

Cardiff LBM workshop

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Abstracts

T1

Paul Dellar, OCIAM, Oxford

Title: Introduction to the lattice Boltzmann method

Keywords:

Abstract: This talk will give an introduction to the lattice Boltzmann method for computing solutions to the nearly incompressible Navier-Stokes equations. The approach will focus on the construction of numerical schemes to solve known sets of partial differential equations. It will emphasise the parallels between discrete kinetic theory and the classical continuous kinetic theory, and the derivation of the Navier-Stokes equations from systems of moment equations.

T2

Peter Coveney, UCL, London

Title: Applications of petascale lattice-Boltzmann simulations in fundamental nanomaterials science, turbulence and cerebro-vascular haemodynamics

Keywords: kinetic lattice-Boltzmann, liquid crystal rheology, turbulence, haemodynamics, computational biomedicine, petascale computing

Abstract: We present various lattice-Boltzmann schemes to investigate fundamental and applied problems in three disparate fields - nanomaterials science, turbulence and cerebro-vascular haemodynamics.

We use a kinetic lattice-Boltzmann algorithm for amphiphilic systems to simulate the self-assembly into and rheology of nanoscale cubic liquid crystals. These materials are rapidly gaining importance in functional materials design for the production of high-efficiency photovoltaic devices, in protein crystallization and as delivery agents for biomedical and consumer products applications. The kinetic lattice-Boltzmann method has been extensively by us to investigate the rheology of these materials and the simulated response is in good agreement with corresponding experimental observations. Performing lattice-Boltzmann simulations on large lattices allows for the treatment of physically realistic, defect-containing liquid crystalline systems in contrast to smaller lattices where, due to finite-size effects, self-assembly of 'perfect crystals' is obtained. In nature, the distribution of defects within a liquid crystal domain is known to play a significant role in its rheology and we aim to gain insight into defect dynamics under shear from these very large lattice sizes.

In our work on fundamental turbulence research, we compute and catalogue principal unstable periodic orbits (UPOs) of the driven Navier-Stokes equations in two and three dimensions which are solved using the lattice-Boltzmann method. UPOs are generic features of driven dissipative systems

exhibiting chaos in low-dimensional dynamical systems, such as the Lorenz equations and shell models of turbulence and in infinite-dimensional systems such as the driven Navier-Stokes equations. These UPOs provide us with a fertile representation of the chaotic dynamics on the attractor of this system and it has been predicted that a relatively small number of UPOs will enable good statistical predictions of turbulent flow from first principles. In this scheme, we implement a variational algorithm which relaxes the periodic orbits to satisfy the driven Navier-Stokes equation, thus extending the parallelism to time in addition to the 3D space parallelization. By computing and cataloguing some of the lowest-period unstable periodic orbits in the driven Navier-Stokes equations, using the novel 4D scheme which is parallel in spacetime, we aim to calculate turbulent averages of observables from first principles.

In the biomedical domain, we use a high-performance lattice-Boltzmann code for haemodynamics simulations coupled with *in situ* visualization, real-time computational steering and other modalities of distributed computing to provide an efficient computational environment to assist interventional neuroradiologists in neurovascular surgery, providing information on patient-specific haemodynamics which would otherwise not be available. The prime aim of this research is to provide these results within clinically relevant time frames: data acquisition to final visualization of results takes 15 to 20 minutes. These simulations are patient-specific since the neurovasculature differs considerably from person to person.

The inherent scalability of the lattice-Boltzmann algorithm has allowed these codes to scale to tens of thousands of cores making this approach suitable for the computationally demanding applications described here. Our computational algorithms combined with software tools for workflow management and analysis have enabled us to perform simulations on the new generation of petascale resources arriving in the US.

T3

Ian Halliday, Sheffield

Title: Lattice Boltzmann equation for multiple immiscible fluids

Keywords: $N > 2$ mutually immiscible fluids, continuum regime, immersed boundary force scheme, adapted multiple relaxation time scheme

Abstract: This presentation will introduce, then briefly analyse, a variant of our lattice Boltzmann equation simulation algorithm for two fluids, based on coupled phase fields and body forces. We will show how key attributes of the new technique allow its generalization to the case of $N > 2$ mutually immiscible, continuum fluids. Subsequent consideration of appropriate interface configurations which emerge in simulation lattice regions which correspond to a three-fluid contact point, and the consistency of these configurations with the Laplace-Young law motivate further developments, which are then discussed. The result in a method which, in principle, accommodates any number of mutually immiscible fluids with properties specified by interfacial tension, contact angle and, of course, kinematic viscosity. The presentation will conclude with brief survey of the advantages and disadvantages of the method.

T4

Kai H Luo, Southampton

Co-authors: Daniel Lycett-Brown, Ernesto Monaco

Title: LBM of multiphase flow

Keywords: Multiple-relaxation-time LBM, entropic LBM (ELBM), multispeed LBM, droplet collisions

Abstract: Multiphase flow is ubiquitous in energy and environmental systems, which presents challenges for almost all types of numerical simulation methods. LBM has unique strengths and weaknesses for simulating multiphase flow. Starting from the basic Shan-Chen multiphase LBM model,

we explore various ways to improve the accuracy and stability of LBM formulations with the ultimate aim of simulating realistic multicomponent, multiphase flow without or with chemical reactions. Using the binary droplet collision as a physical model, we study the capabilities of the various formulations including a multiple-relaxation-time LBM, an entropic LBM as well as effects of equation of state and grid refinement. The current status is reviewed and further work is suggested.

T5

Tim Reis, Oxford

Title: A stochastic sharpening approach for the pinning and facetting of sharp phase boundaries in multiphase lattice Boltzmann simulations

Keywords: pinning; stiff PDEs; multiphase flow

Abstract: We present a model for the pinning and facetting of sharp phase boundaries in multiphase lattice Boltzmann simulations. A discrete Boltzmann equation with an additional source term responsible for the sharpening of phase boundaries is postulated, from which explicit lattice Boltzmann equations (LBEs) are formulated in one and two dimensions. Cubic source terms with two stable fixed points and an unstable (critical) point are considered. Numerical simulations show that, despite being a purely kinematic model, this LBE exhibits the phenomena of pinning and facetting observed in other multiphase lattice Boltzmann models. A modified source term which replaces the critical point with a uniformly distributed random variable is suggested. The statistical average of this method corrects the interface propagation speed.

T6

David R Emerson, STFC, Daresbury

Co-authors: Xiao-Jun Gu, Gui-Hua Tang, Robert W. Barber, Jason M. Reese*, Yong-Hao Zhang*

*Department of Mechanical Engineering, University of Strathclyde, Glasgow

Title: Developing methodologies to capture the flow physics of low-speed rarefied flows – a review and discussion of challenges and some success using the lattice Boltzmann method

Keywords: low-speed flows, MEMS, rarefied gas flow

Abstract: The kinetic pedigree of the lattice Boltzmann method, coupled with its intrinsically mesoscopic nature, makes it an ideal approach to explore the physics of rarefied gases at very low speeds. In particular, the rapid development of micro-electro-mechanical systems (MEMS) has created an urgent requirement to understand gaseous transport for devices that incorporate components with extremely small length scales (ranging from 0.1 – 100 microns) but operating at atmospheric pressure. Under such conditions, gases exhibit rarefaction phenomena and the conventional Navier-Stokes equations begin to break down. We will review the challenges associated with modelling non-equilibrium (rarefied) gas behaviour and present some recent results obtained using the lattice Boltzmann method and other numerical strategies, such as the Method of Moments and direct simulation Monte Carlo (DSMC).

T7

Yonghao Zhang, Strathclyde

Co-author: Jianping Meng

Department of Mechanical Engineering, University of Strathclyde, Glasgow

Title: High-order lattice Boltzmann approach and discrete velocity method for non-equilibrium gas dynamics

Keywords: non-equilibrium flow, rarefaction, kinetic theory, discrete velocity method

Abstract: A theoretical frame was established by Shan et al. (2006) to develop high-order lattice Boltzmann models to capture rarefaction effects in non-equilibrium gas flows. Both high-order Hermite expansion and Gauss-Hermite quadrature are required to describe non-equilibrium phenomena. Here, we show that this approach is essentially equivalent with the

discrete velocity method of directly solving the linearised Bhatnagar-Gross-Krook (BGK) equation if the same Gauss-Hermite quadrature is used. Our theoretical and numerical analysis confirm that the order of Hermite expansion is not correlated with the approximation order in terms of the Knudsen number. The Gauss-Hermite quadrature has most significant effect on the model accuracy.

Shan X, Yuan X-F, and Chen H (2006) Kinetic theory representation of hydrodynamics: a way beyond the Navier-Stokes equation. *J. Fluid Mech.* 550, 413-441.

T8

Jon Summers and Mark Wilson, Leeds

Title: Predictions of dynamic wetting phenomena using a multiphase lattice Boltzmann method

Keywords: Contact line dynamics, wetting failure, hysteresis, droplet dynamics

Abstract: Wetting is a fundamental feature of many natural and engineered processes. As in any practical application, modelling is highly desirable as a means of improving understanding or testing designs, particularly where experimental research is too difficult, dangerous or costly. Despite its practical importance, genuinely predictive modelling of wetting has yet to be achieved. This talk will discuss the length scales affecting wetting behaviour and will outline the difficulties involved in continuum-based modelling that have driven our interest in the lattice Boltzmann method as a potentially more predictive simulation approach, especially for non-uniform surfaces. Preliminary LB results on the prediction of dynamic contact angles, contact angle hysteresis, and wetting failure will be presented, along with some observations of the effect of the liquid-gas interface thickness on the results.

T9

Sauro Succi, IAC-CNR, Rome

Co-authors: M. Bernaschi(1), S. Melchionna(2), Sauro Succi(1,3), and E. Kaxiras(2)

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(2) School of Engineering and Applied Sciences, Harvard University

(3) Initiative in Innovative Computing at Harvard

Title: Lattice Boltzmann simulations of large-scale cardiovascular flows

Keywords: multiscale hemodynamics, parallel and GPU computing

Abstract: The multiscale Lattice Boltzmann-Molecular Dynamics code MUPHY has been recently equipped with the full sequence of computational procedures required for the complete analysis of anatomically accurate cardiovascular flows. Large scale simulations, with up to two hundred millions cells shall be discussed and commented on.

T10

Oliver Henrich, Edinburgh

Title: Lattice Boltzmann studies of blue phases in cholesteric liquid crystals

Keywords: condensed matter, complex fluids

Abstract: Blue Phases (BPs) are equilibrium phases in chiral nematic liquid crystals containing a lattice of disclinations. They are found in thermotropics close to the cholesteric-isotropic transition. While older experiments typically observed BPs only in a very narrow temperature range of about 1 K, more recent ones have created BPs over a strikingly wide temperature range of 50K. This opens up a completely new field of possible future applications. However, for this exciting potential to be fully realised, we need the theoretical understanding of BPs to advance at the same pace. In particular, to study the switching dynamics of real world BP devices, large simulations are necessary as the lengthscale of the disclination network is in the region of visible light.

Here we present extensive lattice Boltzmann simulation results from which we derive a phase diagram of BPs in electric fields. For increasing field strengths the phase diagrams exhibit increasingly large domains of planar and three-dimensional hexagonal BPs. Moreover, by simulating quenches of large systems into the cholesteric phase, we suggest a structure for BPIII (also known as blue fog). Our first supra-unit cell simulations of BPs are strongly in favour of theoretical arguments which suggest BPIII to be an amorphous disclination network, possibly with partially ordered domains.

T11

Paul Dellar, OCIAM, Oxford

Title: Lattice Boltzmann approaches to magnetohydrodynamics and electromagnetism.

Keywords: matrix collision operators, multiple-relaxation-time (MRT) collision operators, moment equations, magnetohydrodynamics, plasmas, electromagnetism

Abstract: We present a review of recent developments in lattice Boltzmann approaches to magnetohydrodynamics and electromagnetism, concentrating on the author's formulation that expresses the magnetic field using a set of vector distribution functions. These distribution functions were first postulated to evolve according to a vector Boltzmann equation with a BGK collision operator. A Chapman-Enskog expansion then leads to the equation that describes the evolution of the magnetic field under resistive magnetohydrodynamics. This formulation has been used in large-scale simulations of magnetohydrodynamic turbulence.

However, resistive magnetohydrodynamics arises from one of the simplest forms of the Ohm's law that relates the electric field to the magnetic and velocity fields. Introducing a complete set of moments for the magnetic distribution functions, we may construct more complex matrix collision operators that allow us to simulate magnetohydrodynamics with current-dependent resistivity (as used to model unresolved plasma microturbulence), Hall magnetohydrodynamics, and even electromagnetic waves. In particular, there are collision operators that allow us to recover the full Maxwell equations together with Ohm's law.

Similarly, by designing a hydrodynamic matrix collision operator that depends upon the magnetic field, we may simulate Braginskii's magnetohydrodynamics with different viscosities parallel and perpendicular to the magnetic field lines.

T12

Yuntian Feng, Swansea

Co-authors: K. Han and D.R.J. Owen
Civil and Computational Engineering Centre, School of Engineering Swansea University

Title: The combined lattice Boltzmann and discrete element method: theory and applications

Keywords: fluid-particle interaction, magnetohydrodynamics

Abstract: Solid particle transport in fluid flows can be found in a wide range of applications in science and engineering. The complexity involved in the physical phenomenon imposes a real challenge to develop effective numerical modelling strategies. This talk aims to review the so called combined Lattice Boltzmann (LBM) and Discrete Element (DEM) approach which appears to provide an ideal numerical simulation framework for the problem, in which LBM is used to model incompressible fluid flows; DEM is to model the motion of and the interaction between the solid particles; and the hydrodynamic interaction between the fluid and particles are accounted for by utilisation of an immerse boundary technique. The methodology has been extended to include additional physical fields such

as thermal and electric/magnetic as well. Several applications in mining operations, biomechanics, smart fluids, and fluidised bed will be demonstrated.

T13

Kevin Stratford, Edinburgh

Title: Shear flow in binary liquids

Keywords: condensed matter, complex fluids

Abstract: I will describe some recent efforts to study shear flow in binary fluids in two and three dimensions. The work has used both 'full' lattice-Boltzmann, and hybrid lattice-Boltzmann finite-difference methods to represent the binary fluid, and is used as a starting point to look at more complex systems. I will also introduce briefly current work to extend the work to sheared particle suspensions.

T14

Xiaowen Shan, Exa Corp., Burlington, MA, USA

Title: Kinetic representation of hydrodynamics: New prospect of lattice Boltzmann method

Keywords: compressible flows, high-Knudsen number flows

Abstract: The lattice Boltzmann method (LBM) has traditionally been developed as a derivative of the somewhat simplistic fluid model known as the Lattice Gas Cellular Automaton. The recently identified kinetic theory connection and reformulation of LB as equivalence to a moment solution to the BGK equation has provided a sound theoretical framework for understanding and analyzing LBM models. Many of the old restrictions of LBM, e.g., limitations in simulating thermodynamic effects, compressible flows, and flows with high Knudsen numbers, have now been lifted and pathways to new application domains paved. In this presentation, I shall give a brief summary of the kinetic theory approach to the LBM and discuss the prospect of LBM as a discrete-velocity kinetic theory method, e.g., its applications in simulations of compressible flows and high-Knudsen number flows beyond the applicable domain of the Navier-Stokes equations.

T15

Alexander Vikhansky, Queen Mary University of London

Title: Lattice-Boltzmann method for non-Newtonian and non-equilibrium flows

Keywords: Bingham liquids, thermal creep, Knudsen compressor

Abstract: We use a unified approach in order to construct LB schemes for non-Newtonian and rarefied gas flows. The results of the calculations are compared with the available analytical solutions (viscoplastic flows) and with the results of the direct Monte Carlo simulations (rarefied gas flows). The LB method is used in order to consider the effect of yield stress on Rayleigh-Bénard convection of a viscoplastic material and the flow of a rarefied gas through Knudsen compressor.

T16

Tim Phillips, Cardiff

Title: Lattice Boltzmann models for axisymmetric flows

Keywords: axisymmetric flows, pipe flow

Abstract: The 2D Navier-Stokes equations in cylindrical coordinates cannot be solved directly using standard 2D lattice Boltzmann methods. However, the inclusion of a spatially and temporally varying source term in the 2D lattice Boltzmann equation allows the axisymmetric Navier-Stokes equations to be recovered in the macroscopic limit. A number of different source terms for achieving this limit have been proposed in the literature. In this paper we will chart the historical development of the subject and describe the main differences between the methods that have been proposed. Some numerical results for benchmark problems will be presented to validate the accuracy of these techniques.

T17

Gareth Wyn Roberts, Cardiff

Title: Non-Newtonian flows

Keywords: generalised Newtonian fluids, variable viscosity, axisymmetric flows

Abstract: A general framework for the simulation of two-dimensional and axisymmetric flows of generalised Newtonian fluids is presented. The software uses lattice-based methods and incorporates Newtonian and generalised Newtonian behaviour. The code is verified in simple geometries by comparison with analytical solutions. We demonstrate the application of the code to the flow of different non-Newtonian fluids in non-trivial geometries and compare results from different rheological models.