3rd Micro and Nano Flows Conference
Thessaloniki, Greece, 22-24 August 2011

Multiscale Modeling of Physical and Biological Systems

George Em Karniadakis george_karniadakis@brown.edu

Professor of Applied Mathematics, Brown University
& Research Scientist of Mechanical Engineering, MIT

In this work I present recent developments on the Dissipative particle Dynamics (DPD) -- a method that bridges the gap between continuum and atomistic scales. In particular, I will first discuss theoretical foundations of DPD and its relation to molecular dynamics (MD) and other coarse-graining approaches, and subsequently I will describe the triple-decker algorithm [1] that interfaces continuum flow regimes with atomistic and mesoscopic regimes. Applications include functionalized surfaces (e.g., polymer brushes, glycocalyx) as well as microflows in physical and biological systems.

DissipativeParticle Dynamics (DPD) [2,3] is a mesoscopic particle method, where each particle represents a molecular cluster rather than an individual atom, and can be thought of as a soft lump of fluid. A first-principles derivation of the DPD method from the Liouville equation is presented in [4], where a direct evaluation of all forces involved was conducted based on companion molecular dynamic simulations (MD). In particular, the DPD governing equations involve three types of forces: conservative, dissipative and random forces, similar to the generalized Langevin dynamics. The first force is computed based on some soft effective potential whereas the dissipative and random pairwise forces constitute the thermostat in the system, which is local unlike the global thermostats used in MD.

Multiscale flow phenomena in microfluidic and biomedical applications require the use of heterogeneous modeling approaches. In the triple-decker algorithm [1], we present a hybrid method based on coupling MD, DPD, and the incompressible Navier-Stokes (NS) equations.MD, DPD and NS are formulated in separate sub-domains and are coupled via an overlapping region by communicating state information at the sub-domain boundaries. Imposition of boundary conditions in the MD and DPD systems involves particle insertion and deletion, specular wall reflection and body force terms. The latter includes a boundary pressure force in order to minimize near-boundary density fluctuations, and an *adaptive* shear force which enforces the tangential velocity component of boundary conditions. The triple-decker algorithm is verified for prototype flows, including simple and multi-layer fluids, using highly accurate reference solutions. A zero-thickness interface is also possible if it is aligned with the flow streamlines. However, it has not been implemented in applications with complex fluids where we have found that modified versions of DPD have been very effective, even at sub-nanometer dimensions.

For example, in two-phase flow, as the distance between two interfaces becomes zero, the continuum model becomes singular and predicts an infinite pressure, while, physically, what happens is that stochastic fluctuations of the interface get into play. Computationally, the occurrence of extremely high pressures in continuum solvers makes the discretized solution inaccurate well ahead of the point where molecular effects set in. A mesoscale approach that represents the continuum scale behavior while accounting for stochastic fluctuations is required to allow continuation of the pinch-off simulation through the singularity. In [5] we used MDPD (Many-Body Dissipative Particle Dynamics) to demonstrate the pinch-off behavior in the canonical capillary and shear breakup cases. In the last part of this work we showed how different hydrophobic or hydrophilic wetting behaviors can be reproduced by tuning the magnitude and/or the range of additional repulsive and attractive forces generated by a solid interface, see Figure 1.

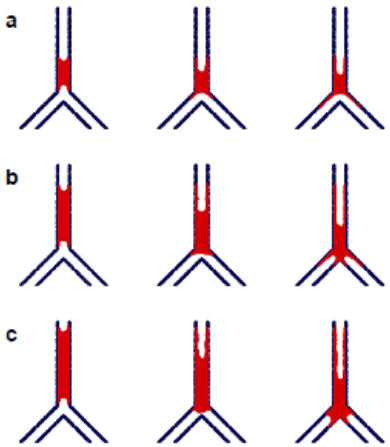

Figure 1: The dynamics of droplets entering an inverted Y-shaped fracture junction as afunction of the droplet size.

A different application is shown is shown in Figure 2, where we use DPD to model an elastic glycocalyx layer and study its compression, the resistance to flow and the slip length at the surface as well as the recoiling behavior after the passing of a white blood cell. The endothelial cell glycocalyx is a macromolecular carbohydrate extracellular matrix, consisting of proteoglycans and glycoproteins that coat the luminal

surface of the endothelial cells. It is now well recognized that the glycocalyx layer is critically involved in many bioprocesses, e.g. as a modulator for permeability in the trans-capillary exchange of water, as a mechanotransducer of fluid shear stress to the endothelial cytoskeleton and as a regulator of blood cells interactions.

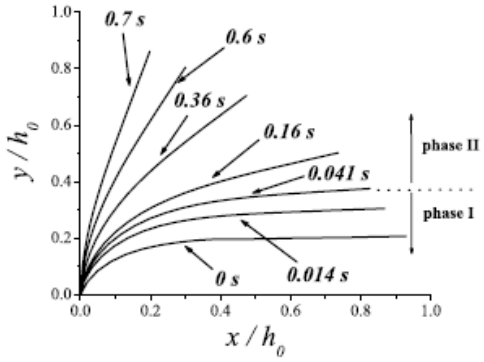

Figure 2: Time-dependent change in the shape of the glycolyx fibre, indicating two distinct phases of restoration.

The last simulation addresses malaria-infected blood flow and the pathogenicity of Plasmodium falciparum (Pf) malaria, which results from the stiffening of red blood cells (RBCs) and their ability to adhere to endothelial cells (cytoadherence). The dynamics of Pf-parasitized RBCs was studied in [6] by 3D DPD simulations of flow in cylindrical capillaries in order to predict the flow resistance enhancement at different parasitemia levels, see Figure 3.

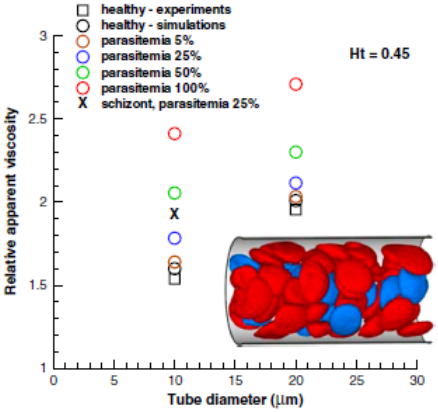

Figure 3: Flow resistance in malaria: Healthy (red) and Pf-RBCs (blue) in Poiseuille flow. Plotted is the relative apparent viscosity of blood in malaria for various parasitemia levels and tube diameters. Symbol “x” corresponds to the schizont stage with a near-spherical shape. Experimental data from the empirical fit by Pries et al. [7].

In addition, the adhesive dynamics of Pf-RBCs was explored for various parameters revealing several types of cell dynamics such as firm adhesion, very slow slipping along the wall, and intermittent flipping. The parasite inside the RBC was modeled explicitly in order to capture phenomena such as “hindered tumbling” motion of the RBC and the sudden transition from firm RBC cyto-adherence to flipping on the endothelial surface. These predictions are in quantitative agreement with recent experimental observations, and thus the three-dimensional DPD modeling method provides new capabilities for guiding and interpreting future in vitro and in vivo studies of malaria.

References

[1] Fedosov, D. and G..E. Karniadakis, *Triple-Decker: Interfacing atomistic-mesoscopic-continuum flow regimes*, J. Comp. Phys., 228:1157-1171, 2009.

[2] Hoogerbrugge, P.J., and J.M.V.A. Koelman, *Simulating microscopic hydrodynamic phenomena with dissipative particle dynamics*, Europhysics Letters 19:155-160, 1992.

[3] Groot, R. D., and P. B. Warren, *Dissipative particle dynamics: Bridging the gap between atomistic and mesoscopic simulation*, J. Chem. Phys., 107:4423-4435, 1997.

[4] Lei, H, Caswell, B., and G.E. Karniadakis, *Direct construction of mesoscopic models from microscopic simulations*, Phys. Rev. E, 81:026704, 2010.

[5] Arienti, M. et al., *Many-body Dissipative Partiocle Dynamics simulation of liquid/vapor and liquid/solid interactions*, J. Chem. Phys., 134:204114, 2011.

[6] Fedosov, D. et al, *Quantifying the biophysical characteristics of Plasmodium-falciparum-parasitized red blood cells in microcirculation*, Proc. Nat. Acad. Sciences, USA, 108:35-39, 2011.

[7] Pries AR, Neuhaus D, Gaehtgens P., *Blood viscosity in tube flow: dependence on diameter and hematocrit*, Am J Physiol 263:H1770–H1778, 1992.