Computational Mechanics: What Do We Do?

An Introduction of Division of Mechanics at CSRC

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Summary

1. Vision, Objectives, and Means
2. Personnel
   - Prof. Xiaolong Deng: DNS of Interfacial Dynamics
   - Prof. Yang Ding: Bio-Mechanics and Complex Fluids
   - Prof. Shujie Li: High-Order Methods, HPC
   - Prof. Weidong Li: Kinetic Methods
   - Prof. Li-Shi Luo: Droplet and Film
3. Some Ongoing Research
   - DNS of Turbulence
   - Modeling/Simulation of Molecular Flows

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Vision

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In classical continuum mechanics of fluids and solids, no need to consider both quantum and relativistic effects, *i.e.*, in the limits of $\hbar = 0$ and $c = \infty$. Quantum ($\hbar = 1$), relativistic ($c = 1$), and other effects may have to be considered ins some non-equilibrium systems.

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It is imperative for us to break the barriers between the "mechanics" and other realms of modern physics so the "*mechanics*" would no longer be just "*continuum*" or "*classical*". This requires multi-disciplinary knowledge.

$\hbar = 1$ $c = \infty$	$\hbar = 1$ $c = 1$
$\hbar = 0$ $c = \infty$	$\hbar = 0$ $c = 1$

Mission

DoM has written a 5-year research plan based on its vision and resources, including the following specific objectives:

- **Mission**: to conduct basic research in the frontiers of modern computational mechanics in its broadest sense — the 3rd Pillar;
- **Character**: interdisciplinary research involving physics, applied mathematics, and computing;
- **Focuses**: modeling and simulation of multi-scale, multi-physics phenomena observed in fluid, soft matter, granular material, and solid, which may or may not be adequately described by macroscopic theories;
- **Education and Training**: our research strength and excellence will drive our educational program to train indigenous students and junior researchers;
- **Exchange**: to build a research platform of international statue which will attract researchers from all over the world, and serve as a center for academic exchange and interaction between domestic and international researchers.

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Research Areas

Modeling and simulation of the following systems:

- thermochemically nonequilibrium flows
- molecular micro flows
- multi-phase and multi-component flows
- interfacial dynamics
- Stokes, incompressible and compressible flows
- multi-scale and multi-physics and complex fluids
- granular flows, bio-mechanics, bio-robotics

Specific Methodologies and Means

General areas:

- PDE's (modeling) and its numerical solutions by means of HPC;
- Large-scale scientific computing, high-performance and parallel computing, emerging computing technology (MIC, GPUs);
- Algorithms and numerical analysis.

Specific methods and techniques:

- Numerical methods for PDEs: finite-volume, finite-difference, spectral and spectral element, discontinuous Galerkin, Stokelets, kinetic methods, high-order/high-resolution methods, ...
- Diffuse-interface and interface tracking methods
- Mesh/grid generation and adaptive mesh refinement
- Discrete element method, Molecular dynamics
- FMM for solving integral equations

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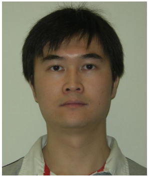
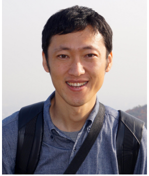
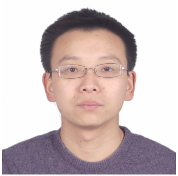
Personnel

			
Prof. Xiaolong Deng	Prof. Yang Ding	Dr. Shujie Li	Dr. Weidong Li

Chair Professor:	**1**
Tenure-track faculty:	**2**
Research faculty:	**2**
Associated members:	**4**
Post-doctoral research associates:	**3**
Graduate students:	**6**
Long-term collaborators/visitors:	...

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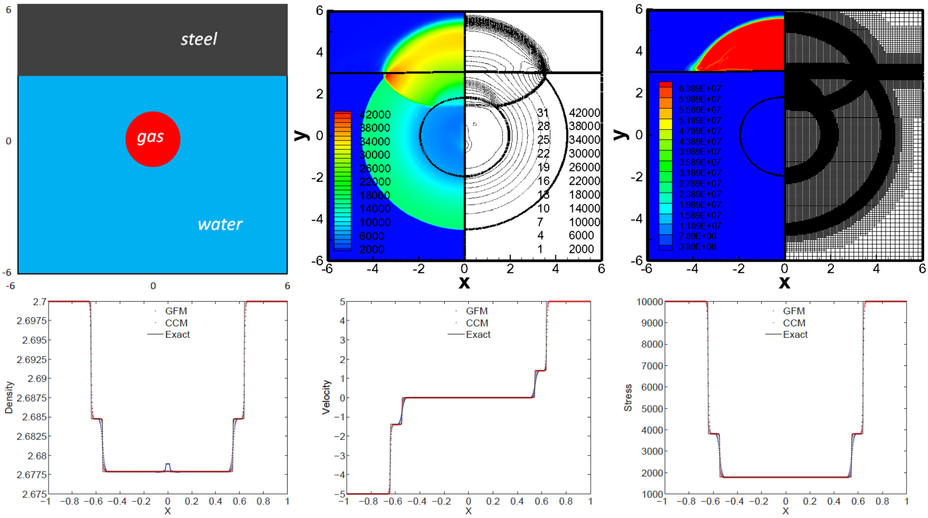
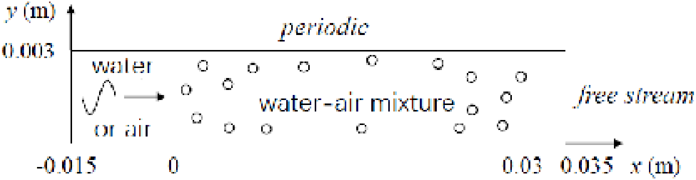
Deng XL: Fluid-Elastic-Perfectly Plastic Interfaces



Deng XL: Sound Speed in Gas-Water Two-Phase Flows



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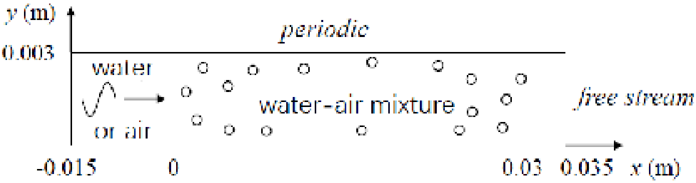
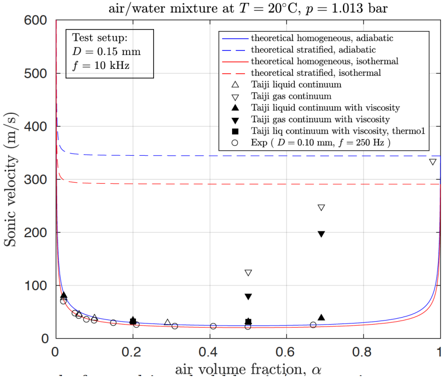
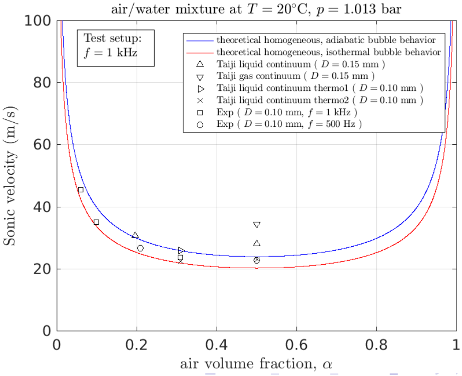


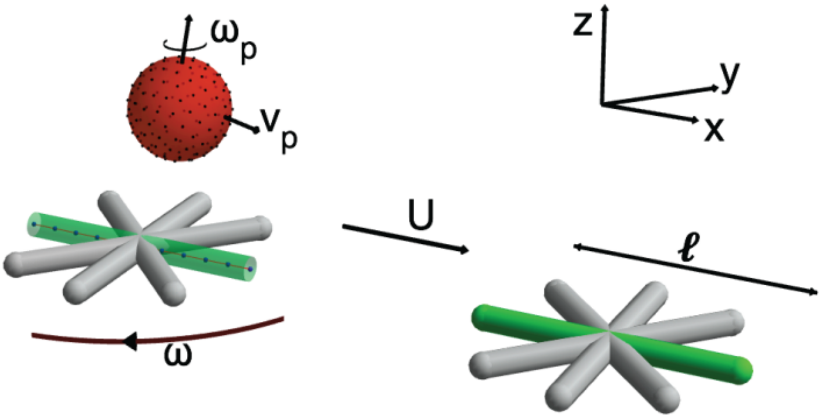




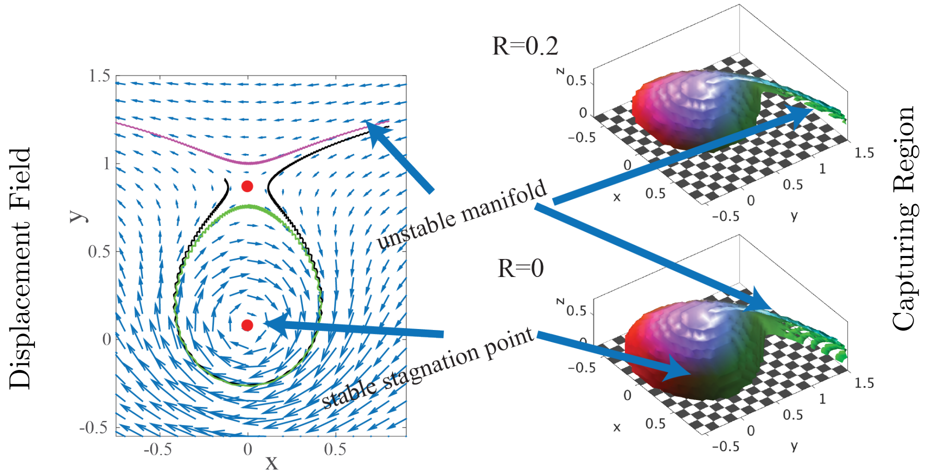
Outline

Ding Y.: Bio/Micro-Fluidics

Numerical study of particle-trapping and transport by a nano-wire:[1]



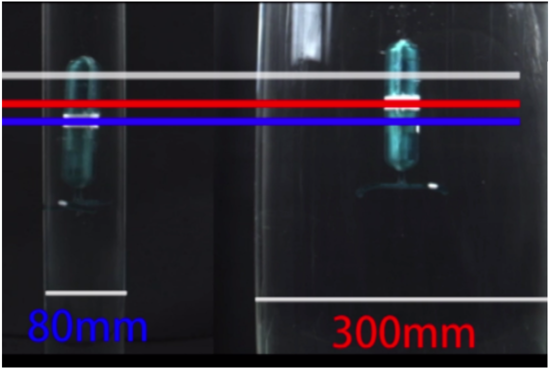
[1] In collaboration with L. Zhao (CWRU) and L. Zhang (CHKU).

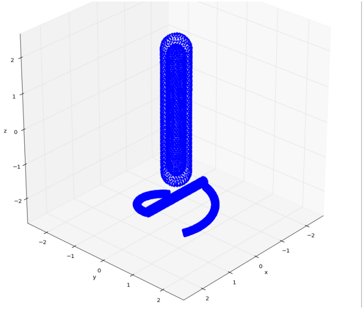


Displacement Field
1.5
1
0.5
0
-0.5
y
-0.5
0
0.5
x
unstable manifold
stable stagnation point
R=0.2
R=0
z
0.5
0
-0.5
0
x
0.5
-0.5
0
0.5
1
1.5
y
Capturing Region

Ding Y.: Bia/Active Fluids

Experimental and numerical study of helix swimmers inside a tube





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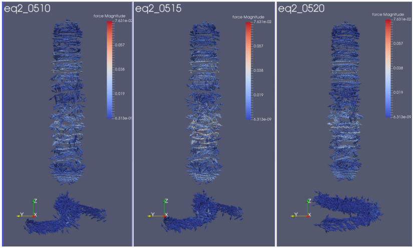

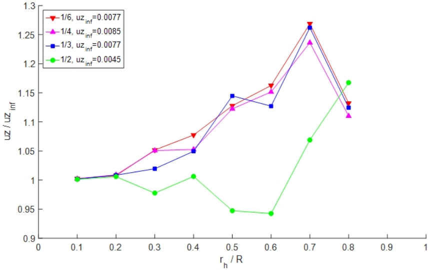

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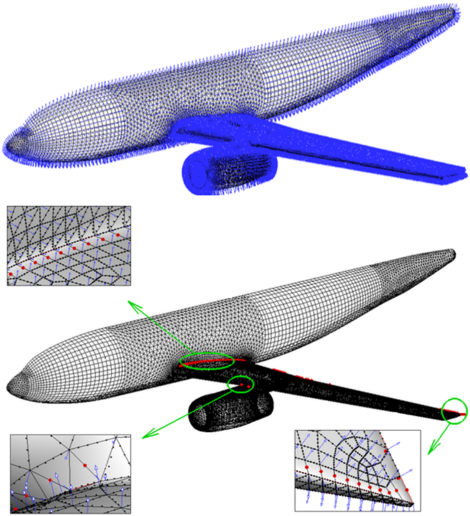
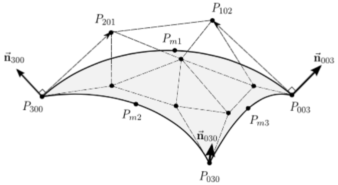
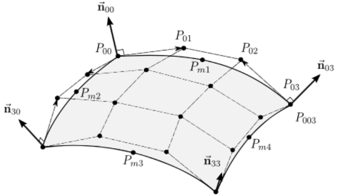
Li Shujie: High-Order Methods on HPC





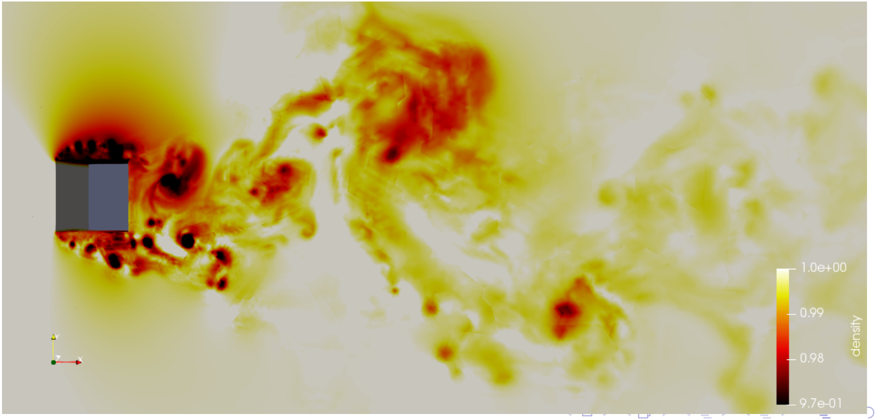
(a) Bézier triangle



(b) Bézier quadrilateral

Li Shujie: High-Order Methods on HPC

- Predictor-Corrector Exponential time integrator scheme (PCEXP) extented to simulate 3D NS equations with varible accuracy
- Implicit LES of turbulence flow past a square cylinder at $\mathrm{Re} = 2,2000$



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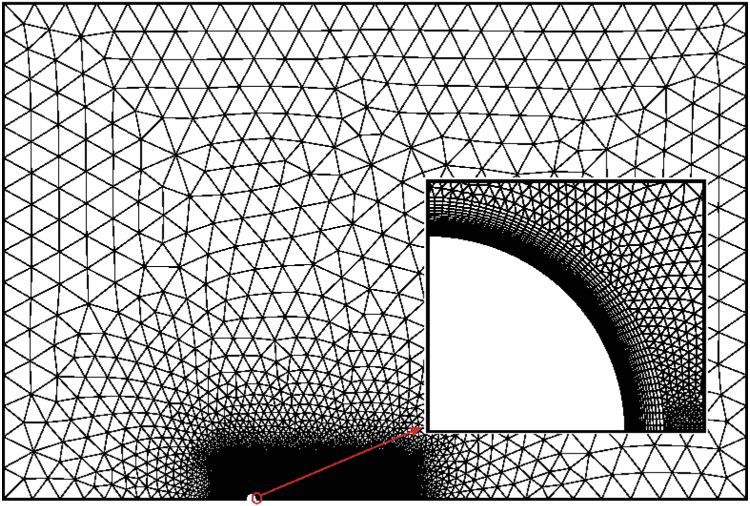
Li WD (李维东): FV-LBE on Unstructured Mesh

Explicit and implicit LBE-FV method on unstructured meshes:[2]



[2] W.D. Li & L.-S. Luo. Commu. Comput. Phys. **20**(2):301–324 (2016); J. Comput. Phys. **327**:503–518 (2016).

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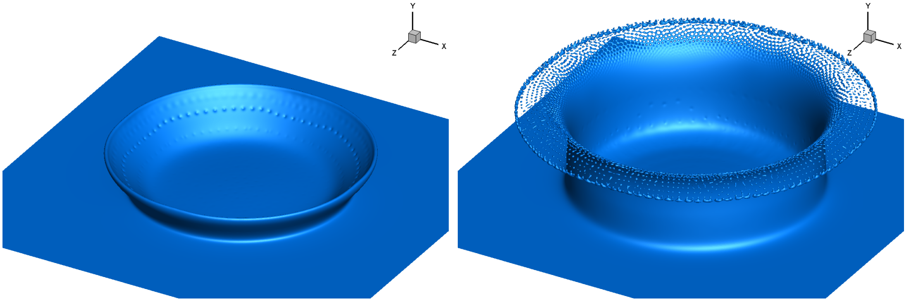
Luo LS: Drop Splashing on a Wet Surface



(a) (b)

Drop impact on a wet surface at $t^* = 2.0$, $R_\rho = 500$, $\mathrm{We} = 8000$, $\mathrm{Re} = 1000$. (a) $R_\mu = 400$; (b) $R_\mu = 40$.

Droplet Coalescence: Simulation *vs.* Experiment

LB numerical *vs.* experimental results

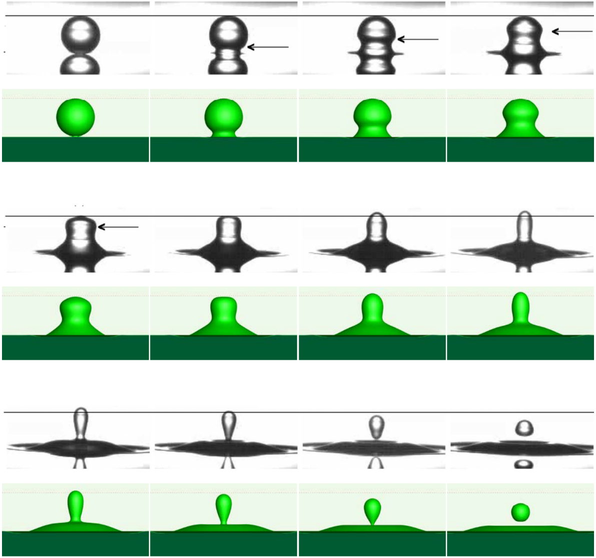
$R_\rho = 1.316$

$R_\mu = 0.5$

$\mathrm{Bo} = 9.59 \times 10^{-2}$

$\mathrm{Oh} = 5.53 \times 10^{-3}$

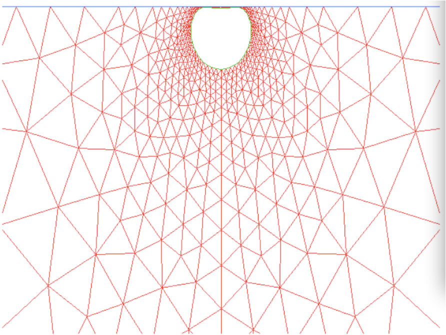
The evolution in $0 \leq t^* \leq 0.890$ with time increament $\Delta t^* = 0.081$, which corresponds to 542 microseconds in experiments [Chen, Mandre, Feng. Phys. Fluids **18**:051705 (2006)].



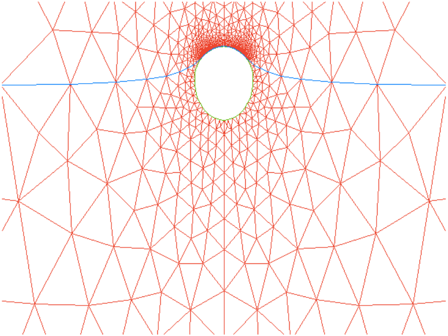
Simulation: Bubble Interact with Interfaces

Objective: To study thin films between interfaces ...

(a) bubble interact with wall



(b) interact with an interface



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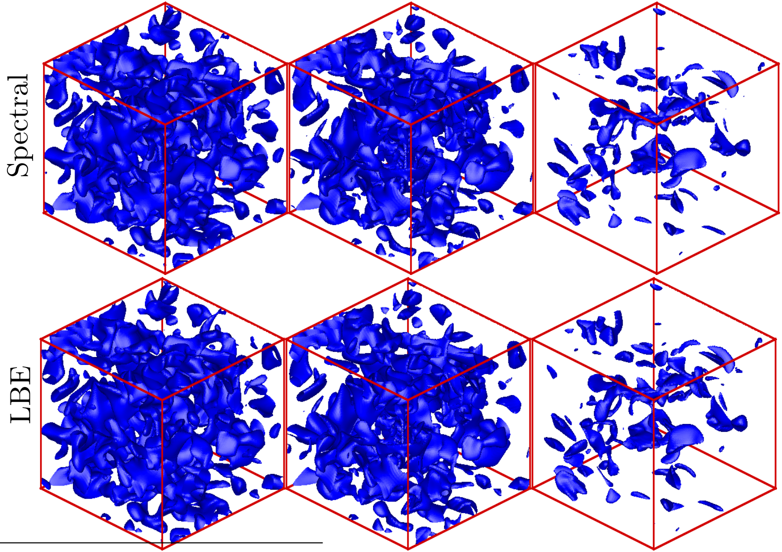
Decaying Homogenous Isotropic Turbulence $\mathrm{Re}_\lambda = 24.37$

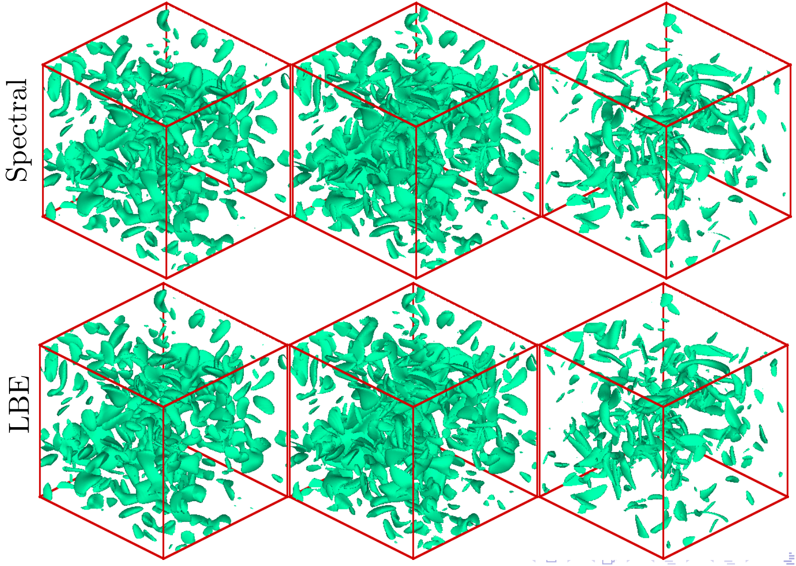
iso-surface of $\|\boldsymbol{u}(t')/u'\| = 2.0$ at $t' = 0.1348$, 0.2359, 0.573:[3]



[3] Y. Peng, W. Liao, L.-S. Luo, L.-P. Wang. Comput. Fluids **39**(4):568–591 (2010).

Decaying Homogenous Isotropic Turbulence $\mathrm{Re}_\lambda = 24.37$

iso-surface of $\|\boldsymbol{\omega}(t')/u'\| = 13.0$ at $t' = 0.1348$, 0.2359, 0.573:



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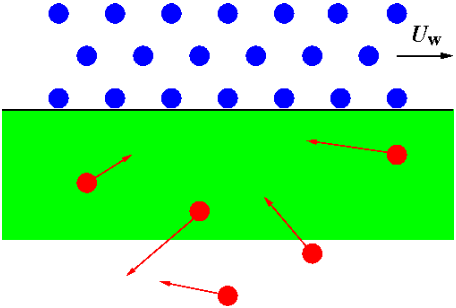
Isothermal Rarefied Couette Flows

Two parallel plate of separation H moving in opposite directions with speed U_{w}, gas and wall molecules are Argon ones with 12-6 Lennard-Jones potential:

$$V(r^*) = 4\epsilon\left(\frac{1}{r^{*12}} - \frac{1}{r^{*6}}\right), \quad r^* := \frac{r_{ij}}{\sigma} = \frac{\|\boldsymbol{r}_i - \boldsymbol{r}_j\|}{\sigma} \tag{1}$$



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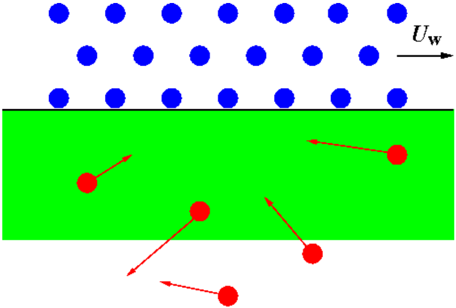
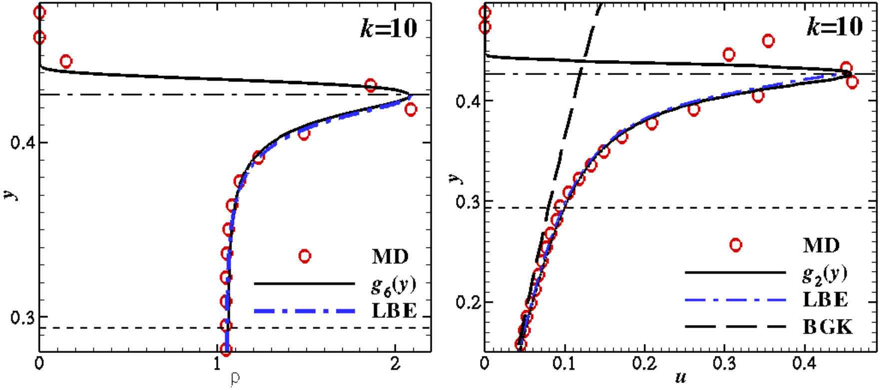


Multi-scale Features:

- Near the walls (greed region) $\left(\frac{1}{2} \geq y \geq \frac{1}{2} - \frac{3\sigma}{2H}\right)$: van der Waals forces dominant molecular flow (σ, ϵ)
- Away from the walls $\left(\frac{H-3\sigma}{2H} \geq y \geq \frac{3\sigma-H}{2H}\right)$: a kinetic problem ($\ell$, Kn)

The results of MD, LBE, and the linearized Boltzmann equation:[4]



CPU times:

MD $\sim O(\text{day}) \gg$ Linearized BE $\approx O(\text{hour}) \gg$ LBE $\lesssim O(\text{minute})$

[4] W. Li, L.-S. Luo, J. Shen. Comput. Fluids **111**:18–32 (2015).

Results: $k = 1.0$

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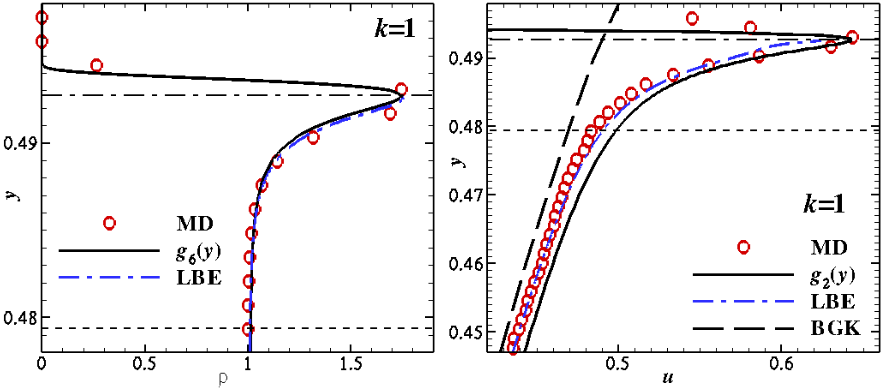

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Thanks! Questions?