Workshop on Numerical Simulations in Engineering

27-28, March, 2018

1. Program

Date	Time	Talk
27-Mar 2018	8:30am – 8:45am	Welcome by **Huilai Li** (Dean of School of Mathematics, Jilin University)
	8:45am – 9:45am	**Nhan Phan-Thien** (Professor, National University of Singapore) SPH modelling of fiber orientation in a 3D printing process
	9:45am – 10:00am	**Coffee break**
	10:00am – 11:00am	**Boo Cheong Khoo** (Professor, National University of Singapore) Flow over shallow dimple arrays
	11:00am – 12:00am	**Heow Pueh Lee** (Associate Professor, National University of Singapore) Membrane-type acoustic metamaterials: towards large-scale noise control applications
	12:00pm – 14:00pm	**Lunch break**
	14:00pm – 15:00pm	**Tiegang Liu** (Professor, Beihang University) Adjoint-based adaptive discontinuous Galerkin method for compressible Navier-Stokes equations
	15:00pm – 16:00pm	**Dingyi Pan** (Associate Professor, Zhejiang University) Pressure control in Dissipative Particle Dynamics and applications in microbubble and droplet simulation
	16:00pm – 16:15pm	**Coffee break**
	16:15pm – 17:15pm	**Yuqiang Fang** (Lecturer, Jilin University) Probing mechanical properties of cells as an early indicator of neurodegeneration
28-Mar 2018	8:45am – 9:45am	**Moubin Liu** (Professor, Peking University) Smoothed particle hydrodynamics - recent development in methodology and applications
	9:45pm – 10:00am	**Coffee break**
	10:00am – 11:00am	**Tong Wang** (Associate Professor, Nanjing University of Aeronautics and Astronautics) Numerical investigation on the transport of non-aggregating and aggregating red blood cells through microvascular bifurcations
	11:00am – 12:00pm	**Ting Ye** (Associate Professor, Jilin University) Simulations of red blood cells in complex microtubes
	12:00pm – 14:00pm	**Lunch break**
	14:00pm – 15:30pm	**International exchange programs**

2. Speaker Biography

1) **Nhan Phan-Thien**, Professor in Mechanical Engineering at National University of Singapore

	2016-present: Mechanical Engineering, NUS, Head 2011-present: National University of Singapore, Professor 2005-2011: Partners in NT Investments (five different LLC in California, USA) 2001-2004: Bioengineering, NUS, founding Head 1991-2001: University of Sydney, Australia, Personal Chair 1989, 90, 92, 95: Los Alamos National Laboratory, External Consultant 1979，University of Sydney, PhD 1975，University of Sydney, BE, 1st Class Hons
Awards:	2016，Fellow of the Asean Academy of Engineering and Technology 2003，Centenary Medal by the Australian Governor General 2002，Fellow of the European Academy of Science 1999，Fellow of the Australian Academy of Science 1997，Gordon Bell Prize
Academic positions:	Physics of Fluids, Associate Editor Journal of non-Newtonian Fluid Mechanics, Editorial Board AIP Advances, Academic Editor
Research areas:	Non-Newtonian Fluid Mechanics Rheology Constitutive & Numerical Modelling of Multiphase and Viscoelastic Fluids Particle-based methods Stochastic simulation methods in viscoelasticity

2) **Boo Cheong Khoo,** Professor in Mechanical Engineering at National University of Singapore

	2012-present: Temasek Laboratories, Director 2011-2012: Temasek Laboratories, NUS, Director of Research 2005-2013: SMA-II, co-Chair of Computational Engineering Program 1999-2004: SMA-I, co-Chair of High Performance Computation for Engineered Systems Program 1998-1999: Institute of High Performance Computing, deputy Director 1989，Massachusettes Institute of Technology, PhD 1984，National University of Singapore, MEng 1980, University of Cambridge, BA, 1st Class Hons
Awards:	Member of the Steering Committee, HPC Asia 1998，Defence Technology Team Prize, Singapore 1980，Royal Aeronautical Prize, UK

Academic positions:	Communications in Computational Physics, Associate Editor Applied Mathematics and Mechanics, Associate Editor American Journal of Heat and Mass Transfer, Editorial Board Ocean Systems Engineering, Editorial Board International Journal of Intelligent Unmanned Systems, , Editorial Board The Open Mechanical Engineering Journal, Editorial Board The Open Ocean Engineering Journal, Editorial Board
Research areas:	Fluid-structure interaction Underwater shock and bubble dynamics Compressible/Incompressible multi-medium flow

3) **Heow Pueh Lee**, Associate Professor in Mechanical Engineering at National University of Singapore

	2012-present: Mechanical Engineering, NUS, Deputy Head 2003-2007, Institute of High Performance Computing, Deputy Executive Director for Research 2002-2003, Institute of High Performance Computing, Deputy Director for Research 1991: Stanford University, PhD 1987，National University of Singapore, MEng 1982，University of Cambridge, BA
Research areas:	Acoustics and Vibration Computational Methods Mechanics in Medicine Biofouling

4) **Tiegang Liu,** Professor in Mathematics at Beihang University

	2007-present, Beihang University, Professor 1999-2007, Institute of High Performance Computing, Research Fellow 1995-1999, National University of Singapore, PhD 1992-1995, Chinese Academy of Sciences, Assistant Professor 1989-1992, Chinese Academy of Sciences, Research Engineer 1986-1989, Peking University, MS 1982-1986, Peking University, BS
Research areas:	Compressible multi-medium and multi-phase flow Fluid-Structure Interaction Shape optimisation design

5) **Dingyi Pan,** Associate professor in Engineering Mechanics at Zhejiang University

2016-present, Zhejiang University, Associate Professor

2014-2016, Zhejiang University, Lecturer

2011-2014, National University of Singapore, Research Fellow

2006-2011, Zhejiang University, PhD

2002-2006, Zhejiang University, B.S.

Research areas: Mesoscale simulation
Multiphase flow
Non-Newtonian fluid mechanics

6) **Yuqiang Fang,** Lecturer in Engineering Mechanics at Jilin University

2015-present: Jilin University, Lecturer

2015, City University of Hong Kong, PhD

2012, Nanjing University of Science and Technology, MEng

2009, Nanjing University of Science and Technology, BS

Research areas: Cell mechanics
Cell modeling

7) **Moubin Liu,** Professor in Mechanical Engineering at Peking University

2014: Peking University, Professor

2009: Chinese Academy of Sciences,

2005, Nanyang Technological University

2004, Idaho National Laboratory,

2003, National University of Singapore, PhD

1996, Xi'an Jiaotong University, MEng

1993, Xi'an Jiaotong University, BS

Awards:	2017, First Prize in Natural Sciences, Ministry of Education 2016, ICACM Fellows Award 2012, Innovation Award, All-China Federation of Returned Overseas 2009, 100 Talent Program Award, Chinese Academy of Sciences 2007, Young Investigator Award, Asia Pacific Association of Computational Mechanics 2005, Lee Kuan Yew （李光耀） Fellowship Award, Nanyang Technological University (NTU)
Research areas:	Computational mechanics Fluid structure interaction Multi-scale modeling

8) **Tong Wang,** Associate Professor in Mathematics at Nanjing University of Aeronautics and Astronautics

2010, Nanjing University of Aeronautics and Astronautics, Assoc. Professor
2009, Texas A & M University, Visiting scholar
2008, University of Houston, PhD
2005, University of Houston, MS
2003, University of Kansas, MS
1992, Tsinghua University, BS

Research areas:	Fluid dynamics Biomedical physics Cell rheology

9) **Ting Ye,** Associate professor in Mathematics at Jilin University

2014-present, Jilin University, Associate Professor
2012-2014, National University of Singapore, Research Fellow
2008-2012, Nanyang Technological University, PhD
2006-2008, Beijing Technological University, MEng
2002-2006, North China University of Water Resources and Electric Power, BS

Research areas:	Computational biomathematics Computational biophysics Computational fluid dynamics

3. Talk Abstract

1) Nhan Phan-Thien (National University of Singapore)

Title: SPH modelling of fiber orientation in a 3D printing process

Abstract: In the first part, a survey of the constitutive modelling of fiber suspensions is given. This is followed by a modelling of the fused deposition process using a Smooth Particle Hydrodynamics (SPH) approach, using a relevant and commonly used fiber suspension constitutive equation. The simulation results for the effects of the fiber aspect ratio and the volume fraction on the fiber orientation state within the deposited layer are discussed. The effects of fibre aspect ratios and volume fractions will be discussed. Our major observation is the existence of a skin/core structure where particles are strongly aligned in the skin region. This is likely to have significant implications in terms of the final part properties and the SPH simulation method represents a promising tool for nozzle design and optimization.

2) Boo Cheong Khoo (National University of Singapore)

Title: Flow over shallow dimple arrays

Abstract: Dimple arrays have been successfully used for heat transfer enhancement because they increase the heat transfer at a relatively smaller penalty in terms of pressure losses compared to traditional heat transfer devices just as fins and pins. Both experiments and numerical simulations have been carried out on shallow round-edged dimple arrays with dimple depth to diameter ratios of 5%. Pressure measurements have been carried out to quantify the drag reduction due to the dimple array in a turbulent channel flow for Reynolds numbers between 5,000 and 37,000, and hot-wire anemometry and Detached Eddy Simulations (DES) have been carried out to understand the flow over the dimples in greater detail. The study shows that the drag due to the dimple array reduces as the Reynolds number increases from 5,000 to 37,000. A drag increase is observed at Reynolds numbers below 13,000, while a drag reduction is observed above this Reynolds number.

The results show that while the streamwise vortices generating spanwise flow near the surface can reduce the skin friction drag, form drag present within the three-dimensional dimples can be significant enough that an increase is observed in the total drag. To optimize the dimple shape and maximize drag reduction, both the skin friction and form drag should be reduced. One possible method to reduce this form drag is through the use of asymmetric dimples, where the deepest point within the dimple is shifted backward, resulting in a shallower wall gradient at the upstream portion of the dimple.

3) Heow Pueh Lee (National University of Singapore)

Title: Membrane-type acoustic metamaterials: towards large-scale noise control applications

Abstract: Recent works have demonstrated the potential of small-scale membrane-type acoustic metamaterials for low-frequency noise control. Such metamaterials are characterised based on the resonant behaviour of the membrane. Considering industrial applications, it is imperative to investigate large-scale design and introduce additional feature to complement the acoustical performance of the membrane-type metamaterials.

The first part of this seminar presents a large-scale membrane-type acoustic metamaterial (or the meta-panel), which was evaluated and verified numerically. Experimental results showed that a broadband sound transmission loss (STL) improvement could be achieved by the incorporated membrane (up to 7.4 dB at 380 Hz). Numerically, parametric studies showed that the broadband STL performance of the meta-panel was due to not only the resonant behaviour of the overhanging membrane but also the resonant behaviour of the sandwiched membrane along the boundaries of the unit cells. If properly designed, this resonant behaviour of the sandwiched membrane could complement membrane-type acoustic metamaterials to achieve an extended good STL performance across a broader frequency bandwidth.

The second part of this seminar focuses on the potential manufacturing issues if large-scale designs are considered. Examples include the spatial consistency of the platelet(s), the uniformity of the membrane pretension, and the durability of the membrane—not to mention stress relaxation. Hence, it is imperative to address the shortcomings for manufacturability. The conceptual design of a membrane-type acoustic metamaterial without the need for pretension and platelet(s) is presented. Additionally, experimental and numerical results showed that the acoustical performance could be complemented by the coupling effect between two enclosed cavities via an orifice. The orifice diameter could serve as a tuning parameter for broadband or narrowband transmission loss at selected frequencies. Consequently, the proposed design could address the shortcomings of membrane-type acoustic metamaterials and complement their acoustical performance with the additional feature.

4) Tiegang Liu (Beihang University)

Title: Adjoint-based adaptive discontinuous Galerkin method for compressible Navier-Stokes equations

Abstract: An adjoint-based high-order h-adaptive direct discontinuous Galerkin method is developed and analyzed for the compressible steady state Navier-Stokes equations. Particular emphasis is devoted to the analysis of the adjoint consistency of the original direct discontinuous Galerkin (DDG) method and the direct discontinuous Galerkin method with interface correction (DDG(IC)). Theoretical analysis shows the extra interface correction term in DDG(IC) method plays a key role in preserving the adjoint consistency. In fact, we prove that the original DDG method is not adjoint consistent, while the DDG(IC) method can be adjoint consistent with appropriate treatment of boundary conditions and correct modification for target functional. The performance of both DDG method and DDG(IC) method is carefully investigated and evaluated through typical test cases. Numerical experiments show that the DDG(IC) method can achieve the optimal order of accuracy with respect to the error in the computed target functional, which clearly indicates its superior potential compared to the original DDG method in the development and implementation of adjoint-based adaptation for simulating compressible flows.

5) Dingyi Pan (Zhejiang University)

Title: Pressure control in Dissipative Particle Dynamics and applications in microbubble and droplet simulation

Abstract: Pressure control is of extensive interest in meso-scopic simulation and particle-based numerical methods. In dissipative particle dynamics (DPD) and many-body DPD (MDPD), a natural thermostat has been already incorporated. Therefore, the barostat for pressure control could be an important part for the (M)DPD application. In current work, the Berendsen barostat from molecular dynamics simulation is applied in both DPD and MDPD simulations. The original Berendsen barostat works well in (M)DPD simulation of single-component system under constant pressure condition. The novel partial Berendsen barostat is proposed for multi-component system simulation with (M)DPD. The displacement rescaling process of Berendsen barostat is only applied on the particles outside the center region, acting as a pressure 'boundary condition'. The center part forms the free zone, in which the interface shape, non-equilibrium dynamic behavior between different phases can be captured properly. Immiscible bubble/droplet in the second fluid under outside pressure condition is studied. A microbubble/droplet model with liquid to gas density ratio up to 10 is created in (M)DPD simulation, and the oscillation of bubble radius is captured and compared with classical Rayleigh–Plesset equation. Bubble oscillation under harmonic pressure wave are also reported in current simulation which may have potential application in the studies on sonoporation and ultrasound bubble dynamics.

6) Yuqiang Fang (Jilin University)

Title: Probing mechanical properties of cells as an early indicator of neurodegeneration

Abstract: The mechanical properties of cells including elasticity, viscosity, morphology, etc., are the inherent characteristics of cells determined by the mechanical components and organization of subcellular structures. The mechanical properties of cells are theoretically potential to indicate any diseased states of cells with subcellular changes. Neurodegenerative diseases, such as Alzheimer's disease and Parkinson's disease, are threating millions of people worldwide. However, efficient biomarkers are still under development, especially for the early stage. Previous studies have demonstrated that cells under neurodegeneration were gradually degenerated accompanying by serial mechanical events including contraction of neurites and shrinkage of cell body. In the following presentation, the progressive states of neurodegeneration will be presented to experimentally evaluate based on the mechanical changes of neuronal cells under neurodegenerative loads, including Ca2+ influx, chemotherapy drug treatment and beta amyloid (Aβ) aggregation. A theoretical model named coarse-gained molecular dynamics model of adherent cells will also be introduced to decipher the correlation between neurodegeneration and cell mechanical properties from molecular events in subcellular components. The presented analysis of neurodegeneration and cell mechanical properties of neuronal cells based on the experimental and simulated approaches aim to develop the potential of cell mechanical properties as a promising biomarker to indicate the progressive states of neurodegeneration.

7) Moubin Liu (Peking University)

Title: Smoothed particle hydrodynamics - recent development in methodology and applications

Abstract: Smoothed particle hydrodynamics (SPH) is a meshfree particle method based on Lagrangian formulation, and has been widely applied to different areas in engineering and sciences. This talk will first introduce the recent advancements in SPH method including a novel particle approximation scheme with higher order accuracy and an efficient coupled dynamic boundary treatment algorithm. The

developed SPH method is then applied to a number of challenging applications in hydrodynamics, environmental flows and problems with material strengths.

8) Tong Wang (Nanjing University of Aeronautics and Astronautics)

Title: Numerical investigation on the transport of non-aggregating and aggregating red blood cells through microvascular bifurcations

Abstract: Blood exhibits a heterogeneous nature of hematocrit, velocity, and effective viscosity in microcapillaries. Microvascular bifurcations have a significant influence on the distribution of the blood cells and blood flow behavior. Under some pathological conditions such as infected by malaria, red blood cells (RBCs) become stiffer and more adhesive than normal. Thus it is even possible that RBCs form aggregates or rouleaux in blood, leading to a change of the hemodynamical behavior of blood flow in microcirculatory system. This study presents a simulation study performed on the two-dimensional motions and deformation of multiple RBCs with and without aggregating force in bifurcated microvessels. Fluid dynamics and membrane mechanics were incorporated. Effects of major factors such as cell shape, hematocrit, cell stiffness, and aggregating strength on rheological behavior of the RBCs and the hemodynamics in the curved bifurcations have been investigated. The simulation results are qualitatively consistent with existing experimental findings. This study may provide fundamental knowledge for a better understanding of hemodynamic behavior of micro-scale blood flow.

9) Ting Ye (Jilin University)

Title: Simulations of red blood cells in complex microtubes

Abstract: In biofluid flow systems, often the flow problems of fluids of complex structures, such as the flow of red blood cells (RBCs) through complex capillary vessels, need to be considered. In this talk, we aim to apply a particle-based method, Smoothed Dissipative Particle Dynamics (SDPD), to simulate the motion and deformation of RBCs in complex micro-tubes. We first present the theoretical models, including SDPD model, RBC-fluid interaction model, RBC deformation model, RBC aggregation model, and boundary treatment model. After that, we show the verification and validation of these models, by comparing our numerical results with the theoretical, experimental and previously-published numerical results. Finally, we provide some simulation cases, such as the motion and deformation of RBCs in rectangular, cylinder, curved, bifurcated, and constricted microtubes, respectively.