# Workshop on Computational Fluid Dynamics and Uncertainty Quantification



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# 1 General Information

## Introduction

Uncertainties are universal in simulation models in science and engineering applications, especially in computational fluid dynamics. They may appear in the model parameters, in the mathematical form of the models, or in the experimental data used to calibrate the models. Uncertainty quantification plays a key role in identifying uncertain sources, characterizing the probability distributions or ranges of uncertain sources. This workshop aims to bring together leading experts and excellent researchers in China to share state of the art research advances in the field of computational fluid dynamics and uncertainty quantification, foster further research collaborations and promote novel and revolutionary research ideas.

### Acknowledgement

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### Date

June 25-26, 2021

### Venue

Room 305, No. 5 Science Building, Minhang Campus, Shanghai Jiao Tong University How to arrive: https://ins.sjtu.edu.cn/contact-us

## **Organizing Committee**

- Shi Jin, Shanghai Jiao Tong University
- Tao Zhou, University of Chinese Academy Sciences
- Wenjun Ying, Shanghai Jiao Tong University

# 2 Schedule

Time	Speaker	Title
08:45 - 09:00		Opening Remarks
09:00 - 09:40	Juan Cheng	High Order Conservative Lagrangian Schemes for
		Radiative Hydrodynamics Equations in The Equi-
		librium Diffusion Limit
09:40 - 10:20	Weiying Zheng	High-order Finite Element Methods for Time-
		moving Interface Problems
10:20 - 10:40		Photots and Coffee Break
10:40 - 11:20	Yuehong Qian	复杂现象和简单模型
11:20 - 12:00	Jianjun Chen	New Technologies for Automatic Hybrid Grid Gen-
		eration
14:00 - 14:40	Zhihui Li	Gas-Kinetic Unified Algorithm for Computable
		Modeling of Boltzmann Equation and Numerical
		Forecast of Reentry Disintegration of Uncontrolled
		Large-scale Spacecraft
14:40 - 15:20	Xiaoquan Yang	鲁棒高效的航空飞行器可压缩湍流数值模拟方法
		及应用
15:20 - 15:40		Coffee Break
15:40 - 16:20	Ling Guo	Normalizing Field Flow: Solving Forward and
		Inverse Stochastic Differential Equations Using
		Physics-Informed Flow Model
16:20 - 17:00	Liang Yan	Adaptive Surrogate Modeling Based on Deep Neu-
		ral Networks for Bayesian Inverse Problems

# 2.1 Day 1, 25 June, Friday

# 2.2 Day 2, 26 June, Saturday

Time	Speaker	Title
09:00 - 09:40	Chuanju Xu	Some New Schemes for the Navier-Stokes Equa-
		tions
09:40 - 10:20	Yanli Wang	Regularized 13-Moment Equations for Inverse
		Power Law Models
10:20 - 10:40		Coffee Break
10:40 - 11:20	Wenjing Yan	Robin-Robin Domain Decomposition Methods for
		The Dual-porosity Model Coupled with Free Flow
		System
11:20 - 12:00	Haibiao Zheng	Some Progress of Domain Decomposition Methods
		for The Coupled Stokes-Darcy Model
14:00 - 17:00		Free Discussion

## 3 Abstracts

### 3.1 Day 1, 25 June, Friday

# High Order Conservative Lagrangian Schemes for Radiative Hydrodynamics Equations in The Equilibrium Diffusion Limit

Juan Cheng, Institute of Applied Physics and Computational Mathematics 09:00 - 09:40

Radiation hydrodynamics describes the interactions between matter and radiation which affect the thermodynamic states and the dynamic flow characteristics of the matter-radiation system. Its application areas are mainly in high-temperature hydrodynamics, including astrophysics, reentry vehicles fusion physics and inertial confinement fusion. In this talk, we will discuss the methodology to construct fully explicit and implicit-explicit (IMEX) high order Lagrangian schemes solving the one-dimensional radiative hydrodynamics equations in the equilibrium diffusion limit respectively, which can be used to simulate multi-material problems with the coupling of radiation and hydrodynamics. The schemes can maintain conservation and uniformly high order accuracy both in space and time. The issue of positivity-preserving for the explicit high order Lagrangian scheme is also discussed. Various numerical tests for the high order Lagrangian schemes are provided to demonstrate the desired properties of the schemes such as high order accuracy, non-oscillation, and positivity-preserving.

#### High-order Finite Element Methods for Time-moving Interface Problems

Weiying Zheng, Chinese Academy of Sciences 09:40 - 10:20

We develop high-order numerical methods for solving advection-diffusion equation and the Oseen equation (linearized Navier-Stokes equations) with time-moving interfaces. The methods are based on unfitted finite element discretization on fixed Eulerian meshes of the domain. The locus of the moving interface is tracked by high-order cubic MARS algorithms. We present thorough error estimates for the methods (orders 2 k 4) by taking full consideration of all errors from interface-tracking, spatial discretization, and temporal integration. Numerical experiments demonstrate the optimal convergence of the methods for k = 3 and 4.

#### 复杂现象和简单模型

Yuehong Qian, Suzhou University 10:40 - 11:20

我们将通过最基本的物理守恒定律来建立相对简单的数学模型,并应用于一些复杂的流动问题和具体的算例。同时我们也会介绍该方法用于描述非流动的一些复杂现象。

#### New Technologies for Automatic Hybrid Grid Generation

Jianjun Chen, Zhejiang University 11:20 - 12:00 In viscous flow simulations, the techniques based on prismatic-tetrahedral hybrid grids represent the best trade-off between ease of use and viscous accuracy. A major performance bottleneck of executing these techniques in real-world examples is how to create a high-quality hybrid grid fully automatically. Automatic hybrid grid generation is key to set up an efficient and scalable viscous flow simulation workflow. To achieve this, its three basic procedures must be automated, as listed below, (1) preparing a valid input geometry, (2) computing an appropriate sizing function, and (3) creating a high-quality grid with the geometry and sizing function as inputs.

In this report, a few new technologies on the three procedures are introduced. In the geometrypreparation procedure, the focus is on how to create a valid surface triangulation on geometries with various errors. A new top-down meshing technique is proposed by first creating a volume mesh and then creating the surface triangulation. Feature preserving are key to the success of this technique and our recent work on this issue will be detailed. In the procedure of sizing function computation, both prior (geometry-based) and posterior (solution-based) techniques are presented, along with a novel sizing-function smoothing algorithm based on nonlinear programming. In the procedure of grid generation itself, a new algorithm is proposed to create high-quality prismatic boundary layer grid. In this algorithm, instead of computing marching directions of layer grids by using heuristic geometric rules, Laplacian-type PDEs are solved by using the boundary element method to provide a marching direction field with smooth transitions.

The above efforts enabled us to set up robust and automatic meshing pipelines for various simulations, including but beyond viscous flow simulations. Grid examples with configurations of a complication level experienced in industry will be selected to demonstrate the capability of the developed technologies.

#### Gas-Kinetic Unified Algorithm for Computable Modeling of Boltzmann Equation and Numerical Forecast of Reentry Disintegration of Uncontrolled Large-scale Spacecraft

#### Zhihui Li, China Aerodynamics Research and Development Center 14:00 - 14:40

To study aerodynamics of spacecraft reentry covering various flow regimes, a Gas-Kinetic Unified Algorithm (GKUA) has been presented by computable modeling of the collision integral of the Boltzmann equation over tens of years. On this basis, the rotational and vibrational energy modes are considered as the independent variables of the gas molecular velocity distribution function, a kind of Boltzmann model equation involving in internal energy excitation is constructed by decomposing the collision term of the Boltzmann equation into elastic and inelastic collision terms under the conservation of the summation invariant and the H-theorem, in which the inelastic collision term is divided into translational-rotational and translational-rotationalvibrational energy relaxation according to a certain relaxation rate. Then, a set of controlling equations involving vibrational non-equilibrium effect can be got by introducing three reduced velocity distribution functions to cut back the number of independent variables. The gas-kinetic numerical scheme is constructed to capture the time evolution of the discretized velocity distribution functions by developing the discrete velocity ordinate method and numerical quadrature technique. The gas-kinetic boundary conditions in thermodynamics non-equilibrium and numerical procedures are implemented by directly acting on the discretized velocity distribution functions, and then the unified algorithm of the Boltzmann model equation involving thermodynamics non-equilibrium effect is presented for the whole range of flow regimes.

#### 鲁棒高效的航空飞行器可压缩湍流数值模拟方法及应用

Xiaoquan Yang, Shanghai University 14:40 - 15:20

针对航空飞行器可压缩湍流数值模拟中的鲁棒性差、收敛缓慢、计算效率低等问题,发展了 鲁棒高效的隐式有限体积和间断伽辽金可压缩湍流数值模拟方法,具体包括:高效的多重网 格方法、预处理方法、时间谱方法、基于精确 Jacobian 矩阵的 LU-SGS 方法和 LU-SGS 预 处理的 GMRES 方法、粘性间断的处理方式 DDG 格式,两步四阶时空耦合方法 (GRP)等; 并通过航空飞行器典型算例验证了方法的精度、收敛性和计算效率;典型算例包括:直升机 旋翼悬停和前飞流场数值模拟、固定翼飞机增升装置流场数值模拟、航空发动机内流数值模 拟等。此外,报告还讨论了 FVM 和 DG 方法在求解复杂构型湍流问题时存在的问题以及将 来的发展方向。

# Normalizing Field Flow: Solving Forward and Inverse Stochastic Differential Equations Using Physics-Informed Flow Model

Ling Guo, Shanghai Normal University 15:40 - 16:20

In this talk, we will introduce a Normalizing field flow model (NFF) to quantify uncertainty propagation in a unified framework for forward, inverse and mixed stochastic problems based on scattered measurements. We first build the NFF model for stochastic field by constructing a bijective transformation between Gaussian random filed and the target stochastic field. Then we train the invertible networks by maximizing the sum of the log-likelihood. Furthermore, to solve the SDEs, we encode the known physics, i.e., the form of the stochastic differential equation (SDE), into the architecture of NFF model and learn the unknown stochastic terms in the equations from data. We will demonstrate the performance of the new NFF model with several numerical examples. This is joint work with Hao Wu and Tao Zhou.

#### Adaptive Surrogate Modeling Based on Deep Neural Networks for Bayesian Inverse Problems

Liang Yan, Southeast University 16:20 - 17:00

Surrogate models are often constructed to speed up the computational procedure of the Bayesian inverse problems (BIPs), as the forward models can be very expensive to evaluate. However, due to the curse of dimensionality and the nonlinear concentration of the posterior, traditional surrogate approaches are still not feasible for large scale problems. This talk will survey our recent works in designing surrogate models using deep learning techniques. Several fast and efficient algorithms based on deep neural networks (DNN) to solve BIPs will be covered, including adaptive multi-fidelity surrogate modeling and local approximations. Numerical examples are presented to confirm that new approaches can obtain accurate posterior information with a limited number of forward simulations.

### 3.2 Day 2, 26 June, Saturday

#### Some New Schemes for the Navier-Stokes Equations

Chuanju Xu, Xiamen University 09:00 - 09:40

In this talk I will discuss a number of numerical methods for the Navier-Stokes equations, including traditional time-space discretizations and some recently developed schemes based on auxiliary variable reformulation. Our objective is to compare and analyze different schemes, and propose improved methods which overcome some of the shortcomings of the existing schemes.

#### Regularized 13-Moment Equations for Inverse Power Law Models

Yanli Wang, Beijing Scientific Research Center 09:40 - 10:20

We propose a systematic methodology to derive the regularized thirteen-moment equations in the rarefied gas dynamics for a general class of linearized collision models. Detailed expressions of the moment equations are written down for all inverse power law models as well as the hardsphere model. By linear analysis, we show that the equations are stable near the equilibrium. The models are tested for shock structure problems to show its capability to capture the correct flow structure in strong nonequilibrium. This is joint work with Zhenning Cai.

# Robin-Robin Domain Decomposition Methods for The Dual-porosity Model Coupled with Free Flow System

Wenjing Yan, Xi'an Jiao Tong University 10:40 - 11:20

In this talk, we propose and analyze domain decomposition methods to decouple the large system arisen from the dual-porosity-Stokes model. The recently developed model describes a complicated dualporosity-conduit system which uses a dual-porosity/permeability model to govern the flow in porous media coupled with free flow via four physical interface conditions. First of all, Robin boundary conditions are applied to decouple the coupling conditions on the interface. Then, Robin-Robin domain decomposition methods are established based on the two decoupled sub-problems. Convergence analysis is demonstrated and a geometric convergence order is obtained. Optimized Schwarz methods are proposed for the dual-porosity-Stokes model and optimized Robin parameters are derived to improve the convergence of proposed algorithms. Numerical experiments are presented to illustrate the accuracy and applicability of the proposed algorithms.

# Some Progress of Domain Decomposition Methods for The Coupled Stokes-Darcy Model

Haibiao Zheng, East China Normal University 11:20 - 12:00 In this talk, we will introduce some progress of Domain Decomposition methods for the coupled Stokes-Darcy model. One is the fully mixed parallel domain decomposition method, with the newly constructed Robin-type boundary conditions, the present method adopts modified weak formulation to decouple the original problem into two independent subproblems. The equivalence between the original problem and the decoupled subproblems is derived under some compatibility conditions. With some suitable choice of parameters, both mesh-dependent and mesh-independent convergence rates are proved rigorously. The other are two-grid Robin-type domain decomposition methods, which firstly adopt the existing Robin-type domain decomposition methods are further constructed on the fine grid by utilizing the framework of two-grid methods to enhance computational efficiency, via replacing some interface terms by the coarse grid information.