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Discrete simulation of fluid dynamics: applications

Luca Biferale, Peter V. Coveney, Stefano Ubertini and Sauro Succi

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PREFACE

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The present two back-to-back theme issues of *Philosophical Transactions of the Royal Society A* collect a selection of papers presented at the Discrete Simulation of Fluid Dynamics (DSFD 2010) conference. This meeting was the most recent in a time-honoured series of 19 to date, which was inaugurated with the 'historical' conference at Los Alamos in 1989 [1]. DSFD 2010 took place in the central premises of the Italian National Research Council (CNR) in Rome on 5–8 July 2010. Opened by CNR President and former Director of the European Organization for Nuclear Research (CERN), Prof. Luciano Maiani, it attracted about 180 participants, with 118 presentations and 20 invited and keynote talks, making it one of the most successful to date in this series.

The DSFD series of conferences has a long and distinguished tradition. Two decades down the line, it is still a vigorous and steadily growing sector of computational physics and computational science more generally, with applications to virtually all branches of fluid dynamics, especially its growing interfaces with allied disciplines, such as chemistry, materials science, engineering, biology and most recently, both basic and clinical medicine.

Despite the numerous discoveries and technical advances that have come into existence in these two decades, many of which have been first reported at DSFD conferences, the 'spirit of DSFD' remains intact in its drive to capture the complexity of fluid flow behaviour by letting such complexity emerge naturally from the underlying micro-dynamics of appropriately simplified particle models. This bottom-up approach stands in vivid contrast with the mainstream of computational fluid dynamics, which is based on the discretization of the appropriate set of partial differential equations (PDEs) of continuum fluid mechanics (Navier–Stokes and generalizations thereof).

The DSFD approach shines most intensely whenever continuum PDE models do not exist, are theoretically unviable, or just very hard to solve on a computer, typical examples in point being multi-phase/multi-component flows, with highly space–time-dependent interfaces, and flows in complex geometries. The various advantages of the DSFD approach have been widely emphasized in the literature, and need not be revisited here.

Rather, as approaches to the discrete simulation of fluid now enter a vigorous maturity, we believe that a new synthesis best describes their place in computational fluid dynamics. Despite their many merits, discrete simulation methods are obviously not a panacea. In fact, many notions and concepts from

One contribution of 25 to a Theme Issue 'Discrete simulation of fluid dynamics: applications'.

PDE discretization have proven extremely valuable in boosting their quality and overall performance, a statement that is particularly true for the widely popular Lattice Boltzmann (LB) method, de facto a powerful blend of particle and grid methods.

This Theme Issue provides the reader with a record of the state of the art in the field and contains a wide range of contributions, covering many aspects relevant to the physics of complex flows, across many scales of motion and type of applications.

This Theme Issue is specifically devoted to applications of discrete simulation methodologies. A series of papers deals with applications of the LB method to a variety of fluid problems in science and engineering, such as turbulence, combustion, flow in porous media, suspensions of charged colloids, multi-phase flows, soft-flowing systems involving lamellar and glassy-like states with highly non-Newtonian rheology.

The remarkably broad spectrum of applications reported herein bears testimony to the amazing versatility of LB methods in addressing different applications across many scales of motion, from macroscopic turbulence, all the way down to micro and nanofluidics. A notable emerging domain embraces multi-scale haemo-dynamics, in which LB has recently demonstrated extreme scalability on petascale supercomputers, up to literally 10^5 cores, for flows of realistic complexity, such as the human arterial system. This permits simulation of full-scale arterial geometries at red-blood-cell resolution, thereby opening entirely new scenarios for clinical applications.

Besides the LB method, new applications of allied particle methods, typically dissipative particle dynamics (DPD) and smoothed particle hydrodynamics, are reported for a wide range of applications including injection moulding, together with molecular dynamics applications to nanoscopic flow problems involving DNA translocation in nanopores.

These examples further confirm versatility of particle methods to address flows whose complexity is hardly harnessed at all within the framework of continuum mechanics. On the other hand, the problem of bridging the gap to match scales of experimental interest, especially in time, still stands out as a major challenge in the field.

To this end, further multi-scale physics schemes, combining different families of methods, such as molecular dynamics or DPD with LB or Navier–Stokes solvers, need to be developed in order to attack a new class of problems, which would otherwise be inaccessible to any of these methods alone. The potential of novel multi-scale methods to tackle a qualitatively new class of problems, accounting for relevant microscopic physics within the scales of interest to modern engineering design (nanoresonators, carbon nanotubes, nanocomposites and so on) cannot be overestimated. We believe that discrete simulation approaches will have a special role to play in this important context for many years to come.

The pervasive nature of fluid flows—the fact that they are key to virtually all human activities, but also to life itself (air, water, blood)—is one of the compelling aspects of the field, as well as one of its major strengths. Just as complex fluids research is characterized by common underlying problems, so computational methods, algorithms and implementations must transcend disciplinary divides, hence the need of the new synthesis discussed earlier on in this Preface.

It is our fervent hope that physicists, mathematicians, engineers, computer scientists and, in general, all scientists working in allied fields where fluids play a major role, will be able to build on the work and experiences reported here, in order to advance their own research field.

A successful project must necessarily close with a list of grateful acknowledgements.

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Luca Biferale[1,*], Peter V. Coveney[2], Stefano Ubertini[3] and Sauro Succi[4,5]

[1] *Department of Physics and INFN, University of Roma, Tor Vergata, Via della Ricerca Scientifica 1, 00133, Roma, Italy*

E-mail address: biferale@gmail.com

[2] *Centre for Computational Science, University College London, 20 Gordon Street, London WC1H 0AJ, UK*

[3] *University of Naples 'Parthenope', DiT – Dipartmento per le Tecnologie, Isola C4 – Centro Direzionale, 80143 Napoli, Italy*

[4] *IAC-CNR, via dei Taurini 19, 00185, Roma, Italy*

[5] *Freiburg Institute for Advanced Studies, Freiburg, Germany*

*Author for correspondence.

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