

Conference Agenda

Session Overview

Date: Monday, 24/July/2023

8:00am	On-site registration
9:00am - 10:30am	SC1: Short Courses 1 Location: Mount Qingcheng Grand Hotel-Growth Hall 9:00am - 10:30am Gas kinetic schemes in CFD Weidong Li^{1,2} ¹ Hypervelocity Aerodynamics Institute, CARDC, Mianyang, China; ² Laboratory of Aerodynamics in Multiple Flow Regimes, CARDC, Mianyang, China In the literature, there are several kinds of gas kinetic schemes, such as the lattice Boltzmann method (LBM), the gas kinetic BGK scheme (GKS), the unified gas kinetic scheme (UGKS), the discrete unified gas kinetic scheme (DUGKS), the gas kinetic Lax-Wendroff scheme (GKLWS) and so on. The gas kinetic schemes are based on the gas kinetic theory, which gives them some advantages over conventional CFD schemes, including the satisfaction of the entropy condition, the positivity preservation, the asymptotic preserve property, and so on. Therefore, gas kinetic schemes have achieved much success and received a lot of attention in recent years. In this short course, an introduction to the basic gas kinetic theory and the principles for developing these gas kinetic schemes will be given. Specifically, this course consists of four parts: part 1 introduces the basic gas kinetic theory, which lies a solid foundation of gas kinetic schemes. By following part 1, part 2 and part 3 elaborate on the gas kinetic schemes for incompressible and compressible flows in the continuum regime, respectively. After that, part 4 further discusses the extensions of the gas kinetic schemes for continuum flows to unified schemes for multiscale flows. Finally, this lecture is summarized.
10:30am - 10:50am	Coffee Break
10:50am - 12:20pm	SC2: Short Courses 2 Location: Mount Qingcheng Grand Hotel-Growth Hall 10:50am - 12:20pm Magic two-relaxation-time lattice Boltzmann schemes as macroscopic finite difference schemes for the Navier-Stokes equations Paul John Dellar University of Oxford, United Kingdom Lattice Boltzmann schemes replace Boltzmann's binary collision operator with a model using linear relaxation of the distribution functions towards their equilibrium values. Examples of these models include linearisations of lattice gas collision operators, the single-relaxation-time or BGK collision operator, and various multiple-relaxation-time collision operators designed to optimize different measures of accuracy or stability. The two-relaxation-time collision operator groups the discrete particles velocities into anti-parallel pairs, called "dumb-bells" in the theory of lattice gas collision operators, and assigns different relaxation times to the odd and even combinations of anti-parallel velocities. This is equivalent to assigning different relaxation times to the odd and even moments of the distribution functions. For example, momentum flux is an even moment while heat or energy flux is an odd moment. A particular "magic" combination of the two relaxation rates has good properties for computing Poiseuille flow parallel to one of the coordinate axes. The point of zero velocity is then located precisely halfway between lattice points. We will describe a different interpretation of the two-relaxation-time collision operator that assigns different relaxation times to the forward-propagating and backward-propagating parts of each anti-parallel pair of discrete velocities. The "magic" combination sets the forward-propagating distribution function to equilibrium in this interpretation. The distribution function at any lattice point and time level thus depends only on the distribution function propagating in the reverse direction at the previous time level, and on the equilibrium distributions that are known functions of the fluid density and velocity. By considering two successive lattice Boltzmann timesteps, and hence two reversals of direction, we can extend this to show that the distribution function at any lattice point and time level depends on the same distribution function at the same lattice point two-time levels earlier, and on the equilibrium distributions. This allows us to construct closed finite difference schemes for evolving the fluid density and velocity alone across three-time levels. The discrete evolution across three-time levels can be thought of as a discrete approximation to partial differential equations with second derivatives with respect to time. However, we prefer to interpret them as a discrete approximation to a first-order system, the expected conservation laws for mass and momentum, and separate evolution equations for the mass and momentum fluxes. The latter depends only on the fluid density and velocity, so we retain just enough kinetic behavior to simulate a Maxwell fluid with a finite stress relaxation time. Our approach also extends to include bounce-back boundary conditions with a one-timestep delay, the natural implementation based on a halo of "ghost" cells outside the computational domain. We will show numerical experiments including a vortex dipole colliding with a rigid boundary, and the flow driven by an oscillating boundary.
12:20pm - 2:00pm	Lunch
2:00pm - 3:30pm	SC3: Short Courses 3 Location: Mount Qingcheng Grand Hotel-Growth Hall 2:00pm - 3:30pm Some essentials of the LBE Li-Shi Luo^{1,2} ¹ CSRC, People's Republic of China (PRC); ² Old Dominion University, USA This lecture aims to cover some basics of the lattice Boltzmann method (LBM), it consists of three parts: (1) the most popular collision models in the lattice Boltzmann equation (LBE), (2) test problems (both

	analytic and not), and (3) the means to analyze the LBE. In the first part, we will discuss the collision models with multiple-relaxation times (MRT), two-relaxation times (TRT), and single-relaxation time (SRT) or the lattice BGK model, and the original entropic model (ELBE). In the second part, we will use the Poiseuille flow as an example to illustrate the effect of the collision model on the boundary conditions. Additional examples are the lid-driven cavity flow in 2D and the flow past porous media in 3D. These examples are used to illustrate the necessity of the collision model with at least two relaxation times. Finally, in the third part, we will briefly discuss the methods used to analyze the LBE: the Chapman-Enskog analysis, the asymptotic analysis, the equivalent-equation analysis, and the linear analysis (Fourier analysis).
3:30pm - 3:50pm	Coffee Break
3:50pm - 5:20pm	<p>SC4: Short Courses 4 Location: Mount Qingcheng Grand Hotel-Growth Hall</p> <p>3:50pm - 5:20pm</p> <p>Kinetic modelling and multi-scale simulation of rarefied gas dynamics</p> <p>Lei Wu Southern University of Science and Technology, China, People's Republic of</p> <p>This short course will cover the recent development on the kinetic modelling and multiscale simulation of rarefied gas flows. First, we will talk about the problem of DSMC in the simulation of polyatomic gas, and our solution to remedy it. Second, we will introduce the general synthetic iterative scheme (GSIS) to find the steady-state solutions of the kinetic equations within dozens of iterations at any Knudsen number. Rigorous mathematical proof and challenging numerical simulations will be carried to demonstrate the accuracy and efficient of our theory and numerical method.</p>
5:20pm - 6:20pm	<p>Poster Session</p> <p>The p-DSMC modeling of radiation effect in high enthalpy rarefied gas flow under hybrid mesh</p> <p>Quanshun Yang¹, Ming Fang¹, Yanguang Yang² ¹China Aerodynamics Research and Development Center, Hypervelocity Aerodynamics Institute, Mianyang 621000, China; ²China Aerodynamics Research and Development Center, Mianyang 621000, China</p> <p>The high temperature in the extremely supersonic flow's shock layer excites internal energy modes and causes thermal radiation. This temperature can cause complete dissociation of air molecules, with atomic components contributing over 80% to the resulting radiation. This study employs an optimized atomic radiation model and the photon tracing direct simulation Monte Carlo (p-DSMC) method to investigate wall radiation heating of a three-dimensional FIREII model during hypersonic re-entry in a rarefied flow region based on flow field right angles mesh and surface triangles unstructured hybrid mesh technology. The study yields wall pressure and heating results that incorporate excited radiation effects. At an inflow condition of standard atmosphere at 80 km, the resulting wall heat flow aligns well with CFD simulation results, particularly in the stagnation point region. Subsequently, it was discovered that at 86 km, the convective heat approaches the model's edge as the angle of attack increases. While the radiation heat flow does approach the model's edge when considering radiation effects, the maximum radiation heat value remains very close to the stagnation point region. Moreover, for re-entry with an angle of attack, the radiative heating near the stagnation point region is markedly greater than the convective heating. The radiation heat results of the FIREII model under different re-entry conditions indicate that the magnitude of radiation heat is closely related to the head radius, incoming flow velocity, and angle of attack.</p> <hr/> <p>An improved macroscopic computational model for thermal non-equilibrium flow in near-continuum regime</p> <p>Yubin JIA, Jihui OU, Jie CHEN Department of Mechanics, Tianjin University, Tianjin 300072, China</p> <p>Accurate prediction of aerothermodynamics is of great importance for the design and development of hypersonic vehicles. When a vehicle flies at moderate and high altitudes, the rarefied non-equilibrium effect is significant and the accuracy of the Navier-Stokes-Fourier (NSF) equations is questionable. The Direct Simulation Monte Carlo (DSMC) method has been widely applied for rarefied non-equilibrium flows, but its computational cost is still unbearable due to its huge computational cost in the near-continuum regime. Recently, an extended continuum model, i.e., DSMC data-improved Navier-Stokes (DiNS), has been proposed by Ou and Chen (2019) for hypersonic near-continuum flows and it showed a pretty good performance in aerodynamics predictions. However, it is only available for the perfect gas. In this paper, the DiNS model is extended to diatomic gas with thermal non-equilibrium effects. First, the rarefied Couette flow of diatomic gas considering thermal non-equilibrium effects are simulated by the DSMC method. The profiles of velocity and temperature as well as shear stress and heat flux under different Mach numbers and Knudsen numbers are obtained. Secondly, based on the DSMC results, effective viscosity and thermal conductivity are calculated using the linear constitutive relation and the modified Eucken factor proposed by Mason & Monchick (1962) based on the Wang Chang and Uhlenbeck (WCU,1951) equation. The functions of these coefficients with respect to a shear non-equilibrium parameter are obtained and the modified model of linear constitutive relation for the diatomic gases is established. Finally, the modified model is embedded into the macroscopic thermal non-equilibrium model and is employed to simulate hypersonic flows over a flat plate and a cylinder in near-continuum regimes. The results show that the surface shear stress and heat flux obtained by the proposed model agree well with the DSMC results.</p> <hr/> <p>An efficient mesoscopic approach to simulate three-dimensional compressible turbulence</p> <p>Yiming Qi¹, Lian-Ping Wang² ¹Peking University, China; ²Southern University of Science and Technology, China</p> <p>We provide an effective mesoscopic method using the total-energy double-distribution-function formulation requiring only 40 discrete velocities when simulating three-dimensional (3D) compressible turbulence. To</p>

achieve complete agreement with the Navier-Stokes-Fourier system, two sets of 3D off-lattice discrete particle velocity models are used: a 27 discrete velocity model with the seventh-order Gauss-Hermite quadrature (GHQ) accuracy (D3V27A7) and a 13 discrete velocity model with the fifth-order GHQ accuracy (D3V13A5). Our modified Boltzmann-Bhatnagar-Gross-Krook system has source terms designed to arbitrarily modify the bulk-to-shear viscosity ratio and Prandtl number. In addition, for the initial and boundary conditions, a lifting relation is needed to associate the distribution functions with the hydrodynamic variables. Unphysical numerical oscillations may occur for certain non-uniform initial flow field if the lifting relation does not match the GHQ accuracy of the applied discrete velocity models. In order to recover the Navier-Stokes-Fourier system, we construct a completely consistent and numerically stable lifting relation based on the Hermite expansion of the conserved and non-conserved moments. Compressible decaying homogeneous isotropic turbulence and Taylor-Green vortex flows are simulated with different initial conditions and Ma numbers to validate our approach. The simulation results are found to be in good agreement with those in the literature.

Study on transport characteristics of gas mixture in shock wave based on gas kinetic theory

Peng Aoping, Wu Junlin

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In order to study the flow mechanism of the transport phenomenon of gas mixture in all flow regimes, a multi relaxation collision model equation suitable for gas mixture was developed from Boltzmann equation, which is the basic equation of gas kinetic theory, and the expression of collision relaxation frequency correspond with DSMC method was established. In order to simulate the range of collision between different gases, for common gases, numerical results of integral expressions in collision cross sections were obtained for exponents of inverse power law from 3 to 15, which was the first report in open references. Then under the framework of Gas Kinetic Unified Algorithm, a multi-component one-dimensional shock wave structure problem with high particle mass and mole fraction ratios was simulated, and compared with DSMC results. The results showed that the present model equation can simulate the macroscopic parameter changes of the gas mixture and its components in the shock wave, and can be used to simulate and analyze the diffusion rules of each component of the gas mixture. These results verified the validity and correctness of the multi relaxation model equation. It was found that the diffusion effects of the component with the smallest molecular weight was the most significant, and it is less affected by other components. Moreover, the non-equilibrium effect of flow is mainly generated by the component with the largest molecular weight.

Research on the parameters and conversion method of aeroheating environment

Jinshan Zhao, Zhigang Zhang, Yilei Shi, Ting Chen, Yu Xiao, Siyao Su, Yong Wang, Junhao Liao, Zhiyu Peng

China Aerodynamics Research and Development Center, China

Wind tunnel experiment was a key means to research and predict aero-heating for hypersonic vehicles. The flow field parameters and model scales in wind tunnel are different from flight condition, owing to the limitation of its simulation capability. Even under the condition that the Mach number and Reynolds number are exactly the same, the flow field parameters of different wind tunnels are quite different, which may cause inconsistent heat flux data. The aero-heating data obtained from wind tunnel experiments can not be directly used for the aero-heating prediction and thermal protection system design in flight condition. So the method to predict the aero-heating environment on flight condition, by using the wind tunnel experimental data, has been a technically difficult problem. In the past, the correlation and extrapolation method of wind tunnel aero-heating experiment data for specific aircrafts has a strong directionality, because of this method is a kind of data fitting based on aero-heating data and does not take into account the specific parameters of aero-heating. It has certain limitations and is difficult to extrapolate to other shapes of aircraft. For solving the problem of the wind tunnel experimental data extrapolation, the aero-heating results of a calibration model in different hypersonic wind tunnel flow field parameters are compared in this paper, and the fundamental reason of the difference between flight and wind tunnel conditions is analysed. Then, the main parameters of the influence of aero-heating were analyzed based on the dimensionless Navier-Stokes equations and boundary layer approximation theory, and the correlation and extrapolation method was developed for laminar and turbulence conditions by deducing the approximate solution of the aero-heating. Because of the parameters of the local boundary layer edge can be taken into consideration, the correlation method has strong universality. Finally, the correlation analysis and validation for the calibration model was accomplished, the wind tunnel experimental data was extrapolated to flight condition by the correlation method in this paper, good results are obtained.

Effect of catalysis on the aerodynamic heating over an ablating hypersonic blunt cone

Leibao Han, Yufeng Han, Wei Cao

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Severe aerodynamic heating associated with high-temperature hypersonic flow typically involves complex gas-surface interactions, the profound understanding of which allows optimization of the thermal protection system design. In this work, the effect of catalysis on the aerodynamic heating over an ablating hypersonic blunt cone is investigated numerically. The results show that all three ablation reactions, i.e., oxidation, nitridation, and sublimation, inhibit the effect of O-catalytic recombination on aerodynamic heating by suppressing its intensity. In particular, the oxidation and sublimation reactions have a stronger effect, while the nitridation reaction has a weaker effect. The inhibitory effect of oxidation reaction on O-catalytic reaction is mainly determined by its surface reaction kinetics, in contrast, the nitration reaction is mainly through the gas-phase reaction kinetics of nitridation products. The inhibition caused by the sublimation reaction is determined by a combination of the kinetics of the surface reaction and the kinetics of the gas-phase reaction of its products, and both are strong. In addition, nitridation and sublimation reactions restrain the intensity of the N-catalytic reaction, reducing the effect of the N-catalytic combination on the aerodynamic heating, while the inhibition caused by the oxidation reaction is negligible. The nitration reaction inhibits the N-catalytic reaction mainly through its surface reaction kinetics, while the gas-phase reaction kinetics of the nitration product plays a promoting role. In addition, both the surface reaction kinetics of the sublimation reaction and the gas-phase reaction kinetics of the sublimation products play an inhibitory role.

Control effects of a high-frequency pulsed discharge on a hypersonic separated flow

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The control effects of a high-frequency pulsed discharge on a hypersonic separated flow induced by a 42° compression ramp are studied with high-speed Schlieren imaging. A discharge is generated between an electrode pair upstream of the ramp to introduce strong disturbances into the boundary layer. The discharge frequencies used are $f_d = 10, 20, 30,$ and 40 kHz, with corresponding single-pulse energies $E_{sp} = 22.2, 20.3, 12.0,$ and 8.7 MJ. The results show that the discharge can reduce the separation area, especially with relatively low frequencies of 10 or 20 kHz. The flow mechanism induced by the discharge is scrutinized using a reduced-order method based on the information from time-resolved Schlieren images, including proper orthogonal decomposition and dynamic mode decomposition. The results identify an unsteady mode representing regular energetic eddies within the shear layer of the separation zone. This model has the same characteristic frequency as the discharge. These eddies enhance the mixing of the shear layer and the main flow stream, accelerating the destruction of the shear layer and reducing the separation zone size. The control effectiveness correlates with the scale of the energetic eddies. At 10 or 20 kHz frequencies, the discharge is more conducive to attenuating the separation because large-scale eddies, excited by higher single-pulse energy, are enhanced as they propagate downstream in the shear layer. By contrast, the control effectiveness deteriorates when the discharge frequency is 30 or 40 kHz because the induced eddies have smaller scales and decay during propagation.

Large-eddy simulation of turbulent channel flow based on the discrete unified gas kinetic scheme

Lin Guo, Hui Gao, Lian-Ping Wang

Southern University of Science and Technology, China, People's Republic of

During the past few decades, large-eddy simulation (LES) combined with mesoscopic kinetic schemes, such as lattice Boltzmann method, gas-kinetic scheme, and discrete unified gas kinetic scheme (DUGKS), has become an increasingly popular tool for numerical studies of turbulent flows. Among various mesoscopic scheme-based LES methods, the DUGKS-LES is of particular interest due to its finite-volume framework and the resulting superior numerical stability together with its flexibility in utilizing non-uniform grids. In this work, we focus on turbulent channel flow simulations with moderate to high friction Reynolds numbers using a parallel DUGKS-LES framework. The effects of sub-grid scale models, including Smagorinsky model coupled with van Driest damping function, Wall-Adapting Local Eddy Viscosity (WALE), Vreman model, and implicit LES model, are explored. The numerical stability and accuracy of different SGS models in the DUGKS framework are discussed in terms of turbulence statistics verified against those reported in literatures. The computational efficiency with each examined SGS models is also compared in this study.

Morphological analysis for thermodynamic of cavitation collapse near fractal solid wall

Yu Yang¹, Ya Zhang²

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In this paper, a fractal geometric boundary with natural wall features is introduced into a hybrid LBM multiphase model. The physical model of cavitation bubble collapse near the irregular geometric wall is established to study the thermodynamic characteristics of the bubble collapse. Due to the lack of periodicity, symmetry, spatial uniformity and obvious correlation in the LBM simulation of the bubble collapse near the fractal wall, the morphological analysis based on Minkowski functional is introduced into the thermodynamic investigation of cavitation bubble for the first time in order to analyze and obtain the effective information. The results show that the Minkowski functional method can study the temperature information in complex physical fields hierarchically and quantitatively. The high/low temperature region of the cavitation flow is explored and thermal effect between irregular and fractal geometric wall and cavitation bubble can be revealed. It illustrates that LBM and morphological analysis complement each other, and morphological analysis can also be used as an optional and potential tool in the research field of complex multiphase flow.

Effect of random roughness on microchannel flow resistance evaluated by large-scale simulations

Junchao Wang, Mingshan Yang, Xiangyu Li

Southwest Jiaotong University

In complex microfluidic devices, micrometer-scale channels with rough surfaces significantly alter flow resistance and, consequently, can have a significant effect on the design goals. Here, we used the lattice Boltzmann method to simulate fluid flow in microchannels with rough surfaces and established a formula that relates the size and shape of the rough surface to changes in channel flow resistance. Using this formula, we were able to determine the equivalent scheme of smooth channel and rough channel flow resistance, so that the design parameters of the microfluidic chip can be adjusted according to the processing technology and equipment parameters. To minimize the impact of the rough surface's randomness, we performed over 5000 simulations. In short, our research mitigates the effects of roughness during manufacturing, guaranteeing that the microfluidic chip's individual channel properties conform to the design criteria. This research has promising applications in microfluidic equipment design and fabrication.

Study of heat transfer modification in particle-laden thermal flow using the lattice-Boltzmann method

Hongcheng Wu, Kairzhan Karzhaubayev, Hui Gao, Lian-Ping Wang

Southern University of Science and Technology, China

In the field of thermal multiphase flow research, a significant inquiry revolves around the alterations in heat transfer phenomena resulting from the presence of solid particles of finite size. Depending on the specific flow conditions, fluid media laden with particles can observe either augmentation or degradation of the efficiency of heat transfer. This study focuses on investigating the influence of dispersed finite-size particles on heat transfer phenomena in the Rayleigh-Bénard convection, considering different volume fractions of the solid phase and various Rayleigh numbers. The present work utilizes the double

distribution function-based Thermal Lattice-Boltzmann method (TLBM), the implementation of which enables successful simulations of multiphase fluid-thermal interactions. The moving boundary of the solid particles is handled by the interpolated bounce-back scheme. Additionally, Galilean invariant momentum exchange and heat exchange approaches are employed for hydrodynamic force and heat transfer calculation at the solid boundaries. The accuracy of current method is verified with several benchmark cases, including two- and three-dimensional single-phase Rayleigh-Bénard flows, as well as the settling of hot and cold spherical particles in a three-dimensional enclosure. Furthermore, we explore the modulation of Rayleigh-Bénard flows due to the presence of either fixed or freely moving finite-size particles. The simulations are conducted on a distributed memory cluster with a 3D domain decomposition technique facilitated by the MPI library. A brief discussion on the parallel performance of the simulations is provided for both particle-laden and single-phase flow scenarios.

Numerical study of droplet impacting on flexible substrates

Yufei Ma, Haibo Huang

University of Science and Technology of China, China, People's Republic of

We numerically study the impact of a droplet on superhydrophobic flexible plates, aiming to understand how the flexible substrate influences the maximum spreading of the droplet. In our simulations, the phase-field lattice Boltzmann method (LBM) is adopted for solving the two-phase fluid flow, and the finite element method is adopted for solving the solid deformation and movement. The flexible substrate in the flow is a deformable moving boundary. To impose this boundary, a modified bounce-back method is used. The external force exerted on the substrate from the fluid can be obtained through the momentum exchange method. Besides, a weighted least squares method is adopted to impose the wettability boundary of the substrate. Our simulation results show that, compared with the rigid case, the vertical movement of the flexible substrate due to droplet impact reduces the maximum spreading. Besides, the average acceleration a during droplet spreading changes significantly. Arising from energy conservation, we rescale the acceleration a for cases with different bending stiffness K_B and mass ratio M_r . Based on a , a formula between the total energy of the flexible substrate at the maximum spreading and the initial kinetic energy of the droplet is obtained. Moreover, through theoretical analysis, we propose a scaling for the droplet's maximum spreading diameter ratio β_{\max} . In the scaling, based on the derived a , an effective Weber number We_m is well defined, which accounts for the substrate properties without any adjustable parameters. In the (β_{\max}, We_m) plane, the two-dimensional (2-D) numerical results of different K_B , M_r and rigid cases all collapse into a single curve, so do the experimental and three-dimensional (3-D) results.

The lattice Boltzmann simulation for the droplet motion in multiphase Rayleigh-Bénard convection

Xiang Li, Ying-Yan Li, Zhi-Qiang Dong, Peng Yu

Southern University of Science and Technology, China, People's Republic of

An aqueous droplet immersed in conduction oil commonly occurs in industrial processes, but the droplet motion and its underlying effect on heat transfer have not been understood. This numerical study presents a simple but effective way to simulate the heat transfer problem in multiphase Rayleigh-Bénard convection, which employs a triple-distribution function strategy to evolve the density, velocity, interface, and temperature fields. The corresponding lattice Boltzmann equations are equivalent to the Navier-Stokes equations for flow properties, the Cahn-Hilliard equation with a mass correction term for the interface between aqueous droplet and conduction oil, and the convection-diffusion equation for heat transfer. To confirm the computational accuracy in temperature field, we first validate the Rayleigh-Bénard convection in single phase flow, which demonstrates that the present numerical model can produce reliable results that are consistent with published data. Then, the different parameters, i.e., density ratio, viscosity ratio, thermal conductivity etc., have been numerically investigated to explore the effect of aqueous droplet motion on heat transfer process. These numerical results and the underlying mechanisms of multiphase Rayleigh-Bénard convection could provide a guideline to industrial design on heat transfer device.

Date: Tuesday, 25/July/2023

8:00am	On-site registration
8:00am - 8:15am	S0-Welcome Location: Mount Qingcheng Grand Hotel-Tianfu Hall
8:15am - 9:00am	Invited speaker #1 Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. Qibing Li , Tsinghua University Simulation of multiscale transport Kun Xu Hong Kong University of Science and Technology, Hong Kong S.A.R. (China) This talk will discuss the direct modelling for the development of numerical algorithms for multiscale transport. This framework is about to model the physical laws directly in a discretized space, where the transport dynamics depends on the cell resolution, such as the so-called cell's Knudsen number. With the variation of local cell's Knudsen number, multiscale transport can be obtained automatically, such as the capturing of particle free transport and continuum wave propagation at the same time in different numerical cells according to the local cell's Knudsen number. The multiscale algorithms, such as the unified gas-kinetic scheme (UGKS) and unified gas-kinetic wave-particle (UGKWP) method, have been successfully used in rarefied gas dynamics, radiative and neutron transfer, plasma physics, and gas-solid particle multiphase flow. This talk will present the application of the unified method in rarefied gas dynamics and gas-particle two phase flow.
9:00am - 10:00am	S1-Algorithms and implementations-I Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. Qibing Li , Tsinghua University 9:00am - 9:20am A p-multigrid geometric multigrid acceleration technique for high-order compact gas-kinetic scheme Xing Ji Xi'an Jiaotong University, Xi'an, China In this presentation, the high-order compact gas-kinetic scheme (CGKS) on three-dimensional unstructured mesh is further developed with the p-multigrid geometric multigrid technique for steady-state acceleration. The high-order CGKS is used to evolve the cell-averaged conservative flow variables and their first derivatives on the finest mesh. The parallel mesh agglomeration algorithm in this paper have two characteristics. Firstly, random hash algorithm is used to select the cell interfaces which may be deleted. Secondly, the geometric skewness factor is used to evaluate whether the selected cell interface should be deleted. Two types of characteristics guarantee its mesh coarsening speed. The final iterative updating method becomes numerically accurate and computationally efficient. The effectiveness of the p-multigrid geometric multigrid method is validated in subsonic, transonic and supersonic flow simulations in three-dimensional unstructured mesh. 9:20am - 9:40am Which one, reconstruction or flux , is more important for high-order scheme : Insights from fifth-order finite volume Schemes. Chengxiang Li^{1,2}, Lian-ping Wang¹, Kun Xu², Xing Ji³ ¹ Department of Mechanics and Aerospace Engineering, Southern University of Science and Technology, Shenzhen 518055, Guangdong, China; ² Department of Mathematics, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China; ³ School of Aerospace Engineering, Xi'an Jiaotong University, 710049 Xi'an, China Most high-order computational fluid dynamics (CFD) methods for compressible flows are based on Riemann solver for the flux evaluation and high-order interpolation or reconstruction such as the weighted ENO (WENO) scheme for spatial accuracy. This combination is advantageous due to its ease of implementation and ability to achieve the required spatial accuracy. However, there has been limited research published related to high-order solvers. Gas-kinetic scheme (GKS), which has been developed considerably in recent years, is well-known for its capacity to nonlinearly combine spatial and temporal evolution in flux evaluation. In this paper, the performance of different flux solvers using the same reconstruction is compared on a structured rectangular mesh with fifth-order finite volume method. Different reconstruction methods are also compared, including the successful target ENO scheme and classic WENO-Z reconstruction. The Lax-Friedrichs (LF) Riemann solver, HLLC solver, and Gas-kinetic schemes are used as solvers. Results from the Blast wave test indicate that using higher-dissipation reconstruction (WENO5-Z) with GKS solver produces the same accuracy as lower-dissipation reconstruction (TENO8) with LF solver. In the Titarev-Toro test, WENO5-GKS and TENO5-GKS schemes seem to have better resolution than LF and HLLC solvers with WENO5 or TENO5 reconstruction. Lastly, potential developments to flux solver, particularly the ability of shock and vortex capture for Compact Gas Kinetic Scheme, will be discussed.
	9:40am - 10:00am Efficient neutron transport UGKS on unstructured polyhedral mesh Shuang Tan, Junxia Wei, Yibing Chen, Zhiming Gao Institute of Applied Physics and Computational Mathematics, Beijing, China The neutron transport equation is a high-dimensional Boltzmann-type equation with complex mathematical properties. In 3D simulations, the efficient, accurate, and robust neutron transport methods have important research value. We focus on the deterministic SN methods for neutron transport. In the former work, the Unified Gas Kinetic scheme (UGKS) for neutron transport on the 3D structured mesh was constructed based on the finite volume (FV) method, which has shown good numerical performance. On the other hand, the unstructured mesh show good application prospects in practical applications with complex

geometric structures. Thus, in order to improve the application ability of neutron transport UGKS in practical problems, the efficient scheme for 3D unstructured polyhedral mesh is studied in this paper. In order to be implemented in complex grids, the spatial discretization of neutron UGKS is designed based on the discontinuous finite element method. The scheme is marked as IUGKS-DG in the following. Compared with the FV scheme, the stencil of IUGKS-DG is compact. IUGKS-DG is more suitable for the calculations of 3D unstructured mesh with arbitrary geometry, especially for parallel computations. To improve the computation efficiency of IUGKS-DG, in time discretization, the efficient and low storage implicit algorithms are designed based on the characteristics of the neutron transport evolution solution. In the analysis, it is demonstrated that IUGKS-DG keeps good asymptotic preservation (AP) properties in the diffusion limits on unstructured mesh. Besides, the computational accuracy and efficiency of IUGKS-DG are tested with a series of typical numerical cases. Furthermore, we conducted detailed comparisons with neutron transport IUGKS-FV and FEM-SN schemes qualitatively and quantitatively. The results show that due to the AP properties of the scheme and the multi-scale characteristics of UGKS flux, the neutron transport IUGKS-DG exhibits ideal numerical performances on 3D unstructured mesh under a wide range of computational conditions.

10:00am - 10:35am	Coffee Break & Take Picture
10:00am - 10:35am	Poster Session
10:35am - 11:20am	<p>Invited speaker #2 Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. Haihu Liu, Xi'an Jiaotong University</p> <p>Coupled lattice Boltzmann method and discrete element method enabling discrete simulation of gas-solid flows</p> <p><u>Limin Wang</u> Institute of Process Engineering, Chinese Academy of Sciences, China</p> <p>Two kinds of coupled lattice Boltzmann method and discrete element method (LBM-DEM) approaches are presented for modeling gas-solid two-phase flows at different levels (different time-spatial scales and accuracy), namely lattice Boltzmann based particle-resolved direct numerical simulation (LB-based PR-DNS)[1] and lattice Boltzmann based discrete particle simulation (LB-based DPS)[2]. LB-based PR-DNS where particle size is much larger than lattice size, can directly simulate the flow and detailed dynamic interaction at gas-solid interface, while LB-based DPS where lattice size is much larger than particle diameter, achieves a good balance between computational accuracy, time consumption and computational efficiency, and it can obtain local information such as particle trajectories, as well as the macro information such as time-averaged flow field. Finally, both LB-based DNS and DPS are powerful tools in exploring gas-solid two-phase flows, which enabled development of lattice-based multi-fluids dynamics (LMFD) simulation software and a new drag correlation is proposed with consideration of scale-dependence[3].</p> <p>References:</p> <p>[1] Wang, L., Zhou, G., Wang, X., Xiong, Q. and Ge, W., Direct numerical simulation of particle-fluid systems by combining time-driven hard-sphere model and lattice Boltzmann method, <i>Particuology</i>, 8:379-382, 2010.</p> <p>[2] Wang, L., Zhang, B., Wang, X., Ge, W. and Li J., Lattice Boltzmann based discrete simulation for gas-solid fluidization, <i>Chem. Eng. Sci.</i>, 101:228-239, 2013.</p> <p>[3] Liu, X, Ge, W. and Wang, L., Scale and structure dependent drag in gas-solid flows, <i>AIChE J.</i>, 66:e16883, 2020.</p>
11:20am - 12:00pm	<p>S2-Complex fluids: multi-phase, interfacial flows-I Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. Haihu Liu, Xi'an Jiaotong University</p> <p>11:20am - 11:40am</p> <p>Sedimentation of an elliptical squirmer in a vertical channel</p> <p><u>Yuxiang Ying</u>¹, <u>Deming Nie</u>¹, <u>Tongxiao Jiang</u>¹, <u>Kaixuan Zheng</u>¹, <u>Jianzhong Lin</u>² ¹China Jiliang University, Hangzhou, China; ²Key Laboratory of Impact and Safety Engineering (Ningbo University), Ministry of Education, Ningbo 315201, China</p> <p>We used a two-dimensional lattice Boltzmann method to simulate the sedimentation motion of an elliptical squirmer in a vertical channel and considered both circular and elliptical squirmers, aiming to more realistically simulate the swimming of microorganisms in nature. The study in this was divided into two phases. The first phase comprised the numerical calculations of an elliptical squirmer with an aspect ratio of $c = 2.0$ and revealed three typical motion modes: steady inclined motion, wall-attraction oscillation, and large-amplitude oscillation. It was found that the formation of these three motion modes and transitions between modes are related to the pressure distribution formed between the elliptical squirmer and wall. In addition, significant differences exist between the motions of elliptical and circular squirmers. The force generated by the interaction between the elliptical squirmer and wall does not all point towards its center of mass, resulting in an additional torque on the elliptical squirmer; this is not the situation for the circular squirmer. The second phase of the study simulated squirmers with different aspect ratios ($c = 1.0$, $c = 3.0$). It was found that for an elliptical squirmer with an aspect ratio $c = 3.0$, the large-amplitude oscillation mode (among the above three motion modes) no longer exists. By combining the motion modes of a circular squirmer in the channel, it can be observed that as the aspect ratio c increases, the squirmer's head direction tends to be more vertical to reduce the drag force during swimming.</p> <hr/> <p>11:40am - 12:00pm</p> <p>Sedimentation of a spherical squirmer in a square tube under gravity</p> <p><u>Tongxiao Jiang</u>, <u>Yuxiang Ying</u>, <u>Kaixuan Zhen</u>, <u>Deming Nie</u> China Jiliang University, China</p> <p>In this study, we used the lattice Boltzmann method to simulate the settling motion of a spherical squirmer in a square tube under the effect of gravity. A three-dimensional squirmer model with chirality was chosen to simulate the motion of a real microswimmer in a three-dimensional space and to systematically analyze its kinematic properties. According to the results of this study, we identified seven different motion modes: diagonal plane large-amplitude oscillation, central stable sedimentation, bidirectional spiral motion, rebound motion, unidirectional spiral motion, corner stable motion, and near-wall attraction oscillation. It is</p>

shown that the formation of different motion modes is caused by the effects of squirmer-type factor and chirality. squirmer-type factor determines the stable motion position of the squirmer in the channel. Chirality makes the head direction of the squirmer more susceptible to change, thus changing the motion trajectory of the squirmer. In addition, it was found that the self-repelling strength determines the speed of squirmer's motion, which affects the motion frequency of squirmer's periodic oscillations.

12:00pm - 2:00pm

Lunch

2:00pm - 2:45pm

Invited speaker #3

Location: **Mount Qingcheng Grand Hotel-Tianfu Hall**

Session Chair: **Prof. Kun Xu**, Hong Kong University of Science and Technology

2:00pm - 2:45pm

Nonlinear coupled constitutive relations derived from the Boltzmann kinetic equation based on balanced closure and mesoscopic methods

Rho Shin Myong

School of Mechanical and Aerospace Engineering and ACTRC, Gyeongsang National University, Jinju, Gyeongnam 52828, South Korea

Rarefied and microscale gases are present in a wide range of scientific and technological problems. Well-known examples are external flows around re-entry (or gliding) vehicles flying through layers of Earth's atmosphere at hypersonic speed and internal flows through micro-channels, micro-pumps, and computer hard disk drives. Various computational methods have been developed to investigate these flows. The most prominent approaches are computational fluid dynamics (CFD) methods based on the Navier-Stokes-Fourier (NSF) constitutive equations or equivalent kinetic equations, and the direct simulation Monte Carlo (DSMC) method. However, the classical description based on the first-order linear NSF constitutive laws is known to suffer from serious limitations when predicting the flow in strong thermal nonequilibrium states. To overcome these shortcomings, the present lecture first introduces the second-order constitutive equations for monatomic, diatomic, and polyatomic gases that are systematically derived from the Boltzmann-Curtiss kinetic equation. They are developed under two tenets: Myong's closing-last balanced closure [1] and Eu's modified moment method [2], which is based on the cumulant expansion and fully complies with the second law of thermodynamics, ensuring the non-negativity of the probability distribution function and nonequilibrium entropy production. Next, it introduces two computational methods to solve the second-order nonlinear coupled constitutive relation (NCCR) in conjunction with conservation laws in a three-dimensional setting: a mixed modal discontinuous Galerkin scheme [3] and the FVM-based nccrFOAM suite in an open-source framework. The methods are also extended to gases with the vibrational degree of freedom [4]: first proposing a modified Boltzmann-Curtiss kinetic equation that includes the vibrational mode of energy and then deriving the second-order constitutive equations in the two-temperature formulation from the kinetic equation. The computational solvers are then applied to various gas flows in a wide range of rarefied regimes: the viscous inner structure of shock waves for all Mach numbers, hypersonic flows past cylinder and sphere, the impingement of a nozzle jet onto a surface at the near-vacuum condition like the lunar surface and a hypersonic flow around a suborbital re-entry vehicle. The computational results show that the second-order constitutive model describes the second-order physical effects, such as stress constraint between the viscous shear and excess normal stresses [4], and provides an improved solution than the first-order NSF constitutive laws.

ACKNOWLEDGEMENTS

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2:45pm - 3:45pm

S3-Rarefied and non-equilibrium compressible flows-I

Location: **Mount Qingcheng Grand Hotel-Tianfu Hall**

Session Chair: **Prof. Kun Xu**, Hong Kong University of Science and Technology

2:45pm - 3:05pm

Numerical study on adsorption and transport of rarefied gas flow in porous media

Ziyang Xin¹, Yue Zhang¹, Zhaoli Guo²

¹State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan 430074, China; ²Institute of Interdisciplinary Research for Mathematics and Applied Science, Huazhong University of Science and Technology, Wuhan 430074, China

The adsorption and transport processes of rarefied gas within porous media play a crucial role in various industrial applications, including purification, separation, catalysis, and more. In this study, a numerical method based on the discrete unified gas-kinetic scheme (DUGKS) is presented to capture the non-equilibrium effect of rarefied gas flow in porous media, where the system involves a wide range of characteristic lengths and transport time scales relative to molecular mean free paths and adsorption-desorption times. In the model, the Shakhov model and Langmuir kinetic model are employed for rarefied gas bulk flow and adsorption-desorption in solid surfaces, respectively. The model is valid within the range of the continuum regime to the rarefied regime and has been verified by the results of the analytical solution and some previously published works. We first investigated the influence of gas physical properties, including gas rarefaction, the initial values of surface coverage, and temperature, on the temporal evolution of adsorption amount and adsorption rate within a single pore channel. It is found that as gas rarefaction increases, the influence of the initial surface coverage on the adsorption surface coverage and flux during the adsorption process is strengthened, indicating the presence of the non-equilibrium effect. Furthermore, we examine the effects of pore structure and pore size distribution on adsorption and transport processes, enabling us to predict both the adsorption capacity and apparent permeability of porous media.

3:05pm - 3:25pm

Natural model reduction for kinetic equations

Zeyu Jin, Ruo Li

Peking University, Beijing, China

A novel framework of model reduction for kinetic equations is proposed, which employs Riemannian geometry and results in first-order symmetrizable hyperbolic equations that preserve properties including hyperbolicity, conservation laws, entropy dissipation, and linear stability. The relationship between the H-theorem for kinetic equations and stability conditions for reduced systems is discussed rigorously, determining the choice of Riemannian metrics involved in the model reduction. The framework is widely applicable to the model reduction of many kinetic models.

3:25pm - 3:45pm

A global-adaptive velocity space for multi-scale flow simulations

Jianfeng Chen, Sha Liu, Rui Zhang, Chengwen Zhong

Northwestern Polytechnical University, Xi'an, China

The modeling and numerical prediction of multiple-regime flows are crucial for the aerodynamic design of spacecraft, ultra-low orbital vehicles and plumes. The deterministic methods, such as the discrete velocity method (DVM) and unified methods, may accurately capture complicated and non-equilibrium velocity distribution functions (VDFs) by including a discrete velocity space (DVS). The extremely steep slope and great concentration of the VDFs in DVS, however, necessitate a high resolution, and there are a lot of discrete velocity points in a Cartesian velocity space (CVS). Additionally, as the DVS must cover a bigger region at high Mach numbers, the number of discrete velocity points likewise rises. The description of high-speed flows with CVS is therefore exceedingly expensive for deterministic approaches. Consequently, adaptive velocity space (AVS) is necessary for the deterministic solvers to be effective in complex rarefied and multi-scale flows. The AVS method receives two improvements in this paper, which are then incorporated into general deterministic frameworks like the unified gas-kinetic scheme. First, to preserve the program's high level of parallelism, a global velocity mesh rather than a local velocity mesh is used. More crucially, the gradient of the VDFs must be employed to compute the microscopic fluxes at the interface when the local velocity mesh is inconsistent on both sides of the physical interface, which poses stability and computational problems. The robust global velocity mesh, in contrast, does not require interpolation. Second, the DVS is recorded using a tree data structure, and the VDFs are recreated on the new DVS using a "consanguinity" relationship. In other words, the VDF of a split child node is the same as that of its parent, and the VDF of a merged parent node is equal to the average of its children's VDF. Contrary to the earlier approach of rebuilding the VDFs on a new DVS by interpolation, which necessitates computing the gradient of VDFs, the "consanguinity" method is less computationally complex and more reliable. The discrete deviation of the equilibrium distribution functions of the new DVS and old DVS is used to maintain the proposed method's conservative property. Additionally, a suitable set of adaptive parameters is created to boost the effectiveness of the suggested approach. Finally, several numerical experiments are conducted to verify the proposed method.

3:45pm - 4:05pm

Coffee Break

3:45pm - 4:05pm

Poster Session

4:05pm - 5:05pm

S4-Applications of AI in nonequilibrium flows

Location: **Mount Qingcheng Grand Hotel-Tianfu Hall**

Session Chair: **Prof. Jun Zhang**, Beihang University

4:05pm - 4:25pm

Flow field super-resolution construction based on physics-informed neural networks.

Qingyi Lin, Xuhui Meng, Zhaoli Guo

Huazhong University of Science and Technology, Wuhan, China

High-resolution flow field information is essential for engineering applications in areas such as aerospace, combustion, and fluid machinery. However, the acquisition of high-quality flow field data is often challenging due to sparse and unevenly distributed measurement data. Moreover, traditional methods for solving macroscopic fluid equations, like the Navier-Stokes equations, typically require complete boundary and initial conditions, which are frequently unavailable in engineering scenarios. To overcome these challenges, researchers have recently explored the use of deep learning techniques, which have demonstrated great potential in capturing complex nonlinear relationships and providing effective solutions for inverse problems. Furthermore, as fluid flow is governed by physical laws, incorporating them into the super-resolution reconstruction process of the flow field can be beneficial.

In this study, we proposed a unified framework for flow field super-resolution reconstruction that integrates the flow governing equation into the training process of Physics-Informed Neural Networks (PINNs). By leveraging a limited set of low-resolution measurements and employing the Boltzmann equation applicable to all flow regimes, we reconstructed super-resolution flow fields. The effectiveness of our proposed method was demonstrated on various benchmark problems. By combining the Bhanagar-Gross-Krook (BGK) model with PINNs, we first achieved super-resolution reconstruction of continuum and rarefied flows. Then, by incorporating the RTE model with PINNs, we obtained more accurate results for radiation heat transfer. Overall, our approach has the potential to facilitate the super-resolution reconstruction of flow field and enable more accurate and efficient flow field measurement and simulation, which can provide valuable guidance for engineering system design and optimization.

4:25pm - 4:45pm

Data-driven discovery of unknown constitutive relation for non-equilibrium flow using dimensional homogeneity constrained gene expression programming

Wenjun Ma, Linying Zhang, Jun Zhang

Beihang University, Beijing, China

The conventional governing equations for fluid flows are the Navier-Stokes Fourier (NSF) equations, which are derived based on conservation laws and the empirical assumptions of linear constitutive relations for the viscous stress and heat flux. However, in strong non-equilibrium flows, these linear constitutive relations would break down and thus NSF equations are no longer applicable. To deal this issue, some

high-order constitutive relations were derived based on kinetic theory, but the applicability of them is still very limited. In this work, we propose to mine the unknown constitutive relations from the molecular simulation data using a novel symbolic regression algorithm, which is referred to as dimensional homogeneity constrained gene expression programming (DHC-GEP). DHC-GEP can simultaneously discover the function forms and coefficients of underlying equations using basic mathematical operators and physical variables, without requiring pre-assumed candidate functions. We first validate the effectiveness of DHC-GEP in two benchmark cases, the governing equations of which are known theoretically. It is found that DHC-GEP can discover the correct equations, and is robust to the hyperparameters of models, the noise level and the size of datasets. Then, we further employ DHC-GEP to discover the unknown constitutive relations of two representative non-equilibrium flows, including one-dimensional shock wave and rarefied Poiseuille flow. Galilean invariance and the second law of thermodynamics are imposed as constraints to enhance the reliability of the obtained constitutive relations. Comparisons, both quantitative and qualitative, indicate that the derived constitutive relations are more accurate than the conventional Burnett equations in a wide range of Knudsen number and Mach number, and are also applicable to the cases beyond the parameter space of the training data. This work proves that DHC-GEP combined with molecular simulations is a promising and alternative method to establish the constitutive relations of non-equilibrium flows and complex fluids.

4:45pm - 5:05pm

Physics-informed neural networks for solving rarefied gas flows combined with discrete velocity method

Linying Zhang, Wenjun Ma, Jun Zhang

Beihang University, Beijing, China

Kinetic equations are essential to accurately characterize low-speed rarefied gas flows in microelectronic devices. Specifically, the linearized Bhatnagar-Gross-Krook (BGK) equation is a suitable model for such flows, which can be solved numerically using deterministic methods such as the discrete velocity method (DVM). Besides, over the past few years, Physics-informed Neural Networks (PINNs) have emerged as a promising tool in the field of solving complex partial differential equations. In this paper, we propose a new surrogate model, referred to as PINN-DVM, which combines PINNs and DVM for simulating rarefied gas flows. The linearized BGK equation is directly encoded into the residual of an artificial neural network. A new loss function of boundary condition is also proposed, based on the Maxwell diffuse model and impermeable boundary condition, to accurately capture velocity slip and temperature jump. PINN-DVM overcomes the limitations of conventional numerical methods, such as complex mesh generation and derivative calculations. Furthermore, the proposed model is enhanced by a self-adaptive strategy based on the neural tangent kernel (NTK) to adaptively adjust the loss weight for each component of the loss function. Four representative cases are employed to demonstrate the superiority of PINN-DVM in accurately solving rarefied gas flows compared with original PINNs, including Couette flow, Fourier heat transfer flow, triangular duct flow, and cavity flow. The results indicate that the proposed PINN-DVM model shows great potential for further development and practical applications in rarefied gas flows.

5:05pm - 6:15pm

S5-ICMMES Awards

Location: [Mount Qingcheng Grand Hotel-Tianfu Hall](#)

Session Chair: [Prof. Li-Shi Luo](#), CSRC

Session Chair: [Prof. Zhaoli Guo](#), Huazhong University of Science and Technology

5:05pm - 5:40pm

Study on the thermo-chemical non-equilibrium effects of gas-kinetic unified algorithm based on Boltzmann model equations

Junlin Wu^{1,2}, Zhihui Li³, Aoping Peng^{1,2}, Xinyu Jiang³

¹Hypervelocity Aerodynamics Institute, China Aerodynamics Research and Development Center,

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Reentry into the atmosphere of the space vehicles, such as the capsule, will undergo the whole complex varying process from free molecular regime to continuum. The "rarefied gas effect" and the "high-temperature real gas effect" due to hyper-velocity flying make great effects on the aerodynamic and thermal characters of the vehicles. Thus, correlative theory and numerical method need to be developed for computation and analyzation of the high-temperature thermochemical non-equilibrium gas flows. The main subject of this paper is to construct the numerically computational methods covering various flow regimes for the thermo-chemical non-equilibrium effects.

Boltzmann equation can describe multi-scale gas flow problems covering various regimes including the rarefied and transition flow regimes. Based on the skeleton frame of the Gas-kinetic Unified Algorithm (GKUA), the fundamental thought of this thesis is to solve Boltzmann model equations by Discrete Velocity Ordinate Method (DVOM) to analyze the gas flow features in rarefied flow regime. The central work of this thesis, however, is to develop Boltzmann-type model equation involving thermochemical non-equilibrium effect, and to develop the computational models for complex physical-chemical processes including the chemical reaction, dissociation and recombination. Concretely, we will focus on the gas-kinetic models of molecular rotational energy, the excited vibrational energy involving discrete quantum effect, on the chemical reaction model for two-component displacement reaction and on the Boltzmann model equation for the dissociation and recombination reactions for high-temperature gas.

A Boltzmann-type gas-kinetic model equation for continuously distributed rotational energy and discrete quantum vibrational energy is constructed by combining the Morse model for quantum internal energy and the model for continuously distributed energy based on the analysis of the rotational and vibration energy. By integrating over the rotational energy modes, the number of independent variables of this model equation is decreased, while discrete quantum vibrational energy levels hold back. According to analysis of the normalization principle, this model is equal to the continuously distributed energy model when the quantum vibration level up to $+\infty$, and the truncation error is obtained when the number of levels is finite. This expression of the truncation error has great significance for numerical simulation of the model equation because it can be used to judge the number of vibrational energy levels. Besides, the mass, momentum and energy conservation properties are proved as well as the H theorem, and the balance equations on vibrational energy levels and macroscopic balance equations involving excited internal energies are derived by moment method. Through computing and comparing of the classical supersonic and hypersonic flows past a cylinder, the validities of the construction of this model equation and

numerical solving process are shown. By comparing with simple gas model, Rykov model involving only the rotational energy and the continuously distributed energy model, the influence of the discrete quantum effect to the numerical results and aerodynamic and thermal characters of the cylinder surface is analyzed, and the distribution laws of the functions on excited vibrational energies are also shown.

Then, by analyzing the gas-kinetic theory of multicomponent chemical reaction and introducing the thought of constructing the consistent Boltzmann model equation, a kind of Boltzmann model equation involving two-component chemical reaction is built based on the elastic collision relaxation feature of the hard-sphere and the thought of dealing with the chemical reaction rate in DSMC. The normalization principle, the mass, momentum and energy conservation properties, and the H theorem for forward endothermic reaction are all proved. Finally, the reliability of the chemical reaction model to describe the endothermic and exothermic reaction processes is validated by simulating the steady supersonic flow involving endothermic reaction and the transient flow involving exothermic reaction. It is shown that GKUA based on the deterministic equation is better for simulating unsteady flows than the probabilistic DSMC method. Besides, the influence of the chemical reaction to numerical simulation of the mixture gas flows is also analyzed.

The dissociation and recombination reactions of high-temperature gas are studied, and a practical chemical reaction model involving the excited internal energies of polyatomic gases is constructed. Then, this model equation is simplified by the reduced rotational and vibrational distribution functions, whose normalization principle and conservation properties are ensured. The correctness of this model and the solving process is validated by numerically computing the hypersonic flow past a cylinder. In future, the engineering applications of the GKUA and continuous developments of the gas-kinetic theory need to be continuously extended.

5:40pm - 6:15pm

Model reduction on Boltzmann equation and Hermite spectral method

Yanli Wang

Beijing Computational Science Research Center, Beijing, China

As one of the main governing equations in kinetic theory, the Boltzmann equation is widely utilized in aerospace, microscopic flow, etc. Its high-resolution simulation is crucial in these related areas. However, due to the high dimensionality of the Boltzmann equation, high-resolution simulations are often difficult to achieve numerically.

In this talk, we will introduce the basic properties of the Boltzmann equation, the model reduction on Boltzmann, and the highly efficient scheme in the framework of the Hermite method. This is a joint work with Prof. Ruo Li from Peking University and Dr. Zhenning Cai from the National University of Singapore.

8:30am	On-site registration
8:30am - 9:15am	<p>Invited speaker #4 Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. François Dubois, CNAM Paris and Univ. Paris-Saclay</p> <p>8:30am - 9:15am</p> <p>Nanoscale modelling of evaporative flows</p> <p>Shaokang Li¹, Wei Su², Livio Gibelli¹, Yonghao Zhang³ ¹School of Engineering, The University of Edinburgh, UK; ²The Hong Kong University of Science and Technology, Hong Kong, China; ³Institute of Mechanics, Chinese Academy of Sciences, Beijing, China</p> <p>Non-equilibrium evaporation is ubiquitous in nature and has numerous applications in nanoscale devices, such as chip cooling and nano-assemblies, where the bulk of the vapour and liquid phases are well described by the hydrodynamic equations at the macroscopic scale, while the interface has a complex structure that still requires experimental and theoretical investigation. The macroscopic variables are subject to strong variations in the interface region which comprises a vapour-liquid interface of the order of the molecular diameter, and a Knudsen layer of the order of the mean free path. The traditional kinetic treatment of evaporation processes is limited to the Knudsen layer described by the Boltzmann equation. The structure of the liquid-vapour interface is not resolved and the molecular exchange process with the liquid phase is described by a phenomenological boundary condition. A more thorough description of the evaporation processes is provided by the Enskog-Vlasov (EV) equation, which is capable of treating both the liquid and vapour phases, including the interfacial region. However, this kinetic equation is computationally demanding, making it impractical for real-world applications. In this work we report a molecular kinetic model that maintains a similar level of accuracy to the EV equation, but is significantly more efficient to solve. We will present the results of our model on capturing the evaporating rate, the liquid-vapour coexistence curve, and the evaporation process into a vacuum.</p>
8:30am - 9:15am	<p>Invited speaker #7 Location: Mount Qingcheng Grand Hotel-Growth Hall Session Chair: Prof. Lian-Ping Wang, Southern University of Science and Technology</p> <p>8:30am - 9:15am</p> <p>Simulations of turbulence and turbulent heat transfer near complex wall geometries by the lattice Boltzmann method</p> <p>Kazuhiko Suga Osaka Metropolitan University, Japan</p> <p>I introduce reliable schemes for turbulence simulations by the lattice Boltzmann method (LBM) such as the D3Q27 MRT LBM, the regularized D3Q19 thermal LBM and the imbalance correction local mesh refinement methods which were developed by our group. After showing the improved simulation accuracy of those schemes, several DNS/LES studies for turbulence and turbulent heat transfer over rough/porous walls are introduced. The results explain how turbulence and turbulent heat transfer are affected by the wall roughness and or the wall permeability via the Kelvin-Helmholtz instability.</p>
9:15am - 10:15am	<p>S6-Algorithms and implementations-II Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. François Dubois, CNAM Paris and Univ. Paris-Saclay</p> <p>9:15am - 9:35am</p> <p>Macroscopic entropy-increasing models with second-order non-equilibrium effect for convection-diffusion problems</p> <p>Jinhua Lu Technical University of Munich, Germany</p> <p>Through von Neumann stability analysis, it is found that the thermal lattice Boltzmann equation (TLBE) has excellent numerical stability at large mesh Fourier numbers. On the contrary, the explicit discretization scheme of the governing equation has an upper limit for the mesh Fourier number, 1/2 and 1/6 for 1D and 3D situations, respectively. Good numerical stability is an intrinsic advantage of TLBE over conventional numerical schemes. Our recent work interprets the mechanism of good numerical stability as the entropy-increasing mechanism and numerical dissipation terms. Consequently, the present work proposes macroscopic entropy-increasing models with second-order non-equilibrium effects for convection-diffusion problems. Numerical investigations and von Neumann stability analyses validate their excellent numerical stability and good accuracy. In addition, the macroscopic entropy-increasing models consist of only local algebraic operations and partial derivatives, which enables them to be easily solved on nonuniform meshes, whereas implementing TLBE on nonuniform meshes is relatively complicated.</p> <hr/> <p>9:35am - 9:55am</p> <p>The force term treatment in the high-order regularized lattice Boltzmann model</p> <p>Xuhui Li¹, Xiaowen Shan² ¹Harbin Engineering University, Harbin, China; ²Southern University of Science and Technology, Shenzhen, China</p> <p>In the present work, the force term is firstly derived in the spectral multiple-relaxation-time (SMRT) high-order regularized lattice Boltzmann model. The force term in the Boltzmann equation is expanded in the temperature rescaled central moment space (RCM) and truncated to second order. For the collision operator in RCM space, the force term is incorporated directly. Through the Chapman-Enskog expansion, the compressible thermal Navier-Stokes-Fourier equation with force term can be recovered.</p> <hr/> <p>9:55am - 10:15am</p>

A fourth-order compact finite difference lattice Boltzmann method based on non-uniform grids

Qitong Chen, Hefang Jing, Zhe Zhang, Yujie Yang

North Minzu University, Yinchuan, China

Lattice Boltzmann method (LBM) has been increasingly used to simulated various complex flow phenomenon, and it has some advantages compared with traditional computational fluid dynamics methods. However, as LBM usually is of lower order accuracy and it difficult to deal with non-uniform grid.

In this paper, a fourth-order accurate compact difference scheme is developed to discretize the spatial derivative term in the lattice Boltzmann equation (LBE) with the Bhatnagar-Gross-Krook (BGK) approximation. The time derivative term is discretized using a fourth order Runge-Kutta method. At the boundary, a fourth-order one-sided difference approximation is used to calculate the unknown macroscopic variables and non-equilibrium parts of the fluid, and the equilibrium part at the boundary is calculated using the macroscopic variables. Furthermore, inhomogeneous grid is adopted.

Finally, the new method is applied to simulate the flow in a lid-driven cavity Comparison between the new method and other methods indicates that the new method exhibited good stability and accuracy.

9:15am - 10:15am

S7-Turbulence

Location: **Mount Qingcheng Grand Hotel-Growth Hall**

Session Chair: **Prof. Lian-Ping Wang**, Southern University of Science and Technology

9:15am - 9:35am

Direct numerical simulation of homogeneous shear turbulence laden with finite-size particles using the lattice Boltzmann method

Cheng Peng¹, Lian-Ping Wang², Li Ji¹

¹Shandong University, Jinan, China; ²Southern University of Science and Technology, Shenzhen, China

Shear turbulence laden with finite-size particles exists in many natural processes and engineering applications. While the lattice Boltzmann method (LBM) successfully simulated a few particle-laden turbulent flows, achieving single-phase or particle-laden homogeneous shear turbulence (HST) with a periodic boundary condition has never been reported. In this work, we propose a scheme to handle the shear periodic boundary and use it for the direct numerical simulations of both single-phase and particle-laden HST. In order to preserve the second-order spatial accuracy of LBM, the interpolated-bounce-back scheme and the moment-exchange method are selected to handle the no-slip condition on the particle surfaces and the fluid-particle interactions, respectively. The validation tests confirm that the proposed scheme successfully preserves the second-order accuracy of LBM and handles the simulations with dense particle suspensions. The comparisons between the single-phase and particle-laden HST show how the presence of finite-size particles modifies the flow structures and turbulence statistics.

9:35am - 9:55am

The influence of particle density and diameter on the interactions between the finite-size particles and the turbulent channel flow

Jie Shen¹, Cheng Peng², Zhiming Lu¹, Lian-Ping Wang^{3,4}

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Particle-resolved direct simulation of particle-laden turbulent channel flow is performed based on the mesoscopic lattice Boltzmann method (LBM), and the particle-fluid interface is treated using the interpolated bounce back scheme. The friction Reynolds number (Re_{τ}) of the single phase turbulent channel flow is 180, and the particle volume fraction is fixed at 1%. Three particle-fluid density ratios and three particle diameters are considered, and five particle-laden simulations are performed to investigate the influence of particle density and diameter on the interactions between the particles and the carrier turbulence. Results show that the streamwise velocity of the solid phase is larger than that of the fluid phase in the near-wall region, and the velocity difference between the two phases decreases with increasing particle density, but increases with increasing particle diameter. The probability density functions (PDFs) of particle velocity and angular velocity depend on the distance between the particles and the wall, but the PDFs of particle acceleration and angular acceleration are not spatially dependent. The distribution of particle Reynolds number follows the Gamma distribution within the buffer region and viscous sublayer. The solid phase concentration is high in the near-wall region, and the largest solid-phase concentration in this region occurs in the case with particles of intermediate density. Two aspects of the turbulence modulation are explored, i.e., the streamwise velocity and the turbulent kinetic energy (TKE). The presence of finite-size particles typically increases the streamwise velocity in the near-wall region and reduce the streamwise velocity outside this region. The trend is similar for TKE, but the TKE attenuation mainly occurs in the buffer region. The modulation to the streamwise velocity is analyzed using the streamwise momentum balance equation. It is found that the streamwise velocity modulation is dominated by the weighted Reynolds stress, but the different modulation in the near-wall region is due to the difference in weighted particle-induced stress, whereas the different modulation outside the near-wall region is due to the change in weighted Reynolds stress. Through TKE budget analysis, it is found that the enhancement of TKE source in the viscous sublayer increases with increasing particle density and diameter and the attenuation of TKE source in the buffer region increases with increasing particle density and diameter, which is consistent with the TKE modulation for different cases.

9:55am - 10:15am

Effect of thermal fluctuations on compressible decaying isotropic turbulence

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For more than a century, it has been widely believed that microscopic molecular motions have negligible influence on macroscopic turbulent motions. However, recent numerical investigations have demonstrated that thermal fluctuations resulting from molecular motions have significant impacts on turbulence small-scale statistics. To further clarify the ongoing debate on this topic, we employ two particle-based simulation methods, i.e., the direct simulation Monte Carlo (DSMC) method and the unified stochastic particle (USP) method, to simulate the two-dimensional (2D) and three-dimensional (3D) compressible decaying isotropic turbulence. Compared to DSMC, USP can be implemented with larger time steps and cell sizes as it couples the effects of molecular movements and collisions. Our findings reveal that the turbulent spectra of velocity and thermodynamic fields are significantly changed by thermal fluctuations below spatial scales comparable to the turbulent dissipation length scale. By applying the Helmholtz decomposition to the velocity field, the effects of thermal fluctuations on the spectra of solenoidal and compressible velocity components are studied separately under different turbulent Mach number conditions. In addition to the turbulence statistics, we discuss the impact of thermal fluctuations on the predictability of turbulence.

10:15am - 10:35am	Coffee Break
10:15am - 10:35am	Poster Session
10:35am - 11:20am	Invited speaker #5 Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. Yonghao Zhang , Institute of Mechanics, Chinese Academy of Sciences 10:35am - 11:20am Lattice Boltzmann gas-liquid two-phase flow and fluid-solid coupling Haibo Huang University of Science and Technology of China, Hefei, China This report aims to introduce the research progress of lattice Boltzmann gas-liquid two-phase flow and fluid-solid coupling. It includes the development of relevant two-phase flow methods, the exploration of the universal laws of the dynamics of the two-phase moving contact line and contact angle hysteresis on heterogeneous wall surfaces, and the maximum spreading law of liquid droplets in the coupling motion of liquid droplets/soft walls.
10:35am - 11:20am	Invited speaker #8 Location: Mount Qingcheng Grand Hotel-Growth Hall Session Chair: Prof. Rho Shin Myong , Gyeongsang National University 10:35am - 11:20am The modification of the Cercignani-Lampis-Lord (CLL) model under thermal non-equilibrium conditions Hui Wu, Weifang Chen School of Aeronautics and Astronautics, Zhejiang University, Hangzhou 310027, China Scattering kernels are of paramount importance in modeling gas-surface interactions for rarefied gas flows. However, the classical Cercignani-Lampis-Lord (CLL) model is restricted to the accommodation coefficients and fails to fully depict the reflection of gas molecules under highly non-equilibrium conditions. To overcome the deficiency, a modified CLL model, namely the GCLL model, with independent momentum, energy, and thermal accommodation coefficients is proposed based on the training results of an unsupervised machine learning model. The presented comparisons have demonstrated the superiority of the GCLL model in matching with MD results, including the velocity correlation distributions and the relevant outgoing velocity probability density function. Compared with the CLL model, the accuracy of the predicted reflection velocity and temperature of gas molecules is significantly improved. Furthermore, the direct simulation Monte Carlo (DSMC) simulations with different gas-surface interaction models are utilized to simulate the two-dimensional hypersonic flow over the sharp flat plate. The reliability of the modified model is verified by comparing it with the results of the traditional scattering model. It is indicated that the GCLL model can be employed as a promising strategy for simulations encountered with highly non-equilibrium.
11:20am - 12:00pm	S8-Complex fluids: multi-phase, interfacial flows-II Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. Yonghao Zhang , Institute of Mechanics, Chinese Academy of Sciences 11:20am - 11:40am Morphological transformation of flexible non-Brownian filaments at low Reynolds number Yetao Lu, Haibo Huang University of Science and Technology of China, Hefei, China A numerical method of fluid-structure interaction combining lattice Boltzmann method, finite element method and immersed boundary method is presented. The behavior of a three-dimensional, non-Brownian flexible filament in a low Reynolds number shear flow was investigated through theoretical and numerical analyses. Four primary motion modes of the filament were identified: Rigid, C-buckling, U-turn, and S-turn. A theoretical model was developed to explain the S-turn mode, and we discovered that the critical flow strength for the transition from U-turn to S-turn was approximately $Z_c = 4900$. Our numerical simulations confirmed this transition value. Furthermore, we observed that the rheological properties of the solution were directly linked to the filament's motion modes, demonstrating a scaling transition. 11:40am - 12:00pm An efficient and vectorized platform of coupling Deep Reinforcement Learning and Lattice Boltzmann Method Chengyun Wang, Haibo Huang University of Science and Technology of China, China, People's Republic of Deep Reinforcement Learning (DRL) has emerged as a powerful approach for optimizing decision-making in nonlinear and high-dimensional problems. However, applying DRL to fluid environments presents

significant challenges due to their continuous interaction and computational requirements. In this study, we address these challenges by developing an in-house platform based on the Lattice Boltzmann Method, integrating DRL for flow control and optimization problems in fluid mechanics. The platform enables efficient data transmission between the agent and the fluid environment using sockets, facilitating distributed computation across multiple devices. Leveraging Cartesian grids and the immersed-boundary method, our platform offers fast and vectorizable solutions, eliminating the need for remeshing and enabling concurrent simulations on CPU clusters. We demonstrate the feasibility and effectiveness of our approach by applying a single-step DRL algorithm to optimize wake stabilization. Specifically, we determine the optimal spatial location and length of a downstream splitter plate to suppress vortex shedding behind a cylinder. Although research on control problems is ongoing, our findings provide valuable insights into the potential of DRL in fluid mechanics and are expected to greatly accelerate both academic and industrial applications in this field.

<p>11:20am - 12:00pm</p>	<p>S9-Rarefied and non-equilibrium compressible flows-II Location: Mount Qingcheng Grand Hotel-Growth Hall Session Chair: Prof. Rho Shin Myong, Gyeongsang National University</p> <p>11:20am - 11:40am Implicit high-order gas-kinetic scheme on unstructured meshes Yaqing Yang, Liang Pan Beijing Normal University, Beijing, China High-order gas-kinetic schemes (HGKS) have achieved successes for unsteady flows on three-dimensional unstructured meshes. To accelerate the rate of convergence for steady flows, the implicit non-compact and compact HGKSs are developed. For non-compact scheme, the simple weighted essentially non-oscillatory (WENO) reconstruction is used to achieve the spatial accuracy. Incorporate with the nonlinear generalized minimal residual (GMRES) method, the implicit non-compact HGKS is developed. In order to improve the resolution and parallelism of non-compact HGKS, the implicit compact HGKS is developed with Hermite WENO (HWENO) reconstruction. A variety of numerical examples are presented to validate the accuracy, robustness and efficiency of both inviscid and viscous flows.</p> <hr/> <p>11:40am - 12:00pm Analysis of effects on energy accommodation of reflected gas molecules on flow structures during reentry of expired spacecraft Yong-Dong Liang^{1,2}, Zhi-Hui Li^{1,2}, Jie Liang¹, Jia-Zhi Hu^{1,2} ¹China Aerodynamics Research and Development Center, China; ²National Laboratory for Computational Fluid Dynamics, Beihang University, Beijing 100191, China With regard to the influence of energy accommodation of scattering gas molecules on flow fields in the process of the reentry of large expired spacecraft, a more elaborated gas-surface interaction model, compared with the full Maxwellian diffuse model, is implemented in implicit algorithms based on the Boltzmann model equation. By comparing the characteristic distributions in different fluid regimes around the cylinder in terms of implicit algorithms, Navier-Stokes solver, and DSMC method, the consistency of these results is verified. It is confirmed that the algorithms are capable to simulate flow fields around objects covering various fluid regimes. The results reveal that under current conditions set in the paper, pressure, and temperature are proportional to wall activation but their variation amplitudes differ with wall activation in different fluid regimes. As for the effects of energy accommodation coefficients, pressure, and temperature profiles vary in a linear way with them in different wall states at different trajectory points. However, the variation ranges of these characteristics in different fluid regimes are diverse. These results favor the construction of efficient software that combined exterior ballistics with aerothermodynamics to predict the flight path of large defunct spacecraft.</p>
<p>12:00pm - 2:00pm</p>	<p>Lunch</p>
<p>2:00pm - 2:45pm</p>	<p>Invited speaker #6 Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Haibo Huang, University of Science and Technology of China</p> <p>2:00pm - 2:45pm Theoretical considerations of Boltzmann-equation based CFD methods for continuum flows Lian-Ping Wang Southern University of Science and Technology, Shenzhen, China Boltzmann-equation based methods such as the lattice Boltzmann method and the discrete unified gas kinetic scheme now play a major role in computational fluid dynamics, due to their simplicity in formulation, feasibility in incorporating microscopic physics, low numerical dissipation, and advantages in parallel implementation. In most cases, they are used to simulate continuum flows, namely, as an alternative approach for solving the Navier-Stokes-Fourier system or multiphase flow systems. In this sense, Boltzmann-equation based methods are methods deigned in a high-dimensional configuration space, which bear both advantages and drawbacks. The design of the model Boltzmann equations for the interior nodes, the implementation of hydrodynamic boundary conditions at the boundary nodes, and the proper and efficient initialization in the case of turbulent flow simulation are the major considerations that determine their capabilities, accuracy, computational efficiency and numerical stability. The design details are not unique, and merits and issues in these should be carefully analyzed. In this talk, I shall discuss and illustrate these aspects and our recent progress from theoretical viewpoints, together with various simulation results.</p>
<p>2:00pm - 2:45pm</p>	<p>Invited speaker #9 Location: Mount Qingcheng Grand Hotel-Growth Hall Session Chair: Prof. Chengwen Zhong, Northwestern Polytechnical University</p> <p>2:00pm - 2:45pm Gas-kinetic unified algorithm by computable modeling of Boltzmann equation and application platform of high performance computation for near-space irregular flows Zhihui Li^{1,2}, Yongdong Liang^{1,2}, Aoping Peng¹, Junling Wu¹, Kun Xu³</p>

¹China Aerodynamics Research and Development Center, Mianyang 621000, China; ²National Laboratory for Computational Fluid Dynamics, Beijing 100191, China; ³Hong Kong University of Science and Technology, Kowloon, Hong Kong, China

Abstract: Severe aerodynamic heating and high temperature non-equilibrium effects are caused by the extremely hypersonic flows during spacecraft re-entry processes, especially the vibrational energy of the detached shock wave, and the quantum effect of vibrational energy can not be neglected. It has been becoming necessary and urgent to consider how to start from the Boltzmann equation, which describes the transport phenomena of gas molecules covering various flow regimes, and the Boltzmann model with translational-rotational-vibrational energy excitation needs to be designed and the aerodynamic thermal effects need to be simulated. Wherefore, the development of accurate and efficient numerical methods for extremely hypersonic flows at all regimes is important for the design, manufacture, and end-of-life re-entry flight track prediction of the spacecraft. In this report with the framework of the gas-kinetic unified algorithm for physical analysis and computable modeling of the collision integral of the Boltzmann equation, the translational, rotational, and vibrational relaxation models of internal degrees of freedom were introduced, using the total molecular conservation of angular momentum as a new collision invariant, based on the energy model partition function and the inelastic collision relaxation number, a two-time-scale collision frequency expression describing the elastic and inelastic collision relaxation of polyatomic molecules has been derived. The collision integral model of the Boltzmann equation is transformed into the elastic and inelastic collision terms, the inelastic collision term is decomposed into translational-rotational energy relaxation and translational-rotational-vibrational energy relaxation according to a certain relaxation rate, it has been proved by the normalization, conservation, and H-theorem. The discrete velocity ordinate method and the numerical integration rule of the real-time determination of the discrete velocity space have been developed for hypersonic flow simulation at any Mach number, which satisfies the conservation condition of the Boltzmann equation. An implicit parallel gas-kinetic numerical scheme for the evolution of discrete velocity distribution functions has been constructed by using the extended finite difference method (LU-SGS). In accordance with the conservation of mass flux on the surface and the relationship between molecular translational energy and internal energy balance, the unified mathematical model and numerical treatment method have been developed for hypersonic flow field boundary-surface interaction based on the evolution update of the gas molecular velocity distribution function, which takes account of thermodynamic non-equilibrium effects. The unified Boltzmann model for characterizing the effects of multiscale rarefaction and high-temperature non-equilibrium viscous real gases has been presented for extremely high Mach spacecraft flows and the new gas-kinetic unified algorithm for solving hypersonic non-equilibrium flows over large-scale and complex structure aircrafts has been developed for near-earth space flight environment. A large-scale parallel computing strategy based on the domain decomposition of two phases in physical and velocity space has been established with the quasilinear speed-up ratio, the parallel efficiency is more than 90% when the parallel algorithms have been tested on 64~1024, 1024~8000, 4950~20625 CPUs and 500 ~ 45000 processors of multi-core heterogeneous computers. To integrate the frontier basic research into engineering requirements, a high-performance parallel computation platform and the numerical prediction software system for the hypersonic aerodynamic/thermal flow problems of spacecraft with complex structures have been established. The algorithm validation of the large-scale parallel computation with the comparison of the DSMC, N-S/DSMC, (slip)N-S solvers, UGKS, and the wind-tunnel tests for aerodynamic and thermal flows around the two-capsule vehicle of Tiangong aircraft, spacecraft re-entry module, the wing-body assembly aircraft, and cavity. It has been indicated from the results and application in Figure 1 that the computational results are in high resolution of the flow fields, and match well with the related results of theoretical, DSMC, N-S/DSMC, Slip N-S, UGKS, and the experimental measures, in manifesting the high accuracy of the present algorithms and providing practical applications on computable modeling of the Boltzmann equation for near-earth space irregular flows and aerothermodynamic problems with multi-scale rarefied and high-temperature non-equilibrium effects covering all flow regimes.

2:45pm - 3:45pm

S10- Complex fluids: multi-phase and porous media flows-I

Location: **Mount Qingcheng Grand Hotel-Tianfu Hall**

Session Chair: **Haibo Huang**, University of Science and Technology of China

2:45pm - 3:05pm

Dynamics of CO₂ density-driven flows in fractured porous media

Peiyao Liu¹, Zhaoli Guo²

¹State Key Laboratory of Coal Combustion, Huazhong University of Science and Technology, Wuhan, China; ²Institute of Interdisciplinary Research for Mathematics and Applied Science, Huazhong University of Science and Technology, Wuhan, China

Dissolution trapping is an essential process in carbon dioxide (CO₂) sequestration. In this study, we use a discrete unified gas kinetic scheme to simulate the behavior of dissolved CO₂ under various fracture scenarios in CO₂ density-driven flows. The effects of single horizontal fracture in both the two-dimensional (2D) and three-dimensional (3D) domain, and single vertical and intersecting fractures in the 2D domain are systematically investigated. The detailed flow characteristics within the fractures are presented for the first time. The results show that the fractures serve as the preferential pathways for CO₂-rich plumes, causing CO₂ fingers to flow along the fracture. Within the fracture, the local circulation flows occur, which may cause adjacent fingers to merge, reducing the number of fingers. Furthermore, the results also show that the single horizontal fracture generates a negative impact on CO₂ trapping, while the single vertical and intersecting fractures induced positive feedback, accelerating CO₂ dissolution.

3:05pm - 3:25pm

Investigating the influence of hydrophobic microstructure on saturated water content and streamline tortuosity of carbon paper in steady-state solid-liquid two-phase flow using the pseudo-potential lattice Boltzmann method

Chaogang Chen, Yuan Gao

Tongji University, Shanghai, China

Carbon paper serves as a crucial substrate material in fuel cell gas diffusion layers. However, the understanding of binder distribution characteristics within carbon fibers remains insufficient. In this study, a microstructure reconstruction method was employed to generate various spatial distributions of binders, while the Lattice Boltzmann Method (LBM) was utilized to investigate the flow characteristics of two-phase gas-liquid flow. During the carbon fiber reconstruction process, a series of convolution kernels with distance judgment functions were employed to incorporate binders into the fiber layer, leading to the

generation of a range of microporous structures by controlling the spatial distribution of the resin. The pseudo-potential LBM method was employed to simulate the gas-liquid two-phase flow of water within these structures. The primary focus is to compare the variations in water saturation during the liquid discharge process for different binder spatial distribution structures, summarize the influence of hydrophobic structures within mesoporous structures on steady-state water saturation in two-phase flow, calculate the tortuosity of steady-state streamlines, and explore the impact of mesoporous structures on streamlines within the overall structure.

3:25pm - 3:45pm

The study of pore doublets and porous media backflow based on lattice Boltzmann method

Yuhang Huang, Haihu Liu

Xi'an Jiaotong University, Xi'an, China

The displacement of multiphase fluid flow in a pore doublet is a fundamental problem, critical for understanding the transport mechanisms of multiphase flows in porous media. During the displacement of immiscible two-phase fluids in a pore doublet, the transport process is influenced not only by capillary and viscous forces but also by channel geometry. In this study, we investigate the unique phenomenon of backflow in immiscible two-phase flow through pore doublets and porous media, along with its underlying flow mechanism, using the LBM color gradient model. In the case of pore doublet imbibition, the capillary force and viscous force compete as the fluid flows through the two-branch pipe. At low capillary numbers, the capillary force dominates, leading to a higher capillary driving force in the fine pipe, promoting faster fluid flow. The pressure step results in a negative pressure difference with a steeper gradient. Simultaneously, under constant inlet flow rate conditions, the inlet flow rate fails to fully supplement the high flow rate in the fine pipe, resulting in flow rate compensation by the thick pipe and inducing backflow. This paper examines the influence of capillary number, viscosity ratio, and diameter ratio on the backflow effect. The backflow effect is most pronounced in pore doublets with low capillary numbers, viscosity ratios, and specific diameter ratios. However, when studying the porous medium, the backflow effect is considerably weaker. The main distinction between the porous medium and the pore doublet lies in the complex pore throat structure of the porous medium. It is revealed that the insignificant backflow effect in the porous medium is primarily due to the capillary valve effect. In conclusion, this work provides valuable insights into backflow dynamics and can be utilized for engineering design and inhibiting displacement fluid backflow.

2:45pm - 3:45pm

S11- - Algorithms and implementations-III

Location: **Mount Qingcheng Grand Hotel-Growth Hall**

Session Chair: **Prof. Chengwen Zhong**, Northwestern Polytechnical University

2:45pm - 3:05pm

Modeling the radiation of non-gray gas with steady discrete unified gas kinetic scheme

Xinliang Song, Zhaoli Guo

Huazhong University of Science and Technology, Wuhan, China

Radiative heat transfer plays a significant role in hypersonic reentry environment, combustion system, and many other areas. Many methods have been proposed to solve the thermal radiation. In the present work, a steady discrete unified gas kinetic scheme (SDUGKS) is developed to model the radiation of non-gray gas. With the coupling of the scattering, absorbing and emitting along the characteristic line of the radiative transfer equation (RTE) in reconstructing the cell interface intensity, the SDUGKS can obtain more accuracy results with coarser mesh. The SDUGKS has achieved great success for gray radiative heat transfer problems. Due to the wide range of the spectral absorption coefficient of non-gray gas, the line-by-line (LBL) model and weighted-sum-of-gray-gases (WSGG) model is adopted to simulate several multidimensional problems. The results demonstrate that the SDUGKS is a reliable and efficient tool for the radiation of non-gray gas.

3:05pm - 3:25pm

Spatial second-order positive and asymptotic preserving filtered PN schemes for nonlinear radiative transfer equations

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A spatial second-order scheme for the nonlinear radiative transfer equations is introduced in this paper. The discretization scheme is based on the filtered spherical

harmonics (FPN) method for the angular variable and the unified gas kinetic scheme (UGKS) framework for the spatial and temporal variables respectively. In order to keep the scheme positive and second-order accuracy, firstly, we use the implicit Monte Carlo (IMC) linearization method in the construction of the UGKS numerical boundary fluxes. This is an essential point in the construction. Then, by carefully analyzing the constructed second-order fluxes involved in the macro-micro decomposition, which is induced by the FPN angular discretization, we establish the sufficient conditions that guarantee the positivity of the radiative energy density and material temperature. Finally, we employ linear scaling limiters for the angular variable in the PN reconstruction and for the spatial variable in the piecewise linear slopes reconstruction respectively, which are shown to be realizable and reasonable to enforce the sufficient conditions holding. Thus, the desired scheme, called the PFPN-based UGKS, is obtained. Furthermore, we can show that in the regime $\epsilon \ll 1$ and the regime $\epsilon = O(1)$, the second-order fluxes can be simplified. And, a simplified spatial second-order scheme, called the PFPN-based SUGKS, is thus presented, which possesses all the properties of the non-simplified one. Inheriting the merit of UGKS, the proposed schemes are asymptotic preserving. By employing the FPN method for the angular variable, the proposed schemes are almost free of ray effects. Moreover, the above-mentioned way of imposing the positivity would not destroy both AP and second-order accuracy properties. To our best knowledge, this is the first time that spatial second-order, positive, asymptotic preserving and almost free of ray effects schemes are constructed for the nonlinear radiative transfer equations without operator splitting. Therefore, this paper improves our previous work on the first-order scheme which could not be directly extended to high order, while keeping the solution positive. Various numerical experiments are included to validate the properties of the proposed schemes.

3:25pm - 3:45pm

Sparse grids based DUGKS for non-equilibrium flow

Shuyang Zhang¹, Zhaoli Guo²

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Discrete Unified Gas Kinetic Scheme (DUGKS) is a finite-volume method for non-equilibrium flows based on kinetic models [1]. With the coupling of particle collision and transport processes in the reconstruction of interface flux, DUGKS can accurately describe flow behaviors from continuum to free molecule regimes. For highly non-equilibrium flows, a large discrete velocity set is required in practical computations, which suffers from the so-called curse of dimensionality especially in 3-D case. The computational cost and storage requirements grow exponentially with the dimensionality of the problem. The Sparse Grids Method has been proposed to ease the curse [2], which reduced the number of velocity space grid points by an order of magnitude. With this technique, a Sparse Grids based DUGKS (DUGKS(SG)) is proposed in this study. A number of numerical tests, including the 2-D Riemann problem, etc are performed to validate the DUGKS(SG). The comparisons with benchmark data demonstrate that the present DUGKS(SG) is a reliable and efficient method for non-equilibrium flows. Particularly, it is found that the computational cost of DUGKS(SG) can be much reduced to obtain the accuracies of the same order for the velocity space grid compared with the original DUGKS, and the computational efficiency is much improved.

[1] Guo Z, Xu K, Wang R. Discrete unified gas kinetic scheme for all Knudsen number flows: Low-speed isothermal case[J]. Physical Review E, 2013, 88(3): 033305.

[2] Bungartz H J, Griebel M. Sparse grids[J]. Acta numerica, 2004, 13: 147-269.

3:45pm - 4:05pm

Coffee Break

3:45pm - 4:05pm

Poster Session

4:05pm - 5:25pm

S12-HPC and other hardware-I

Location: **Mount Qingcheng Grand Hotel-Tianfu Hall**

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

4:05pm - 4:25pm

Taichi-LBM3D: an open-source massive parallel lattice Boltzmann code

Xin Xiong^{1,2}, Jianhui Yang³, Tom-Robin Teschner², Liang Yang¹

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This article presents a lattice Boltzmann solver: Taichi-LBM3D. Taichi-LBM3D is a three-dimensional Lattice Boltzmann Method (LBM) solver based on the Multi-Relaxation-Time (MRT) D3Q19 model. It can solve both single-phase flow and multi-phase flow problems, where the latter is based on the color gradient model that solves an additional advection equation of the scalar phase field. Additionally, the Taichi Language significantly improves the solver's performance based on different backends such as CUDA, OpenGL, and many-core CPUs [1]. The test case of single-phase flow, such as Stokes flow and lid-driven cavity flow, shows good agreement with the analytical solution based on this solver. Moreover, the test case of multi-phase capillary fingering also shows good agreement with the reference results compared to the width of the finger. The solver's performance can reach 900 Million Lattice Updates per Second (MLUPS), which is a modified version of MLUPS with an NVIDIA A100 GPU [2]. The solver is easy to understand and use, which has been proven to apply to many engineering applications such as the external flow of a vehicle, single-phase porous medium, and two-phase porous medium flow of the drainage process. The feature of sparse storage of memory in the porous medium is also one of the reasons for the performance increase. The solver was further extended with distributed memory using the MPI4py library, developed in PyEFEM code [3].

Acknowledgment: This work was supported by ARCHER2 Embedded CSE (eCSE) Programme, UK.

References:

[1] https://github.com/yjhp1016/taichi_LBM3D

[2] Yang, Jianhui, Yi Xu, and Liang Yang. "Taichi-LBM3D: A Single-Phase and Multiphase Lattice Boltzmann Solver on Cross-Platform Multicore CPU/GPUs." *Fluids* 7.8 (2022): 270.

[3] Nillama, Loic Balazi Atchy, Jianhui Yang, and Liang Yang. "An explicit stabilized finite element method for Navier-Stokes-Brinkman equations." *Journal of Computational Physics* 457 (2022): 111033.

4:25pm - 4:45pm

Performance of GPU-based discrete unified gas kinetic scheme for DNS of turbulent flows

Kairzhan Karzhaubayev¹, Lian-Ping Wang¹, Dauren Zhakebayev²

¹Southern University of Science and Technology, Shenzhen, Guangdong, China; ²National Engineering Academy, Almaty, Kazakhstan

In this talk, we present a successful implementation of the Discrete Unified Gas Kinetic Scheme (DUGKS) on GPU systems, utilizing the CUDA Fortran programming language. We introduce a memory usage reduction technique that significantly decreases memory consumption by a factor of 3 compared to our original CPU-based implementation. Moreover, we couple this new implementation with an improved approach for computing cell face flux using trilinear interpolation. Analytical comparisons of truncation errors reveal the enhanced accuracy of the interpolation-based flux calculation over the original DUGKS method. We share the initial simulation results obtained using this enhanced approach, demonstrating that the application of trilinear interpolation can yield slightly improved DNS results, particularly on relatively coarse meshes. Through example applications, we showcase the improved GPU-based DUGKS method for both laminar and turbulent flows in periodic and wall-bounded boundary configurations. Furthermore, we present performance comparison between the GPU and CPU implementations. The GPU implementation achieved a maximum speedup of 7.64x when compared to a 32-core CPU, utilizing a desktop-level GPU. These findings highlight the accelerated performance and increased accuracy

achieved by leveraging GPU capabilities for turbulent flow simulations with the Discrete Unified Gas Kinetic Scheme.

4:45pm - 5:05pm

Efficient display of LBM simulations through combined LOD and octree-based techniques

Chao Xu

Zhejiang University, Hangzhou, China

The Lattice Boltzmann Method (LBM) is a powerful computational fluid dynamics technique used to simulate fluid flow behavior. However, the visualization of large point datasets generated by LBM simulations can be computationally intensive. In this study, we propose a novel approach to accelerate the visualization process by combining Level of Detail (LOD) techniques and octree-based spatial partitioning. By employing octree or spatial partitioning data structures, the point data from LBM simulations are organized into a hierarchical representation, facilitating efficient spatial queries. To manage the visualization, a LOD management scheme is implemented, dynamically selecting and displaying the appropriate level of detail based on the user's viewpoint and the data of interest. This ensures that only the necessary data is processed and rendered, optimizing the visualization performance. The combined LOD and octree-based technique allows for selective rendering of points, reducing the computational load and improving rendering performance. By adapting the LOD levels based on available resources and performance requirements, the visualization remains interactive and responsive. The results demonstrate that the proposed approach efficiently displays LBM simulations, providing a streamlined visualization experience while maintaining the overall accuracy and quality of the visualization. This approach has the potential to significantly enhance the understanding of fluid flow behavior and facilitate in-depth analysis in various domains, such as engineering, environmental sciences, and biophysics.

5:05pm - 5:25pm

Parallel Jacobian-free Newton Krylov discrete ordinates method for neutron Boltzmann transport equation

Yangyi Zhang, Xiaofeng Zhou, Zhaoli Guo

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The neutron transport Boltzmann equation (NBTE) describes the complicated and multiscale neutron transport process in the nuclear reactors, and the solution of which is usually used in the reactor simulation to analyze the power distribution. The NBTE is the distribution function for the angular neutron fluxes as a function of position, transport direction, energy and time, which makes it challenging to be efficiently and accurately solved. Thus, the solution of neutron transport models with large scales, complex structures and high accuracy requirement consumes a lot of computing resources and time. The discrete ordinates method (Sn) has the advantage of high accuracy and good parallel performance for large-scale models, and it has been one of the most popular solutions for the NBTE. But it suffers the efficiency problem because of the poor convergence of the original nested power iteration (PI) and source iteration (SI). To accelerate the solution, the efficient Jacobian-Free Newton Krylov method (JFNK), which combines the nonlinear Newton iterative method, the linear Krylov subspace method and Jacobian-free method, is employed to solve the Boltzmann equation. The parallel JFNK-Sn method is proposed, which makes full use of the good efficiency of the JFNK framework and the high accuracy of the Sn method, and it is applied in multi-dimensional multi-group pin-by-pin neutron transport models. The k-eigenvalue and the scalar fluxes (rather than the angular fluxes) are chosen as the global solution variables of the JFNK method, and the residual functions are evaluated by the Koch-Baker-Alcouffe (KBA) sweep algorithm with the spatial domain decomposition in the parallel Sn framework. Unlike the original Sn iterative strategy, only one sweep is required for the JFNK strategy, rather than the power iteration with nested inner source iterations. Finally, the comeSn_JFNK code is developed in C++ language and, the numerical solutions of the 2-D/3-D KAIST-3A benchmark problems and the 2-D/3-D full-core MOX/UOX pin-by-pin models with different control rod distribution show that comeSn_JFNK method can obtain significant efficiency advantage compared with the original power iteration method (comeSn) for the parallel simulation of the large-scale complicated pin-by-pin models.

4:05pm - 5:25pm

S13-CFD applications-I

Location: **Mount Qingcheng Grand Hotel-Growth Hall**

Session Chair: **Prof. Kazuhiko Suga**, Osaka Metropolitan University

4:05pm - 4:25pm

Numerical investigations of the deformable capsules in a Poiseuille flow with Newtonian/viscoelastic matrix

Hua Zhang^{1,2}, Lian-ping Wang², Chang Shu¹

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Cell manipulations, such as focusing, concentration and separation, play important roles in medical and engineering applications. Compared to active manipulations, such as imposing acoustic and magnetic force fields, passive manipulations control the cells using flow-induced lift and drag forces, which can often be affected by the cell size and deformability, the device size and the fluid properties. In recent years, the motion of particles (non-deformable objects) and capsules (deformable objects) in viscoelastic fluids has attracted much attention since the coupling of viscoelasticity-induced lift and inertia-induced lift can potentially expand the range of equilibrium configurations of particles and capsules. In this talk, an immersed boundary-lattice Boltzmann flux solver (IB-LBFS) incorporating a finite difference method (FDM) or finite element method (FEM) is presented to investigate the lateral migration and dynamic behavior of deformable capsules in Poiseuille flows at finite Reynolds numbers, with a Newtonian or viscoelastic fluid matrix. The work builds on our recent study on the dynamics of deformable capsules in a shear flow. In a Poiseuille flow, the velocity gradient, i.e., the local shear rate, varies across the cross-section of the channel. Shear-induced and wall-induced lift forces are key factors affecting the lateral migration of the flows with Newtonian fluids. However, in the viscoelastic fluid flows, the elastic lift stemming from the first normal stress difference is also important. Therefore, the effects of viscoelasticity on the capsule behaviors should also be considered.

4:25pm - 4:45pm

Lattice Boltzmann modeling of convective heat transfer and phase transitions in additive manufacturing

Wenbin Zhang¹, Dong Li¹, Zhenhua Chai², Dongke Sun¹

¹School of Mechanical Engineering, Southeast University, Nanjing, China; ²School of Mathematics and Statistics, Huazhong University of Science and Technology, Wuhan, China

Metal additive manufacturing (AM) technology represents a significant breakthrough, as it enables the direct formation of three-dimensional parts through discrete-stacking overlays, overcoming the limitations imposed by conventional manufacturing methods. However, the uncertain quality of formed parts poses a substantial barrier to the widespread industrial adoption of AM. To address this, a thorough understanding of heat and mass transfer behavior during the part formation process is essential. This paper focuses on the simulation of the prevailing metal AM process using a lattice Boltzmann coupled model. The model incorporates convection heat and mass transfer, as well as phase transition phenomena. For the flow part, a lattice Boltzmann model for free surface gas-liquid two-phase flow is employed. The solid-liquid phase change is modeled using the lattice Boltzmann total enthalpy method. To validate the model's accuracy, classical benchmarks of flow and heat transfer are simulated quantitatively. Additionally, the model investigates the characteristics of convective heat transfer within the AM melt pool. These include simulations of electron beam selective melting, wire arc AM, and based on the continuous deposition of metal droplets. The investigation focuses on the non-equilibrium convective heat transfer, phase transition, and the rapid solidification behavior of the melt pool. The results demonstrate the significant potential and advantages of the computational model in accurately simulating the intricate process of metal AM, which is of great importance for industrial applications of metal AM.

4:45pm - 5:05pm

Numerical Study on mechanism of air entrainment in resin transfer molding using a phase-field lattice Boltzmann model

Wenqiang Chen^{1,2}, Yumei Yong¹, Hanyang Mo^{1,3}, Jialin Dai^{1,2}, Chao Yang^{1,2}

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Defects are easy to occur due to air entrainment and poor infiltration in resin filling process in resin transfer molding (RTM). Studying the characteristics of resin filling and infiltration and the mechanism of air entrainment in a fiber preform is very important for reducing the defects in composites. In this paper, a phase-field lattice Boltzmann method (PFLBM) for immiscible multiphase flows with large density and viscosity ratios was developed. Since the viscosity of the resin varies with the shear rate, the non-Newtonian viscosity rheological model was introduced to reflect the non-Newtonian properties of resin in the framework of the PFLBM. In order to accurately apply the contact angle of variable curvature surface, the curve equation gradient method (CEGM) was used to dynamically capture the normal intersection of solid grids and physical boundaries. Two cases, i.e. droplet spreading on an ellipse and non-Newtonian Bingham two-phase flow in a pipeline, were used to verify the correctness and accuracy of the proposed contact angle introduction method for variable curvature boundary and the non-Newtonian two-phase flow model in this paper. Based on the established mathematical model, the process of resin displace gas in the complex channel was simulated. The influences of preform geometry and surface properties, non-Newtonian rheological properties, two-phase physical properties and technological conditions on the two-phase flow pattern and air entrainment mechanism were investigated, which provided theoretical basis for the optimization of RTM process.

5:05pm - 5:25pm

Phase behavior of lattice Boltzmann fluids with interface curvature

Jingwei Huang¹, Xiaolong Yin²

¹China University of Geosciences (Wuhan), Wuhan, China; ²Ningbo Eastern Institute of Technology, Ningbo, China

Vapor-liquid phase behavior of lattice Boltzmann fluids is a topic that has received significant past attention. When the vapor-liquid interface is flat, several models can produce phase behaviors in excellent agreement with that from the underlying equation of state. When the interface is curved, it is known that the phase equilibrium of a real fluid is changed due to the Laplace pressure. Does the phase behavior of lattice Boltzmann fluids change correctly with interface curvature? We found that the effect of Laplace pressure on phase equilibrium is only quantitatively correct at high reduced temperatures. At low temperatures, moderate-to-significant discrepancies were noted. For the tested pseudopotential model, tuning its potential parameters reduced the discrepancies. Our tuning suggests that the source of the discrepancies is interface thickness and lattice effects. Evaluating the phase behaviors of lattice Boltzmann fluids with interface curvature also generated the length scale of the lattice spacing. After relating the interfacial tension of the simulated fluid to that of a real fluid, the lattice spacing of the tested models is found to be on the order of several molecular diameters. The interface thickness is, therefore, several nanometers, on par with molecular simulations.

8:30am - 9:15am	<p>Invited speaker #10 Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. Lei Wu, Southern University of Science and Technology</p> <p>8:30am - 9:15am</p> <p>Multiscale and low-noise particle simulation for non-equilibrium gas flows</p> <p>Jun Zhang, Hao Yang, Kaikai Feng, Peng Tian Beihang University, Beijing, China</p> <p>The simulation of non-equilibrium gas flows has garnered significant interest in modern engineering problems. In aerospace engineering, the prediction of aerodynamic properties for high-speed rarefied gas flows has been successfully achieved using the direct simulation Monte Carlo (DSMC) method. However, due to limitations in cell sizes and time steps, DSMC requires extraordinary computational resources when simulating near-continuum flows. Recently, a unified stochastic particle (USP) method has been proposed. In comparison to DSMC, the USP method allows for the use of much larger time steps and cell sizes by effectively coupling molecular movements and collisions. This presentation will highlight a couple of typical applications of the USP method to high-speed flows, which involve internal energy exchange across different flow regimes. For low-speed rarefied gas flows in micro-electro-mechanical systems, the application of DSMC is restricted by statistical scatter issues. As a promising alternative, the information preservation (IP) method is known for its ability to mitigate statistical scatter in DSMC simulations, offering low noise properties. In this talk, I will present a rigorous theoretical framework for the IP method based on kinetic theory. Specifically, the macroscopic transport equations of the IP method are established by introducing a velocity-information joint distribution function. Numerical simulations of various gas flows will be presented to demonstrate that the IP method can achieve similar accuracy to DSMC but with a much smaller sampling size.</p>
8:30am - 9:15am	<p>Invited speaker #13 Location: Mount Qingcheng Grand Hotel-Growth Hall Session Chair: Dr. Paul John Dellar, University of Oxford</p> <p>8:30am - 9:15am</p> <p>Construction and analysis of lattice Boltzmann schemes</p> <p>François Dubois CNAM Paris and Univ. Paris-Saclay, France</p> <p>This lecture is divided into three parts.</p> <p>First, we recall the numerical framework for the construction of multiple relaxation times lattice Boltzmann schemes, in the spirit proposed by Lallemand, d'Humières et Luo [1, 2]. Secondly, we analyze the one-dimensional D1Q3 scheme when it is used for the approximation of acoustic problems. With this study, we use the Taylor expansion method proposed in [3]. In the third part, we explain how the general "ABCD" framework [4] can be used to study the question of the approximation of the compressible Navier-Stokes equations with a single distribution [5].</p> <p>References:</p> <p>[1] D. d'Humières, "Generalized Lattice-Boltzmann Equations", in Rarefied Gas Dynamics: Theory and Simulations, volume 159 of AIAA Progress in Astronautics and Astronautics, 1992.</p> <p>[2] P. Lallemand, L.-S. Luo, "Theory of the Lattice Boltzmann Method: Dispersion, Dissipation, Isotropy, Galilean Invariance, and Stability", Physical Review E, volume 61, 6546, 2000.</p> <p>[3] F. Dubois, "Equivalent partial differential equations of a lattice Boltzmann scheme", Computers and Mathematics with Applications, volume 55, p. 1441-1449, 2008.</p> <p>[4] F. Dubois, "Nonlinear fourth order Taylor expansion of lattice Boltzmann schemes", Asymptotic Analysis, volume 127, pages 297-337, 2022.</p> <p>[5] F. Dubois, P. Lallemand. "On single distribution lattice Boltzmann schemes for solving Navier Stokes equations", Communications in Computational Physics, accepted, April 2023.</p>
9:15am - 10:15am	<p>S14-Rarefied and non-equilibrium compressible flows-III Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. Lei Wu, Southern University of Science and Technology</p> <p>9:15am - 9:35am</p> <p>An asymptotic accurate and preserving time-relaxed Monte Carlo method for multi-scale gas flows</p> <p>Fei Fei School of Aerospace Engineering, Huazhong University of Science and Technology, Wuhan, China</p> <p>Multi-scale gas flows widely exist in aerospace and micro-electro-mechanical systems. In a continuum flow regime, a gas flow near the equilibrium state can be simulated by a gas dynamic scheme, such as computational fluid dynamic (CFD) based on Euler or Navier-Stokes equations. Conversely, in a rarefied flow regime, a gas flow departs far from thermodynamical equilibrium, and a kinetic approach, which tracks molecular motions and collisions individually, is necessary. However, if the Knudsen number varies over several orders of magnitude in the flow field, neither the dynamic nor the kinetic treatment is appropriate. In this talk, a new time-relaxed Monte Carlo (TRMC) method is introduced to overcome this deficiency. Compared to the standard TRMC scheme, the proposed method performs the same convection operator, however, divides the collision operator by a micro-macro decomposition. The continuous part of the collision operator is constructed based on the first-order Chapman-Enskog expansion and solved by an explicit second-order scheme, while the numerical solution of the rest nonequilibrium part is still provided by the standard TRMC scheme. In this way, the new TRMC method demonstrates the same accuracy as the standard TRMC scheme in the kinetic limit, however, preserves Navier-Stokes asymptotics and the second-order accuracy in the fluid limit. Several numerical results show that this stochastic particle method is useful and efficient for simulations of multiscale gas flows ranging from rarefied to continuum regimes.</p>

	<p>9:35am - 9:55am</p> <p>Research on information exchange technology of N-S/DSMC hybrid algorithm based on Bayesian estimation</p> <p>Zhonghua Li, Leining Dang, Junlin Wu China Aerodynamics Research and Development Center, Mianyang, China</p> <p>N-S/DSMC hybrid algorithm is an engineering practical numerical method in the transitional flow region, which can get relatively accurate aerodynamic characteristics in a wider Kn number range. In the process of hybrid calculating, significant statistical fluctuations of DSMC due to small sample size would affect the solving process of N-S equations. In the existing hybrid algorithm, to overcome the effect of DSMC fluctuations, the 'sub-relax' technique is adopted, which can effectively inhibit the propagation of fluctuation to the N-S solution region. In the sub-relax technique, weighted average method is used. Low weight factor is given to DSMC results, and the information exchange efficient is not high. In order to solve this problem, the Bayesian estimation method is considered. Bayesian estimation method is an artificial intelligence method, which can get relatively accurate value through small sample estimation. Using the method of conjugate prior distribution of function, the information exchange technology of N-S/DSMC hybrid algorithm based on Bayesian estimation is preliminary established. The conjugate prior distribution function of normal distribution is used for density, velocity/translating temperature, and the conjugate prior distribution of Gamma distribution is used for rotation and vibration temperature. Based on the DSMC samples, the posterior distribution of different parameters is obtained, and the Bayesian estimation of parameters is given. Taking the estimation as the DSMC result, information is exchanged with N-S solution. The proposed hybrid algorithm is used to simulate the hypersonic thermo-chemical non-equilibrium flow of cylinder and the hypersonic flow of aircraft in the transitional flow region. It is verified that in the case of large variance, the results of Bayesian estimation and sub-relax are good agreement by selecting suitable super parameter.</p> <hr/> <p>9:55am - 10:15am</p> <p>A direct unified wave-particle method for simulating non-equilibrium flows</p> <p>Sha Liu¹, Junzhe Cao¹, Sirui Yang¹, Chengwen Zhong¹, Kun Xu² ¹Northwestern Polytechnical University, Xi'an, Shaanxi, China; ²Hong Kong University of Science and Technology, Hong Kong, China</p> <p>In this work, the Navier-Stokes (NS) solver is combined with the direct simulation Monte Carlo (DSMC) solver in a direct way, under the wave-particle formulation [J. Comput. Phys. 401, 108977 (2020)]. Different from the classical domain decomposition method with buffer zone for overlap, in the proposed direct unified wave-particle (DUWP) method, the NS solver is coupled with DSMC solver on the level of algorithm. Automatically, in the rarefied flow regime, the DSMC solver leads the simulation, while the NS solver leads the continuum flow simulation. Thus advantages of accuracy and efficiency are both taken. At internal flow regimes, like the transition flow regime, the method is accurate as well because a kind of mesoscopic modeling is proposed in this work, which gives the DUWP method the multi-scale property. Specifically, as to the collision process, at $t < \tau$, it is supposed that only single collision happens, and the collision term of DSMC is just used. At $t > \tau$, it is derived that $1-\tau/\Delta t$ of particles should experience multiple collisions, which will be absorbed into the wave part and calculated by the NS solver. Then the DSMC and NS solver can be coupled in a direct and simple way, bringing about multi-scale property. Different from the original wave-particle method, in the proposed DUWP method, the wave-particle formulation is no more restricted by the Boltzmann-BGK type model and the enormous research findings of DSMC and NS solvers can be utilized into much more complicated flows, like the thermochemical non-equilibrium flow, which is essential for the aerodynamic design of hypersonic vehicle and spacecraft. Furthermore, this work provides a new route for modeling and numerical simulation of multi-scale problem and complex scientific problem. In this work, cases in monatomic argon gas are preliminarily tested.</p>
<p>9:15am - 10:15am</p>	<p>S15-Complex fluids: multi-phase, interfacial flows-V Location: Mount Qingcheng Grand Hotel-Growth Hall Session Chair: Dr. Paul John Dellar, University of Oxford</p> <p>9:15am - 9:35am</p> <p>The effect of droplet volume fraction on the modulation of turbulent channel flow laden with finite-size droplets</p> <p>Xiusong Chen¹, Jun Lai^{2,1}, Lian-Ping Wang¹ ¹Southern University of Science and Technology, Shenzhen, Guangdong, China; ²Peking University, Beijing, China</p> <hr/> <p>9:35am - 9:55am</p> <p>Inverse design of mesoscopic methods for two-phase flows</p> <p>Jun Lai^{1,2}, Lian-Ping Wang², Zuoli Xiao¹ ¹Peking University, Beijing, China; ²Southern University of Science and Technology, Shenzhen, Guangdong, China</p> <hr/> <p>9:55am - 10:15am</p> <p>Phase-field-based lattice Boltzmann model for two-phase flows with swirling and phase change</p> <p>Chunhua Zhang¹, Hantao Liu¹, Hong Liang², Zhaoli Guo³ ¹North university of China, Taiyuan, China; ²Hangzhou Dianzi University, Hangzhou, China; ³Huazhong University of Science and Technology, Wuhan, China</p>
<p>10:15am - 10:35am</p>	<p>Coffee Break</p>
<p>10:15am - 10:35am</p>	<p>Poster Session</p>
<p>10:35am - 11:20am</p>	<p>Invited speaker #11 Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Dr. Wei Su, The Hong Kong University of Science and Technology</p>

	<p>10:35am - 11:20am</p> <p>Study on heterogeneous parallel algorithms for SPH based on MPI</p> <p>Hong Chen, Hao Zhou, Jiawei Huang, Yi Li, Shengwei Lan</p> <p>China Aerodynamics Research and Development Center, Mianyang, China</p> <p>In smoothed particle hydrodynamics (SPH) applications, the precision and the scale of simulated problem can be enhanced effectively by increasing the particle numbers, and parallel computing is the necessary method to solve large scale SPH simulation. Based on the CPU-GPU heterogeneous structure of high performance computer, a heterogeneous parallel algorithm for SPH using message passing interface (MPI) is developed. Hierarchical partitioning is used in this algorithm, and the computer is divided into different levels, such as a CPU in one-way, multi CPUs in a computing node, and multi computing nodes. By optimizing the assignment of the subdomain, the localization is ensured, the high speed internal bus is used at higher priority for the communication between subdomains, the communication between computing nodes is minimized, thus to increase the communication speed. The algorithm support CPU-GPU heterogeneous structure, in which some of the subdomains are using CPUs, while other subdomains are using GPUs. The CPU processes and the GPU processes can maintain load balance. In the GPU computing, the pipeline technique is used to minimize the time cost of data copy between CPU and GPU. During the SPH integration, the difference between serial computing and parallel computing is avoid by using unified update mechanism.</p>
<p>10:35am - 11:20am</p>	<p>Invited speaker #14</p> <p>Location: Mount Qingcheng Grand Hotel-Growth Hall</p> <p>Session Chair: Dr. Fei Fei, Huazhong University of science and technology</p> <p>10:35am - 11:20am</p> <p>Status and future of DSMC research in hypervelocity aerodynamics institute</p> <p>Ming Fang¹, Langquan Li¹, Quanshun Yang¹, Hao Jin²</p> <p>¹Hypervelocity Aerodynamics Institute, Chinese Aerodynamics Research and Development Center, Mianyang 621000, China; ²School of Aeronautics, Northwestern Polytechnical University, Xi' an 710071, China</p> <p>The direct simulation Monte Carlo (DSMC) method of Bird has become the standard computational tool for the simulation of gas flows in which molecular effects become important. Our institute started the research work of DSMC in 1992. After more than 30 years of development, it has accumulated a lot of research results in DSMC and formed a relatively comprehensive DSMC capability system mainly reflected in three aspects, namely, adaptability, efficiency, and simulation ability. For adaptability, a hybrid grid system suitable for DSMC: uniform Cartesian background cells and unstructured triangle cells of body surface has been designed which can be applied to complex geometric features and a large variety of conditions, and large grid technology was developed that allowed DSMC to simulate flows in the near-continuum regime with an acceptable runtime and to dramatically decrease the computational time in other regimes. On the other hand, a parallel DSMC program based on MPI was developed by decomposing the physical domain into chain partitioning which can be used with any number of processors. At the same time, dynamic load-balancing technology has been developed to ensure high parallel efficiency. In order to expand the simulation ability and applicable scenarios of DSMC, some studies about the model are carried out, among which the representative ones are ionization reaction, atoms radiation effects of a rarefied gas and radiative equilibrium temperature boundary condition, etc. The relevant models have been successfully applied to predict the communication blackout altitude range during the Chinese capsule reentry and the surface heat value range of hypersonic aircraft. Based on the accumulation of the team's research on DSMC, DSMC software integrating pre-processing, flow field calculation, and post-processing has been developed. In future studies, work related to the coupling of DSMC with MD and extending DSMC parallel computing to GPU will be considered.</p>
<p>11:20am - 12:00pm</p>	<p>S16-HPC and other hardware-II</p> <p>Location: Mount Qingcheng Grand Hotel-Tianfu Hall</p> <p>Session Chair: Dr. Wei Su, The Hong Kong University of Science and Technology</p> <p>11:20am - 11:40am</p> <p>Scalable multi-GPU implementation of thermal lattice Boltzmann simulations in transitional flows</p> <p>Xing Xiang, Limin Wang</p> <p>Institute of Process Engineering, Chinese Academy of Sciences, Beijing, China</p> <hr/> <p>11:40am - 12:00pm</p> <p>SPH-ASR simulation of liquid film cooling</p> <p>Huan Li, Xiufeng Yang</p> <p>Beijing Institute of Technology, Beijing, China</p>
<p>11:20am - 12:00pm</p>	<p>S17-Rarefied and non-equilibrium compressible flows-V</p> <p>Location: Mount Qingcheng Grand Hotel-Growth Hall</p> <p>Session Chair: Dr. Fei Fei, Huazhong University of science and technology</p> <p>11:20am - 11:40am</p> <p>Numerical study of hypersonic near-continuum flows by improved continuum model</p> <p>Bocheng Deng, Jihui Ou, Jie Chen</p> <p>Department of Mechanics, Tianjin University, Tianjin, China,</p> <hr/> <p>11:40am - 12:00pm</p> <p>Effects of bio-inspired herringbone riblets on the turbulent boundary layer and its interaction with shock wave at supersonic flows</p> <p>Gang Wang^{1,2}, Pengcheng Quan³, Ke Zhu^{1,2}, Yanguang Yang^{2,4}</p> <p>¹China Aerodynamics Research and Development Center, Hypervelocity Aerodynamics Institute, Mianyang, 621000, China; ²Laboratory of Aerodynamics in Multiple Flow Regimes, China Aerodynamics</p>

Research and Development Center, Mianyang, 621000, China; ³National University of Defense Technology, Changsha/Nanjing, 410000/210000, China; ⁴China Aerodynamics Research and Development Center, Mianyang, 621000, China

12:00pm - 2:00pm	Lunch
2:00pm - 2:45pm	Invited speaker #12 Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. Limin Wang , Institute of Process Engineering, Chinese Academy of Sciences 2:00pm - 2:45pm Initialization from lattice Boltzmann to multi-step finite difference methods: modified equations and discrete observability Thomas Bellotti Ecole polytechnique, France Latitude on the choice of initialization is a shared feature between one-step extended state-space and multi-step methods. In the first case, the initial data are known exclusively on the conserved variables, whereas they remain arbitrary for the non-conserved moments. In the second case, the schemes need to be supplemented by some starting procedure. This work focuses on lattice Boltzmann schemes, which can be interpreted as examples of both previous categories of numerical schemes. We propose a modified equation analysis of the initialization schemes for lattice Boltzmann methods, determined by the choice of initial data. These modified equations provide guidelines to devise and analyze the initialization in terms of order of consistency with respect to the target Cauchy problem and time smoothness of the numerical solution. In detail, the larger the number of matched terms between modified equations for initialization and bulk methods, the smoother the obtained numerical solution. This is particularly manifest for numerical dissipation. Starting from the constraints to achieve time smoothness, which can quickly become prohibitive, we explain how the distinct lack of observability for certain lattice Boltzmann schemes—seen as dynamical systems on a commutative ring—can yield rather simple conditions and be easily studied as far as their initialization is concerned. This comes from the reduced number of initialization schemes at the fully discrete level. These theoretical results are successfully assessed on several lattice Boltzmann methods.
2:00pm - 2:45pm	Invited speaker #15 Location: Mount Qingcheng Grand Hotel-Growth Hall Session Chair: Prof. Zhaoli Guo , Huazhong University of Science and Technology 2:00pm - 2:45pm Angular momentum conservation in vector lattice Boltzmann formulations for hydrodynamics Paul John Dellar University of Oxford, United Kingdom Standard lattice Boltzmann formulations for hydrodynamics evolve a discrete set of scalar distribution functions. The fluid density is represented by the zeroth moment (or sum) of these distribution functions, the momentum vector by the first moment, and the momentum flux by the second moment. The momentum flux is thus a symmetric tensor by construction, so all these formulations satisfy the Boltzmann axiom. A conservation law for angular momentum, therefore, follows from the conservation law for linear momentum. Some lattice Boltzmann formulations instead represent a vector quantity as the sum of a set of vector-valued distribution functions. The vector quantity evolves through the divergence of the first moment of the vector-valued distributions. This is a general tensor, not necessarily symmetric. This vector approach has long been used to evolve the magnetic field in lattice Boltzmann formulations for Maxwell's equations and magnetohydrodynamics, for which an asymmetric, indeed almost antisymmetric, flux tensor is essential. Only in the last few years has the vector approach been extended to describe hydrodynamics. It proved necessary to change the scaling relation between the mass and momentum densities and their corresponding fluxes to ensure stability. The momentum flux in this formulation is not a symmetric tensor. These formulations reproduce the expected Navier–Stokes momentum equation, but they do not reproduce the expected angular momentum conservation equation, even in the incompressible limit. We will show, and confirm through numerical experiments, that they instead satisfy a more general angular momentum equation with a source term related to the antisymmetric part of the momentum flux. This source term can be absorbed into a redefined angular momentum flux, to the Navier-Stokes level of accuracy, using the same procedure used to construct the symmetric momentum flux tensor from the canonical momentum flux in electromagnetism. We also present a lattice Boltzmann formulation with a modified collision operator that symmetrizes the original momentum flux.
2:45pm - 3:45pm	S18-Algorithms and implementations-V Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. Limin Wang , Institute of Process Engineering, Chinese Academy of Sciences 2:45pm - 3:05pm A systematic study of hidden errors in the bounce back scheme and their various effects in the lattice Boltzmann simulations Zhi-Qiang Dong^{1,2}, Lian-Ping Wang¹, Xiang Li¹, Peng Yu¹ ¹ Southern University of Science and Technology, China; ² Harbin Institute of Technology, Harbin, China The bounce back scheme, the most popular mesoscopic boundary treatment, constitutes the main framework of the lattice Boltzmann method (LBM) together with the lattice Boltzmann equation itself. The lattice Boltzmann equation at interior nodes is used to reproduce the Navier-Stokes equations under the Chapman-Enskog (C-E) approximation, while the unknown distribution functions reconstructed by a bounce back scheme at boundary nodes may not maintain a complete consistency with the C-E approximation for interior nodes. This local inconsistency, referred as “hidden errors” in the present work, would reduce overall numerical accuracy and stability, and could lead to various negative effects in LBM simulations, such as the already-known non-physical slip velocity, grid-scale velocity, pressure noises, less-known local inconsistency with the Navier-Stokes equations, incorrect frequency spectrum of vortex shedding, and instability issues in wall-bounded turbulent flows. A systematic study of the hidden errors and their undesirable effects is provided in this work. We first derive the explicit structure of the distribution function for interior nodes under different collision models, and then identify the hidden errors by directly

contrasting the bounce back scheme to the structure of the distribution function for interior nodes. It is shown that the hidden errors can be explicitly expressed as a function of the hydrodynamic variables and relaxation parameters in the collision operator. For low-Reynolds-number viscous flows, there is an optimal parameter setting under strict physical constraints, which can suppress or eliminate most of these undesirable effects. For high-Reynolds-number wall-bounded turbulent flows, the negative effects cannot be fully eliminated by optimizing parameters alone, hence implementing a bounce back scheme with smaller hidden errors will be another option. Finally, a set of well-designed comparative simulations, including unidirectional, non-uniform and wall-bounded turbulent flow, are conducted to demonstrate that the magnitude of the hidden errors can significantly affect the numerical accuracy and stability.

3:05pm - 3:25pm

Modeling compressible flows using a central-moment-based discrete Boltzmann method

Chuangdong Lin, Xianli Su

Sun Yat-sen University, Shenzhen, China

Compressible flows refer to the movement of fluids that experience remarkable changes in density, temperature, pressure, and velocity as they move through different regions of flow. This type of flow is typically encountered at high velocities, supersonic and hypersonic speeds, and in aerospace and combustion applications. Understanding compressible flows is crucial to improve the design and performance of modern aircraft, rockets, engines, and other advanced technologies. In fact, compressible flows generally encompass a wide variety of nonlinear, unsteady, and nonequilibrium processes, both hydrodynamic and thermodynamic nonequilibrium influences are usually prominent, and the range of timescales involves several orders of magnitude. To probe the dynamic process, a central-moment-based discrete Boltzmann model (CDBM) is developed for compressible flows. Via the Chapman-Enskog analysis, the CDBM is demonstrated to recover Navier-Stokes (NS) equations in the hydrodynamic limit. Moreover, it provides quantification of thermodynamic nonequilibrium effects beyond the NS equations. Based on the CDBM, the nonequilibrium effects of compressible flows related to the thermal fluctuation can be obtained. The capability of the CDBM is demonstrated through simulations of sound wave, thermal Couette flow, sod shock tube, and shock reflection. This work is helpful in studying physical mechanisms and characteristics of compressible flows with essential hydrodynamic and thermodynamic effects.

3:25pm - 3:45pm

An approach to determine the solid volume fraction near solid boundaries for partially saturated method within the LBM framework

Xiang Li

Zhejiang University, Hangzhou, China

Within the LBM (Lattice Boltzmann Method) framework, PSM (Partially Saturated Method) is a quite straightforward approach for dealing with the solid boundaries. Additionally, PSM also has the advantages of exactly mass-conserving and no fresh node problem. There have been numerous successful implementations of PSM in processing the fluid-solid interactions in the previous investigations. In PSM, calculating the solid volume fraction in cubic LBM grids near solid boundaries is an indispensable prerequisite. However, the methods adopted in the previous work should have quite low efficiency in determining the solid fraction for complex boundary. Additionally, most of the PSM-LBM investigations concentrate on the boundary with rather simple geometry (e.g., the sphere in 3D and circle in 2D). Therefore, an approach based on projection method is proposed in this paper to accurately and efficiently determine the solid volume fraction of complex boundary in a cubic grid. To demonstrate the capability of our proposed approach, the calculation results of the solid volume fraction are compared with the theoretical solution of a spherical solid and the subdivision method. The comparison results show that this approach has quite good performances in terms of accuracy and efficiency. Subsequently, the proposed approach is incorporated into PSM-LBM to simulate the flow over a stationary obstacle with the relatively regular shape (including sphere, cube and ellipsoid) and the quite complex geometry (the rearview mirror) for further verifying the ability of the proposed approach. The fairly favorable consistency between the current simulation results and the literature data can ulteriorly validate the feasibility of this approach in processing fluid-solid interaction involving complex boundaries.

2:45pm - 3:45pm

S19-Algorithms and implementations-VI

Location: **Mount Qingcheng Grand Hotel-Growth Hall**

Session Chair: **Prof. Zhaoli Guo**, Huazhong University of Science and Technology

2:45pm - 3:05pm

Lattice Boltzmann simulations of noise induced by a moving cylinder

Jian Song, Feng Ren

School of Marine Science and Technology, Northwestern Polytechnical University, Xi'an, China

3:05pm - 3:25pm

Modeling and simulation of concrete with the cumulant lattice Boltzmann method

Konstantin Kutscher, Martin Geier, Manfred Krafczyk

TU Braunschweig, Germany

3:25pm - 3:45pm

An advanced TVD-filtering PFLBM model for large density-ratio multiphase flow with conduction-dominated mass transfer considering phase equilibrium

Hanyang Mo^{1,2}, Yumei Yong², Wenqiang Chen², Jialin Dai², Chao Yang^{1,2}

¹Institute of Chemical & Environmental Engineering, China University of Mining and Technology-Beijing, Beijing 100083, China.; ²CAS Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China.

3:45pm - 4:05pm

Coffee Break

3:45pm - 4:05pm

Poster Session

4:05pm - 5:25pm

S20-Complex fluids: multi-phase, interfacial flows-III

Location: Mount Qingcheng Grand Hotel-Tianfu Hall
Session Chair: Dr. Cheng Peng, Shandong University

4:05pm - 4:25pm

Modeling droplet dynamics with contact angle hysteresis by using cascaded lattice Boltzmann method

Shengting Zhang¹, Jing Li¹, Zhangxin Chen², Keliu Wu¹

¹China University of Petroleum, Beijing, China; ²University of Calgary, Alberta, Canada

Understanding droplet dynamics, including deformation and sliding on a solid surface, is significant to numerous applications in industrial fields, such as enhanced oil recovery (EOR). In such a process, contact angle hysteresis (CAH) is inevitable. In detail, many physical parameters at a microscopic scale could primarily affect the performance of the CAH, such as the properties of rock surface (heterogeneity, structure, and roughness) and the properties of fluids (interface tensions, droplet Viscosity). Hence, characterizing the CAH during droplet deformation and sliding is essential for understanding the microscopic mechanisms in processes such as EOR. In this work, we developed a multicomponent multiphase (MCMP) cascaded lattice Boltzmann model to simulate droplet dynamics considering CAH. Particularly, the Peng-Robinson (PR) equation of state is added to one component to improve the density ratio of the model; as well as achieved thermodynamic consistency and independent adjustment of the surface tension by improving its fluid-fluid interaction forces scheme. We also implement the modeling of CAH by applying geometric wetting boundaries and using the concept of a "hysteresis window" to control the strength of CAH. Based on this model, we simulated pinning droplets in inclined microchannels with different CAH windows. Similar to Berejnov's experiments, three types of stabilization patterns of pinning droplets were observed, which are (1) the contact line is stable against any inclination angle; (2) the contact line locally displaces to a new static configuration; (3) the contact line globally displaces to a new static configuration. We further used LBM to determine the critical inclination angle at the onset of droplet sliding for different CAH windows and Bond numbers (Bo), and our results are in general agreement with theoretical results.

4:25pm - 4:45pm

Simulation of Flow past a squirmer at low Reynolds numbers

Siwen Li, Deming Nie, Jingwen Wang, Yuxiang Ying, Tongxiao Jiang, Kaixuan Zheng

China Jiliang University, Hangzhou, China

We simulated the flow around a circular squirmer at low Reynolds numbers using the lattice Boltzmann method (LBM). We investigate the effects of Reynolds number (Re), the squirmer-type factor (β), the self-propelled strength (α), and particle head direction angle (θ) on the streamline structure and drag coefficient (CD) of the circular squirmer when $Re \leq 1$. The simulation results reveal that a distinct up-down symmetric recirculation zone is generated on the surface of the squirmer, which varies significantly for pusher ($\beta < 0$), neutral squirmer ($\beta = 0$), and puller ($\beta > 0$). This difference is attributed to the pressure distribution on the particle surface. Furthermore, as α increases, an up-down symmetric recirculation zone is formed near the wall, leading to a linear increase in the drag coefficient (CD), while changing Re has no effect on the flow field structure but negatively correlates with CD. Additionally, variations in the head direction of the particle also affect CD.

4:45pm - 5:05pm

A fractional step lattice Boltzmann method for magnetic multiphase flows

Xiang Li, Zhi-Qiang Dong, Peng Yu

Southern University of Science and Technology, Shenzhen, China

To simulate the complex interfacial behaviors of ferrofluids, a magnetic field coupling fractional step lattice Boltzmann (FSLB) method is proposed. The present FSLB method employs the Chapman-Enskog expansion analysis to reconstruct the convection and diffusion terms of the macroscopic governing equations and uses the equilibrium and non-equilibrium distribution functions to establish the predictor-corrector step. The present FSLB method inherits the excellent performance of kinetic theory from the conventional lattice Boltzmann method and the good numerical stability from the matured fractional-step method. This work successfully performs the first rigorous numerical simulation on the Rosensweig instability, which accurately captures the spikes forming at the surface of a ferrofluid under an applied magnetic field. Moreover, for the first time we numerically reproduce the falling ferrofluid droplet impacted on the solid surface. Intriguingly, our simulation results reveal that the falling velocity of the ferrofluid droplet is slightly accelerated by the elongation, although the direction of the magnetic field is opposite to that of the gravity. All the results for the interfacial behavior and the magnetic interaction highlight the comparative stability, accuracy, and capability of the present magnetic field coupling FSLB method.

5:05pm - 5:25pm

Inertial migration of spherical and oblate particles in triangular microchannels

Junqi Xiong, Haibo Huang

University of Science and Technology of China, Hefei, China

In this study, the lattice Boltzmann method and immersed moving boundary method are used to numerically investigate the inertial migration of particles in a triangular channel. The effects of the blockage ratio (β), Reynolds number (Re), and particle shape on inertial migration are primarily considered. For spherical particles, two equilibrium positions are observed within the cross-section of the channel, the face equilibrium position (FE) and the corner equilibrium position (CE). We quantitatively study the movement of these two positions with respect to β and Re. The process of particle migration can be divided into two stages. The first stage is migrating in the horizontal direction. In the second stage, particle trajectories are attracted to an equilibrium manifold whose shape closely resembles the cross-section of the channel. Moreover, the transition between FE and CE is investigated, and the phase diagram in the (Re, β) parameter plane is given. For oblate particles, there are two modes when particles reach the equilibrium position, tumbling and log-rolling. A similar equilibrium manifold has been observed, but it has a different shape. We study the effects of Re and β on particle migration, a critical β is found to change the equilibrium position. However, the effect of Re on inertial migration is irrelevant, mainly works by suppressing the initial tumbling motion of particles at high Re. Finally, the effect of particle aspect ratio (Ar) on migration is investigated. We show there is a critical Reynolds number (Rets) that can change the

equilibrium positions for small particles ($\beta < 0.2$). As Ar increases, Rets decreases. For large particles ($\beta > 0.4$), the transition of two equilibrium positions occurs within the range of $0.5 < Ar < 1$. These results can aid in the design of microfluidic devices for triangular channels.

4:05pm - 5:25pm

S21-Complex fluids: multi-phase and porous media flows-II

Location: Mount Qingcheng Grand Hotel-Growth Hall
Session Chair: Dr. Konstantin Kutscher, TU Braunschweig

4:05pm - 4:25pm

An analytical equilibrium equation of state for the phase field model for two-phase flow with soluble surfactants

Shi-Ting Zhang, Yang Hu

Beijing Jiaotong University, Beijing, China

In this paper, we proposed a fully logarithmic free energy-based phase field model for two-phase flow with soluble surfactants. Contrary to existing phase field models which use the Cahn-Hilliard free energy for the phase field, the free energies for phase and concentration fields are expressed by the logarithmic potential functions. Most importantly, the signed distance function is introduced to control the spatial distribution of energy. The analytical equilibrium equation of state between surface tension and surfactant concentration is derived based on the free energy functional. A multiple-relaxation-time (MRT) lattice Boltzmann (LB) scheme is utilized to numerically solve the governing equations of the flow, phase, and concentration fields. Laplace law is demonstrated to validate the validity of the analytical equilibrium equation of state. As a result, the numerical results are in good agreement with the analytical results. This study provides a theoretical basis for experiments measuring the surface tension of two-phase flows with soluble surfactants.

4:25pm - 4:45pm

Numerical simulation of miscible fluid displacement with dissolution reaction in a homogeneous porous medium

Aoyu Xu^{1,2}, Gaojie Liu^{1,2}

¹School of Energy and Power Engineering, University of Shanghai for Science and Technology, Shanghai 200093, China; ²Shanghai Key Laboratory of Multiphase Flow and Heat Transfer in Power Engineering, University of Shanghai for Science and Technology, Shanghai 200093, China

Miscible fluid displacement with fluid-solid dissolution reaction in a porous medium is an important mechanism of enhanced oil recovery, mineral transport in soil and the mixing of salt and fresh groundwater. As is well known, the dissolution reaction can change the structure of the porous medium, which will have a great influence on the miscible displacement process.

In this study, the miscible fluid displacement with dissolution reaction in a homogeneous porous medium is simulated by a lattice Boltzmann method (LBM), and the influence of fluid-solid dissolution reaction on displacement efficiency and fluid-fluid interfacial instability is studied. The simulation results show that when the viscosities of the fluids are the same, the dissolution reaction dissolves the framework of the porous medium, thus the porosity of the porous medium is increased. Compared with the case without dissolution reaction, the displacement efficiency is increased with dissolution reaction. When the viscosity of the displacing fluid is smaller than that of the displaced fluid, due to the viscosity difference between the two fluids, there will be a viscous fingering phenomenon at the front end of the displacement. It is found that the optimal displacement efficiency can be obtained when the Damköhler number is small (Damköhler number reflects the relationship between the reaction rate and the mass transfer diffusion coefficient). With the further increase of the Damköhler numbers, the displacement efficiency decreases. This is because when the Damköhler number is increased, the dissolution reaction will generate cracks in the porous medium, resulting in that part of the displacing fluid cannot be swept, and the displacing fluid leaves the porous medium along the cracks, resulting in the reduction of displacement efficiency.

Acknowledgments

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4:45pm - 5:05pm

Phase change heat transfer mechanism and effective thermal conductivity model for the mixed CPCMs

Jialin Dai^{1,2}, Yumei Yong¹, Hanyang Mo^{1,3}, Wenqiang Chen^{1,2}, Chao Yang^{1,2}

¹CAS Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China; ²School of Chemical Engineering, University of Chinese Academy of Sciences, Beijing 100049, China; ³Institute of Chemical & Environmental Engineering, China University of Mining and Technology-Beijing, Beijing 100083, China

The phase change heat transfer mechanism and effective thermal conductivity (ETC) of composite phase change materials (CPCMs) determine the design and performance of the phase change exchanger. So the phase change mechanism and ETC model for the mixed CPCMs are explored by numerical simulation. Firstly, A double-distribution-function (DDF) thermal LB model is built. The non-equilibrium heat transfer on the interface of substrate and PCMs is described by two temperature equations. Then the flow, phase change and heat transfer processes of mixed CPCMs are simulated on the particle scale. Convection diffusion Robin boundary is introduced for the thermal resistance of the material interface, and the thermal resistance method is extended to the enthalpy-based LB thermal model. A new interpolation scheme is applied to solve the material interface with a large curvature. The effects of the shape, size and arrangement of PCMs particles and thermal resistance between PCMs and substrate on the phase change, heat change and flow characteristics are investigated. The phase change mechanism of mixed CPCMs is analyzed, and the ETC is obtained. Finally, a new ETC model considering PCMs particle characteristics and thermal resistance for the mixed CPCMs is built. The validity and efficiency of the thermal LB model, thermal resistance model, and ETC numerical method are tested by the phase change inside a cavity, the thermal conduction with a circular material interface, and ETC for the mixed CPCMs.

5:05pm - 5:25pm

Numerical study on miscible displacement in an inclined anisotropic porous medium

Gaojie Liu^{1,2}, Yongqiang Wang^{1,2}

¹School of Energy and Power Engineering, University of Shanghai for Science and Technology, Shanghai 200093, China; ²Shanghai Key Laboratory of Multiphase Flow and Heat Transfer in Power Engineering, University of Shanghai for Science and Technology, Shanghai 200093, China

The miscible displacement of one fluid to another in an anisotropy porous medium is widely used in practical engineering applications, such as oil recovery, groundwater pollution, pipeline lubrication, chemical industry processes, etc. The miscible displacement process is affected by many factors, for example, when the viscosity of the displacing fluid is less than that of the displaced fluid, viscous fingering may occur, and as the fingerings develop, displacement efficiency is also affected; In addition, the anisotropy of porous medium will also affect the displacement efficiency. In this work, we use the lattice Boltzmann method to analyze the influence of the inclination angle of porous medium and viscosity ratio on displacement process. The research results indicate that, under a fixed inclination angle, the phenomenon of fingering becomes more pronounced as the viscosity ratio increases, resulting in a faster growth rate of fingering and an increase in displacement efficiency.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (Grant No. 51806142).

8:30am - 9:50am	<p>S22-Rarefied and non-equilibrium compressible flows-VI Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Dr. Gang Wang, China Aerodynamics Research and Development Center</p> <p>8:30am - 8:50am Numerical simulation of shock-microscale vortex interaction Yan Lv, Qibing Li Tsinghua University, Beijing, China</p> <hr/> <p>8:50am - 9:10am Linear stability analysis of hypersonic near-continuum flows over a blunt cone Chenyue Wang, Jihui Ou, Jie Chen Department of Mechanics, Tianjin University, Tianjin 300072, China</p> <hr/> <p>9:10am - 9:30am A high-precision pseudo arc-length method based on the TV splitting Chentao Wang Chinese Aeronautical Establishment, Beijing, China</p> <hr/> <p>9:30am - 9:50am Spatio-temporal evolution of pulsed discharge plasma in hypersonic flow field and its application Jie Wang, Huacheng Qiu Hypervelocity Aerodynamics Institute, China Aerodynamics Research and Development Center, People's Republic of China</p>
9:50am - 10:10am	Coffee Break
9:50am - 10:10am	Poster Session
10:10am - 12:10pm	<p>S23-CFD applications-II Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. Xiaolong Yin, Ningbo Eastern Institute of Technology Session Chair: Thomas Bellotti, Ecole polytechnique</p> <p>10:10am - 10:30am Numerical simulation of a neutrally buoyant particle motion in a double-lid-driven square cavity Qinglan Zhai¹, Lin Zheng², Song Zheng³ ¹Chaohu University, Hefei, China; ²Nanjing University of Science and Technology, Nanjing, China; ³Zhejiang University of Finance and Economics, Hangzhou, China</p> <p>A neutrally buoyant circular particle motion in a double lid-driven cavity flow (LDCF) is investigated by immersed moving boundary based lattice Boltzmann method, where the top and bottom walls move with constant velocities. To understand the mechanism of particle motion in double-LDCF, the influence of moving wall velocity ratio u_{wr}, initial position, particle size, and Reynolds number on the trajectory and limit circle of the neutrally buoyant circular particle motion in double-LDCF is systematically studied. The results show that the trajectory of the particle is obviously different with afore impactors. As u_{wr} varies, the limit circle is changed accordingly. The limit circle of particle motion is insensitive to initial position with $u_{wr} < 0$ except for initial location of the particle at the center of the cavity with $u_{wr} = -1$, where the particle is stationary all the time. When u_{wr} becomes positive, due to more complex fluid structure or vortices in cavity, three limit circle modes of the particle motion are observed by u_{wr} varied from 0 to 1 with $Re=1000$ and particle size $d_r=0.1$, namely, the limit circle of the particle motion is only present in the upper primary vortex, the limit circle of the particle motion is present in the lower primary vortex or can shuttle back and forth between the upper and lower primary vortices depending on its initial position, and the limit circle of the particle motion can shuttle back and forth between the upper and lower primary vortices. Especially, when the initial position of the particle is located at the center line in the horizontal direction in the cavity with $u_{wr}=1$, the transient trajectories of particle motion are the horizontal straight line and the particle is finally stationary at the left wall boundary. When particle size increases, the confinement of cavity is enhanced. The limit circle shrinks to the center of the cavity, and it can be greatly changed with different particle size for $u_{wr} > 0$. With the increment of Reynolds number, the flow is strengthened, and the influence domain and the strength of secondary vortices are enhanced, where the limit circle of particle motion is pushed away from the secondary vortices generated in cavity. However, the limit circle mode of particle motion is insensitive to the Reynolds number varied from 500 to 5000.</p> <hr/> <p>10:30am - 10:50am Mesoscopic modelling of microfluidic emulsions using the lattice Boltzmann method Gang Wang, Umberto D'Ortona, Pierrette Guichardon Aix-Marseille Univ., CNRS, Centrale Marseille, M2P2, Marseille, France</p> <p>This work focuses on two major issues that emerge in the simulation of microfluidic emulsion using the lattice Boltzmann pseudopotential multicomponent model. These two issues are the wetting curved wall boundary condition (since many microfluidic devices have complex channel geometries) and the droplet coalescence in the dense emulsion. Currently, in most previous works, the simple bounce-back (BB) method together with the fluid-solid interaction is used to simulate the contact angle. This method is accurate for a flat wall. But when it comes to curved or complex walls, it is not accurate enough since the wall is only a staircase approximation. Thus, we have proposed an improved partially saturated method to solve this problem. This is a curved wall boundary condition, and it is exactly mass conservative. This</p>

method outperforms the BB method in terms of modeling the static contact angle and the movement smoothness of the wetting droplet on the curved walls. The main objective of the microfluidic emulsion is to produce the micro-droplets at the desired size as rapidly as possible, which leads to soft flowing crystals, where droplets are in high concentration and in close contact with each other. Experimentally, the addition of a surfactant is necessary to prevent these closely packed droplets from merging. Numerically, the droplets in contact naturally merge when the original pseudopotential model is applied due to the absence of the repulsive force at the contacting droplet interfaces, which can mimic the effect of the surfactant. Thus, we propose a simple method to introduce the contacting interface repulsion, such that the droplets in close contact will never merge. With all these improvements, we are able to reproduce all the flow regimes observed in the experiment, especially the dense dripping regime of the soft flowing crystal.

10:50am - 11:10am

Mechanisms for various swimming patterns of a confined squirmer under gravity

Kaixuan Zheng¹, Deming Nie¹, Yuxiang Ying¹, Tongxiao Jiang¹, Jingwen Wang¹, Siwen Li¹, Jianzhong Lin²

¹China Jiliang University, Hangzhou, China; ²Zhejiang University, Hangzhou, China

The interaction between a squirmer and a nearby boundary is a well-studied phenomenon. However, the interaction between the typical distributions of squirmers in pressure regions and walls has not been studied. The kinematics of a squirmer in a two-dimensional vertical channel was studied within the framework of the squirmer model in this study. The improved bounce-back boundary and lattice-Boltzmann method were applied to implement the squirmer boundary. The sedimentation of different types of squirmers in a vertical channel of various widths and initial orientations was simulated. Four typical locomotion modes were identified based on the terminal stage of squirmer trajectories, which are related to their typical distributions of pressure regions. The way in which the torque determines the orientation of squirmers, was discussed. We proposed a correlation between the incidence angle and the locomotive mode of the squirmer.

11:10am - 11:30am

A lattice Boltzmann investigation of viscosity and wettability effects on the evolution of an attached-wall cavitation bubble

Xiaolong He¹, Haonan Peng²

¹Sichuan University, Chengdu, China; ²Laboratory for Waste Management, Paul Scherrer Institute, CH, 5232, Villigen PSI, Switzerland

The thermal lattice Boltzmann pseudo-potential model is employed to explore wall wettability and liquid viscosity effects on the evolution of an attached-wall cavitation bubble. A conversion method based on the parameters of a non-ideal equation of state and surface tension is proposed. From force analysis at the contact point, it is found that the dynamic contact angle is larger than the equilibrium contact angle throughout the evolution process for a wetting wall, which results in a hysteresis effect during the growth stage due to the unbalanced Young's force and accelerates the contact point retraction velocity in the collapse stage. For non-wetting walls, the unbalanced Young's force accelerates the expansion of the contact radius, resulting in a larger maximum contact radius than for a bubble on a wetting wall. The hysteresis effects caused by the unbalanced Young's force slow down the retraction of the contact points in the early collapse stage and accelerate the retraction in the final collapse stage because of dramatic interface deformation. The bubble is punctured over a larger volume with a non-wetting wall than with a wetting wall, resulting in a smaller collapse intensity. An exponential relationship between the microjet volume and the cosine function of the equilibrium contact angle at the collapse point is found. Furthermore, the increase in viscosity leads to a decrease in the jet volume at the collapse point and delays the collapse time. Finally, the instant dimensionless temperature distribution indicates that the wetting wall leads to a smaller dimensionless low-temperature region during the growth stage, while the high heat flux peaks are larger at the collapse point than for a non-wetting wall, which is more desirable for enhancing the heat transfer efficiency between the high-temperature fluid and low-temperature wall.

11:30am - 11:50am

The influence of particle distribution range on droplet coalescence process: A lattice Boltzmann study

Hanlin Zhou, Haihu Liu

Xi'an Jiaotong University, Xi'an, China

This study aims to investigate the dynamics of droplet coalescence with loaded particles by focusing on the impact of the distribution range of particles on the coalescence process. Numerical simulations based on the Lattice Boltzmann (LBM) color gradient model are conducted under specific conditions. The findings reveal that besides the expected hindering effect of particles on droplet deformation, the dense initial dispersion of particles surprisingly exerts a significant influence on droplet deformation and internal kinetic energy dissipation, even when no particles are present in the growth region of the liquid bridge. Moreover, it is observed that the initial range of particle distribution can alter the oscillation pattern of the droplet as the ambient viscosity increases. The steady-state time of droplets shows a decrease with dense particle dispersion at low ambient viscosities, while the opposite trend is observed at high viscosities. The increased damping ratio in droplet coalescence resulting from the range of particle distribution has a similar effect to augmenting the internal viscosity of the droplet compared to a clean droplet. Furthermore, as the contact angle changes, the particles arrange themselves differently during droplet fusion. Notably, a sharp increase in the damping effect is observed once the particles form a tightly packed arrangement. The investigation sheds light on the complex interplay between particle distribution, droplet deformation, and internal dynamics during the fusion process, providing insights into the underlying mechanisms that govern droplet-particle interactions.

11:50am - 12:10pm

DNS of cylindrical particle-laden channel turbulence using LBM and DEM

Zehua Zhang¹, Cheng Peng², Yu Guo³, Lian-Ping Wang¹

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Turbulence flows laden with non-spherical particles are widely present in natural phenomena and engineering applications, but research on such flows is still in its early stages. In this talk, we will present direct numerical simulations of the turbulent channel flow laden with cylindrical particles. The flow domain is resolved by the lattice Boltzmann method (LBM), the shape and motion of cylindrical particles are modeled using the discrete element method (DEM). The particle density is assumed to be equal to the fluid density and gravity effects are neglected. From the results gathered in three cases with cylinders of different aspect ratios, we found that the particles increase the turbulence drag. Moreover, their orientation shows large anisotropy near the channel wall. And the pattern and rate of particle rotation show distinct differences across different aspect ratios. The study provides insights into the statistical characteristics and structural features of wall-bounded turbulent flow laden with cylindrical particles.

12:10pm - 12:30pm	Closing Location: Mount Qingcheng Grand Hotel-Tianfu Hall Session Chair: Prof. Li-Shi Luo , CSRC
12:30pm - 2:00pm	Lunch