V European Conference on Computational Fluid Dynamics
ECCOMAS CFD 2010
J. C. F. Pereira and A. Sequeira (Eds)
Lisbon, Portugal,14-17 June 2010

A 3D FINITE ELEMENT APPROACH FOR MESOSCOPIC FLUID-STRUCTURE INTERACTION

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Key words: Intermolecular & surface interaction, fluctuating hydrodynamics, Brownian motion, mesoscopic fluid-structure interaction, finite element method

Abstract.

A 3D finite element approach to fluid-structure interaction (FSI) on the mesoscopic scale allows to study a wide range of problems from engineering, biophysics and statistical mechanics, e.g. the stability of colloidal suspensions, membrane adhesion or biophysical self-assembly processes. The atomistic nature of fluid and solid becomes noticeable on the mesoscopic scale and requires, in contrast to macroscopic fluid-structure interaction, the consideration of further physical phenomena such as intermolecular & surface interaction, Brownian motion and mesoscopic ion transport.

We present a dynamic 3D finite element formulation derived from microscopic dynamics for intermolecular & surface interaction (I&SI) of multiple flexible structures as well as Brownian motion. The finite element formulation of Browian motion is based on a "Fluctuating Hydrodynamics" approach. Both finite element formulations are combined with an EXtended Finite Element Method (XFEM)-based FSI approach and an Arbitrary Lagrangian Eulerian FSI formulation.

Future work will concentrate on the integration of ion transport in mesoscopic fluid-structure interaction by coupling to the Nernst-Planck-Poisson equation.

1 INTRODUCTION

A variety of interesting fluid-structure interaction (FSI) problems from engineering, biophysics and statistical physics can be studied on the mesoscopic scale. Important fields of application include e.g. the simulation of colloidal suspensions such as red blood cell suspensions, membrane adhesion, transport processes through porous media, nano coating, the investigation of efficient swimming techniques of microswimmers and microrobots or biophysical self-assembly processes.

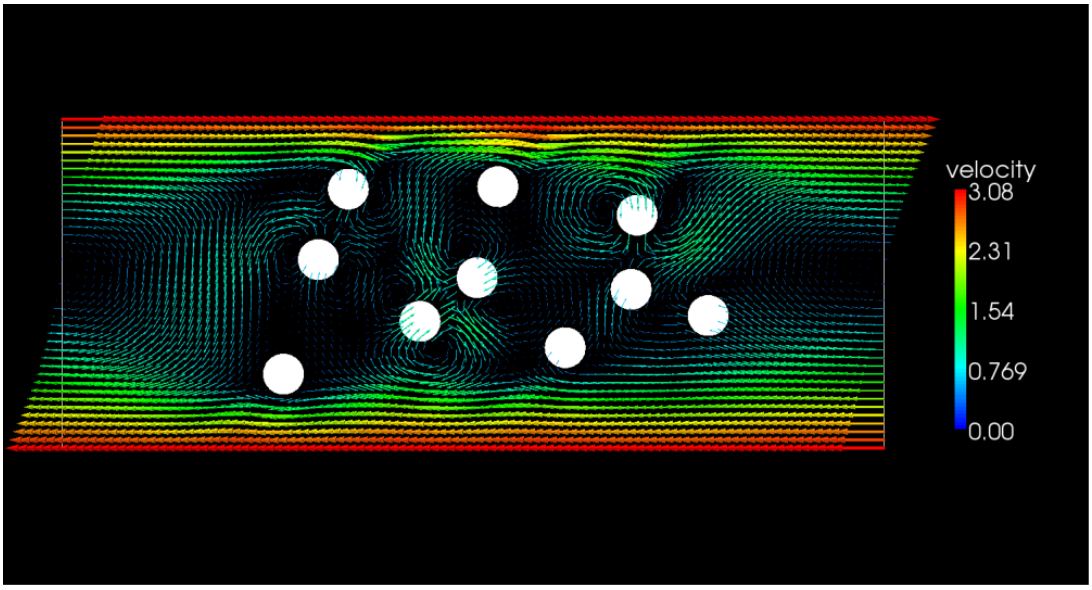
Since the atomistic nature of fluid and solid becomes already noticeable on the mesoscopic scale, further physical phenomena such as intermolecular & surface interaction (I&SI), Brownian motion and mesoscopic ion transport have to be integrated into a mesoscopic fluid-structure interaction approach.

We propose a 3D finite element formulation for I&SI interaction[1] and Brownian motion, the latter being based on a "Fluctuating Hydrodynamics" approach. Both formulations may be derived from microscopic dynamics in order to capture the underlying atomistic physics accurately. Under certain circumstances, repulsive surface interaction of structures very close to contact may be extended or approximated by a macroscopic dual mortar contact formulation[2]. Both finite element formulations allow a straightforward integration into most FSI-approaches. We combined them with a 3D higher-order XFEM FSI approach[3], and an Arbitrary Lagrangian Eulerian (ALE) FSI formulation[4], which allows the simulation of arbitrarily moving and deforming structures. The resulting monolithic linearized system for each FSI method can be solved by any state-of-the-art partitioned or monolithic fluid-structure coupling algorithm[4].

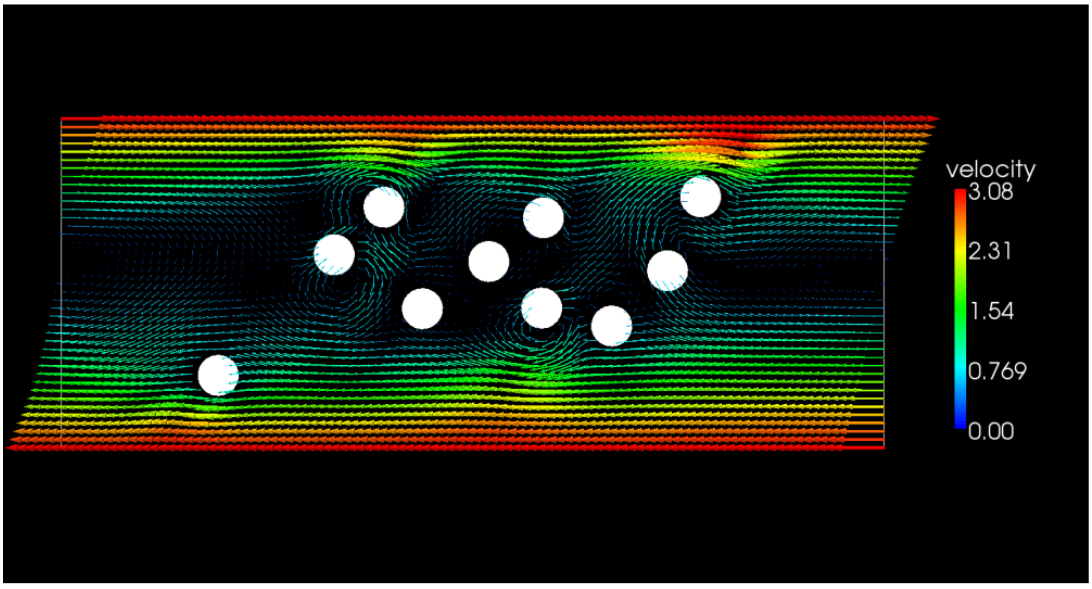
2 INTERMOLECULAR & SURFACE INTERACTION

We present a 3D dynamic finite element formulation for intermolecular & surface interaction (I&SI) of multiple flexible bodies embedded in fluid flow[1]. The coarse-grained continuum formulation may be derived from microscopic dynamics to demonstrate that its underlying atomistic nature is captured precisely. The generality of the finite element formulation allows the integration of intermolecular volume interaction forces as well as a variety of long- or short-ranged attractive as well as repulsive surface forces to model the physical interaction effect of choice. We focused so far on attractive Van-der-Waals forces screened by the surrounding fluid as well as electrostatic repulsion, which constitute the most important interaction phenomena in fluid flow according to the DLVO (Derjaguin, Landau, Verwey, Overbeek) - theory. Under certain circumstances, short-ranged repulsive forces between structures very close to contact may be extended or approximated by a macroscopic dual mortar contact formulation [2].

Figure 1 illustrates how Van-der-Waals adhesion between particles in shear flow leads to a certain pattern formation.



a)



b)

Figure 1: Self-assembly of particles in shear flow due to attractive Van-der-Waals forces. a) Velocity field and particle distribution at an earlier point in time. b) Velocity field and particle distribution at a later point in time.

3 FLUCTUATING HYDRODYNAMICS AND BROWNIAN MOTION

The thermal agitation of water molecules is the second atomistic effect that we include into the mentioned fluid-structure interaction methods based on a "Fluctuating Hydrody-

namics" approach. The erratic motion of structures, which are hit by thermally agitated water molecules is referred to as Brownian motion.

A mesoscopic "Fluctuating Hydrodynamics" approach is realized by including a stochastic stress term in the Navier-Stokes equation. Derivation from microscopic dynamics leads to a stress term which is modelled by white noise in space and time and has a non-Gaussian distribution due to nonlinear nonequilibrium effects. A semi-implicit stochastic time integration method is applied to perform time integration of the resulting stochastic partial differential equation.

This "Fluctuating Hydrodynamics" method itself may already be applied to a variety of mesoscopic flow problems such as the simulation of nanojets and microscopic mixing in a driven cavity. Figure 2 shows the streamline plot in a driven cavity for the deterministic solution of the Navier-Stokes equation and a driving velocity $v = 1\,\mathring{A}/ps$ at the left boundary (3 a)) contrasted with the stochastic solution based on the same boundary conditions (3 b)). Non-smooth streamlines illustrate the affect of fluctuations on the flow. For a smaller driving velocity (in 3 c)) the deterministic circular flow is almost nullified by fluctuations. The extent of mixing in such a microscopic mixer is then affected by the magnitude of the fluctuations.

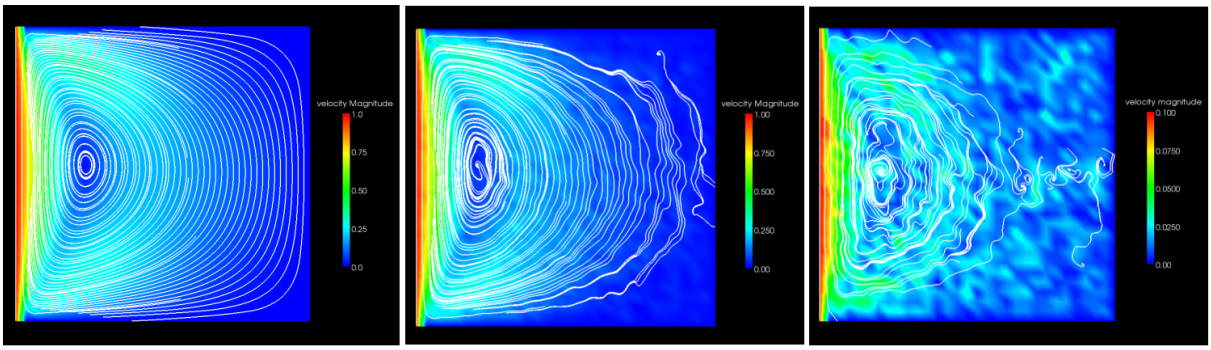


Figure 2: Velocity distribution and streamline plot for water in a driven cavity. a) Streamline plot without fluctuations with $v = 1\ \mathring{A}/ps$. b) Streamline plot including fluctuations with $v = 1\ \mathring{A}/ps$. c) Streamline plot including fluctuations with $v = 0.01\ \mathring{A}/ps$.

The additional inclusion of the stochastic stresses into the fluid-structure coupling conditions leads naturally to Brownian motion of arbitrarily shaped and deforming structures. Fluctuating hydrodynamics may be also coupled to the Nernst-Planck-Poisson equation to simulate mesoscopic ion transport.

4 MESOSCOPIC FLUID-STRUCTURE INTERACTION

The finite element formulation for intermolecular & surface interaction and Brownian motion may be integrated into most FSI-approaches. We combined them with a 3D higher-order XFEM FSI approach[3] and an Arbitrary Lagrangian Eulerian (ALE) FSI

formulation[4], which allow the simulation of arbitrarily moving and deforming structures. An exact interface representation allows to capture flow pattern around structures, which may move and deform now also due to intermolecular & surface forces and Brownian motion. For both FSI-methods, linearized monolithic systems of equations are derived. The linearized systems can be solved by any state-of-the-art partitioned or monolithic fluid-structure coupling algorithm[4].

5 CONCLUSIONS

We present a 3D finite element approach for mesoscopic fluid-structure interaction including intermolecular & surface interaction (I&SI) and Brownian Motion of multiple flexible structures. The finite element formulation for intermolecular & surface interaction allows to simulate the structural movement and deformation due to attractive and repulsive forces. Brownian Motion is realized based on a fluctuating hydrodynamics approach, where a stochastic stress tensor is added to the Navier-Stokes equation and integrated in the fluid-structure coupling conditions. Both finite element formulations are derived from microscopic dynamics to capture the underlying molecular nature accurately. Future work will concentrate on extending the macroscopic ion transport formulation[5] to mesoscopic ion transport by solving the Poisson equation in addition to the Nernst-Planck equation and by coupling to fluctuating hydrodynamics.

REFERENCES

[1] U.M. Mayer and W.A. Wall, A finite element approach to 3D intermolecular & surface interaction of multiple flexible mesoscopic structures in fluid flow, *in preparation*, (2010).

[2] U.M. Mayer, A. Popp, A. Gerstenberger and W.A. Wall, 3D fluid-structure-contact interaction based on a combined XFEM FSI and dual mortar contact approach, *Computational Mechanics*, DOI: 10.1007/s00466-010-0486-0, (2010).

[3] W.A. Wall, A. Gerstenberger and U.M. Mayer, Advances in fixed-grid fluid structure interaction, *ECCOMAS Multidisciplinary Jubilee Symposium - New Computational Challenges in Materials, Structure and Fluids*, **14**, 235–249 (2008).

[4] M. Gee, U. Küttler and W.A. Wall, Truly monolithic algebraic multigrid for fluid-structure interaction, submitted for publication in *Int. J. Numer. Methods Eng.*, (2010).

[5] G. Bauer, V. Gravemeier and W.A. Wall. A 3D finite element approach for the coupled numerical simulation of electrochemical systems and fluid flow, submitted for publication in *Int. J. Numer. Methods Eng.*, (2010).