

Hydrodynamic Fluctuations in Soft-Matter Simulations

PRATO, ITALY
FEBRUARY 9 – 12, 2016

The meeting “Hydrodynamic Fluctuations in Soft-Matter Simulations” [1, 2] was co-sponsored by Monash University (Melbourne, Australia), the CECAM Node “Soft Matter and Statistical Mechanics” located in Mainz, Darmstadt, and Stuttgart (Germany), and the DFG Collaborative Research Center “TRR 146: Multiscale Simulation Methods for Soft Matter Systems” (Mainz). It was co-organized by Ravi Prakash Jagadeeshan (Monash), Burkhard Dünweg (MPI for Polymer Research, Mainz) and Friederike Schmid (University of Mainz). It took place during the second week of February 2016 at the Monash University Prato Center, which is a conference center and training site in the historic Palazzo Vaj in the old town of Prato (Tuscany) near Florence. The 49 participants came from fifteen different countries from Europe, Asia, and the USA. Organizers and participants considered the meeting highly successful and fruitful. The format was a combination of an initial two-day school that was followed by a two-day research workshop.

While usual hydrodynamics is a macroscopic (thermodynamic) theory, the small length scales involved in soft-matter systems force us to take thermal fluctuations into account. This is either done via a top-down approach (Langevin noise added to the Navier-Stokes equations, simulated on a lattice or via particles), or bottom-up modeling. In the latter case (Dissipative Particle Dynamics, Multi-Particle Collision Dynamics, Lattice Boltzmann) there are additional (non-hydrodynamic) degrees of freedom, and the noise is applied to those.

To successfully apply these methods, one needs not only an efficient computer implementation, but also a thorough understanding of the underlying theory, which is typically fairly complex and advanced. The meeting recognized the need to foster communication between the various groups who typically are familiar just with one of these approaches, and also to teach the younger generation of researchers. The combined school and workshop took both of these aspects into account.

Firstly, the school comprised a cast of leading international experts who provided a thorough overview of the field. Introductory lectures on basic hydrodynamics, Langevin theory, and Landau-Lifshitz fluctuating hydrodynamics were given by Burkhard Dünweg. Piotr Szymczak then gave a detailed lecture on Brownian Dynamics with hydrodynamic interactions, including a discussion of advanced methods where high-order approximations to the interaction tensors are used. This was further elaborated by Mike Graham, who put emphasis on the general theory of Stokesian flow and the associated Green's functions, which enables the derivation of new advanced algorithms. Tony Ladd gave an introduction to Lattice Boltzmann methods, while Alexander Wagner discussed thermal fluctuations in this context. Marco Ellero gave a comprehensive lecture on “Dissipative Particle Dynamics and Smoothed Dissipative Particle Dynamics,” while Thomas Ihle explored the subtleties of “Multi-Particle Collision Dynamics”. Alejandro Garcia gave an exhaustive lecture on the old-



Figure 1: Group photo of the participants of the meeting.

This is an extract of the complete reprint-pdf, available at the Applied Rheology website <http://www.appliedrheology.org>

er (but still useful and successful) “Direct Simulation Monte Carlo Method”. In his lecture, Rafael Delgado-Buscalioni discussed the development of advanced algorithms for fluctuating hydrodynamics (grid-based Navier-Stokes solvers) with emphasis on methods to account for fluid-particle coupling. Finally, this program was complemented by Ravi Prakash Jagadeeshan's lecture on theoretical approaches to the development of closure approximations for the dynamics of polymer solutions with hydrodynamic interactions, highlighting its application to nonlinear rheology. All in all, the school provided a unique chance for graduate students and postdocs to learn about the field from amongst the foremost practitioners.

Secondly, the workshop provided an opportunity for exchange of new ideas and results, in terms of further developments of the methods, their theoretical foundations, as well as of their applications to intricate problems in soft-matter dynamics. A highlight in new method development was the talk by Robin Ball, who invented an exciting new approach to the calculation of hydrodynamic interactions by means of wavelets. Further methodological advances were provided by Aleks Donev, who discussed the coupling of Brownian Dynamics to on-the-fly Stokes solvers. Theoretical foundations were explored and refined in the talks by Pep Espanol (relation between the theory of Brownian motion and the concept of coarse-graining, with emphasis on interpolation schemes to couple “point” particles to grid solvers), Giovanni Ciccotti (rigorous theory of Non-Equilibrium Molecular Dynamics and its relation to hydrodynamics), and Thomas Ihle (kinetic theory for systems of active particles). There were several talks

on the new and emerging field of active particle suspensions (by Suzanne Fielding, Holger Stark, Thomas Ihle), while more traditional but still unresolved questions in the suspension dynamics of colloids, blood cells, and star polymers were discussed by Marco Ellero, Mike Graham, and Rafael Delgado-Buscalioni. Alexander Wagner re-visited the topic of Lattice Boltzmann simulations of spinodal decomposition, with an outlook to block copolymer systems, while Alejandro Garcia discussed intricate problems in the field of electrokinetics. Piotr Szymczak presented his recent results on the equilibrium conformations of aggregated chiral filaments, and Tony Ladd investigated the formation of caves and similar geological structures due to water flow. These contributions highlighted the importance of hydrodynamic fluctuations in soft-matter dynamics, and even more the fact that the field of non-equilibrium hydrodynamic phenomena in soft-matter systems is vast and to a large extent still poorly understood.

All in all, it was a highly enjoyable and instructive meeting, and the organizers aim to run a similar conference in a few years time.

[1] <https://www.cecarn.org/workshop-o-12o8.html>

[2] <http://users.monash.edu.au/~rprakash/cecarn2016/home.html>

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