Conference Agenda

The Sixteenth International Conference for Mesoscopic Methods in Engineering and Science

Date: Monday, 22/Jul/2019

9:30am - 10:45am	**SC1: Short Courses 1**
Wolfson Room, 2nd Floor	

On the structure of the distribution functions in kinetic schemes for continuum flows

Wang, Lian-Ping
SUSTech, China, People's Republic of

This short course gives a self-consistent introduction of the structure of the distribution functions in kinetic schemes. Starting from the continuous Boltzmann equation with the BGK collision model and an external force field, the structure of the distribution functions, in terms of the macroscopic variables, is derived by combining the Chapman-Enskog expansion and Gauss-Hermite quadrature. The results reveal basic requirements for a kinetic scheme to reproduce the hydrodynamic equations of the continuum flows at different levels of approximation. Next, the structures of distribution functions solved in discrete schemes, such as the lattice Boltzmann method and the discrete unified gas kinetic scheme, are derived. The derivations provide insights on how to properly implement the external force in kinetic methods, the implementation of no-slip boundary conditions, and the level of numerical dissipation in discrete kinetic methods.

9:30am - 12:00pm	**On-site registration**
PG01	
10:45am - 11:00am	**Coffee Break**
PG01	
11:00am - 12:15pm	**SC2: Short Courses 2**
Wolfson Room, 2nd Floor	

Orthogonalization in lattice Boltzmann models with multiple relaxation rates

Geier, Martin
TU Braunschweig, Germany

Lattice Boltzmann method with multiple relaxation times have been proposed with many different moment bases. It is generally agreed that moments relaxing with different rates should be independent of each other which lead to a wide range of different orthogonalization techniques. The disagreement between these methods in literature is due to an unprecise objective as to what the orthogonalization is supposed to achieve. In this lecture we review some of these techniques. In particular we contrast weighted and unweighted orthogonalization with self-orthogonalizing cumulants.

12:15pm - 1:45pm	**Lunch**
PG01	
1:45pm - 3:00pm	**SC3: Short Courses 3**
Wolfson Room, 2nd Floor	

Lattice Boltzmann algorithms using vector distribution functions - theory and applications

Dellar, Paul John
University of Oxford, United Kingdom

This short course will describe lattice Boltzmann algorithms for a fluid coupled to a system best described by a set of vector-valued distribution functions, analogous to replacing the usual point particles with populations of small magnets. It will survey initial applications to fluids coupled to electromagnetic fields, then cover recent extensions to model suspensions of orientable particles, including fibre suspensions, ferrofluids, active matter and liquid crystals. The machinery that makes these possible is based on the Strang splitting approach to discretising the Boltzmann equation that can accommodate a wide range of more complex and nonlinear collision operators, including coupling the vector degrees of freedom to the hydrodynamic strain field via moments of the non-equilibrium distributions.

2:00pm - 6:00pm **Poster**

PG01

Modelling double emulsion formation in planar flow-focusing microchannels

Wang, Ningning[1]; Semprebon, Ciro[2]; Liu, Haihu[3]; Zhang, Chuhua[3]; Kusumaatmaja, Halim[1]

[1]Department of Physics, Durham University, South Road, Durham DH1 3LE, UK; [2]Smart Materials and Surfaces Laboratory, Department of Mathematics, Physics and Electrical Engineering, Ellison Place, Northumbria University, Newcastle upon Tyne, NE1 8ST, UK; [3]School of Energy and Power Engineering, Xi'an Jiaotong University, Xi'an 710049, China

Double emulsion formation in a hierarchical flow-focusing channel is systematically investigated using a free energy ternary lattice Boltzmann model. A three dimensional formation regime diagram is constructed based on the Weber number of the inner phase, and the capillary numbers of the middle and outer phases. The results show that the formation diagram can be classified into periodic two-step region, periodic one-step region, and non-periodic region. By varying Weber number of the inner phase and the capillary number of the middle phase, different morphologies are obtained in the two- step formation region, including the regular double emulsions, decussate regimes with one or two alternate empty droplets, and structures with multiple inner droplets contained in the continuous middle phase thread. Bidisperse behaviors are also frequently encountered in the two-step formation region. In the periodic one-step formation region, scaling laws are proposed for the double emulsion size and for the size ratio between the inner droplet and the overall double emulsion. Furthermore, we show that the interfacial tension ratio can greatly change the morphologies of the obtained emulsion droplets, in agreement with experimental observations.

Reference:

[1] N. Wang, C. Semprebon, H. Liu, C. Zhang and H. Kusumaatmaja, submitted (2019).

3D flow through flexible vessels using a hybrid lattice Boltzmann-finite element method

Wang, Haifeng[1]; Krüger, Timm[2]; Varnik, Fathollah[1]

[1]The Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), RUB, Germany; [2]School of Engineering, University of Edinburgh, Scotland, UK

A variety of important biological and industrial processes involve transport of fluids in rigid or elastic tubes. Blood flow through an artery (tubular organ) is one of the prominent examples. In this work, the lattice Boltzmann method (LBM) is combined, via the immersed boundary approach, with the finite element method (FEM) to account for fluid-structure interactions. The LBM is used for solving fluid dynamics and the FEM for wall mechanics. The accuracy of the hybrid method in recovering both the Poiseuille solution for steady flow and the Womersley solution for pulsatile flow in a circular rigid tube is demonstrated. Furthermore, the deformation behavior of a flexible tube under the effect of Laplace pressure is studied and tested by comparison, in the limit of low strain, to an independent numerical solver, SimVascular, which is based on a simple linear elastic model. The model is then applied to study time-dependent flow through flexible vessels with heterogeneous elastic properties.

Differential diffusivity effects on dissolution-driven density instability of reactive flow in porous media

Lei, Timan; Luo, Kai H.

University College London, United Kingdom

Dissolution-driven density instability (DI) occurs when a species A dissolves into a host fluid and introduces a buoyantly unstable stratification. This instability accompanied by convection can drive efficient mass and heat transport, which is encountered in diverse fields like groundwater management, enhanced oil recovery, and carbon dioxide sequestration. During dissolution, species A may react with solute B in the host fluid to yield product C, and these three chemical species may have different dissolution coefficients. Such a reaction can subsequently modify the density field and influence the development of density fingering in porous media. For this phenomenon, some investigations have been previously carried out based on the representative elementary volume models, but pore-scale studies are still very rare. Besides, in previous numerical simulations, these chemical species were always assumed to diffuse at the same rate, even though differential diffusion may play an important role.

The lattice Boltzmann (LB) method is an attractive alternative to conventional solvers for studying various fluid flows at pore scale. This attributes to its simple implementation, high parallelism, and ability to handle complex boundary conditions. To fill the gaps in existing numerical investigations, the LB method is applied to simulate the dissolution-driven DI coupled with chemical reaction A+B→C and differential diffusivity effects in porous media at pore scale. Different types of density profiles (or fingering dynamics) are classified based on the Rayleigh numbers and diffusion coefficients of three chemical species. The influence of differential diffusivity on fingering behaviours is quantified by the mixing length, the reaction rate, the dissolution flux of species A, and the total amount of stored A in the host fluid. The numerical results show that varying the diffusion coefficients of three chemical species can significantly influence the development of density fingering and the storage of species A.

3:00pm - 3:15pm **Coffee Break**

PG01	
3:15pm - 4:30pm	**SC4: Short Courses 4**
Wolfson Room, 2nd Floor	

Simulation of rarefied gas flows using half-range quadratures

Ambrus, Victor E.
West University of Timisoara, Romania

In kinetic theory, boundary conditions at solid walls can be prescribed only for the distribution of particles travelling back towards the fluid. Since the particles travelling towards the wall are essentially arbitrarily distributed, a discontinuity develops in the distribution function f at the level of the velocity space. This course is focussed on employing half-range quadratures to discretise the velocity space, highlighting the dramatic increase in simulation efficiency compared to the case when full-range quadratures are employed. Since access to higher order moments of f are required to describe the Knudsen layer physics, the velocity set must be enlarged as the Knudsen number Kn increases. Since exact streaming becomes problematic, one has to resort to finite difference techniques to compute the advection.

4:30pm - 5:45pm	**SC5: Short course 5: Short Course 5**
Wolfson Room, 2nd Floor	

Gas-kinetic schemes for continuum and multiscale flows

Wang, Lian-Ping[1]; Guo, Zhaoli[2]
[1]SUSTech, China, People's Republic of; [2]Huazhong University of Science and Technology, China, People's Republic of

Gas kinetic schemes (GKS's) are a class of CFD methods based on kinetic theory, and have gained much success in flow simulations ranging from continuum compressible flows to rarefied non-equilibrium flows. As a type of kinetic method, GKS's have rich dynamics beyond the classical CFD methods based on the Euler and Navier-Stokes equations. This lecture gives an introduction of the GKS methods, including the original GKS for continuum flows and its recent variants for multiscale flows. Specifically, the lecture consists of four parts: Part 1 reviews the GKS for continuum flows, which is a finite-volume scheme where the numerical flux at cell interface is constructed based on the particle distribution function. With the Chapman-Enskog approximation of the distribution function, only macroscopic flow variables are required to be updated in this GKS. Some analysis of the dissipative property of the GKS is also provided. Part 2 briefly introduces the recently developed Unified Gas Kinetic Scheme (UGKS) for multiscale flows, which is an extension of the original GKS, In UGKS both macroscopic flow variables and distribution functions with discrete velocities are updated, and no Chapman-Enskog approximation is invoked. Part 3 gives an introduction of another UGKS for multiscale flows, namely the Discrete UGKS (DUGKS), which combines the advantages of GKS and the lattice Boltzmann equation (LBE) method. With a discrete representation of the distribution function, DUGKS is much simpler and easier to code than the UGKS. Some comparisons between DUGKS, UGKS, and LBE are also reported. Part 4 focuses on the implementation details of the DUGKS, and a sample code for the cavity flow is provided. Numerical results for some multiscale flows are also shown in this part. A brief summary and some key references are given finally.

5:45pm - 7:00pm	**Q&A for short courses: Questions and Discussions**
PG01	

Date: Tuesday, 23/Jul/2019

9:30am - 9:50am	**Welcome**
PG01	Session Chair: **Baixin Chen**, Heriot-Watt University Session Chair: **Li-Shi Luo**, CSRC
9:30am - 1:00pm	**On-site registration**
PG01	
9:50am - 11:10am	**Phase-Field othe Other Methods for Complex Fluids**
Wolfson Room, 2nd Floor	Session Chair: **Baixin Chen**, Heriot-Watt University

Thermodynamically consistent phase-field modelling for two-phase flows and moving contact line problems and their energy law preserving computational methods

Lin, Ping
University of Dundee, United Kingdom

We develop a phase-field model for the binary incompressible (quasi-incompressible) fluid with thermocapillary effects, which allows for the different properties (densities, viscosities and heat conductivities) of each fluid component while maintaining thermodynamic consistency. The governing equations of the model including the Navier-Stokes equations with additional stress terms, Cahn-Hilliard equations and energy balance equation are derived within a thermodynamic framework based on entropy generation, which guarantees thermodynamic consistency. A sharp-interface limit analysis is carried out to show that the interfacial conditions of the classical sharp-interface models can be recovered from our phase-field model. Energy law preserving finite element methods are developed for the variable density case. The modelling and computational method are also applied to moving contact line problems. A few illustrative computational examples will be presented as well.

A Comparative Study of Phase-Field LBM and ALE interface-conforming FEM for Interface Dynamics

Zhang, Changjuan; Fakhari, Abbas; Li, Jie; Luo, Li-Shi; Qian, Tiezheng
CSRC, China, People's Republic of

We conduct a comparative study for two methods for interfacial flows: an arbitrary Lagrangian-Eulerian (ALE) finite-element method (FEM) on interface-conforming meshes and a phase-field lattice-Boltzmann method (LBM) on Cartesian meshes with quadtree adaptive mesh refinement (AMR). The methods are validated by simulations of a bubble without and with buoyancy force. In particular, the dynamics of an oscillating bubble due to its initial nonequilibrium shape and a rising bubble driven by buoyancy force are simulated to compare two methods quantitatively. Simulations of the breakup of a rising bubble and the bubble interaction with a horizontal plate are used to quantify the efficacy and efficiency of the two methods. It is observed that the phase-field LBM is more dissipative due to the nature of the diffuse-interface method used to capture the interfaces. Overall, the results obtained from both methods agree well with each other when the effects due to the numerical artifacts intrinsic to the diffuse-interface method can be neglected. Also, the LBE method is in general far more efficient and easier to parallelized.

Phase-field-based lattice Boltzmann model for immiscible incompressible N-phase flows

Yuan, Xiaolei[1,2]; Liang, Hong[3]; Chai, Zhenhua[1,2]; Shi, Baochang[1,2]
[1]School of Mathematics and Statistics, Huazhong University of Science and Technology, Wuhan, 430074, China; [2]Hubei Key Laboratory of Engineering Modeling and Scientific Computing, Huazhong University of Science and Technology, Wuhan, 430074, China; [3]Department of Physics, Hangzhou Dianzi University, Hangzhou, 310018, China

In this paper, we develop an efficient lattice Boltzmann (LB) model for simulating immiscible incompressible N-phase flows $(N \geq 2)$ based on the Cahn-Hilliard phase field theory. In order to facilitate the design of LB model and reduce the calculation of the gradient term, the governing equations of the N-phase system are reformulated, and they satisfy the conservation of mass, momentum and the second law of thermodynamics. In the present model, $(N-1)$ LB equations are employed to capture the interface, and another LB equation is used to solve the Navier-Stokes (N-S) equations, where a new distribution function for the total force is delicately designed to reduce the calculation of the gradient term. The developed model is first validated by two classical benchmark problems, including the tests of static droplets and the spreading of a liquid lens, the simulation results show that the current LB model is accurate and efficient for simulating incompressible N-phase fluid flows. To further demonstrate the capability of the LB model, two numerical simulations, including dynamics of droplet collision for four fluid phases and dynamics of droplets and interfaces for five fluid phases, are performed to test the developed model. The results show that the present model can successfully handle complex interactions among N ($N \geq 2$) immiscible incompressible flows.

11:10am - 11:30am	**Coffee Break**

PG01

11:30am - 1:10pm

PG01

Method and Analysis I

Session Chair: **Paul John Dellar**, University of Oxford

Studying the Settling Behaviour of Arbitrarily Shaped Particles with a Homogenised Lattice Boltzmann Approach

Trunk, Robin[1,2]; Nirschl, Hermann[2]; Krause, Mathias J.[1,2,3]

[1]Lattice Boltzmann Research Group (LBRG), KIT, Germany; [2]Institute for Mechanical Process Engineering and Mechanics (MVM), KIT, Germany; [3]Institut for Applied and Numerical Mathematics 2 (IANM2), KIT, Germany

The investigation of particle settling with results relevant for applications requires flexible methods capable of efficient simulations taking the actual shape of particles into account. To produce reliable results high resolutions, for correct depiction of the particles, are required as well as large computational domains to consider large quantities of particles. With the definition of particle shape parameters like sphericity or elongation, dependencies are deducted by a statistical investigation of the simulation results. This enables finally to increase separation efficiency and selectivity in industrial processes.

The object of this investigation are symmetrical shapes generated according to simplified surface parameterization described by Vogelgesang [1].

Here the revisited homogenised lattice Boltzmann method (HLBM) proposed by Krause et al. [2], which considers objects as moving porous media, is applied. The method, recently extended for 3D simulation of suspensions with arbitrarily shaped particles [3], allows the automated processing of surface geometry data, e.g. gained from the processing of computer tomography scans. All computations have been performed with the open-source library OpenLB [4].

In the improved method, the coupling between fluid and object is handled by a local exchange of momentum, leading to a momentum-conserving two-way-coupled system. The computational method is validated by means of comparisons of exemplary simulations to results in literature, e.g. considering the terminal settling velocity of a spherical particle, as well as a sophisticated convergence analysis.

REFERENCES

[1] R. Vogelgesang, Global Surface Parameterization by Smooth Facet Selection, Journal of Computational and Theoretical Nanoscience 8 (2011) 1—8

[2] M. J. Krause, F. Klemens, T. Henn, R. Trunk, H. Nirschl, Particle Flow Simulations with Homogenized Lattice Boltzmann Methods, Particuology 34 (Supplement C) (2016) 1—13

[3] R. Trunk, J. Marquardt, G. Thäter, H. Nirschl, M.J. Krause, Towards the Simulation of arbitrarily shaped 3D particles using a homogenised lattice Boltzmann method, Computers & Fluids 172 (2018) 621—631

[4] OpenLB, Open Source Lattice Boltzmann Code, http://www.openlb.net

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General third order Chapman-Enskog expansion of lattice Boltzmann schemes

Dubois, François

Univ. Paris Sud, Orsay, France

With the general framework of multi relaxation times lattice Boltzmann schemes, we follow in this contribution the Chapman-Enskog formalism proposed by Chen-Doolen and Qian-Zhou. We suppose that there is some infinitesimal parameter and we expand the nonconserved moments as differential nonlinear function of

the conserved variables and we suppose that a multi-scale approach is present for the time dynamics.

Then we prove that the conserved quantities follow the following multi-time dynamics :

dW/dt1 + G1 = 0, dW/dt2 + G2 = 0, dW/dt3 + G3 = 0.

The differential operators G1(W), G2(W) and G3(W) of this expansion are recursively determined. They are exactly the ones derived in our fourth order expansion of lattice Boltzmann schemes with the Taylor expansion method ("Nonlinear fourth order Taylor expansion of lattice Boltzmann schemes", Hal archives ouvertes hal-02081116 and arXiv 1903.12417, march 2019).

The author thanks Bruce Boghosian and Pierre Lallemand for enlighting disussions in Medford (MA, USA) in July 2018 and in Paris (France) in April 2019.

A new coupled HMC constitutive model with consideration of swelling and dissolution based on mixture coupling theory

Ma, Yue; Chen, Xiaohui; Stewart, Doug; Yu, Hai-sui

School of Civil Engineering, University of Leeds, UK

Modelling of coupled hydro (H)-mechanical (M)-chemical (C) processes in Geomaterials has tract attention because of many important engineering applications (e.g. nuclear waste disposal, carbon capture and storage). The molecular scale interaction between fluid and solid (e.g. swelling and dissolution,) has significant influence on the mechanical behaviour of the materials, but are rarely incorporated into the HMC framework. This paper has extended mixture coupling theory establishing

a new HMC framework by including hydration swelling and dissolution of minerals. Helmholtz free energy is used to give the relationship between solids and fluid. The evolution of stress and pore volume fraction are obtained by analysing the free energy density of the wetted matrix. Entropy is used to give the dissipation of the fluids transport process. Using classic continuum mechanics, the final governing equation has been derived. A simple numerical simulation has been given to illustrate the influence of combined swelling and dissolution, shows the combination of swelling and dissolution strongly affects the stress and displacement variations

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Reduced Order Statistical Emulator for Turbulent flows

Gairola, Abhinav; Bindra, Hitesh
Kansas State University, United States of America

Natural systems described by the canonical partial differential equations often reside in a high dimensional space. However, each individual trajectories of the system which carry an important aspect of the behavior of the system may itself reside in a low dimensional space. For the case of Navier-Stokes equation each particle trajectory in a lagrangian systemtend to follow some scaling law (K-41 predicts $\frac{5}{3}$ scaling of energy spectrum in the inertial range and the analytically derived $\frac{4}{5}$ law for the third order structure function) in the inertial range. This behavior changes in the viscous dissipative regime where the small scale turbulent flow structures show non-Gaussian behavior and intermittency. This leads to a regime where the K-41 theory does not seem to predict the correct scaling of the structures present in the velocity signal. Therefore, it can be perceived that a turbulent signal contains a complicated interaction of micro, meso and macro-scales. We exploit these physical characteristics of the turbulence and to build a meso-scopic description of it by constraining a non-linear Langevin equation directly on the data via Kramers-Moyal expansion method. For the stationary signal this will give a statistical surrogate of the velocity signal itself. The lost micro-scales which tend to smooth the velocity signal are absent in this developed surrogate--to overcome this limitation a simple Gaussian smoothing was provided by a convolution operation.

Recasting Navier-Stokes Equations

Dadzie, S Kokou; Lakshminarayana Reddy, M. H.
Heriot-Watt University, United Kingdom

Experiments show that liquid flows through nano-scale structures can be four to five order of magnitude faster than predicted by conventional fluid flow theory. A convincing physical explanation of these high fluid velocities through the nano-tubes is still lacking. Adding solid nano-particles into liquids dramatically increase the fluid thermal conductivity so that the Fourier's law of heat transfer alone is insufficient to understand their transport properties. The meaning of a fluid velocity in the derivation of the conventional flow equations has been severely questioned over the past decade. Meanwhile, several models have been proposed to substitute the Navier-Stokes. Some of these are, for example, Volume Diffusion (or Bi-velocity hydrodynamic models, Ghost effect system Navier-Stokes equations and many others. Here, starting with the conventional Navier-Stokes equations, we introduce a transformation technique similar in nature to Lorentz transformation. It involves transforming the velocity field variable within the standard fluid flow equations. In doing so, we show the existence of a class of systematically thermo-mechanically consistent mass diffusion type of fluid flow set of equations. Our new models are more complete form of those previously proposed to substitute the original Navier-Stokes. The new class of equations appear better suited for: compressible flows, flow involving thermal stresses and other transport processes. As an illustration, our new model for compressible flows is applied to the description of shock wave profiles in a monatomic gas where the Navier-Stokes is well-known to fail. Two other of the new models termed "pressure-diffusion" and "thermal-diffusion" Navier-Stokes are also used to re-interpret experimental data of Rayleigh-Brillouin light scattering in gases.

1:10pm - 3:00pm **Lunch**
PG01

3:00pm - 4:40pm **Multiphase and Porous Media Flows etc.**
PG01
Session Chair: **Martin Geier**, TU Braunschweig

Pore-scale modelling of gas flow in shale rocks - beyond lattice Boltzmann method

Zhang, Yonghao
University of Strathclyde, United Kingdom

Extraction of shale gas poses a new research challenge: understanding and quantifying the gas flow in exceptionally low permeability porous media with pore spaces as small as a few nano-meters across. To uncover the gas transport physics and to predict flow properties of porous media, we utilise high-resolution images of the pore structures of ultra-tight porous media and directly perform pore-scale simulations using lattice Boltzmann method (LBM) and discrete velocity method (DVM). As a computationally-efficient solver, LBM is best used to obtain Darcy permeability while the DVM is able to predict apparent permeability by capturing rarefaction effects. A highly-efficient multi-level parallel solver has been developed, which enables practical pore-scale simulations. This new computational tool may transform the commonly-used heuristic approaches, which rely on empirical Darcy-type models with a few arbitrary tuneable parameters.

Mesoscopic simulation of droplet coalescence in fibrous porous media

Wang, Fang; Schiller, Ulf D.

Clemson University, United States of America

Flow phenomena in porous media are relevant in many industrial applications including fabric filters, gas diffusion membranes, and biomedical implants. For instance, nonwoven membranes can be used as filtration media with tailored permeability range and controllable pore size distribution. However, predicting the structure-property relations that arise from specific porous microstructures remains a challenging task. Theoretical approaches have been limited to simple geometries and can often only predict the general trend of experimental data. Computer simulations are a cost-effective way of validating semi-empirical relations and predicting the precise relations between macroscopic transport properties and microscopic pore structure. To this end, multiscale simulation techniques have proven particularly successful in solving numerically the coupled partial differential equations for the complex boundary conditions in porous media. In this talk, I will present simulations of multiphase flow in fibrous porous media based on a multiphase lattice Boltzmann model for water droplets in oil. We study the effect of fibrous structures and their surface properties on the coalescence behavior of water droplets. We will discuss how the insights can be used to design optimized materials for diesel fuel filters and other filtration devices.

Lattice Boltzmann Simulations of Kinetic Impacts of the Surface Acoustic Wave on a Drop

Burnside, Stephen Burrell; Khajepor, Sorush; Chen, Baixin

Heriot-Watt University, United Kingdom

Over the past few years, there has been a move towards integrating complete laboratory chemical analysis procedures on to the surface of a microfluidic chip, known as Lab-on-a-Chip (LOC) [1]. When scaling the processes down to the micro scale, there are some technical problems such as the pumping of fluids becomes increasingly more difficult as viscous and capillary forces become more dominant. Additionally, mixing of chemical or biological materials at small scale can be inefficient and tedious due to the large time and length scales required.

Recently, Surface Acoustic Waves (SAW) have been shown to demonstrate features that could have positive implications for the development of microfluidic devices. Pumping, mixing, jetting and nebulisation of microdroplets can all be induced through manipulation of the applied power of the SAW. As the acoustic wave propagates in the path of a liquid droplet, the energy is transferred into the liquid medium causing the aforementioned phenomena to occur. This interaction mechanism between the SAW and the fluid is not yet fully understood, hence further investigation is required.

Lattice Boltzmann (LB) is a recent method which has shown great flexibility and performance in the simulation of complex fluid flows. Both mass and momentum conservation are satisfied by a linear stream-collision equation. In this study, the Multipseudopotential interaction (MPI) [2], a new two-phase scheme which ameliorates Shan-Chen (SC) model [3] in different aspects and removes the inconsistency of SC model, is applied to investigate the impacts of the SAW on a droplet.

The current results show the capability of MPI scheme for studying and simulating the streaming, deformation, jetting and breakup of drop arising as a consequence of the attenuation of the sound wave in the liquid. The effects of SAW excitation power/frequency, droplet sizes, and surface wettability are studied. Under SAW actions, the simulated drop changes shape at Weber number (We, based on the drop size) about We~0.45 and intends to break up at We~1.2, respectively. It is identified that deformation and breakup of the drop are due to the interactions between a pair of vortices and among multiple vortices that are formed inside the drop, respectively. Further increase of the SAW power separates the drop from the surface and breaks up the drop. The results show a good agreement with the previous reports in the literature.

REFERENCES:

1. Mark D. ‘Microfluidic lab-on-a-chip platforms: Requirements, characteristics and applications’ Chemical Society Reviews. 2010. 39(3):1153-82

2. Khajepor S. and Chen B. ‘Multipseudopotential interaction: A consistent study of cubic equations of state in lattice Boltzmann models’ Physical Review E. 2016. 93:013303.

3. Shan X. and Chen H. ‘Lattice Boltzmann model for simulating flows with multiple phases and components’ Physical Review E. 1993. 47:1815-9.

Microfluidic numerical diagnostics for the interpretation of lab-on-a-chip mineral precipitation experiments

Mahrous, Mohamed[1,3]; Poonoosamy, Jenna[2]; Curti, Enzo[1]; Churakov, Sergey[1,3]; Prasianakis, Nikolaos[1]

[1]Paul Scherrer Institut, Switzerland; [2]Jülich Research Center, Germany; [3]University of Bern, Switzerland

Minerals precipitation is one of the most widespread processes in many subsurface systems, including enhanced oil recovery, geothermal energy exploitation, carbon dioxide sequestration, and disposal of radioactive waste. Modeling of such a process cannot be fully captured with use of macroscopic

models, since they lack the description of pore-level dependent mechanisms that occur within the pore network. We have developed a reactive transport pore scale model to describe precipitation process within porous media. In this model, solutes are transported by advection and diffusion through a porous medium using the Lattice Boltzmann method with full geochemical speciation. Geochemical speciation is required at every timestep at every voxel, for the accurate calculation of mineral saturation index, which is the driving force of precipitation. The GEMS thermodynamic modelling package is used for the speciation calculations. A sub-grid model is used to integrate sub-micrometer nucleation processes. The classical nucleation theory is used to predict the nucleation of minerals from supersaturated solutions (induction time). Moreover, it gives an estimate of the involved reactive surfaces areas for homogeneous and heterogeneous nucleated precipitates, allowing to predict the mineral growth rates. The model is used to describe the processes occurring in a specifically designed microfluidic lab on a chip experiment, with focus in mineral precipitation in confined spaces. The methodology we follow allows to validate numerical models, and at the same time to explain at an unprecedented detail the experimental observations relevant to crystal growth [1]. Future challenges will be discussed.

[1] Poonoosamy, J., Westerwalbesloh, C., Deissmann, G., Mahrous, M., Curti, E., Churakov, S.V., Klinkenberg, M., Kohlheyer, D., Von Lieres, E., Bosbach, D., Prasianakis, N.I., A microfluidic experiment and pore scale modelling diagnostics for assessing mineral precipitation and dissolution in confined spaces (In Review 2019)

4:40pm - 5:00pm **Coffee Break**

PG01

5:00pm - 6:40pm **Algorithms and Implementations etc.**

PG01

Session Chair: **Christian Obrecht**, INSA Lyon

Performance evaluation of implicit coupling between the immersed boundary and lattice Boltzmann methods on GPU

Klinkovský, Jakub; Fučík, Radek

Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Czech Republic

The lattice Boltzmann method (LBM) is an efficient numerical method capable of simulating fluid flow in the laminar as well as turbulent regime. In order to simulate flow over complex immersed bodies or interactions with elastic structures, it can be coupled with the immersed boundary method (IBM). An efficient implementation of the implicit velocity correction--based IB-LBM coupling proposed by Wu and Shu (2009, 2010) is challenging because large linear systems of equations have to be solved in each time step. In our recent work, we proposed a modification of the method to improve the conditioning of the linear systems, which leads to faster convergence. In this talk, we will focus on the efficient implementation of the linear system solver for GPUs, where the explicit LBM is very efficient. We consider several numerical methods, preconditioners, and libraries such as CUSPARSE and TNL (Template Numerical Library), and present the impact of each approach on the overall performance.

A modified immersed boundary-lattice Boltzmann method for simulating incompressible fluid flow in 2D and 3D on GPU

Eichler, Pavel; Fučík, Radek

FNSPE, CTU in Prague, Czech Republic

Fluid-solid interaction in 2D and 3D is an important topic in fluid dynamics and accurate simulations are desirable in the field of applications dealing with this phenomenon, e.g., blood flow across the aortic valve, air flow in the boundary layer, etc. To accurately represent the position of the solid obstacle, immersed boundary method (IBM) based on the Lagrangian description was introduced. The advantage of this method is that it does not depend on the numerical method used for the fluid simulations and thus modern numerical method such as Cascaded lattice Boltzmann method (CLBM) in 2D and Cumulant lattice Boltzmann method (CuLBM) in 3D can be used.

In this contribution, a computational study on optimal spacing of Lagrangian nodes discretizing a rigid and immobile immersed body boundary in 2D and 3D is presented to show how the density of the Lagrangian points affects the numerical results of the Immersed Boundary–Lattice Boltzmann Method (IB–LBM). The study is based on the implicit velocity correction-based IB–LBM proposed by Wu and Shu (2009, 2010); however, this method often fails for densely spaced Lagrangian points. Thus, we introduce a modification that improves the stability of the original method and compare the performance of both methods using several benchmarks problems. In these problems, we show how the spacing of the Lagrangian points affects the numerical results, mainly the overall drag force and the permeability of the discretized body boundary.

Direct numerical simulations of turbulent flows over periodic hill with lattice Boltzmann method on multi-GPU cluster

Lin, Wei-Jie; Lin, Chao-An

Department of Power Mechanical Engineering, National Tsing Hua University, Taiwan

Turbulent channel flows over the periodic hill were simulated with multiple-relaxation-time lattice Boltzmann method at a wide range of Reynolds numbers. The simulation was conducted on multi-GPU cluster with two-dimensional domain decomposition using message passing interface (MPI). The pressure-driven flow was simulated by adding an external force to the flow field in the streamwise direction and the curved boundary was mimicked by a modified bounce back formulation.

Numerical simulations of 3D wave transformation based on lattice Boltzmann method

Liu, Guang-wei; Zhang, Qing-he; Zhang, Jin-feng; Liu, Run

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In the present work, a 3D numerical wave tank (NWT) based on the modified lattice Boltzmann scheme of Guangwei Liu et al. [1] is developed. The active absorption wave-making boundary condition is implemented to make waves. A depth dependent wave-absorption boundary condition is developed to absorb non-linear waves. In order to obtain a stable and accurate simulation of waves, a D3Q27 MRT collision model is proposed based on the D3Q19 MRT collision model of Janssen C. et al. [2]. The performance of the NWT on wave-making and wave-absorption is validated through simulations of solitary, Stokes and cnoidal waves. Numerical experiments of some of the interesting physical processes in coastal engineering show that the 3D NWT exhibits good performance in simulating wave diffraction, reflection, refraction, runup and breaking.

[1] Liu G, Zhang Q, Zhang J. Numerical wave simulation using a modified lattice Boltzmann scheme. Comput Fluids. 2019;184:153-64.

[2] Janssen C, Krafczyk M. A lattice Boltzmann approach for free-surface-flow simulations on non-uniform block-structured grids. Comput Math Appl. 2010;59:2215-35.

Three-dimensional Lattice Boltzmann simulation of boiling using a non-orthogonal multiple-relaxation-time scheme

Fei, Linlin[1]; Luo, Kaihong[2]

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We present a series of high-resolution numerical simulations of phase change and convection in multiphase flows based on a non-orthogonal multiple-relaxation-time Lattice Boltzmann model. Three dimensional simulations of boiling are conducted under realistic conditions. The change of heat flux with increasing wall superheat is shown and the classical three boiling stages (nucleate, transition, and film boiling stage) are reproduced. The bubble footprint area probability is then measured and verified against some empirical formulations. Finally, we investigate the effect of the buoyant bubble on the small-scale properties of velocity and temperature fields.

7:00pm - 9:00pm	**Reception and Social at Marriot Courtyard Hotel**
Marriott Courtyard Hotel	

Date: Wednesday, 24/Jul/2019

9:30am - 11:10am | **Kinetic Methods etc.**
PG01 | Session Chair: **Paul John Dellar**, University of Oxford

On local kinetic models for fluid flows -- Boltzmann vs. BGK

Babovsky, Hans
Technical University of Ilmenau, Germany

There are a couple of standard techniques to include mesoscopic effects (typically described by some Boltzmann collision operator) into the (macroscopic) description of fluid flows. Common procedures include the Chapman-Enskog expansion and the application of simplified collision or relaxation models e.g. for the adjustment of boundary layers. In a number of situations simplifying models are not appropriate since they tend to suppress local features with an impact on the full fluid flow.

The key observation is that moment perturbations to maxwellians ``survive'' in the case of the full nonlinear Boltzmann collision operator longer than for linearized and BGK systems. As a result, the nonlinear description provides fluids which are locally composed of different components with different macroscopic moments.

As a consequence, perturbations arising from boundaries may penetrate into the fluid in the full model which otherwise are stuck to the boundary layer. Taking this into account helps e.g. to explain some seeming paradox in the context of an evaporation condensation problem [1] or to model effects not possible using the conventional techniques.

In the talk we sketch a general mathematical ansatz applicable in a variety of situations and illustrate it with some numerical experiments obtained with Discrete Velocity Models. We discuss its implications, e.g. for the derivation of Navier-Stokes correction terms, or for the formulation of boundary conditions in the presence of permeable moving walls.

[1] H. Babovsky. Macroscopic limit for an evaporation-condensation problem. European Journal of Mechanics B/Fluids, 63:106--112, 2017.

Analysis of Knudsen layer phenomena using half-range quadratures

Ambrus, Victor E.[1]; **Luo, Li-Shi**[2]
[1]West University of Timisoara, Romania; [2]Old Dominion University, USA

We consider the analysis of Knudsen layer phenomena at the level of the linearised Boltzmann-BGK equation. We highlight the dramatic increase in simulation efficiency when half-range quadratures are employed for the discretisation of the velocity space, compared to that of schemes based on full-range quadratures.

Lattice Boltzmann simulation of gas-liquid flow interacting with a moving geometry

Luo, Tianpei[1,2,3]; **Xia, Jun**[1]; **Liu, Yangwei**[4]; **Zhang, Jiaxian**[2,3]; **Liu, Ruimin**[2,3]; **Yang, Sifeng**[2,3]; **Zhao, Hua**[1]
[1]Department of Mechanical and Aerospace Engineering & Institute of Energy Futures, Brunel University London, Uxbridge UB8 3PH, UK; [2]Beijing Institute of Aerospace Testing Technology, Beijing 100074, China; [3]Beijing Engineering Research Center of Aerospace Testing Technology and Equipment, Beijing 100074, China; [4]National Key Laboratory of Science and Technology on Aero-Engine Aero-Thermodynamics, School of Energy and Power Engineering, Beihang University, Beijing 100191, China

For spray research, although good understanding of fuel spray dynamics following the liquid-fuel ejection out of the nozzle has been achieved in recent years and difficult tasks such as predicting spray combustion emissions can be attempted using high-fidelity simulation and modelling techniques, the internal flow dynamics inside the fuel injector remains poorly understood, although it plays a dominant role in determining spray combustion performance by dictating the upstream boundary conditions at the nozzle exit. It has proven difficult to investigate the internal flow problem using measurement and conventional computational methods, largely due to the complex flow physics of cavitation interacting with a moving needle valve inside the fuel injector featuring a complex geometry. In this paper, we have attempted to use the lattice Boltzmann method (LBM) to analyse cavitating flow interacting with a moving geometry, mimicking flow conditions in a simplified fuel injector. The Bhatnagar-Gross-Krook (BGK) algorithm coupled with the immersed boundary method and Shan-Chen multiphase flow model was employed and further developed. Firstly, the performance of the immersed boundary method and Shan-Chen multiphase flow model was independently tested in a case where an oscillating cylinder moves according to a sine function in water and an inside-nozzle cavitating flow case, respectively. In order to improve the Shan-Chen model on its limitation of the density ratio, so to be used in realistic multiphase flow, the Peng-Robinson equation of state and Exact Difference Method force scheme were adopted. In addition, the interaction force has been upgraded under the guidance of the Taylor expansion to achieve thermodynamic consistency and improve mechanical stability. Through comparisons with the Maxwell construction and experimental data, the upgraded model proved to be effective on improving numerical stability at low temperatures and large density ratios. Finally, the cooperation of the improved Shan-Chen model and immersed boundary has been achieved under the lattice Boltzmann framework. It should be pointed out that, in addition to fuel

spray processes, the further developed LBM can be readily extended to other spray processes and spraying devices extensively used in medical and materials applications.

Chemical-Potential Multiphase Model with Superlarge Density Ratio

Wen, Binghai
Guangxi Normal University, Guilin, China

Chemical potential, as an important thermodynamic quantity, has been popularly used in thermodynamic modeling for complex systems, especially for those involving the phase transitions and chemical reactions. Here we present a chemical-potential multiphase lattice Boltzmann model, in which the nonideal force is directly evaluated by a chemical potential. The chemical potentials of the popular equations of state are derived from the free-energy density function. An effective chemical-potential boundary condition is also implemented to investigate the wettability of a solid surface, and the contact angle can be linearly tuned by the surface chemical potential. Then, three technologies enhance the computational accuracy of the multiphase model. Firstly, decoupling the mesh space from the momentum space stretches the steep liquid-gas transition region into a gentle curve, and then the dense lattices provide more accurate raw data for the derivative calculations. Secondly, the high order difference supports that the gradient computations of density and chemical potential obtain very high precisions. Thirdly, the nonideal force is incorporated into the lattice Boltzmann equation by the forcing term technology of the exact difference method. The simulation computations show that the model can work at very low temperatures, at which the liquid-gas density ratios are superlarge, namely more than 1013, while the model fully satisfies thermodynamic and dynamic Galilean invariance.

9:30am - 1:00pm **On-site registration**
PG01

11:10am - 11:30am **Coffee Break**
PG01

11:30am - 1:10pm **Thermal and Compressible Flows etc.**
PG01
Session Chair: **Lian-Ping Wang**, SUSTech

Simulation of three-dimensional compressible turbulence and compressible heat transfer using discrete unified gas kinetic schemes

Wang, Lian-Ping[1,2]; Wen, Xin[2]; Chen, Tao[1,3]; Guo, Zhaoli[4]
[1]Southern University of Science and Technology, China; [2]University of Delaware, USA; [3]Peking University, China; [4]Huazhong University of Science and Technology, China

The discrete unified gas-kinetic scheme (DUGKS) is a finite-volume formulation of the Boltzmann equation. It has two major advantages over the lattice Boltzmann method (LBM) in that it can simulate compressible (and even non-continuum) flows, and can naturally incorporate a non-uniform mesh. Recently, we have successfully simulated three-dimensional (3D), incompressible turbulent flows including homogeneous isotropic turbulence (Phys. Rev. E., 94, 043304, 2016) and turbulent channel flow (Computers & Fluids, 2017, 155: 9-21). In this talk, we present some results on using DUGKS for the simulation of compressible isotropic homogeneous turbulence, as well as compressible heat transfer in a cavity. The relevant issues in simulating 3D compressible flows using DUGKS include the choice of the set of discrete velocities, efficient and accurate numerical integration method, method to treat local discontinuity, and parallel implementation. In this talk, we incorporated WENO in DUGKS to simulate compressible isotropic homogeneous turbulence and compare results with those obtained from high-order compact finite-difference methods. Also, as another example, the problem of compressible heat transfer is also studied by DUGKS. Methods for flow initialization and the implementation of boundary conditions are re-examined and developed in order to achieve these flow simulations.

A Semi-Lagrange Gas Kinetic Scheme for Compressible Flows

Li, Weidong; Zhao, Zhangyan
Wuhan University of Technology, China, People's Republic of

In this work, a semi-Lagrange gas kinetic scheme for compressible flows is proposed. Not as the conventional gas kinetic scheme, the present scheme is constructed from the characteristic solution rather than the formal integral solution of the BGK model equation, and based on the characteristic solution of the BGK model equation, the present gas kinetic scheme has an implicit form. Moreover, thanks to the collision invariant, the implicitness of the proposed gas kinetic scheme can be easily converted into explicitness and therefore, the proposed scheme can be much simpler than the conventional gas kinetic scheme. To demonstrate the accuracy of the proposed scheme, several compressible benchmarks are simulated by the proposed scheme and numerical results show that the present scheme has second-order accuracy and good robustness. Thus, the proposed scheme can be a reliable simulation tool for compressible flows.

Simulation of a laser melting additive manufacturing process by using the lattice Boltzmann method

Cheng, Ming; Li, Hongying; Lou, Jing
Institute of High Performance Computing, Singapore

Additive manufacturing (AM or 3D printing), which produces parts in layer-by-layer manner from a variety of materials, has been rapidly gaining popularity as a digital manufacturing process in recent years. Laser beam and powder-based AM process is a typical one, in which, the beam scans the powder bed surface, the melted powder forms a liquid pool and then re-solidifies to build up the bulk part. The process includes a lot of physical phenomena such as the beam absorption in the powder bed, phase change, diffusive and convective heat conduction in the melt pool. The phase change and highly dynamic flow accompanying the material transformation have been attracted both experimental and theoretical interest because of their intrinsic complexity and practical importance. Many researchers have put their efforts toward understanding the AM process and improving its performance. This paper presents a numerical modelling for simulating an additive manufacturing process (laser beam melting and re-solidification of the melt pool). Our approach is based on the lattice Boltzmann method. The numerical scheme is tested on different benchmark problems. Comparison with results obtained by other methods and experiments shows that the present approach can capture the typical flow characteristics in the complex AM processes, and could be adapted as an effective tool for the AM processes optimization.

Adaptive relaxation times for aeroacoustic simulations.

Marié, Simon[1]; Gloerfelt, Xavier[2]
[1]Conservatoire National des arts et métiers, France; [2]Ecole Nationale Supérieure d'arts et Métiers, France

In the lattice Boltzmann framework, several collision operators can be used to investigate a wide range of physical phenomenon. Each of them have their own particularities and have been developed to overcome some of the original BGK limitations. However, these limitations often appears in some specific region characterized by high gradient levels. In contrast, the BGK-model still holds and is largely enough to simulate uniform fow regions. Then it could be tempting to use each of the prescribed models only in some specific regions.

In this study, we introduce some adaptive relaxation times in the MRT framework [1] in order to be able to switch from BGK to MRT when it is needed. The idea is to use the shear selectivity introduced in previous work [2] to recompute the relaxation times at each grid point. This approach will be validated in a 3D turbulent fow such as Taylor-Green vortex and tested for an acoustic application such as the noise radiated by a cylinder where good stability is need in sheared regions and low dissipation is needed in acoustic regions.

[1] D. d'Humière, I. Ginzburg, Y. Krafczyk, P. Lallemand, and L.S. Luo. Multiple relaxation time lattice Boltzmann models in three dimensions. Phil. Trans. R. Soc. Lon. A , 360 :437-451, 2002.

[2] S. Marié ,X. Gloerfelt. Adaptive FItering for the lattice Boltzmann method. Computational Physics , 333C :212-226, 2017.

Effective Thermal Conductivity of Hydrate-Free Permafrost Sediments: Experimental Study and Development of a Predictive Numerical Model

Vasheghani Farahani, Mehrdad; Hassanpouryouzband, Aliakbar; Yang, Jinhai; Tohidi, Bahman
Heriot-Watt University, United Kingdom

In this communication, we report systematic measurements of the effective thermal conductivity (ETC) of hydrate-free permafrost sediments at wide ranges of temperature (-10 to 10 °C), pore pressure (2.75 to 14 MPa), and effective overburden stress (1.4 to 9.75 MPa) utilizing a high-pressure Unsteady State Needle Probe. Four sets of experiment were designed and performed to measure the ETC of hydrate-free sediments and investigate the effect of pore pressure, overburden stress, temperature, and degree of water/ice saturation. It was observed that depending on the pore pressure of the system and degree of saturation, such increase in the effective overburden stress could typically result in more than 10% increase in the ETC (from 2.2 W/mK to 2.5 W/mK above the freezing point and from 3.8 W/mK to 4.2 W/mK below the freezing point). Moreover, it was found that the pore water distribution regimes (hydration, pendular, funicular, and capillary) directly control the magnitude of the ETC. We also developed a numerical model for the effective thermal conductivity, where Free-energy-based Lattice Boltzmann Method is firstly employed to set the two phases of water and gas (N2) in a 2D Single Cubic (SC) medium consisting of two same size semicircles with respect to the temperature, pore pressure, degree of saturation, and wettability characteristics. The Hertz contact equation is also used to find the contact radius as a function of the effective overburden stress. The ETC is calculated via applying a renormalization method on the domain. The experimental data were compared with the predictions made by the developed numerical model and the other predictive models available in the literature. Despite the others, our model is able to consider two phenomena which significantly impact

the magnitude of the ETC: 1) Thermal contact resistance as a function of the overburden stress, 2) Unfrozen water at temperatures below the freezing point. Therefore, as expected and confirmed via calculation of the average relative error (ARE) values, our predictions are more accurate than those of the other models.

1:10pm - 3:00pm **Lunch**

PG01

3:00pm - 4:40pm **Multiphase Flows: Modelling and Simulation**

PG01 Session Chair: **Manfred Krafczyk**, TU Braunschweig

Modelling ternary fluid flows with free energy lattice Boltzmann method

Kusumaatmaja, Halim
Durham University, United Kingdom

I will present a free energy lattice Boltzmann approach to simulate multicomponent fluid flows. Focusing on ternary fluid systems, I will discuss models where the density is the same for all fluids [1], and where high density ratios between the liquid and gas components can be achieved [2]. I will then discuss several applications. First, I will discuss the dynamics of drops moving across liquid infused surfaces [3]. These are liquid repellent surfaces made by infusing a lubricant into porous or rough solid surfaces. Second, I will present collision dynamics between two immiscible drops [2]. We are able to capture bouncing, adhesive and insertive regimes, in agreement with experimental observations. Third, I will show our numerical study on generating emulsion droplets using a microfluidic channel [4]. I will demonstrate the rich morphologies that can be achieved by varying the fluid surface tensions and flow rates.

[1] C. Semprebon, T. Krüger and H. Kusumaatmaja, Physical Review E 93, 033305 (2016).

[2] M. Wörhwag, C. Semprebon, A. Mazloomi M., I. Karlin and H. Kusumaatmaja, Physical Review Letters 120, 234501 (2018).

[3] M. S. Sadullah, C. Semprebon and H. Kusumaatmaja, Langmuir 34, 8112–8118 (2018)

[4] N. Wang, C. Semprebon, C. Zhang, H. Liu and H. Kusumaatmaja, http://arxiv.org/abs/1906.01034 (2019).

A pseudopotential Lattice Boltzmann model of liquid-liquid dissolution

Wei, Wei; Khajepor, Sorush; Pasieczynski, Kimal; Chen, Baixin
Heriot-Watt University, United Kingdom

In this study, a pseudopotential lattice Boltzmann model is developed for simulations of liquid-liquid dissolution and tested for CO2 droplet dissolution in water. A pseudopotential is introduced to predict the interparticle interaction of solutes and solvent driven by chemical potential. The interface between the solute and solvent is monitored by solubility, which indicates the moving of interface as solute dissolving. An equation of state (EOS) of real liquids is implemented to the model for both liquids to calculate the thermodynamic properties. Moreover, instead of using an additional Lattice that is requested by the existed LBM diffusion models, the further dispersion of dissolved solutes is attached to the Lattice of solvent, which made the both the cost of computing and memory size significantly reduced. The proposed model is calibrated by the data of Lab experiment of dissolution of CO2 droplet in water at a state of CO2 geological storage about 1000m depth. The numerical predictions are well agreement with data from lab experiment.

Wetting boundaries for high density ratio ternary Lattice Boltzmann

Bala, Neeru[1]; Pepona, Marianna[2]; Karlin, Ilya[3]; Kusumaatmaja, Halim[2]; Semprebon, Ciro[1]
[1]Department of Mathematics, Physics and Electrical Engineering, Northumbria University, Newcastle upon Tyne, UK, NE1 8ST; [2]Department of Physics, Durham University, Durham, UK, DH1 3LE;
[3]Department of Mechanical and Process Engineering, ETH Zurich, CH-8092 Zurich, Switzerland

The physics and dynamics of a ternary fluid system are of special interests for a variety of practical applications, including combustion engines, ink-jet printing, and oil recovery. We recently developed a novel ternary free energy lattice Boltzmann method to address problems where inertial forces dominate [1]. The model can reproduce two liquid phases and one gas phase having a density contrast of order 1000 and proved to convincingly simulate the impact of immiscible drops for a wide range of interfacial properties.

To study problems involving interaction of ternary fluids with a solid wall we have introduced various schemes for wetting boundary conditions[2]. In this contribution, I will present three alternative implementations of boundary methods and systematic benchmark of static and dynamic properties. Furthermore, by simulating the self-propelled motion of a train of drops in a channel, we are able to evaluate the dynamic properties of the contact line for the ternary fluids.

[1] M. Wöhrwag, C. Semprebon, A. Mazloomi Moqaddam, I. Karlin, and H. Kusumaatmaja. Ternary free-energy entropic lattice boltzmann model with a high density ratio. Phys. Rev. Lett., 120:234501, Jun 2018.

[2] N. Bala, M. Pepona, I. Karlin, H. Kusumaatmaja, and C. Semprebon. Wetting boundaries for high density ratio ternary lattice boltzmann method. https://arxiv.org/abs/1904.06881

Collective self-propulsion of multiple flapping plates in viscous fluids

Huang, Haibo; Zhang, Chengyao; Lu, Xi-Yun
University of Science and Technology of China, China, People's Republic of

Here we study the collective behaviour of multiple self-propelled plates in tandem and side-by-side configurations, which are driven by harmonic flapping motions of identical frequency

and amplitude. Typical stable configurations were observed. The Lighthill conjecture that orderly configurations may emerge passively from hydrodynamic interactions was verified on a larger scale with up to eight plates. The whole group may consist of subgroups and individuals with regular separations. Hydrodynamic forces experienced by the plates near their multiple equilibrium locations are all springlike restoring forces, which stabilize the orderly formation and maintain group cohesion. For the cruising speed of the whole group, the leading subgroup or individual plays the role of 'leading goose'.

4:40pm - 5:00pm **Coffee Break**
PG01

5:00pm - 6:40pm **Algorithm and Applications**
PG01
Session Chair: **Martin Geier**, TU Braunschweig

LAMBReX: Configurable lattice Boltzmann with adaptive meshes

Brown, Oliver T; Nash, Rupert W
EPCC, University of Edinburgh, United Kingdom

In this poster we present ongoing work in the development of an adaptive mesh code for lattice Boltzmann calculations. It is built on the AMReX adaptive mesh refinement library [1]. In addition to providing high-level structures for managing multiple levels of refinement in the calculation, AMReX also handles parallelisation using both MPI and OpenMP. At present only a D3Q15 velocity set with a multiple relaxation time collision operator is implemented, however, we intend to make both components fully configurable. It is open source and available on GitHub [2], and written in modern C++, with templating eventually being used to allow compile time composition of specific models. We present initial results from the current version, as well as our planned next steps. This work is part of HiLeMMS, a project which aims to produce a domain specific language (DSL) for writing lattice Boltzmann CFD simulations. The DSL will provide an intuitive way to express physical problems, and produce performant, parallel C++ code.

[1] The AMReX Development Team, A. Almgren, V. Beckner, J. Blaschke, C. Chan, M. Day, B. Friesen, K. Gott, D. Graves, M. Katz, A. Myers, T. Nguyen, A. Nonaka, M. Rosso, S. Williams, W. Zhang, M. Zingale, AMReX: Software Framework for Block Structured AMR (May 2019). doi:10.5281/zenodo.2555438.

[2] O. T. Brown, R. W. Nash, LAMBReX: Lattice Boltzmann code built on AMReX (May 2019). URL https://github.com/otbrown/LAMBReX

Investigation of Pseudopotential Forces and Their Effects on Multiphase Flow Simulations

Pasieczynski, Kimal; Chen, Baixin
Heriot-Watt University, United Kingdom

In this study, we investigated the performance of the forcing schemes of single- and multi-pseudopotential interactions in pseudopotential Lattice Boltzmann models (LBM). For single-pseudopotential interaction (SPI) scheme, the cubic and piecewise-linear (PL) equation of state (EOS) are tested. For multi-pseudopotential interactions (MPI), the scheme is extended to the multiple relaxation time (MRT) as the first attempt. A hybrid scheme is constructed to calculate the pseudopotential in the regions above the upper spinodal point for both schemes of SPI and MPI.

The performance is assessed: a) at the saturated points; b) across the phase envelope at a constant temperature. It is found that the SPI with PL-EOS is the only scheme that has physically meaningful pseudopotential crossing the phase envelope, especially at the states of liquid saturation. Meanwhile, it is identified that the interparticular force distribution that is generated by the schemes, plays the key role on both the simulation stability and the generation of the sporous velocity.

Finally, the schemes were assessed for simulations of phase separation. The results show that both schemes performance well with similar final morphology when bulk viscosity is identified to kinematic viscosity, however, are different when bulk viscosity is larger than kinematic viscosity.

Acoustical analysis of fluid structure interaction using the Cumulant lattice Boltzmann method

Gorakifard, Mohsen[1]; **Cuesta, Ildefonso**[1]; **Salueña, Clara**[1]; **Kian far, Ehsan**[2]
[1]Rovira i Virgili University, Spain; [2]The University of Manchester, United Kingdom

Noise reduction is a critical part of transportation industries through limiting the operation, disturbing passengers, and polluting environment. As a result, a better understanding of noise emitting process is required substantially. A typical case of aerodynamic noise is The Aeolian Tone. One of the self adaptive devices to control the actual flow conditions and sound is splitter plates attached to the cylinder base and look like hair. The flexible flaps reduce the vortex shedding and net drag. The direct numerical simulation of the sound waves stimulated by controlling devices is a sophisticated task since the sound pressure is much smaller than the whole pressure variation. In addition, the acoustic fields spread in a large region and it is a time-consuming process. For example, the direct numerical simulation of sound waves based on Navier-Stokes equations needs schemes of fifth-order accuracy in space and fourth-order accuracy in time [1]. However, Cumulant Lattice Boltzmann method (LBM) shows a stable and powerful method at high Reynolds numbers and can carry out these simulations accurately.

In this work, Cumulant Lattice Boltzmann method [2] as a fluid flow solver is coupled with a Finite Element structural mechanics solver to predict the consequence of hairy flaps on the noise generated by cylinders in a turbulent flow. Moreover the spectral modification and possible acoustic damping impact of such flaps and sound propagation through interactions between acoustic waves and solid walls and between acoustic waves and shear layers is studied. To outline, the tonal noise generated by vortex shedding from one and two circular cylinders for three Reynolds numbers is studied; the Strouhal numbers and the sound pressure spectra (SPL) with and without flaps are presented. The results have a good agreement with experimental data. The mean drag and lift force is reduced by a changed vortex separation mechanism. In addition, the hairy flaps alter the phase of the vortex shedding cycle and decrease the transversal distance from the center line of the shed vortices. Thus hairy flaps control the wake generated behind a cylinder and have an effective impact on decreasing structural vibrations and sound generation.

1. O. Inoue and N. Hatakeyama, Sound generation by a two-dimensional circular cylinder in a uniform flow, J.Fluid Mechanics, 471, 2002, pp.285-314.

2. E. Kian Far, M. Geier, and M. Krafczyk, Simulation of rotating objects in fluids with the cumulant lattice Boltzmann model on sliding meshes, J. Computers & Mathematics with Applications, 2018.

Meshless approach for lattice Boltzmann methods on irregular point clouds

Pribec, Ivan; Fattahi, Ehsan; Becker, Thomas
Technical University of Munich, Germany

Meshless methods represent the latest paradigm in discretization methods for solving PDEs, offering geometric flexibility, tunable accuracy, simple implementation and opportunity for large-scale parallel computing. These advantages can be put to use in off-lattice Boltzmann methods (OLBM) providing access to a wider range of kinetic models than their on-lattice counterparts, including models for thermohydrodynamics and compressible flow, viscoelastic flow, nonlinear acoustics and even elastodynamics. Pursuant to this approach, we propose a characteristic-based meshless lattice Boltzmann method (MLBM) using the strong form of the discrete Boltzmann equation in combination with monomial and radial basis trial functions for derivative approximation. Decoupling the physical and lattice symmetry allows us to use nonuniform point clouds, useful for local refinement of boundary layers. The accuracy and computational efficiency of the proposed method are studied using the lid-driven cavity benchmark. The flexibility with respect to lattice models is demonstrated on the case of flow through a periodic array of cylinders, where we probe the rotational invariance of several two-dimensional velocity lattices and the influence of different boundary conditions. Together, our results show that the meshless paradigm is a promising method for Boltzmann-based kinetic simulations.

Central moment LBM accuracy of the advection-diffusion equation in 1D

Straka, Robert
Czech Technical University - Faculty of Nuclear Sciences and Physical Engineering, Czech Republic

We analyze higher order error terms (greater than second order) in the central moment/cascaded lattice Boltzmann method (CLBM) for one conservation law -- the advection-diffusion equation in one dimension using the D1Q3 lattice model. To inspect behavior of the error terms we derive an equivalent finite difference equation (EFDE). The EFDE is obtained from the recurrence formulas of the lattice Boltzmann equations for the CLBM and is subsequently analyzed by standard analytical techniques. We will show relations of the relaxation times which could cancel some of the higher order terms, making the method more accurate. The detailed derivation of the EFDE and higher order terms' pre-factors will be presented together with results for BGK & MRT LBMs in order to validate our approach. We believe that EFDE is the closest approach of what we really compute when using LBM in the numerical codes run by computers.

Date: Thursday, 25/Jul/2019

9:30am - 11:10am | **LBM and Complex Flows**
PG01 | Session Chair: **Li-Shi Luo**, CSRC

Lattice Boltzmann simulations of liquid crystals: blue phases and active gels

Marenduzzo, Davide
University of Edinburgh, UK

I will discuss lattice Boltzmann simulations of the hydrodynamics of liquid crystalline fluids. First, I will review work on blue phases, topological phases made up of defect lattices in cholesterics. This work includes the proposal of a new structure for blue phase III, or the 'blue fog', a phase experimentally observed long ago bit never fully understood theoretically. I will then show how simulations can be used to uncover the exotic dynamics of active nematics, new materials which can be built by mixing cytoskeletal filaments and molecular motors.

Lattice Boltzmann model for miscible mixtures: application to the viscous fingering instability

Vienne, Lucien; Marié, Simon; Grasso, Francesco
Cnam, France

In the first part of the presentation, we introduce a lattice Boltzmann model for miscible gases. In this model, the standard lattice Boltzmann algorithm is employed for each species composing the mixture. First, the diffusion between species is modeled by means of a force derived from kinetic theory of gases, and the complex diffusion dynamics predicted by the Maxwell-Stefan equations is recovered for a purely diffusive flow. Second, the model relies on transport coefficients calculated by an approximation of the relations obtained from kinetic theory. Third, species having different molar masses are simulated using a force term avoiding costly interpolations or an increase in the velocity set. The model is validated against analytical, experimental, and numerical results. One of the advantages of the proposed forcing approach is the easiness of implementation. Since collision is not altered, our method can easily be introduced in any other lattice Boltzmann algorithms in order to take into account complex diffusion among species.

The second part of the talk is dedicated to the simulation of the viscous fingering instability with the aforementioned lattice Boltzmann model. This challenging mixture dynamic takes place when a less viscous fluid displaces a more viscous fluid in a porous medium. Previous studies only consider a binary mixture with Fick-like diffusion behavior. Here, we focus on a mixture composed of three species in different proportions. In this case, the flow may exhibits complex diffusion behavior such as diffusion reversal, diffusion barrier, and osmotic diffusion. These phenomena are not predicted by Fick's law and their effects on the development of the fingers are presented.

Rheology of dense suspensions in shear flow via simulations with an immersed boundary lattice Boltzmann method

Srinivasan, Sudharsan[1,2]; Van den Akker, Harry[1,2,3]; Shardt, Orest[1,2]
[1]Synthesis and Solid State Pharmaceutical Centre (SSPC), University of Limerick, Limerick V94T9PX, Ireland; [2]Bernal Institute, University of Limerick, Limerick, V94T9PX, Ireland; [3]Transport Phenomena Lab, Department of Chemical Engineering, Delft University of Technology, Van der Maasweg 9, Delft, 2629 HZ, The Netherlands

Direct numerical simulations of dense suspensions of monodisperse spherical particles in simple shear flow have been performed at particle Reynolds numbers between 0.1 and 0.5. In these simulations, the flow of the interstitial Newtonian carrier liquid is solved using the lattice Boltzmann method. The no-slip boundary condition at the surface of each particle is implemented by means of an immersed boundary method. Simulations are three dimensional and parallelised using the Message Passing Interface (MPI) library with full 3D domain decomposition. The particles translate, rotate, and collide under the influence of the applied shear and lubrication forces (normal and tangential) and torques over sub-grid scale distances. We compute the relative apparent viscosity of the simulated suspensions for solids volume fractions up to 35%, corresponding to a mass fraction of 65% for a density ratio (solid over liquid) of 3.5. We present a study of the factors that affect the apparent viscosity of the suspension, emphasising the effects of variation (over time) of shear rate, particle size, and concentration. We assess the individual contributions of interparticle collision forces (spring) as well as normal and tangential lubrication forces and torques on the observed viscosity, comparing the simulation results with experimental and theoretical values. The choice of interparticle collision forcing scheme affects the rheology when the solids volume fraction exceeds 30%.

Accurate particulate flow simulations with a coupled lattice Boltzmann - discrete element method

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As a cost- and time-efficient alternative to laboratory experiments, engineers have become increasingly interested in applying computer simulations to investigate particulate flows numerically as they can provide more detailed information about the individual particles and the fluid flow. Among the available simulation techniques, only direct numerical simulations (DNS) can represent geometrically fully resolved particles and flow structures. Thus such a fully resolved DNS is the method of choice to investigate particulate systems from first principles and in order to gain more insight into the underlying physical phenomena.

In this talk, we will present our DNS approach. The fluid dynamics is represented by the lattice Boltzmann method and is coupled to a particle simulation, performed by the discrete element method (DEM). The fluid-particle coupling mechanism is based on the momentum exchange between the particulate and the fluid phase. By considering a settling sphere that impacts on a wall, we thoroughly investigate the influence of different LBM collision models and DEM parameters on the sphere's trajectory. Detailed comparisons with experimental data serve to validate the coupled simulation. This constitutes the basis for accurate predictions with particulate flow simulations and lets us formulate valuable guidelines for designing such simulations. Finally, illustrating examples from environmental engineering will be presented, such as studies of the onset of sediment motion in riverbeds.

9:30am - 1:10pm	**On-site registration**
PG01	
11:10am - 11:30am	**Coffee Break**
PG01	
11:30am - 1:10pm	**Method and Analysis II**
PG01	Session Chair: **François Dubois**, Univ. Paris Sud, Orsay

Implicit versus explicit LES: Taylor-Green vortex benchmark

Geier, Martin; Lenz, Stephan; Schönherr, Martin
TU Braunschweig, Germany

We compare implicit and explicit Large Eddy Simulations (LES) with the cumulant lattice Boltzmann method. The explicit turbulence model is realized by a Wall Adaptive Local Eddy (WALE) model. For the implicit LES either no model or a ghost mode limiter is applied. The cumulant lattice Boltzmann model with fourth order convergent diffusion and improved fourth order convergent velocity correction shows the smallest deviation from the reference solution. The benchmark is conducted in both diffusive and acoustic scaling and little influence of the scaling is observed for the fourth order convergent method while the regularized method shows the known deterioration with smaller time steps.

The WALE model shows no advantage over no model in the investigated case. The filter eliminates the higher wave numbers from the simulation such that it behaves like a no-model simulation run on a coarser grid.

We also compare to results from a low Mach number Gas Kinetic Scheme (GKS). The GKS shows the desired improvement for shorter time steps missing in the regularized lattice Boltzmann method. In general, the GKS results are inferior to those of the lattice Boltzmann method.

Investigation of Different Lattice Boltzmann Fluid-Structure Interaction Approaches for Vortex-Induced Vibrations

Haussmann, Marc; Raichle, Florian; Nirschl, Hermann; Krause, Mathias J.
Karlsruhe Institute of Technology, Germany

The present work compares fluid-structure interaction (FSI) approaches for the lattice Boltzmann method (LBM) to study vortex-induced vibrations (VIV). Two classes of FSI approaches, namely the partially saturated methods (PSM) (Noble et Torczynski [1; 2], Krause et al. [3; 4]) and moving boundary methods (MBM) (Bouzidi et al. [5; 6], Yu et al. [7], Guo et al. [8] and Filippova et Hänel [9; 10; 11]), are investigated. First, the Galilean invariance of aerodynamic coefficients obtained by each scheme is examined. Therefore, the Bhatnagar-Gross-Krook (BGK) LBM is used to simulate a eccentrically positioned cylinder in a transient Couette flow. In addition, various refill methods for MBM and volume approximation techniques for PSM are tested. Beside different error norms and a grid independence study of each method also the Galilean invariance violating frequencies are determined. These results are used to chose for each class a representative to simulate vortex shedding. The VIV test case describes a transverse oscillation of a cylinder in a freestream at a Reynolds number of 100. The cylinder oscillation is prescribed by a fixed frequency and amplitude. Known phenomena as lock in and lock out zones are studied and compared to results obtained by finite volume methods.

[1] D. Noble, J. Torczynski, A lattice-boltzmann method for partially saturated computational cells, International Journal of Modern Physics C 9 (08) (1998) 1189–1201.
[2] D. J. Holdych, Lattice Boltzmann methods for diffuse and mobile interfaces, Ph.D. thesis, University of Illinois at Urbana-Champaign (2003).
[3] M. J. Krause, F. Klemens, T. Henn, R. Trunk, H. Nirschl, Particle flow simulations with homogenised lattice boltzmann methods, Particuology 34 (2017) 1–13.
[4] R. Trunk, J. Marquardt, G. Thäter, H. Nirschl, M. J. Krause, Towards the simulation of arbitrarily shaped 3d particles using a homogenised lattice boltzmann method, Computers & Fluids 172 (2018) 621–631.
[5] M. Bouzidi, M. Firdaouss, P. Lallemand, Momentum transfer of a Boltzmann-lattice fluid with boundaries, Physics of fluids 13 (11) (2001) 3452–3459.
[6] P. Lallemand, L.-S. Luo, Lattice boltzmann method for moving boundaries, Journal of Computational Physics 184 (2) (2003) 406–421.
[7] D. Yu, R. Mei, W. Shyy, A unified boundary treatment in lattice boltzmann method, in: 41st Aerospace Sciences Meeting and Exhibit, 2003, p. 953.
[8] Z. Guo, C. Zheng, B. Shi, An extrapolation method for boundary conditions in lattice Boltzmann method, Physics of Fluids 14 (6) (2002) 2007–2010.
[9] O. Filippova, D. Hänel, Grid refinement for lattice-bgk models, Journal of Computational physics 147 (1) (1998) 219–228.
[10] R. Mei, L.-S. Luo, W. Shyy, An accurate curved boundary treatment in the lattice boltzmann method, Journal of computational physics 155 (2) (1999) 307–330.
[11] R. Mei, W. Shyy, D. Yu, L.-S. Luo, Lattice boltzmann method for 3-d flows with curved boundary, Journal of Computational Physics 161 (2) (2000) 680–699.

A block triple-relaxation-time lattice Boltzmann model for nonlinear anisotropic convection-diffusion equations

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A block triple-relaxation-time (B-TriRT) lattice Boltzmann model for general nonlinear anisotropic convection-diffusion equations (NACDEs) is proposed, and the Chapman-Enskog analysis shows that the present B-TriRT model can recover the NACDEs correctly. There are some striking features of the present B-TriRT model: firstly, the relaxation matrix of B-TriRT model is partitioned into three relaxation parameter blocks, rather than a diagonal matrix in general multiple-relaxation-time (MRT) model; secondly, based on the analysis of half-way bounce-back (HBB) scheme for Dirichlet boundary conditions, we obtain an expression to determine the relaxation parameters; thirdly, the anisotropic diffusion tensor can be recovered by the relaxation parameter block that corresponds to the first-order moment of non-equilibrium distribution function. A number of simulations of isotropic and anisotropic convection-diffusion equations are conducted to validate the present B-TriRT model. The results indicate that the present model has a second-order accuracy in space, and is also more accurate and more stable than some available lattice Boltzmann models.

Fully coupled multiscale lattice Boltzmann-discrete element model for dense reactive particulate flows

Maier, Marie-Luise[1]; Patel, Ravi Ajitbhai[2]; Prasianakis, Nikolaos[2]; Churakov, Sergey[2]; Nirschl, Hermann[1]; Krause, Mathias J.[1]

[1]Karlsruhe Institute of Technology, Germany; [2]Paul Scherrer Institute, Switzerland

Systems with reactive dense particulate suspensions are of importance in a wide range of practical applications in process engineering such as the biomass conversion in photobioreactors, chemical catalytic reactors, fluidized bed reactors and filtering systems. The motivation of this study is the optimization of the P-RoC process, that stands for phosphorus recovery by calcium silicate hydrate (C-S-H) and crystallization. The process targets to model the removal of phosphate from water using C-S-H solvated calcium ions from the particle surface. The phosphate ions bind to the C-S-H particle

surface by adsorption. The goal is to obtain the knowledge of how the process boundary conditions are to be chosen to obtain an optimal uptake on the particles by numerical simulation.

Models for fully resolved simulations in which particles-fluid interactions are explicitly resolved, are computationally very intensive. Here we present a novel fully coupled lattice Boltzmann-discrete element model in which the fluid flow and reactive transport processes are not resolved around particles but rather treated in a continuum framework through a volume averaging procedure. The fluid flow and the reactive mass transport are governed by volume-averaged Navier-Stokes which recovers the Darcy-Brinkman equations in systems with a sufficiently slow fluid flow and volume averaged advection-diffusion-reaction equation, respectively. The dynamics of the suspended particles are modelled by the discrete element method (DEM). Special treatment and care has to be taken to have a correct coupling between the models to ensure a grid convergent solution. The governing equations of fluid flow and the reactive mass transport are computed using a novel two relaxation time Lattice-Boltzmann method which recovers correctly both governing equations upon the Chapman-Enskog expansion. The coupling to the particles is performed by a forcing term that considers the relation between averaged fluid velocity and particle velocity. For the mass transport equation, the effect of porosity and specific surface area due to the movement of the particles is included in a reaction term and diffusion/dispersion coefficients.

We finally demonstrate the ability of the developed model by a multi-particle simulation in a cavity filled with water and particles, that settle down. The settling is affected by the fluid as particle and fluid are two-way coupled. In another simulation, a reaction is included.

Local Kinetic Computation of Skew-Symmetric Velocity Gradient Tensor using Double Distribution functions-based Lattice Boltzmann Schemes on Standard Lattices

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[2]Department of Mechanical Engineering, University of Tobruk, Tobruk, Libya

Computation of the skew-symmetric velocity gradient tensor, and hence the vorticity, in conjunction with the strain rate tensor play an important role in flow simulations in their classification and the identification of vortical structures, and in the modeling of various complex fluids. For simulating flows along with the transport of a scalar field, which is represented by a convection-diffusion equation, double distribution functions (DDF)-based lattice Boltzmann (LB) methods are commonly used. We present a new local computation method for the skew-symmetric velocity gradient tensor by introducing an intensional anisotropy of the scalar flux in the third order, off-diagonal moment equilibria of the LB scheme for the scalar field, and then combining the second order non-equilibrium components of both the LB schemes. As such, any pair of lattice sets in the DDF formulation that can independently support the third order off-diagonal moments would enable local determination of the complete flow kinematics, with the LB schemes for the fluid motion and the transport of the passive scalar, respectively, providing the necessary moment relationships to determine the symmetric and skew-symmetric components of the velocity gradient tensor. The resulting formulation is completely kinetic and local in nature and does not involve a finite-difference approximation of the velocity gradient components, and hence naturally facilitates their implementation on parallel computers. Based on a Chapman-Enskog analysis, the necessary moment relationships to determine all the components of the velocity gradient tensor are derived for various standard lattices. In particular, we will present the local computation formulas of the complete velocity gradient tensor in two-dimensions (2D) using a pair of D2Q9 lattices for both the fluid motion and the scalar transport, and in three-dimensions (3D) using a D3Q15 lattice for the scalar field, and either a D3Q15, D3Q19 or D3Q27 lattice for the velocity field. Simulations of various benchmark flows demonstrate good accuracy of the predicted skew-symmetric velocity gradient tensors or the vorticity fields obtained using our approach against some benchmark analytical solutions with a second order grid convergence.

1:10pm - 2:20pm	**Lunch**
PG01	
2:20pm - 4:00pm	**CFD and Bio Fluids**
PG01	Session Chair: **Baixin Chen**, Heriot-Watt University

Feeding the baby: a multiscale model of placental transport

Jensen, Oliver[1]; Erlich, Alexander[2]; Pearce, Philip[3]; Chernyavsky, Igor[1]
[1]University of Manchester, United Kingdom; [2]Universite Grenoble Alpes, France; [3]MIT, USA

The human placenta presents many challenges in multiscale modelling, in having an elaborate hierarchical structure that is a strong determinant of its function. As the primary exchange organ of a developing fetus, it performs multiple simultaneous roles including supplying nutrients and removing waste products. I will describe recent work in which imaging data inform computational models of placental transport, and discuss the use of homogenization approximations for spatially disordered media.

Lattice Boltzmann-finite element based simulation of blood flow in aneurysms

Wang, Haifeng[1]; **Krüger, Timm**[2]; **Varnik, Fathollah**[1]
[1]Interdisciplinary Center for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany; [2]School of Engineering, University of Edinburgh, Scotland, UK

Hemodynamic parameters such as blood pressure and wall shear stress (WSS) play a crucial role in the formation, enlargement and rupture of aneurysms. Using a hybrid lattice Boltzmann-finite element model [Krüger, Varnik, Raabe. 2011], we investigate how aneurysm size and wall stiffness affect intra-aneurysm flow characteristics and WSS. Based on simulation results, we conclude that there are at least two independent mechanisms controlling the intra-aneurysm flow properties: (i) size and (ii) deformability of the aneurysm dome. The effects of these competing mechanisms on the phase shift between blood pressure and WSS are also investigated. We also discuss the importance of the latter aspect for triggering certain biological processes.

References:

Krüger T, Varnik F, Raabe D. Efficient and accurate simulations of deformable particles immersed in a fluid using a combined immersed boundary lattice Boltzmann finite element method. Comput Math with Appl. 2011;61:3485-3505.

Noise reduction of flow MRI measurements using a lattice Boltzmann based topology optimisation approach

Klemens, Fabian; Thäter, Gudrun; Krause, Mathias
Karlsruhe Institute of Technology, Germany

In this talk, the coupling of magnetic resonance imaging (MRI) measurements and computational fluid dynamics (CFD) simulation for the application on porous media, e.g. filters, will be investigated.

Using a lattice Boltzmann method based topology optimisation approach, the method can be described as a Navier-Stokes filter for flow MRI measurements.

The main objective of this talk is to analyse the proposed CFD-MRI method for its ability to reduce measurement noise.

For this, real MRI data is analysed and used as basis for artificially generated data. Thus, the ground truth is available and a thorough analysis can be performed. The results show a very high agreement with the ground truth, even with highly noisy images and limited informations available.

Microvascular Sodium Transport Under Complex Endothelial Glycocalyx Structure: A Large-Scale Molecular Dynamics Simulation

Jiang, Xizhuo; Ventikos, Yiannis; Luo, Kai H.
University College London, United Kingdom

The endothelial glycocalyx layer is the first barrier in direct contact with blood flow, and it plays a pivotal role in regulating microvascular transport. Such a layer with a thickness of 50 to 500 nm is featured for its highly negative charges, and intensively interacts with sodium ions. Study of ions and EGL interactions would help to advance understanding and cure of endothelial glycocalyx-related vascular diseases.

In this research, large-scale molecular dynamics simulations were conducted to investigate the interactions of Na+ ions with the EGL under physiological flow conditions. Results show that an increasing blood flow velocity can benefit the outward transport of sodium ions from the endothelial glycocalyx layer to the main flow region. The relationship between the glycocalyx constituent conformations and the ions was then studied. Results suggest that a corner structure of the glycocalyx confines Na+ ions whereas the stretching structure facilitates Na+ ion movement. Based on the findings, an improved Starling principle was proposed. This research provides new insights into the ion-EGL interactions, which adds to our understanding of microvascular fluid exchange.

4:00pm - 4:20pm **Coffee Break**
PG01

4:20pm - 6:00pm **ICMMES Awards etc.**
PG01
Session Chair: **Manfred Krafczyk**, TU Braunschweig
Session Chair: **Li-Shi Luo**, CSRC

Applications of the lattice Boltzmann method in studying particle-laden turbulent flows

Peng, Cheng[1]; **Wang, Lian-Ping**[2,3]
[1]the Pennsylvania State University, United States of America; [2]Southern University of Science and Technology, China; [3]University of Delaware, United States of America

Turbulent flows laden with finite-size solid particles, liquid droplets, and gas bubbles are encountered in a variety of industrial and environmental applications. So far, the only rigorous approach to study details of particle-laden turbulent flows is to numerically resolve the disturbance flow around each particle, known as the interface-resolved simulations (IRS). The key to conduct IRS is to enforce no-slip boundaries on the particle surfaces accurately and efficiently. Due to its flexibility in boundary treatments, the lattice Boltzmann method (LBM) has great potentials to become a mainstream method for IRS. However, certain issues still remain. In this talk, we will give a comprehensive review of LBM

in particle-laden turbulent flow studies. The no-slip boundary treatment methods in LBM, including the immersed boundary method (IBM) and the bounce-back schemes (BBS), and their advantages and potential problems will be discussed. Several examples of LBM simulations of particle-laden turbulent flows will also be given.

Sound propagation through a rarefied gas: kinetic theory, high-order LBM, and moment equations

Wu, Lei
University of Strathclyde, United Kingdom

While computational fluid dynamics based on continuum approach is the fundamental tool for analysing gas dynamics, it fails in the area of rarefied gas dynamics. The primary reason is that the molecular nature of the gas can no longer be ignored when the characteristic length scale of a flow is small and/or the characteristic time scale is short. At the micro/nano-scale, molecular collisions are too infrequent to fully thermodynamically equilibrate the gas, causing the velocity 'slip' and temperature 'jump' at solid surfaces, and the 'Knudsen layer' of nonlinear stress/strain-rate behaviour. In this talk, the sound propagation through a rarefied gas is investigated based on the gas kinetic theory, macroscopic equations such as Navier-Stokes, regularized 13 and 26 moment equations, as well as high-order LBM. It is found that macroscopic equations can only describe the sound propagation in certain parameter regions, and the reason why moment equations and higher-order LBM cannot capture the rarefied gas dynamics is explained at the mesoscopic level.

General synthetic iteration scheme: non-linear case

Zhu, Lianhua; Su, Wei; Zhang, Yonghao; Wu, Lei
James Weir Fluid Laboratory, University of Strathclyde, United Kingdom

Numerical schemes designed for gas kinetic equations, which can describe non-equilibrium gas flows, often encounter difficulties in near-continuum flows. Such as the severe limitations that the grid and time resolutions need to resolve the mean free path and relaxation time, and the notoriety slow convergence of iterative schemes for near-continuum flows. In our recent work, a general synthetic iteration scheme (GSIS) has been developed that can obtain the steady-state solutions of general rarefied gas flows within dozens of iterations at any Knudsen number, using linearized kinetic equations. This work extends the GSIS further to nonlinear cases involving compressible flows in the entire range of Knudsen number.

7:30pm - 10:30pm	**Conference Dinner**
Howies Waterloo Place	

Date: Friday, 26/Jul/2019

9:30am - 10:50am | **LBM for MHD and Other Complex Flows**
PG01 | Session Chair: **Timm Krueger**, University of Edinburgh

Lattice Boltzmann formulations for complex and active fluids based on Jeffery's equation

Dellar, Paul John
University of Oxford, United Kingdom

Jeffery's equation describes a rigid axisymmetric immersed in an ncompressible Stokes flow with a uniform velocity gradient far from the particle. It expresses the evolution of the particle's orientation due to the vorticity and strain rate in the surrounding flow. The particle shape is captured by the single Bretherton parameter. Jeffery's equation reduces to known special cases in the relevant limits of this parameter. Spherical particles rotate with the local fluid vorticity, and elongated slender particles align themselves with the local velocity gradient like material vector fields.

Jeffery's equation forms the basis for modelling dilute and semi-dilute suspensions of many particles. Brownian effects are negligible for sufficiently large particles, so one may simply treat the orientation as a vector field, and the time derivative in Jeffery's equation as a Lagrangian time derivative. The evolution equation for the vector field that is the product of the orientation vector and the fluid density in a compressible fluid resembles the magnetohydrodynamic induction equation, since the orientations of slender particles behave like material vector fields, with additional terms involving the divergence of this vector field, and the strain rate in the surrounding fluid. These terms arise because the vector field describing the particles' orientations has unit length, but not zero divergence. We construct a pure lattice Boltzmann formulation with no additional finite difference approximations. The necessary terms are obtained from the non-equilibrium parts of the orientational and hydrodynamic distribution functions during collisions.

The stress in a suspension of slender rods in a Newtonian fluid contains an additional contribution involving the component of the fluid's strain rate aligned with the orientation vector. This may be significant even at low particle concentrations if the particles' aspect ratio is sufficiently large. A mathematically equivalent stress arises in magnetohydrodynamic models of strongly magnetised plasmas, in which momentum transport across magnetic field lines is suppressed, and can be implemented using the same anisotropic collision operator for the momentum flux. In addition, active particles exert an active stress analogous to the Maxwell stress in magnetohydrodynamics, and propel themselves relative to the fluid around them. Both effects are included.

A theoretical model to study ionizing radiation driven colloidal particles

Wilson, Graham; Bahadori, Amir; Bindra, Hitesh
Kansas State University, United States of America

Kinematics of colloidal particles propelled by ionizing radiation is studied by developing radiation force term for the Lagrangian colloidal particle framework. Using Langevin dynamics

and a random walk model, a theory has been developed to describe the motion of a

radioactively-driven colloid. This theory shows a special case of anomalous di usion. Numerical

simulations have substantiated the theory. It is shown that alpha-particle emission

can signicantly a ect the motion of a radioactive microparticle, although a short-lived radioisotope

is required. Using Brownian dynamics, a second theory has been developed to

describe the motion of a radioactive Janus particle. Non-Gaussian behavior is shown in

addition to the special case of anomalous di ffusion for alpha-emitting radiation colloids.

A lattice Boltzmann model for anisotropic radiative transport problems

Mink, Albert; Nirsch, Hermann; Krause, Mathias J.
Karlsruhe Institute of Technology

With its roots in kinetic theory, the lattice Boltzmann method (LBM) can not only be applied to complex fluid flows, but also to radiative transport in participating volume. Until now, existing radiative transport lattice Boltzmann methods are either derived directly from the radiative transport equation or accordingly to the target equation, obtained by the P1-Approximation. While the first shows its limitation in the high numerical effort, the second fails to model general anisotropy effects.

We show an anisotropic radiative transport LBM by choosing a new equilibrium function. This approach merges the benefits of precise mesoscopic modeling and an intuitive collision step, which implements anisotropy natively. By validation against Monte--Carlo data, the derived LBM is shown to resolve anisotropy close to the radiative source properly. Then, the simulation of the radiative energy density in a microalgae culture, which is illuminated by a large number of LED spots, emphasis the need of accurate anisotropy modeling.

10:50am - 11:10am	**Coffee Break**
PG01	
11:10am - 12:50pm	**Boundary conditions, their implementations, etc.**
PG01	Session Chair: **Victor E. Ambrus**, West University of Timisoara

An improved coupled Immersed-Boundary-Lattice-Boltzmann Solver for the simulation of Particulate Flows

Falagkaris, Emmanouil; Krüger, Timm
The University of Edinburgh, United Kingdom

Fluid-particle systems are commonly encountered in a wide range of disciplines such as medical sciences (blood flow) and chemical engineering (fluidised beds). However, our present understanding of the fundamental physical mechanisms of particle-fluid interactions is far from complete.

We focus on the accurate computation of the hydrodynamic forces and torques, as well as the no slip condition on the boundary using different lattice-Boltzmann collision operators (such as BGK and cascaded) for the solution of the flow field and a multi-direct forcing (MDF) immersed-boundary method for the fluid-structure interaction. We found that previous MDF schemes can become unstable after a certain number of iterations. The source of the instability has been identified in the iterative computation of the boundary force. Here, we propose an alternative iterative scheme that significantly enhances the numerical stability by allowing the boundary force computation to relax at a different rate.

The numerical accuracy and stability of the proposed scheme is demonstrated by simulating flows laden with moving finite-size particles, including a particle in shear flow and the sedimentation of single spherical and non-spherical particles in a cavity. Good agreement between the present results and other schemes is obtained. Furthermore, the sedimentation of two particles in a channel (drafting-kissing-tumbling) is examined, demonstrating the importance of the accurate boundary force computation on the particle motion and dynamics.

Diffuse bounce back condition for lattice Boltzmann method

Liu, Geng; Lee, Taehun
City College of New York, United States of America

The lattice Boltzmann method has been widely used in curved and moving boundary fluid simulations. Both explicit and implicit treatments are studied to recover proper boundary conditions on Cartesian grids. These methods can describe curved boundaries more accurately and more smoothly than the staircase approximation. However, to improve the order of accuracy and to reduce the fluctuation of force, complicated modifications have been applied to the collision step of lattice Boltzmann equation. In this study, a new boundary scheme based on diffuse geometry is proposed for lattice Boltzmann method. The scheme is derived by directly incorporating the bounce back condition into the weak form of the streaming step of discretized Boltzmann equation. The new method does not change the collision operator. Therefore it can be easily combined with complex collision models. Although diffuse boundary is introduced, this scheme recovers exact bounce back condition at sharp boundary limit, regardless of the shapes and motions of the boundaries. Numerical tests show that the accuracy of this method is first order and depends on several lattice Boltzmann parameters and the boundary thickness. In moving boundary problems, the fluctuation of force can be largely reduced compared to popular sharp boundary conditions because it does not require extrapolation to fulfill the unknown information of the newly generated fluid nodes around the boundaries.

An Approach to Treat Boundary Nodes of Complex Porous Media for Conservative Phase-Field Lattice Boltzmann Method

Zarareh, Amin; Khajepor, Sorush; Burnside, Stephen B; Chen, Baixin
Heriot-Watt University, United Kingdom

In this study, an approach based on the Sobel operator is introduced to identify the direction of the unit vector normal at each of the boundary nodes required for calculation of order parameter. Combination of Sobel operator with the conservative phase-field enables the model to simulate two-phase immiscible flow in complex geometries.

The phase-field model is validated by the case of free droplet in comparison with the Laplace's law, as well as the contact angle with the analytical solution obtained from mass conservation. Finally, in order to evaluate the capability of proposed approach in dealing with complex geometries, the droplet penetration into a porous media with realistic geometry is investigated.

Effects of associated non-dimensional numbers including the Reynolds number, Weber number, Froude number, and density ratio as well as wettability condition of porous media on the droplet's penetration, spreading, and deformation are studied. Overall, not only does this study manifest the capability of conservative phase-field combined with Sobel operator but also illuminates the dynamics of droplet impingement into a complex porous media.

Comparison of Boundary Conditions for thermal LBM

Klaß, Friedemann[1]; Gabbana, Alessandro[2]; Bartel, Andreas[1]
[1]University of Wuppertal, Germany; [2]University of Ferrara, Italy

The adoption of appropriate Boundary Conditions (BC) is a crucial aspect for the realization of accurate and numerically

stable LBM simulations. The role of BC is possibly even more prominent when thermal flows are taken into consideration.

In this work we present the implementation and comparison of a few selected BC for a thermal multi-speed LBM, based on the D2Q37 model.

We compare a naive approach, where the equilibrium distribution function is prescribed at the boundary nodes, with

diffusive BC [1] and Chapman-Enskog based BC (CEBC) [2].

We perform simulations of a thermal Couette flow and Rayleigh-Benard cells to numerically assess

the different cases, making use of coarse grids in order to enhance the impact of the BC.

With respect to the other two BC here analyzed, the CEBC ensure mass conservation down to machine precision,

at the price of a significantly higher level of complexity from both the analytical and computational point of view.

We also present a slightly modified version of CEBC that comes from reinterpreting the post streaming mass,

which is shown to be more accurate in prescribing macroscopic values of velocity and temperature at the boundary layers [3].

References:

[1] Ansumali, S., Karlin, I.V., Kinetic boundary conditions in the lattice Boltzmann method, Phys. Rev. E 66, 2002.

[2] Scagliarini, A., Biferale, L., Sbragaglia, M., Sugiyama, K., Toschi, F., Lattice Boltzmann Methods for thermal flows: continuum limit and applications to compressible Rayleigh-Taylor systems. Phys. Fluids. 22, 2010

[3] Klaß, F., Investigations of boundary conditions for thermal lattice Boltzmann models, Master's thesis, University of Wuppertal, 2019.

A Lattice Boltzmann Scheme for Two-phase Flow Based on a Sharp Interface Phase Field Model

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The lattice Boltzmann method based on phase field model is an effective method to simulate multiphase flow. It can calculate complex multiphase flow with good numerical stability, even for large density ratio problems. However, the interface width involved need to be much larger than the grid spacing by using continuous free energy definition if one want to obtain reliable numerical results. This will naturally lead to large computational time, in addition, the artificial pinning on the grid will appear when the interfaces move. To solve the problem, a new lattice Boltzmann method based on phase-field model for large-density-ratio two-phase flows is proposed by using a new free energy calculation formula which is intrinsically discrete. In this method, sharp-interfaces are resolved with essentially one grid point and an accurate rotational invariance can be achieved. As demonstrated by the numerical experiment results, the interfacial kinetic properties can be reproduced accurately with much less ratio of the interface width to the grid spacing compared with the results obtained by existing models in the literature.

12:50pm - 2:00pm **Lunch**
PG01

2:00pm - 3:40pm **Multiphase, Suspensions, Biofluids, etc.**
PG01
Session Chair: **Baixin Chen**, Heriot-Watt University

Modelling and simulation of soft tissue mechanics and fluid-structure interaction

Luo, Xiaoyu
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In this talk I will report my research on fluid-structure interaction (FSI) problems involving soft tissue mechanics. I will use two examples to illustrate different approaches we use. The first example is on the collapsible behaviour of a vessel conveying viscous flows subject to external pressure, a scenario that could occur in many physiological applications. The vessel is modelled as a three-dimensional cylindrical tube of nonlinear hyperelastic material. To solve the fully coupled FSI, we adopt a novel approach based on the Arbitrary Lagrangian–Eulerian (ALE) method and the frontal solver. The

method of rotating spines is used to enable an automatic mesh adaptation. We study the behaviour of the tube under a mode-3 buckling and reveal its complex flow patterns under various external pressures. To understand these flow patterns, we show how energy dissipation is associated with the boundary layers created at the narrowest collapsed section of the tube, and how the transverse flow forms a virtual sink to feed a strong axial jet.

In the second example, we build a dynamic mitral valve (MV) model with FSI that includes physiologically detailed descriptions of the mitral leaflets and the chordae tendineae. Three different chordae models — complex, “pseudo-fibre”, and simplified chordae — are compared to determine how different chordae representations affect the dynamics of the MV. The leaflets and chordae are modelled as fibre-reinforced hyperelastic materials, and FSI is modelled using an immersed boundary-finite element (IB/FE) method. The MV model is used to simulate MV dynamics under physiological pressure conditions. Interesting flow patterns and vortex formulation are identified.

Lattice-Boltzmann model for soft particles with tunable contact angle in multi-component fluids

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Soft particles at fluid interfaces play an important role in many aspects of our daily life, such as food, paints, and medicine. On the one hand, analytical methods are not capable of describing the emergent non-linear effects of the complex dynamics of suspensions of multiple soft particles. On the other hand, experiments typically either only capture bulk properties or require invasive methods. Computational methods, however, are ideally suited to complement experimental work.

Until recently, no efficient and reliable numerical method was available to simulate multiple soft particles at fluid interfaces. Here we present a method to simulate soft particles with tunable contact angle in a multi-component fluid. The numerical model is based on the Shan-Chen lattice-Boltzmann method for the fluids, a finite-element method for the elastic particles, and bounce back for the fluid-structure interaction.

We show benchmark tests with a single deformed particle at an interface, including an analysis of the error stemming from the fluid-structure coupling. Furthermore, we characterise the influence of the preferential contact angle and softness on the particle shape and location relative to the interface. We also demonstrate the model's capability by simulating the covering of a droplet suspended in another fluid by soft particles.

5:00pm - 6:40pm	**Closing**
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