Discrete simulation of fluid dynamics: methods

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This Theme Issue of *Philosophical Transactions of the Royal Society A* collects 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 the welcome speech of CNR President, and former Director of CERN, Prof. Luciano Maiani, it attracted over 180 participants, with 118 presentations and 20 invited and keynote talks, making it one of the most successful meetings of this series.

The tradition of the DSFD series of conferences is long and distinguished. 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 in 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 simply do not exist, or are 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 realistically complex geometries.

The 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 are now entering their 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 PDE discretization have proven extremely valuable in boosting their quality

One contribution of 26 to a Theme Issue 'Discrete simulation of fluid dynamics: methods'.

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 collects specific contributions to methodological advances. A substantial group of papers presents innovative developments of the LB method, targeted to a variety of subjects, such as new types of boundary conditions, transport of passive and active scalars, thermodynamic consistency, improvements of the stability using both the single-time relaxation version (Lattice Bhatnagar–Gross–Krook), as well as its multiple-time relaxation variant. Other advances concern the formulation of new LB models for Brownian suspensions and polymer flows, thermal fluctuations in multi-phase flows and haemodynamic flows with suspended biological bodies. The LB method is not limited to classical fluids, as witnessed by a few exploratory papers, dealing with relativistic quantum mechanics and even general relativity (LB on manifolds). Whether or not the success met with classical fluids can indeed be replicated in these new arenas, only time will tell. In any case, the prospects are exciting, with many potential applications, from astrophysics to cold atom research.

In addition, discrete simulation of fluid dynamics is far more than LB! Besides advances in particle/grid computational fluid mechanics, such as particle-mesh methods on multi-core graphics processing unit architectures, exciting developments in allied particle methods, typically smoothed particle hydrodynamics, particle-mesh methods for fluid flows, as well as constrained molecular dynamics, are also reported. A new class of four-dimensional (space–time) variational algorithms, tracking the unstable periodic orbits of high-dimensional nonlinear dynamical systems are described, which may disclose new avenues in computational studies of turbulence.

The pervasive nature of fluid flows—the fact that they are key to virtually all human activities, life itself in the first place (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 major wish and 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.

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

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