Conference Agenda

The Fifteenth International Conference for Mesoscopic Methods in Engineering and Science

Date: Monday, 09/Jul/2018

8:00am - 11:00am **Rodney Room, Perkins Student Center**	**On-site registration: Rodney Room, Perkins Student Center** 325 Academy St, Newark, DE 19716
9:00am - 10:15am **Rodney Room, Perkins Student Center**	**SC1: Short Courses 1**
	9:00am - 10:15am **Conditioning for the Lattice Boltzmann Method** **Geier, Martin** TU-Braunschweig, Germany Explicit numerical schemes are sensitive to round-off errors. This applies in particular to the lattice Boltzmann method due to its utilization of the velocity distribution function. The relevant hydrodynamic information is hidden in statistical moments or cumulants of the distribution function and these moments have different scales. The problem is of relevance in particular in large simulations involving many space and time scales, especially if slowly moving fluid is studied. To mitigate the problem of accumulation of round-off errors a set of measures can be applied which is referred to as conditioning. Conditioning is indispensable for high fidelity fluid dynamic simulations, especially if single precision data types are used as is often done in the case of GPU computing. Conditioning involves relatively obvious measures like centering variables around zero as well as complicated procedures involving asymptotic analysis for the separation of variables by scale. Conditioning is the art to write down a mathematical statement such that the computer can evaluate it with the highest possible precision. In this short course, we will explain the problem of doing computation with variables of different scales. We show how operations should be order to minimize the impact of round-off errors and discuss how asymptotic analysis is applied to determine scale differences in variables.
10:15am - 10:45am **Rodney Room, Perkins Student Center**	**Coffee Break**
10:45am - 12:00pm **Rodney Room, Perkins Student Center**	**SC2: Short Courses 2**
	10:45am - 12:00pm **LBM on GPUs: a tale of many cores** **Obrecht, Christian** INSA Lyon, France During the last decade, graphics processing units (GPUs) have shown to be very effective hardware platforms for general-purpose high-performance computing. Their area of use now include a considerable number of cardinal scientific computing applications as well as data mining and deep learning applications. Because of their intrinsic data parallelism and explicitness, mesoscopic methods such as the LBM are especially well suited for GPUs. The use of recent GPUs for LBM simulations makes it possible to go beyond 1000 MLUPS per GPU whereas performance of parallel implementations on modern multicore CPUs are of the order of 100 MLUPS per processor. GPU programming remains however an often challenging task, their massively parallel architecture leading to a very specific programming paradigm. This short course will comprise two main parts. In the first one, we will introduce the hardware architecture of modern GPUs as well as present general programming principles and some current programming technologies, namely CUDA and OpenCL. The second part will focus on LBM implementation, introducing programming guidelines and optimisation techniques. Some insight on multi-GPU programming will be given as a conclusion.
12:00pm - 1:30pm **Lunch**	**Lunch**
1:30pm - 2:45pm **Rodney Room, Perkins Student Center**	**SC3: Short Courses 3**
	1:30pm - 2:45pm

Mesoscopic sharp-interface implementation of a moving solid boundary in a viscous fluid

Wang, Lian-Ping
University of Delaware, United States of America

In this short course, we will review various issues related to the implementation of a moving solid boundary in the lattice Boltzmann method. In general, the moving boundary could be handled by an immersed boundary method or an interpolated bounce-back method. Implementation details of different methods will be discussed and contrasted. The question is whether the second-order accuracy and the sharpness of the fluid-solid interface can be maintained. Several benchmark examples will be used to illustrate the details, subtle issues, and relevant open questions.

2:45pm - 3:15pm

Rodney Room, Perkins Student Center

Coffee Break

3:15pm - 4:30pm

Rodney Room, Perkins Student Center

SC4: Short Courses 4

3:15pm - 4:30pm

Gas-kinetic schemes for continuum and multiscale flows

Guo, Zhaoli
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 give 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.

4:30pm - 5:15pm

Rodney Room, Perkins Student Center

Questions and Discussions
Session Chair: **Lian-Ping Wang**, University of Delaware

Date: Tuesday, 10/Jul/2018

8:00am - 12:30pm
Rodney Room, Perkins Student Center

On-site registration: Rodney Room, Perkins Student Center
325 Academy St, Newark, DE 19716

8:45am - 9:00am
Rodney Room, Perkins Student Center

Welcome
Session Chair: **Lian-Ping Wang**, University of Delaware
Session Chair: **Li-Shi Luo**, CSRC

9:00am - 10:40am
Rodney Room, Perkins Student Center

Multiphase and suspension Flows
Session Chair: **Lian-Ping Wang**, University of Delaware

9:00am - 9:50am

Simulation Methods for Particulate Flows and Concentrated Suspensions

Maxey, Martin
Brown University, United States of America

Fluids with solid particles suspended in a gas or liquid are an important area of multiphase flows. The range of conditions vary from low Reynolds number viscous flows to turbulence and cover a wide range of applications such as materials handling, food manufacturing and geophysical contexts. At the bulk level, the goal is often to develop macroscopic equations of motion that describe the dynamics at the level of mixture momentum, volume fractions of the particles and the fluid, and fluid-particle forces or stresses. However we often need a more fundamental understanding that comes from simulations that resolve the motion of individual particles and how they interact with each other and with the suspending fluid.

This presentation will give an overview of the simulation methods currently in use and their range of application [1]. This will include various forms of fictitious domain schemes such as the immersed boundary method as well as developments with lattice Boltzmann methods where the aim is to resolve the particle-fluid boundaries. Often a partial resolution of the particles is sufficient as with the force coupling method supplemented with short-range lubrication hydrodynamics. There is always a trade-off between the level of resolution of the particles and the number of particles or scale of the flow that can be considered. Finally, some comment will be made regarding meshless methods for simulating particulate multiphase flows.

[1] Maxey MR. Annual Review Fluid Mechanics. 49:171-193, 2017

9:50am - 10:15am

An Efficient Numerical Model of Capsule Deformation

Peng, Yan; Armstrong, Charles
Old Dominion University, United States of America

Models of capsule deformation are of interest to the medical community where they can be used to study phenomena such as the deformation of red blood cells. Here we improve the efficiency of a pre-existing model of a capsule in shear flow by implementing a lattice Boltzmann multigrid method. The capsule membrane is modelled as an infinitely thin shell suspended in a fluid domain. A finite element method is used to compute the forces exerted by the elastic nature of the capsule membrane. The fluid field is computed using the lattice Boltzmann method and the interaction between the fluid and the membrane is modelled using the Immersed Boundary method. Implementation of the Full Approximation Storage multigrid method during the computation of the fluid field allows for an increased time step for the capsule, which results in efficiency gains of a full order of magnitude. The deformation for spherical and biconcave capsules are presented and the efficiency of the model is discussed.

10:15am - 10:40am

LBM study of flocculation of monosized spherical particles in homogeneous isotropic turbulence

Wang, Guichao[1]; Wan, Dongdong[2]; Peng, Cheng[3]; Wang, Lian-Ping[1,3]
[1]Department of Mechanics and Aerospace Engineering, Southern University of Science Technology, China, People's Republic of; [2]Key Laboratory of High-efficiency and Clean Mechanical Manufacture, National Demonstration Center for Experimental Mechanical Engineering Education, Shandong University, Jinan, Shandong 250061, P. R. China; [3]Department of Mechanical Engineering, 126 Spencer Laboratory, University of Delaware, Newark, DE 19716-3140, USA

Flocculation of small particles is commonly encountered in many industrial processes including water purification, mineral beneficiation and dewatering, and biological separation processes [1-3]. The efficiency of such processes often depends on the rate and extent of flocculation and subsequently the size and structure of the aggregates formed in the suspension. An optimum energy input can be achieved in getting rid of insufficient mixing and generating a flow field where flocs can form to their optimum size and strength simultaneously. Particle-fluid and particle-particle interactions play an important role in flocculation process. It is desirable to understand the formation and dynamics of flocs in a turbulent field of different intensities.

The influence of energy input and kinetic energy dissipation rate on flocculation behaviour and the resulting effect on yield stress of a concentrated colloidal suspension was investigated. To simulate particle interactions, the non-contact surface force and the contact force were taken into account using the well-known Derjaguin-Landau-Verway-Overbeek (DLVO) theory and the soft-sphere model, respectively. The model was built based on the lattice Boltzmann method (D3Q19, three-dimensional nineteen discrete velocities) incorporating a sharp-interface treatment of no-slip condition on particle surfaces. Bounce-back schemes were used to treat no-slip boundary conditions with minimal numerical dissipation. In this study, an interpolated bounce-back scheme designed by Lallemand et al. [4] was adopted to treat the interaction

of the fluid with moving solid surfaces. The multiple-relaxation time (MRT) collision model was selected for its better numerical stability over the single-relaxation time (SRT) model. We apply the well-known stochastic forcing scheme of Eswaran and Pope [5] to drive the turbulent flow for the advantage of predictable energy input. In the current work, a LBM model for flocculation of monosized spherical particles has been developed and the simulation results of the flocculation hydrodynamics, fluid–particle interactions, and particle–particle collision behaviour will be reported.

[1] C. Wang, D. Harbottle, Q. Liu, Z. Xu, Current state of fine mineral tailings treatment: A critical review on theory and practice, Miner. Eng. 58 (2014) 113-131.

[2] D. Vandamme, I. Foubert, K. Muylaert, Flocculation as a low-cost method for harvesting microalgae for bulk biomass production, Trends Biotechnol. 31 (2013) 233-239.

[3] J. Bratby, Coagulation and flocculation in water and wastewater treatment, IWA publishing2006.

[4] P. Lallemand, L.-S. Luo, Lattice Boltzmann method for moving boundaries, Journal of Computational Physics 184 (2003) 406-421.

[5] V. Eswaran, S.B. Pope, An examination of forcing in direct numerical simulations of turbulence, Computers & Fluids 16 (1988) 257-278.

10:40am - 11:00am

Rodney Room, Perkins Student Center

Coffee Break

11:00am - 12:40pm

Rodney Room, Perkins Student Center

Method and Analysis I

Session Chair: **François Dubois**, Universite Paris Sud

11:00am - 11:25am

Fourth order Galilean invariant lattice Boltzmann models

Geier, Martin

TU-Braunschweig, Germany

Finite velocity models like the lattice Boltzmann equation suffer from incomplete Galilean invariance. The analysis of this problem is rather involved, in particular for high order schemes, as it requires a non-linear asymptotic analysis. Cumulants provide a drastic short cut in the determination of the critical terms. Setting the equilibrium cumulants to zero up to a given order leads to Galilean invariance at the corresponding order. Lattice Boltzmann models on standard lattices usually lack the necessary number of degrees of freedom to ensure Galilean invariance beyond second order. In the talk we present minimal conditions for Galilean invariance of fourth order and show three different approaches to obtain fourth order Galilean invariance with minimal velocity sets.

11:25am - 11:50am

The Efficiency of the Lattice Boltzmann Multigrid Method

Armstrong, Charles Leland; Peng, Yan

Old Dominion University, United States of America

A Full Approximation Scheme multigrid method has been shown to improve the convergence properties of the D2Q9 BGK lattice Boltzmann method for steady flows. In this paper we extend the method to the multiple relaxation time collision model due to its improved stability. The method is then extended to the D3Q19 lattice Boltzmann method and validated using lid driven cavity flow. Multiple smoothers and multigrid schedules are employed and the resulting efficiencies in two and three dimensions are reported for various parameters.

11:50am - 12:15pm

On the computation of surface sensitivities by the adjoint-LBM method for aerodynamic applications

Cheylan, Isabelle Christine[1]; Sagaut, Pierre[2]; Fritz, Guillaume[1]; Ricot, Denis[1]

[1]Renault, France; [2]M2P2 Laboratory, Aix-Marseille Université, France

Shape optimization is a widely used tool in structural mechanics, which has spread to CFD in the past few decades and more recently to LBM-based simulation tools for fluid dynamics. The work presented here focuses on shape optimization using the Lattice-Boltzmann Method (LBM) applied to aerodynamic cases. The adjoint method is used to calculate the sensitivities of the aerodynamic force (drag, lift, side force …) with respect to the design parameters (the position of the nodes of the surface mesh). The main advantage of the adjoint method is its cost, since it is independent from the number of optimization parameters. Here, the continuous adjoint method is developed by deriving the LBM discretized in space, time, and velocities.

The first test case addressed is a sphere in a steady 3D flow, computed using the D3Q19 LBM-BGK collision operator. The continuous steady adjoint equation of the LBM is established, with a focus on the source term which depends on our case-specific cost functional (drag force). The adjoint LBM also includes grid refinements and the Ginzburg interpolation for the wall boundary conditions. Sensitivities obtained with the adjoint method are then compared to those obtained by finite differences. The last step in the optimization loop is performed using an external software to morph the sphere surface mesh according to the surface sensitivities obtained with the adjoint LBM solution. The usefulness of the method is finally assessed with several optimization loops until the drag force reaches a plateau and our criteria is met.

The second test case, that is a more complex case, is closer to an industrial case. The geometry of the previous case is reused, and the Reynolds number is increased, leading to the occurrence of an unsteady vortex shedding. Therefore, an unsteady adjoint method should now be used, but the full recording of the primal flow is of course very demanding in terms of memory storage. An alternative method would be to use a steady adjoint based on a steady time-averaged primal flow solution. Results obtained with this approached adjoint are finally compared once again to finite differences.

Finally, the application of the continuous adjoint to a fully developed 3D turbulent flow is discussed for future use, as well as stability issues that can arise from industrial applications. Last but not least, the cost reduction associated with the use of the adjoint method is highlighted, compared to optimization methods relying on ensemble-based computation of the solution gradient.

12:15pm - 12:40pm

LB-Overset Approach for Moving Boundary Problem

Lallemand, Pierre; Luo, Li-Shi
CSRC, China, People's Republic of

We present the theory and numerical implementation of the lattice Boltzmann method (LBM) with overset technique to treat boundary boundary problem in the nearly incompressible flows. In the overset approach, the moving body, which may have a complicated sharp, is fixed with a mesh of regular boundary, thus the data communication between the moving mesh and the underlying fixed mesh becomes a simpler problem than directly treating the moving body directly with respecting the fixed mesh.

We first present the theory of transferring moments between moving and fixed meshes in 2D. The proposed LB-overset scheme is tested with a cylinder moving with a prescribed motion in a retangular domain with periodic boundary conditions in y direction, and fully-developed flow boundary conditions in x direction. This approach drastically reduces the numerical artifact due to the movement of moving-boday boundary with respect to the underlying Cartesean mesh.

12:40pm - 2:00pm **Lunch**

1:00pm - 6:00pm

Rodney Room, Perkins Student Center

Poster: Poster Exhibit

Study on the Micro-Scale Effection Micro-nano Throat of Shale Reservoir

Wu, Zisen[1]; Dong, Pingchuan[2]; Yuan, Zhongchao[3]
[1]China university of petroleum-Beijing, China; [2]China university of petroleum-Beijing, China; [3]CNOOC Research Institute,china

The micro-scale effect occurs in gas flow through shale reservoirs with small organic pores. Based on the lattice Boltzmann model, which incorporates the bounce-back and specular-reflection boundary conditions, the gas flow through two parallel plates driven by differential pressures was simulated, which in turn verified the model. Considering the slippage effect, surface diffusion and adsorption effect, gas flow in organic channels was simulated based on the proposed modified LB model. It is shown that the micro-scale effect is significant in gas flow through micro-scale channels. The compression effect leads to the nonlinear distribution of pressures along the centerline of the flow channels, and the nonlinearity enhances with the increase in the pressure difference between the two sides of the flow channel. Gas flows in organic pores ,the adsorption effect lead to the decreasing of free-gas velocities and with the decreasing of pore sizes, the reduction of average velocity duo to adsorption effect is increased. The slippage effect and surface diffusion have important influence on the free-gas velocity mass flow. Compared with slippage effect, surface diffusion has a greater contribution to the gas mass flow in organic pores. The increasing of the Knudsen number leads to intensified slippage effect and surface diffusion, growth in the mass flow.

Implementation of local grid refinement based on the general rectangular lattice Boltzmann method in viscous flows

Chen, Songying; Wei, Xuesong; Xiang, Longhao
Shandong University, China, People's Republic of

Local grid refinement of the general rectangular lattice Boltzmann method is established to compute the viscous flow problems. Within the frame of the multi-relaxation time model, all nine moments are related to transfer the parameters on the fine and coarse blocks in D2Q9 model. The fine block keeps shifting with the particle moving, the information at the newly created nodes are initialized with interpolations. Two computed results are presented to validate the proposed method. For an asymmetrical placed moving particle in the Couette flow, the fluctuations of the forces, torque and stresses acting on the moving particle boundary are simulated with uniform coarse grid, uniform fine grid and rectangular refining block. For lid driven cavity flow, refining blocks are set to cover the singular domain, velocity and stress profiles on the middle plane, pressure contour are computed. The computational results show that the dynamic fluctuations are significant suppressed comparing the benchmark.

Micromechanical modeling of the transition from shear thickening to shear thinning in a granular media-fluid suspension

Johnson, Daniel Hunter
Mississippi State University, United States of America

Shear thickening occurs when the viscosity of a fluid drastically increases as the strain rate or shear stress increases. At some point the viscosity starts to decrease as a function of strain rate, a phenomena referred to as shear thinning. The transition from shear thickening to shear thinning is important because at this range of applied shear stresses the system begins to weaken leading to undesired results. The main objective of this study is to micromechanically characterize the transition from shear thickening to shear thinning in a granular media-fluid suspension. For this purpose, we use a micromechanical model built by coupling the Discrete Element Method (DEM) and Lattice Boltzmann Method to simulate the behavior of granular media-fluid suspension undergoing shear thickening and shear thinning. The DEM models the inter-particle contacts, and the LBM approximates the Navier-Stokes equations for incompressible fluids. A previous study has demonstrated that the DEM-LBM can properly capture and effectively model shear thickening phenomenon. In this study, we employ the DEM-LBM model to investigate the zone of applied shear stress (or strain rate) where the system transitions from shear thickening to shear thinning. By increasing the normal stiffness of the boundary, the maximum stress where shear thickening occurs is increased. The effects of other parameters and variables such as inter-particle friction, particle fraction, and particle stiffness are also evaluated.

Phase-Field Modeling of Complex Fluids using Lattice Boltzmann Methods

Fakhari, Abbas; Sinno, Talid; Diamond, Scott
University of Pennsylvania, United States of America

Numerical study of multiphase flows is important in a variety of engineering disciplines, spanning droplet and bubble dynamics, shear flow instabilities, three-phase contact-line motion, mixing and reactive transport in porous media, blood flow in vessels, etc. Despite significant advancements in the field, accurate and efficient modeling of complex fluids is still challenging. The main difficulty is in devising a reliable, and numerically stable, interface tracking method that can tackle rapid topological changes such as coalescence and breakup. The most popular interface tracking schemes, namely the volume-of-fluid, front-tracking, level-set, and phase-field methods, are all macroscopic models which rely on the continuum assumption. Given that the interphase between different fluids is on the order of nanometers, microscopic and mesoscopic approaches are ideal for interfacial phenomena. Lattice Boltzmann Method (LBM) is one of such mesoscopic schemes. The phase-field LBM is particularly advantageous in simulation of immiscible multiphase flows in complex geometries, in studying contact line dynamics, and in modelling biofilm growth and blood flow, among others.

We present a state-of-the-art LB solver, which can be effectively equipped with an Adaptive Mesh Refinement (AMR) technique, for direct numerical simulation of multiphase flows. We consider a variety of fundamentally important phenomena in fluid dynamics and engineering, such as rising bubble and falling droplet, droplet splashing on a wet surface, partial coalescence of a liquid drop at a liquid-liquid interface, and other classical examples. We also use a curved boundary model for dealing with contact line dynamics within the diffuse-interface modeling framework to conduct some numerical simulations of drop impact dynamics on superhydrophobic, cylindrical surfaces.

A Coupled Volume Penalization-Thermal Lattice Boltzmann Method for heat transfer

Cui, Xiongwei[1]; Yao, Xiongliang[1]; Liu, Huimin[2]
[1]Harbin Engineering University, China, People's Republic of; [2]Heilongjiang Branch Pingfang Sub, Bank of China, Harbin, China

In this article, a coupled Volume Penalization-Thermal Lattice Boltzmann method (VP-TLBM) is proposed to solve the thermal flow problem. An external thermal penalization heat source term is introduced into the energy equation to enforce the temperature field at the boundaries satisfied the temperature Dirichlet boundary condition. The modified energy equation is solved by the Thermal Lattice Boltzmann method with the external heat source term. Coupled with the Lattice Boltzmann-Volume Penalization method, which is used to simulated athermal flow past obstacles, the thermal flow problem can be solved. Besides, performing the Volume Penalization-Thermal Lattice Boltzmann method on a certain point, only the variables of this point are needed, which means the present method can be conducted parallelly. Here, we use the proposed VP-TLBM to study the heat transfer between two concentric circular cylinders problem, in which the accuracy of the present method is also studied. Good agreement between the present results and the analytical solution in is achieved.

The Fluid-Fluid Interactions in Pseudopotential Lattice Boltzmann Models – the effects of forcing schemes and fluid properties

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

A wide range of lattice Boltzmann (LB) multiphase models has been proposed and developed [1-6]. The objective of this study is to investigate the details of the pseudopotential model [2, 3] in order to find out the best strategies for simulating multiphase fluids. The investigated schemes include collision operators, implementations of equations of state (EOS), and forcing schemes. The criteria for the assessment of the schemes are based on the following key performance indicators (KPIs): the physics of real fluids recovered by the Maxwell equal-area construction [7]; interfacial interaction in the form of surface tension; spurious velocities; interfacial thickness; and the independent adjustment of density ratio and fluid viscosities (both the kinematic and bulk viscosities). Multiple relaxation time (MRT) models [8] are used instead of simpler Bhatnagar-Gross-Krook (BGK) models [9] to expand the physical envelope within which the simulations are stable and accurate. MRT allows independent adjustment of symmetric and antisymmetric relaxation modes and control of bulk viscosity separate from kinematic viscosity.

The following suggestions are made in this study: the MRT collision operator is more suitable than the BGK collision operator for multiphase simulations; the Huang and Wu forcing scheme [10] is more suitable for larger interfacial tension values; the Li-Luo forcing scheme [11, 12] is preferred for smaller surface tension values. The piecewise linear EOS [13] was found to perform better than the Yuan and Schaefer method of EOS inclusion [14] at high density ratios when the kinematic viscosity is high. The piecewise linear EOS encountered problems achieving equilibrium at lower kinematic viscosities. Imposing a kinematic viscosity ratio between the phases almost eliminated the sensitivity of spurious velocities to the density ratio and allowed the piecewise linear EOS to reach equilibrium at low kinematic viscosities.

In terms of numerical stability, it is found that density ratio, viscosity, interfacial tension and interface thickness all contribute to the creation of spurious velocities. However, viscosity has a greater effect than density ratio. Spurious velocities are inversely proportional to the kinematic viscosity, which is observed for both the YS method and the piecewise linear EOS. Changing the density ratio from 100 to 1000 increases spurious velocities 2.5 times when the YS method is used. The piecewise linear EOS was found to be even less susceptible to increasing the density ratio.

It was confirmed that the optimal value of the MRT magic parameter for multiphase simulations is 1/12 and that setting the bulk viscosity to multiple times the value of the kinematic viscosity can help to increase stability.

References

[1] Gunstensen, Rothman, Zaleski, and Zanetti, "Lattice Boltzmann model of immiscible fluids," Physical review. A, Atomic, molecular, and optical physics, vol. 43, no. 8, p. 4320, 1991.

[2] X. Shan and H. Chen, "Lattice Boltzmann model for simulating flows with multiple phases and components," Physical Review E. Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics, vol. 47, no. 3, pp. 1815-1815, 1993.

[3] X. W. Shan and H. D. Chen, "Simulation of Nonideal Gases and Liquid-gas Phase-transitions by the Lattice Boltzmann-equation", Physical Review E, Article vol. 49, no. 4, pp. 2941-2948, Apr 1994.

[4] Swift, Osborn, and Yeomans, "Lattice Boltzmann simulation of nonideal fluids," Physical review letters, vol. 75, no. 5, p. 830, 1995.

[5] M. R. Swift, E. Orlandini, W. R. Osborn, and J. M. Yeomans, "Lattice Boltzmann simulations of liquid-gas and binary fluid systems," Physical Review E, vol. 54, no. 5, pp. 5041-5052, 11/01/ 1996.

[6] X. He, S. Chen, and R. Zhang, "A Lattice Boltzmann Scheme for Incompressible Multiphase Flow and Its Application in Simulation of Rayleigh–Taylor Instability," Journal of Computational Physics, vol. 152, no. 2, pp. 642-663, 1999/07/01/ 1999.

[7] Boltzmann, Lectures on gas theory / by L. Boltzmann. 1964.

[8] D. d'Humieres, "Generalized lattice-boltzmann equations," vol. 159(Progress in Astronautics and Aeronautics: AIAA, 1994, pp. 450-450.

[9] P. L. Bhatnagar, E. P. Gross, and M. Krook, "A Model for Collision Processes in Gases. I. Small Amplitude Processes in Charged and Neutral One-Component Systems," Physical Review, vol. 94, no. 3, pp. 511-525, 05/01/ 1954.

[10] R. Huang and H. Wu, "Third-order analysis of pseudopotential lattice Boltzmann model for multiphase flow," Journal of Computational Physics, vol. 327, pp. 121-139, 2016.

[11] Q. Li, K. H. Luo, X. J. Luo, and X. J. Li, "Lattice Boltzmann modeling of multiphase flows at large density ratio with an improved pseudopotential model," Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, vol. 87, no. 5, 2013.

[12] Q. Li and Q. Luo, "Achieving tunable surface tension in the pseudopotential lattice Boltzmann modeling of multiphase flows," Physical Review E - Statistical, Nonlinear, and Soft Matter Physics, vol. 88, no. 5, 2013.

[13] C. E. Colosqui, G. Falcucci, S. Ubertini, and S. Succi, "Mesoscopic simulation of non-ideal fluids with self-tuning of the equation of state," Soft Matter, 10.1039/C2SM06353K vol. 8, no. 14, pp. 3798-3809, 2012.

[14] P. Yuan and L. Schaefer, "Equations of state in a lattice Boltzmann model," Physics of Fluids, vol. 18, no. 4, 2006.

2:00pm - 3:40pm

Rodney Room, Perkins Student Center

Multiphase and Porous Media Flows

Session Chair: **Martin Geier**, TU-Braunschweig

2:00pm - 2:50pm

Mesoscopic simulation of transport phenomena 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. 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. Mesoscopic 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 review some lattice-based modeling approaches for mesoscopic simulation of flow in porous media. The techniques employed include the lattice Boltzmann method, link-flux method for electrokinetic transport, and moment propagation methods for advection-diffusion. I will then discuss how these techniques can be combined to simulate porous materials with realistic morphology based on experimental data. Results for permeability measurements will be presented to illustrate how the simulation data can provide feedback to experiment in order to optimize the materials properties of nonwoven fibrous membranes.

2:50pm - 3:15pm

Thermally stratified porous media flow simulations using a central moment lattice Boltzmann method

Hajabdollahi, Farzaneh; Premnath, Kannan
University of Colorado Denver, United States of America

Thermal dispersion and flow through porous media arise in a number of geophysical applications and engineering settings, including geothermal reservoirs, chemical and petroleum refining processes, solar energy-based heat exchangers, and subsurface contaminant transport. In this work, we present a central moment based cascaded lattice Boltzmann (LB) method for simulation of thermally stratified flows through porous media. The averaged flow and thermal energy transport at the representative elementary volume scales are represented by means of the macroscopic Brinkman-Forchheimer-Darcy (BFD) equation and the energy equation, with the latter coupled to the former via the buoyancy force. The fluid motion represented by the BFD equation is solved by means of a cascaded LB scheme on a D2Q9 lattice, where the linear and nonlinear drag force of the medium as well as the buoyancy force are incorporated via a symmetrized operator splitting based approach. The moment equilibria in this scheme are constructed to depend on the porosity and augmented with corrections to eliminate cubic velocity errors parameterized by porosity to recover the BFD equation on the standard D2Q9 lattice. The advection-diffusion equation for the temperature field is solved using another cascaded LB scheme, with its equilibria dependent on the heat capacity ratio and augmented with additional corrections parameterized by porosity to consistently represent the energy equation. Simulations of various benchmark buoyancy-driven flows validate the proposed cascaded LB schemes for fluid convection in porous media.

3:15pm - 3:40pm

Effects of the lubrication force model on turbulence modulation by finite-size particles

Wan, Dongdong[1,3]; Wang, Lianping[2,3]; Wang, Guichao[3]; Peng, Cheng[2]; Chen, Songying[1]
[1]Shandong University, China, People's Republic of; [2]University of Delaware, United States of America; [3]Southern University of Science and Technology, China, People's Republic of

In recent years, more and more interface-resolved simulations of a turbulent flow laden with finite-size solid particles have been reported. A general issue is how to handle the near-field hydrodynamic interactions of two solid particles when they are close to each other. The flow in the narrow gap between the solid particles may not be resolved and a lubrication force model is needed. In general, there are mainly two classes of lubrication force models: (a) an unphysical repulsive force model designed to prevent particle overlap and (b) a physical lubrication force model based on the Stokes flow solution. There are also variations of details in these models. It is not clear if and when the lubrication force model affects the physical results of the bulk turbulent flow and dynamics of solid particles. In the present work, several reported models of lubrication force are compared in detail to study their impact on the modulation of turbulent flow by finite-size non-sedimenting particles. We consider a homogeneous isotropic turbulent flow laden with neutrally buoyant solid particles. The flow is solved using the multiple-relaxation-time lattice Boltzmann method. Flow statistics, such as turbulent kinetic energy, energy spectrum, dissipation rate, r.m.s. component fluctuation velocity, Kolmogorov length scale, eddy turnover time, etc. as well as the conditional statistics near the solid particle surface are presented. The differences between the results based on different lubrication force models are analyzed to illustrate the limitations and open questions related to the treatment of the short-range hydrodynamic interactions in interface-resolved direct numerical simulations.

3:40pm - 4:00pm

Rodney Room, Perkins Student Center

Coffee Break

4:00pm - 5:40pm

Rodney Room, Perkins Student Center

CFD and GPU implementations

Session Chair: **Ulf Schiller**, Clemson University

4:00pm - 4:25pm

DNS of Passive Scalar Transport in Turbulent Channel Flow using the Lattice-Boltzmann Method on Massively Parallel GPU Architectures

Pachalieva, Aleksandra[1]; Niedermeier, Christoph A.[2]; Tschirschnitz, Gustav[2,3]; Indinger, Thomas[1]; Adams, Nikolaus A.[1]

[1]Technical University of Munich, Chair of Aerodynamics and Fluid Mechanics, Boltzmannstr. 15, 85748 Garching bei München, Germany; [2]FluiDyna GmbH, Edisonstr. 3, 85716 Unterschleißheim, Germany; [3]Technische Universität Dresden, 01062 Dresden, Germany

We present a framework for the simulation of turbulent flows with passive scalar transport using the lattice-Boltzmann method (LBM) on massively parallel GPU architectures. We apply the double-distribution-function (DDF) lattice-Boltzmann method to solve the Navier-Stokes Equations (NSE) for the flow field and the Advection-Diffusion Equation (ADE) for the scalar field. The improved Bhatnagar-Gross-Krook (BGK+) collision operator introduced by Geier et al. together with a D3Q27 lattice velocity set is used for the flow field and the BGK collision operator together with a D3Q7 lattice velocity set is used for the scalar field. To validate the framework, we perform Direct Numerical Simulation (DNS) of fully developed turbulent channel flow with passive scalar transport at Re_tau = 180 and at different Prandtl/Schmidt numbers. The results are in very good agreement with reference data and show that our GPU-based LBM framework is well-suited for this type of simulations.

4:25pm - 4:50pm

lbmpy: A Flexible Symbolic Toolkit for Lattice Boltzmann Methods with Code Generation for CPUs and GPUs

Bauer, Martin; Rüde, Ulrich

University Erlangen-Nuremberg, Germany

There are many different lattice Boltzmann methods (LBM), starting from the well-known single-relaxation-time scheme with its multi-relaxation-time (MRT) generalization, up to recently proposed entropic or cumulant methods.

We present a symbolic toolkit that enables the user to formulate, analyse and run all these different LB schemes using a Python-based interface. For example, one can define a custom MRT LB method by choosing a set of moments with corresponding equilibrium descriptions, analyse it by running an automated Chapman-Enskog expansion, improve the scheme, and finally execute it efficiently on the GPU, all inside a user friendly, interactive Python environment. Our toolkit allows the definition and modification of a LB method on different levels of complexity. For example, relaxation times can be defined as a function of local flow properties. With this mechanism, extensions like non-Newtonian effects or LES models can be easily incorporated into LB schemes by choosing relaxation times as functions of local shear stresses.

Having the LB method available in symbolic representation allows us to use a set of transformations that simplify and optimize the formulation of the method. Depending on the scenario at hand and the target architecture, different optimization steps are automatically applied. Transformations propagate constants, eliminate common subexpressions, improve cache characteristics by utilizing non-temporal stores, or automatically determine optimal CUDA block sizes for GPU kernels. This optimized formulation is then compiled to a highly efficient compute kernel, that can be called directly from the Python environment. In addition, the generated LB kernels can also be integrated into the waLBerla C++ framework [1] to run massively parallel MPI simulations on block-structured grids.

[1] http://walberla.net

4:50pm - 5:15pm

The GeLB domain-specific programming language -- a new tool for lattice Boltzmann modeling

Chirila, Dragos Bogdan[1]; Lohmann, Gerrit[1,2]

[1]Alfred Wegener Institute, Helmholtz Centre for Polar and Marine Research (AWI), Germany; [2]University of Bremen

Unlike general-purpose programming languages (which are flexible-enough for implementing arbitrary applications), domain-specific languages (DSLs) are focused on a particular range of applications. The (intentional) loss in flexibility is usually compensated for by significant gains in ease-of-use and expressiveness (for example, by minimizing the amount of boilerplate code required). Although a large body of work exists related to DSLs for other application domains (e.g. well-known software build-systems such as Make and CMake, or operating-system-level virtualization technologies such as Docker), so far this approach has not been used extensively for creating high-performance computing (HPC) applications. We present the generic lattice Boltzmann (GeLB) DSL, as a new tool for researchers who develop and use lattice Boltzmann (LB) algorithms. In the context of LB research, the main design-goals of GeLB are (a) to decrease the effort required from researchers to implement and test existing or new LB algorithms, and (b) to isolate most of the technical implementation side-issues away from the core numerical kernels. The second benefit is particularly valuable, given the recent trends towards fragmentation of computing hardware (e.g. accelerators such as GPUs and FPGAs). After presenting the GeLB DSL, we discuss how this new tool can facilitate sharing and more objective comparisons (regarding arithmetic intensity and performance bottlenecks) of the computational kernels corresponding to various classes of LB algorithms, such as the multiple-relaxation-times (MRT) or the cumulant LB methods.

5:15pm - 5:40pm

Pore scale modeling of hydraulic fracture process

Chen, Zhiqiang; Wang, Moran
Tsinghua University, China, People's Republic of

Hydraulic fracturing is one of primary engineering techniques to improve well productivity especially for unconventional reservoirs. Generally, there are two kinds of numerical models for hydraulic fracture simulation, continuum-based models and discontinuum-based models.In continuum-based models governing equations based on continuum theory are solved with single planar fracture assumption. However, in unconventional reservoirs this assumption breaks down, which results in the predictions by continuum-based models are not consistent with experiments.

In this work we develop a more accurate hydro-mechanical coupled discontinuum-based model, where the solid deformation and fracture behavior are simulated by discrete element method (DEM) and the fluid flow is solved directly by lattice Boltzmann method (LBM) at pore scale. To validate current hydro-mechanical coupled model, sphere sedimentation in Newtonian fluid is simulated, and the results agree well with the previous work in literature. Then hydro-fracturing is simulated, attempting to answer the inconsistence between continuum-based model predictions and experiment observation.

6:00pm - 7:30pm	**Reception and Social at Klondike Kate's Restaurant & Saloon**

Date: Wednesday, 11/Jul/2018

8:30am - 10:30am
Rodney Room, Perkins Student Center

On-site registration: Rodney Room, Perkins Student Center
325 Academy St, Newark, DE 19716

9:00am - 10:40am
Rodney Room, Perkins Student Center

CFD and Bio Fluids
Session Chair: **John Abraham**, San Diego State University

9:00am - 9:50am

Coupling Lattice-Boltzmann and Langevin Dynamics to Explore the Complex Nature of Blood Flow

Aidun, Cyrus K; Zhu, Yuanzheng; Liu, Zixiang
Georgia Tech, United States of America

Including the cells and proteins suspended in blood present a complex system for computational analysis. In particular, the red blood cell (RBC) is highly deformable and forms nearly half of the blood volume. Where RBC and platelets have a length scale of few microns, the proteins in blood, such von Willebrand factor (vWF), are in the nanoscale with significant Brownian motion. We show that treatment of the nanoscale particles with Langevin Dynamics coupled to the lattice-Boltzmann platform provides an effective approach for large-scale exploration of blood flow complexities. We discuss recent progress and challenges in blood flow simulation and application to important cardiovascular diseases, such as thrombosis, where interaction of platelets and RBC with vWF and other proteins is of particular interest.

9:50am - 10:15am

A comparative study of forcing schemes in a multicomponent lattice Boltzmann model

Küllmer, Knut[1]; Krämer, Andreas[2]; Wilde, Dominik[1]; Joppich, Wolfgang[1]; Reith, Dirk[1]; Foysi, Holger[3]
[1]Bonn-Rhein-Sieg University of Applied Sciences, Sankt Augustin, Germany; [2]National Heart, Lung, and Blood Institute, Bethesda, United States; [3]University of Siegen, Siegen, Germany

In this contribution, we investigate the diffusion characteristics in pseudopotential-based lattice Boltzmann models for multicomponent systems [Shan & Doolen: J. Stat. Phys. 81, 379 (1995)]. The influence of different forcing schemes on the macroscopic diffusion coefficients is analysed using the Shan-forcing scheme [Shan & Chen: Phys. Rev. E 47, 1815 (1993)], the He-forcing scheme [He et al.: Phys. Rev. E 57, R13 (1997)], the Guo-forcing scheme [Guo et al.: Phys. Rev. E 65, 046308 (2002)] and the exact difference method from Kupershtokh et al. [Kupershtokh et al.: Comput. Math. Appl. 58, 965 (2009)]. We show that these can lead to a shift in the diffusion characteristics [Küllmer et al.: Phys. Rev. E 97, 023313 (2018)], which indirectly impacts the interfacial properties (spurious velocities, static contact angles). On this basis, a consistent way to compare different model variations (and potential functions within a model formulation) is introduced, which relies on reduced diffusion-related variables. To verify our theory, we present results for simulations of static contact angles, decaying concentration waves and static droplets using the different model variations and different potential functions (including commonly used and new ones).

10:15am - 10:40am

Exploring turning strategies for biomimetic underwater propulsors

Demirer, Ersan; Yeh, Peter; Alexeev, Alexander
Georgia Tech, United States of America

Fish employs multiple fins to perform gradual turn or escape maneuver. In the case of robotic fish, it can advantageous to use a single flapping propulsor to generate forward thrust and control navigation. Here we use three-dimensional computer simulations that are based on fluid-structure interaction method integrating lattice Boltzmann and lattice spring models to examine turning strategies for a biomimetic oscillating elastic rectangular plate propulsor that is submerged in a viscous Newtonian fluid. The elastic plate is actuated near the first natural frequency at the leading edge. We examine two kinematic actuation patterns to produce both pitching and yaw moments. In the first scenario, we use periodic plunging with asymmetric velocities on the upstroke and downstroke to create pitching moment. In the second case, we combine sinusoidal plunging and twisting motion to induce yaw moment. We find that both strategies generate net lateral forces and turning moments. For the first case, we find that the magnitudes of the force and turning moment increase with increasing velocity ratio between the upstroke and downstroke. For the second case, our simulations reveal a range of optimal phase angles and twisting amplitudes that lead to the maximum yaw moment. We show that optimal turning, the phase need to be tuned such that the instant of time during the maximum propulsor rotation coincides with the instant of the maximum force production. Furthermore, we find that the plate bending is primarily normal to the plunging plane with negligible twisting.

10:40am - 11:00am
Rodney Room, Perkins Student Center

Coffee Break

11:00am - 12:40pm
Rodney Room, Perkins Student Center

Thermal and Compressible Flows
Session Chair: **Paul Dellar**, University of Oxford

11:00am - 11:25am

Simulate the thermal Navier Stokes equations with a single particle distribution ?

Dubois, François[1,2]; Lallemand, Pierre[3]

[1]Universite Paris Sud, France; [2]LMSSC, CNAM, Paris; [3]Beijing Computational Science Research Center, Haidian District, Beijing 100094, China

In a previous contribution [2], we have observed the difficulties to simulate the thermal Navier Stokes equations with two particle distributions : one for mass and momentum, a second distribution for total energy. In particular, the heat transfer due to viscous dissipation is a priori impossible to simulate when we follow the initial framework of multiple relaxation schemes [3] of the lattice Boltzmann method [4]. With an extension of the Taylor expansion method [1] that will be detailed during the conference, we are able to write in a direct and straightforward way the equivalent partial differential equations of any nonlinear lattice Boltzmann scheme. In particular conservation laws including conservation of mass, momentum and energy, with a single particle distribution, as in [5, 6]. During the conference, we will present our results for various lattice Boltzmann schemes and in particular the algebraic difficulties to recover the thermal Navier Stokes equations and in particular the viscous work.

References

[1] F. Dubois. “Equivalent partial differential equations of a lattice Boltzmann scheme”, Computers and Mathematics with Applications, vol. 55, p. 1441-1449, 2008.

[2] F. Dubois, B. Graille, P. Lallemand. “Recovering the full Navier Stokes equations with lattice Boltzmann schemes”, 30th International Symposium on Rarefied Gas Dynamics, Jul 2016, Victoria, BC, Canada. American Institute of Physics Proceedings, vol. 1786 (040003), pp.40003 - 40003, 2016.

[3] D. d’Humières, “Generalized Lattice-Boltzmann Equations”, in: AIAA Rarefied Gas Dynamics: Theory and Applications, Progress in Astronautics and Aeronautics, vol. 159, AIAA, Washington, D.C., p. 450-458 (1992).

[4] P. Lallemand, L.S. Luo. “Theory of the lattice Boltzmann method: Dispersion, dissipation, isotropy, Galilean invariance, and stability”, Physical Review E, vol. 61, p. 6546-6562, (2000).

[5] P. Lallemand, L.-S. Luo. “Theory of the lattice Boltzmann method: Acoustic and thermal properties in two and three dimensions”, Physical Review E, vol. 68, p. 036706, 2003.

[6] P. Lallemand, F. Dubois, “Comparison of Simulations of Convective Flows”, Communications in Computational Physics, vol. 17, p. 1169-1184, 2015.

11:25am - 11:50am

Study of compressible natural convection in an enclosure with discrete unified gas kinetic scheme

Wen, Xin; Wang, LianPing

Department of Mechanical Engineering, University of Delaware, Newark, DE 19716, USA

The buoyancy driven natural convection in an enclosure plays an important role in both flow structure study and practical applications such as energy storage systems and air conditioning systems. One of the major control parameters in such study is the temperature difference which governs the level of flow compressibility. When the temperature difference is small enough the Boussinesq assumption is valid, researchers have provided both two-dimensional and three-dimensional benchmark solutions for the natural convection in a cavity under the Boussinesq assumption. However, with large temperature differences, such convection flows are compressible and complex due to stronger coupling between velocity field and temperature field and a larger range of system parameters such as the Rayleigh number, Prandtl number, cavity aspect ratio, temperature difference.

The previous studies on compressible natural convection are limited to two-dimensional simulations and low Rayleigh numbers, and most of the works are conducted under a low Mach number assumption. In this study, we perform the simulations with discrete unified gas-kinetic scheme (DUGKS) developed by Guo et al, [1, 2]. Instead of discretizing the Navier-Stokes equations directly as done by conventional Computational Fluid Dynamics (CFD), DUGKS treats the fluid motion through the kinetic approach by solving a model Boltzmann equation. As a finite-volume method, the non-uniform mesh can be easily employed by DUGKS, the steep gradient of the velocity and temperature near the wall can then be well resolved. The discrete unified gas-kinetic scheme is constructed based on the BGK Shakhov model, the full compressible Navier Stokes equation can be recovered. We will investigate the influence of the temperature difference on the flow structure and heat transfer rate by the simulations of natural convection in a square cavity with the large temperature difference at moderate Rayleigh numbers.

[1] Z. L. Guo, K. Xu and R. J. Wang, Phys. Rev. E 88, 033305 (2013).

[2] Z. L. Guo, R. J. Wang and K. Xu, Phys. Rev. E 91, 033313 (2015).

11:50am - 12:15pm

A discrete unified gas kinetic scheme with force term for flows in different regime

Shen, Jie[1,2]; Lu, Zhiming[1]; Wang, Lian-Ping[2]

[1]Shanghai University, CHINA; [2]University of Delaware, USA

The discrete unified gas kinetic scheme is a multiscale method designed for flows in all regimes including compressible flow and non-continuum flow regimes. External force term often occurs in realistic physical problems, but was considered only briefly in previous studies. In this paper we include a general force term into the Boltzmann BGK-Shakhov model using the Hermite expansion. With no further approximation made to the force term, the current scheme is valid in all flow regimes. To validate the scheme, we simulate the Rayleigh Benard convection, forced Taylor Green vortex flow in the continuum regime and standing shear wave problem with different Knudsen numbers. The numerical results show that the current scheme can be used in different flow regimes.

12:15pm - 12:40pm

Modeling Fouling Process on Tubes with Lattice Boltzmann Method and Immersed Boundary Method

Tong, Zi-Xiang; Li, Ming-Jia; He, Ya-Ling
Xi'an Jiaotong University, China, People's Republic of

In the waste heat recovery heat exchangers, the flue gas always carries fly ashes, which can deposit on the surface of the heat exchangers, generate porous fouling layers and degrade the performance of the system. Therefore, it is important to study the fouling process on heat exchangers. The growth of the fouling layer moves the flow boundary and complicates the traditional method based on dynamic meshes.

In the present work the immersed boundary method (IBM) is coupled with lattice Boltzmann method (LBM) to simulate the fouling processes on tubes. A large-eddy simulation based multiple-relaxation-time LBM is used to model the air flow and the Lagrangian particle tracing method is used to study the motion of particles. A subgrid Brownian force is added to the particle motion to consider the effects of subgrid fluctuations. The energy analysis is used to determine the particle deposition criterion and the force and momentum analyses are employed for the removal criterion. For the boundary of the fouling layer, the IBM is adopted and the shape of the boundary is evolved according to the amount of deposited particles. Based on the proposed numerical model, the evolution of the shape of fouling layer is obtained. The effects of the parameters, such as air velocity, particle diameter, tube shape and arrangement, on the growth of fouling layer are also studied. The proposed numerical model can be further used to predict the fouling processes on heat exchangers and facilitate the design of heat exchangers.

12:40pm - 2:00pm — **Lunch**

2:00pm - 3:40pm
Rodney Room, Perkins Student Center

Multiphase Flows: Modelling and Simulation

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

2:00pm - 2:50pm

Multi-scale modeling of polydisperse multiphase flows using quadrature-based moment methods

Fox, Rodney
Iowa State University, United States of America

Quadrature-based moment methods (QBMM) are employed to solve kinetic and population balance equations and are especially useful for systems far from equilibrium. Examples include highly compressible and disperse multiphase flows. Starting from the closed mesoscale model, the unclosed moment equations are formulated and closed using QBMM. The order of the closure is controlled by the order of the moments used in QBMM. For example, dilute particle-laden flows can be described by a kinetic equation for the particle-phase velocity distribution function (VDF), and successfully closed with velocity moments up to fourth order.

The numerical algorithms used to solve moment equations must be consistent with the mesoscale model. For example, the numerical methods employed to solve the spatial advection terms and the source terms must guarantee that the moments remain realizable (i.e., they must correspond to a VDF). This can be accomplished with kinetic-based finite-volume methods. With QBMM, the VDF is represented by a finite set of weighted delta functions, similar to the lattice-Boltzmann method, but with velocities that vary in space and time. Using applications from disperse multiphase flows, I will discuss how QBMM are applied to solve mesoscale models using the OpenQBMM.org software.

2:50pm - 3:15pm

Phase-field lattice Boltzmann modelling and its application in the oil & gas sector

Mitchell, Travis Ryan[1]; Leonardi, Christopher Ross[1]; Towler, Brian[2]; Firouzi, Mahshid[2]
[1]School of Mechanical and Mining Engineering, The University of Queensland, Australia; [2]School of Chemical Engineering, The University of Queensland, Australia

A prominent example of applied multiphase flows is in the oil and gas industry where the extraction and transport of hydrocarbons is of primary concern. Understanding phase interactions at the bubble scale is essential when looking to up-scale to models that capture the system dynamics of wells and piping networks. At the system level, the liquid hold-up, flow regime and ultimately the pressure gradient are the primary outputs desired for making predictions and operational decisions. \\

In order to determine the flow dynamics within piping systems, the most common approaches used in the oil and gas industry consist of either mechanistic models or 1D multi-fluid (Euler-Euler) type formulations. These models do not directly simulate the interaction of different fluids, but approximate them with closure relations allowing their set of governing equations to be solved. Historically, these relations have been generated experimentally or from simplified analytical derivations. Both of these methods can cause issues when extrapolating models to different geometrical configurations or fluid types, as evidenced in the unconventional gas literature \cite{ref1}.\\

Recently, a multiphase lattice Boltzmann model (LBM) \cite{ref2, ref3} was proposed based on the conservative phase-field model \cite{ref4} and the work of Zu and He \cite{ref5}, which has provided the foundation for this work. The LBM has been shown to be computationally efficient on parallel architectures in comparison to other phase-field based solvers, and capable of accurately capturing high density ratio and Reynolds number scenarios. This presentation will look to highlight liquid-gas closure relations previously incorporated into mechanistic pipe flow models; their applicability to unconventional gas wells and how the proposed LBM can improve on these, often empirically formulated, closures.

\begin{thebibliography}{00}

\bibitem{ref1} Firouzi, M., Towler, B., Rufford, T., \textit{Developing new mechanistic models for predicting pressure gradient in coal bed methane wells}, Journal of Natural Gas Science and Engineering \textbf{33}, 961-972, 2016.

\bibitem{ref2} Fakhari, A., Mitchell, T., Leonardi, C., Bolster, D., \textit{A robust phase-field lattice Boltzmann model for immiscible fluids at high density ratios}, Physical Review E \textbf{96}, 053301, 2017.

\bibitem{ref3} Mitchell, T., Leonardi, C., Fakhari, A., \textit{Development of a three-dimensional phase-field lattice Boltzmann method for the study of immiscible fluids at high density ratios}, International Journal of Multiphase Flow, In press.

\bibitem{ref4} Geier, M., Fakhari, A., Lee, T., \textit{Conservative phase-field lattice Boltzmann model for interface tracking equation}, Physical Review E \textbf{91}, 063309, 2015.

\bibitem{ref5} Zu, Y. and He, S., \textit{Phase-field-based lattice Boltzmann model for incompressible binary fluid systems with density and viscosity contrasts}, Physical Review E \textbf{87}, 043301, 2013.

\end{thebibliography}

3:15pm - 3:40pm

Lattice Boltzmann Simulations of Particle Motion in a Turbulent Channel Flow

Jebakumar, Anand Samuel[1]; Premnath, Kannan Nandha[2]; Magi, Vinicio[3]; Abraham, John[1,4]

[1]Purdue University, United States of America; [2]University of Colorado, Denver, United States of America; [3]University of Basilicata, Italy; [4]San Diego State University

Particle-resolved direct numerical simulations (PR-DNS) of particle-laden turbulent flow in a channel are carried out to understand the effect of particle Stokes number (St) on their motion. The study focuses on particles which are larger than the Kolmogorov scale. The forces that impact this motion are factored into the discussion. The lattice-Boltzmann method (LBM) is employed for the simulations. The scheme employed is able to resolve the surface of the particle and a method is adopted to account for the exchange of momentum

between the particles and fluid as the particles move on fixed lattices. The simulations show that particles with relatively lower St move preferentially toward the wall while those with higher St exhibit a relatively uniform concentration.

3:40pm - 4:00pm

Rodney Room, Perkins Student Center

Coffee Break

4:00pm - 5:40pm

Rodney Room, Perkins Student Center

Algorithm and Applications

Session Chair: **Travis Ryan Mitchell**, The University of Queensland

4:00pm - 4:25pm

Multistep Integration in the Lattice Boltzmann Method: Application and Limitations

Wilde, Dominik[1]; Krämer, Andreas[1]; Küllmer, Knut[1]; Foysi, Holger[2]; Reith, Dirk[1]

[1]Bonn-Rhein-Sieg University of Applied Sciences, Germany; [2]University of Siegen, Germany

One of the several ways for deriving the lattice Boltzmann method (LBM) is making use of the trapezoidal rule [He et al.: Phys. Rev. E, 57, 1 (1998)], an implicit multistep scheme of second order.

The question arises, whether higher order time discretizations are possible and beneficial. In this work, we therefore present a generalized framework for the incorporation of implicit multistep methods of arbitrary order and demonstrate both the advantages and the limitations of this approach.

According to the analysis of Dahlquist, A-stable multistep methods can only reach an order of convergence of two and among these methods, the trapezoidal rule used generally within the lattice Boltzmann method (LBM) has the smallest error rate [Dahlquist: BIT Numerical Mathematics, 3, 27-43(1963)]. Thus, relaxing the stability restriction makes it possible to increase the temporal order of accuracy within LBM simulations. To evaluate the developed multistep LBM, our ansatz has been chosen as follows: The stability issues are investigated in a linear stability analysis. Additionally, a 2D Taylor Green vortex is simulated with a third-order accurate Adams-Moulton method and a second-order backward differentiation formula (BDF) to prove the applicability of multistep methods.

It is shown, that the multistep LBM framework principally improves the temporal order of the method, in accordance with theoretical predictions.

However, this leads to a higher error rate of one magnitude for the BDF and a limited stability region for the Adams-Moulton scheme.

A discussion of situations where such an approach will be beneficial nevertheless, is going to be presented at the conference.

4:25pm - 4:50pm

A Semi-Lagrangian Finite Volume Discrete Boltzmann BGK Model on an Unstructured Triangular Mesh

Chen, Leitao; Schaefer, Laura

Rice University, United States of America

As an emerging alternative to the conventional lattice Boltzmann method (LBM), the discrete Boltzmann method (DBM) displayed the great advantage of incorporating an unstructured mesh in order to capture the complex boundaries that are very common in fluid flow problems. A new model that solves the BGK discrete Boltzmann equation (DBE) with a finite volume method on an unstructured triangular mesh is developed in the present work. The new model uses the information along the characteristic microscopic velocities of the particle distribution functions (PDFs) to calculate the implicit Maxwellian distribution function as well as the PDF flux during the step of finite volume integration. The tests on several numerical cases have shown improvement for instability and accuracy over our existing model.

4:50pm - 5:15pm

Direct numerical simulation of the three-dimensional Taylor-Green vortex using the link-wise artificial compressibility method

Obrecht, Christian[1]; Asinari, Pietro[2]; Kuznik, Frédéric[1]

[1]Univ Lyon, CNRS, INSA-Lyon, Université Claude Bernard Lyon 1, CETHIL UMR5008, F-69621, Villeurbanne, France; [2]Politecnico di Torino, Department of Energy, 10129 Torino, Italy

The link-wise artificial compressibility method (LW-ACM) is a recent implementation of the artificial compressibility method which can be expressed in both a finite-difference framework and a link-wise framework, the latter showing strong analogies with the lattice Boltmann method (LBM). Similarly to the LBM, the LW-ACM proves to be well-suited to parallel computations, with the additional benefit of a significantly reduced memory consumption and, consequently, improved performance in memory-bound contexts.

In this contribution, we present direct numerical simulations of the three-dimensional decaying Taylor-Green vortex using the LW-ACM. The computations were carried out using OpenCLAMP (OpenCL Link-wise ACM on Many-core Processors), a recent OpenCL implementation of the LW-ACM which yields high computational performance on both CPU-based and GPU-based platforms. Simulation results such as the energy dissipation rate are compared to reference values from literature as well as LBM simulations.

5:15pm - 5:40pm

Investigating the laminar-turbulent transition delay with compliant coating

Banari, Amir; Rung, Thomas
Technical university of Hamburg, Germany

Study the transition from laminar to turbulent flow has been the subject of many researches because of its importance on the drag of moving objects. The drag coefficient profile clearly shows the significant impact of the turbulent transition on increasing the frictional force.Therefore, manipulating the flow field for the results of transition delay can result in a huge drag reduction.

In low-disturbance environments, the transition is induced the growth of boundary-layer instability modes, such as Tollmien-Schlichting (T-S) waves, which are produced from the interaction of free stream disturbances with the boundary layer (receptivity). These T-S waves are amplified as they travel downstream until they get large enough to trigger the transition to turbulence via non-linear processes

The most simple and straightforward transition delay method is to damp the TS waves before they are amplified. This damping procedure can be achieved either using active methods such as blowing and

suction wall, or with passive methods such as using viscoelastic coating materials on

the wall.

In this study we investigate transition delay above a flat plate by using a coating layer above the plate.

Lattice Boltzmann method has been chosen for simulating the flow filed while fourth order Runge–Kutta method is used for solving the viscoelastic coating layer. The flow field and the coating layer is coupled through the velocity and pressure boundary condition.

By doing a series of simulations and test different coating properties such as Young's modulus, thickness, damping coefficient, density. We aim to find a suitable coating layer which would lead to a significant delay in transition.

Date: Thursday, 12/Jul/2018

8:30am - 10:30am
Rodney Room, Perkins Student Center

On-site registration: Rodney Room, Perkins Student Center
325 Academy St, Newark, DE 19716

9:00am - 10:40am
Rodney Room, Perkins Student Center

Simulation for Complex Flows
Session Chair: **Paul Dellar**, University of Oxford

9:00am - 9:50am

Algorithms for Eulerian plasma simulations: from ion to electron kinetic scales
Valentini, Francesco
University of Calabria, Italy

The numerical description of the kinetic dynamics of turbulent non collisional plasmas in multi-dimensional phase-space geometry is nowadays a great challenge for scientists. However, the impressive rate of increase in the computational capabilities of modern super-computers gives us today the opportunity of attacking fundamental problems through complex algorithms, whose use was absolutely unthinkable just ten years ago.

Eulerian codes for the description of kinetic plasmas are designed to integrate numerically on a fixed grid in phase space the multi-dimensional Vlasov equation for the particle distribution function coupled to Maxwell's equations for electromagnetic fields.

Here, we present and discuss in detail the characteristics (pro and cons) of the so-called Hybrid Vlasov-Maxwell code, an explicit finite volume algorithm suitable for the simulation of plasmas in the range of ion kinetic scales. Hints on the strategy of algorithm parallelization will be also given, together with a brief discussion on the latest results achieved in the field of space physics.

Finally, future developments will be presented concerning the ongoing implementation of a novel Vlasov-Darwin algorithm, suitable for the description of both ion and electron kinetic physics under the so-called Darwin approximation for fields, consisting in neglecting the propagation of light waves.

9:50am - 10:15am

GPGPU-Implementation of a Gas-Kinetic Scheme on quadtree like Cartesian meshes
Lenz, Stephan; Geier, Martin; Krafczyk, Manfred
TU Braunschweig, Germany

Gas-kinetic schemes (GKS) are kinetic Finite-Volume approaches to fluid dynamics. The fluxes are computed as moments of a time dependent particle distribution function which is derived from a formal solution of the BGK-Boltzmann equation. The initial particle distribution is reconstructed to the first order Chapman-Enskog expansion, utilizing the derivatives of the macroscopic quantities. The time dependent distribution function is formulated essentially in terms of products of a local Maxwellian and the particle velocity. Therefore, the moments of this time dependent distribution function (i.e. the fluxes) can be evaluated analytically. No further discretization of the velocity space or expansions of the equilibrium distribution are required. Hence, the GKS is able to capture the compressible Navier-Stokes equation. We focus on thermal compressible flows with natural convection and without shocks.

As a Finite-Volume method GKS can in general be implemented on arbitrary boundary conforming meshes. The mesh generation of boundary conforming meshes requires much manual work, though. Hence we present a GKS on Cartesian meshes with a quadtree like refinement, where mesh generation can be automated. Second order accurate flux evaluation at the coarse to fine interface is achieved by the use of ghost cell interpolation around the interface. The conservation property of the scheme is preserved. We also present a concept for the treatment of complex boundaries. In order to exploit synergies with Lattice-Boltzmann grid generation, we propose a morph cell approach, that generates boundary conforming meshes based on sub grid distances of a Lattice-Boltzmann grid.

The GKS algorithm is fully explicit by nature. Hence, it thrives on massive parallel hardware, such as GPGPUs. The present scheme is implement in CUDA and delivers a performance of nearly a billion cell updates per second for fully compressible two-dimensional flows.

10:15am - 10:40am

Numerical investigation on the radiometric force on a solid plate in a closed narrow channel
Guo, Zhaoli; Zhu, Liahua
Huazhong University of Science and Technology, China, People's Republic of

Radiometric gas flow is generated as the temperatures of two surfaces of a solid plate are different under rarefied conditions. The force on the plate is influenced by a number of factors such as the Knudsen number, the temperature difference, the size of the plate. In practice, the plate is usually placed in a closed space with bounded walls, and the radiometric flow can be influenced by the outer boundaries. In previous studies, the flow behaviors in large closures have been analyzed. In the present study, we will investigate numerically the flow and radiometric force in a two-dimensional narrow channel with width comparable to the length of the plate via the discrete unified gas-kinetic scheme (DUGKS). The size effects on the flow pattern and force are analyzed under different Knudsen numbers.

10:40am - 11:00am
Coffee Break

11:00am - 12:15pm
Rodney Room, Perkins Student

Method and Analysis II
Session Chair: **Frédéric KUZNIK**, INSA LYON

Center

11:00am - 11:25am

Improving the discrete unified gas kinetic scheme for efficient simulation of three-dimensional compressible turbulence

Wang, Lian-Ping[1,2,3]; Guo, Zhaoli[2]; Wang, Jianchun[3]

[1]University of Delaware, United States of America; [2]Huazhong University of Science and Technology, China; [3]Southern University of Science and Technology, China

The discrete unified gas-kinetic scheme (DUGKS) is a relatively new, 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, doi: 10.1016/j.compfluid.2017.03.007). Preliminary results on using DUGKS for the simulation of compressible isotropic homogeneous turbulence were reported at ICMMES-2017. 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, numerical limiter to treat local discontinuity, and parallel implementation. In this talk, we proposed two modifications to the previous DUGKS implementations. The first is to use the standard Maxwellian equilibrium but adjust the heat flux to achieve variable Prandtl numbers, as done in the unified gas kinetic schemes. The second and more important improvement is to introduce a method (L. Mieussens, J. Comp. Phys. 162, 429-466) to restore the physically correct entropy balance. We test the consequences of these two modifications in terms of physical accuracy, numerical stability, and computational efficiency. A series of test simulations will be reported for both decaying and forced compressible turbulences.

11:25am - 11:50am

A comparative study of interpolated bounce-back schemes and the immersed boundary methods for treating no-slip boundary in the lattice Boltzmann method

Peng, Cheng[1]; Ayala, Orlando M[2]; Wang, Lian-Ping[1,3]

[1]University of Delaware, United States of America; [2]Old Dominion University, United States of America; [3]Southern University of Science and Technology, China

The lattice Boltzmann method (LBM) is a promising numerical method for studying turbulent flows laden with finite-size solid particles due to its flexibility in treating no-slip moving solid boundary. In the recent years, many applications of LBM incorporating either the immersed boundary methods (IBM) or interpolated bounce-back schemes (IBB) have been reported in simulating particle-laden turbulent flows. However, careful comparisons of the two categories of boundary treatments in terms of the accuracy and efficiency are largely missing. In this study, we carefully compare and benchmark the accuracy and efficiency of some popular IBM and IBB schemes in both laminar and turbulent flows. Specific focuses are given to the calculation of velocity, hydrodynamic force, and the local dissipation rate.

Some representative new developments of IBM and IBB are also included in this study. The purpose of this study is to provide a convincing and objective assessment on the performance of these schemes and to offer guidance for choosing the appropriate boundary treatment schemes for the future applications of particle-laden turbulent flows laden with finite-size particles.

11:50am - 12:15pm

Lattice Boltzmann simulations of high-order statistics in isotropic turbulent flows

Jin, Guodong

Institute of Mechanics, Chinese Academy of Sciences, China, People's Republic of

The lattice Boltzmann method (LBM) is coupled with the multiple-relaxation-time (MRT) collision model and the three-dimensional 19-discrete-velocity (D3Q19) model to resolve intermittent behaviors on small scales in isotropic turbulent flows. The high-order scaling exponents of the velocity structure functions, the probability distribution functions of Lagrangian accelerations, and the local energy dissipation rates are investigated. The self-similarity of the space-time velocity structure functions is explored using the extended self-similarity (ESS) method, which was originally developed for velocity spatial structure functions. The scaling exponents of spatial structure functions at up to ten orders are consistent with the experimental measurements and theoretical results, implying that the LBM can accurately resolve the intermittent behaviors. This validation provides a solid basis for using the LBM to study more complex processes that are sensitive to small scales in turbulent flows, such as the relative dispersion of pollutants and mesoscale structures of preferential concentration of heavy particles suspended in turbulent flows.

12:15pm - 2:00pm **Lunch**

2:00pm - 3:40pm

Rodney Room, Perkins Student Center

Theory of kinetic methods

Session Chair: **Li-Shi Luo**, CSRC

2:00pm - 2:50pm

Deterministic Solution of the Boltzmann Equation: Fast Spectral Methods for the Full Boltzmann Collision Operator

Hu, Jingwei

Purdue University, United States of America

The Boltzmann equation, an integro-differential equation for the molecular distribution function in the physical and velocity phase space, governs the fluid flow behavior at a wide range of physical conditions. Despite its wide applicability, deterministic solution of the Boltzmann equation presents a huge computational challenge, and often the collision operator is simplified for practical reasons. We introduce a fast Fourier spectral method for the Boltzmann collision operator which leverages the convolutional and low-rank structure of the collision integral. We show that the framework is quite general and can be applied to arbitrary collision kernels. We then couple the fast spectral method in the velocity space with

the discontinuous Galerkin discretization in the physical space to obtain a highly accurate deterministic solver for the full Boltzmann equation. Standard benchmark test cases including rarefied Fourier heat transfer, Couette flow, and thermally driven cavity flow at different Knudsen numbers have been studied and the results are compared against direct simulation Monte Carlo (DMSC) solutions.

2:50pm - 3:15pm

Lattice Boltzmann formulation for ferrofluids

Dellar, Paul
University of Oxford, United Kingdom

We present a lattice Boltzmann formulation for a continuum description of ferrofluids, suspensions of tiny ferromagnetic particles in insulating liquids, for timescales comparable to the magnetisation relaxation time, but much longer than the viscous spin relaxation time (typically 10^-11 seconds).

Rosensweig's evolution equation for the magnetisation vector in a compressible ferrofluid is written in terms of the divergence of an antisymmetric tensor, as in magnetohydrodynamics, plus further terms involving the divergence of the magnetisation vector and the hydrodynamic strain rate. These are both readily available from the non-equilibrium parts of the magnetic and hydrodynamic distribution functions. The full magnetisation gradient matrix is no longer required, which makes this formulation far more stable at higher magnetisations than the author's earlier formulation. The kinetic system of partial differential equations is discretised using the Strang splitting formulation, which readily accommodates complicated nonlinear source terms for the rotation of the magnetisation vector by the background magnetic field. This approach is again far simpler than an earlier formulation based upon integrating the unsplit kinetic equations along characteristics.

3:15pm - 3:40pm

Link-Wise ACM, regularized LBM and LBM: a study of numerical stability

Vergnault, Etienne[1]; Kuznik, Frédéric[2]; Wang, Feng[2]
[1]Université Claude Bernard Lyon 1, France; [2]INSA Lyon, France

Link-wise artificial compressibility method (LW-ACM) [1], which come from the wide family of Lattice kinetic schemes (LKS), is an innovative method to simulate fluid flows and recover the Navier- Stokes behavior of incompressible Newtonian fluids. This methods exhibits strong similarities with the Lattice Boltzmann method (LBM), which is widely used for engineering fluid dynamics problems. LW- ACM exhibits the algorithmic simplicity of LBM with less variables ! Consequently, LW-ACM is appealing and offers a high potential for high performance computing [4].

The LW-ACM is a relatively new approach and its behavior in the asymptotic limit of linear stability analysis remains unexplored. Some numerical artifacts coming from its original expression have been identified [5, 2]. The LW-ACM also shares some similarities with pre-collision regularization methods for the LBM [3] and can be expressed as a special regularization. This regularization does not recover the same stress tensor as in [3]. A numerical linear stability analysis is performed and some improve- ments are proposed for the regularization process. LBM, LW-ACM and regularized LBM are compared with respect to numerical stability.

Références

[1] Asinari, P., Ohwada, T., Chiavazzo, E., and Di Rienzo, A. (2012). Link-wise artificial compressibility method. Journal of Computational Physics, 231(15) :5109–5143.

[2] Dubois, F., Lallemand, P., Obrecht, C., and Tekitek, M. M. (2017). Lattice boltzmann model ap- proximated with finite difference expressions. Computers Fluids, 155 :3 – 8. ICMMES2015.

[3] Latt, J. and Chopard, B. (2006). Lattice Boltzmann method with regularized pre-collision distribu- tion functions. Mathematics and Computers in Simulation, 72(2) :165–168.

[4] Obrecht, C., Asinari, P., Kuznik, F., and Roux, J.-J. (2014). High-performance implementations and large-scale validation of the link-wise artificial compressibility method. Journal of Computational Physics, 275 :143–153.

[5] Suzuki, K. and Inamuro, T. (2014). An Improved Lattice Kinetic Scheme for Incompressible Viscous Fluid Flows. International Journal of Modern Physics C, 25(01) :1340017.

3:40pm - 4:00pm — **Coffee Break**

4:00pm - 5:40pm — **Rodney Room, Perkins Student Center**

CFD and applications

Session Chair: **Li-Shi Luo**, CSRC

4:00pm - 4:25pm

MPI-LB 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]. Unfortunately, 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 which 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 coupled into the liquid medium causing the aforementioned phenomena to occur. This coupling 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 a 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) [2-3], a new two-phase scheme which ameliorates Shan-Chen (SC) model [4] 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, 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, which is put on a wettable surface, changes the 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 which 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.

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

[2] Khajepor S, Chen B. Multipseudopotential interaction: A consistent study of cubic equations of state in lattice Boltzmann models. Physical Review E. 2016; 93:013303.

[3] Khajepor S, Wen J, Chen B. Multipseudopotential interaction: A solution for thermodynamic inconsistency in pseudopotential lattice Boltzmann models. Physical Review E. 2015; 91:023301.

[4] Shan X, Chen H. Lattice Boltzmann model for simulating flows with multiple phases and components. Physical Review E. 1993; 47:1815-9.

4:25pm - 4:50pm

Assessment of thermal heat losses from solar cavity receiver with Lattice Boltzmann Method

Sediki, Ezeddine[1]; Msaddak, Ayoub[1]; Ben Salah, Moheddine[2]; Tekitek, Mohamed Mahdi[3]

[1]Thermal Radiation Research Unit, Faculty of Sciences of Tunis. University of Tunis El Manar TUNISIA, Tunisia; [2]Thermal Process Laboratory, Center of Research and Energy Technology, 2050 Hammam Lif, Tunisia; [3]EDP Laboratory. Faculty of Sciences of Tunis. University of Tunis El Manar TUNISIA, Tunisia

Efficiency of concentrating solar power system (CSP) can be significantly reduced by heat losses from the receiver. So, the assessment of heat losses is the key to improve its thermal performance. This paper attempts to present a numerical method able to estimate convective and radiative heat losses from specified cavity receiver using Lattice Boltzmann method (LBM). Double distribution functions (D2Q9-D2Q4) with different relaxation times are used to predict dynamic and thermal fields. Distribution functions at the boundaries and pointing outside fluid domain are known from the streaming process, while those pointing inside the fluid domain are unknown and must be defined on all boundaries, including the open boundary. For the no-slip boundary condition, the full bounce back scheme with second order accuracy is applied.

Several calculations have been firstly performed to analyze numerically combined natural convection and surface radiation inside cavity receiver assimilated to a 2D open square cavity. Second, we focus on the assessment of thermal heat losses from solar cavity receiver. The cavity wall facing the opening is subjected to a constant temperature or to a parabolic temperature profile while the other walls are insulated. Cavity walls are assumed to be diffuse, gray and opaque while the open boundary is assumed to be a fictitious black surface at ambient temperature.

Results are presented in terms of isotherms, streamlines, and Nusselt number. Effects of surface radiation, operating temperature, inclination angle and aspect ratio on heat losses from the hot wall inside the cavity is analyzed and discussed. Results of coupled convective and radiative fluxes show that the total Nusselt number increases with increasing surface emissivity and Rayleigh number. It was also found that convective heat loss is largely increasing by increasing the inclination angle. An increase of surface emissivity from 0.2 to unity leads to a four fold thermal radiation heat losses, whereas convective heat loss was marginally reduced. It was also found that the magnitude of total heat losses from the cavity absorber is closely related to the choice of operating temperature and cavity aspect ratio.

4:50pm - 5:40pm

Phase-Field Modeling of Complex Fluids using Lattice Boltzmann Methods

Fakhari, Abbas; Sinno, Talid; Diamond, Scott

University of Pennsylvania, United States of America

Numerical study of multiphase flows is important in a variety of engineering disciplines, spanning droplet and bubble dynamics, shear flow instabilities, three-phase contact-line motion, mixing and reactive transport in porous media, blood flow in vessels, etc. Despite significant advancements in the field, accurate and efficient modeling of complex fluids is still challenging. The main difficulty is in devising a reliable, and numerically stable, interface tracking method that can tackle rapid topological changes such as coalescence and breakup. The most popular interface tracking schemes, namely the volume-of-fluid, front-tracking, level-set, and phase-field methods, are all macroscopic models which rely on the continuum assumption. Given that the interface between different fluids is on the order of nanometers, microscopic and mesoscopic approaches seem to be ideal for interfacial phenomena. Lattice Boltzmann Method (LBM) is one such mesoscopic scheme. The phase-field LBM is particularly advantageous in simulation of immiscible multiphase flows in complex geometries, in studying contact line dynamics, and in modelling biofilm growth and blood flow, among others.

We present a state-of-the-art LB solver, which can be effectively equipped with an Adaptive Mesh Refinement (AMR) technique, for direct numerical simulation of multiphase flows. We consider a variety of fundamentally important phenomena in fluid dynamics and engineering, such as rising bubble and falling droplet, droplet splashing on a wet surface, partial coalescence of a liquid drop at a liquid-liquid interface, and other classical examples.

5:45pm - 10:30pm **Conference Dinner**

Conference dinner at the Chesapeake Inn in Chesapeake City.

Date: Friday, 13/Jul/2018

9:00am - 10:40am

Rodney Room, Perkins Student Center

Efficient and intelligent algorithms

Session Chair: **William H Matthaeus**, UD

9:00am - 9:50am

Rise of Intelligent Algorithms in Science and Industry

Karimabadi, Homa

Analytics Ventures, United States of America

All learning, whether human or machine, is fueled by data. While human knowledge saturates as a function of size of data, deep learning algorithms offer the possibility to grow unbounded. As a result, deep learning has in a very short time emerged as one of the most important technologies of our time. Its impact is widespread and touches every field of science and engineering. Such algorithms have now achieved superhuman performance in a number of areas. This talk provides a brief history of artificial intelligence and an overview of the underlying algorithms. Of particular interest is the recent merging of concepts from disparate fields of artificial intelligence, physics, and statistics that are leading to new types of neural nets. The power and usability of these techniques shall be presented partly based on my personal journey in algorithm development in the areas of scientific visualization, petascale simulations, big data, and commercial applications in medical imaging, financial trading, IoT, among others. We will discuss the current limitations of the artificial intelligence techniques and ongoing efforts to overcome them.

9:50am - 10:15am

A new Open Boundary Condition in a Lattice Boltzmann Model for the Shallow Water Equations Applied to the 2014 Iquique (Chile) Tsunami

Salinas, Álvaro[1]; Torres, Claudio E.[1,2]; Ayala, Orlando Manuel[3]

[1]Universidad Técnica Federico Santa María, Valparaíso, Chile; [2]Centro Científico Tecnológico de Valparaíso (CCTVal), Valparaíso, Chile; [3]Old Dominion University, United States of America

In recent decades, the lattice Boltzmann method (LBM) has proven to be an efficient and accurate tool in numerical simulations of shallow water flows. However, a little analysis has been done for open boundary conditions (OBC). Open boundaries are usually required in numerical coastal simulation so that outgoing waves pass to the exterior of the computational domain minimizing the reflection back to the interior. In this study, we propose a new OBC and we analyze it computationally. A real scenario is presented and comparisons of reflecting waves are made between simulations in domains with different sizes. The size reduction is performed by removing an entire edge-to-edge section, and therefore bringing closer the open boundary to the initial water lifting. The purpose of this study is to present the developed model as a good approximation of open boundaries that allows to reduce the computational domain without suffering perturbations caused by the reflections of outgoing waves. We also present a special treatment for corner nodes sharing several boundary conditions

10:15am - 10:40am

A high order non-splitting conservative semi-Lagrangian Discontinuous Galerkin Method for two-dimemsional transport simulations

Cai, Xiaofeng

University of Delaware, United States of America

In this talk, we will introduce a high order non-splitting conservative semi-Lagrangian (SL) discontinuous Galerkin (DG) method for the two-dimensional transport simulations. The proposed method relies on a characteristic Galerkin weak formulation and a high order characteristics tracing mechanism. Unlike many existing SL methods, the high order accuracy and mass conservation of the method are realized in a non-splitting manner. Thus, the detrimental splitting error, which could significantly contaminate long term transport simulations, will be not incurred. One key ingredient in the scheme formulation is the use of Green's theorem which allows us to convert volume integrals into a set of line integrals. The resulting line integrals are much easier to approximate with high order accuracy, hence facilitating the implementation. To assess the numerical performance, we benchmark the proposed SLDG schemes for simulating several transport problems, the nonlinear Vlasov-Poisson system, incompressible Euler equations and the Vlasov Guiding center model. The efficiency and efficacy of the proposed scheme are numerically verified when compared with other prominent transport solvers such as the Eulerian DG methods combined with Runge-Kutta time integrators.

10:40am - 11:00am

Coffee Break

11:00am - 11:50am

Rodney Room, Perkins Student Center

Boundary conditions and implementations

Session Chair: **Li-Shi Luo**, CSRC

11:00am - 11:25am

On the accuracy of boundary condition of 2D lattice Boltzmann method when modeling High frequency acoustic waves

Louati, Moez[1]; Tekitek, Mohamed Mahdi[2]; Lallemand, Pierre[3]; Ghidaoui, Mohamed[1]

[1]The Hong Kong University of Science and Technology; [2]University Tunis El Manar, Tunisia; [3]Beijing Computational Science Research Center, China

The multiple-relaxation-times lattice Boltzmann method (LBM) is used (cf. [1]) to model acoustic wave propagation in water-filled conduits (i.e., water hammer applications).The results show that LBM is

capable to model WH applications with high accuracy and performance at low frequency cases; however it looses performance for high frequency (HF) cases. This work investigates the causes of LBM performance deterioration at HF.

The investigation is performed by a detailed analysis of acoustics waves for the simple 2-dimensional D2Q9 model in the linear regime. This analysis shows that the high order terms of the equivalent macroscopic equations and the direction of the propagation of the waves have a small effect on the diffusivity. It turns out that the main cause of diffusivity is due to the bounce-back (BB) boundary condition used to model the rigid pipe wall boundary. This finding is demonstrated throughout a numerical test case where an acoustic wave is sent in a 2D square domain with BB at its boundaries. The variations of damping due to BB boundary versus the wave frequency as well as the angle of propagation are investigated. Then by evaluating of the modes of the wave equation a dependency of the damping no frequency and the angle of the propagation is given. The results show that the damping due to BB boundary conditions is much more important then the damping caused by the propagation in the internal domain. This work conclude that, when modeling HF acoustic waves, the accuracy of the boundary scheme is more important then reducing diffusivity of the LBM scheme by using quartics parameters (cf. [2]).

References

[1] M. Louati, M. M. Tekitek and M. S. Ghidaoui, Computers & Fluids, under review, (2017).

[2] F. Dubois, P. Lallemand, Towards higher order lattice Boltzmann schemes, Journal of Statistical Mechanics: Theory and Experiment, (2009).

11:25am - 11:50am

Investigation of the internal mass effect of the immersed boundary-lattice Boltzmann method for FSI problems involving deformable body

Cai, Yunan[1]; Lu, Jianhua[1,2]; Li, Sheng[1,2]

[1]State Key Laboratory of Structural Analysis for Industrial Equipment, School of Naval Architecture, Faculty of Vehicle Engineering and Mechanics, Dalian University of Technology, Dalian 116024, China;

[2]Collaborative Innovation Center for Advanced Ship and Deep-Sea Exploration, Shanghai 200240, China

In the framework of the immersed boundary method (IBM), the fluid inside the solid domain has insignificant influences in accurately calculating the solid motion, especially for the FSI problems involving deformable body, as the solid motion and fluid field are strongly coupled. In this paper, a coupled immersed boundary-lattice Boltzmann method (IB-LBM) and the smoothed point interpolation method (S-PIM) is adapted to the deformable body involved FSI problems, in which the fluid domain is solved by the lattice Boltzmann method, the solid domain is modeled by the S-PIM based on realistic nonlinear constitutive law. The internal mass effect is investigated on the IB-LBM for problems. To consider the internal mass effect, a force term is introduced to the solid calculation in the coupled IB-LBM and S-PIM by the Lagrangian points approximation approach. The efficiency of the present numerical scheme is validated through several numerical experiments including flows around an oscillating circular cylinder, sedimentations of an circular disk and an elliptical disk. It is shown that the results obtained by the present method have significant accuracy improvement compared with those without considering the mass effect. Moreover, soft disk sedimentations are also simulated which demonstrates the efficiency of the present method for deformable body involved FSI problems.

12:00pm - 1:30pm **Lunch**