orientation of the cylindrical holes in the forms was found to greatly affect the turbulent wake. Pressure on the surface of the forms explain the increase in drag force observed for forms with holes normal to the flow direction.

Acknowledgments

The authors thank all those involved in the organization of OFW16 and to all the contributors that will enrich this event. We acknowledge the Utah Center For High Performance Computing for technical support. Funding for this work was provided by the DRI Foundation.

References

[1] R. Falkenstein-Smith and K. McGrattan, "Determining flow resistance through vegetation canopy," *Fire and Materials*, 05 2020.

[2] J. A. Gillies, V. Etyemezian, and G. Nikolich, "Trapping of sand-sized particles exterior and interior to large porous roughness forms in the atmospheric surface layer," *Boundary-Layer Meteorology*, vol. 170, no. 3, pp. 443–469, nov 2018.

TRI-PERIODIC FIXED BEDS OF SPHERICAL PARTICLES

FLORENCIA FALKINHOFF[1], LIONEL GAMET[1], JEAN-LOU PIERSON[1],
ROMAIN VOLK[2] and MICKAEL BOURGOIN[2]

[1]*IFP Energies Nouvelles, Solaize, France*
Florencia.Falkinhoff@ifpen.fr, Lionel.Gamet@ifpen.fr, Jean-Lou.Pierson@ifpen.fr

[2]*Ecole Normale Supérieure de Lyon, Laboratoire de Physique, France*
Romain.Volk@ens-lyon.fr, Mickael.Bourgoin@ens-lyon.fr

Keywords: *Fixed beds, DNS, DEM, Periodic packed bed of spheres, Heat transfer, Thermal Energy Storage*

Advanced Adiabatic Compressed Air Energy Storage (AA-CAES) is an efficient technology for storing intermittent energy, for example wind-turbine generated energy. Energy is stored under the form of compressed air at high pressure. In classical compressed air systems, a large amount of the heat generated during the compression process is lost. In AA-CAES, the heat released during the compression is stored in adiabatic containers and reused during the expansion stages, thus minimizing global losses. Stored compressed air can later be converted back, for example to electricity through turbines and generators. Containers consist in packed beds of solid particles able to store thermal energy.
A fundamental description of the hydrodynamics and heat exchange inside a bed of fixed particles is necessary to establish 1D models of the full system, which will be useful for dimensionning installations at the industrial scale. This is done by simulating a representative volume of the packed bed and performing averaging and statistics on this volume. Direct Numerical Simulations (DNS) are conducted on fixed beds in tri-periodic domains, focusing on the hydrodynamics of the flow and on the heat exchange between the particles and the flow. The first results presented here focus only on the hydrodynamics.

Numerical methods

As many other works on fixed bed simulation [1, 2, 3, 4, 5], our hydrodynamics workflow is based on coupling a Discrete Element Method (DEM) package, namely Grains3D [6, 7], and the single phase steady-state solver `simpleFoam`. Meshing is done with the utility `snappyHexMesh`. A uniform cubic background grid topology is first generated with `blockMesh`. The spheres are input as `searchableSphere` in the `geometry` section of the `snappyHexMeshDict`, the centre and radius of the spheres being calculated by the DEM solver Grains3D. A surface based refinement level (typically 1 or 2) is used on all the surfaces of the spheres. A global `gapLevelIncrement` (typically value 1) was used to ensure a correct capture of thin gaps in regions where the spheres are tangent. As the spherical particles packing can intersect the 3-periodic domain bounds, special care was taken to acurately match the so generated intersection edges. Explicit features `eMesh` files were thus included in `snappyHexMeshDict` in order to capture and refine properly the circular intersection edges of the spheres with the cyclic boundaries. `cyclicAMI` boundary conditions are used on all periodic boundary conditions and no-slip walls on the spheres.
The steady state incompressible Navier-Stokes equations are solved using the SIMPLE algorithm (solver `simpleFoam`). In order to compensate the pressure gradient in the bed along the main flow direction, a volumic source term is added to the momentum equations. To that purpose, the function `meanVelocityForce` is used in `fvOptions`. This function computes a volumic source term such that the mean velocity accross the whole domain reaches the specified mean velocity target `Ubar` in `fvOptions`. In our cases, the flow direction was chosen as z.

Results and discussion

The workflow is first validated on ordered periodic arrays of spheres for low to moderate Reynolds numbers, following the articles of Zick [8] and Hill [9, 10]. Simple Cubic (SC) and Face Centered Cubic (FCC) arrangements are computed, containing respectively 1 and 4 spheres per cubic periodic block. The figure 1 presents the total force applied by the fluid to the sphere versus solid volume fraction (left) and Reynolds number (right) in the SC configuration. The force has been made

STUDY OF THE OVERSET APPROACH FOR SIMULATING CYCLOIDAL ROTORS AND COMPARISON TO OTHER RIGID MESH MOTION APPROACHES

JOHANNES GANZMANN[1], LOUIS GAGNON[2]
[1]*Johannes Ganzmann, Institute of Aerodynamics and Gas Dynamics, University of Stuttgart, ganzmannjohannes@gmail.com*
[2]*Louis Gagnon, Institute of Aerodynamics and Gas Dynamics, University of Stuttgart, gagnon@iag.uni-stuttgart.de*

Keywords: *cyclogyros, overset, overset-extend, motion, rotor*

The interest in unmanned aerial vehicles (UAVs) and micro air vehicles (MAVs) is growing continuously. Not only economically, but technologically as well [1]. Drones can carry out different tasks, that would not be possible with any other kind of vehicle or without the risk of endangering the pilot. Nowadays these vehicles exist mainly with conventional propellers. These propellers tend to be sluggish when maneuvering and are susceptible to winds and gusts. An alternative means of propulsion is a cyclorotor. Cyclorotor technology is being revived lately [2], [3]. A cyclocopter uses cylindrically arranged rotating wings which can change their pitch. This results in lift, good maneuverability and vertical take-off and landing capability.

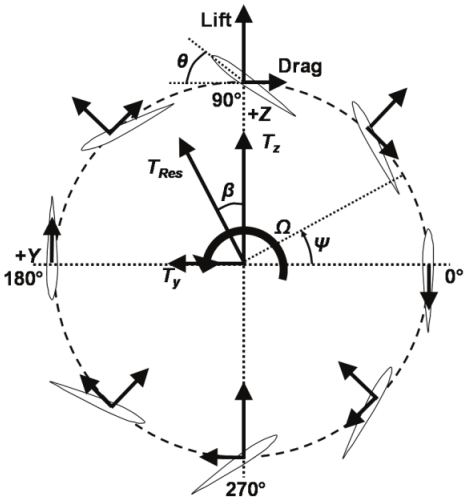


Figure 1: Blade kinematics of a hovering cyclorotor [4].

Cyclorotors need to be well researched before they can enter the market safely. Therefore it is important to understand the aerodynamics behind this technology. Aerodynamic research of these rotors is widely conducted via computational fluid dynamics (CFD) simulations. This presentation discusses the usage of OpenFOAM Overset and Foam-extend Overset to investigate the aerodynamics of a cyclorotor. Overset, which is also known as Chimera, uses multiple overlaid meshes. These overlaid meshes allow complex motions without altering any mesh. The Arbitrary Mesh Interface (AMI) on the other hand, consists of multiple meshes with interpolated values at their mesh fringes. Simulations on cyclorotors have been conducted already with AMI [5], [6], [7], [8] and the Overset mesh motion method [9], [10]. Compared to Overset, AMI runs quicker whereas Overset delivers conservative results at the cost of more simulation time. The scope of the presentation is to explain the usage of OpenFOAMs and Foam-extends Overset and to verify its results compared to an AMI simulation. The process of setting up of an Overset case begins with generating a mesh, creating the motion for each mesh and setting up the entire file structure needed to run a simulation. The results of these simulations are introduced and further investigations on parallel processing efficiency as well as a comprehensive comparison between AMI, OpenFOAM and Foam-Extend is conducted. Overset is a strong tool given its ability to handle complex motion. This makes it universal and useful to analyze the aerodynamics of a cyclorotor.

TOPOLOGY OPTIMIZATION OF INCOMPRESSIBLE TURBULENT FLOW CONSIDERING THE CONTINUOUS ADJOINT METHOD

LUIS FERNANDO GARCIA RODRIGUEZ[1], CESAR KIYONO[2], EMILIO CARLOS NELLI SILVA[3]
[1]*Mechanical Engineering Department, University of Sao Paulo. Av. Prof. Luciano Gualberto, 380. São Paulo, Brazil, ingarcia1703@usp.br*
[2]*Mechanical Engineering Department, University of Sao Paulo. Av. Prof. Luciano Gualberto, 380. São Paulo, Brazil, ckiyono@gmail.com*
[3]*Mechanical Engineering Department, University of Sao Paulo. Av. Prof. Luciano Gualberto, 380. São Paulo, Brazil, ecnsilva@usp.br*

Keywords: *topology, optimization, turbulent, flow, incompressible.*

Topology optimization of turbulent flow has been tackled at the continuous adjoint approach by considering frozen turbulence and the Spalart Allmaras turbulence model without solving the near-wall distance calculation. At this research, the method is extended by including not only the Eikonal equation for the near-wall distance calculation but also, replacing the steepest descent optimizer by considering advanced optimization techniques used at structures optimization: the method of moving asymptotes (MMA) and Topology Optimization of Binary Structures (TOBS), which behaves in the discrete form to improve the solid-fluid boundary definition. Promissory results are obtained at incompressible turbulent regime, by optimizing pipes in 2D and 3D considering coarse meshes. It diminishes considerably the computational cost of previous assumptions and extends the Topology Optimization of fluids applications to industrial regimes.

1. INTRODUCTION

"Topology optimization (TO)", has achieved efficient designs of fluid slow passages by changing the permeability of the volume cells in a domain considering a material distribution (ALEXANDERSEN [1]). The technique combines Computational Fluid Dynamics (CFD) and optimization method libraries based on derivatives that maximize objective functions like minimizing the energy dissipation through the domain. The adjoint code obtained by the continuous adjoint approach is performed by hand, and considering the developments of PAPOUTSIS [2], YOON [3], BUENO [4], KIYONO [5], and PICELLI [6], the method is extended at the current research for incompressible turbulent regime in FVM. The scientific contribution is given by considering TOBS optimizer and 3D optimization in coarse meshes.

1.1. Topology Optimization Formulation for Incompressible Turbulent Flow

$$\boldsymbol{Minimize}\left\{F=\int_{\Gamma}\left(p+\frac{1}{2}u^2\right)\boldsymbol{u}\cdot\boldsymbol{n}\,d\Gamma\right.$$

$$\boldsymbol{subject\ to}\begin{cases}0<\gamma<1\\ R^{p}=\dfrac{\partial\overline{u}_i}{\partial x_i}=0\\ R^{u}=\dfrac{\partial\left(\overline{u}_i\overline{u}_j\right)}{\partial x_j}+\dfrac{1}{\rho}\dfrac{\partial\bar{p}}{\partial x_j}-\left[(\nu)\left(\dfrac{\partial\overline{u}_i}{\partial x_j}+\dfrac{\partial\overline{u}_j}{\partial x_i}\right)-\overline{u_i'u_j'}\right]+\underbrace{\alpha_u\overline{u}_i}_{\substack{Penalization\\ term}}=0\\ R^{\tilde{\nu}_t}=v_j\dfrac{\partial\tilde{\nu}}{\partial x_j}-\dfrac{\partial}{\partial x_j}\left[\left(\nu+\dfrac{\tilde{\nu}}{\sigma}\right)\dfrac{\partial\tilde{\nu}}{\partial x_j}\right]-\dfrac{c_{b2}}{\sigma}\left(\dfrac{\partial\tilde{\nu}}{\partial x_j}\right)^2-\tilde{\nu}P(\tilde{\nu})+\tilde{\nu}D(\tilde{\nu})+\alpha_t\tilde{\nu}_t=0\\ R^{\Delta}=\dfrac{\partial\left(\dfrac{\partial\Delta}{\partial x_j}\Delta\right)}{\partial x_j}-\Delta\dfrac{\partial^2\Delta}{\partial x_j^2}-1+\alpha_{\Delta}\Delta=0\\ \overline{V}_{frac}\geq\dfrac{\int_{\Omega}\gamma d\Omega}{\int_{\Omega}d\Omega}-V_{tar}\end{cases}\tag{1}$$

2. METHODOLOGY

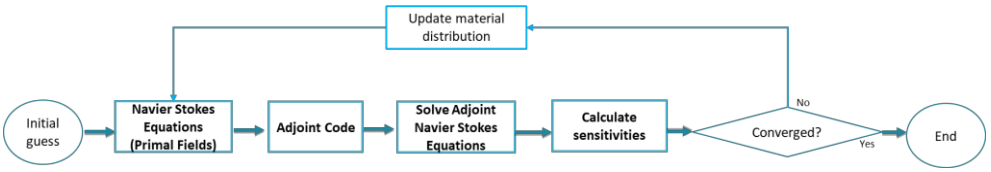


Figure 1: Topology Optimization Flowchart [Author]

COMPARISON OF VOF AND LEVEL SET METHODS FOR SIMULATING SHIP SELF–PROPULSION IN FULL SCALE

Inno Gatin[1], Sanijo Đurasević[2], Hrvoje Jasak[3]
[1]*University of Zagreb, Croatia, igatin@fsb.hr*
[2]*University of Zagreb, Croatia, sdurasevic@fsb.hr*
[3]*University of Zagreb, Croatia, hjasak@fsb.hr*

Keywords: *VOF, Level Set, Self–propulsion, Full–scale*

Comparison of the Volume of Fluid (VOF) and Phase–field based Level Set methods for interface capturing is presented in this paper in terms of calculating self–propulsion characteristics of a car carrier ship. In both cases the Ghost Fluid Method is used for modeling the free surface boundary conditions, i.e. to take into account the density jump across the interface [1]. The VOF approach uses implicit discretisation of the volume fraction advection equation with interface compression [1, 2]. The Level Set method used in this work is based on the Phase Field equation with implicit re–distancing as described in [3]. The propeller of the vessel is modeled using the actuator disc theory for efficiency [4], which uses open water characteristics of the propeller to calculate the propeller delivered power based on the thrust force required to satisfy the net zero sum of forces acting on the vessel. The two-equation $k-\omega\ SST$ turbulence model is used in both simulations.

Table 1 shows the main ship particulars used in this study. The computational grid was generated using cfMesh software and it comprises 2.4 million cells. Figure 1 depicts the grid at the stern and bow of the vessel. Figure 2 shows the free surface and dynamic pressure on the hull surface in the VOF simulation. Table 2 shows the result comparison between VOF and Level Set for various items. For most items, the relative difference is around 1.5% to 2.5%, with dynamic sinkage and trim being outliers mostly due to their small absolute values. The delivered power P_Q, which is of primary interest, shows a difference of 2.3%. This difference is not large but cannot be neglected either, which is why a deeper investigation will be performed to identify its cause.

Table 1: Main ship particulars

Item		**Value**	**Unit**
L_{pp}	Length between perpendiculars	188.7	m
L_{oa}	Length over all	198	m
B	Maximum breadth	32.26	m
D	Total vessel height	33	m
T_D	Draft	6.235	m
m	Displacement	20846.9	t
LCG	Longitudinal centre of gravity	90.49	m
v	Speed	21.25	kt
F_r	Froude number	0.254	

Acknowledgments

The authors thank the financial support from the CEKOM project from the European regional development fund, Referent number KK.01.2.2.03., sub–projects IRI 2 and IRI 6, in scope of which this study is conducted.

References

[1] V. Vukčević, H. Jasak, and I. Gatin, "Implementation of the Ghost Fluid Method for free surface flows in polyhedral Finite Volume framework ," *Computers & Fluids*, vol. 153, pp. 1 – 19, 2017.

A NEW FREE-SURFACE ADAPTIVE GRID REFINEMENT METHOD FOR MARINE APPLICATIONS

PAOLO GEREMIA[1], KEVIN J. MAKI[2], DANIEL DEISING[3]
[1] *ENGYS S.R.L., p.geremia@engys.com*
[2] *University of Michigan, kjmaki@umich.edu*
[3] *ENGYS GmbH, d.deising@engys.com*

Keywords: *AMR, VOF, Ship Hydrodynamics, 6DoF*

Accurate prediction of calm-water resistance represents probably one of the most successful application examples of Computational Fluid Dynamics (CFD) methods applied to ship hydrodynamics, both in the early stage and in the final phases of the engineering development process. To this end, fully non-linear viscous RANS based on the Volume-Of-Fluid (VOF) method [1] has been used for free-surface flows for more than two decades due to its proven accuracy in predicting drag force, as opposite to traditional potential flow methods which do not account for the viscous boundary layer and could potentially lead to non-optimized hull-forms. In this context, one of the main bottlenecks of the VOF method applied to calm-water prediction is the high computational cost to resolve the flow field around the hull as well as the wave pattern on the free-surface in order to accurately predict the wave-making resistance component. In addition, the creation of the computational grid can be challenging if we consider the ship motion due to the change of attitude when operating at different speeds, thus the free-surface shape can change as a function of the testing speed and potentially different grid refinements would be required. For these reasons, having an efficient mesh strategy for ship hydrodynamics is not trivial compared to external aerodynamics applications, where usually the grid is refined only around the body and in the wake region and not in the far field for which a coarser mesh size can be employed without compromising in terms of accuracy of the resolved flow features. Different methods have been implemented in CFD software packages to account for body motion, including for example 6 Degrees of Freedom (6DoF) mesh deformation libraries [2] and overset grids [3]. Both these methods are robust and accurate, however for large wave elevation the total number of cells of the grid can become excessively high to achieve an accurate solution and yet very often complex workflows are required to setup and create the mesh volumetric refinements based on a given operating condition [4]. In previous works [5] the authors employed a 6DoF rigid-body motion library based on OpenFOAM for maneuvering applications to address ship motion. The method solves accurately the six-degree-of-freedom equations of motion in an earth-fixed reference frame including tensor of added masses and body constraints and as a result the entire domain translates and rotates with the hull geometry [6]. One of the main drawbacks, however, is the potentially high number of cells required in case of large motion of the ship, for example high values of pitch angles for a planing craft at high Froude numbers. To tackle this issue, a newly developed Adaptive Mesh Refinement (AMR) method for accurate resolution of the free-surface flow is developed and presented in this work [7].
In the work detailed here, the newly developed AMR method is coupled to the 6DoF rigid-body motion library and tested on calm-water resistance prediction for displacement hulls. To assess the efficiency of the method over the traditional mesh strategies, an even keel condition with suppressed motion is firstly considered and results compared to the experiments.

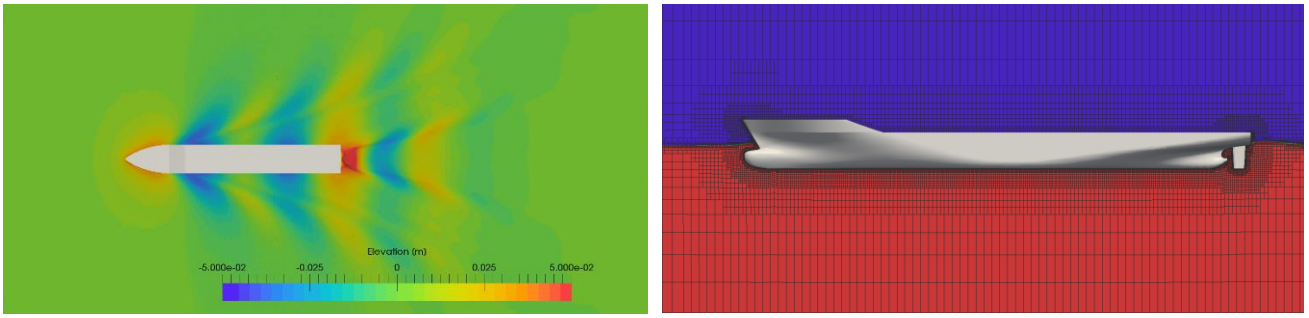


Figure 1: Free-surface elevation (left) and close up of the grid using AMR (right) for a test hull

Finally, the method is validated against a moving hull with sinkage and trim and accuracy of the results with respect to the experimental data and the efficiency of the method are discussed.

CONSISTENCY BETWEEN AVERAGE CELL STRESSES AND NEUMANN BOUNDARY CONDITIONS IN SOLID MECHANICS

PAVEL GRUBER[1,2], MARTIN ISOZ[2,3]
[1]*CARDAM s.r.o., Pražská 636, 252 41 Dolní Břežany, pavel.gruber@cardam-solution.cz*
[2]*Institute of Thermomechanics, Academy of Sciences of the Czech Republic, Dolejškova 1402/5, 182 00, Prague, Czech Republic, isozm@it.cas.cz*
[3]*Department of Mathematics, UCT Prague, Technická 5, 166 28, Prague, Czech Republic*

Keywords: *solid mechanics; explicit dynamics; neumann boundary conditions; finite volume method; OpenFOAM*

The presented research is motivated by the necessity to simulate a component material response under laser shock peening (LSP) conditions using the finite volume method (FVM) as implemented in the OpenFOAM library. LSP is an innovative surface treatment for strenghtening metallic materials. Modeling LSP comprises simulation of a material dynamic response to a high-intensity pressure pulse applied over a finite area of the component [1]. Thus, a physically accurate implementation of the traction boundary condition is of utmost importance.
In numerical simulations of solids based on the FVM [2, 3, 4, 5], dealing with traction vectors on cell faces is crucial. Under infinitesimal strain settings, its semi-discrete form on a cell face f with unit outer normal n_f is expressed as

$$t_f = n_f \cdot \sigma_f = \underbrace{\mu_f \left(n_f \cdot \nabla u_f\right)}_{\substack{\text{(a) face normal contraction} \\ + \\ \text{"in face" shear effects}}} + \underbrace{\mu_f \left(\nabla u_f \cdot n_f\right)}_{\substack{\text{(b) face normal contraction} \\ + \\ \text{"out off face" shear effects}}} + \underbrace{\lambda_f \left(\nabla \cdot u_f n_f\right),}_{\substack{\text{(c) face normal contraction} \\ + \\ \text{transverse contractions}}} \tag{1}$$

where σ_f is a stress tensor on the face depending on displacement u_f spatial derivatives according the Hooke's material law. The Lamé's first (λ_f) and second (μ_f) parameters vary on cell faces from material natural heterogeneity reasons or as a result of a material nonlinear response. In the "standard" cell-centered FVM, a full-discrete form of (1) involves spatial derivatives of displacements in tangential directions to faces in an average sense [3, 6, 7]. On internal faces, the averaging can be performed sufficiently by interpolating cell average displacement gradients. However, on boundary faces this approach cannot be applied. Consequently, shear effects and mainly transverse contraction effects on boundary faces are over- and underestimated, respectively.
Assume a boundary cell with a volume V_c bounded by internal faces $f \in C_\mathrm{i}$ and boundary faces $f \in C_\mathrm{b}$ with areas S_f and $C = C_\mathrm{i} \cup C_\mathrm{b}$. The standard boundary condition treatment leads to inconsistency between the cell average stress

$$\overline{\sigma}_c = \sum_{f \in C} \overline{\mu}_f \left(n_f u_f\right) + \sum_{f \in C} \overline{\mu}_f \left(u_f n_f\right) + \sum_{f \in C} \overline{\lambda}_f \left(n_f \cdot u_f\right) \mathrm{I}, \quad \overline{\mu}_f = \frac{\mu_f S_f}{V_c}, \quad \overline{\lambda}_f = \frac{\lambda_f S_f}{V_c} \tag{2}$$

and traction vectors on a face set $f \in N \subseteq C_\mathrm{b}$ with a prescribed Neumann boundary conditions. The above mentioned problem can be overcome by directly connecting the cell average stress (2) to the boundary traction vectors as

$$t_n = n_n \cdot \overline{\sigma}_c = \sum_{f \in C} \left[\overline{\mu}_f \left(n_n \cdot n_f\right) \mathrm{I} \cdot u_f + \overline{\mu}_f \left(n_f n_n\right) \cdot u_f + \overline{\lambda}_f \left(n_n n_f\right) \cdot u_f\right] = \sum_{f \in C} \left(A_{nf} \cdot u_f\right), \quad \forall n \in N, \tag{3}$$

leading to a system of linear equations

$$\sum_{f \in N} \left(A_{nf} \cdot u_f\right) = t_n - \sum_{f \in C \setminus N} \left(A_{nf} \cdot u_f\right), \quad \forall n \in N, \tag{4}$$

for unknown displacements u_f on faces $f \in N$ with prescribed traction vectors.
A new boundary condition based on the proposed approach (4) was implemented in OpenFOAM, and the obtained behavior on a simple LSP-motivated numerical experiment can be compared with the standard treatment on Figure 1.

A BENCHMARKING AND COMPARATIVE STUDY OF DIFFERENT LINEAR SOLVERS AND PRECONDITIONERS IN OPENFOAM, PETSC, AND FLUBIO

JOEL GUERRERO[1], EDOARDO ALINOVI
[1]*University of Genova, joel.guerrero@unige.it*
[2]*University of Genova, edoardo.alinovi@gmail.com*

Keywords: *linear solvers, preconditioners, convergence rate, parallel computing*

Hereafter, we present a benchmarking and comparative study of the different linear solvers and preconditioner methods available in OpenFOAM. We also make use of PETSc-FOAM [1], and we compare PETSc [2] linear solvers with OpenFOAM built-in linear solvers. In addition, we also compare OpenFOAM against the Open-Source CFD solver FLUBIO [3], which is a parallel, unstructured, finite-volume based solver for the solution of the Navier–Stokes equations and convection-diffusion like equations, recently developed by the authors. FLUBIO is written using modern Fortran (2003+ standard), it is object-oriented, and it leverages PETSc.

In this study, we first explore the performance of different linear solver in academic problems, where besides measuring the performance of the linear solvers and preconditioners, we also look at the matrices and compute the condition number and spectral radius of convergence. The aim is to construct a database of the linear solvers' behavior for the problems studied and developed guidelines on how to choose the linear solvers according to the characteristics of the linear system arising from the discretization of the problem studied.

In the second part, we simulate industrial applications using large meshes, and we compare the performance of OpenFOAM and FLUBIO using different linear solvers and preconditioners. It is important to mention that in order to conduct a fair comparison between both solvers, the same mesh data structure is used. We also look at any possible improvement in computational efficiency between a solver written in C++ and a solver written in Fortran (aspirational goal). Additionally, using the guidelines proposed and the knowledge gathered in the previous step, we choose the best linear solver.

Acknowledgments

The authors thank all those involved in the organization of OFW16 and to all the contributors that will enrich this event. The authors kindly acknowledge the PETSc development team for the helpful support received through their mailing list.

References

[1] https://gitlab.hpc.cineca.it/openfoam/petsc-foam/

[2] S. Balay, S. Abhyankar, M. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, A. Dener, V. Eijkhout, W. Gropp, D. Karpeyev, D. Kaushik, M. Knepley, D. May, L. McInnes, R. Mills, T. Munson, K. Rupp, P. Sanan, B. Smith, S. Zampini, H. Zhang, H. Zhang. PETSc Users Manual: Tech. Rep. ANL-95/11 Revision 3.13. Argonne National Laboratory (2020). URL https://www.mcs.anl.gov/petsc

[3] E. Alinovi, J. Guerrero/ FLUBIO—An unstructured, parallel, finite-volume based Navier–Stokes and convection-diffusion like equations solver for teaching and research purposes. SoftwareX, Volume 13, 2021, https://doi.org/10.1016/j.softx.2020.100655.

COMPUTATIONAL FLUID DYNAMICS SIMULATIONS OF ENERGY-SAVING VORTEX RING THRUSTER USING COANDA EFFECT

YOUNGMIN HEO[1], WOOCHAN SEOK[2], SHIN HYUNG RHEE[3]
[1]*Seoul National University, Seoul, Korea, heoym1@snu.ac.kr*
[2] *Research Institute of Marine Systems Engineering, Seoul National University, Seoul, Korea, swc@snu.ac.kr*
[3]*Seoul National University, Seoul, Korea, shr@snu.ac.kr*

Keywords: *Vortex ring thruster, Propulsion efficiency, Coanda effect*

One of the jet propulsion systems, a Vortex Ring Thruster (VRT), has better propulsion performance than other propulsion systems at low speeds. It is also economical in terms of cost and relatively small volume, making it suitable for unmanned underwater vehicles (UUVs) (Mohseni, 2006).

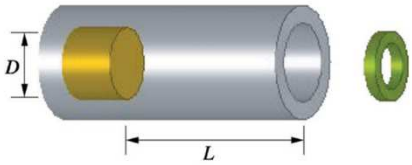


Figure 1 Schematic of the piston-cylinder mechanism

The VRT is a piston-cylinder mechanism, as shown in Figure 1. Various studies using such a piston-cylinder mechanism have been conducted. Gharib et al. (1998) conducted experiments about the vortex ring, which occurs in piston shapes with a diameter of D and a length of L. The vortex ring was observed by setting the ratio of piston length to diameter, dubbed stroke ratio, and various ranges. It was confirmed that a leading vortex ring was clearly observed in the wake region, and the trailing jet did not occur in the range of stroke ratio less than 4. Rosenfeld et al. (1998) carried out computer fluid dynamics (CFD) simulations to investigate the generation and evolution of vortex rings. For the evaluation of the propulsion performance of VRT, Zhang et al. (2020) systematically studied the generation and evolution of vortex rings and the propulsion efficiency using a piston-nozzle computational model.

The governing equations are the continuity equation and Navier-Stokes equation for incompressible, which was expressed as follows:

$$\nabla u_i = 0 \tag{1}$$

$$\frac{\partial u_i}{\partial t} + (u_i \cdot \nabla)u_i = -\nabla p + \nu \nabla^2 u_i \tag{2}$$

where u_i is velocity in three-axis directions $(i = x, y, z)$, ∇ is divergence operator, ∇^2 is Laplacian, and ν is the fluid kinematic viscosity. The second-order implicit scheme was used for temporal discretization, and the second-order central finite difference scheme was used for spatial discretization. Dynamic mesh techniques were used to control piston motion. The PIMPLE algorithm was applied for the pressure-velocity coupling, which is a combination of both the semi-implicit method for pressure-linked equations (SIMPLE) and the pressure implicit with the splitting of operators (PISO) algorithm (Chen et al. 2014).

The main purpose of this study was to design a more propulsion-efficient VRT than a conventional VRT, using the Coanda effect. Numerical simulations were conducted on two VRT: VRT, which has only a primary jet, and VRT, which has a primary jet with a Coanda jet. The computational domains and boundary conditions of the conventional VRT and VRT considering the Coanda effect (hereafter referred to as CVRT) are shown in Figure 2. Dimensions of the piston and nozzle were exactly the same as experiments of Gharib et al. (1998). The whole computational domains were axisymmetric. The diameter (D) of the nozzle is 0.0254m, and the total length of the piston is 0.4m. The computational domain size is 20D × 3D in the x-, y-directions, respectively.

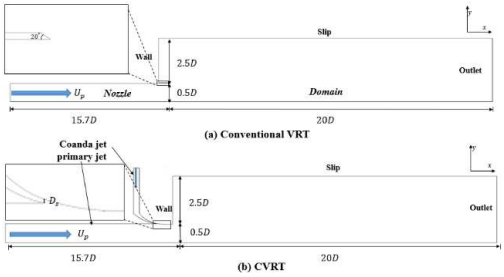


Figure 2 Domain dimensions and boundary conditions of conventional VRT and CVRT

CFD STUDY OF DE LAVAL NOZZLE - COLD SPRAY PROCESS APPLICATIONS

M. HERNANDEZ-HERNANDEZ
[1]*Cátedras CONACYT-COMIMSA, Calle Ciencia y Tecnología No. 790, Saltillo 400, 25290, Saltillo, Coahuila, México, maricruz.hdz@comimsa.com*

Keywords: *Cold spraying, OpenFOAM, de Laval nozzle, computational fluid dynamics, process numerical simulation*.

Cold spray is a coating technology process with the ability to form characteristic layers of specific materials onto engineering components to augment different properties and the possibility of their applications. Among the projection techniques, cold spray has a high potential, both for the generation of coatings, and for the additive manufacturing techniques. One of the main components of this equipment is the spray gun, its configuration is highly important in the control of the final characteristics of the coating, and in the efficiency of the process. The gun is composed of a Laval type nozzle, which is a device consisting of a converging and a divergent section with the ability to accelerate compressible fluids at supersonic speeds. In this work, the geometrical features of the convergent-divergent de Laval nozzle employed in the Cold spray process are numerically analysed. Computational fluid dynamics has been a study tool used to have a more extensive understand of the different geometries and performance of the flow phenomena in Cold spray process. The simulation model used is based on the reactingParcelFoam solver of OpenFOAM. This transient solver uses the PIMPLE algorithm for the solution of the compressible Navier–Stokes equation and allows the consideration of Lagrangian tracer particles [1].

Acknowledgments
The author acknowledges the support through projects CONACYT-CB A1-S-23339 and Cátedras-CONACYT 850.

References

[1] K.-H. Leitz, M. O'Sullivan, A. Plankensteiner, T. Lichtenegger, S. Pirker, H. Kestler, and L. S. Sigl, OpenFOAM modeling of Particle Heating and Acceleration in Cold Spraying, J. Therm. Spray Technol., 2018, 27, p 135–144.

SIMULATION OF PARTICLE TRANSPORT IN VISCOPLASTIC FLUIDS

PATRICK HÖHN[1], ROGER ARAGALL[2], JOACHIM OPPELT[3],
[1]*Clausthal University of Technology, Drilling Simulator Celle, patrick.hoehn@tu-clausthal.de*
[2]*Baker Hughes, Celle Technology Center, roger.aragall@bakerhughes.com*
[3]*Clausthal University of Technology, Drilling Simulator Celle, joachim.oppelt@tu-clausthal.de*

Keywords: *particle transport, eulerian-lagrangian, non-Newtonian fluids*

Drilling is essential for the recovery and storage of sub-surface energy, such as oil, gas and geothermal. It typically accounts for large parts of the project costs. In the case of deep geothermal wells, drilling alone accounts for at least 50% of the total project budget [1]. Large shares of these costs are due to non-productive time during the drilling process caused by stuck pipe events, damage to underground equipment or borehole integrity issues. These can result in several days lost to pull out the drill string and trip it in again, or in re-conditioning the borehole. For optimal drilling operations it is required to achieve an efficient transport of cuttings from the drill-bit to the surface. As drilling often reaches several thousand meters below the surface, in-situ measurements of drilling parameters are very challenging. Therefore, limited field knowledge about the underlying phenomena exists and many investigations rely on simplified laboratory setups and detailed software-based simulations.

Previous work reported extensive simulations under various conditions. However, to the knowledge of the authors, open questions remain related to phenomena taking place in large wellbores with critical inclinations, around 30 to 60° with respect to the vertical.

The authors already presented in the previous two OpenFOAM workshops a solver [2, 3] integrating solver cfdemSolverPiso for particle transport from CFDEMcoupling [4, 5] as additional fluid model in the fluid-structure-interaction library solids4foam by Cardiff *et al.* [6]. Despite OpenFOAM flavors already implementing different non-Newtonian fluid models, the particle-fluid interaction in CFDEMcoupling does not yet consider non-Newtonian fluid properties. Unlike previous work by the authors, the current implementation is based on the upstream branch of CFDEMcoupling, which is compatible with OpenFOAM-5.x. The new developments aim to extend the particle transport models by implementing closure relations published by Akhshik *et al.* [7] to consider viscoplastic fluid behavior. The implemented solver will then be validated using data from the literature [7, 8]. Lastly, it is intended to integrate the newly developed and validated feature in the own fork [2, 3].

References

[1] W. Bauer, "Exploration Strategies," Strasbourg, France, Oct. 2018.

[2] P. Höhn, R. Aragall, and J. Oppelt, "Analysis of lateral drill string vibrations using fluid-structure interaction and particle simulations," 14th OpenFOAM Workshop, Duisburg, Germany, Jul. 2019.

[3] ——, "Improved Solver for coupled fluid-structure interaction and particle simulations," 15 th OpenFOAM Workshop, Virtual, Jun. 2020.

[4] C. Goniva, C. Kloss, N. G. Deen, J. A. Kuipers, and S. Pirker, "Influence of rolling friction on single spout fluidized bed simulation," *Particuology*, vol. 10, no. 5, pp. 582–591, Oct. 2012.

[5] C. Kloss, C. Goniva, A. Hager, S. Amberger, and S. Pirker, "Models, algorithms and validation for opensource DEM and CFD-DEM," *Progress in Computational Fluid Dynamics, An International Journal*, vol. 12, no. 2/3, p. 140, 2012.

[6] P. Cardiff, A. Karač, P. De Jaeger, H. Jasak, J. Nagy, A. Ivanković, and Ž. Tuković, "An open-source finite volume toolbox for solid mechanics and fluid-solid interaction simulations," *arXiv e-prints*, Aug. 2018.

[7] S. Akhshik, M. Behzad, and M. Rajabi, "On the particle–particle contact effects on the hole cleaning process via a CFD–DEM model," *Particulate Science and Technology*, vol. 34, no. 6, pp. 736–743, Nov. 2016.

[8] P. Tomren, A. Iyoho, and J. Azar, "Experimental Study of Cuttings Transport in Directional Wells," *SPE Drilling Engineering*, vol. 1, no. 01, pp. 43–56, Feb. 1986.

NUMERICAL STUDY ON VORTEX-INDUCED VIBRATION SUPPRESSION OF A FLEXIBLE TENSIONED RISER WITH SPANWISE GROOVES

Hao Hu, Di Deng, Decheng Wan[*]
Computational Marine Hydrodynamics Lab (CMHL), School of Naval Architecture, Ocean and Civil Engineering, Shanghai Jiao Tong University, Shanghai 200240, China
[*]Corresponding author: dcwan@sjtu.edu.cn

***Keywords**: vortex-induced vibration suppression; viv3D-FOAM-SJTU; uniform flow; spanwise grooves*

1. INTRODUCTION

The vortex-induced vibration (VIV) is well-recognized when the riser is exposed to current. The multi-mode vibrations and mode transitions of the riser structure caused by VIV are the important sources of fatigue damage. Therefore, the numerous investigations have been conducted to seek the VIV suppression methods. Due to no additional energy input, The passive control methods are extensively applied and studied in ocean engineering. In recent decades, many researchers are beginning to modify the shape of cross section to suppress the VIV of the cylinder instead of installing additional passive devices. Law and Jaiman (2018) carried out simulations to investigate the effect of VIV suppression with the staggered groove and the helical groove, and the results indicated that the staggered groove showed better VIV suppression performance. Zhao et al (2020) numerically studied VIV responses of the grooved cylinder with different current angles, they found that the vibration amplitude was increased by the variation of current angles. In this paper, the VIV of a flexible riser with two-start spanwise grooves exposed to uniform flow is numerically investigated by the in-house solver viv3D-FOAM-SJTU. The depths (d) of spanwise grooves in the simulation are 0.08, 0.12 and 0.16 riser diameter (D), respectively.

2. CFD METHOD

2.1 Hydrodynamic Numerical Method

For the incompressible flow field, the Reynolds-averaged Navier-Stokes (RANS) equations are commonly selected as the governing equations, and the continuity and momentum equations are given as follows:

$$\frac{\partial \overline{u_i}}{\partial x_i} = 0 \tag{1}$$

$$\rho \frac{\partial}{\partial t}(\overline{u_i}) + \rho \frac{\partial}{\partial x_j}(\overline{u_i u_j}) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}(\mu\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right) - \rho\overline{u_j' u_i'}) \tag{2}$$

where ρ is the density of fluid, p is the pressure, and μ is dynamic viscosity coefficient of fluid.

In order to close the RANS equations, the shear stress transport (SST) *k-ω* is used to compute the Reynolds stress $\rho\overline{u_j' u_i'}$ in the momentum equation. The transport equations of turbulence kinetic energy k and turbulence dissipation rate ω have the following forms:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_j k)}{\partial x_j} = \tau_{ij}\frac{\partial u_i}{\partial x_j} - \beta^*\rho\omega k + \frac{\partial}{\partial x_j}\left[(\mu + \sigma_k \mu_t)\frac{\partial k}{\partial x_j}\right] \tag{3}$$

$$\frac{\partial(\rho\omega)}{\partial t} + \frac{\partial(\rho u_j \omega)}{\partial x_j} = \frac{\gamma}{\mu_t}\tau_{ij}\frac{\partial u_i}{\partial x_j} - \beta\rho\omega^2 + \frac{\partial}{\partial x_j}\left[(\mu + \sigma_\omega \mu_t)\frac{\partial \omega}{\partial x_j}\right] + 2(1 - F_l)\frac{\rho\sigma_{\omega 2}}{\omega}\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j} \tag{4}$$

where $\tau_{ij} = \rho\overline{u_j' u_i'}$, $\mu_t = \frac{\rho a_1 k}{\max(a_1\omega, \Omega F_2)}$ represents the eddy viscosity, F_l is the blending function; β^*, σ_k, γ, β, σ_ω, $\sigma_{\omega 2}$, a_1 represent the empirical coefficients in the turbulence model.

MODELLING OF VENTED CORN STARCH DUST EXPLOSION USING OPENFOAM

CHEN HUANG[1], ANDREI LIPATNIKOV[2]
[1]*Department of safety and transport, RISE Research Institutes of Sweden, chen.huang@ri.se*
[2]*Department of Mechanics and Maritime Sciences, Chalmers University of Technology, andrei.lipatnikov@chalmers.se*

Keywords: *premixed turbulent combustion, corn starch, dust explosion, OpenFOAM, CFD*

Introduction

Dust explosion is a constant threat to the industries which deal with combustible powders such as pellets producers, food industry, metal industry, pharmaceuticals and additive industries. It is a complicated chemical and physical process, when very fine combustible particles well mixed with air in a confined equipment are ignited, resulting in a violent and explosive combustion. Once the dust explosion occurs, the generated high-pressure waves, hot flames and extremely radiative heat may cause loss of life and severe economic consequences. Statistics shows that there is one serious dust explosion every day in Europe alone [1].

This work is part of a project which aims at developing a well-verified and well-validated numerical tool based on the OpenFOAM platform for studying dust explosions in the process industry. A dust explosion process resembles the turbulent burning of a gas cloud for very fine organic dust particles with high volatile content [2, 3]. Therefore, to simulate dust explosions within the framework of the present project, a so-called Flame Speed Closure (FSC) model of premixed turbulent combustion has been implemented into OpenFOAM [4]. Note that the FSC model has been quantitatively validated against a wide set of experimental data obtained by various research groups from various gaseous flames under a wide range of substantially different conditions [5-7]. In a previous work [4], implementation of the FSC model into OpenFOAM was verified and the model was validated against Leeds experimental data [3] obtained in well-defined laboratory conditions. In the present work, the tool is applied for simulating a large-scale industrial vented dust explosion and the first results are reported.

Experimental and numerical setups

Corn starch vented explosion experiments were carried out at Rembe Research and Technology Center during 2017 and 2018 with an aim of studying the effect of vent geometry on the vent efficiency [8, 9]. An 11.5 m^3 explosion vessel utilized in those experiments can be equipped with a round, a square, or a rectangular opening with an area of 0.5 m^2, at one end of the vessel. The vent opening is covered with a layer of 70 μm aluminium foil with a static activation overpressure P_{stat} of 0.1 ± 15% bar. The corn starch dust was injected into the vessel from two attached 20 l containers at approximately 20 bar pressure. After an ignition delay time of around 800 ms for corn starch, the dust-air cloud was ignited by a pair of pyro-technique ignitors with a total ignition energy of 10 kJ. The reduced explosion overpressure P_{red} inside of the vessel was measured by two pressure detectors mounted on the wall of the vessel; see Figure 1.

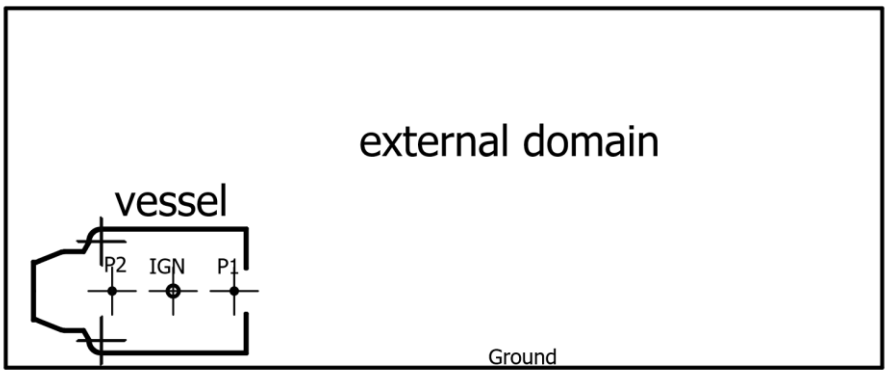


Figure 1: 2D drawing of dimensions of Rembe explosion vessel and the computational domain.

Two sets of computational meshes used for the simulations. The first mesh is used for simulating dust explosion before the rupture of the vent panel, whereas the second mesh covers the volume of the vessel and a volume outside of the vessel to capture the venting process. The explosion is simulated in two stages. The first finer-resolved simulation is stopped when the pressure inside the vessel reaches a critical pressure. Then, the saved results are mapped to the second mesh with the pressure and temperature outside of the vessel equal to 1 atm and 273 K, respectively. The mapped fields provide initial conditions for the second simulations performed for the entire computational domain. Only a half of the vessel and a half of the outside volume are simulated to save computational time by assuming symmetry with respect to the vertical plane. The CAD geometry of the vessel was provided by Rembe as stp files, and the files were read in an open source 3D CAD modelling tool FreeCAD [10]. The detailed geometry of the vessel was obtained in FreeCAD, and the geometry of the vessel shell was exported in a stl file in the ASCII format. The geometry is then imported into the OpenFOAM, and the computational mesh was generated using a so-called snappyHexMesh tool in OpenFOAM.

Results and discussions

Table 1 shows evolution of the computed fields of the mean temperature at different time instants before the rupture of the vent panel. Figure 2 (a) compares the measured (solid line) and computed (dashed line) explosion overpressures at the measurement point P2 in Figure 1. Note that the measured explosion overpressure is an averaged value of two test

AN EXTERNAL CFD STUDY OF THE HYEND N_2ORTH ROCKET

HUGH IRVING[1], PHILIP CARDIFF[1,2,3]
[1]*School of Mechanical and Materials Engineering, University College Dublin, Belfield, Dublin, Ireland*
[2]*Bekaert UTC, School of Mechanical and Materials Engineering, University College Dublin, Ireland*
[3]*SFI I-Form Centre, University College Dublin, Ireland*
hugh.irving@ucdconnect.ie, philip.cardiff@ucd.ie

Keywords: *External Aerodynamics, Compressible Flows, Rocketry, OpenFOAM, CFD*

Many of the advancements in Computational Fluid Dynamics have been within the field of aerospace. Many of the applications in this field have been complex, computationally intensive and have used expensive commercial software or developed proprietary codes [1]. Open-source CFD software has now become a viable option for these problems, allowing expedited design and analysis at a significantly lower cost.

This work is a collaboration between University College Dublin's School of Mechanical and Materials Engineering and the University of Stuttgart's Institute of Space Systems. The University of Stuttgart's Hybrid Engine Development group are concerned with the design, development and manufacture of suborbital rockets using novel hybrid rocket engines. They hold the present European altitude record for a university developed rocket. Their new 'N_2ORTH' vehicle design is more lightweight and higher performing than their previous projects. Due to these more onerous design conditions, the use of computational fluid dynamics (CFD) simulation was thought to be valuable tool in the design and analysis of the vehicle.

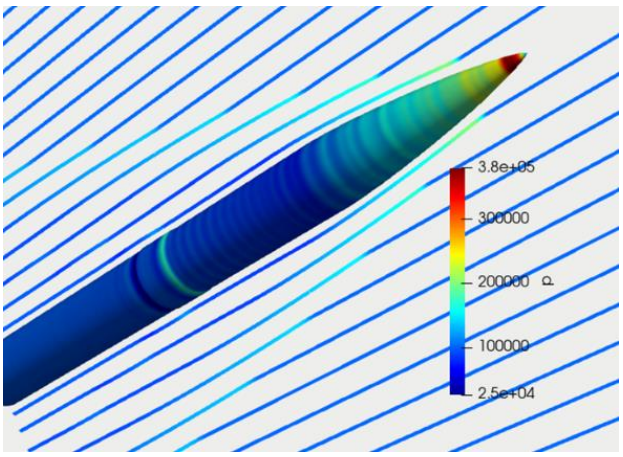


Figure 1: Visualisation of surface pressures (Pa) for flight at Mach 4 and sea level ambient pressure. Streamlines also coloured by pressure.

OpenFOAM has been used in the verification, validation and implementation of an appropriate numerical model. A compressible solver (*rhoCentrlFoam)* was required due to the high velocities of up to Mach 4. The solvers were verified against an analytical solution [2, 3]. Turbulence modelling was also required due to interaction between the exhaust plume and incoming airflow. A RANS approach was used and validated against experimental data [4, 5, 6].
The front section of the vehicle was simulated across a range of flight conditions using a two-dimensional axisymmetric mesh. The full vehicle was then simulated across various flight conditions using a one eighth symmetric mesh, due to the quad fin configuration. The data from these simulations has been analysed and used to inform vehicle design and trajectory analysis. Next steps include experimentation with alternative designs to optimise vehicle performance.

DEVELOPMENT OF THE NEW OPENFOAM SOLVER FOR SHALLOW WATER SIMULATION USING QGD/QHD LIBRARY

ALEKSANDR V. IVANOV[1], TATIANA G. ELIZAROVA[2], MATVEY V. KRAPOSHIN[3],
[1] *Ivannikov Institute for System Programming of the RAS,*
Keldysh Institute of Applied Mathematics RAS, av.ivanov@ispras.ru
[2]*Keldysh Institute of Applied Mathematics RAS, telizar@mail.ru*
[3]*Ivannikov Institute for System Programming of the RAS, m.kraposhin@ispras.ru*

Keywords: *shallow water, OpenFOAM, Regularized Shallow Water Equations, Quasi-Gas Dynamic approach, Finite Volume Method, incompressible flows, RSWEFoam*

Introduction

Hydrodynamic flows simulation in a full three-dimensional formulation allows one to obtain the most accurate numerical solution and study the problem from different angles. However, some problems could be studied using simpler physical and mathematical models, while significantly reducing computational costs. An example of simplification is using a two-dimensional hydrodynamic model such as the shallow water approximation. Shallow water equations are commonly used to model homogeneous currents in which vertical effects can be neglected (tsunamis, reservoirs with unexpressed stratification, fuel fluctuations in tanks, etc.).

Regularized shallow water equations

Shallow water model describes incompressible flows in terms of water depth $h(x, y, t)$ and horizontal velocity vector $\vec{u} = \{u_x(x, y, t), u_y(x, y, t)\}$. Also $b(x, y)$ usually denotes bathymetry function and therefore $\xi(x, y, t) = h(x, y, t) + b(x, y)$ is the level of water surface, see Fig. 1.

Due to instability of numerical solution to solve shallow water equations (SWE) system one usually uses complex numerical

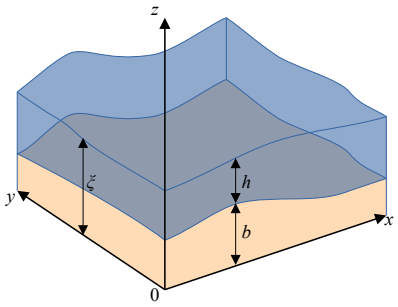


Figure 1: Schematic view of shallow water

schemes which are implicit or semi-implicit. This fact significantly decreases the effectiveness of program parallelization and consequently the computational performance. Otherwise, using fully explicit methods is inappropriate in case of modeling discontinuities (such as hydrodynamic jump) or transcritical flows.

It is well-known that SWE is similar to Euler equations for an inviscid compressible gas. Therefore, numerical algorithms for solving the SWE are based on methods developed for the Euler equations.

By analogy with the construction of the QHD/QGD systems regularized shallow water equations (RSWE) system has been derived [1]:

$$\frac{\partial h}{\partial t} + \operatorname{div} \vec{j}_m = 0, \tag{1}$$

$$\frac{\partial \left(h\vec{u}\right)}{\partial t} + \operatorname{div}\left(\vec{j}_m \otimes \vec{u}\right) + \nabla \frac{gh^2}{2} = -h^* g \nabla b + \operatorname{div} \Pi, \tag{2}$$

IMPROVEMENTS TO LOW Y+ MESH GENERATION IN HELYX

ANDREW JACKSON[1]
[1]*Engys Ltd, a.jackson@engys.com*

Keywords: *helyx, polyhedral mesh generation, low y+*

The mesh generator snappyHexMesh was first introduced at the 3rd OpenFOAM workshop in 2008 [1]. In the 11th OpenFOAM workshop in 2016 a new mesh generation technique to enable full layer coverage was described which was based on a dualised mesh approach [2].

In the current work an alternative full layer coverage mesh generation method is presented which is being developed to allow the generation of low y+ meshes. The new approach will also support the Adaptive Mesh Refinement (AMR) method for which the dual method does not.

In the new mesh generation approach a refined castellated mesh is first generated and for every boundary face a zero sized cell is extruded to leave a single layer of cells over the entire boundary. An optimiser is then used to inflate these zero sized cells to unit aspect ratio. A series of optimisation and error reduction steps are then deployed both during snapping and the final layer addition phase.

Both the dual and new extrude methods generate a full layer coverage mesh and the topological differences between the two methods are show in Figure 1 for a pump case.

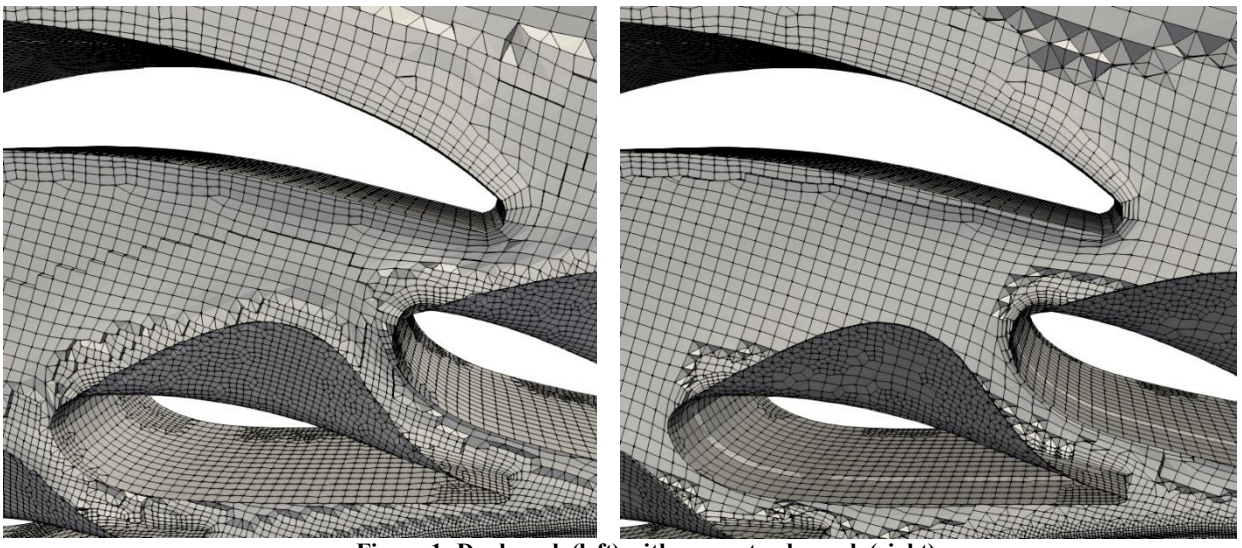


Figure 1: Dual mesh (left) with new extrude mesh (right)

These methods provide a robust framework for the modelling of moderate first cells heights. But as the first cell height is reduced to many orders of magnitude smaller that the local mesh spacing, it can become more challenging to generate an error free mesh.

There are two situations where the current methods can struggle. In the first, because the base mesh in general cannot be aligned with the geometry, the snapped surface elements may become warped because of their poor alignment to the local curvature. If the boundary face warpage is of the order of the specified first cell height, then inverted cells can result. To overcome this the associated hexahedral boundary cell for the warped faces are split into prisms in the direction of maximum surface curvature as shown in Figure 2.

HOW WE MADE OUR BUILD TEN TIMES FASTER

THOMAS A. JAMES[1], OLIVER OXTOBY[2], DANIEL COMBEST[3]
[1]*ENGYS Ltd, t.james@engys.com*
[2]*ENGYS Ltd, o.oxtoby@engys.com*
[3]*ENGYS LLC, d.combest@engys.com*

Keywords: *wmake, DevOps, CMake, Kitware*

Wmake has been the build system of choice for OpenFOAM and its derivatives for many years. As well as promising to simplify the process of writing makefiles, it provides a framework to manage the complex interconnectivity of OpenFOAM libraries and applications. Until recently, wmake was the build system used by HELYX®, a CFD software leveraging portions of the OpenFOAM C++ SDK. In an effort to reduce maintenance costs and increase usability, robustness, and extensibility, wmake has now been replaced in HELYX with a new build system based on CMake [1].

CMake is the de-facto industry standard C++ build tool [2]. As CMake is developed by Kitware Inc., HELYX developers are now only tasked with maintaining one specific implementation of that system. This obviously leads to less time spent on maintenance, but it also allows for the use of existing paradigms and extensions that confer significant advantages. For example, the HELYX build is now parameterised in a single text file (which makes the build much more reproducible), the build order is based on the dependencies of individual targets (which allows elegant handling of optional libraries and strange dependencies), and there is a separate configuration step (which allows for very fast detection of almost all potential failures). Additional improvements can be seen by leveraging the powerful tools available in the CMake ecosystem, such as clangd (which can be used to improve the already adequate IDE support provided by CMake), Google's ninja-build (which can be used instead of make to improve no-op build times), and CMake's built-in support for unity builds (which can reduce build times by an order of magnitude).

In this talk, attendees will be provided an overview of the CMake system and its qualitative benefits. They will be introduced to several third-party tools that enable improved build times, and give a simple quantitative analysis of the speed-ups that can be achieved (for example, see figures 1a and 1b). This is meant as a technical discussion of the success of CMake at ENGYS and the benefits of leveraging modern build tools from outside the OpenFOAM ecosystem.

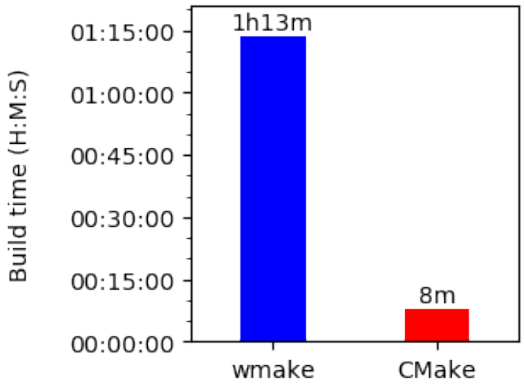


Figure 1a: The time taken for a complete build of HELYX (including waves2Foam and swak4Foam).

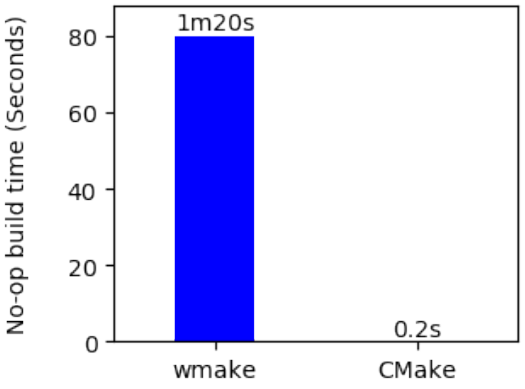


Figure 1b: The time taken for a no-op build (i.e. a build where all files are already compiled).

References

[1] Kitware Inc., CMake: https://cmake.org/

[2] Jetbrains, The State of Developer Ecosystem 2020: https://www.jetbrains.com/lp/devecosystem-2020/cpp/

Simulation of an Electrohydraulic discharge for sand remediation applications

Francisco J. Jimenez[1], Richard D. Sydora[2], Trent S. Hunter[3]
[1]*Department of Physics, University of Alberta, fjimenez@ualberta.ca*
[2]*Department of Physics, University of Alberta, rsydora@ualberta.ca*
[3]*3P Technology Corp., trent@3ptechnologycorp.com*

Keywords: *Plasma, electrohydraulic discharge, shock waves, compressibleInterFoam*

3P Technology Corp. is a Calgary-based company currently developing a new electrohydraulic process described as an innovative sand remediation process. A simplified description is as follows. A large capacitor bank is first charged up to the operational voltage (typically a few kV) while keeping it isolated from the treatment chamber through a spark activated high voltage switch. Once fully charged, the capacitor is suddenly discharged by closing the high voltage switch depositing all of its stored energy directly into the medium to be treated. In practice, two electrodes are used as the main mechanism to assist in this energy deposition process, creating a high power discharge characterized by the sudden appearance of a thin conducting (plasma) cavity channel between the electrodes. A high electrical current (typically on the order of few thousands of amperes) flows through the plasma channel rapidly depositing a large amount of energy into a small volume. As the discharge evolves, the channel grows in response to the characteristics of the discharging circuit, expanding the gas-filled cavity up to the point where internal forces are balanced with the hydrodynamic pressure exerted on the surface of the expanding bubble. The sudden appearance of such cavity, and the subsequent expanding process, creates pressure perturbations within the medium in the form of shock and acoustic waves traveling outwards to the walls of the container. Once the gas cavity has reached the maximum volume, it starts to collapse leading to the generation of more shocks due to cavitation phenomena. The dynamics of subsequent pressure perturbations follow a similar trajectory as the original plasma- based cavity until all energy has been dissipated. During this process, pressure perturbations are converted into mechanical forces that removes the viscous bitumen layer from sand particulates.

In an effort to create a comprehensive model, we have compartmentalized the discharge into three different stages, each dealing with a specific aspect of the process. In this work, we present a coupled plasma-hydrodynamic model to study the impact of geometrical parameters on the pressure dynamics inside a reactor. More details about this work can be found in [1]. The first stage, with a time scale in nanoseconds, deals with the initial expansion of a plasma channel due to the rapid evolution of the electric current. Electrical breakdown in liquids is a complex process and it is beyond the scope of this work, therefore we assume that the plasma channel already exists. This stage is modeled using a simplified approach that consists of a set of ordinary differential equations describing the evolution of energy, mass and momentum within the electric arc [2]. The model includes the effects of the capacitance and parasitic inductance on the system by coupling conservation laws based on a simple RLC electrical circuit (see Figure 1a). The model assumes a cylindrical expanding channel and produces information regarding the dynamic evolution of the cylinder radius, internal pressure, temperature and particle density in the plasma conducting channel. The solution of the ode system is then fed into the second stage, with a time scale in microseconds, which is based on a hydrodynamic model to simulate the evolution of the pressure waves and it is based on the OpenFOAM's compressibleInterFoam solver (v1912). The mesh resolution should be carefully chosen to have the necessary level of refinement to capture the pressure perturbations while keeping manageable execution times. The third stage, time scale in milliseconds, also based on compressibleInterFoam, follows the evolution of the steam bubble that appears once the plasma channel has long ceased to exist.

The computational geometry consist of a cylindrical slab to exploit the inherent cylindrical symmetry of the experimental batch reactor (see Figure 1b). The simulation is initialized by first creating a thin gas-filled channel at the center of the mesh keeping the rest of the geometry filled with water. To bridge the plasma circuit and hydrodynamic model, two simple coupling mechanisms have been explored. The first mechanism treats both phases of the process as separate entities. The coupling is then attained by initializing the parameters in the gas-filled cavity according to the output of the plasma circuit model. For instance, after a successful run of the plasma circuit model, we consider the pressure and plasma radius at the point which the pressure has reached its maximum, and initialize the gas filled cavity with these values. The simulation is then initiated and the pressure perturbation produced by this pressure gradient is followed by the solver. A second approach, currently under development, directly couples the ode system with OpenFOAM by communicating the ode solution results each time step to OpenFOAM. Results from the first approach are in very good agreement with experimental measurements of the pressure

LINEAR STABILITY ANALYSIS OF PLANE POISEUILLE FLOW USING OPENFOAM

RAVI KANT[1] AND ANIRUDH KULKARNI[2]
[1]*Pandit Deendayal Petroleum University, Gandhinagar, India, ravi.kant@sot.pdpu.ac.in*
[2]*Pandit Deendayal Petroleum University, Gandhinagar, India, anirudh.kulkarni@sot.pdpu.ac.in*

Keywords: *Stability analysis, transition, plane Poiseuille flow, modal and non-modal flow instability, OpenFOAM.*

We present the linear stability analysis of plane Poiseuille flow using OpenFOAM. Although the flow instability of plane Poiseuille flow (PPF) is very well understood by the research community [1,2], but the attempt to analyse instabilities of plane Poiseuille flow in OpenFOAM has not been carried out to the best of our knowledge. In this regard, we modify the standard incompressible solver i.e., "icoFoam" and associated libraries in OpenFOAM to get the perturbation fields. We also study the modal analysis and obtain the eigenmodes, which are validated with that of existing benchmark results [3]. Nevertheless, Liu et.al [4] has already studied the structural sensitivity and receptivity of standard lid driven cavity using direct and adjoint Navier-Stokes equations in OpenFOAM. In this paper we solve LNSE (linearized Navier-Stokes equation) around the base flow of PPF utilising the "icoFoam" solver in OpenFOAM.
Flow setup – The plane Poiseuille flow is setup in streamwise direction with nondimensional base flow $U(Y) = 1- Y^2$ as shown in Figure 1. The Reynolds number is defined as UL/μ, where U is the base flow and L is the width between two plates and μ is the kinematic viscosity.

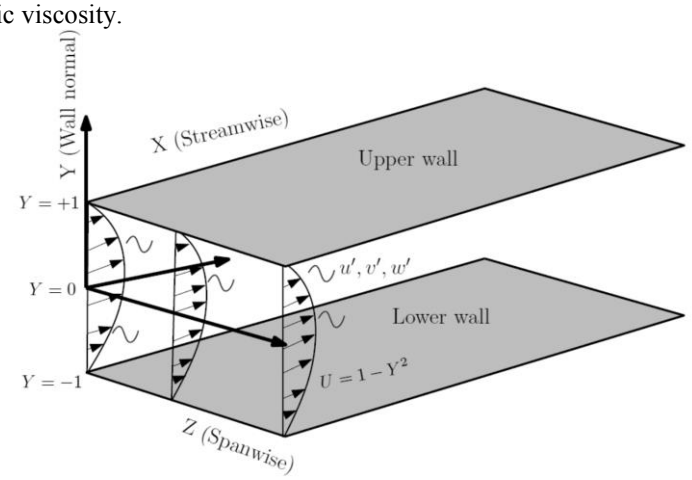


Figure 1: Perturbation field added to the base flow for stability analysis

Governing equation – Perturbed incompressible linear Navier Stokes equation (LNSE) along with the perturbed continuity is written as,

$$\nabla \cdot \boldsymbol{u}' = 0$$

$$\frac{\partial \boldsymbol{u}'}{\partial t} + \boldsymbol{U}.\nabla \boldsymbol{u}' + \boldsymbol{u}'\nabla \boldsymbol{U} = -\nabla p' + \frac{1}{Re}\nabla^2 \boldsymbol{u}'$$

Where $\boldsymbol{u'}$ = [u',v',w'] is the perturbation field and U = [0, 1-y^2,0] is the base flow in cartesian coordinate for plane Poiseuille flow. In compact form, we can write the LNSE as,

$$\frac{\partial \boldsymbol{u}'}{\partial t} = A\boldsymbol{u}'$$

Where $\boldsymbol{A}$ is the LNSE operator. This can be also be formulated as an eigenvalue problem as,

$$A\boldsymbol{u}' = \lambda \boldsymbol{u}'$$

Modification in icoFoam – The LNSE perturbed set of equations are quite similar to the usual Navier-Stokes equation. The standard incompressible icoFoam solver can be easily modified and the perturbation field solutions can sought with no-slip perturbation boundary conditions at walls. In addition to the solution of perturbation field, the eigenmodes are also evaluated and validated with the existing benchmark results [3].

Acknowledgements

The authors thank all those involved in the organisation of OFW16 and to all the contributors that will enrich this event.

EULERIAN MULTI-FLUID MODEL FOR EVAPORATING LIQUID SPRAYS

ROBERT KESER[1], MICHELE BATTISTONI[2], HONG G. IM[3], HRVOJE JASAK[4],
[1]*University of Zagreb, Faculty of Mechanical Engineering and Naval Architecture, robert.keser@fsb.hr*
[2]*Department of Engineering, University of Perugia, michele.battistoni@unipg.it*
[3]*King Abdullah University of Science and Technology, Clean Combustion Research Center, hong.im@kaust.edu.sa*
[4]*University of Zagreb, Faculty of Mechanical Engineering and Naval Architecture, hrvoje.jasak@fsb.hr*

Keywords: *Eulerian multi-fluid model, Multiphase, Polydisperse, Spray, Droplet Flow, Evaporation*

This research aims to develop a numerical model capable of predicting the dynamic behaviour of liquid fuels in dense sprays. In the developed method, the flow's polydisperse nature is handled using the method of classes in the Euler-Euler framework, using the Eulerian multi-fluid model. Therefore, every droplet class is represented with a dedicated phase momentum and phase continuity equation. However, all phases, i.e. all droplet classes and the continuous phase, share the same mixture pressure.

This work represents an update of the previously published model [1, 2, 3], where the developed solver is further updated with evaporation functionality. To implement a functioning evaporation model, the solver required implementation of energy equations for the continuous and the droplet phases to broaden the developed solver's functionality. The continuous and droplet phases are thermally coupled either by the evaporation model or using the Ranz-Marshall correlation (for non-evaporating functionality). To capture more details concerning droplets' internal thermal behaviour, e.g. finite thermal conductivity and internal recirculation within the droplets, the solver utilizes a parabolic temperature profile model [4], which is coupled with the effective thermal conductivity model [5]. Furthermore, the evaporation model required a species transfer equation which was the last prerequisite for adding single component evaporation capability. For describing evaporation of moving droplets, we have selected the Abrazon and Sirignano model [6].

Figure 1 presents the temperatures extracted along a sampling line which goes through a non-evaporating spray (evaporation model is turned off), i.e. cold droplets are injected into a stationary hot gas. As the results suggest, the passing droplets are cooling down the hot gas, and the surface temperature is slightly higher than the volume-averaged droplet temperature. Furthermore, to perform preliminary tests of the implemented evaporation model, Figure 2 gives the penetration curves (both for the liquid fuel, and the fuel vapour) for a similar test case where large droplets (i.e. blobs) are injected into a stationary hot gas, and the evaporation model is turned on.

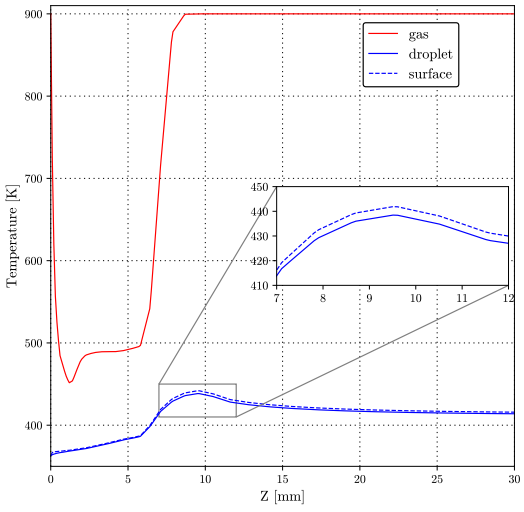


Figure 1: Temperature behaviour.

QGDSOLVER – THE OPENFOAM-BASED FRAMEWORK FOR NUMERICAL MODELLING OF TRANSIENT GAS AND LIQUID FLOWS USING REGULARIZED EQUATIONS

MATVEY KRAPOSHIN[1]
[1]*Ivannikov Institute for System Programming of the RAS, os-cfd@yandex.ru*

Keywords: *regularized equations, gas dynamics, fluid dynamics, finite volume method, numerical modelling, QGD, QHD.*

One of the key to success of OpenFOAM technology is the generality of PIMPLE (PISO-SIMPLE) approach for pressure-velocity coupling. Being applied to variety of flow types (from incompressible to trans- and supersonic, from perfect gases to real gases, multicomponent and even multiphase) this procedure has allowed to develop numerous numerical algorithms that form the basis of OpenFOAM applications for numerical modelling. With the generality, this procedure has some restrictions that do not allow to resolve properly some phenomena or make the development multiphysics applications. For example, while literal application of the procedure to compressible flows has allowed to derive approximation of gas flow equations, the range the Mach numbers where numerical algorithm can operate is bounded by maximum value of 2. As another example of PIMPLE algorithm limitation its iterative nature can mentioned: an introduction of new mechanisms (such as mesh motion, buoyancy, etc) requires additional iterations loops or numerical coupling tricks (for instance, pressure correction equations after mesh motion).
Some problems can be resolved by introduction of approximate Rieman solvers (for example, hybrid PIMPLE-KNP scheme was implemented as rhoPimpleCentralFoam application for numerical simulation of compressible viscous real gas flows). However in some cases the evaluation of Rieman fluxes could be a serious obstacle in the numerical model development process.
As an alternative to conventional approaches, the numerical algorithm based on regularized equations of flow was implemented using OpenFOAM library. The essential idea behind this approach is the application of averaging procedure to convective part of equations which produces additional diffusive terms or tau-terms, named by the multiplier τ with dimensions of time. For gas flows this new equations are called quasi gas dynamics equations (QGD), for fluid flows – quasi hydrodynamics equations (QHD). They posses such important properties as non-negative dissipative function. First variant QGD system was obtained by B.N. Chetverushkin about 30 years ago, then this system was extended to QHD by Yu.V. Sheretov. Nowadays, it is used broadly in Keldysh Institute of Applied Mathematics of the RAS for various problems.
The implementation of OpenFOAM solvers using QGD/QHD approach was started in 2017. Since then, several major improvements were introduced in the QGDsolver library (https://github.com/unicfdlab/QGDsolver) and today it includes next applications:

1. QGDFoam - solver for compressible viscous perfect gas flows in a wide Mach number range - from 0 to infinity
2. QHDFoam - solver for incompressible viscous fluid flows with buoyancy force
3. particlesQGDFOam - solver for compressible viscous perfect gas flows in a wide Mach number range with particles - from 0 to infinity
4. particlesQHDFoam - solver for incompressible viscous fluid flows with buoyancy force with particles
5. SRFQHDFoam - solver for incompressible viscous fluid flows in rotating frame of reference with buoyancy force
6. QHDDyMFoam - solver for incompressible viscous fluid flows in domains with deforming boundary and with buoyancy force
7. interQHDFoam - solver for incompressible 2-phase viscous fluid flows with buoyancy force and surface tension
8. reactingLagrangianQGDFoam - solver for reacting multicomponent compressible viscous perfect gas flows in a wide Mach number range with particles - from 0 to infinity
9. scalarTransportQHDFoam - solver for scalar transport equation to demonstrate the very basics of QGD/QHD equations principles

The main benefits of the implemented approach are:
- absence of flux limiters (they could be used, but they are not required, even for very high speed flows);
- single computational strategy in all regions (for example – QGDFoam can operate at Mach numbers from 0.01 to 100)

Hydrodynamic and thermal characteristics of flow past a 2D and 3D porous square cylinder at moderate Reynolds numbers

Anirudh Kulkarni[1], Ravi Kant[2],
[1]Department of Mechanical Engineering, School of Technology, Pandit Deendayal Petroleum University, Gandhinagar, Gujarat, India, anirudh.kulkarni@sot.pdpu.ac.in
[2]Department of Mechanical Engineering, School of Technology, Pandit Deendayal Petroleum University, Gandhinagar, Gujarat, India, ravi.kant@sot.pdpu.ac.in

Keywords: porous block, onset of three-dimensionality, wake transition, Darcy-Brinkman-Forchheimer model, fluid flow, heat transfer

The onset of three-dimensionality in the flow and heat transfer from a heated porous square cylinder has been studied. A vivid comparison between the results for two-dimensional and three-dimensional hydrodynamic and thermal characteristics of flow behind a solid square cylinder has been made. The porous region is modelled by using the extended Darcy-Brinkman-Forchheimer model. The generic dnsFoam solver of the OpenFOAM 5.0 has been modified to model the porous area along with the consideration of local pore velocity. The parametric simulations are run for Reynolds number range of Re = 10-1000 (with a high resolution in Re) and Darcy number values of $Da = 10^{-6}$ - 10^{-2}. The numerical results show three critical regions wherein existence of secondary wake instability, the discrepancy between 2D and 3D results, and properties of the recirculation regions on the upper and lower side of the solid cylinder is noticed. Critical values of Re for each instability has been highlighted throughout of the article. Moreover, these values significantly change with respect to the various Da values and are explicitly listed in the article. Furthermore, critical values of Da has been listed out for each mode at respective Re values. Also, the validity of the inertial or the Forchheimer term has been tested out thoroughly for the present study to verify if the porous region can be modelled by Darcy-Brinkman model alone.

ACCELERATION OF LARGE DOES FOR MACHINE LEARNING AUGMENTED AUTOMOTIVE AERODYNAMIC DESIGN

NIKOLAOS KYRIAZIS[1], GIAMPAOLO CETRARO[1], JIANBO HUANG[1], GEORGE HOHOLIS[1], GEORGIOS KARPOUZAS[1], EUGENE DE VILLIERS[1]
[1]*Engys Ltd., n.kyriazis@engys.com*

Keywords: *DOEs, volumetric mapping & sampling, coupled solver*

An accelerated platform for vehicle CFD simulations used in AI training is presented. The geometries for creating the large flow field database are based on DrivAer Model [1] and were provided by FCA group in the context of the European Union project UPSCALE. Efficient generation of the flow field database necessitated development and enhancement of pre-processing utilities, CFD solver, and data-extraction tools.

In the pre-processing context of the workflow, the computational grid for each vehicle geometry was constructed by employing the HELYX mesh generator [2], which is an evolved version of snappyHexMesh with improved performance and mesh quality. Since all geometry variants to be used in the study are derived from a single baseline case and their flow fields are expected to be similar, the mapping of initial fields from previous results was adopted instead of potential flow for field initialization. The newly developed mapping technology uses a K-nearest neighbour (KNN) search [3] and it is up to 10 times more efficient than traditional Octree mapping techniques. The way the mapping is performed is either coordinate or wall distanced based. In the coordinate-based map utility, areas of similar location are mapped from the source to the target, whereas in the wall-distance-based approach, areas of similar wall distances are mapped. The latter produces a smoother initial solution as it avoids mapping a solid region into a fluid one or vice versa.

Regarding the CFD solver selected for creating the flow field DOEs, a pressure-based block solver [4], [5] with Algebraic Multi-Grid was employed. In the 3-D steady-state vehicle simulations that were performed as part of this work, the coupled solver was found to converge twice as fast as compared to the heavily optimised segregated counterpart. Due to faster convergence and incremental speed-up per case, the total simulation time was significantly reduced. Furthermore, a new convergence assessment criterium, based on statistical and integral considerations, was applied to terminate the simulation once objective conditions regarding the aerodynamic coefficients were satisfied, so avoiding redundant iterations at the end of the calculation.

As a final step, the CFD solution on the cell centres and the vehicle geometry was sampled in the vicinity of the vehicle, significantly reducing the volume of data that has to be stored for subsequent use with the AI training algorithms. The sampling can be either structured by employing the KNN algorithm or unstructured by making use of OpenVDB technology [6]. In both cases, the computational cost compared to traditional sampling techniques used in OpenFOAM is significantly reduced.

Various permutations of the above detailed workflow are compared in the context of the DrivAer DoE to demonstrate the performance gains that have been achieved.

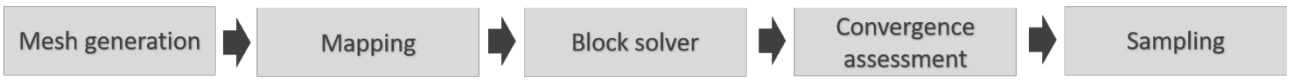


Figure 1: Platform workflow

Acknowledgements

The research leading to these results has received funding from Upscale H2020 programme under GA number 824306. The authors would like to thank Luca Miretti and FCA group for providing the geometry database.

References

[1] A. Heft, T. Indinger, N. Adams: Introduction of a New Realistic Generic Car Model for Aerodynamic Investigations, SAE 2012 World Congress, April 23-26, 2012, Detroit, Michigan, USA, Paper 2012-01-0168.

[2] E. de Villiers, A. Jackson and M. Janssens, Automatic Parallel Polyhedral Mesh Generation on Complex Geometries in OpenFOAM, Third OpenFOAM Workshop, Politecnico di Milano, 2008.

[3] S. Arya and D. M. Mount: Approximate Nearest Neighbor Searching, Proc. 4th Annu. ACM-SIAM Sympos. on Discrete Algorithms (SODA'93), 1993, 271-280.

[4] G.K.Karpouzas: A Hybrid Method for Shape And Topology Optimization in Fluid Mechanics, Ph.D. Thesis, Engys Ltd. - NTUA, 2018.

Turbulent Non-Premixed Combustion in Single Heating Section of an Anode Baking Ring Furnace

D. Lahaye[1], P. Nakate[1], C. Vuik[1], M. Talice[2], F. Juretić[3]
[1] *Delft Institute of Applied Mathematics, Technical University of Delft*
[2] *PMSQUARED Engineering, Cagliari, Italy*
[3] *Creative Fields Ltd., Zagreb, Croatia*

Keywords: *non-premixed combustion, turbulence, radiative heat transfer, conjugate heat transfer, thermal NOx, anode baking furnace*

1 Introduction

Heavy industry relies on hydro-carbon fuels as a primary source of energy. Alternatives that meet power demands are not available. The future use of fossil fuels, however, is met by environmental, economical and geo-political challenges. Measures to combat climate change impose ever stringent requirements on pollutant emissions. The depletion of proper sources renders the Netherlands critically dependent on foreign import. Data-driven insight to formulate guidelines for sustainable and economical use of hydro-carbon fuels is thus urgently required. Ways to introduce fuel blends with hydrogen, synthetic fuels and exhaust gas recirculation to obtain mild combustion regimes will be investigated.

The aim of this project is to deploy digital twins to study the combustion processes in large Dutch industrial installations. A digital twin will mimmic the turbulent mixing of fuel and oxidizer, their chemical reaction, the ensuing heat release and the radiative transport of the heat through the furnace. The furnace and twins will communicate through measured data such as temperature, velocity and chemical species. After a calibration stage, the digital twin will allow to experiment with innovative ways to operate industrial furnace. These include adaption of new burners to obtain better fuel mixing, the recirculation of exhaust gasses to reduce overheating and the injection of new fuel mixtures (including blends with hydrogen). The project is carried out in close collaboration between TU Delft and the company AluChemie in the harbor of Rotterdam.

2 Anode Baking Furnace

In this work we study ring furnaces used in the production of anodes to melt aluminum. The furnaces consists of multiple section of which one is schematically represented in Figure 1 (left). The combustion air enters on the top left, travels through a double U-shaped profile with obstructions and exits on the top right. The gaseous fuel in injected through two burners mounted on top of the furnace. The heat produced by combustion travels through refractory lateral walls and bakes the anode material. We wish to control the combustion process, to arrive at the best possible mixing of air and fuel and to reduce the pollutant formation (such as nitric-oxides and carbon-monoxide) to a lowest possible level. The design parameters that we can control include the type of burner, the locations and size of obstructions in the channel and the amount of hydrogen in the gaseous fuel blend.

Details on the type of furnace, on the geometry and flow conditions considered in this work are given in [5].

3 Non-Premixed Turbulent Combustion Using OpenFoam

OpenFoam offers various solvers to model non-premixed turbulent combustion processes. Here we are primarily interested in capturing the mixing of gaseous fuel and oxidizer to a sufficient level of accuracy. Motivated by earlier work in [2], we choose to employ the chtMultiRegionFoam solver. The turbulence, combustion and radiative heat transfer are modeled using a realizable k-ϵ, an eddy-dissipation and a discrete ordinate model, respectively. Meshes are generated using the cfMesh software. The thermal nitric-oxide concentration is evaluated in post-processing stage.

LAGRANGIAN-BASED NONLINEAR MANEUVERING AND SEAKEEPING PARAMETER IDENTIFICATION USING OPENFOAM

WILLIAM LAMBERT[1], STEFANO BRIZZOLARA[1]
[1]*Virginia Polytechnic Institute and State University, wblambert@vt.edu*
[2]*Virginia Polytechnic Institute and State University, stebriz@vt.edu*

Keywords: *Free-surface, Parameter identification, Added-mass*

Recent work by students at Virginia Tech has resulted in a Lagrangian-based formulation for the maneuvering and seakeeping of autonomous underwater vehicles operating close to a wavy free-surface [1]. Advancements were made to reformulate the model to use state-dependent parameters (depth and pitch) that can be calculated using a time-domain boundary element method [2]. While calculation of parameters in this fashion produces useful results, this process relies on several major model simplifications including the neglect of viscous effects, linearization of free-surface deformation, and ignoring time-dependent memory effects. Attempts to incorporate more nonlinear effects into the model through nonlinear free-surface boundary conditions in the time-domain panel method [3] ultimately led to the realization that full fidelity CFD calculations through OpenFOAM would be necessary to mitigate the errors due to the previously made model simplifications.

The model and subsequent force calculations, based off first principle energy considerations, ultimately come down to the calculation of the system Lagrangian, which is the system kinetic energy minus the system potential energy. The Lagrangian, as proposed by Battista, has a general form similar to:

$$\begin{aligned}\mathcal{L} =& \frac{1}{2}\boldsymbol{\nu}^T(\boldsymbol{M}_b + \boldsymbol{M}_{\mathcal{B}} + \Delta\boldsymbol{M}_{\mathcal{B}}(\boldsymbol{q}) + \boldsymbol{M}_{\mathcal{S}}(\boldsymbol{q},\boldsymbol{\nu}))\boldsymbol{\nu} \\ &+ \boldsymbol{\nu}^T\int_0^t [\boldsymbol{K}_{\mathcal{B}}(\boldsymbol{q}(\tau), t-\tau) + \boldsymbol{K}_{\mathcal{S}}(\boldsymbol{q},\boldsymbol{\nu},\boldsymbol{q}(\tau), t-\tau)]\boldsymbol{\nu}(\tau)d\tau\end{aligned} \tag{1}$$

The second line of this equation is a convolution integral tied to the inclusion of memory terms and is not going to be immediately considered. The first line, however, contains terms that are tied to both the kinetic and potential energy of the rigid body, fluid body, and free-surface interface. There are four mass matrices in this calculation, the rigid-body mass and three other added mass matrices: the deeply-submerged added mass, a correction accounting for the asymmetry of the fluid due to a free-surface, and a last correction for energy contained within a deformable free-surface. The latter two matrices are dependent on position and position/ velocity, respectively.

OpenFOAM is being utilized to develop simulations in order to derive these added mass terms. A succession of three simulations with three different operating conditions is being used to calculate these matrices for a spheroidal body. Understanding the physical nature of these values, one is able to append conditions to the simulations in order to isolate the terms. Figure 1 shows this progression beginning with a forced motion of the body (similar to VPMM tests) in a deeply submerged condition. One then imposes a rigid-wall boundary, with which the body will operate under various orientations and distances with regard to the wall. This will isolate the influence of the asymmetry of the fluid. Lastly, the body is again subjected to a forced motion but now in the proximity of a fully deformable free-surface, isolating the energy contained in the deformations. This series of simulations is conducted both in inviscid and viscous fluids to determine any corrections needed to account for viscous phenomena. The resulting added mass terms (and viscous corrections) will be used within the model to help create a controller for this body when operating in conditions where free-surface effects are important.

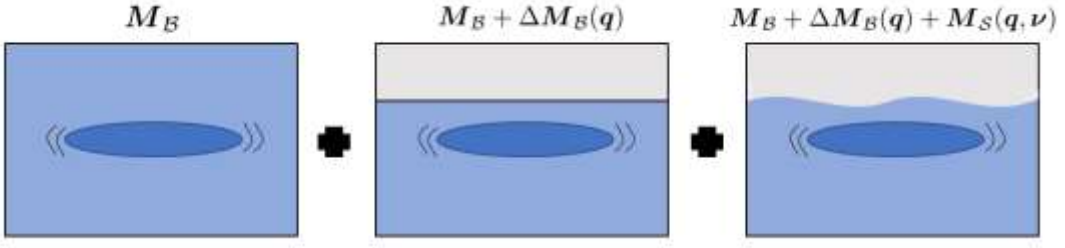


Figure 1: Progression of simulations used in calculation of added-mass parameters

EXTENSION OF THE OVERSET MESH METHOD FOR MODELLING GEOPHYSICAL FLOWS AND MARITIME APPLICATIONS

JAVIER L. LARA[1], ALESSANDRO ROMANO[1], GABRIEL BARAJAS[1], ÍÑIGO J. LOSADA[1]
[1]*IHCantabria - Instituto de Hidráulica Ambiental de la Universidad de Cantabria, Santander, Spain,*
jav.lopez@unican.es, romanoal@unican.es, gabriel.barajas@unican.es, inigo.losada@unican.es

Keywords: *Landlside tsunamis, CFD modelling, water waves.*

Computational Fluid Dynamics (CFD) has become in recent years a crucial means for studying and solving various technical/scientific applications, addressing different and diverse areas of the knowledge, spanning from the dynamics of floating objects to the investigation of complex geophysical flows (e.g. tsunamis). In this work, we present how the application and the extension of the Overset mesh method, coupled with other numerical methods (e.g. porous media approach), can be used to shed light on unresolved phenomena connected to maritime applications. In particular, we focus on the numerical modelling of tsunamis generated by landslides.

The interest in tsunamis generated by landslides in proximity of the coast has risen in the last decades, due to several devastating events (e.g. Lituya Bay, Alaska, Fritz et al., 2009; Stromboli Island, Italy, Tinti et al., 2005; Anak Krakatau, Indonesia, Grilli et al., 2019). Among the tsunami triggering mechanisms, landslides assume a relevant role. The destructive effects caused by the impulsive waves, generated by landslide sources, can be strongly magnified by the characteristics of the so-called confined geometries (e.g. bays, reservoirs, lakes, volcanic islands, fjords, etc.). Complicated physical phenomena (e.g. trapping mechanisms, edge waves, wave runup, etc.) take place as a consequence of the interaction between the generated waves and the local bathymetry and control the tsunami propagation and interaction with the coast, often causing devastating consequences.

To reduce and mitigate the landslide-tsunami hazard a proper comprehension, and modelling, of such complicated phenomena is crucial. Landslide-generated tsunamis have been studied by exploiting experimental, analytical and numerical modelling. Experimental tests are often time and money consuming, especially if 3D models are considered. Large facilities, as well as complicated experimental configurations and sophisticated measurement systems (e.g. Romano et al. 2016), are often needed. Furthermore, not always it is possible to explore in detail the influence of all the involved parameters, in particular those related to the landslide triggering mechanisms and rheology, that have a considerable influence on the wave characteristics in the so-called "near-field".

To this end, numerical modelling can provide a valuable assistance. The new tools offered by the CFD methods represent a valuable means for shedding light on the unresolved aspects. In particular, the 3D CFD modelling techniques appear to be crucial as far as the tsunami characteristics in the near-field, induced by landslide sources, are concerned. Indeed, the accurate reproduction of the energy transfer between the landslide and the water is essential to model the tsunami generation and propagation mechanisms, allowing to explore a large variety of landslide triggering mechanisms and rheology.

In this paper, we present the numerical modelling of tsunamis generated by landslides, both subaerial and submerged, in OpenFOAM by taking advantage of a hybrid approach, based on the combined use of the Overset mesh technique and the porous media approach (Lara et al., 2012). The method has been previously used by Romano et al. (2020) to model submerged landslides of simple shape at a straight coast. In this work both subaerial and submerged landslides are reproduced by exploring the influence of different landslide shapes and shoreline geometries. To this end, two experimental benchmarks are numerically reproduced, namely: I) the experiments carried out by Liu et al. (2005), reproducing a wedge-shaped rigid and impermeable submerged landslide at a straight coast (see Figure 1); II) the benchmark experiments carried out by Romano et al. (2016), reproducing an ellipsoid-shaped rigid and impermeable subaerial landslide, sliding along the flanks of a conical island (see Figure 2).

A detailed description of the numerical approach and an in-depth comparison between experimental and numerical results will be shown at the Conference.

DEVELOPING A GODUNOV-TYPE SCHEME FOR THE VARIABLE-DENSITY ARTIFICIAL-COMPRESSIBILITY EQUATIONS

SHANNON LEAKEY[1], CASPAR J.M. HEWETT[2], VASSILIS GLENIS[3], PAUL F. QUINN[4]
School of Engineering, Newcastle University, United Kingdom
[1]*s.c.leakey2@newcastle.ac.uk*
[2]*caspar.hewett@newcastle.ac.uk*
[3]*vassilis.glenis@newcastle.ac.uk*
[4]*p.f.quinn@newcastle.ac.uk*

Keywords: *multiphase, artificial compressibility, dual time stepping, Godunov-type scheme, Riemann solvers, density-based*

Artificial compressibility

Density-based methods, such as Godunov-type schemes for hyperbolic conservation laws, can be extended to incompressible flow using the idea of artificial compressibility. Artificial compressibility introduces a pseudo-time derivative for pressure, and the solution advances in this pseudo-time until convergence to an incompressible limit [1, 2, 3]. Chorin [4] created the method for steady-state cases, but it has since been generalised to transient cases using dual time stepping, that is, driving the solution to an incompressible limit each real-time step. Multi-stage Runge-Kutta methods [5, 6] are particularly popular for the pseudo-time stepping [7], and local time stepping can be used to speed up the convergence. This is a fundamentally different approach to PISO or SIMPLE as the equations are coupled, not segregated [8]. Moreover, while pressure-velocity iterations are computationally cheaper than pseudo-time steps, these pseudo-time steps are explicit and local, and so the method lends itself to easier parallelisation [9, 10].

Variable density equations

Although the artificial compressibility method is widespread, its application to multiphase flows is not [8]. Kelecy and Pletcher [11] pioneered an approach, which has since been built upon by [12, 13]. The idea is to model the flows as incompressible with variable density and then the air-water interface gets automatically captured by the contact wave in the Riemann solver. As such, no special treatment like in the volume-of-fluid method [14] is required. Adopting the cancellation matrix notation of [7] and denoting the artificial compressibility coefficient by β, this study uses the governing equations

$$\frac{\partial \mathbf{Q}}{\partial \tau} + \mathbf{I}_C \frac{\partial \mathbf{Q}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{B} \tag{1}$$

where $\mathbf{Q} = [\rho, \rho u, \rho v, \rho w, p/\beta]^T$, $\mathbf{I}_C = \text{diag}(1, 1, 1, 1, 0)$, τ is pseudo-time, t is real-time,

$$\mathbf{F} = \mathbf{F}_{inv} - \mathbf{F}_{vis} \tag{2}$$

$$\mathbf{F}_{inv} = \left(\begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uw \\ u \end{bmatrix}, \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vw \\ v \end{bmatrix}, \begin{bmatrix} \rho w \\ \rho uw \\ \rho vw \\ \rho w^2 + p \\ w \end{bmatrix} \right) \tag{3}$$

$$\mathbf{F}_{vis} = \left(\begin{bmatrix} 0 \\ \mu\left(\frac{\partial u}{\partial x} + \nabla u\right) \\ \mu\left(\frac{\partial u}{\partial y} + \nabla v\right) \\ \mu\left(\frac{\partial u}{\partial z} + \nabla w\right) \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ \mu\left(\frac{\partial v}{\partial x} + \nabla u\right) \\ \mu\left(\frac{\partial v}{\partial y} + \nabla v\right) \\ \mu\left(\frac{\partial v}{\partial z} + \nabla w\right) \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ \mu\left(\frac{\partial w}{\partial x} + \nabla u\right) \\ \mu\left(\frac{\partial w}{\partial y} + \nabla v\right) \\ \mu\left(\frac{\partial w}{\partial z} + \nabla w\right) \\ 0 \end{bmatrix} \right), \tag{4}$$

and $\mathbf{B} = [0, \rho \mathbf{g}_x, \rho \mathbf{g}_y, \rho \mathbf{g}_z, 0]^T$. The inviscid fluxes are calculated with a Riemann solver, the equations are updated using an explicit multi-stage Runge-Kutta method for pseudo-time, and the real-time derivative gets updated each pseudo-time step until convergence.

INFLUENCE OF BUBBLE SIZE DISTRIBUTION ON ACOUSTICALLY CAVITATING FLOWS

SERGEY LESNIK[1], GUNTHER BRENNER[2]
[1]*Clausthal University of Technology, Institute of Applied Mechanics, Adolph-Roemer-Straße 2A, 38678 Clausthal-Zellerfeld, Germany, sergey.lesnik@gmail.com*
[2]*Clausthal University of Technology, Institute of Applied Mechanics, Adolph-Roemer-Straße 2A, 38678 Clausthal-Zellerfeld, Germany, gunther.brenner@tu-clausthal.de*

Keywords: *Acoustic Cavitation, Bubble size distribution, Euler-Lagrange, Newton-Raphson method, Helmholtz equation, Dynamic load balancing*

Acoustic cavitation applied in process engineering allows speeding up a wide range of chemical reactions. The geometries of chemical reactors are mostly not customized for such applications. There is a lack of numerical tools, which could deliver simulations suitable for reactors' optimization.
A solver for acoustic cavitation is proposed in foam-extend, which predicts acoustic field inside a reactor taking into account damping effect of cavitation bubbles. Since the time and length scales of the involved physics may differ by several orders of magnitude, a special treatment during the modeling is applied. We use Euler-Lagrange approach to couple acoustics and flow with cavitation bubbles. Eulerian phase accounts for the field quantities such as acoustic pressure or flow velocity. The governing equation for acoustics is the Helmholtz equation that leads to highly indefinite matrices after discretization. Thus, a coupling to the direct solver MUMPS is introduced. Further, a state-of-the-art model for the damping of acoustics due to cavitation bubbles [1] introduces a non-linear problem which is resolved by an implementation of the Newton-Raphson method. The cavitation bubbles represent the Lagrangian phase. Due to cavitational forces, bubbles form clusters that might be dense locally. From the performance view of the solver this leads to an unbalanced load in a parallel run, where few computational units might have to deal with the largest part of the bubble population. The dynamic load balancing from foam-extend is customized to allow rebalancing the number of bubbles per computational core on demand. As a result, the model allows efficient computation of cavitation flows with spatially inhomogeneous bubble distribution.
One of the challenges in order to provide reasonable cavitation model is the correct depiction of the bubble size distribution. Our test cases focus primarily on reactors with immersed ultrasound transducers. We run several numerical experiments with monodisperse bubble populations, where we alter the bubble diameter keeping all other input parameters, especially the void fraction, constant. We also run calculations with polydisperse bubble populations, where the size distribution is set according to the optical measurements from a recent experimental work [2]. According to the results, the non-linear damping model and the different bubble size distributions show a large influence on the ultrasonic field and the flow.

Acknowledgements

We thank all group members of the cavitation research group at the Drittes Physikalisches Institut for support and stimulating discussions. The authors acknowledge the support of Deutsche Forschungsgemeinschaft – Germany under the grant BR 1864/12-2.

References

[1] O. Louisnard, “A simple model of ultrasound propagation in a cavitating liquid. Part I: Theory, nonlinear attenuation and traveling wave generation,” Ultrason. Sonochem., vol. 19, no. 1, pp. 66–76, 2012, doi: 10.1016/j.ultsonch.2011.06.008.

[2] F. Reuter, S. Lesnik, K. Ayaz-Bustami, G. Brenner, and R. Mettin, “Bubble size measurements in different acoustic cavitation structures: Filaments, clusters, and the acoustically cavitated jet,” Ultrason. Sonochem., vol. 55, pp. 383–394, Jul. 2019, doi: 10.1016/j.ultsonch.2018.05.003.

NOVEL FLUID-SOLID INTERACTIONS TECHNIQUES BASED ON MACHINE LEARNING

SCOTT LEVIE[1], PHILIP CARDIFF[1,2,3]
[1] *School of Mechanical and Materials Engineering, University College Dublin, Ireland*
[2] *Bekaert University Technology Centre, School of Mechanical and Materials Engineering, University College Dublin, Ireland*
[3] *SFI I-Form Centre, University College Dublin, Ireland*
scott.levie@ucdconnect.ie
philip.cardiff@ucd.ie

Keywords: *Fluid-solid interaction, machine learning, solids4foam, linear regression, artificial neural networks*

Computational fluid-solid interaction (FSI) techniques are notoriously computationally expensive and time-consuming especially for strongly coupled schemes in partitioned FSI solvers, particularly when large numbers of outer correctors are required for stability. These partitioned solvers involve the use of separate computational fluid dynamics and computational solid mechanics procedures to solve their respective domains before being coupled at the interface. This coupling procedure at the interface iterates within each timestep in order to determine an interface position which satisfies local kinematic and kinetic equilibrium conditions [1]. This project presents a novel supervised regression machine learning model which has been trained to predict the converged (final iteration) interface deflection values from the initial iteration values. This model has been implemented into solids4foam [2], an open-source toolbox for solid mechanics and fluid-solid interactions in OpenFOAM, and tested on the FSI benchmark test case proposed by Richter et al., incompressible channel flow over an elastic beam [3].

An immediate application of this technique is the use of a linear regression model trained on the interface data from a coarse mesh simulation using the Aitken's iterative scheme, to predict the converged interface displacement values of an identical case using a finer mesh. The combined time to run the coarse mesh case, train the predictive model and run fine mesh case using the predictive iterative scheme was 20% lower than solely running the fine mesh case using the Aitken's iterative scheme. This was demonstrated for cases containing both small and large strains (Figure 1).

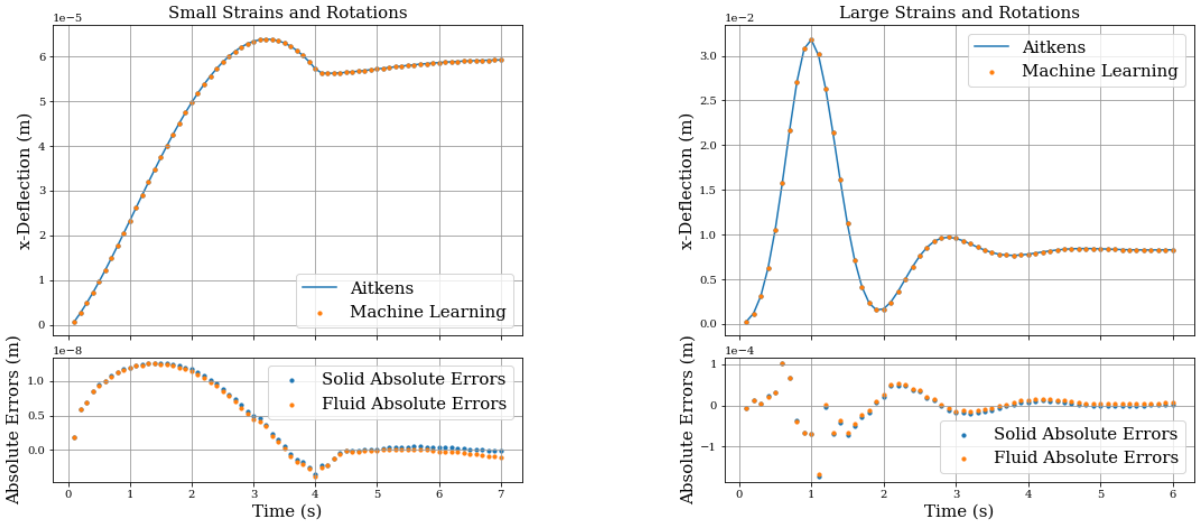


Figure 1: Comparison of point deflections on the fluid/solid interface using the standard Aitken's iterative scheme and the proposed machine learning scheme. The comparison is shown for cases with small strains (left) and large strains (right) [1]

The same linear regression model has been trained on cases of varying Young's modulus, inlet velocity and beam geometry and has been shown to predict the interface behaviour of unseen test cases containing different forementioned parameters for small strains and rotations. Future work will examine the benefit of using artificial neural networks to achieve the same generalisation for cases exhibiting large strains and rotations.

CFD STUDIES OF THE DYNAMICS IN GASTRIC CONTENTS INDUCED BY HUMAN-STOMACH MOTILITY

CHANGYONG LI[1], YAN JIN[1]
[1]*Center of Applied Space Technology and Microgravity (ZARM), University of Bremen, Am Fallturm 2, 28359, Bremen, Germany. changyong.li@zarm.uni-bremen.de, yan.jin@zarm.uni-bremen.de*

Keywords: *human-stomach model; computational fluid dynamics (CFD); gastric motility; gastric pH*

The digestion in stomach is highly complicated and the mechanism needs further understanding. Muscular movements of the stomach play critical roles in the digestive process. A CFD model is developed to better understand the flow dynamics in the process of mixing liquid foods with the gastric juice. The dynamics of stomach muscles, including tonic contraction (TC), antral contraction waves (ACWs), and terminal antral contraction (TAC) are modelled using the method of dynamic mesh. A porous medium model is used to approximate the effect of the wrinkles on stomach inner-surfaces. The gastric juice secretion is modelled as sources of mass and hydrogen ions continually added into the stomach lumen. Gastric emptying rates of different foods are determined according to their calorie content. The numerical results show that the terminal antral contraction (TAC) can considerably increase the kinetic energy in the stomach. The TAC creates retropulsive "jets" and reduces the pH of liquid gastric contents. The mixing efficiency of liquid gastric contents and gastric juice is low, which takes about 40-50 min to approach an acidic environment with a pH of 1.6 inside the stomach lumen. Our simulation results show that the density difference in food/stomach-juice has significant effects on the dynamic spatial distribution of gastric pH. The study shows that the developed model is a helpful tool to better understand the digestion process in human-stomach.

ON THE PERFORMANCE OF OPENFOAM OVERSET MESH SOLVER FOR MODELLING OFFSHORE WIND TURBINE ROTOR AERODYNAMICS

ZAIBIN LIN[1], LING QIAN[2],WEI BAI[3]

[1]*Centre for Mathematical Modelling and Flow Analysis, Department of Computing and Mathematics, Manchester Metropolitan University, Manchester, M1 5GD, United Kingdom, z.lin@mmu.ac.uk*

[2]*Centre for Mathematical Modelling and Flow Analysis, Department of Computing and Mathematics, Manchester Metropolitan University, Manchester, M1 5GD, United Kingdom, l.qian@mmu.ac.uk*

[3]*Centre for Mathematical Modelling and Flow Analysis, Department of Computing and Mathematics, Manchester Metropolitan University, Manchester, M1 5GD, United Kingdom, w.bai@mmu.ac.uk*

Keywords: *Overset mesh solver, aerodynamics, offshore wind turbine rotor, comparative study*

Aerodynamic and hydrodynamic loads on offshore floating wind turbines play a predominant role in determining their fatigue life, optimising power control systems, and predicting the platform stability and survivability under both normal operation and extreme conditions. Therefore, it is of great importance to develop an integrated aerodynamics and hydrodynamics model, which is capable of accurately predicting both loads and associated dynamic motions of an entire offshore wind turbine system. Prior to developing such a model, aerodynamics and hydrodynamics models need to be evaluated individually and systematically in terms of their accuracy and efficiency. In this study, the performance of the overset mesh solver in OpenFOAM for modelling offshore wind turbine rotor aerodynamics is examined in detail. More specifically, the aerodynamics of the National Renewable Energy Laboratory (NERL) 5MW reference turbine, which is designed to be mounted on a semi-submersible platform, is modelled and the results are compared with the frequency-domain Naiver-Stokes Computational Fluid Dynamics solver [1], and open source Blade Element Momentum theory code [2].

To generate the mesh around the rotor blades, as a first step and owing its simplicity, the snappyHexMesh functionality in OpenFOAM has been applied. The details of the local mesh around a rotor blade and the overall overset mesh zone as well as its position in the background mesh are shown in Figure 1 and Figure 2 respectively. In Figure 1, the mesh is well refined by adding boundary mesh layers at the proximity of blade surface in order to capture the details of the turbulent boundary layer flow. Based on this mesh setup, the overset mesh solver in OpenFOAM has been applied to model the flow problem with a wind speed of 11 m/s and a rotor speed of 12 RPM and the numerical results are in good agreement with the results from Ortolani et al. (2020)[3] in terms of rotor thrust and power. Both temporal and spatial refinement tests have also been performed to ensure solution convergence. Due to the isotropic nature of the mesh refinement, which leads to a prohibitively large number of mesh cells in the overset mesh zone, instead of the mesh setup based on snappyHexMesh, mesh optimisation based on the body-fitted mesh and non-isotropic mesh refinement within the overset mesh will be explored. The accuracy and computational efficiency based on the optimised mesh setup will be investigated and compared to those based on preliminary mesh setups in Figures 1 and 2.

Acknowledgments

This work is being funded by the Engineering and Physical Sciences Research Council (EPSRC, UK) projects: Extreme Loading on FOWT Under Complex Environmental Conditions (EP/T004150/1) and A CCP on Wave Structure Interaction: CCP-WSI (EP/M022382/1).

References

[1] M. S. Campobasso, A. Piskopakis, J. Drofelnik, and A. Jackson, "Turbulent navier–stokes analysis of an oscillating wing in a power-extraction regime using the shear stress transport turbulence model," *Computers & Fluids*, vol. 88, pp. 136–155, 2013.

[2] G. Heyman, B. Jonkman, R. Murray, R. Damiani, and J. Jonkman, "Aerodyn: a time-domain wind and mhk turbine aerodynamics module," *National Renewable Energy Laboratory*, 2019.

DEVELOPING SEABED SCOUR ASSESSMENT AND PREDICTION TOOLS USING COMPUTATIONAL FLUID DYNAMICS MODELLING (DEMO)

GARY LITTLER[1], MARK COUGHLAN[2], JENNIFER KEENAHAN[3]
[1]*University College Dublin, gary.littler@ucdconnect.ie*
[2]*University College Dublin/Irish Centre for Research in Applied Geosciences, mark.coughlan@icrag-centre.org*
[3]*University College Dublin, jennifer.keenahan@ucd.ie*

Keywords: *Scour, Renewable, CFD, Hydrodynamics*

Introduction

Seabed hydrodynamics, morphodynamics and scour represent geological risks to the stability of offshore renewable energy installations from an environmental and engineering perspective. Scour is the process of seabed erosion due to the imposed shear stress generated by seabed current and/or waves. Predicting scour can be difficult due to vagaries about hydrodynamic conditions. It represents an environmental constraint on engineering activities such as pipelines, cable routes and anchor foundations. Ireland's only offshore wind farm constructed to date, Arklow Bank, experienced scour issues that resulted in the use of rock armour to mitigate against further scour and turbine instability (Whitehouse et al., 2011). This project uses CFD modelling, validated by traditional seabed mapping results, to better understand seabed hydrodynamics and scour development in the Irish Sea. A scour prediction tool and methodology were developed using CFD which will support sustainable marine infrastructure development and project de-risking.

Initial Approach

Based on a screening exercise, we have selected the wreck of the SS Polwell (Fig. 1) as a suitable site to run CFD simulations to study scour development. This was based on factors such as depth, substrate type, and proximity to MPAs and existing infrastructure. This site has been mapped using multibeam echosounder (MBES) during 3 separate surveys (2015, 2016 and 2019) offering key temporal data on scour development with which to validate outputs.

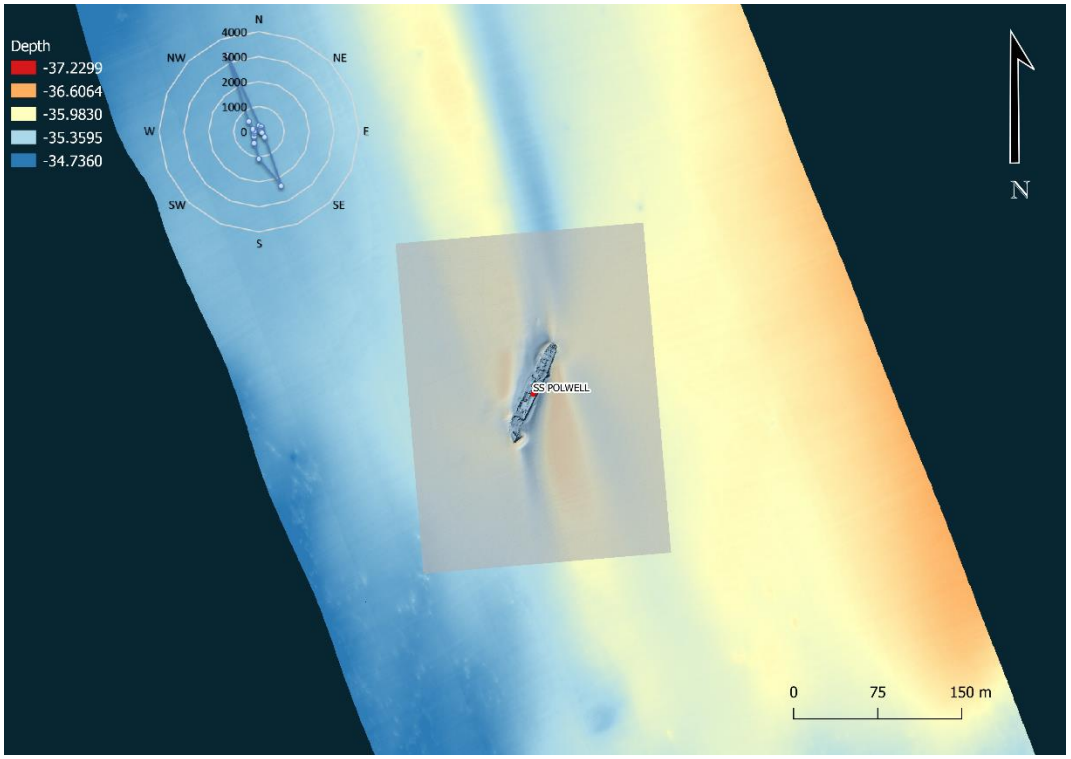


Figure 1 SS Polwell wreck site with bathymetry (water depth) from multibeam echosounder data. Included is current frequency data from Marine Institute ROMS model (Rose plot top left)

DIGITAL-TWIN FOR PARTICLE-LADEN VISCOELASTIC FLUIDS: DEEP LEARNING TO PREDICT THE DRAG COEFFICIENT OF RANDOM ARRAYS OF SPHERES

C. LOIRO[1], C. FERNANDES[1], G. H. MCKINLEY[2], J. M. NÓBREGA[1], S. A. FAROUGHI[2,*]
[1]*Institute for Polymers and Composites, University of Minho, Campus de Azurém, 4800-058 Guimarães, Portugal*
[2]*Hatsopoulos Microfluids Laboratory, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

Keywords: *direct numerical simulations, Giesekus model, fluid-particle force, random arrays of particles, deep neural network*

Efficiently and accurately computing the interphase momentum transfer between a flowing liquid matrix and a solid dispersed phase is a fundamental challenge for simulating particle-laden viscoelastic flows. Here we address this challenge through an Eulerian-Lagrangian Computational Fluid Dynamics-Discrete Element Method (CFD-DEM) formulation which we will apply to simulations of hydraulic fracturing operations. For this purpose, the dependence of the average fluid-particle force on the solid volume fraction and on the rheology of the constitutive model selected to describe the suspending fluid matrix needs to be characterized.
In this work, direct numerical simulations (DNS) (approximately 7000 runs) are being performed to obtain the drag coefficient of random arrays of monodisperse spherical particles translating in shear-thinning viscoelastic fluids, described by the Giesekus model. The normalized average fluid-particle force F is obtained as a function of solid volume fraction $0 \leq \emptyset \leq 0.2$, Reynolds number $\mathrm{Re} \leq 50$, Deborah number $\mathrm{De} \leq 4$, retardation ratio $0 < \beta < 1$ and mobility parameter $0 < \alpha \leq 0.5$. The results generated by these simulations are used to develop a meta-model, obtained by employing deep neural network algorithms, for the fluid-particle drag force. This model can then be employed in a CFD-DEM formulation forming a digital-twin framework, which will significantly enhance the simulation of canonical particle-laden viscoelastic flows, such as the proppant (particle) transport in largescale hydraulic fracturing treatments.

Acknowledgements
This work is funded by FEDER funds through the COMPETE 2020 Programme and National Funds through FCT (Portuguese Foundation for Science and Technology) under the projects UID-B/05256/2020, UID-P/05256/2020 and APROVA-Aprendizagem PROfunda na modelação de escoamentos com fluidos de matriz Viscoelástica Aditivados com partículas (POCI-01-0145-FEDER-016665). The authors would like to acknowledge the Minho University cluster under the project NORTE-07-0162-FEDER-000086 (URL: http://search6.di.uminho.pt), the Minho Advanced Computing Center (MACC) (URL: https://macc.fccn.pt), the Texas Advanced Computing Center (TACC) at The University of Texas at Austin (URL: http://www.tacc.utexas.edu), the Gompute HPC Cloud Platform (URL: https://www.gompute.com) for providing HPC resources that have contributed to the research results reported within this paper.

EXTENSION OF P1 RADIATION MODEL TO PARTICLE-FLUID FLOWS

JELENA MAČAK[1], CHRISTOPH GONIVA[2], STEFAN RADL[3]
[1]*DCS Computing, jelena.macak@dcs-computing.com*
[2]*DCS Computing, christoph.goniva@dcs-computing.com*
[3]*TU Graz, radl@tugraz.com*

Keywords: *radiative heat transfer, granular media, CFD-DEM*

Granular media are found in many high-temperature processes, such as in concentrating solar power units, reactors for biomass pyrolysis, laser sintering, etc. At high temperatures (over $400°C$) all modes of heat transfer occur, including radiation, which is the focus of this work. While air, the most common ambient fluid, remains unaffected by radiation, one particle will radiatively exchange heat with all particles in its unobstructed field of vision. Precise radiation models based on Monte Carlo ray tracing [1] or view factor calculations [2] are generally computationally too demanding for industrial scale simulations.
Aiming for computational efficiency, we use OpenFOAM's P1 radiation model to describe heat transfer in granular media by the means of combined computational fluid dynamics and discrete element method (CFD-DEM). We first derive the equations accounting for radiative particle-fluid and particle-particle heat transfer in P1 model formulation. P1 model is a first-order spherical harmonics approximation of the radiative transfer equation, resulting in a diffusion-like scalar conservation equation. We introduce discrete particles in the radiative intensity conservation equation as source/sink terms.
Major drawback of P1 approximation is the loss of angular dependence, which might lead to inaccurate heat fluxes. We counteract this issue by introducing a scattering function based on attenuation in packed beds [4]. The resulting model formulation allows particles to emit and absorb radiation, while scattering is shared between the phases.
The model is implemented within CFDEMCoupling framework [3] and verified using benchmark test cases. Finally, the model is applied to a complex industrial scale problem.

References

[1] S. Amberger, S. Pirker, and C. Kloss, "Thermal radiation modeling using ray tracing in LIGGGHTS," in *Proceedings of DEM 6*, 2013.

[2] T. Forgber and S. Radl, "A novel approach to calculate radiative thermal exchange in coupled particle simulatons," *Powder Technol.*, vol. 323, pp. 24–44, 2018.

[3] C. Goniva, C. Kloss, N. Deen, J. A. M. Kuipers, and S. Priker, "Influence of rolling friction modelling on single spout fluidized bed simulations," *Particuology*, vol. 10, pp. 582–591, 2012.

[4] Q. Brewster, "Volume scattering of radiation in packed beds of large, opaque spheres," *J. Heat Transfer*, vol. 126, pp. 1048–1050, 2004.

Direct numerical simulations of boiling flows in microchannels

Mirco Magnini[1], Federico Municchi[2], Ismail El Mellas[3], Matteo Icardi[4]
[1]*Faculty of Engineering, University of Nottingham, mirco.magnini@nottingham.ac.uk*
[2]*Faculty of Engineering, University of Nottingham, federico.municchi@nottingham.ac.uk*
[3]*Faculty of Engineering, University of Nottingham, ismail.elmellas1@nottingham.ac.uk*
[4]*School of Mathematical Sciences, University of Nottingham, matteo.icardi@nottingham.ac.uk*

Keywords: *Volume of Fluid; Phase Change; Microchannels; Multiphase Flows*

While the recent advances in manufacturing technology enabled mass production of devices operating at high power densities (e.g., microelectronics, batteries, miniature fuel cells, etc.), they also led to a dramatic surge in the pressure for developing efficient cooling systems. Since such high-power devices tend to produce heat fluxes on the order of several MW/m^2, they require a heat-removal capability beyond that of traditional single phase cooling systems, which is generally bounded to less than 1 MW/m^2 [1]. On the contrary, multiphase flows with phase-change represent a viable technological solution, since additional energy can be dissipated in the form of latent heat. Furthermore, two-phase flows maintain uniform surface temperatures, vital for the correct operation of components; and respond positively and passively, i.e. without the need to increase the mass flux, to localised "hot-spots", as the heat transfer coefficient increases with heat flux.

Despite the large number of experimental studies conducted on boiling heat transfer in microchannels, there is still general disagreement on the underlying dynamics, because the existing experimental techniques cannot yet access the small spatial and temporal scales of the flow with sufficient resolution. On the other hand, numerical simulation methods have advanced rapidly in the last decades and, if computational resources are available, the direct numerical simulation of boiling flows with interface-tracking methods may provide valuable information on fluid dynamics and governing heat transfer mechanisms [2].

In this work, we present an application of both algebraic and geometric VoF (volume of fluid) solvers available in OpenFOAM®to simulate boiling heat transfer in noncircular microchannels, at conditions that are pertinent to industrial applications: low viscosity fluids (water, refrigerants), small capillary numbers ($\mathrm{Ca} = \mu U/\sigma \ll 1$, with μ: liquid viscosity, U: liquid or bubble speed, σ: surface tension), laminar flows, nonuniform heat loads of hundreds of $\mathrm{kW/m^2}$. Thin-film flows within microchannels represent a formidable challenge for interface-capturing methods, owing to the dominant role played by surface tension forces. The thin film trapped between the bubble and the channel wall must be resolved by the mesh, thus requiring high aspect-ratio mesh cells near the wall to limit the computational cost. Also, the VoF method with surface tension forces reconstructed based on volume fraction gradients typically exhibits spurious velocities that scale as $\sim 1/\mathrm{Ca}$, and thus very detrimental in capillary flows where $\mathrm{Ca} = \mu U/\sigma \ll 1$ [3].

As a validation study, we reproduce the isothermal confined bubble flow configuration of de Lózar et al. [4], for aspect ratios $AR = W/H$ (W, H: channel width and height, respectively) in the range $AR = 1-8$. Preliminary results are shown on the left box of Fig. 1. InterFoam reproduces very well the results of de Lózar et al. [4] for square channels ($AR = 1$), whereas increasing deviations appear for higher aspect ratio channels. We observe that such deviations result from poorly accurate surface tension reconstructions in interFoam, whereas coupling the more recent isoAdvector VoF algorithm [5, 6] with a geometric interface curvature calculation yields much more accurate bubble profiles and velocity fields nearby interfaces.

For boiling flows, we begin with a numerical framework based on interFoam, augmented with the solution of the enthalpy transport equation and a phase change model based on the work of Hardt and Wondra [7]. This computational framework was recently utilised to study the impact of the microchannel aspect ratio on boiling heat transfer and emphasised that the thin-film evaporation is the dominant heat transfer mechanism along the channel wall, whereas relatively larger temperatures are measured at the corners, where thick liquid lobes are left [2]; see the right box of Fig. 1. In the present work, this numerical framework is extended with a conjugate heat transfer model, and both static and dynamic contact angle models. Our objective is to close the gap with actual boiling dynamics in microchannels: an embryo vapour bubble is inialised at the corner between the bottom and lateral wall of the channel, as observed in recent experiments [8]; heat is nonuniformly distributed around the channel perimeter, as the source is from the bottom of the evaporator; both pressure and velocity boundary conditions are tested, as the actual condition in experiments of multi-microchannel evaporators is a mixture of the two. We present results of the bubble dynamics for different size of the channel, different mass flow rates, heat fluxes, wall material and wall thicknesses, with the scope of shedding a light to the microchannel configuration that brings the best compromise between heat removal capabilities and compactness of the evaporator.

Shock interface interaction simulation using compressible-compressible ghost fluid method solver developed in foam-extend

Ehsan Mahravan[1], Mohsen Lahooti[2], Daegyoum Kim[3]
[1]*KAIST, mahravan@kaist.ac.kr*
[2]*Imprial college, m.lahooti@imperial.ac.uk*
[3]*KAIST, daegyoum@kaist.ac.kr*

Keywords: *GFM, compressible, shock, bubble*

Ghost Fluid Method (GFM) is a robust and efficient approach for dealing with sharp-interface multiphase flows with highly discontinuous flow field across the interface [1]. The method has been developed and widely used for compressible flows and offers sharp and high-accuracy treatment of the interface [2]. In the GFM approach, the multiphase problem is treated as multiple single-phase problems where each of these single-phase flows are solved over an extended domain containing the grid cells of their phase and a layer of adjacent cells to the interface from other phases, the Ghost cells (Fig. 1). The flow conditions at the ghost cells are defined such that the required kinematic and dynamic conditions at the interface satisfy. Several variants of the GFM approach have been developed and distinguished by how they treated and populated the ghost cells. However, despite the robustness and wide range of their application, non of the GFM methods has been available neither in OpenFOAM official distribution nor in its forks. In the present work, an efficient Ghost fluid method approach is implemented in foam-extend framework, using the modified Riemann-based solver dbnsFoam as the main single-phase solver. Four interface treatments are implemented including original GFM [1], modified GFM [3] and the methods introduced in [4] and [5]. Interface position is sharply captured using Level-Set (LS) method, with 3^{rd} order TVD Runge-Kutta time integration and 5^{th} order WENO discretization of the spatial terms [6]. The solver is validated and verified via several two-phase simulations in one, two, and three-dimensional problems, including shock-tube, bubble explosion and implosion, and shock-bubble interaction.

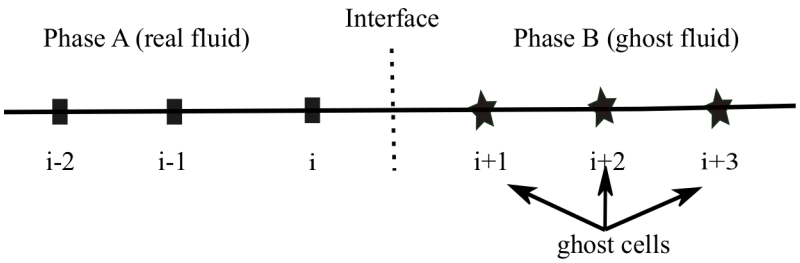


Figure 1: Illustration of GFM real and ghost fluids in one dimension when phase A is being solved. At this instant, phase A is called the real fluid, phase B is ghost Fluid, and cells from phase B are called ghost cells.

References

[1] R. P. Fedkiw, T. Aslam, B. Merriman, and S. Osher, "A non-oscillatory eulerian approach to interfaces in multimaterial flows (the ghost fluid method)," *Journal of Computational Physics*, vol. 152, no. 2, pp. 457–492, Jul. 1999. [Online]. Available: https://doi.org/10.1006/jcph.1999.6236

[2] R. Egan and F. Gibou, "xGFM: Recovering convergence of fluxes in the ghost fluid method," *Journal of Computational Physics*, vol. 409, p. 109351, May 2020. [Online]. Available: https://doi.org/10.1016/j.jcp.2020.109351

[3] T. Liu, B. Khoo, and K. Yeo, "Ghost fluid method for strong shock impacting on material interface," *Journal of Computational Physics*, vol. 190, no. 2, pp. 651–681, Sep. 2003. [Online]. Available: https://doi.org/10.1016/s0021-9991(03)00301-2

poroMechanicalFoam – A Toolbox-Extension for Flow Deformation Analysis in Variably Saturated Porous Media

Denis Maier[1], Héctor Montenegro[2], Bernhard Odenwald[3],
Federal Waterways Engineering and Research Institute
[1]*denis.maier@baw.de*
[2]*hector.montenegro@baw.de*
[3]*bernhard.odenwald@baw.de*

Keywords: *porous media, variable saturation, hydromechanics*

Poromechanics studies the behavior of fluid-saturated porous media. A porous medium consists of a solid matrix permeated by an interconnected network of pores filled with a fluid (liquid or gas). The proposed model assumes both the solid matrix and the pore network to form two interpenetrating continua. Pormechanics plays a significant role in a broad variety of disciplines ranging from reservoir engineering to biomedical applications extending over quite a span of different spatial and temporal scales.

In geotechnical engineering soils are generally considered as water filled porous media consisting of a porous, deformable solid matrix filled with a compressible fluid which may consist of water and entrapped gas bubbles. The so called hydromechanical behavior generally depends on the elastic properties of the solid and the fluid and is central to the performance of many engineering systems. In soils and geomaterials however the degree of saturation can vary over time and space. Commonly, the solid–fluid interaction is strongly-coupled in fully saturated soils while the interaction is less pronounced with decreasing saturation.

The main computational work in a poromechanical analysis involves the solution of a linear system to compute each update. In general, this system is highly ill-conditioned due to non-linearities rising from strong deformation-flow interactions and, in the case of prtial saturation, the dependence of the storage and conductivity properties from the degree of saturation. The OpenFOAM platform has shown to be more than capable of handling such strong nonlinearities and the finite volume approach has been proven to be advantageous not only for the flow but also for the deformation analysis. The proposed poroMechanicalFoam toolbox extends the ability to analyze poromechanical processes seamlessly considering a varying degree of saturation in the voids from complete saturation over small gas entrapments to a continuous unsaturated fluid phase. It seizes major advantages from the fluid-structure interaction solids4Foam toolbox through the integration of the material models established there. The proposed poroMechanicalFoam toolbox aims at the expansion of the well-established "fluid-structure interaction" analysis capabilities of solids4foam to investigate "porous structure – interstitial flow – surface flow interactions".

THE EFFECT OF HDR INFINIBAND AND IN-NETWORK COMPUTING ON OPENFOAM SIMULATIONS

OPHIR MAOR, YONG QIN, GERARDO CISNEROS-STOIANOWSKI, GILAD SHAINER
HPC-AI Advisory Council

Keywords: *InfiniBand HDR, In-Network Computing, Performance*

Abstract

High-performance computing (HPC) technologies are used in the engineering and automotive design and manufacturing industry. One of the applications is the computer-aided engineering (CAE), from component-level design to full analyses such as: crash simulations, structure integrity, thermal management, climate control, modeling, acoustics, and much more. HPC helps drive faster time-to-market, realizing significant cost reductions over laboratory testing and tremendous flexibility. HPC's strength and efficiency depend on the ability to achieve sustained top performance by driving the CPU performance toward its limits. The motivation for high-performance computing has long been its tremendous cost savings and product improvements; the cost of a high-performance compute cluster can be just a fraction of the price of a single crash test for example, and the same cluster can serve as the platform for every test simulation going forward. The recent trends in cluster environments, such as multi-core CPUs, GPUs, and advanced high speed, low latency interconnect with offloading capabilities, are changing the dynamics of cluster-based simulations. Software applications are being reshaped for higher degrees of parallelism and multithreading, and hardware is being reconfigured to solve new emerging bottlenecks to maintain high scalability and efficiency. OpenFOAM Applications are widely used and provide better flexibility, scalability, and efficiency for such simulations, allowing for larger problem sizes and speeding up time to results.
HPC Applications relies on Message Passing Interface (MPI), the de-facto messaging library for high performance clusters that is used for node-to-node inter-process communication (IPC). MPI relies on a fast, unified server and storage interconnect to provide low latency and high messaging rate. Performance demands from the cluster interconnect increase exponentially with scale due in part to all-to-all communication patterns. This demand is even more dramatic as simulations involve greater complexity to properly simulate physical model behaviours.
In this paper we will focus on the value of In-Network computing for HDR InfiniBand Networks for OpenFOAM application.

LINEAR STABILITY ANALYSIS OF BOUNDARY LAYER FLOW USING OPENFOAM

NINAD MAVANI[1], SAMARTH ACHARYA[2] AND RAVI KANT[3]
[1]*Pandit Deendayal Petroleum University, Gandhinagar, India, ninad.mmc17@sot.pdpu.ac.in*
[2]*Pandit Deendayal Petroleum University, Gandhinagar, India, samarth.mmc17@sot.pdpu.ac.in*
[3] *Pandit Deendayal Petroleum University, Gandhinagar, India, ravi.kant@sot.pdpu.ac.in*

Keywords: *Stability analysis, transition, boundary layer flow, modal and non-modal flow instability, OpenFOAM.*

We hereby present the linear stability analysis of boundary layer flow using OpenFOAM. Although there is ample documentation on stability theories, any attempt to analyse such instabilities in OpenFOAM has been very limited. The transition Reynolds number depends on nature and spectrum of disturbance environment, signatures in the shear flow and receptivity. The normal modes concept in instability suggests simple wavelike solutions for linearized Navier-Stokes equation (LNSE), thus expecting a representation of Initial Boundary Value Problem (IBVP) as a sum of normal modes. In correspondence with this, we aim to modify standard solver in OpenFOAM for incompressibility "icoFoam" and several associated libraries in order to get the perturbation fields. We also study the modal analysis and obtain the eigenmodes, which are validated with that of existing benchmark results.

Governing equation – Perturbed incompressible linear Navier Stokes equation (LNSE) along with the perturbed continuity is written as,

$$\nabla \cdot \boldsymbol{u}' = 0 \tag{1}$$

$$\frac{\partial \boldsymbol{u}'}{\partial t} + \boldsymbol{U}.\nabla \boldsymbol{u}' + \boldsymbol{u}'\nabla \boldsymbol{U} = -\nabla \boldsymbol{p}' + \frac{\mathbf{1}}{\boldsymbol{Re}}\nabla^{\mathbf{2}}\boldsymbol{u}' \tag{2}$$

Where $\boldsymbol{u'}$ = [u',v',w'] is the perturbation field and U represents velocity field in a boundary layer over a flat plate. In compact form, we can write the LNSE as,

$$\frac{\partial \boldsymbol{u}'}{\partial t} = A\boldsymbol{u}' \tag{3}$$

Where $\boldsymbol{A}$ is the LNSE operator. This can be also be formulated as an eigenvalue problem as,

$$A\hat{\boldsymbol{u}} = \lambda\hat{\boldsymbol{u}} \tag{4}$$

Modification suggested in icoFoam – The LNSE perturbed set of equations are quite similar to the usual Navier-Stokes equation. The standard incompressible icoFoam solver can be easily modified and the perturbation field solutions can seek with no-slip perturbation boundary conditions at walls. In addition to the solution of perturbation field, the eigenmodes are also evaluated and validated with the existing benchmark results.

Acknowledgements

The authors thank all those involved in the organisation of OFW16 and to all the contributors that will enrich this event.

References

[1] Schmid, P. J., Henningson, D. S., & Jankowski, D. F. (2002). Stability and transition in shear flows. Applied mathematical sciences, Vol. 142. Appl. Mech. Rev., 55(3), B57-B59.

[2] Schmid, P. J., & Brandt, L. (2014). Analysis of fluid systems: Stability, receptivity, sensitivity lecture notes from the flow-nordita summer school on advanced instability methods for complex flows, stockholm, sweden, 2013. Applied Mechanics Reviews, 66(2).

[3] Reddy, S. C., & Henningson, D. S. (1993). Energy growth in viscous channel flows. Journal of Fluid Mechanics, 252, 209-238.

[4] Liu, Q., Gómez, F., Perez, J. M., & Theofilis, V. (2016). Instability and sensitivity analysis of flows using OpenFOAM®. Chinese Journal of Aeronautics, 29(2), 316-325.

INFLUENCE OF SHOCK ON RAE2822 TRANSONIC AIRFOIL USING HISA LIBRARY IN OPENFOAM

ÇAĞRI METİN[1], BARIŞ BİÇER[2], AND, MEHMET ŞAHIN[3]
[1]*Turkish Aerospace, cagrialimseyit.metin@tai.com.tr*
[2]*Turkish Aerospace, baris.bicer@tai.com.tr*
[3]*Istanbul Technical University, msahin@itu.edu.tr*

Keywords: *transonic flow, shock-boundary layer interaction, shock interaction length, density-based HISA solver, OpenFOAM.*

In the transonic regime, the shock-boundary layer interaction plays a crucial role in engineering design, and it is important to understand this nonlinear phenomenon. This complex physics also affects the solution and challenge for many numerical solvers [1]. On the other hand, open-source software has become more popular during the last decades in the industry as well as in the scientific community. OpenFOAM has one of the largest open-source communities and has been contributed by different libraries [2, 3]. Most of the solvers in OpenFOAM are based on the pressure-based algorithm. The capacity of existing density-based solver is limited due to the only explicit time discretization [4]. On the other hand, the HISA library stands out with its local time stepping, the LU-SGS preconditioner and the GMRES matrix solver, and the flux-vector splitting and flux-differencing in a coupled matrix approach [5].

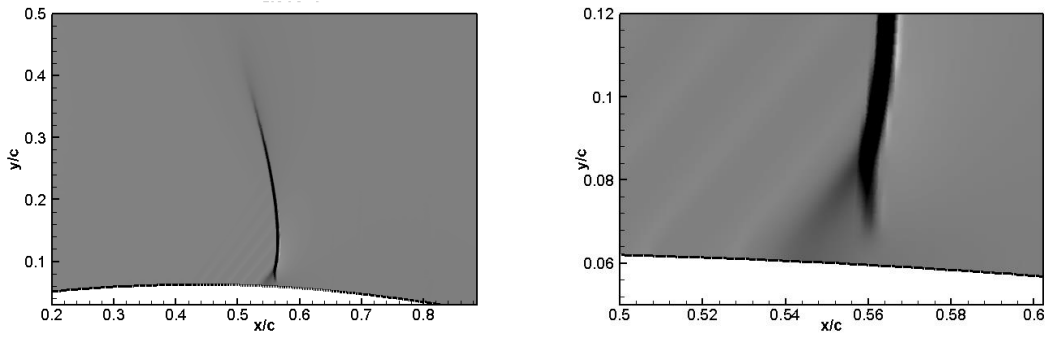


Figure 1: The shock visualization on the transonic regime.

In this study, therefore, we conduct numerical analysis in the transonic regime with the relatively new library HISA in OpenFOAM environment. RAE2822 supercritical profile was investigated in transonic regime using the HISA library integrated into OpenFOAM environment. The HISA solver is coupled density based solver and mostly suitable for transonic and supersonic flow problems. Numerical studies were performed with AUSM+Up flux-vector splitting approach. It is argued that the shock and boundary layer interaction leads to a sudden increasing of the boundary layer and turbulent activities as well. The effect of the shock on the boundary layer was determined by the interaction length against two different scenarios. It is found that increasing shock strength can be observed on the wall by measuring interaction length. The weak shock produces a smaller interaction length, whereas the stronger shock becomes lambda-shock and produces a larger interaction length that may causes separation of the boundary layer.

Acknowledgements
The authors thank to Turkish Aerospace (TAI) for the computer infrastructures that were used in this study.

References

[1] Yamazaki, W., Matsushima, K., & Nakahashi, K. (2008). Drag prediction, decomposition and visualization in unstructured mesh CFD solver of TAS-code. International journal for numerical methods in fluids, 57(4), 417-436.

[2] Weller HG, Tabor G, Jasak H, Fureby C. A tensorial approach to computational continuum mechanics using object-oriented techniques. Comput Phys 1998;12(6):620–31.

[3] H. Jasak, Error Analysis and Estimation for the Finite Volume Method with Application to Fluid Flows, A thesis for the degree of Doctor of Philosophy, University of London, (1996), London. UK.

[4] Shen, C., Xia, X. L., Wang, Y. Z., Yu, F., & Jiao, Z. W. (2016). Implementation of density-based implicit LU-SGS solver in the framework of OpenFOAM. Advances in Engineering Software, 91, 80-88.

[5] Heyns, J. A., Oxtoby, O. F., & Steenkamp, A. (2014, June). Modelling high-speed flow using a matrix-free coupled solver. In Proceedings of the 9th OpenFOAM Workshop, Zagreb, Croatia (pp. 23-26).

TRACKING THE ELECTRODE-ELECTROLYTE INTERFACE IN LIQUID METAL BATTERIES

FEDOR MISIURA[1], PROFESSOR PETER DAVIDSON[2], DR HRVOJE JASAK[3]
[1]*Department of Engineering, University of Cambridge, fm466@cam.ac.uk*
[2]*Department of Engineering, University of Cambridge, pad3@eng.cam.ac.uk*
[N]*Department of Physics, Univeristy of Cambridge, hj348@cam.ac.uk*

Keywords: *Liquid Metal Batteries, Interface, Transition to turbulence*

A 2-phase Navies Stokes solver was used to simulate the flow in a model of a liquid metal battery, with a particular focus on the interface between the liquid metal electrode and electrolyte layer. Liquid Metal Batteries' operation is heavily dependant on the integrity of the electrolyte separating the electrodes and their round-trip efficiency is affected by the electrolyte's thickness, making it important to understand the fluid flows generated due to magneto-hydrodynamic effects. The electrolyte layer was found to be sensitive to varying the strength of the stray magnetic fields and a parametric study outlined an operating envelope. By defining clear operating bounds, the model in question could remain operational by ensuring that the flows are steady and no short circuits can occur due to loss of electrolyte layer integrity.

Acknowledgments

The authors thank all those involved in the organisation of OFW16 and to all the contributors that will enrich this event.

References

FLUID-STRUCTURE INTERACTION ON A FIXED FAN BLADE

SABER MOHAMMADI[1], HÅKAN NILSSON[2], PHILIP CARDIFF[3], DANIEL RUNDSTRÖM[4]
[1]*Chalmers University of Technology, Dept. Mechanics and Maritime Sciences, mohammadisaber@outlook.com,*
[2]*Chalmers University of Technology, Dept. Mechanics and Maritime Sciences, hakan.nilsson@chalmers.se,*
[3] *University College Dublin, School of Mechanical and Materials Engineering, philip.cardiff@ucd.ie,*
[4]*Voith Hydro Company, R&D Centre, Daniel.Rundstrom@voith.com*

Keywords: *Numerical Simulation, Solids4Foam, OpenFOAM, Fan Blade, FSI, CFD*

High global electricity demand is pushing engineers towards providing hydropower electromagnetic generators with more resistant rotary equipment against well-known problems such as fatigue and vibrational cracking. The aim is to make power plants immune against high time and cost consuming refurbishments. In these systems, one of the rotating parts that is most susceptible to such failures is the ventilation fan. It is often an axial fan with blades distributed at one or two ends of the machine. The blades are attached to, and rotating with, the same shaft as the rotor, pushing the air through the rotor and stator towards the cooler. The blades are often manufactured by simple bent plates that are welded to the rotor, to keep the cost at minimum. They operate in an air flow that is highly restricted to the space that is available when the electromagnetic parts of the machine have been designed, causing temporally and spatially varying and non-ideal flow angles. For such conditions it is vital to study fluid-structure interaction on the blades to be able to avoid fan blade failures. Broken fan blades may cause severe damages to other parts of the machine, at enormous costs of repair and down-time. The present work provides a numerical study of the aeroelastic behaviour of a fixed blade resembling a blade of a double-sided axial fan of a hydropower generator. The focus is on flow-induced fluttering and resonance due to vortex shedding. The fluid-structure interaction is captured using the solids4Foam toolbox, which is an open source module for OpenFOAM, including specific solvers for solid and fluid mechanics and fluid-structure interaction. The turbulence is modelled using the scale-adaptive SAS model, which is able to capture vortex shedding with a combination of moderate computational costs and acceptable accuracy.

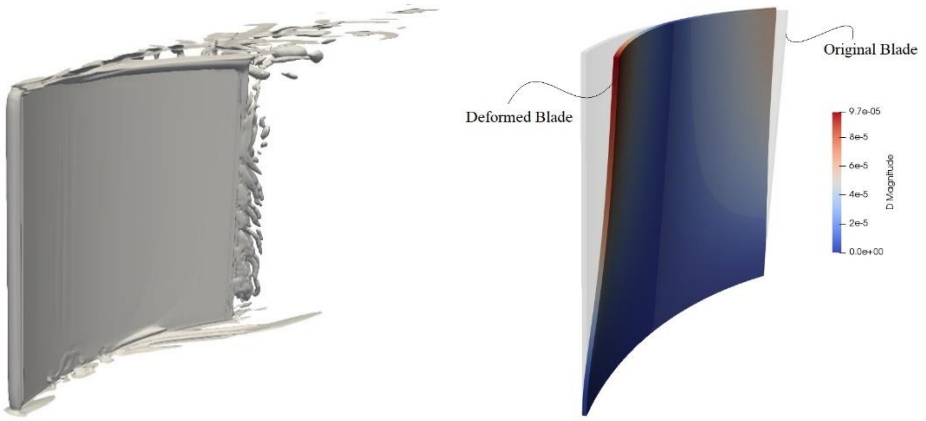


Figure 1: Left) Vortical structures, Right) Instantaneous magnified deformation of the blade

Figure 1 shows the blade geometry, which has an extruded circular arc cross-section that is connected to a base plate at the lower side and has a thin clearance to a cover at the upper side. Iso-surfaces of the Q-criterion in the left picture, show the vortical structures at the tip and trailing edge. In the right picture, an instantaneous exaggerated deformed shape of the blade is shown under the working condition.

Acknowledgements

The research presented was carried out as a part of the Swedish Hydropower Centre (SVC). SVC is established by the Swedish Energy Agency, EnergiForsk and Svenska Kraftnät together with Luleå University of Technology, The Royal Institute of Technology, Chalmers University of Technology and Uppsala University, www.svc.nu. The computations were enabled by resources provided by the Swedish National Infrastructure for Computing (SNIC) at NSC and C3SE, partially funded by the Swedish Research Council through grant agreement no. 2018-05973.

On the solution of the Cahn-Hilliard equation in OpenFOAM: coupled and segregated algorithms

Federico Municchi[1], Ismail El Mellas[2], Matteo Icardi[3], Mirco Magnini[4]
[1]*Faculty of Engineering, University of Nottingham, federico.municchi@nottingham.ac.uk*
[2]*Faculty of Engineering, University of Nottingham, ezxie1@nottingham.ac.uk*
[3]*School of Mathematical Sciences, University of Nottingham, matteo.icardi@nottingham.ac.uk*
[4]*Faculty of Engineering, University of Nottingham, mirco.magnini@nottingham.ac.uk*

Keywords: *Cahn-Hilliard; Phase-Field; Multiphase Flows; Diffuse Interface*

Phase field methods are often employed in science and engineering to model multicomponent and multiphase systems where different fluids are separated by a diffuse interface (i.e., an interface of finite thickness). The phase field method has also been employed to model two (or more) fluids separated by a sharp interface, due to its better performance concerning the production of spurious currents, which constitute a major issue in Volume of Fluid (VoF) methods at milli- and micro-scales [1, 2]. Such issues in the VoF have been recently addressed in the latest versions of OpenFOAM by means of geometric recontruction algorithms, which provide a better estimation of the interface curvature [3].

Unlike the VoF, the phase-field method relies on a consistent thermodynamic formulation based on the free energy of the mixture that results in the well known Cahn-Hilliard equation, which minimizes the interface energy [4]. Coupling with the Navier-Stokes equations is achieved by means of a continuous forcing. However, one of the key features of the Cahn-Hilliard equation is the presence of the fourth order derivative of the phase field, which excites a broad range of lenght scales and can not be discretised implicitly within the finite volume method; at least not in a general-purpose second order code like OpenFOAM. A straightforward solution consists in adding this extra flux explicitly into Cahn-Hilliard equation, which is then solved using an explicit scheme as is done in interFoam [5].

In this work, we present a different approach, where the the Cahn-Hilliard equation is discretized in an implicit manner. Specifically, we illustrate how the mixed formulation, often employed in finite element methods, can be implemented in foam-extend-4.1 using block coupled matrices. We also provide details on a novel segregated approach based on incomplete block Schur preconditioning of the mixed formulation, which transforms the Cahn-Hilliard equation into a non-linear advection-diffusion-reaction equation where only derivatives up to second orders appear. Both methods successfully account for the fourth-order derivative by means of second order derivatives.We applied these methods to a range of cases, including that of spinodal decomposition illustrated in figure 1.

After describing the algorithms in detail, we discuss the coupling with the Navier-Stokes equations and compare different combinations of coupled and segregated methods for a number of test cases. We analyze the accuracy, efficiency and scalability of the segregated algorithms compared to the coupled algorithms. The effects on spurious currents are also discussed.

Acknowledgments

This work is supported by the UK Engineering & Physical Sciences Research Council (EPSRC), through the BONSAI (EP/T033398/1) Programme Grant. We acknowledge the use of Athena at HPC Midlands+, which was funded by the EPSRC grant EP/P020232/1, as part of the HPC Midlands+ consortium. Part of this work is also supported by the European Union's Horizon 2020 research and innovation programme, grant agreement number 764531, "SECURe – Subsurface Evaluation of Carbon capture and storage and Unconventional risks".

References

[1] F. Jamshidi, H. Heimel, M. Hasert, X. Cai, O. Deutschmann, H. Marschall, and M. Wörner, "On suitability of phase-field and algebraic volume-of-fluid OpenFOAM® solvers for gas–liquid microfluidic applications," *Computer Physics Communications*, vol. 236, pp. 72–85, mar 2019. [Online]. Available: https://linkinghub.elsevier.com/retrieve/pii/S0010465518303631

[2] A. Badillo, "Quantitative phase-field modeling for boiling phenomena," *Physical Review E*, vol. 86, no. 4, p. 041603, oct 2012. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevE.86.041603

FLUID-STRUCTURE INTERACTION SIMULATIONS IN OPENFOAM WITH HYPERELASTIC MATERIAL MODELS FOR ANEURYSM MODELING

JOZSEF NAGY[1], VERONIKA M. MIRON[2], ZOLTAN MAJOR[2], PHILIP CARDIFF[3]
[1]*eulerian-solutions e.U., jozsef.nagy@eulerian-solutions.com, Linz, Austria*
[2] *Johannes Kepler University, Linz, Austria*
[3] *University College Dublin, Dublin, Irland*

Keywords: *Fluid-Structure Interaction, hyperelastic, aneurysm*

Understanding physiological processes is key to treat patients, especially in emergency situations. For this reason, the understanding of the creation of aneurysms in the human brain has been the study of research for decades. With a better understanding of the processes involved the treatment of patients can be improved.
Modelling as well as hardware capabilities have improved in the last years to a level, where it is possible to model the fluid-structure interaction (FSI) between the fluid dynamics of the blood flow as well as the structural behaviour of the blood vessel in a reasonable simulation runtime [1,2]. For certain applications, the solid behaviour can be modelled in a simple linear way [2], however in some cases the material behaviour of the blood vessels is more complex. These cases are especially interesting as aneurysm creation is more likely.
For this reason, it is important to model the tissue of the blood vessel with more realistic hyperelastic material models instead of assuming linear elasticity. In this work the widely used hyperelastic structural mechanical models "second order reduced polynomial" as well as "Ogden" are utilized in the framework of OpenFOAM within the user library solids4Foam [1].
Structural mechanic simulations were previously performed to verify compatibility between the models themselves [3]. With the verified models FSI simulations are run of simplified geometries (see figure 1) to identify the dominant influences for the onset of aneurysms (see figure 2).

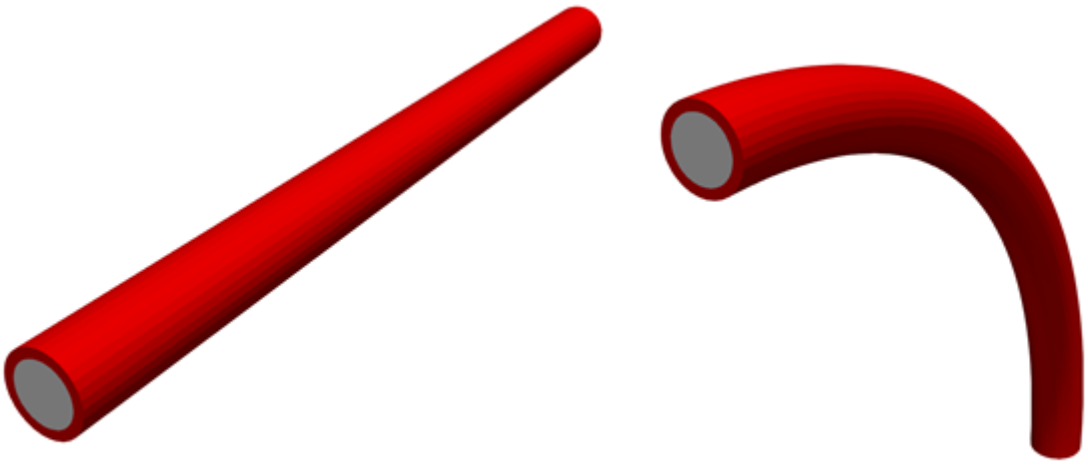


Figure 1: Investigated geometries in FSI simulations: straight channel (left) and 90° bent channel (right) with fluid regions in grey and solid regions in red

With the implemented models as well as the established simulation workflow in the future we hope to simulate the onset conditions for aneurysms in real life vessels.

EFFECT OF DIFFERENT LINEAR ALGEBRA SOLVERS AND DYNAMIC MESH MOTION STRATEGIES ON THE FLOW-FIELD OF A PITCHING FOIL

MUHAMMED NAJVAN[1], BRIJESH K. SUMAN[2], CHANDAN BOSE[3], SACHIN Y. SHINDE[4]
[1]*Department of Mechanical Engineering, Indian Institute of Technology Kanpur, India, najvanm@iitk.ac.in*
[2]*Department of Mechanical Engineering, Indian Institute of Technology Kanpur, India, bksuman@iitk.ac.in*
[3]*Department of Aerospace and Mechanical Engineering, University of Liège, Belgium, chandan.bose@uliege.be*
[4]*Department of Mechanical Engineering, Indian Institute of Technology Kanpur, India, sachin@iitk.ac.in*

Keywords: *Linear Algebra Solvers, Mesh Motion, Flapping Foils, Wake Patterns, Vortex Dynamics.*

This study reports that the choice of a seemingly appropriate linear algebra solver may fail to arrive at the accurate unsteady flow-field solution, leading to non-physical results. To that end, we take up a well studied canonical problem of a periodically pitching airfoil in uniform free-stream condition. Simulations are performed in the low Reynolds number regime using the open-source library OpenFOAM-v7[1]. The simulated flow-field results are compared for different solver set-ups and mesh motion strategies with existing experimental flow visualization results. A benchmark experimental case[2] of a purely pitching NACA 0012 symmetric airfoil is chosen to compare the numerical results. The airfoil pitches about the quarter chord point from the leading edge. The pitching amplitude θ and the non-dimensional reduced frequency ($\kappa = 2\pi fc/U$; c is the airfoil chord-length and U is free-stream velocity) are considered to be the primary control parameters, which govern the wake dynamics. Two different linear solver set-ups are considered. In the first set-up, a Preconditioned Conjugate Gradient (PCG) method with Diagonal Incomplete-Cholesky (DIC) preconditioner is used to solve the pressure equation. The velocity equations are solved using a Preconditioned Bi-Conjugate Gradient method (PBiCG) with Diagonal Incomplete-LU (DILU) preconditioner. In the second set-up, the pressure equation is treated using a Generalized Geometric Algebraic Multigrid (GAMG) method with Gauss-Seidel smoother and a smoothSolver method with symmetric Gauss-Seidel smoother is used for solving the velocity equations.

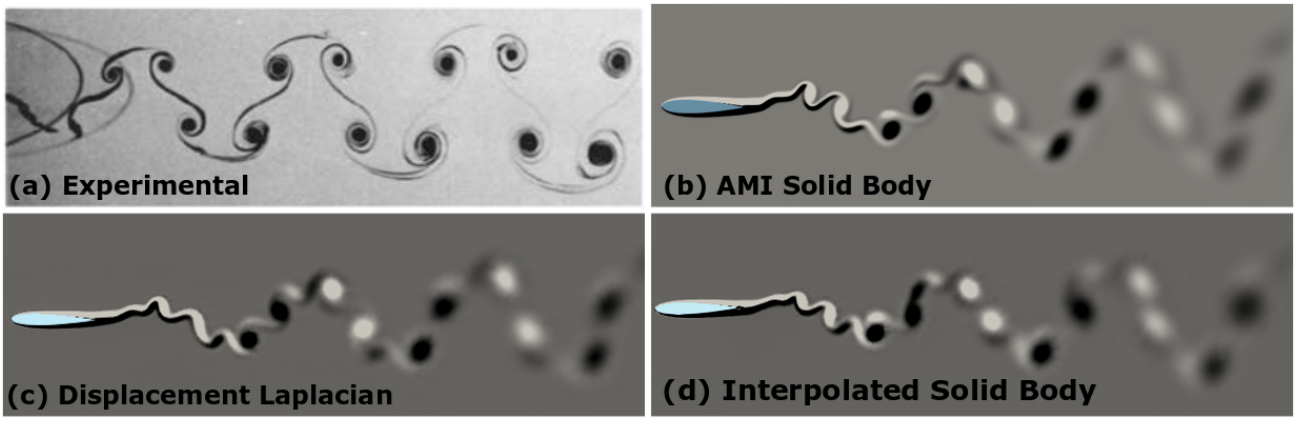


Figure 1: Comparison of instantaneous vorticity field at amplitude, $\theta = 4^\circ$ and reduced frequency, $\kappa = 3.1$ with *Koochesfahani (1989)*.

First, an Arbitrary Mesh Interface (AMI) dynamic mesh motion strategy is used in order to investigate the effect of different linear solver setups. In the present simulations, a circular domain with a radius of $30c$ is chosen based on a domain independence study. The entire domain is divided into two subdomains: one that surrounds the airfoil and rotates along with it as a solid body, known as the rotor ($15c$ radius), and the other is outside the circular rotor and up to the domain boundary, which remains stationary and is known as the stator. The entire computational domain is discretized with 534600 structured grid nodes, chosen through a systematic grid independence study. The AMI solid-body rotation algorithm oscillates the entire

A GREEN COMPUTING SOLUTION FOR COMPUTATIONAL FLUID DYNAMICS

THANH TRI NGUYEN
Qarnot Computing, 40-42 rue Barbès, 92120, Montrouge, thanh-tri.nguyen@qarnot-computing.com

Keywords: *Digital Pollution, Distributed Computing, Cloud Computing, Docker, OpenFoam*

As the world becomes increasingly digital, the impact of pollution from the numerical sector cannot be understated. According to The Shift Project, it accounts for 3.7% of global CO2 emissions in 2019, up from 2.5% in 2013 [1]. To keep up with the increasing need for computational power, stronger processing units have to be produced and bigger data centers have to be built with more energy being used to cool all of the hardware. Computational Fluid Dynamics (CFD) in particular uses copious amounts of computing power, usually with cases running on clusters with considerable amounts of processors. With the coming of higher order simulations, Large-Eddy Simulations (LES) and eventually Direct Numerical Simulations (DNS), the need for computing power will only increase in the future.
Qarnot is proposing an alternative solution with a distributed grid and where the heat output of computers is used to heat houses, offices and warehouses. This way, there is no need to build data centers and the overall carbont footprint is significantly reduced. A scheduler sends the computing load to a terminal that needs to heat up. Qarnot focuses mainly on open source softwares and OpenFoam is used for almost all of the fluid dynamics simulations. However, work is continuously being done on adding more softwares to the platform, even proprietary ones depending on the needs. The software can be customized to the user's preferences and it is packaged into a Docker container for consistent operation across all hardware. The Docker image can then either be stored on Docker Hub or on any other registry (public or private).
To launch a simulation case, a simple Python script can be used. The case that has already been set up needs only to be uploaded to the cloud with a bash file that contains the commands to be launched. The solver is then launched in the aforementioned Docker container which has been deployed on a Qarnot computing node. [2] Finally, the results can be downloaded back locally. If the simulation case is too heavy to be visualized on the local computer because of memory or graphics card constraints, a Paraview instance can also be deployed.

Acknowledgements
The presenter and Qarnot would like to thank Mr. Cardiff and the OpenFoam Workshop organizers for this great event. We want to also thank every researchers and industrials that will attend and present their work for their contributions.

References

1 H. Ferreboeuf, "Towards Digital Sobriety", The Shift Project, Lean ICT, Paris, Ile-de-France, France, March 2019 [Online] Available : https://theshiftproject.org/wp-content/uploads/2019/03/Executive-Summary_Lean-ICT-Report_EN_lowdef.pdf

2 R. Bouzel et al., "Distributed grid computing manager covering waste heat reuse constraints", Qarnot Computing, Montrouge, Ile-de-France, France, Unpublished.

SEMICOUPLED NUMERICAL STRATEGY TO SOLVE LARGE-STRAIN MOTION OF INCOMPRESSIBLE HYPERELASTIC MATERIALS

I. OLIVEIRA[1], Ž. TUKOVIĆ[2], J.L. GASCHE[1], P. CARDIFF[3]
[1]*São Paulo State University (UNESP), School of Engineering, Ilha Solteira, Brazil*
iago.oliveira@unesp.br; jose.gasche@unesp.br
[2]*Department of Energy, Power Engineering and Environment (FSB), University of Zagreb, Zeljko.Tukovic@fsb.hr*
[3]*University College Dublin, School of Mechanical and Materials Engineering, philip.cardiff@ucd.ie*

Keywords: *Computational solid dynamics. Finite-volume method. Coupled solver. Hyperelasticity.*

1 Introduction

Solids that can be modeled as incompressible or nearly incompressible represent a challenge to be solved using traditional numerical methodologies, such as the segregated solution of the vector momentum equation. Bijelonja, Demirdžić, and Muzaferija [1] proposed a "mixed finite-volume" technique based on the decoupling of the material constitutive equation between hydrostatic pressure and displacements that proved to be robust enough to handle all ranges of Poisson's coefficients. Moreover, Tuković, Batistić, Cardiff, *et al.* [2] further used the mentioned mixed finite-volume technique in a coupled numerical framework where the pressure and momentum equations are solved monolithically. However, their work explored only small-strain problems and the linear elastic constitutive law. In this work, we aim at assessing the suitability of the aforementioned technique to handle a material characterized by a nonlinear hyperelastic constitutive law, typically used to model materials in the large-strain regime.

2 Numerical Methodology

The nonlinear constitutive model used in this work is the compressible neo-Hookean model, represented by the following constitutive equation:

$$J\boldsymbol{\sigma} = \frac{\kappa}{2}\left(J^2 - 1\right)\boldsymbol{I} + \mu^{\mathrm{s}}\,\mathrm{dev}\,\boldsymbol{B}^{*}\,, \tag{1}$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, κ is the material bulk modulus, μ^{s} is the first Lamé coefficient, J is the determinant of the deformation gradient, and $\boldsymbol{B}^{*}$ is the isochoric part of the left Cauchy-Green deformation tensor.

The momentum equation in the total Lagrangian formulation is written as:

$$\rho_0 \frac{\partial^2 \boldsymbol{u}}{\partial t^2} = \nabla_0 \bullet \left(J\boldsymbol{F}^{-1} \bullet \boldsymbol{\sigma}\right) + \rho_0 \boldsymbol{b}\,, \tag{2}$$

where $\boldsymbol{u}$ is the solid displacement, ρ_0 is the density of the reference configuration and $\boldsymbol{b}$ represents body forces applied to the body. To numerically solve Eq. (2), a linear term is added in a deferred-correction manner, as follows:

$$\rho_0 \frac{\partial^2 \boldsymbol{u}}{\partial t^2} = \nabla \bullet \boldsymbol{\sigma}_H + \nabla_0 \bullet \left(J\boldsymbol{F}^{-1} \bullet \boldsymbol{\sigma} - \boldsymbol{\sigma}_H\right) + \rho_0 \boldsymbol{b}\,, \tag{3}$$

where $\boldsymbol{\sigma}_H$ is the Cauchy stress tensor for an elastic solid in the small-strain regime:

$$\boldsymbol{\sigma}_H = \mu^{\mathrm{s}}\left(\nabla \boldsymbol{u} + \nabla^{\mathrm{T}} \boldsymbol{u}\right) - \frac{\lambda^{\mathrm{s}}}{\kappa} p \boldsymbol{I}\,, \tag{4}$$

where λ^{s} is the second Lamé's coefficient. The pressure in Eq. (4) is given by

$$-p = \kappa \nabla \bullet \boldsymbol{u}\,, \tag{5}$$

GENERALISED INTERNAL BOUNDARIES APPLIED TO HIGH-SPEED COMPRESSIBLE FLOW

OLIVER OXTOBY[1], NALENDRAN SINGH[2], GEORGIOS KARPOUZAS[3], EUGENE DE VILLIERS[4]
[1]*Engys Ltd, o.oxtoby@engys.com*
[2]*Flamengro, a division of Armscor SOC Ltd, nalendrans@armscor.co.za*
[3]*Engys Ltd, g.karpouzas@engys.com*
[4]*Engys Ltd, e.devilliers@engys.com*

Keywords: *GIB, compressible, density-based, rocket motor, HELYX*

Generalised internal boundaries (GIBs) were developed in the HELYX® CFD code to provide an exact boundary representation for immersed regions in an existing computational mesh, using normal OpenFOAM boundary conditions [1]. So far it has been employed in diverse industrial applications including pumps, moving injectors, mould sealing, trapdoor valves, floating bodies, and grain burnback in solid rocket motors. The latter application has been successfully demonstrated using a pressure-based formulation based on the sonicDyMFoam solver [2]. However, the Courant number restriction imposed on the simulation time-step size places a severe limit on computing speed in these cases due the high Mach numbers encountered.

A more appropriate solver for these high-speed flows would be coupled and density-based, where implicit block-coupling removes the stability criterion on time-step size, and the density-based formulation improves the fidelity of shock wave capturing. One such solver, available in the OpenFOAM framework, is the HiSA (High-Speed Aerodynamic) solver [3]. In this talk, we describe its adaptation to cater for applications in internal ballistics. The modifications to the compressible flow algorithm and code to support GIBs is described, together with appropriate boundary conditions for general Mach numbers as well as verification tests performed. Finally the application of the solver to efficiently calculate grain burnback in three-dimensional solid rocket motor with a finocyl propellant design, is demonstrated.

References

[1] G. K. Karpouzas and E. de Villiers, “Generalized Internal Boundaries (GIB),” 2017. [Online]. Available: arXiv:physics.flu-dyn/1709.05125v2.

[2] A. Steenkamp, W. Rousseau, G. Karpouzas, O. Oxtoby, “Rapid Computational Fluid Dynamics method for SRM grain design using the Geometric Immersed Boundary condition method,” presented at the 14th OpenFOAM Workshop, Duisburg, Germany, Jul. 23–25, 2019.

[3] J. Heyns and O. Oxtoby. “HiSA” https://hisa.gitlab.io (accessed Feb. 11, 2021).

NUMERICAL ASSESSMENT OF THE SONAR DOME ADDED RESISTANCE FOR AN OCEANOGRAPHIC RESEARCH VESSEL USING FULL-SCALE SIMULATIONS

RUBEN J. PAREDES[1], MARIA T. QUINTUNA[1], JOSE R. MARIN[1], TAKANORI HINO[2]
[1]*ESPOL Polytechnic University, Escuela Superior Politécnica del Litoral, ESPOL, Ecuador*
[2]*Yokohama National University, Japan*

Keywords: *Sonar dome. Added resistance. Full-scale simulation. Torque measurement. Sea trial.*

An accurate ship resistance estimation is critical to design the propulsion system and guarantee its design speed. Typically, the dominant resistance components for displacement hulls are viscous and pressure forces. Sometimes, the operational need of the ship owner requires to add a dome appendage to protect the sonar equipment. The sonar dome added resistance could be significant and it is influenced by its wetted surface, shape, and relative length location. Moreover, the propeller performance is expected to be affected by the modified wake field.
In the present study, the hydrodynamic effect of a sonar dome recently added to an oceanographic research vessel, built in 1981, is assessed using the open source CFD software tool, OpenFOAM v7. First, full-scale numerical results of the original 70-meter long vessel configuration, without sonar dome and for the design conditions, were verified and validated following ITTC guidelines, using EHP curve and wake fraction coefficients provided by the propeller manufacturer. Later, the added resistance due to the addition of a sonar dome are estimated through simulations with a fixed hull until a steady state. Furthermore, the speed loss is estimated through an engine-propeller analysis using a 4 blade MAU twin propeller configuration. Preliminary results suggest a speed reduction of about three knots due to an increase of 25 percent of the total resistance and an important modification to the wake field. These results agreed with recent sea trials at partial displacement condition where torque measurements using a telemetry device on the shafts were performed.

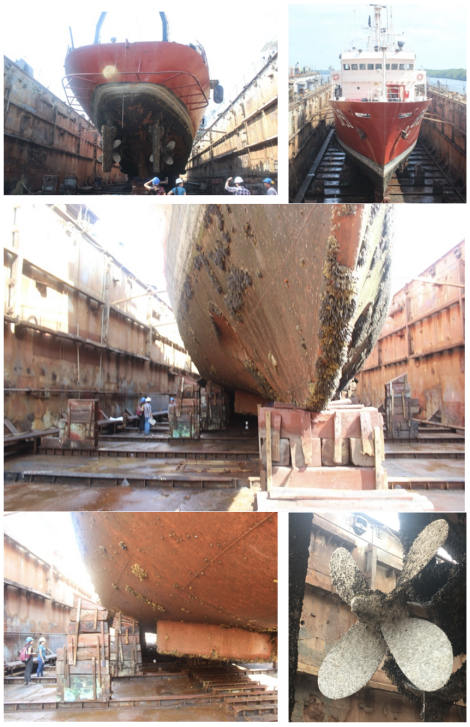


Figure 1: Oceanographic Research Vessel on a dry-dock during an schedule maintenance at 2018

Numerical modelling of Melt pool hydrodynamics and shrinkage of solidified tracks in Powder Bed Fusion processes

Gowthaman Parivendhan[1], Thomas Flint[2], Mike Smith[2], Philip Cardiff[1], Alojz Ivanković[1]
[1] *University College Dublin, I-FORM Advanced Manufacturing Research Centre, gowthaman.parivendhan@ucdconnect.ie*
[2] *Dalton Nuclear Institute, The University of Manchester, thomas.flint@manchester.ac.uk*

Keywords: *Powder Bed Fusion (PBF), Discrete Element Method (DEM), Computational Fluid Dynamics (CFD), Volume of Fluid (VoF), Heat transfer, Residual stresses*

Powder Bed Fusion (PBF) is a layer-wise additive manufacturing technique where the geometry is fabricated in slices. In PBF, the heat generated by a laser or an electron beam is used to melt and fuse powder particles. PBF offers several advantages over conventional manufacturing techniques such as the ability to create complex geometry, rapid prototyping, and lower material wastage. Nonetheless, PBF technology suffers from issues such as processability and repeatability which hinders the rise of PBF as a prominent manufacturing technique. To address these complications, it is necessary to understand the physics involved in PBF processes. Some of these are difficult to observe using experimental techniques due to the temporal and spatial scales involved, this is where numerical models can aid. The objective of the current study is to develop a numerical platform that can model most of the primary mechanisms that take place within PBF processes.

1 Mathematical Model

1.1 Powder Deposition

The particle packing density and distribution during the deposition process is stochastic and random in nature. The particle interaction is modelled using the Discrete Element Method (DEM) within LIGGGHTS. A 'rain-drop' approach is used wherein particles are generated at the top of the domain and allowed to fall to the bed-plate under the influence of gravity. Particles over the desired layer thickness are then removed. The position and size of the particles are then transferred to a volumetric mesh in OpenFOAM by assigning the volume fraction of metal in each cell as shown in Figure 1.

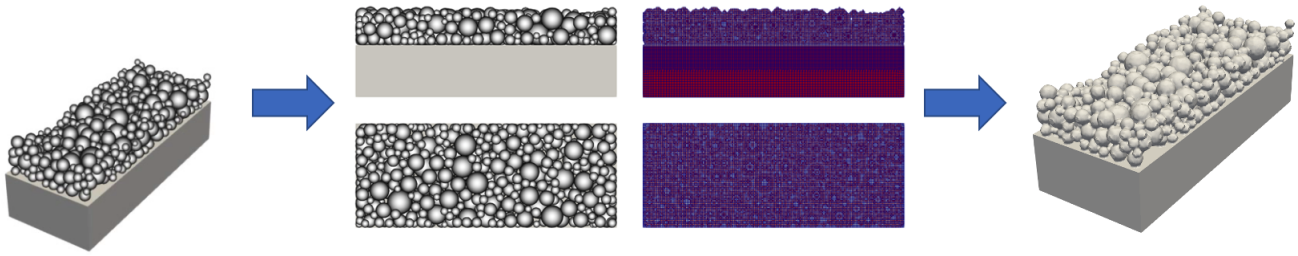


Figure 1: Representation of data transfer from DEM to CFD model.

1.2 Laser Processing

A Volume of Fluid (VoF) based solver has been developed for foam-extend fork of OpenFOAM, to model the thermofluid behaviour of the metal during the PBF process. A modified Navier-Stokes equation is solved to determine the mixture velocity using the volume fraction averaged properties. Flow due to buoyancy, capillary forces, Marangoni convection and recoil pressure are included in the model to emulate the melt pool hydrodynamics during the PBF process. A Carmen-Kozeny source is used to force the velocities to zero in the solid cells.

PREDICTION OF CROSS-FLOW TRANSITION USING γ TRANSITION MODEL COUPLED WITH REYNOLDS STRESS TRANSPORT TURBULENCE MODEL

Naina Pisharoti[1], John Webster[1], Stefano Brizzolara[1],
[1]*Kevin T Crofton Department of Aerospace and Ocean Engineering, Virginia Tech, Blacksburg, VA.*

Keywords: *Reynolds Stress Transport Model, Transition, Cross-flow*

Transition from laminar to turbulent flows is a complex phenomena and is prevalent in various aerodynamic applications like transport aircraft, rotorcraft and turbo-machinery. Based on the operating conditions, different modes of transition can be observed. Natural transition is observed at low free-stream turbulence intensities and occurs due to an amplification in the viscous and acoustic instabilities, while by-pass transition occurs due to high free-stream turbulence levels. Separation-induced transition is observed when there are adverse pressure gradients. Cross-flow transition on the other hand, occurs when there are favorable pressure gradients in 3-dimensional flows and arises due to instabilities caused by cross-flow velocity components.

In the past two decades, there have been various models introduced to predict transition that are also compatible with commercial CFD codes. The most widely used of all is γ-$Re_{\theta t}$, proposed by Menter et al [1]. It is a local correlation based model that is coupled with the k-ω SST model [2]. However, the model has a complex formulation and additionally, lacks Galilean invariance, restricting its usage to stationary wall boundaries. To overcome this, Menter et al [3] introduced a single equation γ model. It is a simplified version of the γ-$Re_{\theta t}$ model that eliminates the transport equation for $Re_{\theta t}$ and the correlations that depend on it. Nie et al [4] later on coupled the γ-$Re_{\theta t}$ model with SSG/LRR-ω, which is a second-order closure, Reynolds stress transport (RST) model introduced by Eisfeld et. al [5], thereby increasing the order of turbulence calculation. Although, by using γ-$Re_{\theta t}$ for transition prediction, the higher order model carried its disadvantages along.

Recently, Pisharoti et. al [6] introduced a transition turbulence model that was formulated using the SSG/LRR-ω, coupled with a single transport equation for intermittency, γ that governs transition. The transition model was inspired by Menter's one equation γ model [3]. The model framework was further calibrated by modifying the production of Reynolds stress and the length-scale governing equation (ω). The complete model was implemented using OpenFOAM-v2006. SSG/LRR-ω-γ uses simplified correlations with tune-able model co-efficients that depend only on local quantities within the boundary layer, making it independent of the free-stream velocity and rendering it Galilean invariant. Apart from the simplicity in its transition formulation, the advantage of the model is that by using a second-order closure turbulence model, it can be applied to complex flows that have strong streamline curvature and strong swirling. Additionally, since it is Galilean invariant, it can be applied to stationary as well as moving walls and also is widely suitable for general purpose CFD codes.

However, currently the model is capable of predicting only stream-wise transition like natural, bypass and separation-induced mechanisms. It does not involve other transition mechanisms like cross-flow transition. For geometries like swept wings, propellers and turbo-machinery, that have 3-dimensional boundary layers, there is a significant amount of cross-flow velocity that can cause a yawing effect and a favorable pressure gradient leading to an earlier transition than TS-instability. Therefore, it is important that the transition turbulence model capture these cross-flow transition effects.

The SST and RST based $\gamma - Re_{\theta t}$ was extended to include cross-flow effects by using the C1-criteria and helicity-based methods [7, 8]. Similarly, Pillai and Lardeau [9] introduced a method that used a combination of both the C1 criterion and effects of the local stream-wise helicity to incorporate cross-flow effects in the SST-based one equation γ model. The current paper is an effort to enrich the SSG/LRR-ω-γ model by extending it to include cross-flow transition. The proposed implementation will be using the helicity-based cross-flow formulation inspired by the RST-based γ-$Re_{\theta t}$ [8]. This has been chosen since helicity was discovered as a major contributor to the cross-flow velocity gradient. The formulation depends on the helicity based Reynolds number, Re_{He}, which is a good indicator to detect cross-flow instabilities. It plays a similar role to the vorticity Reynolds number, Re_v , which detects the onset of instabilities in standard transition formulations.

The transport equations for Reynolds stress (R_{ij}), dissipation rate (ω) and intermittency (γ) fof the SSG/LRR-ω-γ are given in equations (1) (2), (3) respectively.

$$\frac{\partial \rho R_{ij}}{\partial t} + \frac{\partial (\rho U_k R_{ij})}{\partial x_k} = \rho P_{ij} + \rho \Pi_{ij} - \rho \epsilon_{ij} + \rho D_{ij} \tag{1}$$

$$\frac{\partial (\rho \omega)}{\partial t} + \frac{\partial (\rho U_k \omega)}{\partial x_k} = \frac{\alpha_\omega \omega}{k} \frac{\rho P_{kk}}{2} - \beta \rho \omega^2 + \frac{\partial}{\partial x_k} \left[\left(\mu + \sigma_\omega \frac{\rho k}{\omega} \right) \frac{\partial \omega}{\partial x_k} \right] + \sigma_d \frac{\rho}{\omega} max \left(\frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}, 0 \right) \tag{2}$$

OPTIMIZING CFD CODE FOR MEMORY LOCALITY

ILYA POPOV[1], DMITRY ASTAKHOV[2]
[1]*ISTEQ B.V., RND-ISAN, ilya.popov@rnd-isan.ru*
[2]*RnD-ISAN, astakhov@rnd-isan.ru*

Keywords: *CFD, memory locality, performance, cloud computing*

It is well known that CFD performance, including OpenFOAM, is often limited by memory performance. This is especially so for species transport, where operations performed on every data item are relatively simple. On the top level, we have MPI nodes having separate memory. Then each machine has multiple levels of cache, TLBs (translation look-aside buffers) and memory is organized in a NUMA (non-uniform memory access) structure. All of this has to be taken into account for optimal performance. If the amount of data required to solve an equation is larger than cache size, accesses to further cells will be evicting previous cells from the cache. To make maximum reuse of the cache real estate, data access has to be rearranged accordingly. OpenFOAM already provides an utility, renumberMesh, to rearrange the mesh in order to minimize matrix bandwidth. In this work we study further measures one can take to improve performance by taking into account memory organization.
To account for multiple levels of memory organization, we employ multiple levels of reordering. Within one MPI node we use mesh division into microdomains. This microdomains can be processed using threads, for example using OpenMP. However, scheduling of the work between the threads in not trivial. This is especially true for cloud environments, where the user does not have complete control over hardware. For example, if one thread stalls for whatever reason, computation time would double in the case os static equally divided scheduling. A more dynamic approach is needed to avoid that.
The size of microdomains has to be chosen based on sizes of caches and properties of the equation to be solved. Characteristic sizes are memory page size and L1 cache size.
These improvements are benchmarked on model test cases.

Acknowledgments

The work was done in ISTEQ and RnD-ISAN companies.

References

INVESTIGATION OF WETTING UNDER THE INFLUENCE OF TRANSPORT PHENOMENON USING AN ALE-METHOD

RAJU,S.[1], KOCH,B.[2], BOTHE,D.[3], GRÜNDING,D. [4]
[1]*Mathematical Modeling and Analysis, TU Darmstadt, raju@mma.tu-darmstadt.de*
[2]*Mathematical Modeling and Analysis, TU Darmstadt, bastian.koch@stud.tu-darmstadt.de*
[3]*Mathematical Modeling and Analysis, TU Darmstadt, bothe@mma.tu-darmstadt.de*
[4]*Mathematical Modeling and Analysis, TU Darmstadt, gruending@mma.tu-darmstadt.de*

Keywords: *Wetting, ALE method, Finite area method*

Wetting phenomena are basically omnipresent in every machinery or natural process that involve liquids. While a reliable prediction of the basic process itself is already a challenging task, the interaction with transport processes is even less understood. Hence, such fundamental interactions are the focus of the Collaborative Research Centre (CRC) 1194.
This work aims to investigate the interaction between wetting and the influence of transport phenomenon in a region close to the moving contact line. For this purpose, we employ our extension of the Arbitrary Lagrangian-Eulerian method available in OpenFOAM which is going back to [1]. The method can handle general contact line geometries. An example of this approach is shown in Figure 1, where two contact lines - one at the lower wall and another at the triangular prism on the right - are used. The influence of surfactants on the velocity field in the region close to the contact line will be realized using OpenFOAM's finite area method. To resolve the different scales which are relevant for the wetting processes in general, a novel meshing approach has been developed that provides a strongly resolved mesh in the region close to the contact line as shown in Figure 1. Our simulations aim to understand the influences in the velocity field close to the contact line which has been observed in highly resolved experimental measurements from our cooperation partners within the CRC1194.

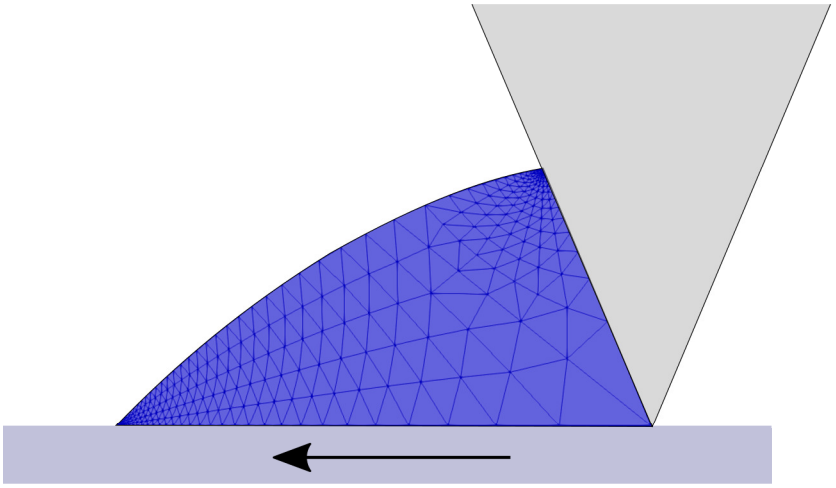


Figure 1: Overview of the experimental setup. The drop (blue) is dragged over a solid moving surface while being attached to a stationary prism (right).

Acknowledgments

The authors thank all those involved in the organisation of OFW16 and to all the contributors that will enrich this event. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-B02 265191195 – SFB 1194. Calculations for this research were conducted on the Lichtenberg high performance computer of the TU Darmstadt.

AN EFFICIENT FRAMEWORK FOR PEDESTRIAN WIND COMFORT ASSESSMENT

S.M. RENDA[1], P. ALEXIAS[2], G. KARPOUZAS[3], E. DE VILLIERS[4]
[1]*Engys Ltd, s.renda@engys.com*
[2]*Engys Ltd, p.alexias@engys.com*
[3]*Engys Ltd, g.karpouzas@engys.com*
[4]*Engys Ltd, e.devilliers@engys.com*

Keywords: *pedestrian comfort, coupled solver, multi-instance, DoE.*

The construction of new high-rise buildings in existing urban landscapes might increase wind speeds at pedestrian level, affecting the type of activities that humans can carry out in the surrounding areas. Computational fluid dynamics (CFD) is widely applied, alongside wind tunnel measurements, in the context of architecture, engineering and construction (AEC) industry to predict the airflow distribution around buildings and to assess pedestrian comfort and safety conditions. Wind studies are performed for various building geometries and configurations, by running multiple CFD analyses at different wind conditions, to determine the feasibility of a new development. Some of the more comprehensive analysis schemes are even necessitated by local regulations to grant planning permission [1], which can add up to a heavy computational burden. A quick turnaround time is often required to make early and effective decisions during design stages. As such, an efficient computational framework can have great benefits, especially if accuracy is not sacrificed.

Recently, a plethora of automated cloud-based solutions have become available in this space. While these solutions provide a convenient way for non-experts to perform wind-comfort analysis, this convenience comes at a cost: black-box automated workflows provide limited means of validation and often come at a significant price premium relative to in-house solutions. Further, such platforms significantly limit the ability of domain experts to add value, by evolving or enhancing the analysis process.

In this work, we demonstrate the performance of our pressure-velocity block-coupled solver algorithm, in combination with a new multi-instance solution framework which can automatically run multiple design conditions in a single execution without the need of external scripting. The presented toolchain can significantly accelerate time to solution and streamlines the process to move from input geometry and climate data to comfort indices (Figure 1). Despite its ease of use, the implementation remains accessible to the end-user, is easily extensible and can form the basis for arbitrary workflows that require design of experiments (DoEs). Sample results are presented for the Niigata benchmark case C, selected from the Architectural Institute of Japan (AIJ) guidebook [2].

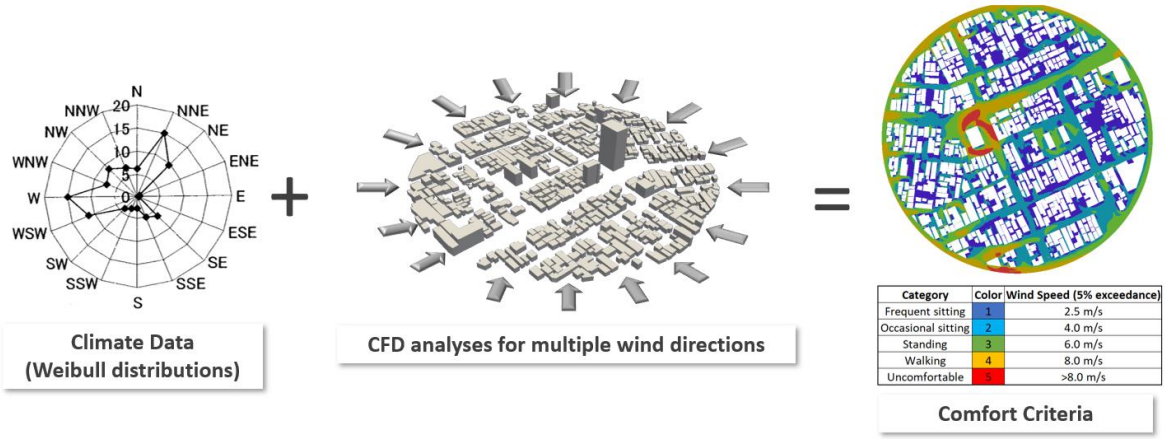


Figure 1: Highlights from typical pedestrian comfort workflow.

References

[1] City of London, RWDI, Wind Microclimate Guidelines for Developments in the City of London, City of London Corporation, 2019.

[2] Architectural Institute of Japan: AIJ Benchmarks for Validation of CFD simulations Applied to Pedestrian Wind Environment around Buildings. AIJ Publish. Tokyo, Japan, Sept. 2016.

A novel elastoplastic material model based on machine learning for finite volume solvers

SIMON RODRIGUEZ[1], MICHAEL CLANCY[1], PHILIP CARDIFF[1]
[1]*School of Mechanical and Materials Engineering, University College Dublin, Ireland.*
simon.rodriguezluzardo@ucdconnect.ie
michael.clancy@ucdconnect.ie
philip.cardiff@ucd.ie

Keywords: *elastoplasticity, machine learning, constitutive law, solid mechanics.*

Within the field of numerical simulation of inelastic problems in solid mechanics, a typical solution loop (omitting the solution of auxiliary equations such as the conservation of energy) involves the following steps [1]:

1. A displacement field is generated from the discretised momentum equation (frequently, this comes from finite element method solution loop).
2. New state variables, i.e. true stress (σ), plastic deformation (ϵ^P) and internal variables (q) are obtained by solving the constitutive equation (material model) considering the history of loading (this is known in the literature as the central problem in plasticity).
3. The momentum equation is solved with the new state variables. If the momentum balance does not hold, the whole process is repeated until convergence.

This project aims to provide an alternative for the solution step 2 which consists of replacing the unknown phenomenological constitutive law relating the strain tensor to the stress tensor by a machine learning (ML) model trained with data from microstructures simulations or Digital Image Correlation (DIC) [2] experiments.

Typically, manufacturing processes such as metal forming have seen its applicability limited by the accuracy of the constitutive law: The quality of the results rapidly degrades as the number of passes increases, however, formulating a material model that accurately captures the experimental behaviour is extremely complex [3] due to reasons such as the necessity of considering the historical loading, the difficulties to experimentally measure parameters in elaborated formulations and others. The approach proposed in this project avoids all this complexity by producing the stress responses based on the "experience" of the machine learning model on similar (real) data. Therefore, potentially, this approach could improve the accuracy of results from the plasticity simulation in general, with an initial focus on the processing and manufacture of high-strength steel wire. Theoretically, this should be achieved by the application of a sequence-to-sequence method from the neural networks realm [4], where a sequence of strain tensors is fed to a model that produces the corresponding stress tensor. Even though deep learning literature seems to be focused on predicting sequences for natural language processing, there is evidence on the capability of these methods to capture the elastoplastic behaviour [5], [6]. This inference is reinforced by the early results of this project which have captured the behaviour of a 1-D isotropic hardening law by applying a recurrent neural network [4] making use of the specialised Keras [7] library for Python, as shown in figure 1.

The next steps are to increase the complexity of the target constitutive model, until the methodology can effectively replace classical 3-D material laws such as the radial return algorithm for J2 plasticity [8]. As stated previously, the solids mechanics numerical simulations have traditionally been based on the finite element method. Nevertheless, once the surrogate model for the constitutive law is generated, it will be incorporated into the solids mechanics framework of OpenFOAM [9], [10]. The idea is that the predicted displacement field in step 1 above is produced by OpenFOAM as part of the finite volume method iterations. That new field will be fed to the machine learning-based model generated in the presented problem, as shown in figure 2.

Acknowledgments

Financial support is gratefully acknowledged from the Irish Research Council through the Laureate programme, grant number IRCLA/2017/45. Additionally, the authors want to acknowledge project affiliates, Bekaert, through the Bekaert

AN UPDATE ON THE LATEST DEVELOPMENTS OF THE ISOADVECTOR GEOMETRIC VOF METHOD IN OPENFOAM

JOHAN ROENBY[1,2], HENNING SCHEUFLER[3], KONSTANTINOS MISSIOS[1] KASPER MØLLER[1], FYNN ASCHMONEIT[1], NIELS JACOBSEN[4]

[1]*Department of Mathematical Sciences, Aalborg University, Denmark, roenby@math.aau.dk*

[2]*STROMNING IVS, Denmark, johan@stromning.com*

[3]*DLR, Germany, Henning.Scheufler@dlr.de*

[4]*Deltares, The Netherlands, Niels.Jacobsen@deltares.nl*

Keywords: *Interfacial flows, multiphase flows, geometric Volume of Fluid, isoAdvector*

IsoAdvector was first introduced in 2016 as a new geometric volume of fluid (VoF) method in OpenFOAM [1], [2]. The key novelty of the isoAdvector method is the idea of modelling the fluid interface as a straight line sweeping over a mesh face during a time step. Based on an initial geometric reconstruction of the fluid interface, the flux of heavy vs. light fluid passing through a cell face during a time step is calculated accurately and efficiently without the expensive and complex polyhedron intersection calculations often required by "traditional" geometric VOF methods. The result is a method that is as efficient as algebraic VoF, and hence applicable for practical engineering simulations, without compromising the sharpness of the interface, boundedness of the volume fraction field or the accuracy of the interface advection. The isoAdvector method was integrated into OpenFOAM-v1706 where it is used by the interIsoFoam solver. Since the initial integration, the method has been extended to work with moving and morphing meshes [3] as well as with automatic mesh refinement. New geometric reconstruction methods were developed to improve the accuracy, particularly on unstructured meshes [4]. And maybe most importantly, the method has found widespread use in many areas of application, see e.g. [5]–[7].

In this presentation, we will give an overview of the latest developments around isoAdvector-based geometric VoF capabilities in OpenFOAM. These include flows through porous media in the spirit of [8], development of a compressible flow solver [9], coupling with phase change models as well as with more accurate surface tension models. We will also discuss strategies for handling the main drawback of the isoAdvector method, namely its explicit nature, limiting it to interface Courant numbers smaller than one. Finally, our plans for further improvements of geometric VoF based interfacial flow solvers in OpenFOAM will be sketched.

Acknowledgements

The presented work was supported by the Independent Research Fund Denmark (InterFlow project, grant no. 9063-00018B) and by Innovation Fund Denmark (FloatStep project, grant no. 8055-00075A).

References

[1] J. Roenby, H. Bredmose, and H. Jasak, 'A computational method for sharp interface advection', *R. Soc. Open Sci.*, vol. 3, no. 11, p. 160405, Nov. 2016, doi: 10.1098/rsos.160405.

[2] J. Roenby, H. Bredmose, and H. Jasak, 'IsoAdvector: Geometric VOF on general meshes', in *OpenFOAM - Selected papers of the 11th Workshop*, Springer, 2018.

[3] OpenCFD, 'OpenFOAM® v1906 release notes'. https://www.openfoam.com/releases/openfoam-v1906/solver-and-physics.php#solver-and-physics-interisofoam-morphing-meshes (accessed Feb. 11, 2021).

[4] H. Scheufler and J. Roenby, 'Accurate and efficient surface reconstruction from volume fraction data on general meshes', *J. Comput. Phys.*, vol. 383, pp. 1–23, Apr. 2019, doi: 10.1016/j.jcp.2019.01.009.

[5] L. Gamet, M. Scala, J. Roenby, H. Scheufler, and J.-L. Pierson, 'Validation of volume-of-fluid OpenFOAM® isoAdvector solvers using single bubble benchmarks', *Comput. Fluids*, vol. 213, p. 104722, Dec. 2020, doi: 10.1016/j.compfluid.2020.104722.

[6] Y. (曹元伟) Cao and R. Macián-Juan, 'Numerical investigation of central breakup of large bubble induced by liquid jet', *Phys. Fluids*, vol. 32, no. 3, p. 033302, Mar. 2020, doi: 10.1063/1.5144975.

[7] E. Laurila, D. Izbassarov, M. Järvinen, and V. Vuorinen, 'Numerical study of bubbly flow in a swirl atomizer', *Phys. Fluids*, vol. 32, no. 12, p. 122104, Dec. 2020, doi: 10.1063/5.0028963.

[8] B. Jensen, N. G. Jacobsen, and E. D. Christensen, 'Investigations on the porous media equations and resistance coefficients for coastal structures', *Coast. Eng.*, vol. 84, pp. 56–72, 2014.

[9] OpenCFD, 'OpenFOAM® v2006: release notes'. https://www.openfoam.com/releases/openfoam-v2006/solver-and-physics.php#solver-and-physics-interIsoFoam (accessed Feb. 11, 2021).

AI DRIVEN MODELS TO PREDICT THE DRAG COEFFICIENT OF A SPHERE TRANSLATING IN SHEAR-THINNING VISCOELASTIC FLUIDS

A. I. RORIZ[1], S. A. FAROUGHI[2,*], G. H. MCKINLEY[2], J. M. NÓBREGA[1], C. FERNANDES[1]

[1] *Institute for Polymers and Composites, University of Minho, Campus de Azurém, 4800-058 Guimarães, Portugal*

[2] *Hatsopoulos Microfluids Laboratory, Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

Keywords: *drag coefficient, viscoelastic fluids, Giesekus model, Random forest, Gradient extreme boosting, Deep neural network*

Non-Newtonian fluid suspensions are widely used in several areas of our daily life, e.g., to produce bags, toys, car components, textiles, etc., and they are also commonly encountered in many advanced manufacturing and industrial operations, such as processing of battery slurries or hydraulic fracturing operations. However, an efficient numerical solver capable of simulating such processes is still missing in the scientific literature. For this purpose, a 3D CFD-DEM viscoelastic solver is developed in this work to handle particle-laden viscoelastic flows using a new approach, based on machine learning and deep learning models, to compute a particulate-phase drag model valid for a wide range of material parameters.

The present work studies the evolution of the drag coefficient of a single sphere translating through a viscoelastic fluid that is described by the shear-thinning Giesekus model. To calculate the drag coefficient, we begin with 3D direct numerical simulations (DNS) of unconfined viscoelastic flows over a wide range of parameters, specifically the Reynolds number $Re \leq 50$, the Deborah number $De \leq 5$, the retardation ratio $0 < \zeta < 1$, and the mobility parameter $0 < \alpha < 1$. A total of approximately 3000 DNS were performed and the results obtained enable the development and validation of deep learning models which relate the input data (specifically *Re, De*, ζ and α) to the output (response) variable, here the dimensionless drag coefficient on the particle. A number of different learning algorithms are considered, including the Random Forest [1], Gradient Extreme Boosting [2] and Deep Neural Network [3]. These physics-based data-driven model can then be integrated into a 3D CFD-DEM viscoelastic solver to enable simulations of particle laden viscoelastic suspensions in more complex 2D and 3D flow fields.

Acknowledgements

This work is funded by FEDER funds through the COMPETE 2020 Programme and National Funds through FCT (Portuguese Foundation for Science and Technology) under the projects UID-B/05256/2020, UID-P/05256/2020, APROVA-Aprendizagem PROfunda na modelação de escoamentos com fluidos de matriz Viscoelástica Aditivados com partículas (POCI-01-0145-FEDER-016665) and HPC-EUROPA3 (INFRAIA-2016-1-730897). The authors would like to acknowledge the Minho University cluster under the project NORTE-07-0162-FEDER-000086 (URL: http://search6.di.uminho.pt), the Minho Advanced Computing Center (MACC) (URL: https://macc.fccn.pt), the Texas Advanced Computing Center (TACC) at The University of Texas at Austin (URL: http://www.tacc.utexas.edu), the Gompute HPC Cloud Platform (URL: https://www.gompute.com) and Consorzio Interuniversitario dell'Italia Nord Est per il Calcolo Automatico (CINECA) for providing HPC resources that have contributed to the research results reported within this paper.

References

[1] A. Liaw and M. Wiener. Classification and regression by random forest. *R news*, 2(3):18-22, 2002

[2] T. Chen and C. E. Guestrin. XGBoost: A scalable tree boosting system. In *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining,* 785-794, 2016

[3] D. F. Specht. A general regression neural network. *IEEE transactions on neural networks*, 2(6):568-576, 1991.

LOWERING THE OBSTACLES FOR SMES TO ADOPT MULTI-PHYSICS BIOMASS FURNACE SIMULATIONS BY PROVIDING A CLOUD BASED SOLUTION

H. RUSCHE[1],
B. PETERS[2], X. BESSERON[2], A. ROUSSET[2],
R. LUKOŠEVIČIUS[3], L. PAUKŠTAITIS[3], L. NARBUTAS[3]
[1] *Wikki GmbH, Ziegelbergsweg 68, 38855 Wernigerode, Germany, h.rusche@wikki-gmbh.de*
[2] *Université du Luxembourg, 2, avenue de l'Université, L-4365 Esch-sur-Alzette, Luxembourg, bernhard.peters@uni.lu*
[3] *Enerstena UAB, Ateities ave. 30A, 52163 Kaunas, Lithuania*

Keywords: *DEM, CFD, biomass furnace, automatic workflow, cloud based solution*

Biomass as a renewable energy source continues to grow in popularity to reduce fossil fuel consumption for environmental and economic benefits. The combustion chamber of a biomass furnace is typically equipped with a forward acting grate that transports the fuel (e.g. wood chips) through the combustion chamber. During the pyrolysis step, the fuel releases hydrocarbons which are burned in the gas phase above the grate. The simulation therefore requires a hybrid four-way coupling between the Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD) complicating the setup, execution and post-processing.
Many manufacturers of biomass furnaces are small to medium sized enterprises (SMEs). Although such simulations could be an important element in the digitalization of their business, the adoption of such technologies requires substantial investment in computer hardware, software licenses and last but of least training of engineering staff. The Cloudifacturing EU project (www.cloudifacturing.eu) aims to democratically boost the competitiveness of such manufacturers by supporting a set of applications where technological and commercial scalability is considered from the beginning. The simulation of biomass furnaces has been selected as one of them.
The core simulator used in the application is based on the extended discrete element method (XDEM) developed at the University of Luxembourg. For the CFD part, FOAM-extend is utilised. The computational work-flow will include a domain-specific user interface based on MS Excel, validation of the input, geometry and mesh generation, case set-up, execution in an high-performance computing (HPC) environment as well as automated reporting and post-processing. The work-flow deals with the DEM and CFD domain in a consistent and unified manner.
The presentation will outline some challenges of biomass furnace simulations, describe the computational work-flow and the choice and design of the user interface. Initial results for Enerstena's biomass furnace will be presented. It will demonstrate how manufacturing SMEs are empowered to compute and solve problems that cannot be tackled without Cloud and HPC technology, making them more competitive by reducing development times for innovative products with better performance.

Acknowledgements

This work received funding from the European Union's Horizon 2020 research and innovation programme through the CloudiFacturing project (Grant No. 768892).

SIMULATION OF KAPLAN TURBINE TRANSIENTS: A NOVEL OPENFOAM FRAMEWORK

SAEED SALEHI[1], HÅKAN NILSSON[2], ERIC LILLBERG[3] , NICOLAS EDH[4]
[1]*Chalmers University of Technology, Gothenburg, Sweden, saeed.salehi@chalmers.se*
[2]*Chalmers University of Technology, Gothenburg, Sweden, hakan.nilsson@chalmers.se*
[3]*Vattenfall AB, Research and Development, Solna, Sweden, eric.lillberg@vattenfall.com*
[4]*Forsmarks Kraftgrupp AB, Östhammar, Sweden, nicolas.edh@vattenfall.com*

Keywords: *Kaplan turbine, transient operation, OpenFOAM, Dynamic mesh*

Introduction

In recent years, there has been a rapid growth in renewable electric energy resources, such as solar and wind energy. These resources are intermittent, meaning they are not always available and may vary even during day time [1]. Fast increase of intermittent resources usage, necessitate transient operation of hydraulic turbines (i.e., variable load conditions) to regulate the electrical grid. Hydraulic turbines are generally designed to continuously work at the best efficiency condition and transient operation causes additional stresses on the turbines and reduces their lifetime. Therefore, developing methodologies for performing an in-depth analysis of hydraulic turbines under such conditions is essential.

Novel OpenFOAM framework

Transient operation of Kaplan turbines involves a change of flow rate, change of guide vane angles, and change of runner blade angles while the runner is rotating around the turbine axis. Hence, the numerical simulation of such transients can be tremendously challenging. From a numerical point of view, different types of mesh motion are needed in the computational domain. The mesh motion of the runner domain consists of simultaneous solid-body rotation and mesh morphing and the guide vane mesh motion includes only mesh deformation due to morphing. Each guide vane and runner blade changes its angle about its own axis, and the runner blade axes also have the solid-body rotation of the runner. While the mesh is deformed, it must slip on arbitrarily shaped surfaces, such as the hub and the shroud, and in some cases even on the blades. This makes the mesh morphing procedure more difficult. Thus, simulations of the flow in Kaplan turbines during transient operation is very challenging and needs special developments.

A general slip boundary condition does not have an implicit implementation that contributes to the coefficient matrix. Instead, it works as an explicit correction. This explicit implementation may work fine for small mesh deformations or surfaces with small curvatures, but it cannot handle large deformations or highly curved surfaces. Slip boundary conditions based on the classical explicit correction are shown to have severe convergence issues on complex geometries [2]. For this reason, in the current study, a novel methodology is developed in OpenFOAM to treat surface slip displacements more robustly. The main idea is to have two different displacement fields and solve the Laplacian equation for each of those fields. The first Laplacian solution gives an intermediate displacement field $\boldsymbol{\delta}_0$ in which a conventional explicit surface slip displacement boundary condition is used to slip points on the curved surfaces. Then the tangential component of the intermediate displacement field is computed and set as a Dirichlet boundary condition for the main displacement field $\boldsymbol{\delta}$. In this way, the points inside the domain *feel* the slip boundary surface and move with the same curvature. A new mesh motion solver is developed in OpenFOAM and the above-described methodology is implemented. In addition, a new boundary condition is implemented to extract the tangential component of $\boldsymbol{\delta}_0$ on the slipped surface and to apply it as a Dirichlet boundary type for the $\boldsymbol{\delta}$ field.

Case-study

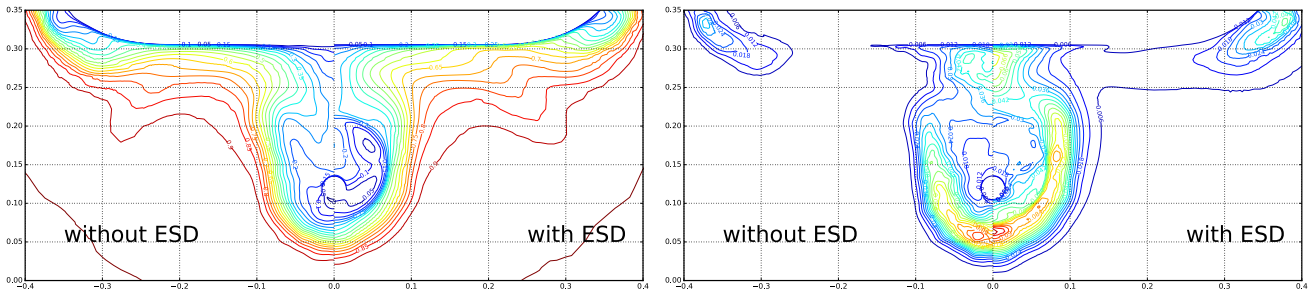
The newly developed OpenFOAM numerical framework is utilized to simulate the flow in the U9-400 Kaplan turbine model, going from an operating condition close to the best efficiency point to a part load condition. The guide vanes and runner blades are rotated around their own axes with a constant rotational speed, and the flow rate is linearly changed with the guide vane angle. The numerical results are used for studying the flow behavior, such as the formation of the rotating vortex rope and the frequencies that occur in the system.

STUDY OF THE UNSTEADY LOADING AND TURBULENCE IN THE WAKE OF SHIP WITH AND WITHOUT ENERGY SAVING DEVICE USING HYBRID RANS-LES MODEL

Sina Samarbakhsh[1], Nikolai Kornev[2]
Chair of modeling and simulation (LeMoS), University of Rostock, 18059 Rostock, Germany
[1] *sina.samarbakhsh@uni-rostock.de*
[2] *nikolai.kornev@uni-rostock.de*

Keywords: *Turbulence modeling, hybrid RANS-LES, Energy saving device*

Hybrid RANS-LES method are enable to solve a practical problem with a reasonable computational cost. In this paper a hybrid RANS-LES method which has been developed in LeMoS and implemented in OpenFOAM is being used. The computational domain in LeMoS hybrid model is dynamically subdivided into the LES and URANS region. The key quantity for this transition are the integral length scale L and the extended LES filter Δ which are computed for each cell of the mesh. L is determined from the formula of Kolmogorov and Prandtl $L = C.k^{3/2}/\epsilon$. The filter Δ is computed as $\Delta = \sqrt{0.5(d_{max}^2 + \delta^2)}$ where d_{max} is the maximal length of the cell edges and δ is the common filter which used in LES. If $L > \Delta$ then the cell is in LES region and the rest is RANS region [1]. LeMoS hybrid model with shielding function (SLH) was also introduced in order to prevent the artificial grid induced separation resulting from ambiguous grid [2].
The ship hull with and without ESD was studied with three different mesh resolution. Coarse grid (3+ Mio), Medium grid (8+ Mio) and fine grid (16+ Mio) have been considered for grid study. The length between perpendiculars in ship model scale is $L_{pp} = 6[m]$, draft $T = 0.35[m]$, beam $B = 1[m]$ and block coefficient $C_b = 0.79$. The study has been performed on the constant velocity of 1.315[m/s] corresponding to the Reynolds number of $Re = 7.4 \times 10^6$ and Froude number of $Fr = 0.169$. Energy saving devices (ESD) such as duct with pre-swirl stators are reliable approach to reduce energy consumption for ship. The energy saving device major role is reducing ship resistance, increasing propulsion efficiency and improving hull-propeller interaction. In this paper the influence of energy saving device on the turbulent kinetic energy and velocity field are investigated. Figure 1 shows the influence of energy saving device on the wake and developing turbulent kinetic energy field. The application of LeMoS hybrid model for prediction of wake and integral forces acting on the ship have been analysed and compared with DES based hybrid models. On the relatively coarse grid (8+ Mio) both DDES SST and IDDES SST failed to predict the unsteadiness of the ship wake region and showing very large grey zone, while LeMoS hybrid model is capable of capturing unsteady effect caused by vortices in the wake region. The transition from RANS to LES branch in DDES and IDDES for this relatively coarse grid has not been achieved correctly. The turbulent kinetic energy in different cross section along the hull was evaluated using LeMoS hybrid model as well as DDES and IDDES. As can be seen in Figure 2 the value of TKE in LeMoS hybrid model is much larger compare to DDES and IDDES due to capability of resolving velocity fluctuations in the wake region.



(a) Isoline of x-component of averaged velocity

(b) Isoline of total turbulent kinetic energy

Figure 1: Influence of energy saving device on velocity field and turbulence kinetic energy, at cross section $x/L_{pp} = 0.977$ (Turbulence model: LeMoS hybrid Model)

Modelling of droplet formation and growth in the turbulent moist-air wind tunnel LACIS-T

SILVO SCHMALFUSS[1], DENNIS NIEDERMEIER[1], JENS VOIGTLÄNDER[1], FRANK STRATMANN[1]
[1]*Experimental Aerosol and Cloud Microphysics Department, Leibniz Institute for Tropospheric Research*

Keywords: *Lagrangian particle tracking, droplet growth, LES*

Clouds play an important role in short term weather forecasts as well as in long term climate predictions. However, some important cloud processes are not fully understood, yet. One open issue in understanding clouds and their behaviour is the influence of turbulence on – among others – the activation and (condensational) growth of cloud droplets from Cloud Condesation Nuclei (CCN) [1]. In the past, cloud processes were mainly studied by means of field measurements – with the drawback, that controlled, reproducible conditions were nearly impossible to achieve [2]. For this reason, cloud simulation chambers were set up. One of them is LACIS-T (Turbulent Leipzig Aerosol Cloud Interaction Simulator), a closed-loop, moist-air wind tunnel for investigating the interaction between cloud microphysics and turbulence [3]. Temperature, humidity, and velocity can be controlled precisely, and defined turbulence is introduced by turbulence grids. Promising results from first experiments demonstrate the high accuracy and broad abilities of LACIS-T [3].
LACIS-T features two flow branches, as can be seen on the left in Fig. 1. For each branch, airflow velocity, humidity, and temperature can be set individually. In the setup described here, both branches are saturated wrt. water (i.e. the relative humidity is 100%), but are set to different temperatures (20 °C and 4 °C). This leads to supersaturation in the mixing region between the two flows. Size-segregated, monodisperse dry sodium chloride particles with a diameter of d_P = 100 nm are injected in this mixing zone and tracked along their trajectories through the tunnel.
To accompany the experiments in LACIS-T, and to help interpreting the gained results, numerical simulations are of great help. Therefore, OpenFOAM's Lagrangian library was extended to allow solid particles to take up water vapour from the carrier fluid and to grow to droplets. The initially solid particles condense or evaporate water corresponding to the prevailing water vapour saturation S in their surrounding, which is described by mass change

$$dm = 2\pi d_P \rho_{v,sat}(S - S^*)dt \tag{1}$$

Here, d_P, $\rho_{v,sat}$, S, S^*, and t refer to particle diameter, water vapour density at saturated conditions, saturation in the gas phase, saturation at the particle surface, and time, respectively. For the calculation of S^*, Koehler-theory is considered, so that the growth behaviour of unactivated (i.e. very small) droplets is captured correctly. Furthermore, for the modelling of the wind tunnel, accounting for conjugate heat transfer is necessary due to the principle and construction details of the wind tunnel. In result, a conjugate heat transfer solver extended by a passively transported humidity field and the aforementioned Lagrangian library was created.
For comparison with experimental data gathered with an optical particle counter, two particle size distributions obtained in two different heights (40 cm and 80 cm below the aerosol inlet) are shown on the right hand side of Fig. 1. The good agreement between measured and simulated size distributions indicates that the microphysical processes of droplet formation and condensational growth inside the wind tunnel are captured reasonably well with the modified library and solver and that this combination can be employed as a useful tool for complementing and interpreting experimental data from LACIS-T.

Acknowledgments

LACIS-T was built in the framework of the Leibniz-SAW-Project Leipzig Aerosol Cloud Turbulence Tunnel (number: SAW-2013-IfT-2) and has received funding by European Union's Horizon 2020 (EUROCHAMP-2020 Infrastructure Activity, grant agreement no. 730997).

References

[1] E. Bodenschatz, S. P. Malinowski, R. A. Shaw, and F. Stratmann, "Can we understand clouds without turbulence?" *Science*, vol. 327, no. 5968, pp. 970–971, 2010.

NEPTUN'S SPAGHETTI – BENDING ACTUATOR LINE MODELS

PÁL SCHMITT[1], DESMOND ROBINSON[2],
[1] *Queen's University Belfast, p.schmitt@qub.ac.uk*
[2] *Queen's University Belfast, des.robinson@qub.ac.uk*

Keywords: *Actuator-Line-Model, Beam-Element, Frame-Analysis, FEA, FSI)*

Actuator Line Methods (ALM), an adaptation of Blade Element Momentum methods to Computational Fluid Dynamics, are commonly used tools for simulating slender bodies like aero/hydrodynamic profiles which would require a very high mesh count to resolve the geometry and whose properties like lift and drag are well known and readily available [1, 2, 3, 4].

Slender, beam-like structures can be assessed efficiently for deformations, strains and stresses using Finite Element Analysis (FEA). Coupling the ALM with an FEA solver thus creates a useful tool and has been used, for example, for designing wind turbine blades.

We implemented a coupling of the ALM implementation originally presented by [5] with a general FEA solver based on Euler–Bernoulli beam theory following [6]. The aim is to create a toolbox not only for the simulation of horizontal axis turbine blades but achieving a flexible and general framework for the simulation of arbitrary slender structures. The FEA solver is implemented from scratch and uses the armadillo library [7].

First validation cases and applications to the design of non conventional offshore renewable devices are presented.

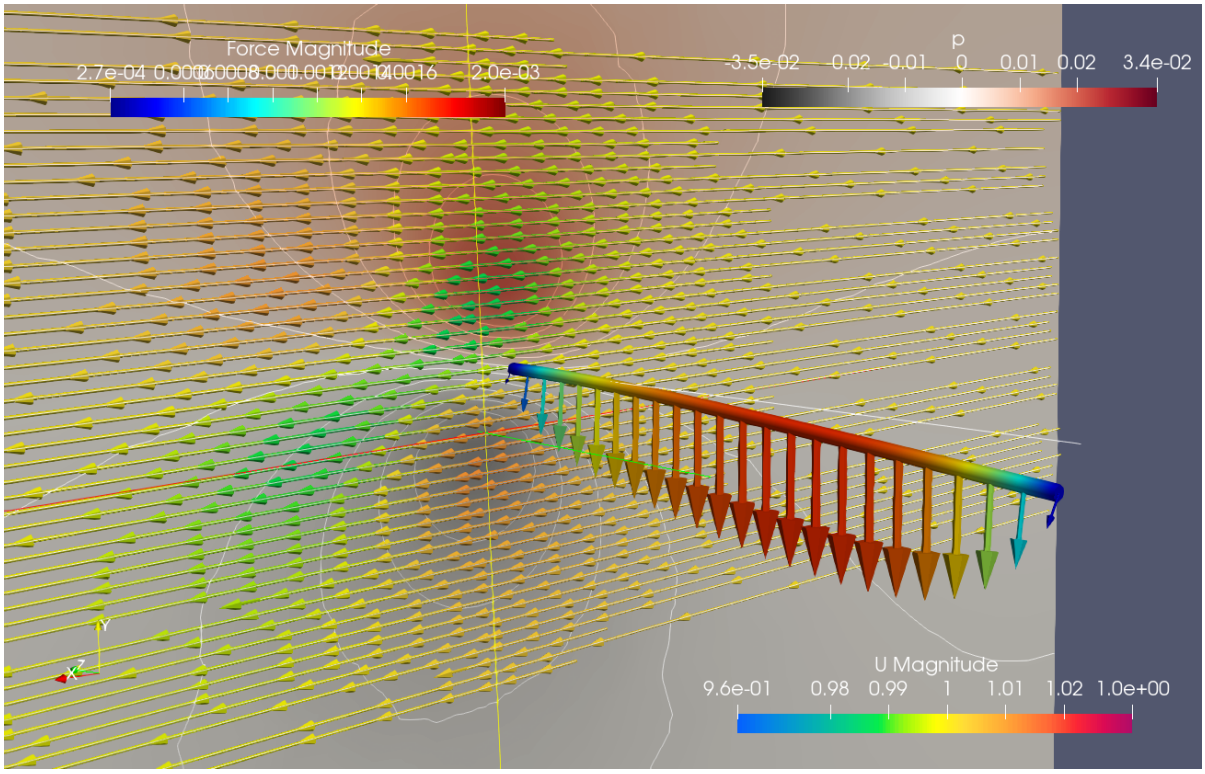


Figure 1: Proof of concept for deforming actuator line model. Beam is deformed

References

[1] M. Ravensbergen, A. Bayram Mohamed, and A. Korobenko, "The actuator line method for wind turbine modelling applied in a variational multiscale framework," *Computers & Fluids*, vol. 201, p. 104465, 2020. [Online]. Available: https://www.sciencedirect.com/science/article/pii/S0045793020300384

RAPID PERFORMANCE ASSESSMENT OF PERIODIC TURBO-MACHINES UNDER INCOMPRESSIBLE FLOW CONDITIONS

GEORGIOS KARPOUZAS[1], THOMAS SCHUMACHER[2]

[1]Engys Ltd., g.karpouzas@engys.com
[2]Engys GmbH., t.schumacher@engys.com

Keywords: *Incompressible block-solver, Turbomachinery*

Turbomachinery design process requires many optimization iterations to get an optimal and robust final design due to the high aerodynamic requirements. The prediction of the turbomachinery design characteristics using Computational Fluid Dynamics (CFD) simulations plays an important role on accelerating the overall design process. In this paper, the solutions of an incompressible turbomachinery application are presented. For the simulations, a pressure-based block solver [1][2][3] are used for the incompressible flow solutions.

In turbomachinery applications, sector models are commonly used for reducing computational cost with the assumption of periodicity between the sectors. The computational cost reduction depends on the number or blades/sectors. For this purpose, the *cyclicPeriodicAMI* related classes, which are used at the boundary between rotating and stationary sector-based interfaces are rewritten to:

- make a consistent, robust and conservative interpolation between the interfaces (figure 1),
- support a near-integer pitch ratio interfaces and
- work in a generic way for segregated and block-based formulations.

The new interface is used in the presented cases and the results are compared with the ones produced using the segregated solvers.

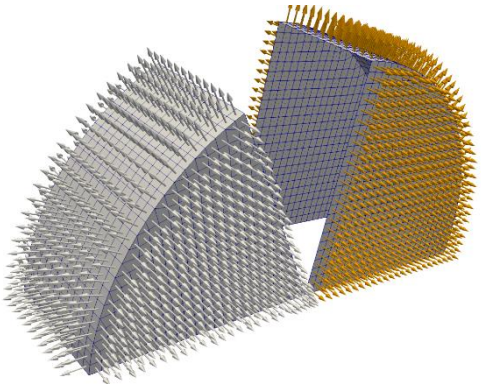


Figure 1: Example of Surface normal vector interpolation from source to target in a 90º-60º sector model.

References

[1] https://engys.com/products/add-ons/helyx-coupled

[2] M. Darwish, I. Sraj and F. Moukalled. A coupled finite volume solver for the solution of incompressible flows on unstructured grids. Journal of Computational Physics. 2009

[3] G. Karpouzas. A Hybrid Method for Shape and Topology Optimization in Fluid Mechanics. PhD Thesis, 2019

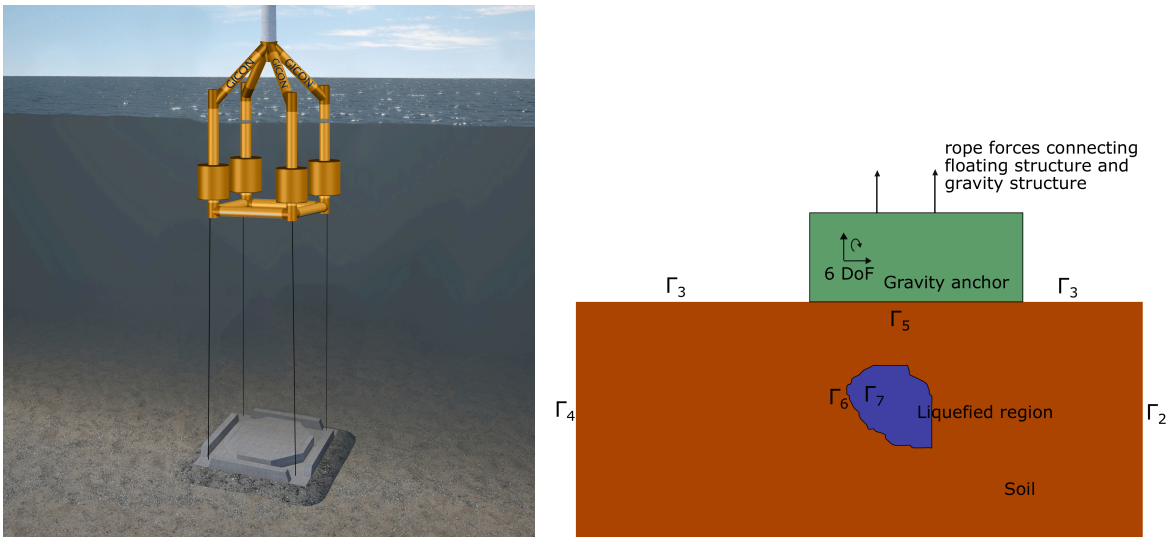
NUMERICAL MODELLING OF LIQUEFACTION AROUND MARINE STRUCTURES

RANJITH KHUMAR SHANMUGASUNDARAM[1,2], HENRIK RUSCHE[2],
CHRISTIAN WINDT[1], NILS GOSEBERG[1]
[1]*Leichtweiß–Institute for Hydraulic Engineering and Water Resources,*
Technische Universität Braunschweig, 38106 Braunschweig, Germany
[2]*WIKKI GmbH, 38855 Wernigerode, Germany*

Keywords: *Seabed liquefaction, Poro–elastic, Soil modelling, Gloating offshore wind, Gravity foundation*

Seabed liquefaction is the phenomenon by which the seabed soil loses its strength and stiffness due to applied stress and behaves as non-Newtonian fluid, which can eventually lead to severe failure of marine structures, such as buried pipelines or coastal breakwaters. For a cost–efficient and durable design of marine structures, detailed knowledge of the hydro-geotechnical processes is required. Gaining this knowledge is a challenging task due to the occurring (non–linear) wave–structure–soil interaction (WSSI).

A number of studies can found in the literature, experimentally investigating the liquefaction around marine structures [1]. In addition to experimental testing, numerical modelling of liquefaction can provide valuable insights into the prevailing WSSI. To that end, e.g. Elsafti and Oumeraci [2] or Li *et al.* [3] propose different modelling frameworks, implemented in the open source CFD toolbox OpenFOAM. However, both models omit the phase change of the soil from solid to liquid (liquefaction) and back to solid (compaction). As part of the NuLIMAS project (numerical modelling of liquefaction around marine structures), this study will present first steps towards a numerical, CFD–based, modelling tool for the analysis of seabed liquefaction around marine structures, including a more complete representation of the hydro-technical processes.



(a) 3D view

(b) Model boundary conditions

Figure 1: Artist's impression of GICON's offshore floating platform.

SHEAR STRESS CHARACTERIZATION IN THE PNEUMATIC ATOMIZATION OF BIOLOGICS USING CFD

P.LINO[1], R.C.SILVA[2]
[1]*Hovione Farmaciência SA, plino@hovione.com*
[2]*Hovione Farmaciência SA, CIEPQPF, Department of Chemical Engineering, Coimbra University, 3004-531 Coimbra, Portugal, rcesar@hovione.com*

Keywords: *atomization, biologics, pneumatic, shear stress*

In the pharmaceutical industry biologics is the fastest growing segment and one of the most challenging due to the intrinsic instable nature of protein molecules. This challenging nature is owed to their higher molecular weights and wide range of composition which results in more intricate structures than smaller conventional pharmaceuticals chemical entities. Variations in temperature, pH, light exposure, agitation, shear stress and presence of organic solvents are some of the factors potentially affecting protein denaturation or aggregation. Due to the inherently susceptibility to unfavourable physicochemical degradation solid dosage form is preferred to liquid formulation, because water molecules tend to mobilize proteins, since they are less prone to shear-related denaturation and agglomeration during manufacturing and storage [1].

Amongst drying strategies to produce solids dosage forms, spray drying, freeze drying, and spray freeze drying are frequently used to isolate proteins and improve stability [2]. Understanding the hydrodynamic flows in biologics solutions during these unit operations is paramount to minimize protein degradation and, particularly for more complex geometries such as nozzles. During atomization velocity gradients resulting from gas-liquid and liquid-rigid surfaces interactions lead to shear stress that can unfold the protein structure and subsequently aggregation and denaturation and ultimately loss of biological activity [3].

Computational Fluids Dynamics (CFD) studies were applied in this ongoing work to characterize shear stress profiles in a pneumatic or two-fluid nozzle (see Figure 1) for different atomization ratios and establish a correlation between the shear, atomization ratios and protein stability. Knowledge gathered from these studies will serve to guide scale-up of biologics spray drying processes.

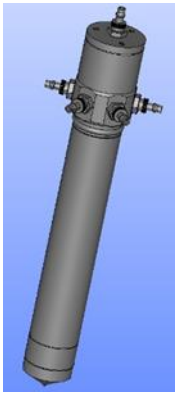


Figure 1: Pneumatic or two-fluid nozzle.]

References

[1] C. Van Der Walle, *Peptide and Protein Delivery*. .

[2] F. Emami, A. Vatanara, E. J. Park, and D. H. Na, “Drying technologies for the stability and bioavailability of biopharmaceuticals,” *Pharmaceutics*, vol. 10, no. 3, pp. 1–22, 2018, doi: 10.3390/pharmaceutics10030131.

[3] Y. A. Haggag and A. M. Faheem, “Evaluation of nano spray drying as a method for drying and formulation of therapeutic peptides and proteins,” *Front. Pharmacol.*, vol. 6, no. JUL, pp. 1–5, 2015, doi: 10.3389/fphar.2015.00140.

DEVELOPMENT OF CFD-DEM COUPLED SOLVER FOR ARBITRARILY-SHAPED PARTICLE-LADEN FLOWS

M. Šourek[1,2], M. Isoz[2,3]
[1]*Department of Chemical Engineering, UCT Prague, Czech Republic, sourekm@vscht.cz*
[2]*Department of Mathematics, UCT Prague, Czech Republic, isozm@vscht.cz*
[3]*Czech Academy of Sciences, Institute of Thermomechanics, Czech Republic*

Keywords: *CFD-DEM, OpenFOAM, HFDIB*

Computational fluid dynamics (CFD) has become a commonly used method to simulate industrial processes. However, it cannot simulate processes, such as sedimentation or fluidization, that involve freely moving larger solid particles. While new methods combining CFD and discrete element method (DEM) have been studied to overcome this constraint, they are mostly focused on spherical particles only. Here, we present a strongly coupled CFD-DEM solver capable of simulating the movement of arbitrarily-shaped particles dispersed in a fluid. The particles are assumed to be large enough to affect the fluid flow and distributed densely enough to interact with both the computational domain boundaries and with each other. The newly introduced solver is intended to simulate fully coupled particle-laden flows with individual particles spanning multiple domain discretization elements. The solid bodies are included in the computational domain via a hybrid fictitious domain-immersed boundary (HFDIB) method built based on previous works by [1], [2] and [3]. In particular, the physical movement of fluid in the solid bodiesv́icinity is enforced via a direct forcing term included in the momentum balance. The forcing term is designed to be directly incorporated into the standard PISO-like CFD algorithms and the overall solution method remains semi-implicit. The movement of individual solids inside the computational domain is described via DEM [4] with effects of environment computed from the outputs of HFDIB and with contact modeled within the framework of the soft DEM, i.e. allowing slight overlaps between different particles.

Computational methods

In case of a body $\mathcal{B}$ freely moving inside the computational domain, the computational cost of frequent remeshing makes standard methods of computational fluid dynamics, in which the computational mesh conforms to the shape and position of the solids, impractical. An alternative is to include the solid bodies in the computational domain fictitiously by modifying terms in the flow governing equations. In general, we are interested in solving balance equations for momentum and mass in a finite open and simply connected domain $\Omega \subset \mathbb{R}^3$ with boundary $\Gamma = \partial\Omega$. Let Ω be split as $\Omega = \Omega_\mathrm{s} \cup \Omega_\mathrm{f} \cup \Gamma_\mathrm{sf}$, where Ω_s represents the part of Ω occupied by a solid phase, Ω_f the part of Ω occupied by the fluid and $\Gamma_\mathrm{sf} = \partial\Omega_\mathrm{s} = \partial\Omega_\mathrm{f}$ is the solid-fluid interface in Ω. In particular, the considered flow governing equations correspond to the standard variant of laminar Navier-Stokes equations for an incompressible Newtonian fluid with added forcing term $\boldsymbol{s}$,

$$\begin{matrix}\mathcal{M}(\boldsymbol{u}) = -\nabla\tilde{p} + \boldsymbol{g} + \boldsymbol{s} \\ \nabla\cdot\boldsymbol{u} = 0\end{matrix}, \quad \mathcal{M}(\boldsymbol{u}) = \frac{\partial\boldsymbol{u}}{\partial t} + \nabla\cdot(\boldsymbol{u}\otimes\boldsymbol{u}) - \nabla\cdot(\nu\nabla\boldsymbol{u}) \tag{1}$$

where $\boldsymbol{u}$ is the fluid velocity, ν kinematic viscosity, $\tilde{p}$ kinematic pressure and $\boldsymbol{g}$ the gravitational acceleration. The forcing term $\boldsymbol{s}$ is constructed in such a way that it generates a fictitious representation of Ω_s inside Ω. It is based on and indicator field λ and defined as

$$\boldsymbol{s} = \mathrm{ceil}\,(\lambda)\tilde{\boldsymbol{s}}\,, \quad \tilde{\boldsymbol{s}} = \mathcal{M}(\boldsymbol{u}_\mathrm{ib}) + \nabla\tilde{p} - \boldsymbol{g}\,, \quad \lambda = \begin{cases} 0 & \text{in} \quad \Omega_\mathrm{f} \\ 1 & \text{in} \quad \Omega_\mathrm{s} \\ \tilde{\lambda}\in(0,1) & \text{in} \quad \Gamma_\mathrm{sf} \end{cases} \tag{2}$$

where $\boldsymbol{u}_\mathrm{ib}$ is the velocity imposed in $\mathcal{B}$. The imposed velocity $\boldsymbol{u}_\mathrm{ib}$ needs to be prescribed such that the prescribed velocity boundary condition is fulfilled on $\Gamma_\mathrm{sf}^{\mathcal{B}}$.

Solid body movement

The solids are included into Ω as described in the previous section. The present section deals with the remaining feature necessary to simulate the flow-induced motion of a dispersed solid phase i.e. updating Ω_s. The commonly used method

A MULTIPHYSICS OBJECT-ORIENTED SOLVER FOR FLUID-STRUCTURE-THERMAL INTERACTION SIMULATIONS

Gabriel St-Onge[1], Mathieu Olivier[2],
[1]*Departement of Mechanical Engineering, Université Laval, gabriel.st-onge.1@ulaval.ca*
[2]*Departement of Mechanical Engineering, Université Laval, mathieu.olivier@gmc.ulaval.ca*

Keywords: *multiphysics solver, fluid-structure interaction, fluid-solid-thermal interaction, interface coupling, strongly coupled schemes*

Introduction

Through the years, multiple solvers have been developed in the OpenFOAM framework to resolve different types of problems in specific fields. However, in some cases, multiphysics interactions between different regions cannot be ignored. In such scenarios, new solvers need to be implemented to account for these interactions. An example of the need to combine multiple solvers is fluid-structure interaction problems. This type of problem is encountered in numerous areas such as engineering or life sciences and involves the coupled solution of the fluid and solid fields. Coupling multiple solvers can be done in two ways: with a loosely coupled scheme or with a tightly coupled scheme. In loosely coupled schemes, fields are solved sequentially and the interaction is treated explicitly, which may break the formal accuracy of implicit schemes. Also, loosely coupled schemes can introduce latency between fluid and solid fields [1] or even produce instability. With tightly coupled schemes, the interaction is computed in a way that ensures the consistency of the time marching scheme at every time steps. These schemes can be implemented through a monolithic or a partitioned approach. The partitioned approach offers a few advantages in the development of a generalized approach since it uses other solvers as black boxes and it is easier to generalize than a monolithic approach. This paper presents a multiphysics framework implemented in OpenFOAM that introduces a coupled scheme based on the partitioned approach to simulate interactions between multiple physics regions. The proposed framework introduces a time-marching procedure in which an iterative outer loop is implemented. The framework also allows easy selection of field-specific solvers and allows strongly coupled fields to be handled through specifically designed interface boundary conditions. Two test cases illustrating the capabilities of this multiphysics solver are briefly presented.

Methodology

The implemented partitioned approach allows physics solvers to be used as black boxes. Since individual solvers are independent of the coupling algorithm, interface boundary conditions are needed to compute the transfer of physical quantities from one region to another. To generalize their implementation and their usage, each physics solver is inherited from the same base class. All fields object and other parameters needed for the simulation of a given region are imbedded in these solver classes. Even if each physical solver may use different algorithmic procedure, the solution process can generally be decomposed in the following steps: solver construction, fields creation and initialization, and time loop operations. The latter includes a pre-solution step, the solution procedure itself as well as convergence verification, and a post-solution step. All these steps are transposed as class methods in the base solver class. This allows the main solver application to manage all solver objects the same way without regard for their physics particularities. The whole partitioned approach is summarized in the algorithm 1. The outer loop executed within each time step ensures the consistency of implicit schemes in all regions upon convergence. The role of the main application is thus to initialize and execute solver objects that are created at run time. Every physical domain is identified as a region which is then associated with a specific user-defined physical solver that includes its own specific fields. Although, the computation process is managed by the main solver application, the interaction between fields is done with boundary conditions. In fluid-structure interaction, Dirichlet-Neumann partitioning is used, that is, a Dirichlet condition is applied to the fluid-solid interface on the fluid side whereas a Neumann condition is applied on the solid side. Boundary conditions interact with region specific fields and, thanks to the modular structure of OpenFOAM, a given interface boundary condition class can be used with more than one physical solver.

Tests cases

The multiphysics solver has been used on several occasions to study the propulsive performance of a flexible flapping plate [2], to study the effect of blade flexibility in energy extraction devices [3], or to assess the performance of the partitioned method

UNSUPERVISED LEARNING OF NUMERICAL SOLUTION IN LINEAR ELASTIC SOLVER

EMAD TANDIS[1,2,3], MICHAEL CLANCY[1,2,3], PHILIP CARDIFF[1,2,3]
[1] *School of Mechanical and Materials Engineering, University College Dublin, Ireland,*
[2]*Bekaert University Technology Centre, School of Mechanical and Materials Engineering, University College Dublin, Ireland*
[3]*SFI I-Form Centre, University College Dublin, Ireland*
emad.tandis@ucd.ie, philip.cardiff@ucd.ie

Keywords: *Machine learning, unsupervised learning, linear elasticity, TensorFlow.*

Recent advances in machine learning techniques have led to significant progress across many scientific disciplines. In the area of computational continuum mechanics, however, machine learning is in its early stages and its full potential is yet to be fully realised in practical simulations. Reviewing the literature reveals that studies in this area can be categorised into two classes: boosting performance of available solvers via incorporating machine learning techniques as a sub-module (DL-enhanced solvers) [1] or network architectures that use prior knowledge of the physical model (model-aware network). As an example of the first approach, some studies aimed to facilitate linking between available software in computational methods and machine learning, e.g. OpenFOAM and TensorFlow [2].

Leveraging the prior knowledge of the physics across machine learning techniques has recently led to the smart design of network architectures which are capable of accomplishing tasks such as data-driven solution and data-driven discovery in the field of physical modeling. Among the works in this context, Physics Informed Deep Learning [3-6], PDE-Net and FEA-Net [7], model-aware autoencoder [8] and many other integrating techniques have been presented as a surrogate for conventional computational algorithms.

The objective of this study is to leverage computational capabilities in OpenFOAM [9] to present an unsupervised machine learning algorithm which is capable of learning physical disciplines across computational domains without requiring prior training solutions. More specifically and for the proof of the concept, we limit this study to linear elastic solid mechanics problems and focus on developing linear operation techniques to define foam-based gradient and divergence operations as a symbolic function of the displacement in TensorFlow. This, consequently, allows for a finite volume-based residual of the momentum equation to be used as a symbolic function within the output of the network. Compared to a numerical approach, a symbolic definition of the loss function conveniently allows the use of automatic differentiation during the back-propagation step [10] which is core component of TensorFlow optimisations procedures. Fig. 1 illustrates the role of linear operation in the network:

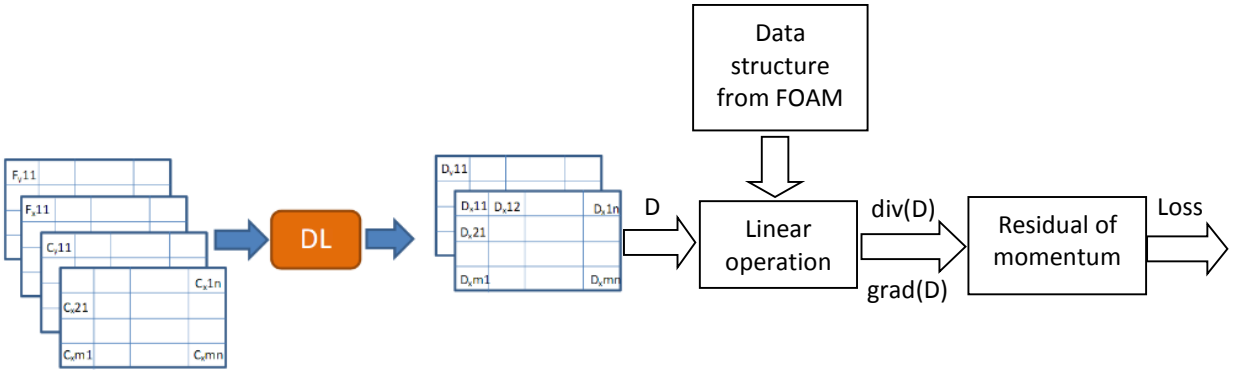


Figure 1: Schematic of the network and loss evaluation

This architecture, unlike in supervised learning, does not require ground-truth data for the sake of training; instead, the physics-based loss function is employed for the backpropagation training procedure. The trained model, then, can be potentially used as surrogate for the linear elastic solvers, especially, when solution of large numbers of cases within a specific parameter space is a desired. Alternatively, the trained model can be employed as an initialiser, or predictor, for the available solvers in OpenFOAM.

Figure 1 demonstrates a qualitative comparison between the results of a prediction by one such network - with 258 K weights and trained on 150 samples - for an unseen specific case with that of OpenFOAM solver.

A dynamic load balancing model with analytical Jacobian for fast combustion simulations in OpenFOAM

BULUT TEKGÜL[1], HEIKKI KAHILA[2], PETTERI PELTONEN[1], MAHMOUD GADALLA[1], OSSI KAARIO[1], VILLE VUORINEN[1]

[1]*Department of Mechanical Engineering, Aalto University School of Engineering, Otakaari 4, 02150 Espoo, Finland, bulut.tekgul@aalto.fi*

[2]*Wärtsilä Finland Oy, Vaasa FI-65101, Finland*

Keywords: *Reacting flows, Combustion, Load balancing, Jacobian*

Direct-integration of chemical kinetics within a reasonable computing time in reactive Computational Fluid Dynamics (CFD) simulations is essential for obtaining fast and accurate results. In finite-rate chemistry, the chemistry problem is treated as a stiff system of ordinary differential equations (ODE) in each computational cell. Due to the operator splitting procedure commonly applied in most reactive CFD solvers (including OpenFOAM), the chemistry in each cell can be treated as an independent problem, making the chemistry problem *embarrassingly parallel*.

Due to the non-linear characteristics of the stiff chemical kinetics, a computational load imbalance may occur in parallel reactive simulations where one or more processes create a bottleneck and increase the simulation time. Using the easy parallelization feature of the chemistry problem, we introduce a novel chemistry model called `DLBFoam` [1] in OpenFOAM to mitigate this imbalance issue. Our novel model restructures the chemistry solution process starting from the computational cell by improving the ODE solver performance and treating the stiff problem more adequately, up to utilizing a dynamic load balancing technique using Message Passing Interface (MPI) routines to mitigate the load imbalance across processes.

First, the chemistry solution in a single computational cell is improved by utilizing a third-party open-source library `pyJac` [2] to replace the standard OpenFOAM's reaction rate and Jacobian calculation. In addition, the ODE solvers of OpenFOAM are improved by using utilizing the well-known `LAPACK` linear algebra library, suitable for dense matrices, in particular for LU decomposition and back-substitution routines required during many implicit ODE solvers provided by OpenFOAM. These changes provide at least an order of magnitude speedup in a single computational cell, depending on the thermochemical state and ODE solver tolerance. Figure 1 demonstrates the effect of utilizing `pyJac` and `LAPACK` on computational performance. It can be seen that utilizing these models reduces the execution time, especially with tighter ODE tolerances (increased accuracy).

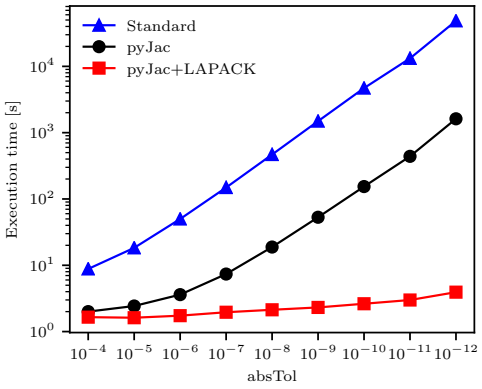


Figure 1: Mean execution time of a 0D chemistry problem involving CH4 oxidation for different ODE convergence tolerance values using OpenFOAM.

Second, a dynamic load balancing model is introduced to balance the computational load of chemistry across processes in multi-processor simulations. In addition, a zonal reference mapping model is presented to map the solution of inactive regions with no fuel present from a computed reference solution. Figure 2 shows the execution time in each processor for Standard

Initialization of volume fractions and signed distances on unstructured meshes from triangulated surfaces

TOBIAS TOLLE[1], DIRK GRÜNDING[2], DIETER BOTHE[3], TOMISLAV MARIĆ[4]
[1]*Mathematical Modeling and Analysis, TU Darmstadt, tolle@mma.tu-darmstadt.de*
[2]*Mathematical Modeling and Analysis, TU Darmstadt, gruending@mma.tu-darmstadt.de*
[3]*Mathematical Modeling and Analysis, TU Darmstadt, bothe@mma.tu-darmstadt.de*
[4]*Mathematical Modeling and Analysis, TU Darmstadt, maric@mma.tu-darmstadt.de*

Keywords: *volume of fluid, triangular surface mesh, signed distances, unstructured mesh*

The Volume-of-Fluid method is a widely used approach for the treatment of multiphase flows and employed in many CFD codes, e.g. Basilisk [1] or the interIsoFoam solver of the OpenFOAM® framework [2]. A crucial prerequisite for meaningful simulation results are accurate initial conditions of the problem at hand. In the case of multiphase flows the initial volume fractions that correspond to the initial interface position, in particular, can be complicated to compute. A variety of different approaches have been proposed in the literature for initialization of volume fractions, e.g. [3, 4]. While the available methods yield very accurate results, to our knowledge they all share a common limitation, namely the requirement for an analytical interface description. However, such a description cannot always be found, especially for more complex interface configurations, e.g. from experimental measurements.

For this purpose, we have developed a novel method that initializes volume fractions from triangulated surfaces, e.g. from an STL file. It is applicable to structured and unstructured meshes with arbitrary cell shapes. Only a consistent triangle normal orientation is required for the triangulated surface. As our method also computes a signed distance field as an intermediate step, it is also possible to initialize signed distances of arbitrary shaped surfaces for the Level Set method.

Our approach utilizes an octree-based search to compute the signed distance between different cell points and the triangular surface mesh. Restricting this computation to a narrow band of user-prescribed thickness around the interface reduces computational complexity. Normals computed at the vertices of the surface mesh are used to robustly determine on which side of the surface points of the volume mesh are located. Based on the signed distance at cell centres and cell corner-points, cells intersected by the surface mesh are identified. For those cells, the volume fraction is calculated either by means of geometrical intersection or by a polynomial approximation in combination with mesh refinement. Volume fractions for the bulk cells are set according to their signed distance. Figure 1 shows a triangular surface (left) and the corresponding volume fractions (right). These results have been obtained with an implementation of our method based on the OpenFOAM® framework. The

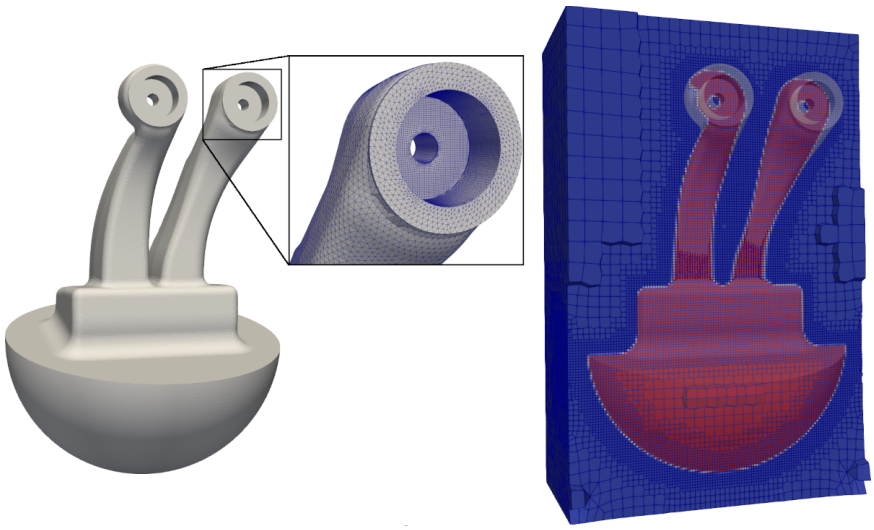


Figure 1: Volume fractions (right) initialized from a triangular surface mesh representing an interface (left).

NUMERICAL INVESTIGATION OF THE TURBULENT FLOW FIELD IN CONFINED IMPINGING JETS

MARIO TOMÉ[1], A. S. CAVADAS[1,2]
[1, 2]*ProMetheus – Escola Superior de Tecnologia e Gestão, Instituto Politécnico de Viana do Castelo, Rua Escola Industrial e Comercial de Nun'Álvares, 4900-347, Viana do Castelo, Portugal,*
[1]*mariotome@estg.ipvc.pt*
[2]*CEFT- Centro de Estudos e Fenómenos de Transporte – Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias s/n, 4200-465 Porto, Portugal, adelioc@estg.ipvc.pt*

Keywords: *Impinging jets, separated flow, Turbulent flow, rectangular duct flow*

High velocity impinging jets are frequently used in industry to cool metals and process food and pharmaceutical products because of the large increases in heat and mass transfer that they promote near the impact surface. The jet may or may not be confined. In this work, a numerical investigation is reported on the isothermal turbulent flow characteristics in a three-dimensional cell. The cell test section is schematically represented in Fig.1. The numerical results are compared with the experimental data for turbulent regime [1] and with the experimental data and numerical data for laminar regime [2].

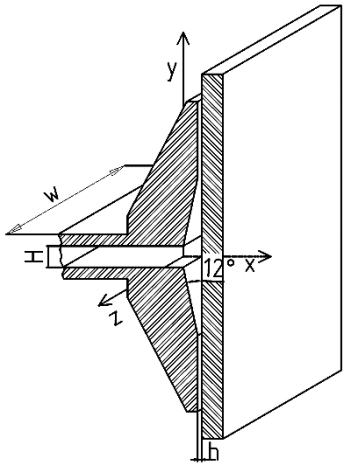


Figure 1: Cell test section

The approach flow is a symmetric fully-developed flow in a rectangular channel of aspect-ratio of 13, that impacts onto a perpendicular wall. The plates opposite the wall are inclined at 12°, thus confining the ensuing wall jets to flow through nozzles before the thin constant width exit channels. The flow is symmetric in the whole geometry and the Reynolds number in the inlet channel was 13750. The 3D numerical calculations were carried out using the OpenFoam software [3]. Preliminary wall-to-wall calculations confirmed that the flow was symmetric relative to the x-y and x-z center planes and consequently the bulk of the numerical simulations were carried out using a computational domain equal to half the physical domain. Near the plane slopping wall there is separated flow that was observed in visualizations studies. Figure 2. Shows vector plots and streamlines of the flow inside the cell.

Modelling woth is based in RANS standard k-epsilon with both OpenFOAM 8.0 and Fluent 21R1 and results are compared and discussed against measured components on the experimental work. Further, some remarks comparing the two tools, from the user view are given.

CFD SIMULATION OF OFF-DESIGN OPERATING POINTS OF A CENTRIFUGAL COMPRESSOR

MATEJ ČORAK[1], TESSA UROIĆ[2], HRVOJE JASAK[3],
[1]*Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Croatia, matej.corak@gmail.com*
[2]*Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Croatia, tessa.uroic@fsb.hr*
[3]*Faculty of Mechanical Engineering and Naval Architecture, University of Zagreb, Croatia, hrvoje.jasak@fsb.hr*

Keywords: *turbomachinery, centrifugal compressor, foam-extend*

CFD simulations of turbomachinery are now a part of the standard approach in the design process. However, CFD as an investigation tool in the later stages of the design process, namely to investigate off–design operating points and fluid flow instabilities are rarely used. The main objective of this work is to investigate the applicability of CFD software, i.e. open–source library `foam-extend` to predict the flow field corresponding to off-design operating conditions of a centrifugal compressor. Since a full rotor geometry is challenging to model due to the size of the computational mesh, we decided to investigate performing the simulations on a single blade passage using cyclic boundary conditions for non–conforming meshes (Generalised Grid Interface – GGI). The mesh is block–structured, created in Pointwise with 7.2 million cells, Fig. 1. A Multiple Reference Frame approach is used to which means that the obtained flow field corresponds to a single rotor position. Start–up of the simulation if very sensitive due to the extreme operating conditions of the nominal operating–point, and it is necessary to change the boundary conditions gradually. Thus, the total pressure ratios and MRF angular velocity are increased progressively to prevent the simulation from crashing due to local extreme velocities and pressure values. To validate the simulation approach, a comparison is made to experimental and numerical data provided in the paper [1]. The final objective is to create a compressor map with the established flow field features corresponding to different operating points, some close surge and choke conditions.

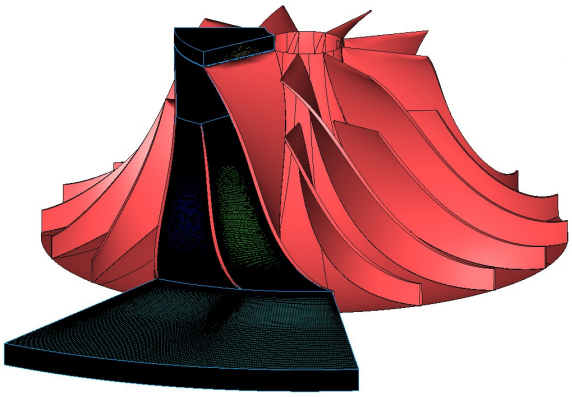


Figure 1: Computational mesh of a single blade passage of a centrifugal compressor.

References

[1] B. Dewar, J. Tiainen, A. Jaatinen-Värri, M. Creamer, M. Dotcheva, J. Radulovic, and J. M. Buick, "Cfd modelling of a centrifugal compressor with experimental validation through radial diffuser static pressure measurement," *International Journal of Rotating Machinery*, vol. 2019, 2019.

NUMERICAL INVESTIGATION OF BREAKING AND BROKEN REGULAR WAVE FORCES ON A SHOAL-MOUNTED CYLINDER

JAN VAN GORSEL[1], AKSHAY PATIL[2], JEREMY BRICKER[1], STUART PEARSON[1], ALISSON RABY[3], DARSHANA DASSANAYAKE[4], ALESSANDRO ANTONINI[1]

[1]*Faculty of Civil Engineering and Geosciences Delft University of Technology, jan_v_gorsel@outlook.com, J.D.Bricker@tudelft.nl, S.G.Pearson@tudelft.nl, A.Antonini@tudelft.nl*

[2]*Stanford University, alpatil@stanford.edu*

[3]*University of Plymouth, alison.raby@plymouth.ac.uk*

[4]*University of Sri Jayewardenepura, darshana.dassanayake@sjp.ac.lk*

Keywords: *STORMLAMP, Wave-impact, isoAdvector, RANS*

INTRODUCTION

Shoal-mounted cylindrical structures such as lighthouses assist in the navigation of vessels, and act as warning systems. Many of these iconic lighthouses are continuously subjected to extreme sea-wave action, made acute by the effects of climate change [1], [2]. Studying the complex hydrodynamic loads acting on such structures surrounded by rocks or emerged shoals can provide valuable insights for addressing their structural integrity, and how much longer these heritage structures can withstand such harsh environments. In this work, the effectiveness of a finite volume-based numerical framework to predict wave loads on such structures is assessed. The proposed numerical investigation is supplemented by the STORMLAMP (STructural behaviour Of Rock Mounted Lighthouses At the Mercy of imPulsive waves) project's experimental data [3] that has been used as a benchmark case to validate the proposed computational framework.

METHODS

The numerical wave tank (NWT) consists of the finite volume framework OpenFOAM® and the waves2Foam toolbox [4]. The recently developed Volume of Fluid (VOF) based isoAdvector algorithm [5] is used to model the multiphase nature of the flow and resolve the sharp discontinuities in the propagation of broken waves. Additionally, to limit the over-production of turbulent kinetic energy (TKE) under breaking waves, the stabilization closure developed by [6] was preferred. To reduce the computational cost and maintain the nonlinear nature of the shallow water waves, the numerical domain consists of an NWT coupled to a nonlinear potential wave model (i.e., OceanWave3D, [7]) as demonstrated by [8] and [9]; this coupled NWT can be seen in Figure 1. The computational grid is generated using snappyHexMesh for both the 2D and 3D NWT. The preliminary 2D model - without the cylindrical structure - is used for the mesh sensitivity analysis and compared to the water surface elevation of the experimental data for validation. The validation indicates that a numerical grid characterized by 15 cells per wave height and an aspect ratio of 1 is sufficient to properly resolve the wave kinematics and therefore the same grid set-up is also applied for the 3D model. Given the 3D NWT's symmetric nature, a symmetry boundary condition along the centre of the domain is applied while the lateral domain walls are modelled through a slip boundary condition, and the bottom boundary is modelled by a wall function prescribed rough no-slip wall.

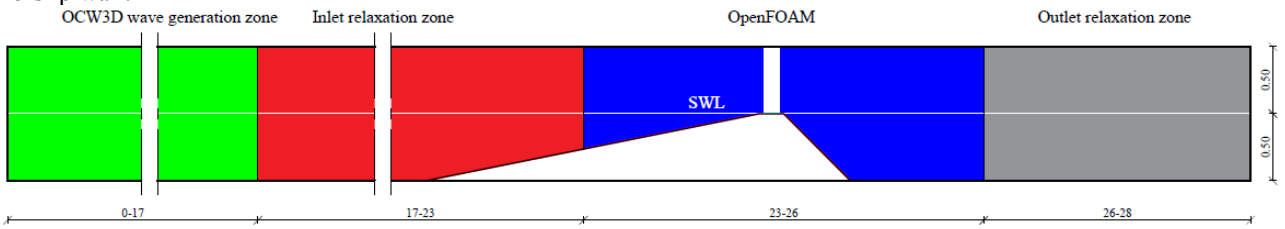


Figure 1: Schematization of the numerical domain used in this investigation indicating the different parts in streamwise direction (in meters) in the NWT. The white horizontal line represents the still water level in the NWT.

RESULTS

The comparison of the 2D numerical surface elevation against the experimental results show good agreement, with a minimum Pearson Correlation Coefficient (PCC) of 0.8 for the time-series analysis and a maximum value of 1 for the ensemble-averaged surface elevation. The surface elevation analysis is complemented with the Root Mean Square Error (RMSE) normalized by the local mean wave height, and shows a maximum value of 0.30, suggesting good agreement in the frequency domain (see Figure 2a). Comparison of the ensemble averaged surface elevation in the time-domain can be seen in Figure 2b, which shows satisfactory agreement between the two datasets. Figure 2c presents the numerical ensemble-averaged force time series compared with the experimental results, in which the ensemble means, and enveloping (1 standard deviation) error bands have been aligned considering the mean peak value and are normalised with the experiment peak value. Figure 2c confirms that the proposed NWT set-up can predict not only the surface

NUMERICAL SIMULATION OF HYDROGEN INJECTION IN HIGH-SPEED CROSSFLOW

ASHISH VASHISHTHA [1,*], DEAN CALLAGHAN [2], CATHAL NOLAN [1],
[1]*Department of Aerospace, Mechanical and Electronics Engineering, Institute of Technology Carlow, IRELAND*
[2]*The Centre for Research and Enterprise in Engineering (engCORE), Institute of Technology Carlow, IRELAND*
[*]*Corresponding author:ashish.vashishtha@itcarlow.ie*

Keywords: *Hydrogen, Jet-in-Crossflow, shock induced combustion, detonation, ddtFoam*

Extended Abstract

Shockwaves can be defined as a compression wave front in front of any object, flying at the local speed more than the speed of sound. Shockwaves can cause jump in flow properties across it, especially jump in pressure and temperature. The rise in temperature across the shock can be utilized for igniting fuel air mixture in air-breathing hypersonic propulsion applications. Further, the shock induced ignited fuel-air mixture may turn into detonation combustion and produce detonation wave at a given appropriate local flow conditions and fuel air mixture composition. Detonation wave differs than deflagration wave as it travels at supersonic speed and pressure and temperature can have higher jump across it [1]. The deflagration wave travels at subsonic speeds and pressure remains almost constant across, only temperature increases across flame. There are few hypersonic propulsion concepts [2] based on detonation combustion (or pressure gain combustion), which have been extensively studied by many researchers in past decades: pulse detonation engine (PDE), oblique detonation wave engine (shock induced combustion ramjet or schramjet) and rotatory detonation engine (RDE). The advantages of detonation based propulsion systems are: it can provide higher rate of energy release, higher thermodynamic efficiency as well as shorter combustion chamber in comparison to conventional deflagration combustion based systems. Among above three, pulse detonation engine has been initially studied extensively and it was found to have operational constraints because of the requirements of: long tubes for detonation transition, ignition source in each cycle and purging of combustion products in each cycle, which leads to lower frequency (few hundreds Hz) operation. The Oblique detonation wave engine has simplest design and can be easily integrated in scramjet engine configuration. It requires a wedge in supersonic premixed stream of fuel-air mixture, which can establish a compression wave as oblique shock wave. Sufficient strength of oblique shock (can be controlled by wedge angle) can ignite fuel-air mixture and may turn it in standing or propagating detonation wave, which can be further accelerated through the nozzle. However, understanding of shock induced combustion and transition to oblique detonation waves, required detailed understanding of affecting operating parameters. The rotary detonation engine (RDE) has annular cylindrical domain, which is advantageous than the PDE as it requires ignition only once and can operate at higher frequencies of the order of 1000s Hz. In RDE, the premixed fuel-air mixture is ignited once and the detonation wave travels in circumferential manner until all the fuel-air mixture is burnt. Initial design, development of the above pressure gain combustion systems are mainly based on premixed fuel-air mixture, a physical ignition source such as spark plug, pre-detonator or shock induced combustion can be very much effective in premixed systems. However, there have been recent interest in non-premixed systems also, due to operational constraints of providing quick premixed mixture during the future long-term operation of such systems. The current study is motivated to develop understanding of fuel jet ignition by direct injection in crossflow of supersonic or hypersonic freestream. The two-dimensional numerical simulations are performed by using ddtFOAM solver at OpenFOAM platform [3].

The ddtFoam solver have been developed by Etter et al. [4], to study 2-D deflagration to detonation transition in obstacle laden tube for hydrogen-air mixture. It utilizes density based solver,approximate Riemann solver using HLLC scheme for solving convective fluxes. The reaction mechanism of hydrogen air combustion is modeled as O'Conaire reaction scheme [5] the deflagration and detonation combustion source terms in transport equation of reaction progress variable are evaluated using two look-up tables: reaction product using mechanism in Cantera [6] and autoignition time delay using Cantera and EDL Toolbox [7]. The Weller model [8] have been used for deflagration combustion modeling and detonation is modeled using autoignition delay time. This study aims to further utilize the ddtFoam solver to study the shock induced ignition mechanism for direct injection of hydrogen in supersonic and hypersonic freestream in crossflow manner. Hydrogen is injected at sonic speeds in supersonic or hypersonic freestream, leads to formation of the bow shock as shown in Fig. 1a. The injected fuel in compressed region mixes with the incoming air. If there is sufficient compression provided by the bow shock, it can raise the

A PRESSURE-BASED COMPRESSIBLE MULTIPHASE CAVITATION SOLVER IN THE OPENFOAM FRAMEWORK

CHANGCHANG WANG[1], GUOYU WANG[1], BIAO HUANG[1]
[1]*School of Mechanical Engineering, Beijing Institute of Technology, Beijing, 100081, China,*
wangchangchang@bit.edu.cn

Keywords: *3 Cavitation; pressure-based solver; OpenFOAM; compressibility*

Due to their significant impact on noise, vibrations and erosion in practical engineering applications, investigation of cavitation has received increasing attention [1], [2]. However, to the best of our knowledge, there is very limited understanding on the compressibility effects in turbulent cavitating flows, in spite of the extensive work on bubble dynamics in compressible liquids where the bubble-wall velocity could be comparable to the velocity of sound in the surrounding liquid [3]. Knowledge of compressibility effects is important for the understanding of bubble dynamics and cavitation instabilities, especially in the process of bubble/cavity collapse. Experimental and theoretical work have proved that cavitating flows experience a significant reduction in sonic speed [4]-[6], the value of which is far lower than that of its constituents, i.e., pure liquid and pure vapor, and increase in fluid comparability. We develop a pressure-based finite-volume method compressible multiphase cavitation solver [8] for turbulent cavitating flows to address the compressibility effects turbulent cavitating flows using a Computational Fluid Dynamics (CFD) tool.

The numerical development and simulation were conducted in the OpenFOAM framework [9]. The governing equations of the present compressible multiphase cavitation solver include continuity equation, momentum equation and energy equation along with a transport equation for the volume fraction.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho U) = 0 \tag{1}$$

$$\frac{\partial \rho U}{\partial t} + \nabla \cdot (\rho UU) = -\nabla p + \nabla \cdot \mathbf{T} + \sigma_S \kappa \nabla \alpha_l \tag{2}$$

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho Ue) + \frac{\partial \rho K}{\partial t} + \nabla \cdot (\rho UK) = \nabla \cdot \mathrm{q} - \nabla \cdot (pU) \tag{3}$$

$$\frac{\partial \rho \alpha_v}{\partial t} + \nabla \cdot (\rho \alpha_v U) = \dot{m}^+ + \dot{m}^- \tag{4}$$

where ρ, U, p, and α_v are the density, velocity vector, pressure, temperature and vapor volume fraction, respectively. $\mathbf{T}$, σ_S, μ, κ, q, e, K (K=0.5$|U|^2$) and q are the stress tensor, surface tension, dynamic viscosity, interface curvature, heat flux density, internal energy and kinematic energy, respectively. The terms "$\dot{m}^+$" and "$\dot{m}^-$" on the right-hand side of Eq. (4) are the cavitation source terms which represents the evaporation rate and condensation rate in cavitating flows which is modelled using Saito's method. More details can be found in [8]. The hybrid SST-SAS (Scale Adaptive Simulation) turbulence model is used to model turbulence effects. The thermodynamic closure relations including Tait equation of state for pure liquid and ideal gas equation of state for pure vapor are used.

$$\frac{p_l + B}{p_{l,sat} + B} = \left(\frac{\rho_l}{\rho_{l,sat}}\right)^N \tag{5}$$

$$p_v = \rho_v R_v T_v \tag{6}$$

where parameters are B=3.06 ×10^8 Pa, N=7.1 and R_v= 461.6 J/(kg.K). The saturated water density in Eq. (5) is taken to be constant as $\rho_{l,sat}$=998.16 kg/(m^3) at T=293.16 K. The compressibility ψ_l and ψ_v is computed as follows

$$\psi_l = \frac{d\rho_l}{dp} = \frac{\rho_l}{(\rho_l/\rho_{l.sat})^N N(p_{l,sat}+B)} \tag{7}$$

$$\psi_v = \frac{d\rho_s}{dp} = \frac{1}{R_g T} \tag{8}$$

The time-dependent vapor saturated pressure is used as

$$p_v = p_c exp\left[\left(\frac{T_c}{T}\right)\sum_1^6 -7.85823\theta + 1.83991\theta^{1.5} - 11.7811\theta^3 + 22.6705\theta^{3.5} - 15.9393\theta^4 + 1.77516\theta^{7.5}\right] \tag{9}$$

with θ=1-T/T_c. The subscript "c" denotes parameters at critical condition. For water, T_c=647.14 K. The SIMPLE algorithm is used for the pressure-velocity coupling. The second-order upwind scheme was used for convective terms and the Gauss-linear second order approach for the diffusion terms. The nonorthogonality correction is applied for the gradients, and a strictly bounded scheme with the second order differencing scheme for the void fraction transport equation. The pressure and velocity residual convergence criterion in each iteration is set small enough equal to 10^{-12}.

Numerical results are presented for the cloud cavitating flows around a NACA66(mod) hydrofoil [10]. Experiment study has been conducted by Leroux et al. [10] and more details about the experiment data can be found in [10]. According to the experiment, cavity cloud collapse is observed to influence the sheet/cloud cavitation evolution frequency accompanying with large pressure magnitude. A cavity shorten phenomenon in certain stage of cavity period which is associated with cavity cloud collapse was observed under the flow conditions of α=6° and σ=1.25. The same

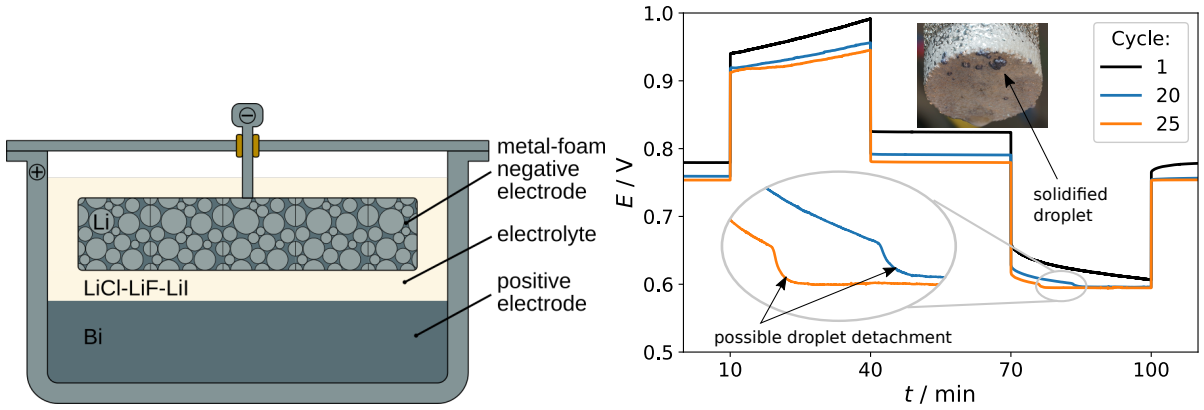
LOCAL SHORT CIRCUITS IN LIQUID METAL BATTERIES – INFLUENCE OF THE CONTACT ANGLE ON THE DROPLET MOVEMENT IN VOF-SIMULATIONS

SABRINA BENARD[1], STEFFEN LANDGRAF[2], NORBERT WEBER[2], TOM WEIER[2]
[1]*LIMSI, CNRS, Bât 508, rue John von Neumann, Campus Universitaire, F-91405 Orsay, France*
[2]*Helmholtz-Zentrum Dresden – Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany*

Keywords: *volume-of-fluid, contact angle, battery, multiphase, magnetohydrodynamics, electrochemistry*

1 Motivation

Liquid metal batteries (LMBs) are discussed as cheap stationary energy storage for wind and solar energy [1]. Li||Bi LMBs consist of a molten Bi-cathode on the bottom and a molten salt electrolyte. The anode material, liquid Li, is contained in a metal foam – as illustrated in fig. 1(a).
While during discharge Li is transferred through the electrolyte into the Bi-electrode, this process is reversed upon charge. Then, Li is transported from the alloy back into the foam-electrode. Due to chemical reactions it might happen that the Li does not wet the foam any more, finally forming Li-droplets below of the foam. If these droplet grow too much, this might lead to localised short circuits, as observed in fig. 1(b) [2].



(a) (b)

Figure 1: Setup of a Li||Bi liquid metal battery (a) and voltage-drop-offs and intermetallic phases formed due to localised short circuits (b).

2 Numerical simulation

The aim of the presentation is to give an overview about Li-droplet formation, their detachment and transport, which finally might lead to a localised short circuit of the battery.
A multiphase model, based on *multiphaseInterFoam* is implemented in OpenFOAM. It includes surface tension and buoyancy as stabilising forces. The droplet detachment is mainly caused by the Lorentz force, which is induced by the battery current. In order to study the interaction of these different forces, the electric potential, current distribution as well as the resulting magnetic field are all modelled using a multi-mesh approach [3]. Special attention is given to an accurate contact angle modelling, as this is essential for correctly describing the detachment of the droplet. Finally, the model is carefully validated using an analytical solution for a stationary droplet shape – as illustrated in fig. 2.

OPEN-SOURCE PEM FUEL CELL MODEL COMBINING THE UNSATURATED FLOW THEORY FOR POROUS MEDIA WITH SPRINGER'S MODEL

NORBERT WEBER[1], LEON KNÜPFER[2],
SHIDONG ZHANG[3], UWE REIMER[3], STEVEN BEALE[3],
ANTONIO M. CHAPARRO[4], PALOMA FERREIRA-APARICIO[4]
[1]*Helmholtz-Zentrum Dresden – Rossendorf, Germany*
[2]*Technische Universität Dresden, Germany*
[3]*Forschungszentrum Jülich, Germany*
[4]*CIEMAT, Spain*

Keywords: *fuel cell, two-phase transport, multiphysics, electrochemistry*

1 Motivation

Proton-exchange membrane (PEM) fuel cells consist of two flow plates with adjacent porous electrodes, which are separated by an ion conducting membrane – as illustrated in Fig. 1. Producing green electricity from oxygen and hydrogen, such cells will make their contribution towards a decarbonised future. Since the seminal paper of Springer [1], hundreds of different fuel cell models have seen the light of day. As most of them are implemented as proprietary code, or in costly commercial software, a comparison, reuse or extension by other researchers is very limited or even impossible [2]. The motivation of this work is therefore the development of an open-source PEM fuel cell model within the framework of OpenFOAM.

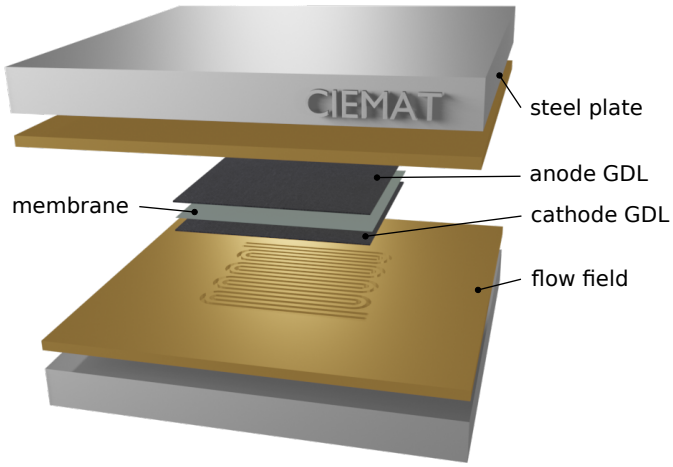


Figure 1: PEM fuel cell operated at CIEMAT as used for this study [3]. The flow fields are gold-covered, containing two 1x1 mm gas channels each.

2 Simulation model & results

The PEM fuel cell model is based on the existing OpenFOAM code "openFuelCell", which has originally been implemented for simulating high-temperature and solid-electrolyte fuel cells [4]. The latter is extended by a membrane model [1], which provides the ionic conductivity as well as the water transport over the membrane due to diffusion and electro-osmotic drag. Phase-change is computed based on the unsaturated flow theory for porous media [5]. The three-dimensional, steady state model solves for temperature on a global mesh, while flow velocity and pressure are determined on two child meshes for

CFD METHOD FOR THE RELATIONSHIP BETWEEN THE RADIUS SIZE OF IMPELLERS AND CROSS-SECTIONAL AVERAGE VELOCITY OF FLOW IN AN OXIDATION DITCH

JIAHAO WEI[1], ZHIQIANG XU[2]
[1]*University College Dublin, jiahao.wei@ucdconnect.ie*
[2]*Xi'an University of Technology, xuzhiqiang@xaut.edu.cn*

Keywords: *Oxidation ditch; radius size of impellers; dimensional analysis; cross-sectional average velocity of flow；CFD*

Introduction

OD process is one of the most important technologies for wastewater treatment, and has been widely used due to its reliability, simplicity of operation and low sludge production[1-2]. Since the flow field structure in OD has an important influence on its operation efficiency. Therefore, many scholars have carried out a large number of experimental studies and numerical simulation to understand the hydrodynamics of the ditch for its successful design.
With a constant rotational speed, the radius size of impellers has an important influence on the flow velocity distribution and flow structure in OD. When the rotational speed of impellers is fixed at a constant, the larger the radius of impellers, the greater is the average velocity over a cross-section. Thus, an appropriate radius for impellers should be proposed for OD to obtain the ideal flow so that the efficiency of water treatment will be increased greatly. Therefore, the objective of this work is to find the variation of average velocity over a cross-section with the radius size of impellers by the dimensional analysis method and the solution of 3D time-averaged Navier-Stokes(N-S) equations along with a RNG k-ε turbulence model, which can provide a reference in the designing of ODs.

Analysis of the simulated results

OD is a structure composed of bend and straight channels. The smaller average velocity of the flow may cause sludge phase retention in an OD, which is adverse to its operation. The radius size of impellers has a great effect on the average velocity over a cross section. Here, the average velocity under different radius sizes, 1.25m，1.85m, 2.50m, 3.12m and 3.75m of impellers was simulated. The simulated velocity fields and streamlines on the horizontal plane with submerged depth to the total water depth of 0.45 are shown in Fig.1.

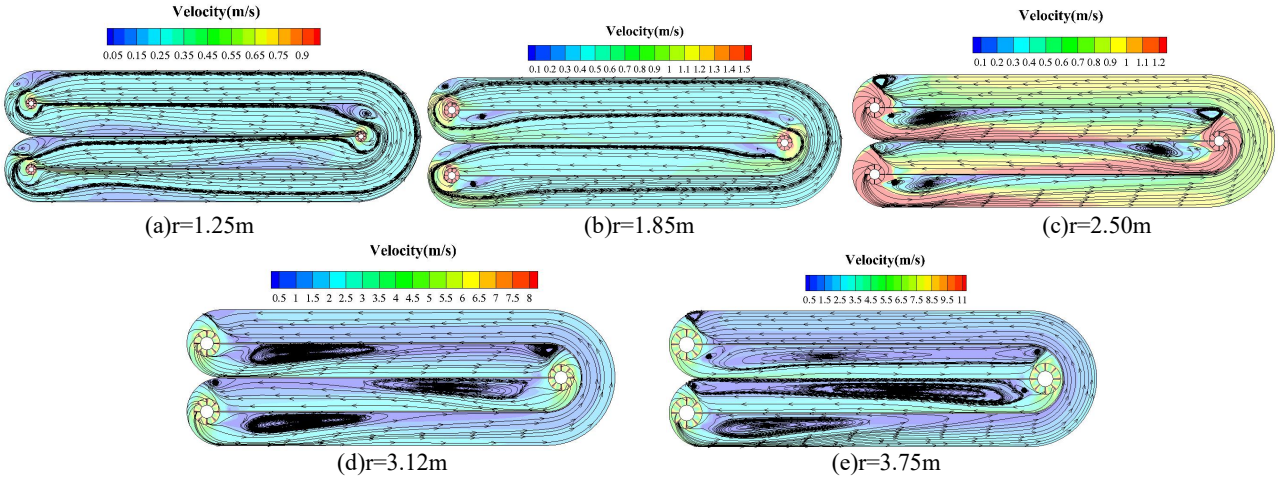


Figure 1: Simulated velocity fields and streamlines on the horizontal plane for different radii

Figure 1 shows that the larger radius of impellers will results in a further uneven velocity distribution at the bend outlets, which leads to a further larger recirculation zone. At the same time, with an increase in the radius size of impellers, the entrainment effect of the surrounding water will be enhanced, which has a great effect on the flow structure of OD. Therefore, it is obtained that a larger radius size of impellers can generate a further uneven velocity distribution so as to forms a larger recirculation zone. Therefore, with a constant rotational speed, the radius size of impellers can be neither

CONVECTION IN LIQUID METAL BATTERIES - COMPARING RESULTS FROM OpenFOAM, Semtex, AND SFEMaNS

PAOLO PERSONNETTAZ[1], TANJA KLOPPER[2], SABRINA BÉNARD[3], NORBERT WEBER[4], TOM WEIER[5]
[1]*Helmholtz-Zentrum Dresden - Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany, p.personnettaz@hzdr.de*
[2]*Helmholtz-Zentrum Dresden - Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany, t.klopper@hzdr.de*
[3]*Ecole Normale Supérieure Paris-Saclay, 4 avenue des Sciences, 91190, Gif-sur-Yvette, France, sabrina.benard@limsi.fr*
[4]*Helmholtz-Zentrum Dresden - Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany, norbert.weber@hzdr.de*
[5]*Helmholtz-Zentrum Dresden - Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany, t.weier@hzdr.de*

Keywords: *Liquid metal batteries, energy storage, solutal convection*

Switching the energy supply from today's dominant fossil sources to mainly variable renewable energies (wind and solar) means a fundamental change. It will entail the transformation from a centralised energy system to distributed generation that needs flexibility options to balance supply and demand across time and space. Transmission grid expansions can only partially account for the resulting variations in supply. Therefore, large-scale stationary storage will gain importance in future energy landscapes.

Among the candidates to meet the growing demand for stationary storage are liquid metal batteries (LMBs) [1]. Their active materials as well as the electrolyte are in the liquid state. The cell interior consists of two layers of liquid metals interspaced by a molten salt electrolyte in stable density stratification (Fig. 1 top left). This conceptually very simple and self-assembling structure has the unique advantage to allow for an easy scale-up at the cell level: single-cell cross sections can potentially reach several square-meters. Such cell sizes enable highly favourable and otherwise unattainable ratios of active to construction material because of the cubic scaling (volume) of the former and the quadratic scaling (surface) of the latter. The total costs should therefore largely be determined by those of the active materials.

While mass transport in most modern battery systems is typically dominated by diffusion and migration in micrometer-scale

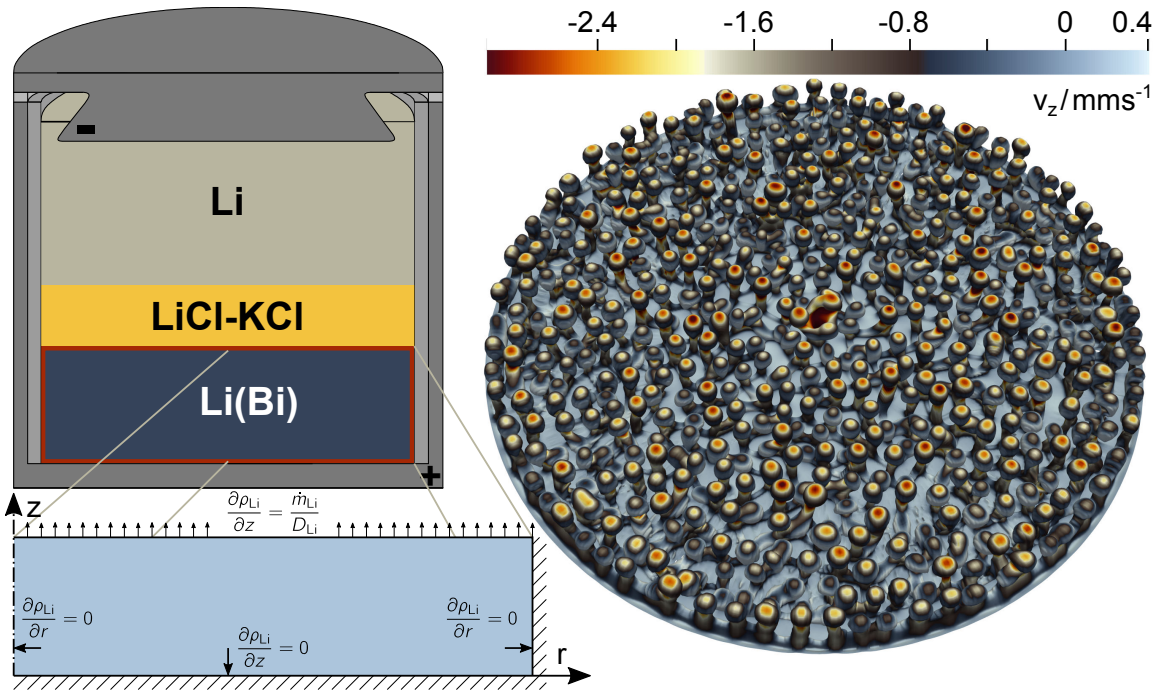


Figure 1: Sketch of a liquid metal battery and of the computational domain (left). Plumes (density iso-contours) of Li-depleted Li(Bi) alloy sinking down during charge. Their surface is colored by vertical velocity (right, view from below).

IMPLEMENTATION OF DAMAGE MECHANICS AND FRACTURE MODELS IN OPENFOAM

ANDREW WHELAN[1], MICHAEL CLANCY[1], VIKRAM PAKRASHI[1], MERT CELIKIN[1], PHILIP CARDIFF[1]

[1] *School of Mechanical and Materials Engineering, University College Dublin, Belfield, D4, Dublin, Ireland, andrew.whelan@ucdconnect.ie , michael.clancy@ucdconnect.ie, vikram.pakrashi@ucd.ie, mert.celikin@ucd.ie, philip.cardiff@ucd.ie*

Keywords: *Damage mechanics, Lemaitre model, GTN model, Phase field, non-local, finite volume method.*

In this presentation, the implementation of various damage and fracture mechanics models are described. To the authors knowledge, these models have not before been implemented using the finite volume method and by extension in OpenFOAM [1]. The canonical Lemaitre damage [2] and GTN models [3] have been implemented and coupled with Lagrangian large strain elasto-plastic solvers [4]. Furthermore, a non-local gradient damage formulation of these models has been implemented to remove mesh size and orientation effects. The more novel phase field model of fracture [5] has also been implemented. This approach involves introducing a phase field partial differential equation to diffuse the sharp crack over a continuum. Herein, the algorithmic implementation of these models is described and verified against test cases from the literature (figure 1).

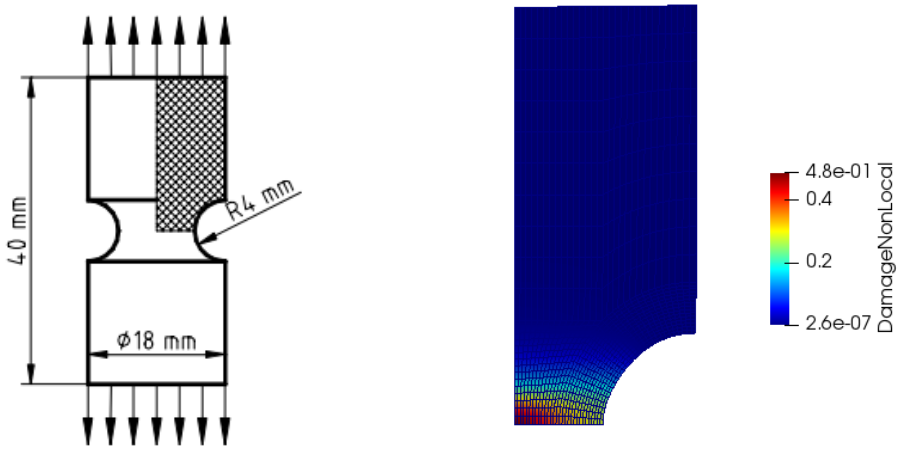


Figure 1: Damage mechanics benchmark case

References

[1] OpenCFD, OpenFOAM: The Open Source CFD Toolbox. User Guide Version 1.4, OpenCFD Limited. Reading UK, Apr. 2007.

[2] J. Lemaitre. A Continuous Damage Mechanics Model for Ductile Fracture. *Journal of Engineering Materials and Technology*, 107(1), pp.83-89., 1985.

[3] M. Achouri, G. Germain, P. Dal Santo and D, Saidane. Numerical integration of an advanced Gurson model for shear loading: Application to the blanking process. *Computational Materials Science, 72, pp.62-67., 2013.*

[4] P. Cardiff, Z. Tukovic, P. De Jaeger, M. Clancy, and A. Ivankovic. A Lagrangian cell-centred finite volume method for metal forming simulation. *International journal for numerical methods in engineering*, 109(13):1777–1803, 2016.

Implementing a Langevin-type turbulent dispersion model for dilute particle-laden flows

Josh Williams, Uwe Wolfram, Ali Ozel
School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, UK, jw144@hw.ac.uk

Keywords: *multiphase flows, large-eddy simulation, turbulent dispersion, channel flow, stochastic modelling.*

Introduction

Turbulent particle-laden flows appear in many medical applications such as inhaler drug deposition. For these applications, drugs are transported as aerosolised solid particles or liquid droplets (henceforth called 'particles') that have low inertia and are strongly influenced by fluctuations in the motion of their carrier fluid. To account for the effect of carrier fluid fluctuations on the particle dynamics, [1] proposed a transport model for the fluid velocity seen by a particle along its trajectory, described by a Langevin model with a deterministic 'drift' term, and a random 'diffusion' term [2]. In this study, we aimed to (i) implement this model in OpenFOAM and (ii) validate it against direct numerical simulation (DNS) results of particle-laden turbulent channel flow [3].

Mathematical modelling

Here we describe the mathematical relations governing our particle-laden channel flow simulations. The fluid phase is modelled with a Large Eddy Simulation (LES) model [4] and the particles are tracked in a Lagrangian fashion by Newton's equations of motion as

$$dx_{p,i} = U_{p,i}\, dt \tag{1}$$

$$dU_{p,i} = \frac{U_{s,i} - U_{p,i}}{\tau_p} dt, \tag{2}$$

where $x_{p,i}$ is the particle position, $U_{p,i}$ is the particle velocity, U_s is the fluid velocity seen by a particle. The particle relaxation timescale is $\tau_p = \rho_p\, d_p^2/18\mu$, where ρ_p is the particle density, d_p is the particle diameter and μ is the fluid dynamic viscosity. The fluid velocity seen by a particle may be modelled with the following stochastic differential (Langevin) equation given by Innocenti et al. [1], written here for a general coordinate system to enable future modelling in complex geometries

$$dU_{s,i} = -\nabla \widetilde{P}\, dt + \nu\, \nabla \cdot \nabla \widetilde{U}_{f,i}\, dt + (\widetilde{U}_{p,i} - \widetilde{U}_{f,i}) \nabla \widetilde{U}_{f,i}\, dt + (U_{s,i} - \widetilde{U}_{f,i})\, G^*_{ij}\, dt + B_{ij} dW_i. \tag{3}$$

Here, $\nabla \widetilde{P}$ is the fluid pressure gradient, ν is the kinematic viscosity, $\widetilde{U}_{f,i}$ is the fluid velocity, $\widetilde{U}_{p,i}$ is the Eulerian solid velocity interpolated at particle position, B_{ij} is the diffusion tensor, dW_i is a vector of independent, random Gaussian variables with variance dt to account for randomness in the turbulence, named a Wiener process. The symbol $(\,\widetilde{\cdot}\,)$ represents a volume-filtered field. For a fluid variable, (e.g. $\widetilde{U}_{f,i}$) this is readily obtained from the LES filtering. Dispersed phase variables (e.g. $\widetilde{U}_{p,i}$) are obtained by mass-averaging over all particles in each computational cell. G^*_{ij} is a second-order tensor based on the ratio between the fluid timescale (T_{sgs}) and fluid velocity seen timescale (T^*_L), and the normal vector of relative transport, $r_i = \widetilde{U}_{r,i}/|\widetilde{\boldsymbol{U}}_{\boldsymbol{r}}|$, that converts the perpendicular and parallel components of T^*_L to a general coordinate system. This is given as

$$G^*_{ij} = -\left(\frac{1}{2} + \frac{3}{4} C_0\right) \frac{\varepsilon}{k} H_{ij} = -\frac{H_{ij}}{T_{sgs}}, \tag{4}$$

where k is the subgrid turbulent kinetic energy, ε is the subgrid dissipation rate, and the model constant C_0 best matches DNS data when $C_0 = 3.5$ for wall-bounded turbulent flows [1]. The orientation matrix (H_{ij}) is found by [5]

$$H_{ij} = b_\perp \delta_{ij} + \big[b_\parallel - b_\perp\big] r_i r_j \qquad b_{\{\parallel,\perp\}} = \sqrt{1 + \beta^2_{\{\parallel,\perp\}}\, |\widetilde{\boldsymbol{U}_{\boldsymbol{r}}}|^2\, 3/2k}, \tag{5}$$

where δ_{ij} is the Kronecker delta. β is the ratio of Lagrangian and Eulerian timescales, where $\beta_\parallel = 0.8$ and $\beta_\perp = 1.6$.
The diffusion tensor (B_{ij}) is found by $B_{ij} = \sqrt{L_{ij}}$, where $L_{ij} = L_\perp \delta_{ij} + \big[L_\parallel - L_\perp\big] r_i r_j$ [5], where the parallel and perpendicular components are

$$L_{\{\parallel,\perp\}} = \varepsilon [C_0\, b_{\{\parallel,\perp\}} + 2(b_{\{\parallel,\perp\}} - 1)/3]. \tag{6}$$

Transient Two-way Molecular-Continuum Coupling with OpenFOAM and MaMiCo: A sensitivity study

Helene Wittenberg[1], Philipp Neumann[2], Piet Jarmatz[3],
[1]*Helmut-Schmidt-Universität Hamburg, h.wittenberg@hsu-hh.de*
[2]*Helmut-Schmidt-Universität Hamburg, philipp.neumann@hsu-hh.de*
[3]*Helmut-Schmidt-Universität Hamburg, jarmatz@hsu-hh.de*

Keywords: *transient, two-way-coupling, molecular-dynamics, CFD, sensitivity*

A molecular dynamics (MD) simulation evaluates the physical processes within a system on the level of atoms and molecules. Thereby one can analyze the trajectory of molecules and understand, e.g., fluid motion on the molecular scale. Considering individual molecules with time steps of femtoseconds results in a high overall computing time. For the application of MD-based methods in research and development, it is necessary to overcome these limitations. Therefore, one approach to assess molecular fluid motion lies in hybrid multiscale simulation schemes, coupling the micro-scale MD simulation with a macro-scale simulation, e.g. a computational fluid dynamics (CFD) simulation.
Our goal is to simulate a process within a continuous domain using two models, and thereby combine the continuous perspective with the discrete perspective on matter. Thus the domain is decomposed into two regions. For a transient two-way-coupling with strong coupling in time (i.e. O(50) MD time steps correspond to one CFD step), it is necessary to exchange information and set appropriate boundary conditions at the domains' interface. Since both simulations rely on different variables and scales in space and time, a challenge lies in physically correct processing of the data.
In my talk, I will present an approach for such a coupling, using the macro-micro-coupling tool (MaMiCo) as interface for the coupling, the in-house code SimpleMD as MD model and OpenFOAM as CFD model. The focus will be on the correct setup of a stable and transient coupling, using an overlapping domain decomposition approach. The system has shown to be quite sensitive to changes in certain parameters, for example the particle insertion algorithm or cell sizes in the continuum simulation. Therefore a coherent setting of every value and algorithm is the key to achieve an accurate hybrid solution.
Besides the physical correctnes of the model, another key aspect is the performance of our coupled simulation. Therefore, we decicded to exchange the data directly, instead of using the classical OpenFOAM concept to write and read files. Consequently we had to add functionality to the icoFoam solver.
For the evaluation of the coupling algorithm we simulate a Couette flow startup. The biggest part of the channel is simulated with the CFD solver. The MD solver is placed in the center of the domain. The figure 1 shows a stable solution for this case, including the analytic solution for comparsion.

Acknowledgments

This work has been supported through the project "MaST: Macro/Micro-Simulation of Phase Separation in the Transcritical Regime" of the center for digitization and technology research of the armed forces (dtec.bw) and the HSU-internal research founding (IFF) project "Resilience and Dynamic Noise Reduction at Exascale for Multiscale Simulation Coupling".

3D THERMAL ANALYSIS OF FOOTWEAR WITH OPEN SOURCE SOFTWARE, OPENFOAM

Muhammad Asad Yamin[1], Nikolai Kornev[2], Irina Cherunova[3]
[1,2,3]*Chair of modelling and simulation (LeMoS), University of Rostock, 18059 Rostock, Germany*
[3]*Don State Technical University, 346500 Shakhty, Russia*
[1]*muhammad.yamin@uni-rostock.de*
[2]*nikolai.kornev@uni-rostock.de*
[3] *i_sch@mail.ru*

Keywords: *thermodynamics of footwear, transport of heat and moisture, modelling of footwear comfort*

Abstract

A mathematical modelling of heat and moisture transport for footwear is implemented in OpenFOAM in- house solver. A model consists of four main physical phenomena which are the conservation of energy for control volume, conservation of mass for water vapour, conservation of mass for water retained in footwear material and conservation of mass for liquid water in footwear material.
A number of simulations are carried out for 3D and 1D scenario, which accumulate the different ambient conditions such as temperature and moisture. A 3D geometry is created from scratch which is nearly resembled to the reality footwear. The results for heat and moisture transport are analysed at different six places around the footwear and compared with the 1D scenario.
In further work, the simulations are performed without considering the moisture transport in the footwear material and results are compared with the previous base model (with moisture transport). The comparison of temperature with and without moisture transport is elaborated around the footwear.

Methodology and Results

The implementation of mathematical model is mostly taken from the PhD thesis of the Chitrphiromsri [1] and Neves2015 [2]. Additionally, this formation considers extra equations for liquid water, mass flow from liquid water to footwear material and vapours and vice versa.

$$\rho_{ef}\, c_{p,ef} \frac{\partial T}{\partial t} - \frac{\partial}{\partial x}\left(k_{ef} \frac{\partial T}{\partial x}\right) - \Delta h_{vap}\left(\dot{m}_{gs} + \dot{m}_{gl}\right) - \Delta h_{sorp}\left(\dot{m}_{ls} + \dot{m}_{gs}\right) = 0 \quad (1)$$

This conservative energy equation (1) which accumulates the energy, heat transfer by conduction and energy associated with sorption and desorption of water between the footwear material, liquid water and gaseous phase.

$$\frac{\partial(\varepsilon_\gamma \rho_v)}{\partial t} - \frac{\partial}{\partial x}\left(D_{ef} \frac{\partial \rho_v}{\partial x}\right) + \dot{m}_{gs} + \dot{m}_{gl} = 0 \quad (2)$$

This continuity equation (2) for water vapour which accumulate the water vapours in pores, vapours diffusion, mass sorption rate of water from gaseous phase to footwear material and liquid water.

$$\rho_w \frac{\partial \varepsilon_{bw}}{\partial t} - \dot{m}_{ls} - \dot{m}_{gs} = 0 \quad (3)$$

This continuity equation (3) is for water retain in footwear material.

$$\rho_w \frac{\partial \varepsilon_l}{\partial t} + \dot{m}_{ls} - \dot{m}_{gl} = 0 \quad (4)$$

This continuity equation (4) is for the liquid water which is present in the pores of footwear material.
A 3D geometry has layer structure formation, each layer composed of different material respectively, socks (cotton), air and shoe (polyester).

AN OPEN SOURCE SHAPE OPTIMIZATION PROCESS FOR AEROSPACE APPLICATIONS

S. YIGIT[1], S. ABUHANIEH[1], B. BICER[1], M. SAHIN[2]
[1]*Turkish Aerospace Industries, Turkey, sahin.yigit@tai.com.tr*
[1]*Turkish Aerospace Industries, Turkey, salehkhairisaleh.abuhanieh@tai.com.tr*
[1]*Turkish Aerospace Industries, Turkey, baris.bicer@tai.com.tr*
[2]*Istanbul Technical University, Turkey, msahin@itu.edu.tr*

Keywords: *Propeller, Shape Optimization, Free-form Deformation, Dakota, Mimmo, OpenFOAM, SnappyHexMesh*

Shape optimization is immensely important for aerospace industry to design efficient air vehicles and components such as propellers. However, the shape optimization process is quite expensive cycle even for a single propeller with experimental analysis since it needs considerable number of steps. Therefore, a numerical based shape optimization process can be an efficient tool to overcome extra experimental costs. Accordingly, in the present study, an open-source shape optimization framework (involving the combined use of CFD solver, optimization solver, Free-form Deformation Tool and mesh generator) is combined to optimize the shape of a generic propeller. Figure 1 shows the component of our optimization cycle which consists of OpenFOAM [1], Dakota (an open-source optimization tool) [2] and MiMMO (an open source C++ library for manipulation and morphing of surface and its mesh) [3] and SnappyHexMesh[1].

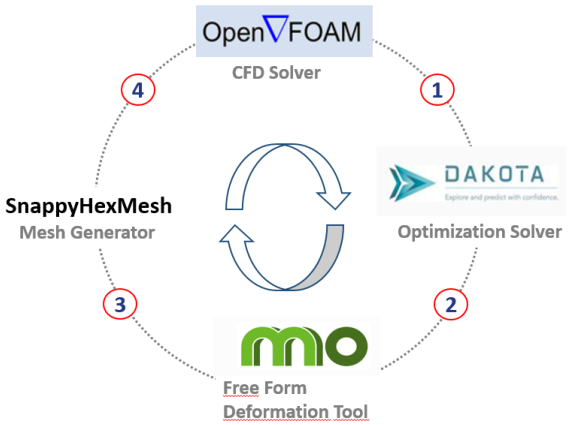


Figure 1: The schematic scheme of open-source shape optimization.

The steady compressible OpenFOAM solver (i.e. rhoSimpleFOAM-v2006) has been used with MRF (Multi Reference Frame) for modelling a generic propeller in both hover and forward flight conditions. The numerical results of (i.e. thrust and torque values) are compared with experimental results (in-house experimental test-facilities of Turkish Aerospace Industries). After numerical modelling of the propeller flow dynamics, in the step 1 of the above cycle, the torque and thrust results obtained from OpenFOAM solver are optimized in Dakota by using different methods (e.g. gradient based, surrogate-based optimization). In the step 2, Dakota produces new displacement values for the MiMMO. In step 3, MiMMO deforms the propeller geometry and its surface mesh (i.e. gives a new stl file). In step 4, SnappyHexMesh generates new volume mesh for the new fluid domain for OpenFOAM solver to find new thrust and torque values for new propeller design. This cycle is continued until certain level of enhancement achieved in the efficiency of the propeller.

It has been found that shape optimization cycle is developed in the current study performs sufficiently well for the shape optimization of a propeller. The detailed results will be presented in the OFW16 organisation.

Acknowledgements

The authors gratefully acknowledge that in-house cluster of Turkish Aerospace Industries have been used in the current analysis.

References

[1] OpenCFD, OpenFOAM: The Open Source CFD Toolbox. User Guide Version 1.4, OpenCFD Limited. Reading UK, Apr. 2007.

An in-situ characterization of coherent structures in two-phase flow simulations

J. Miguel Zavala-Aké[1], Niclas Jansson[1], Mohamad Rezaei[1], Marco Atzori[1], Philipp Schlatter[1] and Erwin Laure[1,2]
[1]*KTH Royal Institute of Technology, Stockholm, Sweden*
[2]*Max Planck Computing and Data Facility Garching, Germany*

Keywords: *in-situ visualization/analysis, high performance computing, two-phase flow*

This paper describes a parallel algorithm which allows an in-situ characterization of the time evolution of coherent structures in 3D incompressible two-phase flow simulations. In general, the evolution of coherent structures could be divided in two main stages: cluster analysis and time tracking. The first stage, coherent structures are spatial localized and characterized. For this purpose, at any time, structures are identified by regions in the domain with values below a certain threshold. Then, these regions are grouped in sub-sets (clusters), each of them characterized by an unique number along with geometrical properties as its area, volume or center of mass. In the second stage, the tracking of each of these structures through the time is performed. In this point, a searching for overlappings between clusters belonging to different time steps is performed. Clusters are considered connected if overlapping between them exist. The searching for overlappings could be (ideally) repeated each time step, so that connections found enable a high resolution time tracking of each cluster.

The implementation of the algorithm above described has been performed by means of a *real time* handling of the computer graphics algorithms available in the Visualization Toolkit (VTK) software [1, 2]. Coherent structures are identified by using the *vtkContourFilter* class which, given a threshold, allows an isosurface extraction. For the clustering, the *vtkConnectivityFilter* class makes use of a recursive algorithm which allows to extract data based on geometric connectivities. Sets of extracted cells are identified through an unique number which is used to separate the isosurface in clusters. Once clustering is performed, time tracking could be established by identifying temporal connectivities between clusters allocated in different times steps. These connectivities are determined in three steps. Firstly, each cluster is confined within its smallest bounding box. Then, a searching for overlappings is performed between a bounding box belonging to the current time step and bounding boxes held in a previous time step. Finally, if two bounding boxes (allocated in different time steps) overlap, then a boolean operation is performed between the clusters contained by each bounding box. Specifically, the intersection between these clusters is found by using the *vtkBooleanOperationPolyDataFilter* class. A positive result of the boolean intersection of these clusters means that overlapping between them exist. This overlapping is understood as that a temporal connection exists between these two clusters. This algorithm is available as a modification of the catalyst plugin in OpenFOAM-v1806 however, it is worth nothing that, by means of an appropiated in-situ instrumentation, it could be used in any code.

The validation of this algorithm has been performed by using a simulation of boiling flow. The main goal is to identify and characterize the coherent structures generated during vaporization. At the begining of the simulation, a cubic centimer of water at 378.15 degrees Kelvin is subjected to a temperature difference of 100 degrees, see Figure 1. Under this set-up, at some point, nucleation starts so that bubbles of vapor emerge from random points on the heated surface. In this simulation, the volume-of-fluid (VoF) solver implemented in OpenFOAM is used to model the phase change [3]. Ten thousand time steps of the multi-phase Navier-Stokes equations are solved in one millon cells. Results are shown in Figures 2 and 3.

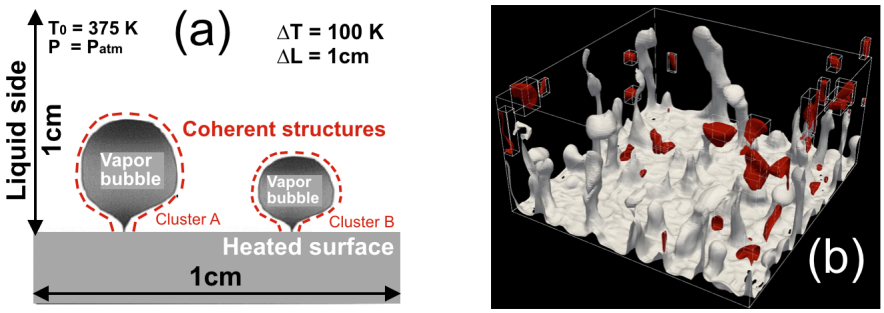


Figure 1: (a) Simulation setup. (b) Tridimensional view of coherent structures (volume fraction field $\alpha = 0.6$) generated at t=1.0.

A 3D NUMERICAL STUDY ON THE AERODYNAMIC PERFORMANCE OF A BRIDGE DECK

YUXIANG ZHANG[1], PHILIP CARDIFF[2], JENNIFER KEENAHAN[3]
[1]*School of Civil Engineering, University College Dublin, yuxiang.zhang1@ucdconnect.ie*
[2]*School of Mechanical and Materials Engineering, University College Dublin, philip.cardiff@ucd.ie*
[3]*School of Civil Engineering, University College Dublin, jennifer.keenahan@ucd.ie*

Keywords: *bridge aerodynamics, bridge deck, CFD, RANS, wind tunnel test*

The Rose Fitzgerald Kennedy Bridge is an extrados bridge. It has a main span of 230 m, the longest span of its kind. It is currently the longest bridge in Ireland to date with a full length of 887 m. Wind actions were considered critical for this bridge. Wind tunnel experiments [1] were performed to determine the aerodynamic coefficients of the cross section which are used to compute global forces and moments on a unit length segment of the bridge deck. This study is proposed to apply CFD simulations to investigate the aerodynamic performance of the bridge by replicating the wind tunnel tests using OpenFOAM.

The focus of this study is on the estimation of aerodynamic coefficients of the bridge deck at different angles of attack. The geometry of the bridge deck is shown in Figure 1. Configurations of angles of attack are shown in Figure 2.

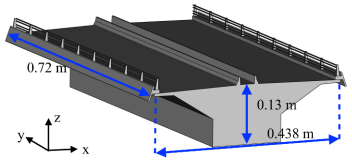


Figure 1: Bridge deck geometry

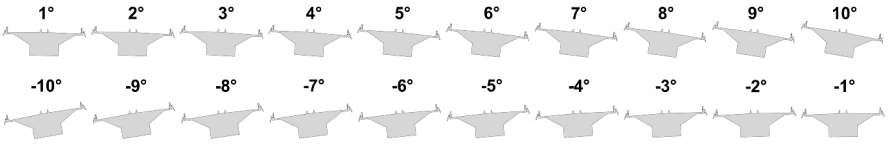


Figure 2: Configurations of different angles of attack

The computational mesh is shown in Figure 3, generated using *SnappyHexMesh.* Regional refinement is applied around the bridge geometry with 6 levels. There are 5 buffer layers between two adjacent levels. Eight layers of cells were placed on the bridge surface to resolve the viscous sublayer, with the thickness of 0.5 mm; which corresponds to a maximum and mean y^+ values of 1.3 and 0.35 respectively at the bridge surface. The total mesh contained approximately 35 million cells, depending on the angles of attack.

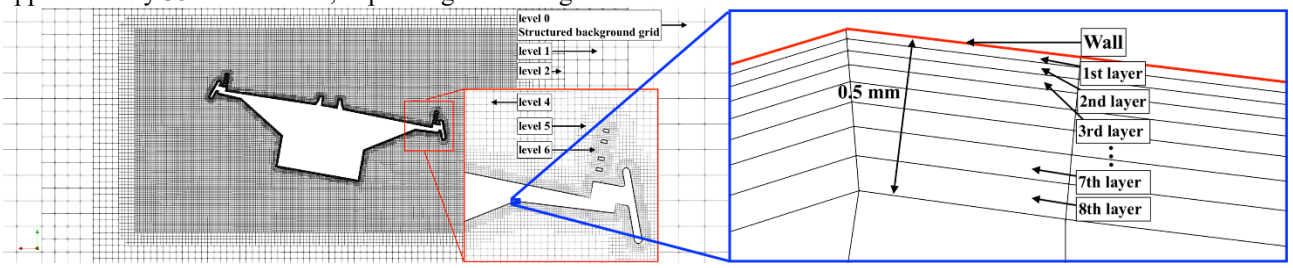


Figure 3: Sectional view of the computational mesh

In this study, all simulations employ the SIMPLE algorithm [2](Patankar & Spalding 1972) to perform the pressure-velocity coupling (simpleFoam solver in OpenFOAM-v6). All terms in the Reynolds-averaged Navier-Stokes (RANS) equations are discretised using the nominally second-order cell-centred finite volume method [3](Jasak 1996), where gradient and Laplacian terms are discretised using Gaussian integration with linear interpolation. Convection terms are discretised using a second-order accurate linear-upwind scheme.

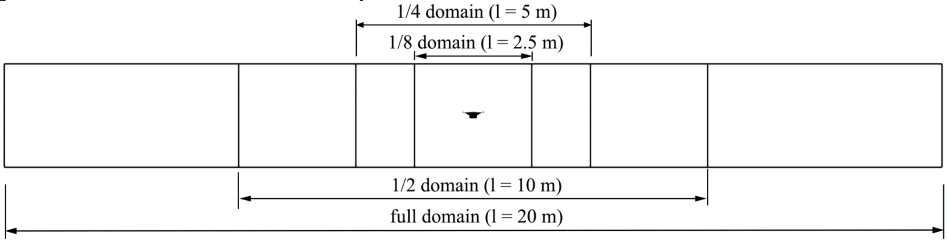


Figure 4: Domain sizes considered in the domain sensitivity study

When replicating wind tunnel tests using CFD simulations, using a smaller computational domain can reduce the cell count in the mesh, thereby saving on the computational power. However, the use of smaller computational domains

Numerical Study on Coupled Aeroelastic Performance of Wind Turbines Considering Blade Deformation

Jiancai Zheng, Yang Huang, Decheng Wan*
Computational Marine Hydrodynamics Lab (CMHL), School of Naval Architecture, Ocean and Civil Engineering, Shanghai Jiao Tong University, Shanghai 200240, China
*Corresponding author: dcwan@sjtu.edu.cn

Keywords: *Blade Deformation; Structural Dynamic Responses; Aeroelastic Actuator Line Model.*

INTRODUCTION

Blade enlargement has become a major trend of future development in the wind turbine manufacturing industry. This leads to the significant structural deformation of blades in wind turbines (Mo et al., 2015). Furthermore, because of the variation in aerodynamic performance due to the structural deformation, which will further disturb the downstream wind turbines in a wind farm. Therefore, the study on the performance of wind turbines considering deformation and disturbance effect is becoming a key issue in loads predicting and wake interference effect.
In the present work, an elastic actuator line model combined with Euler-Bernoulli beam theory is developed to perform aeroelastic simulations for wind turbines. The coupled aeroelastic performance includes the aerodynamic loads, deformation of the structure of blades, and wake field characteristics. Moreover, the interference effect in the downstream wind turbine is also discussed when the aeroelastic is considered.

NUMERICAL METHOD

The actuator line model (ALM) was an effective method, which is proposed by Sørensen and Shen (2002). The aerodynamic loads and the wake and vortex are captured through the way to use the virtual actuator lines to replace the blades in wind turbines. However, the deformation of blades has not been considered during the operation of the wind turbine. In order to the aeroelastic responses of blades are computed, an elastic actuator line model (EALM) is proposed, which combined the ALM and Euler-Bernoulli beam theory (Bauchau et al., 2009). In the EALM, the aerodynamic characteristics are calculated by the ALM and the blade deformation is predicted by the finite element method (FEM).

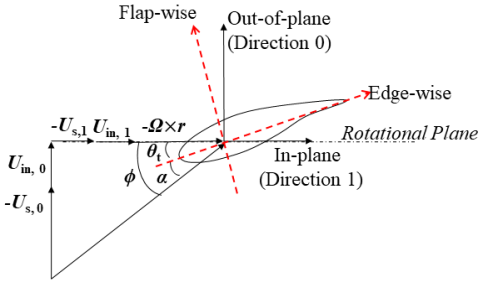
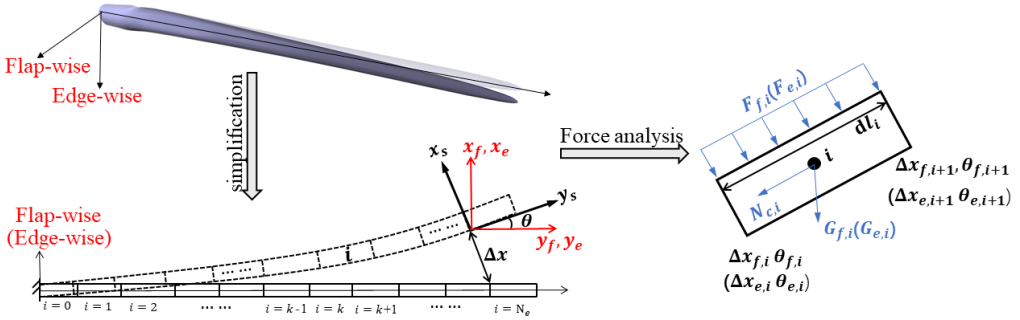


Fig.1 Velocity triangle seen locally on a blade section

The relationship of the velocity vectors is shown in Figure 1, in which the relative wind speed vectors can be resolved by the following equation:

$$U_{rel} = U_{in} + U_B + U_s \quad (1)$$

in which the inflow wind speed is represented as U_{in}. The rotational velocity of the rotor is expressed as U_B. U_s is donated by the additional velocities induced by structural deformation. Meanwhile, the slender blade is simplified into a cantilever beam in the EALM. Therefore, the deformation can be solved by EBM theory. The equivalent beam model is discretized by the one-dimensional FEM method, and the deformation is solved by the two-node, four-degree-of-freedom beam element.



VALIDATION OF A 3D COMPUTATIONAL FLUID DYNAMICS MODEL AND WIND TUNNEL TEST RESULTS FOR THE QUEENSFERRY CROSSING: MESH SENSITIVITY AND DOMAIN STUDY

LICHENG ZHU[1], DANIEL MCCRUM[2], JENNIFER KEENAHAN[3]
[1] *School of Civil Engineering, University College Dublin, licheng.zhu@ucdconnect.ie*
[2] *School of Civil Engineering, University College Dublin, daniel.mccrum@ucd.ie*
[3] *School of Civil Engineering, University College Dublin, jennifer.keenahan@ucd.ie*

Keywords: *Computational fluid dynamics; aerodynamic; wind tunnel test*

Abstract

The study of bridge aerodynamics is essential in ensuring the safety and acceptable performance of long-span bridges are vulnerable to the effects of wind. Traditionally, aerodynamic studies were carried out in the wind tunnel facilities, however the opportunities of using CFD modelling for wind assessments are significant. Previous studies have largely focused on two-dimensional (2D) models, and three-dimensional (3D) analyses of wind effects on bridges have rarely been performed. There are also few studies that consider the presence of vehicles on the bridge. In this study, 3D CFD models are developed in OpenFOAM using the k-ω-SST turbulence model for the Queensferry Crossing bridge, containing wind shields and sample vehicles. The study focuses on the effect of mesh sensitivity and domain size on determining the aerodynamic coefficients. The models are then validated by comparing results with wind tunnel test data for the same configuration. Results are very promising and show good agreement between results from the CFD models and the wind tunnel tests, this creating a pathway for further development in the use of CFD models for analysing wind effects on long span bridges.

PERFORMANCE ASSESSMENT OF A FLOATING PLATFORM SURROUNDED BY ELASTIC ICE PLATES

CHONGWEI ZHANG[1], QIANZE ZHUANG[1], LUOFENG HUANG[2], DEZHI NING[1]
[1]*State Key Laboratory of Coastal and Offshore Engineering, Dalian University of Technology,*
chongweizhang@dlut.edu.cn
0_0zqz@mail.dult.edu.cn
dzning@dlut.edu.cn
[2]*Dept. of Mechanical Engineering, University College London, ucemlhu@ucl.ac.uk*

Keywords: *Arctic Engineering, Floating Platform, Hydroelasticity, Sea Ice, OpenFOAM.*

Oil and gas resources are abundant in the Arctic. In recent decades, with global warming and the melting of polar ice coverages, the Arctic marginal ice zone (MIZ) has gradually expanded, particularly in summer [1]. It is therefore more accessible to carry out oil and gas exploitation in the region. However, different from open water, the design of floating platforms in a polar sea state must consider the influence of floating ices. Previous studies have shown that the existence of elastic ice floes has complex effects on the water wave characteristics [2], [3]. Thus, for ensuring the structural safety of polar floating platforms, it is essential to assess the hydrodynamic loads combining with sea ice effects.
Until now, there is little research on wave-ice-structure interactions. The majority of previous work relied on analytical methods [4], [5], including two-dimensional linear potential flow theory and linear elastic theory. Meanwhile, studies on the interaction between waves and ice floes have made considerable progress [6], [7]. For the last several years, numerical approaches have been significantly developed and show the potential to improve the accuracy by accounting for nonlinear features that are excluded in analytical solutions.
In such a context, this study establishes a two-dimensional numerical structure-ice-wave interactive model based on OpenFOAM. The layout of the model is shown in Figure 1. Water waves are generated from the left-hand side and propagate towards the right-hand-side. A two-way fully fluid-structural coupling algorithm is applied to simulate the interaction between elastic floating ice floes and waves [8], [9]. The associated hydrodynamic effects on the floating platform are investigated systematically, considering different distribution modes and stiffness of elastic ice floes and incident wave frequencies. More detailed results will be presented in the full-length paper.

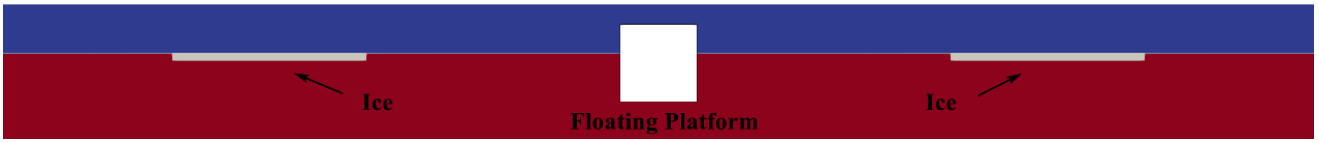


Figure 1: Layout of the structure-ice-wave tank

Acknowledgements

This study is supported by the National Natural Science Foundation of China (Grant Nos.51709038 and 51739010), the Project funded by China Postdoctoral Science Foundation (No.2018M630289 and 2019T120209).

References

[1] C. Strong and I. G. Rigor, "Arctic marginal ice zone trending wider in summer and narrower in winter," *Geophys. Res. Lett.*, vol. 40, pp. 4864–4868, Sep. 2013.

[2] L. G. Bennetts, N. R. T. Biggs and D. Porter, "A multi-mode approximation to wave scattering by ice sheets of varying thickness," *J. Fluid Mech.*, vol. 579, pp. 413–443, May 2007.

[3] C. Wang, M. Song, C. Guo, S. Wang, T. Tian and W. Luo, "Experimental Study of Sea Ice Motion in Waves." *J. Cold Reg Eng.*, vol. 34, pp. 04020010, Jun. 2020.

[4] Z. Li, Y. Shi and G. Wu, "Interaction of wave with a body floating on a wide polynya," *Phys. Fluids*., vol. 29, pp. 097104, Sep. 2017.

[5] Z. Li, Y. Shi and G. Wu, "A hybrid method for linearized wave radiation and diffraction problem by a three dimensional floating structure in a polynya," *J. Comput. Phys.*, vol. 412, pp. 109445, Apr. 2020.

[6] L. G. Bennetts, M. A. Peter, V. A. Squire and M. H. Meylan, "A three-dimensional model of wave attenuation in the marginal ice zone," *J. Geophys. Res.*, vol. 115, pp. C12043, Dec. 2010.