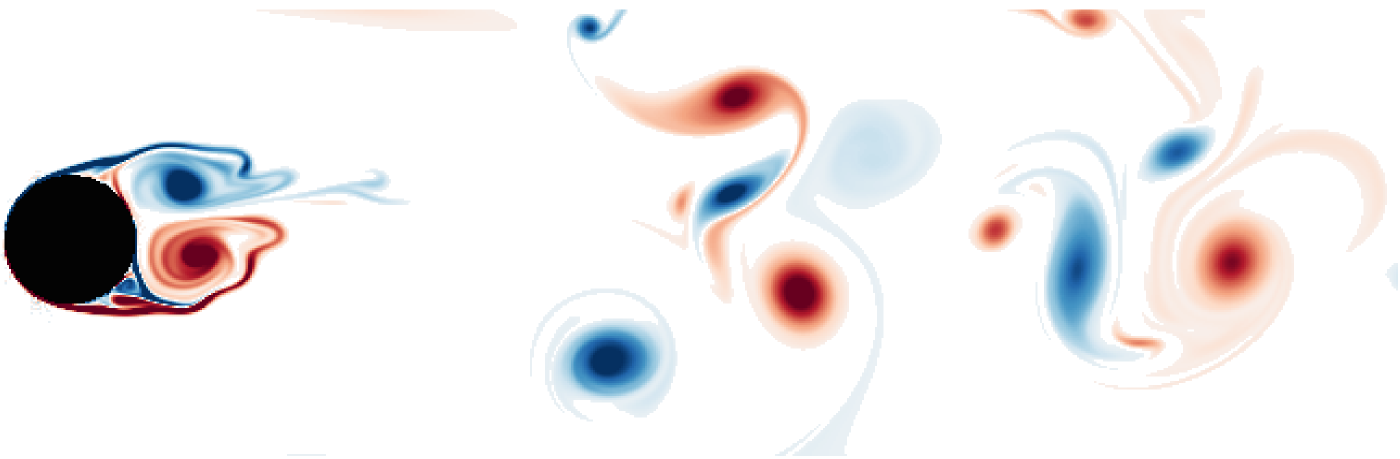
Australasian Conference on Particle Approaches and Applications in Fluids

1st - 2nd February 2024



ACKNOWLEDGEMENT OF TRADITIONAL OWNERS

QUT acknowledges the Turrbal and Yugara, as the First Nations owners of the lands where QUT now stands. We pay respect to their Elders, lores, customs and creation spirits. We recognise that these lands have always been places of teaching, research and learning.

QUT acknowledges the important role Aboriginal and Torres Strait Islander people play within the QUT community.

Queensland University of Technology

1st Australasian Conference on Particle Approaches and Applications in Fluids (ACPAAF)

Conference Booklet

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Foreword

I am pleased to welcome you to the 1st Australasian Conference on Particle Approaches and Applications in Fluids (ACPAAF) hosted by the Queensland University of Technology (QUT)!

The conference is a forum for researchers and practitioners to share their latest developments and practical applications of particle-based methods in various fields of science and engineering. Particle-based methods are becoming increasingly popular for studying fluid dynamics, particularly for simulating complex systems where traditional macroscopic methods based on continuum assumptions may not be practical. Particle methods have shown great promise in accurately simulating fluid flow in a wide range of applications, from microfluidics to macroscopic systems.

The conference brings together researchers from academia, industry, and government agencies to share their latest research findings, exchange ideas, and network with colleagues. This inaugural event includes 3 outstanding keynote speakers, 1 ECR keynote session and 31 presentations over 2 full days.

I would like to thank the Local Organising Committee for their hard work in setting up all the aspects of the conference. I also thank the invited keynote and ECR speakers as well as all the contributing authors, presenters, and participants for establishing the foundation of a long-lasting event on particle-based methods for fluid flows in the Australasia region.

The conference is organised with the support of the Australasian Fluid Mechanics Society (AFMS), the School of Mechanical, Medical and Process Engineering (MMPE) and the Laboratory for Advanced Modelling and Simulation in Engineering and Science (LAMSES) at QUT, Leap Australia, HEXAGON and SCx Solutions. Finally, we would like to thank QUT in providing access to the Science & Engineering precinct as the ideal venue for hosting the conference.

It is an honour to inaugurate this initiative and wish you all an enjoyable and fruitful stay in Brisbane and Queensland.

Emilie Sauret

Conference Chair

Organisation

QUT Organising Committee

Professor Emilie Sauret

Dr Zhongzheng Wang

Mr Jiachen Zhao

Dr Vedad Dzanic

Associate Professor David Holmes

Scientific Committee

Dr Christopher From (University of Manchester)

Dr Charith Rathnayaka (University of the Sunshine Coast)

Dr Ryan (Qiuxiang) Huang (Queensland University of Technology)

Associate Professor Fangbao Tian (University of New South Wales, Canberra)

Associate Professor Christopher Leonardi (University of Queensland)

Dr Travis Mitchell (University of Queensland)

Sponsors

Queensland University of Technology, School of School of Mechanical, Medical and Process Engineering. https://www.qut.edu.au/

Australasian Fluid Mechanics Society. https://www.afms.org.au/

Laboratory for Advanced Modelling and Simulation in Engineering and Science. https://research.qut.edu.au/lamses

LEAP Australia. https://www.leapaust.com.au/

LEAP supports local academic researchers and engineers working in industry to adopt computer-aided engineering software to optimise the performance of critical equipment and develop digital twins using Ansys simulation (incl. Fluent and Rocky DEM) as well as CAD/PLM, Internet of Things (IoT) & Augmented Reality (AR) technologies from PTC.

Hexagon. https://hexagon.com/products/product-groups/computer-aided-engineering-software/cradle-cfd

Hexagon is a leader in modelling technologies with strong academia focus. Its Cradle CFD enable users to visualise the complex gas/liquid flow to predict the products performance, particularly strong at coupled simulations.

SCx Solutions. https://scx-solutions.com/

SCx is Hexagon's partner, focusing on airflow modelling inside/outside of buildings to optimize design and operation of HVAC.

Conference Venue

The conference will be held in **QUT Gardens Point (GP) campus in P-Block room P- 419**. The registration desk will be located outside at the front of the P-Block entrance.

Program Overview

Day 1 – 1st February 2024		Day 2 – 2nd February 2024	
8:30	Registration	9:00 – 10:00	Keynote speaker presentation
9:15 - 10:15	Keynote speaker presentation	10:00 – 11:00	Session 4
10:15 – 10:45	Morning tea break	11:00 – 11:30	Morning tea break
10:45 – 12:15	Session 1	11:30 – 12:45	Session 5
12:15 – 13:15	Lunch break	12:45 – 13:45	Lunch break
13:15 – 14:15	Keynote speaker presentation	13:45 – 15:15	Invited Early Career Researcher (ECR) presentations
14:15 – 15:30	Session 2	15:15 – 16:15	Session 6
15:30 – 16:00	Afternoon tea break	16:15 – 16:45	Afternoon tea break
16:00 – 17:30	Session 3	16:45 – 17:15	Closing ceremony and awards
18:00 – 20:30	Conference dinner		

Keynote Speakers

The organising committee is pleased to welcome our invited keynote speakers:

Assoc. Prof Christophe Coreixas

University of Geneva

Christophe Coreixas is an aeronautical engineer who graduated in 2014 from ISAE-SUPAERO in Toulouse, France. His master's thesis was dedicated to evaluating the capabilities of 'ProLB', a lattice Boltzmann (LB) commercial software, for computational aeroacoustics simulations of cavity and landing gear noise emissions during the landing phase of an airplane. He obtained his Ph.D. in Fluid Dynamics from INP Toulouse while working at CERFACS from 2015 to 2018. His doctoral thesis focused on extending ProLB's capabilities for high-speed flow simulations through novel collision models and compressible LBMs. Christophe continued to broaden his horizons by joining in 2018 the Computer Science department of the University of Geneva in Switzerland. First as a PostDoc and later as a Senior Researcher, he worked on the GPU acceleration of open-source LB solvers, such as Palabos, and their application to multiphysics and biomedical fields. In early 2024, Christophe became a Research Associate Professor at the Institute of Advanced Study of UIC in Zhuhai, China. In this capacity, he develops Octree-based GPU-accelerated computational fluid dynamics solvers dedicated to the aeronautical and automotive sectors.

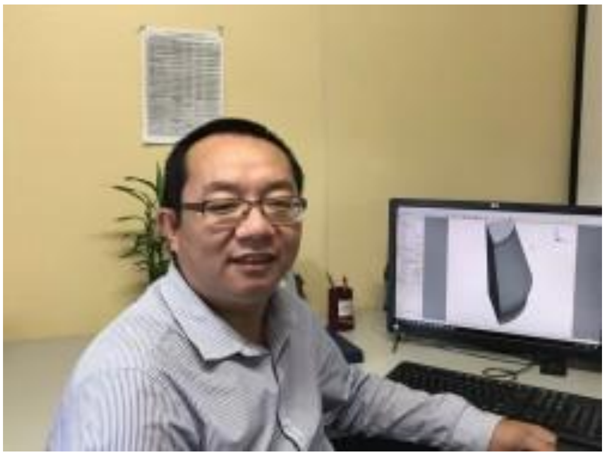
Lattice Boltzmann methods (LBMs): From fundamentals to industrial and GPU-accelerated applications.

LBMs are memory-bound which makes them particularly interesting for high-performance computing based on either CPUs or GPUs. They rely on Cartesian grids with Octree-based refinement methodologies, kinetic boundary conditions, and can easily include subgrid-scale or wall modelings to simulate overnight realistic flow conditions past complex geometries. This explains why, over the past three decades, LBMs have progressively gained recognition as promising alternatives to NSF solvers.

Nonetheless, LB solvers come with a number of practical limitations. For instance, their inherent link to non-body-fitted Octree grids poses challenges in accurately simulating wall-bounded turbulent flows without the assistance of advanced wall models. Additionally, the explicit-in-time nature of LB schemes makes them less suitable for steady-state flow simulations than time-implicit NSF solvers.

The purpose of this presentation is to provide essential insights into understanding the strengths and limitations of LBMs. Additionally, it will provide an overview of their applications across various industrial sectors (automotive, aeronautics, wind energy, oil & gas, etc). Special attention will also be devoted to the GPU acceleration of LBMs, which has the potential to significantly reduce their computational costs and energy consumption.

Keynote Speakers



Dr Shibo Kuang

Monash University

Dr. Shibo Kuang currently holds the position of Senior Research Fellow at Monash University within the ARC Research Hub for Smart Process Design and Control, where he leads one of the five primary research areas. His research primarily focuses on computational process engineering, with the goal of advancing our understanding and control of multiphase transportation and processes. This research encompasses fundamental elucidation, theory and method development, exploration of new technologies, and process optimization. Dr. Kuang's approach involves the development and application of mechanistic models and data-driven AI models. The key research areas he covers include particle transportation, particle separation, and multiphase reacting flows. Through his work, Dr. Kuang has authored over 140 papers, with more than 120 of them indexed by ISI Web of Science. He has been invited to present over 30 lectures, including 15 keynote and plenary speeches, at international venues. Additionally, he holds the position of an editorial board member for Metallurgical and Materials Transactions B and plays a role equivalent to that of an associate editor.

Multiscale analysis of non-Newtonian suspension flows

Non-Newtonian fluid suspensions are common in both natural phenomena and various industrial applications. Despite their prevalence, our understanding of these complex flow systems remains limited. As a result, there is a significant lack of comprehensive constitutive relationships to effectively describe essential aspects of non-Newtonian suspension flows, including particle-fluid interactions, fluid rheology, and fluid turbulence. This knowledge gap poses challenges for scaling, designing, controlling, and optimizing flow systems for diverse applications. To bridge this knowledge gap, we have developed and validated models based on the Discrete Element Method (DEM) to study non-Newtonian fluid suspension flows. Our approach combines numerical simulations with physical laboratory experiments. In this modelling framework, particle motion is described using DEM, while non-Newtonian fluid flow is analysed using either the Lattice Boltzmann method or the finite volume method, each with its specific rheological models. We also employ both resolved and unresolved methods for modelling particle-fluid interactions. The resolved method directly simulates these interactions, while the unresolved method relies on specific correlations. To demonstrate the practical applicability of these developments, we explore applications such as mine tailing management, sewage treatment, and sand retention.

Keynote Speakers

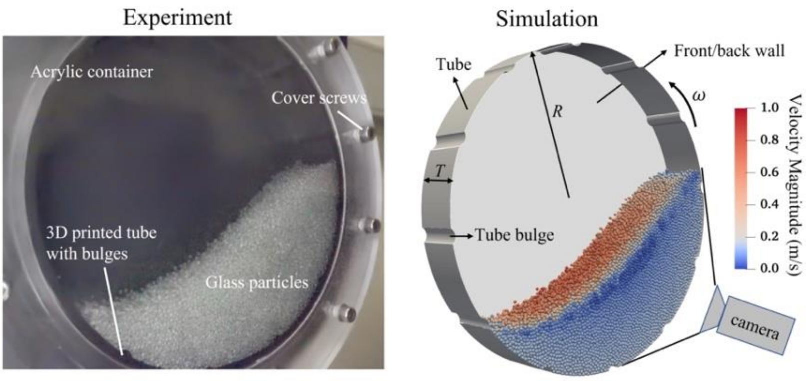
A/Prof Yixiang Gan

The University of Sydney

Dr Yixiang Gan is currently Associate Professor and Associate Head of School (External Engagement) at the School of Civil Engineering and Deputy Director of Sydney Nano Institute, The University of Sydney, Australia. He received his Dr.-Ing (with summa cum laude) from Karlsruhe Institute of Technology, Germany. After joining The University in 2010, he has been developing his research group with unique data-driven modelling and experimental capabilities to optimise engineering solutions for energy storage. His research contains a balance between engineering applications addressing grand challenges and curiosity-driven topics transforming fundamental understanding. He has been an active researcher in the mechanics and physics of granular materials from microstructure-informed approaches. His research areas include mechanics of granular and porous media, mechanics of interfaces, and energy geotechnics. He was a recipient of ARC Discovery Early Career Researcher Award (DECRA), SOAR Fellowship, and Endeavour Leadership Awards.

Granular Flow in a Rotating Drum from Dry, Partially Saturated to Submerged Conditions

Granular flows are common in various natural and industrial processes, such as landslides, mineral handling, and food processing. We investigated rheological and segregation behaviour of granular media in a rotating drum, which exhibits dependency on interstitial fluids. From dry, partially saturated to submerged conditions, we conduct experiments and numerical simulations to study granular flows in rotating drums. For modelling the granular systems, we employed the discrete element method (DEM), volume of fluids (VOF) and CFD-DEM methods for respective conditions. For fully dry or wet (submerged) conditions, VOF and CFD-DEM results show excellent match with experimental observations from mono- and binary systems, whilst revealing the internal dynamics, such as shear zones and pore pressure. In partially saturated conditions, we focus on varying the strength of cohesion (surface tension) and rotation rate within the modes of rolling flow and cascading flow. We extract statistical information on the formation of clusters within the flow and find a power law relation between the cluster size distribution and its probability, which indicates that stronger cohesion can promote the formation of larger clusters. Finally, we will discuss how intestinal fluids impact on the flow and segregation of granular media and its implications on industrial processes.



Invited Early Career Researcher (ECR) Speakers

The organising committee is delighted to welcome our invited Early Career Researchers (ECR):

Dr. Xinying Liu (University of Sydney)

Model validation on peristalsis and application to gastric mixing using smoothed particle hydrodynamics.

Dr. Liu is a Research Associate at the School of Chemical and Biomolecular Engineering, University of Sydney, specializing in Computational Fluid Dynamics (CFD), Fluid-Structure Interaction (FSI), and multiphysics simulation for biomedical engineering problems. Her research focuses on revolutionizing healthcare technologies and improving patient outcomes by developing advanced modelling and simulation techniques for complex fluid systems. With expertise in cardiovascular hydrodynamics and gastric flow systems, she contributes to a deeper understanding of physiological processes and the development of innovative medical treatments.

Dr Charith Rathnayaka (University of the Sunshine Coast)

New horizons for smoothed particle hydrodynamics and coarse-grained approaches for multiphase phenomena, multiphysics and morphological characteristics associated with soft matter.

Dr Charith Rathnayaka is currently a Lecturer in the School of Science, Technology and Engineering at University of the Sunshine Coast (UniSC) and a Senior Fellow of the Higher Education Academy (SFHEA). Charith's research vision is to explore sustainable solutions to the grand challenges of food security and climate change through transdisciplinary research in the domains of computational mechanics, machine learning and food engineering. In a broader scale, his work focuses on developing and understanding environmentally, technically and economically sustainable processes for food, energy and power, which are all critical for our civilisation and survival. In doing so, Charith utilises state-of-the-art computational modelling and experimental techniques with the aid of High-Performance Computing (HPC).

Dr Methma Rajamuni (UNSW Canberra)

An immersed boundary-regularised lattice Boltzmann method for acoustic simulations of fluid-structure interaction (FSI) problems

Dr Methma Rajamuni is a Research Scientist, Applied Mathematician, and Mechanical Engineer with expertise in computational fluid dynamics, numerical analysis, systems and control, and optimization. Her research interests are ember storm modelling, fluid-structure interaction, bluff-body aerodynamics, wake stability and control, numerical methods, bio-mathematics, bio-mechanics and environmental flows. Methma received her PhD in Engineering from Monash University, Australia and her MSc by research in Applied Mathematics from Texas Tech University, the USA. She is a passionate tertiary lecturer in Mechanical & Aerospace Engineering, Mathematics and Statistics, with more than 10 years of experience.

Detailed Program

1st February 2024	
8:30	**Registration**
9:00-9:15	**Welcome & Introduction**
9:15 - 10:15	**Keynote I, Dr Christophe Coreixas** **Chair**: Prof Emilie Sauret **Lattice Boltzmann methods (LBMs): From fundamentals to industrial and GPU-accelerated applications.**
10:15 – 10:45	Morning tea break
10:45 – 12:15 Session 1 **Chair**: Dr Christophe Coreixas	**IB-LBM for high Reynolds numbers** Li Wang, Fang-Bao Tian*
	Study of Film Dynamics Over a Planar and Topographical Surface Using Lattice Boltzmann Method Garima Singh*, Naveen Tiwari
	Solid-liquid phase transition under hypergravity Yinnan Zhang*, Chaofeng Lu, Emilie Sauret, Yuantong Gu
	Towards Optimal Accuracy and Efficiency in Lattice Boltzmann Simulations of Multiphase Flows in Rough Fractures Dmytro Sashko*, Travis Mitchell, Lukasz Laniewski-Wołłk, Christopher Leonardi
	Investigation on electrohydrodynamic suppression of viscous fingering using a hybrid lattice Boltzmann and finite difference method Jiachen Zhao*, Zhongzheng Wang, Emilie Sauret
	A simple and efficient LBM-based (bush)fire model using volumetric heating source Seyed Mohsen Hashem Zadeh, Li Wang, John Young, Fang-Bao Tian*
12:15 – 13:15	Lunch break
13:15 – 14:15	**Keynote II, Dr Shibo Kuang** **Chair**: Assoc Prof Yixiang Gan **Multiscale analysis of non-Newtonian suspension flows**
14:15 – 15:30 Session 2 **Chair**: Dr Charith Rathnayaka	**Efficient multiphysics computations on modern GPU-based architectures using Lattice Boltzmann Method coupled with Discrete Element Method** Lukasz Laniewski-Wołłk*
	Large-scale handling and transportation simulations of granular materials in the GPU-DEM framework Patricio Jacobs-Capdeville*, Shibo Kuang, Aibing Yu

	Arbitrary grid implementation of the LBM on GPU for efficient simulation of microporous structures Travis Mitchell*, Jakub Gałecki, Łukasz Łaniewski-Wołłk
	Developing a Physics-Informed Machine Learning (PIML) Predictive Framework for Pollutant Dispersion in the Atmosphere P.G.K.B. Ranathunga*, Y.T. Gu, C.M. Rathnayaka
	Physics-informed data-driven RANS turbulence modelling for particle-laden jet flows with various Stokes numbers Xinchen Zhang*, Zhen Zhang, Alfonso Chinnici, Zhiwei Sun, Javen Qinfeng Shi, Graham J. Nathan, Rey C. Chin
15:30 – 16:00	Afternoon tea break
16:00 – 17:30 Session 3 **Chair**: Assoc Prof Christopher Leonardi	**LBM-DEM simulation of the flow of particle suspensions through rough, narrow fractures** Lukasz Laniewski-Wołłk, Nathan J. Di Vaira, Christopher R. Leonardi*
	In Silico Exploration of Binary Packed Beds: Coupled CFD-DEM Analysis of Thermofluidic Characteristics Angelo Christakakis*, Lewis Clark, David Fletcher, Nish Joseph
	Effect of particle shape on tribocharging in pneumatic conveying Fayuan Huang*, Shibo Kuang, Ruiping Zou, Aibing Yu
	Particle-resolved simulations of the interaction between turbulent flow and subaqueous bedforms Aman G. Kidanemariam*, Markus Uhlmann
	Shear Induced Lift and Rotation on MicroFiber Deposition in Low Reynolds Number Flows Lin Tian*, Jiang Li
	Aerosol extraction from inkjet print-zones S. G. Mallinson*, G. LLanes, A.F.V. de A. Aquino, T.J. Barber, C.M. de Silva
18:00 – 20:30	**Conference dinner** **Restaurant**: Ahmet's Turkish Restaurant **Address**: 10/168 Grey St, South Brisbane, QLD 4101

Detailed Program

2nd February 2024	
9:00 – 10:00	**Keynote III, Assoc Prof Yixiang Gan** **Chair**: Dr Shibo Kuang **Granular Flow in a Rotating Drum from Dry, Partially Saturated to Submerged Conditions**
10:00 – 11:00 Session 4 **Chair**: Dr Qiuxiang Ryan Huang	**Revised Macroscopic and Mesoscopic Models for Convective Transport in Newtonian and Non-Newtonian Nanofluids** Gholamreza Kefayati*
	Development and validation of a phase-field lattice Boltzmann method for non-Newtonian Herschel-Bulkley fluids in three dimensions Bryce Hill*, Travis Mitchell, Łukasz Łaniewski-Wołłk, Christopher Leonardi, Saiied Aminossadati
	Simulating Bingham Plastics in a Cavity: Integrating Internal and External Natural Convection with Lattice Boltzmann Method Gholamreza Kefayati*
	Influence of plasticity on inertialess viscoelastic instabilities using a hybrid lattice Boltzmann model Vedad Dzanic*, Christopher Soriano From, Emilie Sauret
11:00 – 11:30	Morning tea break
11:30 – 12:45 Session 5 **Chair**: Dr Methma Rajamuni	**Resolving bubble dynamics in molten media bubble columns using a phase-field lattice Boltzmann model** Nicholas Paraskevas*, Travis Mitchell
	Computing sessile droplet shapes on arbitrary surfaces with a new pairwise force smoothed particle hydrodynamics model Riley M Whebell*, Timothy J Moroney, Ian W Turner, Ravindra Pethiyagoda, Scott W McCue
	Enhancement of the flow boiling heat transfer in microchannels by a Flow-induced vibrating cylinder Mohammed Fouad Kamel Ibrahim*, Methma Rajamuni, Li Chen, John Young, Fangbao Tian
	Immersed boundary method and its applications for the fluid-structure interaction in blood flow and insect flight

	Qiuxiang Ryan Huang*, Jingtao Ma, Zhengliang Liu, Li Wang, FangBao Tian, Zhiyong Li
	Effects of bio-inspired flaps on the aerodynamics of an airfoil Mohammad Ghaffari*, Sridhar Ravi, John Young, Joseph C.S. Lai, Fang-Bao Tian
12:45 – 13:45	Lunch break
13:45 – 15:15 **Chair**: Dr Zhongzheng Wang	**ECR Keynote I, Dr Xinying Liu** **Model validation on peristalsis and application to gastric mixing using smoothed particle hydrodynamics**
	ECR Keynote II, Dr Charith Rathnayaka **New horizons for smoothed particle hydrodynamics and coarse-grained approaches for multiphase phenomena, multiphysics and morphological characteristics associated with soft matter**
	ECR Keynote III, Dr Methma Rajamuni **An immersed boundary-regularised lattice Boltzmann method for acoustic simulations of fluid-structure interaction (FSI) problems**
15:15 – 16:15 Session 6 **Chair**: Dr Xinying Liu	**CFD modelling of mixing zone during extracorporeal membrane oxygenation (ECMO) treatment** Dhayananth Kanagarajan*, Van Dau, Jo Pauls, John Fraser, Geoff Tansley
	Viscoelastic Fluids-based Microfluidic Devices and Applications Dan Yuan*
	Stretchable Microfluidics for cell manipulation and separation Jun Zhang*, Hedieh Fallahia, Hang Thu Ta, Nam-Trung Nguyen
	Microflows in alveolar cells Jun Dong, Huimin Lv, Yue Yang, Yonggang Zhu*
16:15 – 16:45	Afternoon tea break
16:45 – 17:15	Closing ceremony and awards

IB-LBM for high Reynolds numbers

Li Wang [1], Fang-Bao Tian [1]

[1] SET, UNSW Canberra

This work presents our recent work on the immersed boundary-lattice Boltzmann method (IB-LBM) for high Reynolds number flows involving complex geometries. The IB-LBM is based on lattice-Boltzmann method (LBM) considering incompressible or weakly compressible flows, with immersed boundary method (IBM) for implementing the velocity boundary conditions at the fluid-structure interface. Three collision models, i.e., single relaxation time (SRT), multi-relaxation time (MRT) and recursive regularized (RR) collision models are implemented. For high Reynolds number turbulence flows, the wall modelled large eddy simulation (WMLES) is incorporated with the feedback IBM. To improve the computational efficiency involving complex moving structures, a multi-block geometry-adaptive mesh strategy with dynamically updated features is also implemented. A few validation cases will be presented.

Study of Film Dynamics Over a Planar and Topographical Surface Using Lattice Boltzmann Method

Garima Singh [1], Naveen Tiwari [1]

[1] Indian Institute of Technology Kanpur, India

In this work, the dynamics of a spreading liquid film on a planar and topographical substrate are numerically modeled using the phase-field lattice Boltzmann approach (PFLBM). A two-phase interface is inherently mesoscopic in nature, making the PFLBM a suitable technique for modeling. Interfacial patterns generated using PFLBM perfectly match the experimental and analytical results obtained within the lubrication assumption. PFLBM simulations uncovered that steady-state solutions are not possible for large topographies and the fluid-fluid interface results in a series of droplets, leaving the topographical feature in the downstream direction. A decrease in viscosity ratio (bottom to top fluid) increases the height of the capillary ridge formed, making the film more prone to instability. We also explore the effect of multiple obstacles on the capillary ridges formed by each and obtain the condition of independent obstacles. Finally, a detailed analysis will be presented for the effect of aspect ratio (film thickness away from contact point versus capillary length) on planar surfaces with contact-line spreading. Our study unveils that at a critical value of the aspect ratio, the maximum value of dimensionless capillary ridge height reaches unity, and this critical value is found to be independent of the inclination angle. On further increasing the value of this parameter, a nose-like structure appears near the contact point, which is strongly dependent on contact angle values.

Solid-liquid phase transition under hypergravity

Yinnan Zhang [1,2], Chaofeng Lu [1,3], Emilie Sauret [2], Yuantong Gu [2]

[1] College of Civil Engineering and Architecture, Zhejiang University, Hangzhou 310058, P. R. China.

[2] School of Mechanical, Medical and Process Engineering, Queensland University of Technology, Brisbane, QLD 4000, Australia.

[3] Center for Mechanics Plus under Extreme Environment, Ningbo University, Ningbo 315211, P. R. China.

The solid-liquid phase change under hypergravity can be widely found in the manufacture of high-performance materials, substance extraction from solutions, and laboratory experiments based on the scaling laws of hypergravity. Various experiments have shown that the morphology of the solid phase will be significantly influenced by the gravity level and direction. However, the effects of hypergravity have not yet been revealed theoretically.

This work aims to incorporate hypergravity effects into the two-dimensional cavity freezing/melting process, analyze the fluid motion and temperature transfer characteristics, examine the evolution of the solid-liquid interface under hypergravity, and set up the scaling law of hypergravity for this phenomenon. The governing equations that couple the fluid field, temperature field and gravity field are formulated. We use the lattice Boltzmann method to simulate this process, and an enthalpy-based method is employed to induce heat release and absorption when phase transition occurs and separate the solid and liquid regions. Results show that the effects of hypergravity include enhancing the flow, promoting the solidification process, and altering the shape of the solid-liquid interface. The increasing gravity leads to a corresponding rise in buoyancy-driven force, thereby enhancing fluid flow and heat transfer. Consequently, stronger gravity causes the solid-liquid interface to evolve more quickly. Moreover, the scaling laws of hypergravity can be defined such that when the length scale decreases by a factor of n, gravity needs to increase by n cubed to maintain the same average solid-liquid interface. This work will benefit the application of hypergravity in manufacturing, providing theoretical support for material preparation under hypergravity. Furthermore, the scaling laws can be applied in small-scale lab experiments to mimic large-scale solid-liquid phase transitions and help determine the selection of experimental parameters.

Towards Optimal Accuracy and Efficiency in Lattice Boltzmann Simulations of Multiphase Flows in Rough Fractures

Dmytro Sashko [1], Travis Mitchell [1], Lukasz Laniewski-Wołłk [1,2], Christopher Leonardi [1]

[1] School of Mechanical and Mining Engineering, The University of Queensland

[2] Institute of Aeronautics and Applied Mechanics, Warsaw University of Technology

In the field of natural gas production, understanding the impact of fracture geometry, such as roughness, surface correlation, and aperture size, on hydraulic properties during multiphase flows is crucial for estimating production rate. The randomness and complexity of fracture surfaces make the application of traditional numerical modelling approaches challenging. The lattice Boltzmann method (LBM) is a potential alternative, due to its inherent parallelism and simplicity in treating complex boundaries. Recent developments in multiphase LBM models, such as phase-field methods, allow for simulating flows with large density and viscosity contrast, commonly occurring during natural gas extraction.

On naturally curved fracture surfaces, the proper implementation of the wetting boundary conditions and specifying appropriate mesh resolution have a critical effect on the flow behaviour. Two common approaches for wetting boundary conditions both require non-local data access, thus impacting the performance of the solver. Mitigating the negative effects of the staircase approximation on curved fracture surfaces can further decrease the computational speed.

This research investigates an optimal balance between solver accuracy and efficiency on a wide range of fracture geometries and flow parameters. We apply several variants of the wetting boundary conditions to multiphase flows in rough fractures using phase-field LBM, and additionally study the impact of mesh resolution and staircase approximation. The obtained computational setup can be used to obtain new insights into two-phase flows in rough fractures through large-scale stochastic studies.

Investigation on electrohydrodynamic suppression of viscous fingering using a hybrid lattice Boltzmann and finite difference method

Jiachen Zhao [1], Zhongzheng Wang [1], Emilie Sauret [1]

[1] School of Mechanical, Medical and Process Engineering, Faculty of Engineering, Queensland University of Technology, QLD 4001, Australia

Viscous fingering is a widely observed interfacial instability in multicomponent fluid flow, where a finger-like shape is formed when a more viscous fluid is displaced by a less viscous fluid. In many practical applications, viscous fingering is undesirable. For example, the efficiency of enhanced oil recovery by water flooding is dramatically decreased due to viscous fingering, causing a significant amount of oil to be trapped underground. Similarly, this interfacial instability also drastically affects the displacement efficiency of geological CO_2 sequestration. Here, we study the influence of an electric field on the viscous fingering of perfect dielectric fluids by using the hybrid lattice Boltzmann method (LBM) and finite difference method (FDM). It is shown that the development of viscous fingering can be delayed under a horizontal electric field and completely suppressed when the electric field strength exceeds a certain value. Based on the force balance, a non-dimensional parameter ϕ is defined to reflect the relative importance of stabilising and destabilising stress by taking into account the electrical, capillary, and viscous stress on the fluid interface. Results from extensive simulations show that under different fluid properties and flow conditions, ϕ can well characterise the transition of viscous fingering from unstable to stable regime.

A simple and efficient LBM-based (bush)fire model using volumetric heating source

Seyed Mohsen Hashem Zadeh [1], Li Wang [1], John Young [1], Fang-Bao Tian [1]

[1] School of Engineering and Technology, University of New South Wales, Canberra, ACT 2600, Australia

To study the role of bushfires-enhanced wind load on structures, a simple fire model, known as the volumetric heating source (VHS) model has been incorporated in a hybrid finite difference method-lattice Boltzmann method (FDM-LBM). Despite its simplicity, the model was found in excellent agreement with the experimental studies of indoor and outdoor fires. The model also shows superior efficiency compared to combustion-based fire models.

Efficient multiphysics computations on odern GPU-based architectures using Lattice Boltzmann Method coupled with Discrete Element Method

Lukasz Laniewski-Wołłk [1,2]

[1] School of Mechanical and Mining Engineering, The University of Queensland

[2] Faculty of Power and Aeronautical Engineering, Warsaw University of Technology

Over the past three decades, the lattice Boltzmann method (LBM) has emerged as an important part of the landscape of numerical methods employed for computational fluid dynamics (CFD). The fine mesh and relatively inexpensive explicit iterative scheme makes it a perfect candidate for highly resolved computation of single- and multi-component flows in complex geometries. To fully realise the benefits offered by the LBM, it is imperative to employ efficient parallel implementation of the computations, lest the required grid size and number of iterations become intractable.

This presentation will introduce the open-source LBM solver, TCLB, which allows for efficient execution of any explicit LBM or finite difference scheme on modern GPU architectures. The solver was designed to provide a simple interface for implementation and testing of new physics models, while simultaneously offering highly-parallel execution on high-performance computing (HPC) infrastructure. To maximise performance, the code uses CUDA on nVidia GPUs, HIP on AMD GPUs, and OpenMP when executed on CPUs (achieving the inter-node communication via MPI). Furthermore, the solver is coupled with a number of discrete element method (DEM) solvers, such as LIGGGHTS and ESyS-Particle.

This presentation will also detail recent improvements of TCLB, and associated performance tests, completed in cooperation with the Pawsey Supercomputing Centre as a part of a Pawsey Centre for Extreme Scale Readiness (PaCER) project. These include the improved particle indexing for DEM-LBM coupling, improved branching in the GPU code, and the lessons learned while porting the TCLB codebase to AMD GPUs on the largest HPC system in Australia, Setonix.

Large-scale handling and transportation simulations of granular materials in the GPU-DEM framework.

Patricio Jacobs-Capdeville [1,2], Shibo Kuang [1], Aibing Yu [1]

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Handling and transportation processes of granular materials are crucial in various engineering fields such as agricultural, pharmaceutical, and mining industries. The flow behaviour of grains plays a key role in the performance of such processes. Thus, the understanding of the mechanical properties of granular assemblies is of paramount importance for the optimal performance and design of handling and transportation equipment. The discrete element method (DEM) is a powerful particle-scale modelling technique that has been widely applied to study the mechanical behaviour of granular materials. In DEM, individual particles are explicitly modelled, and their interactions with surrounding particles and handling equipment walls can be traced spatially and temporally. Despite its suitability for modelling granular flows, the DEM is computationally expensive, and simulating large-scale systems can be prohibitive for industrial applications. The adoption of high-performance computing technologies such as the graphical processing unit (GPU) parallelization model for DEM, poses a potential solution to upscale particle method simulations. This talk will present the development of our in-house GPU-DEM simulator and its application to industrial-scale handling and transportation processes in the ironmaking industry. The model can significantly improve the computation time of DEM simulations, up to 70 times faster compared to the CPU counterpart. Additionally, it allows the consideration of wide particle size distributions, as well as modelling various aspects of particle-wise interactions such as particle breakage, wear of equipment walls and energy consumption. The model is applied to simulate polydisperse granular materials and evaluate the effects of the mixture composition, equipment geometrical properties and operational parameters in hoppers, transfer chutes and the full model of the blast furnace charging system. The full model includes the surge hopper charging, belt conveyor and chute transfer to the parallel hoppers and the discharge to the rotating chute into the blast furnace throat.

Arbitrary grid implementation of the LBM on GPU for efficient simulation of microporous structures

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Microporous electrodes play a critical role in various energy storage and conversion systems. In particular, gas diffusion electrodes (GDE) facilitate rapid mass transfer enabling technologies such as polymer electrolyte membrane fuel cells (PEMFC), and are currently being studied for carbon dioxide (CO2) electrolysis to produce value-added chemicals and fuels from captured CO2. Yet, the transport phenomena of reactants and products in GDEs is not well understood and hard to probe experimentally. The complex structural morphologies of GDEs present significant challenges in the simulation for conventional computational fluid dynamics due to infeasible meshing requirements. Lattice Boltzmann methods are well suited to simulate flow through complex geometries but are often implemented on large, structural Cartesian grids, encompassing the whole flow domain. For simulations of flow through complex geometries, or materials with low porosity, this can result in wasted computational effort and memory usage in non-fluid regions.

This research aims to facilitate the efficient simulation of microporous electrodes by developing an alternative lattice implementation for the open-source code, TCLB. The new structure, called arbitrary grid, will allow the user to run existing model kernels without modification, on complex unstructured meshes with arbitrary connectivity. The newly implemented data structure was designed to achieve high efficiency on modern accelerator hardware (GPUs), which have wide memory buses and SIMD groups. At the cost of a moderate increase in per-node memory bandwidth requirements, the arbitrary grid formulation limits the computational domain to the physical region of interest. Comparative analyses with traditional methods showcased significant reduction in computational time and required memory resources, especially in simulating highly complex microporous electrodes. The arbitrary grid extension to the TCLB code streamlines simulation processes and opens new horizons for exploring transport behaviour in microporous materials for various energy applications, promising advancements in energy storage, electrolysis, and beyond.

Developing a Physics-Informed Machine Learning (PIML) Predictive Framework for Pollutant Dispersion in the Atmosphere

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Background

Air pollution has major adverse effects on health and climate. Air pollutant concentration can exhibit significant fluctuations over short spatial distances due to unevenly spread emission sources, meteorological conditions, physical characteristics of pollutants, particles and chemical processes. The increasing concern over atmospheric pollution demands strong predictive models for pollutant dispersion. Traditional models including mechanism-based methods, statistics-based machine learning methods and even chemical transport models often face limitations in capturing complex atmospheric dynamics accurately. Air pollution prediction with Physics Informed Machine Learning (PIML) show potential in overcoming these challenges by combining data-driven techniques with a strong foundation in physics.

Objectives

The primary objective of the research is developing a comprehensive PIML model for simulating air pollutant dispersion and transport. A secondary objective involves enhancing accuracy and applicability of the developed PIML model by incorporating real world data sources.

Methods

The first phase of the methodology involves leveraging advection-diffusion equations as the governing equation, utilizing the Eulerian method to predict pollutant concentrations spatially. By incorporating physical constraints into the learning process, the models will better capture the underlying dynamics of atmospheric pollutant dispersion.

Expected Results

Expected results anticipate a significant advancement in predictive accuracy for spatial distributions for air pollutants compared to traditional machine learning models.

Significance and Impact

The integration of advection-diffusion equation with PIML represents a significant advancement as a predictive model for atmospheric dispersion. This potentially ground-breaking approach holds promise for further refining atmospheric pollutant dispersion predictions.

Physics-informed data-driven RANS turbulence modelling for particle-laden jet flows with various Stokes numbers

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In this study, with the assistance of deep learning (DL), we present a framework for augmenting turbulence models in unsteady Reynolds-averaged Navier–Stokes (URANS) simulations for particle-laden flows. A complete workflow is illustrated from the identification of input flow and particle quantities to the final prediction of the instantaneous flow and particle fields. The framework incorporates a deep neural network model into the momentum equations of the Euler–Lagrangian gas–solid flow system. A data-driven, physics-informed DL approach is employed to predict the turbulent eddy viscosity fields for URANS, which are formulated as functions of the instantaneous flow quantities. In the training stage, such eddy viscosity functions are trained by an existing high-fidelity direct numerical simulation database. In the predicting stage, the trained model is then used to predict the instantaneous local eddy viscosity to update the closure term and to solve the URANS equation and particle equation of motions in an iterative manner.

Assessments of the model are performed for a series of round turbulent particle-laden co-flow jets with various Stokes numbers on the order of 0.1 to 10 to represent practical computational fluid dynamics applications. For the URANS of such inhomogeneous and multiphase flows, the proper input flow features (i.e., the instantaneous flow and particle quantities) and the effective form of the closure term (i.e., the turbulent eddy viscosity) are discussed to identify the suitable input and target variables for the DL model. In such an identification process, the physical domain knowledge is taken into account to establish a proper regression system. Finally, a posteriori tests were conducted using the same conditions as the training data set and those outside the range of conditions employed for training to evaluate the performance and robustness of the DL-URANS framework.

LBM-DEM simulation of the flow of particle suspensions through rough, narrow fractures

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The flow of particle suspensions through narrow and uneven slots is an important component of many engineering and scientific problems. One example is the propagation of proppant particles through natural and induced rock fractures. The proppant particles are injected to improve the permeability of the rock matrix after depressurisation and their even distribution in the complex fracture network is crucial to successful deployment.

To simulate this propagation at large-scales, one needs accurate knowledge of the behaviour of such suspensions at the fracture scale. To achieve this knowledge, we employ a computational methodology based on the coupling of the lattice Boltzmann Method (LBM) for the simulation of fluid flow with the

discrete element method (DEM) for the integration of the equations of motion of the particles. The resulting computational framework is applied to execute highly-resolved simulations of particle laden flows in small cells of random, rough fractures, providing data for the fracture network scale models. The fracture geometries themselves are generated using a statistical description fitted to data acquired from real rough surfaces of coal samples.

This presentation will detail the employed methodology and the new insights into fracture flows that can be gained through such simulations. It will also introduce the workflow management system, Snakemake, which was used to manage the large number of interdependent computation steps that are needed to collate the presented data.

In Silico Exploration of Binary Packed Beds: Coupled CFD-DEM Analysis of Thermofluidic Characteristics

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Packed beds are ubiquitous in the processing industry, with a wide variety of applications. Typically used for the large-scale manufacturing and treatment of chemicals, packed beds are an integral component in blast furnaces, distilleries, catalyzers, and chemical looping systems, among others. Historically, efforts have been put towards the estimation, through empirical correlations, of pressure drop and permeability, residence time, as well as mass and heat transfer characteristics. The accuracy of such models being critical to the optimal design of packed bed systems. Over time, the continual increases in available computational power, has allowed for the extension upon the capabilities of traditional analytical representations of multiphase systems, through the utilization of numerical approaches. In particular, coupling between Finite Volume-based Computational Fluid Dynamics (CFD) and Discrete Element Method (DEM) solvers have been successfully applied to study systems of both fluids and dispersed solids. However, studies on thermofluidic analyses of packed bed systems which utilize the coupled CFD-DEM approach are relatively scarce, particularly for those which include beds of heterogeneously sized particles. In this work, an existing CFD-DEM coupling strategy, based on a porous media approach, is utilized to extract packing performance, heat extraction behaviour, and flow characteristics through a binary packed bed, with varying size ratio. Further, the computational model is validated against the Ergun equation for a monospherical case. Finally, the CFD-DEM results are compared against prior experimental and computational work, for both homogenous and binary packed spherical beds.

Effect of particle shape on tribocharging in pneumatic conveying

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The tribocharging phenomenon in the pneumatic conveying process, arising from repeated particle-particle and particle-wall interactions, can lead to numerous issues, including particle clustering, adhesion to pipe walls, and potentially even fires and explosions. This phenomenon is greatly influenced by the particle shape. Until now, challenges persist in investigating tribocharging behaviour during pneumatic conveying, particularly when dealing with particles of various shapes, due to equipment limitations and the absence of numerical models. This study offers a numerical investigation of the tribocharging process by employing particles with different shapes during pneumatic conveying, accomplished by integrating computational fluid dynamics (CFD) and the discrete element method (DEM). The condenser model considering the frictional charge is incorporated into an in-house CFD-DEM model developed through continuous efforts. This model takes into account impact charge, frictional charge, and electrostatic interactions between the pipe wall and particles of varying shapes. It is firstly validated by comparing the simulation results with the specific charge measurements in different applications. The model is then used to investigate particle tribocharging behaviour under various particle shapes, gas velocities, solid concentrations, and pipe orientations and geometries. The cumulative charge and its effect on the performance of pneumatic conveying are investigated, and the effect of particle tribocharging on pipe wall wear is quantified. Furthermore, the flow characteristics are analysed to understand the charging phenomena of particles of different shapes. This study highlights the substantial effect of tribocharging in pneumatic conveying and provides insights into optimizing pneumatic conveying systems to mitigate these effects.

Particle-resolved simulations of the interaction between turbulent flow and subaqueous bedforms

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When a body of water flows over a sediment bed, erosion takes place which over time leads to a change in the morphology of the bed itself. Once the motion of sediment particles is initiated, a complex interplay between the grains and the carrier fluid ensues which often results in the formation of bedforms. An accurate prediction of the formation process is highly important from an environmental or engineering point of view. The aim of our work is to contribute to the understanding of the complex fluid-sediment interaction processes, and the mechanisms involved, at the grain level. To this end, we have numerically investigated the phenomenon in an open-channel flow configuration involving a thick, freely evolving, subaqueous sediment bed. The fluid-solid interaction has been faithfully accounted for via particle-resolved direct numerical simulations, while the sediment bed has been represented by a large number of mobile finite-size spherical particles. The numerical method used to carry out the simulations is based upon the immersed boundary technique for the treatment of the fluid-solid interactions, while the inter-particle collision process is described via a discrete element model based on the soft-sphere approach. Based on the information gained from these unique simulations, we will present key aspects of the mutual interaction mechanisms between the shearing flow and the evolving sediment bed. Specifically, we will discuss in detail the spatio-temporal correlation of the boundary shear stress and the particle flow rate, which is an essential ingredient of many sediment transport models.

Shear Induced Lift and Rotation on MicroFiber Deposition in Low Reynolds Number Flows

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Lateral migration is of significant importance to fiber deposition in wall-bounded flows, especially when there is an absence of other active external physical transport mechanisms in the process. Due to great technical difficulty, investigation on this phenomenon is limited to fundamentals of theoretical and experimental derivation, and the implication to particle deposition has not been fully explored. To fill the gap, this study investigated the shear induced lift and rotation on microfiber transport and deposition in low Reynolds number flows. Transport and deposition of non-neutrally buoyant ellipsoidal fibers in Poiseuille flow in horizontal and vertical channels is systematically examined numerically, and the various lateral migration scenarios are carefully investigated. It was found out that, in absence of the sideway gravity, shear induced lift and rotation cause the fibers to drift across the main streamlines in the vertical channel. This lateral movement is either the driving force for fiber deposition in a downward flow, or it pushes the particles toward the channel center in an upward flow configuration. The lateral migration velocity in the vertical channel is found to correlate positively with fiber length and the shear rate. Lateral migration is present, however negligible, in a horizontal channel where the sideway gravity is dominant. Current study clearly identified the presence of fiber transport scenarios where lateral migration driven by the shear induced lift and rotation is the major contributor for fiber deposition in wall-bounded flows. The finding is of particular significance to practical applications, as frequently, they involve a combination of these transport scenarios either actively or passively. The study also provided additional insights to examine the spherical equivalency of fiber dynamics to the spherical particles.

Aerosol extraction from inkjet print-zones

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Inkjet printers produce waste aerosols due to the production of small satellite droplets during the ejection and break-up process. Much of the waste aerosol impacts the media, which can cause printing defects, but there can be a substantial amount which leaves the print zone, and which can cause issues with surface fouling, causing both operator and media staining, and operator health and safety, due to ingestion of the aerosols. For home and office use, the volume of waste aerosols produced is usually very small and does not pose issues, but in industrial printing systems, the problem is much greater, and industrial systems typically include an aerosol management system (AMS) which captures as much of the waste aerosol as possible.

Here, we investigate the effect of the AMS design on the waste aerosol capture efficiency using numerical simulations which track Lagrangian particles in the domain. Our simulation models have been validated against experimental data from the literature and from a specialized printing rig which permits simultaneous printing and flow visualization. The effects of the nozzle width and angle relative to the paper motion have been examined, with the most efficient configuration identified. Then the effects of not sealing the print zone on capture efficiency are examined.

Revised Macroscopic and Mesoscopic Models for Convective Transport in Newtonian and Non-Newtonian Nanofluids

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Over the past two decades, the modeling and simulation of nanofluids using the two-phase model proposed by Buongiorno has been predominant (2006). However, this model is limited to Newtonian nanofluids. Recently, Bnsch (2019) highlighted that this model lacks thermodynamic consistency and subsequently enhanced the model, particularly in the momentum and energy equations. Furthermore, when considering the application of nanofluids in intricate geometries and porous structures, researchers found it necessary to account for additional crucial factors like the deposition rate, nanoparticle thermal dispersion, and hydrodynamic interactions around the nanoparticles within the Buongiorno model. Nevertheless, these aspects were incorporated and examined in isolated studies, without an assessment of thermodynamic equilibrium in the applied models. Thus, it underscores the need for the development of a comprehensive new two-phase model for nanofluids that encompasses all these previously overlooked elements and maintains thermodynamic consistency. For tackling the recently introduced macroscopic model, a lattice Boltzmann method has been devised. This method possesses the capability to incorporate all of the newly introduced parameters, along with capturing the non-Newtonian characteristics of nanofluids, encompassing both shear-thinning and viscoplasticity trends (2021,2022). Additionally, we incorporated a reexamined local thermal non-equilibrium (LTNE) condition to investigate the temperature contrast between the carrier fluid and nanoparticles. This involved introducing a novel correlation for the thermal conductivity of both the solid and liquid phases under LTNE conditions, taking into account potential particle aggregation (2022).

Development and validation of a phase-field lattice Boltzmann method for non-Newtonian Herschel-Bulkley fluids in three dimensions

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The behaviour of non-Newtonian fluids, and their interaction with other fluid phases and components, is of interest in a diverse range of scientific and engineering problems. In the context of the lattice Boltzmann method (LBM), both non-Newtonian rheology and multiphase flows have received significant attention in the literature. This work builds on that work by presenting the development and validation of a phase-field LBM which combines these features in three-dimensional flows. Specifically, the model presented herein combines the simulation of Herschel-Bulkley fluids, which exhibit both a yield stress and power-law dependence on shear rate, interacting with a Newtonian fluid. The developed model is verified and validated using a diverse set of rheological properties and flow conditions, which in their totality represent an additional contribution of this work. Comparison with steady-state layered Poiseuille flow, where one fluid is Newtonian and the other is non-Newtonian, showed excellent correlation with the corresponding analytic solution. Validation against analytic solutions for the rise of a power-law fluid in a capillary tube also showed good correlation, but highlighted some sensitivity to initial conditions and high velocities occurring early in the simulation. A demonstration of the model in a microfluidic junction highlighted how non-Newtonian rheology can alter behaviour from cases where only Newtonian fluids are present. It also showed that significant changes in behaviour can occur when making small and smooth changes in non-Newtonian parameters. To summarise, this work broadens the range of physical phenomena that can be captured in computational analysis of complex fluid flows using the LBM.

Simulating Bingham Plastics in a Cavity: Integrating Internal and External Natural Convection with Lattice Boltzmann Method

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This study numerically investigates the natural convection behavior of Bingham plastics within a cavity with differentially heated walls and an internal heat source. The dimensional and non-dimensional macroscopic equations governing the phenomenon are presented, along with the constitutive equation based on an exact Bingham model. The lattice Boltzmann method utilized in the study is explained, and the derivation of the governing equations is demonstrated. The code's accuracy is validated and confirmed through comparison with previous research, showing good agreement. The results are presented and discussed for a range of non-dimensional parameters. The maximum (or critical) Yield number is identified within the studied parameters and reported.

Influence of plasticity on inertialess viscoelastic instabilities using a hybrid lattice Boltzmann model

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Many important practical applications involving porous media, cosmetics, biological systems, and food processing involve the transport of non-Newtonian fluids, which possess non-linear material properties. Elastoviscoplastic fluids are indeed a complex example, simultaneously involving viscous, elastic, and plastic properties. In this study, we conduct numerical simulations of elastoviscoplastic fluids using a hybrid lattice Boltzmann solver in order to investigate the impact of plasticity, characterized by the Bingham number, on inertialess viscoelastic instabilities at high Weissenberg numbers. Results obtained using the four-roll mill and cellular-forcing scheme benchmark cases, which produce a strong elongational flow regime, reveal the emergence of three distinct flow states over time. The transition and behavior between the different flow states are found to strongly depend on the interplay between elasticity and plasticity. Moreover, we demonstrate that the general effect of the Bingham number is to increase the unyielded regions in the flow, which ultimately laminarize and suppress the flow fluctuations in the late stages.

Resolving bubble dynamics in molten media bubble columns using a phase-field lattice Boltzmann model

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Hydrogen production through methane pyrolysis is gaining traction as an effective method for generating clean, cost-effective hydrogen for both energy and chemical industries. Methane pyrolysis offers a compelling advantage by producing hydrogen with solid carbon as the sole by-product, thereby eliminating direct greenhouse gas emissions. This technology has shown promising results in lab-to-pilot-scale settings; however, challenges, such as the continuous removal of carbon products, have inhibited their commercial feasibility.

Molten-media bubble column reactors (MMBCRs) have emerged as a promising solution to this challenge. These reactors leverage molten media to continuously remove carbon deposits, thus allowing for continuous operation. The efficiency of MMBCRs is intricately linked to bubble dynamics since the pyrolysis reaction occurs primarily at the gas-liquid interface. Despite their potential, the complexity of bubble dynamics in molten-media environments remains poorly understood.

Traditional experimental methods fail to capture the high-temperature bubble dynamics within MMBCRs, leading to over-reliance on empirical correlations that do not accurately reflect the flow regime transitions. Numerical modelling provides a promising approach for elucidating phenomena observed in experimental environments that are difficult to probe. The phase-field lattice Boltzmann method (PFLBM) has been highlighted for its ability to simulate the complex bubble behaviour and flow regime changes within MMBCRs.

In this study, the simulation results from the PFLBM were compared with lab-scale findings of argon injection into a molten iron column. The extreme density ratio of this environment (ρ^*=27,000) and the potentially high gas flow rates pose numerical challenges, indicating further avenues of research. Using a lower density ratio, it was observed that the PFLBM could reasonably recover the reported gas holdup profile in the molten column and capture the natural formation of different flow regimes. These findings highlight the need for improved numerical models to guide the upscaling process of MMCBRs.

Computing sessile droplet shapes on arbitrary surfaces with a new pairwise force smoothed particle hydrodynamics model

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The study of the shape of small droplets has applications in multiple industries, from agrichemical spraying to inkjet printing. For these real-world applications, solutions for droplet shapes on complex substrates -- rough and chemically patterned surfaces -- are desired. Grid-based discretisations in axisymmetric coordinates are well-established numerical solution methods in this area, but when the problem is not axisymmetric, the shape of the contact line and the distribution of the contact angle around it are unknown. Recently, particle methods, such as pairwise force smoothed particle hydrodynamics (PF-SPH), have been used to conveniently forego the explicit enforcement of the contact angle. The pairwise force model, however, is far from mature. Specifically, there is no consensus in the literature on the choice of pairwise force profile. We propose a new pair of polynomial force profiles with a simple motivation and validate the PF-SPH model in both static and dynamic tests. We demonstrate its capabilities by computing droplet shapes on a physically structured surface, a surface with a hydrophilic stripe, and a virtual wheat leaf with both microscale roughness and variable wettability. We anticipate that this model can be extended to dynamic scenarios, such as droplet impaction, in the future.

Enhancement of the flow boiling heat transfer in microchannels by a Flow-induced vibrating cylinder

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Microchannel flow boiling is gaining great attention due to its high heat dissipation with a small temperature difference, which is particularly beneficial in cooling systems. This work numerically studies the flow-boiling heat transfer in microchannels enhanced by flow-induced vibrations (FIV). Simulations are conducted by an immersed boundary-lattice Boltzmann method. In this method, the boiling flow is solved by using the pseudopotential multiphase lattice Boltzmann model, the flow-induced vibration of the cylinder is modelled by a mass-spring-damping system, the heat transfer equation is solved by the finite difference method, and the boundary condition at the fluid-cylinder interface is handled by a feedback-immersed boundary method. Three groups of simulations are examined: a clear channel, a channel with a stationary cylinder, and a channel with a flow-induced vibrating cylinder. Various parameters are varied, including Reynolds number, heat flux, surface wettability, and blockage ratio. In the case of flow over a fixed cylinder with a blockage ratio of 3.0, the induced vortex achieved an enhancement of about 20% in the rates of flow boiling heat transfer in the intermediate region of heat flux compared to the clear channel. Moreover, in the high heat flux region, there is a substantial improvement in heat transfer, exceeding 23.455%, 22.97%, and 25.881% for Reynolds numbers of 600, 800, and 1000, respectively. The presence of the induced vortex effectively delayed the onset of the dryout condition at the critical heat flux point. Additionally, decreasing the blockage ratio enhances the rates of heat transfer. When the vibrating cylinder is positioned near the wall with a low blockage ratio, notable enhancements in heat transfer in moderate range of heat flux. Therefore, this study provides an efficient solution for flow boiling problems without using any additional external power source for evaporative cooling systems of the high-powered applications.

Immersed boundary method and its applications for the fluid-structure interaction in blood flow and insect flight

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The fluid-structure interaction (FSI) problems are common in nature, particularly in engineering and biological applications. Nevertheless, a comprehensive study of such problems remains a challenge due to their strong nonlinearity and multidisciplinary nature. The immersed boundary method has attracted growing interest in the computational fluid dynamics research community due to its simplicity in dealing with moving boundaries. The lattice Boltzmann method is an alternative and promising numerical scheme for fluid flow simulations due to its advantages of simplicity, explicit calculation, and intrinsic parallel nature. A high-fidelity and in-house FSI solver for simulating blood flow and insect flight will be presented. The developed FSI solver is based on the immersed boundary-lattice Boltzmann method (IB-LBM), which has gained popularity in various fields, including biofluid dynamics and engineering applications. Its ability to handle complex geometries makes it a valuable tool for a wide range of scientific and engineering simulations. The IB-LBM is first introduced into the study of collapsible blood flow, which shows high efficiency with strong robustness compared with conventional CFD methods. The IB-LBM promotes the first full-domain numerical simulations of large-amplitude self-excited oscillations of collapsible blood vessels. It's a very promising numerical method for further extension to the simulation of blood cells, heart valves, and heart murmurs due to the disturbances in blood flow caused by stenosed vessels.

Effects of bio-inspired flaps on the aerodynamics of an airfoil

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Long-time evolution has resulted in superior flight performance of aerial animals. Observation of flying mammals has shown their ability to cope with chaotic and turbulent flows and perform complex maneuvering in different scenarios like high-speed flight, prey hunting, and short-distance landing which the manufactured machines are not capable of imitating. Feathers are believed to play a significant role in adapting flow patterns near wings and customizing flow configurations for the bird to perform such targeted maneuvering. Given the intricate behavior of feathers and the complexity involved with their modeling, they have been mainly ignored in past research. Present work has been motivated by the lack of knowledge and understanding of the aerodynamics of feathers and strived to develop a robust framework to numerically model this fluid-structure interaction phenomenon and to investigate this nature-inspired mechanism. In our framework, the Lattice Boltzmann Method is used for modeling the fluid, the Finite Element Method is used for solving the structural dynamics, and the feedback-immersed boundary method is employed for the coupling. To study the aerodynamic behavior, the feathers are modeled as highly flexible and deformable flaps covering the top section of the airfoil. It is found that feathers are capable of enhancing the leading-edge suction peak by mitigating flow separation and reducing wake size and drag. Further study will be conducted to correlate the structural properties of feathers with aerodynamic performance.

CFD modelling of mixing zone during extracorporeal membrane oxygenation (ECMO) treatment

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Background: Veno-Arterial Extracorporeal Membrane Oxygenation (V-A ECMO) is a critical care support for patients with severe cardiac or cardiopulmonary failure. When lung failure patients are supported with V-A ECMO, there is a mixing of LV blood with low oxygen levels and ECMO blood with high oxygen levels in the aorta, which is termed as mixing zone. This phenomenon feeds the upper body with blood above mixing zone and lower body with blood below mixing zone, resulting in harlequin syndrome. Recently, pulsatile flow has been introduced in V-A ECMO, and several in vitro and animal studies have demonstrated benefits, namely cerebral oxygenation, cardiac unloading, and end organ perfusion.

Aims: This study aims to model the mixing zone in a patient-specific aorta during pulsatile flow ECMO application and calculates its movement during various ECMO pulse timings.

Methods: Numerical simulations were performed in a geometrically accurate aorta model by solving continuity and Navier-Stokes equations. To model the mixing zone, a non-reactive species transport equation for oxygen was solved. The non-Newtonian nature of blood flow was modelled using the Carreau model. The aortic root was applied with flow waveform from a heart failure patient, the femoral artery was applied with ECMO flow waveform, and all the outlets were provided with three-element Windkessel model. The CFD model was validated against particle image velocimetry data.

Results: For various position of ECMO pulse in a cardiac cycle, the mixing zone was positioned between 9.0 cm and 9.6 cm from aortic root. But some of the aortic arch branches were supplied with blood from LV.

Significance and Impact: This study shows that pulsatile flow ECMO partly oxygenate the upper body but fails to supply oxygen-rich blood to heart and brain. This shows the need for intervention to prevent harlequin syndrome during V-A ECMO treatment, even in pulsatile mode.

Viscoelastic Fluids-based Microfluidic Devices and Applications

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Manipulation and separation of micro/nano-objects such as cells are indispensable and crucial in disease diagnostics, environmental science, and chemical and biological assays. Microfluidic techniques have emerged as efficient and powerful tools for particle/cell manipulation due to their unique advantages of lower cost with higher efficiency and accuracy. However, most of these manipulating methods are performed and studied in Newtonian fluids (whose viscosity does not change with the flow conditions such as water). In fact, non-Newtonian fluids (whose viscosity changes with the flow conditions leading to unique properties) such as blood, saliva, cytoplasm, and many other body fluids, are very ubiquitous in our daily life and in real world issues. Therefore, it is important to investigate particle migration in non-Newtonian fluids to develop a deep understanding of cell behaviours in these body fluids. The unique advantages of particle/cell manipulation using viscoelastic microfluidics were explored, and cutting edge microfluidic technologies for particle and cell manipulation including 3D particle focusing, separation and on-chip cell washing was developed, and their usefulness in both environment and biomedicine was demonstrated.

Stretchable Microfluidics for cell manipulation and separation

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Inertial microfluidics is a promising approach for particle separation because of the superior advantages of high throughput, simplicity, precise manipulation, and low cost. However, the rigid geometrical dimensions of current systems limit their ability to isolate and separate particles of different sizes. This study introduces a proof of concept for a stretchable and flexible inertial microfluidic technology that can be elongated to control channel dimensions, allowing the device to adapt to different particle sizes. By changing the channel dimensions, the device can be adapted to different particle sizes and flow rate ratios. We successfully demonstrated this approach with the separation of a mixture of 10 and 15 µm particles. Stretching the device could significantly improve the focusing and separation efficiency of the specific particle sizes. In addition, we have applied the stretchable inertial microfluidics for the separation of cancer cells and blood cells. Stretchability allows for the fine-tuning of the separation cut-off size in real time, adapting separation threshold to separate the cells of interest. We evaluated the focusing efficiency, flow behaviour, and the positions of cancer cells and white blood cells (WBCs) in an elongated channel. Finally, the performance of the device was verified by isolating cancer cells from WBCs which revealed a high recovery rate and purity. In summary, the proposed new concept of stretchable inertial microfluidics enables onsite modification of the dimensions of a microchannel leading to a precise tunability in separation threshold and resolution.

Microflows in alveolar cells

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Investigation on the dynamics of airflow and mechanism of particle transport in the deep lung is important for understanding the lung functions and the cause of many lung diseases. This study aims to develop an alveolar microfluidic chip for investigating the fluid flow and particle transportation in the pulmonary alveolar cells. The alveolar chip was fabricated using the standard soft lithography technique. The system for velocity measurement mainly consists of a pump system and a micro particle image velocimetry (MicroPIV) system. One syringe pump channel was used to control the cyclic oscillating flow in the alveolar duct, and the other one was applied to control the pressure of a chamber to achieve rhythmic alveolar expansion and contraction. A particle tracking system is also used for tracking micro-particles in alveolar cells with air under various forces. Dimensionless numbers, i.e., Reynolds number (Re), Womersley number (Wo), Stokes number (Stk), Gravity number (H), and Peclet number (Pe) are used for dynamic matching of fluid flow and particle transport. In the study, radial flow patterns and recirculating flow patterns in the alveolar cells are presented. There is a saddle point in the recirculating flow, which is first found by experiment. The gravity plays a significant role in particle deposition for large particles, while drag force determines the deposition regions. Particles that are close to the alveolar ducts have a chance to enter the alveolar cells for high Re. The particles always enter the alveoli against the wall from the distal side of the alveolar opening.

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