2017 NETL Workshop on Multiphase Flow

Statistical Analysis on Large-scale Direct Numerical Simulation of Gas-solid Flow

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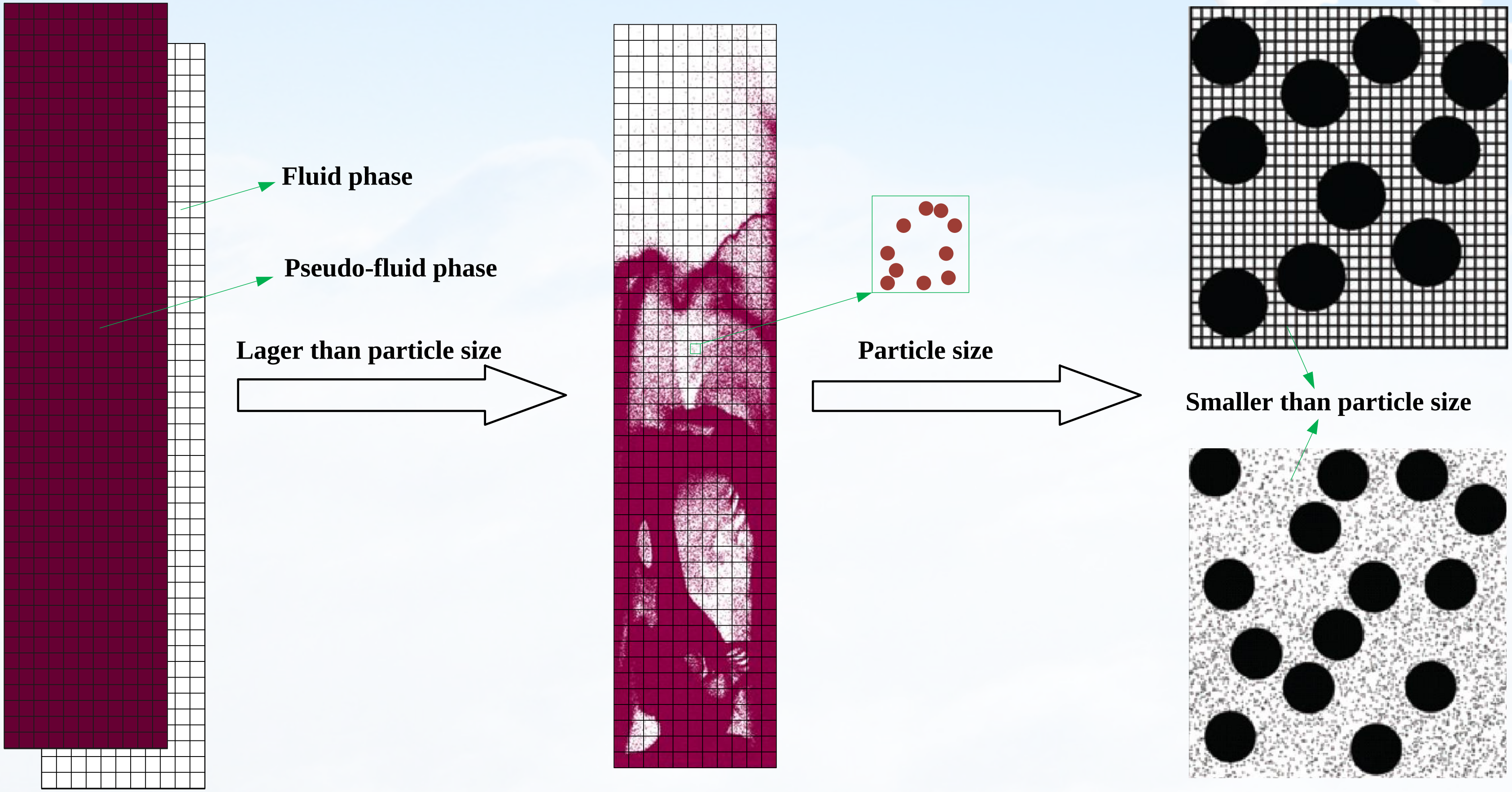
Morgantown, WV ·2017.8.8

Outline

- → **Background**
- **Enabling Large-scale DNS**
- **Numerical Results**
- **Conclusions**

Multi-scale Modelling for Gas-solid Flow



Fluid phase

Pseudo-fluid phase

Lager than particle size

Particle size

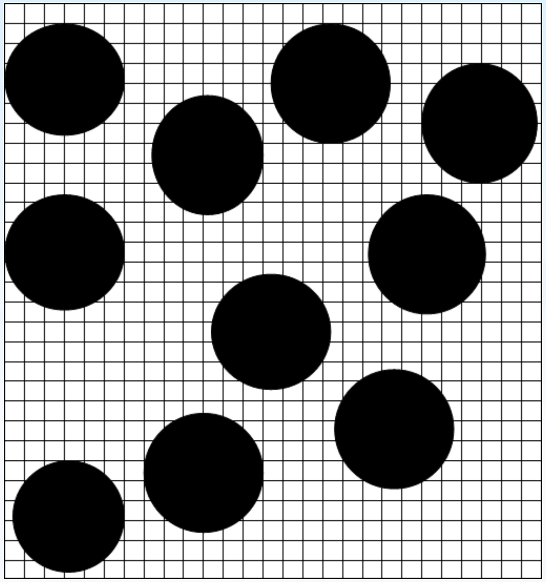
Smaller than particle size

Two-fluid Model
(TFM)

Discrete Particle Model
(DPM or CFD-DEM)

Direct Numerical Simulation
(DNS)

Particle-resolved DNS

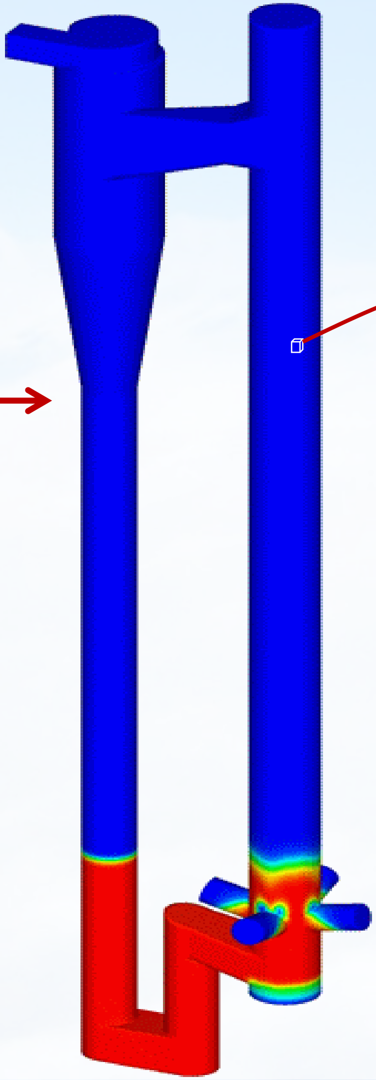


Computational grid $h \ll d_p$ **Particle diameter**

The mesh is reduced to below the size of particle, and the flow field around particle is fully resolved. The fluid-solid interaction force is directly obtained by integrating the viscous stress on the surface of the particles.

DNS can be regarded as the most accurate method, but it's huge computational cost leads to small-scale simulation domain

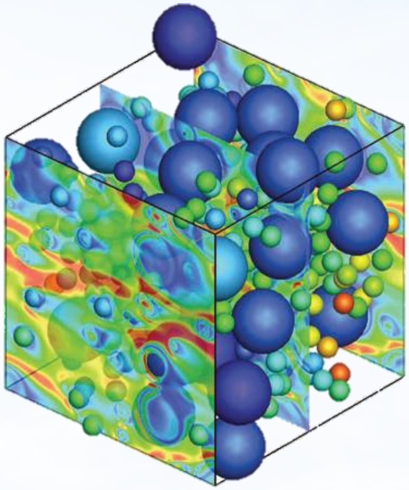
DNS *VS* Real Constitutive Laws



Real gas-solid flows

A computational grid

$N_p \sim O(10^5)$

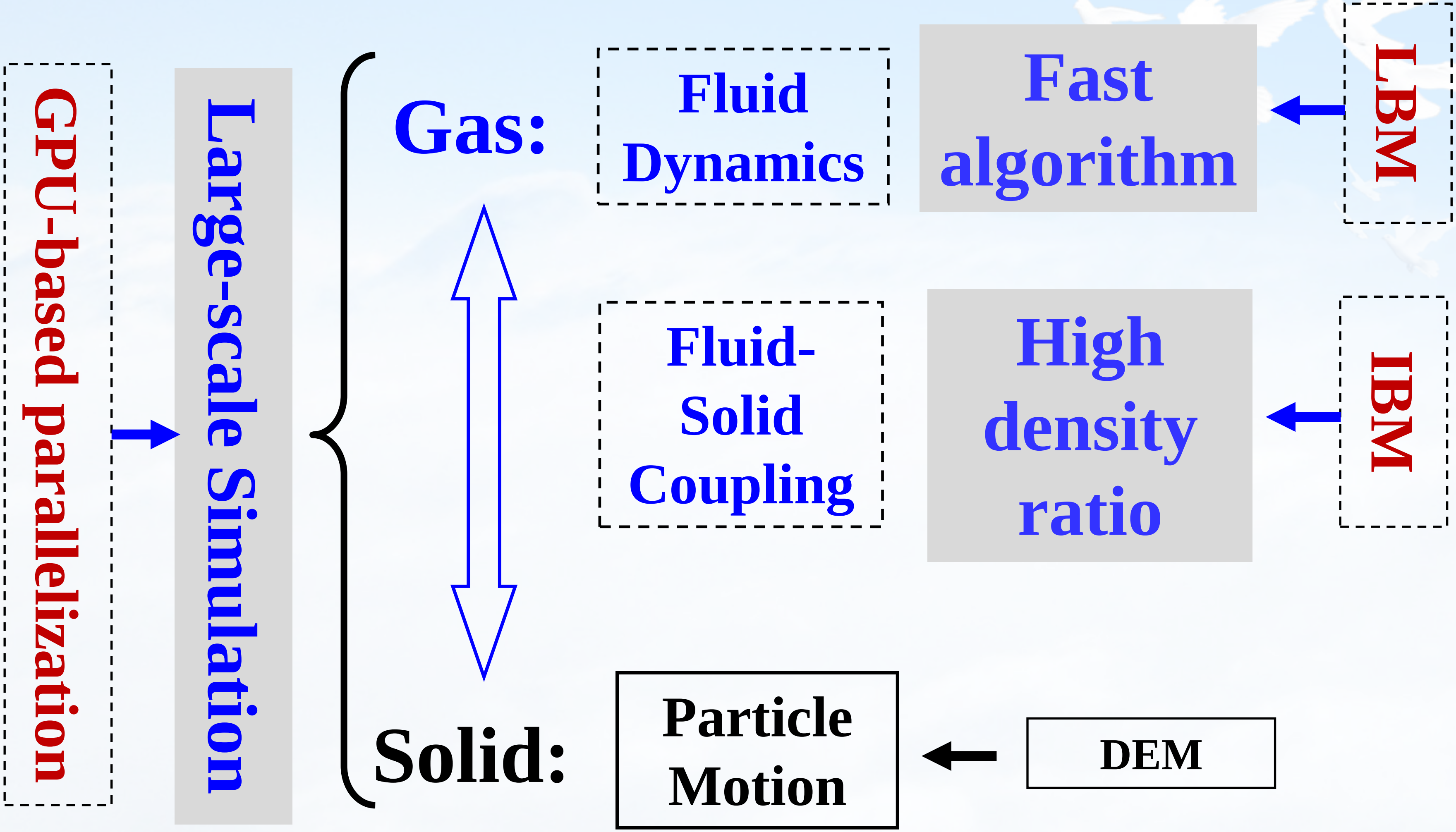


(S Tenneti , S Subramaniam. ***Annu. Rev. Fluid Mech.*** 2014, 46:277-286)

Particle-resolved DNS

$N_p \sim O(10^2)$

Strategies for Enabling Large-scale DNS



GPU-based parallelization

Large-scale Simulation

Gas:

Fluid Dynamics

Fast algorithm

LBM

Fluid-Solid Coupling

High density ratio

IBM

Solid:

Particle Motion

DEM

Wang L*, Zhou G, et.al. ***Particuology***, 2010, 8(4): 379-382.

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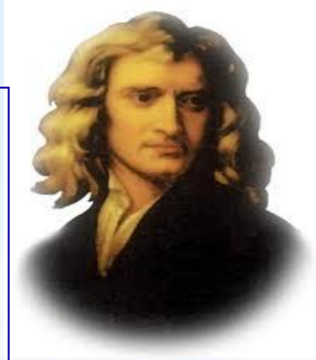
Discrete Modeling of Particle-Fluid System

Particle

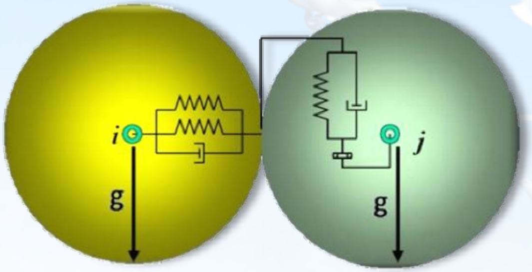


Issac Newton
(1643.1.4-1727.3.31)

Newton's second law

$$\mathbf{F}=m\mathbf{a}$$

Inter-particle collision



Gas

Ludwig Edward Boltzmann
(1844.2.20-1906.9.5)

Boltzmann equation

$$\frac{Df}{Dt}=\frac{\partial f\left(t,\mathbf{x},\mathbf{v}\right)}{\partial t}+\mathbf{v}\frac{\partial f\left(t,\mathbf{x},\mathbf{v}\right)}{\partial \mathbf{x}}=\Omega$$

Discrete form

$$f\left(\mathbf{x}+\mathbf{e}_i\Delta t,t+\Delta t\right)-f\left(\mathbf{x},t\right)=\Omega_i$$

Strategy 1
LBM

Improved Solution for Gas Flow

Navier-stokes equation

$$\rho \frac{d\mathbf{u}}{dt} = -\nabla p + \mu \Delta \mathbf{u} + \rho g$$

Implicit, Serial, Euler

parallelization

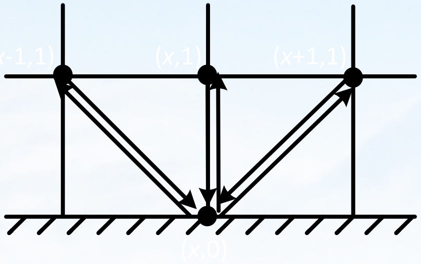
Lattice Boltzmann equation

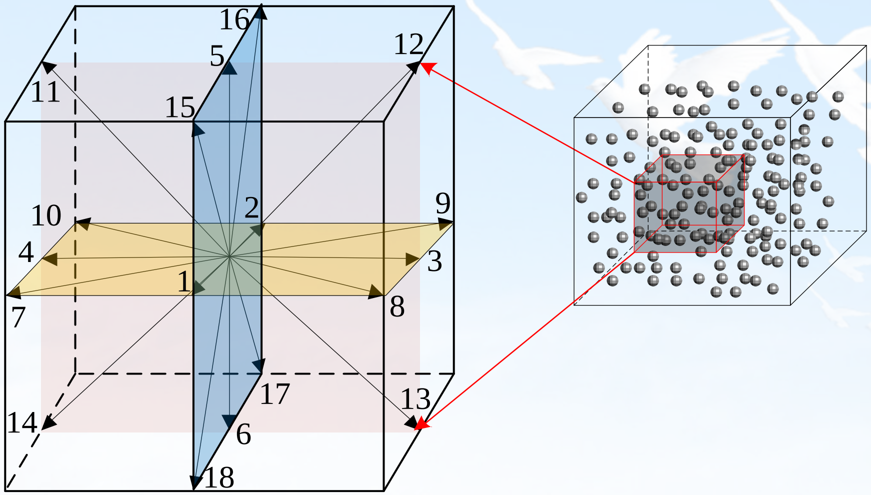
$$f\left(\boldsymbol{x} + \boldsymbol{e}_i \Delta t, t + \Delta t\right) - f\left(\boldsymbol{x}, t\right) = \Omega_i$$

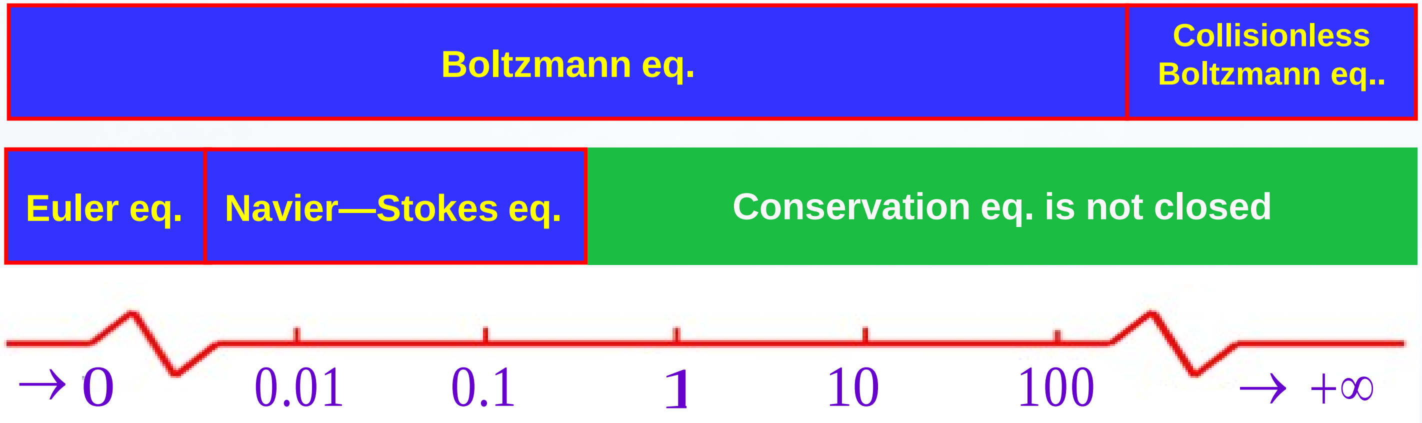
Explicit, Parallel, Lagrange

Lattice Boltzmann method

Simple rule:
bounce-back boundary condition







Molecular Model

Boltzmann eq.

Collisionless Boltzmann eq..

Continuous Model

Euler eq.

Navier—Stokes eq.

Conservation eq. is not closed

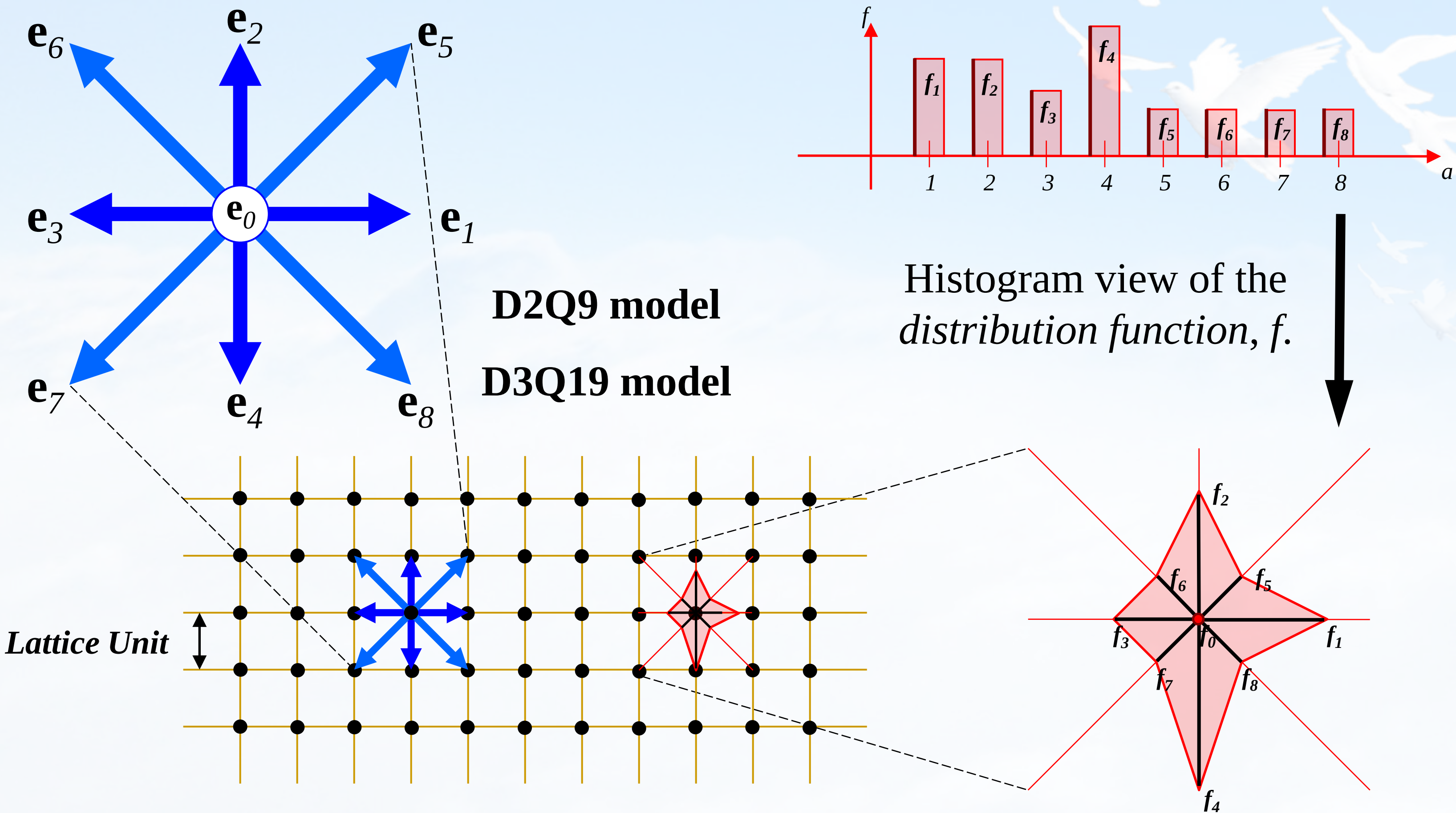
$$Kn = \frac{\bar{\lambda}}{L}$$

→ 0 | 0.01 | 0.1 | 1 | 10 | 100 | → +∞

Inviscid flow

Free molecular flow

Collision and Streaming Steps



D2Q9 model

D3Q19 model

Histogram view of the *distribution function*, *f*.

Discrete velocities $\mathbf{e}_i$

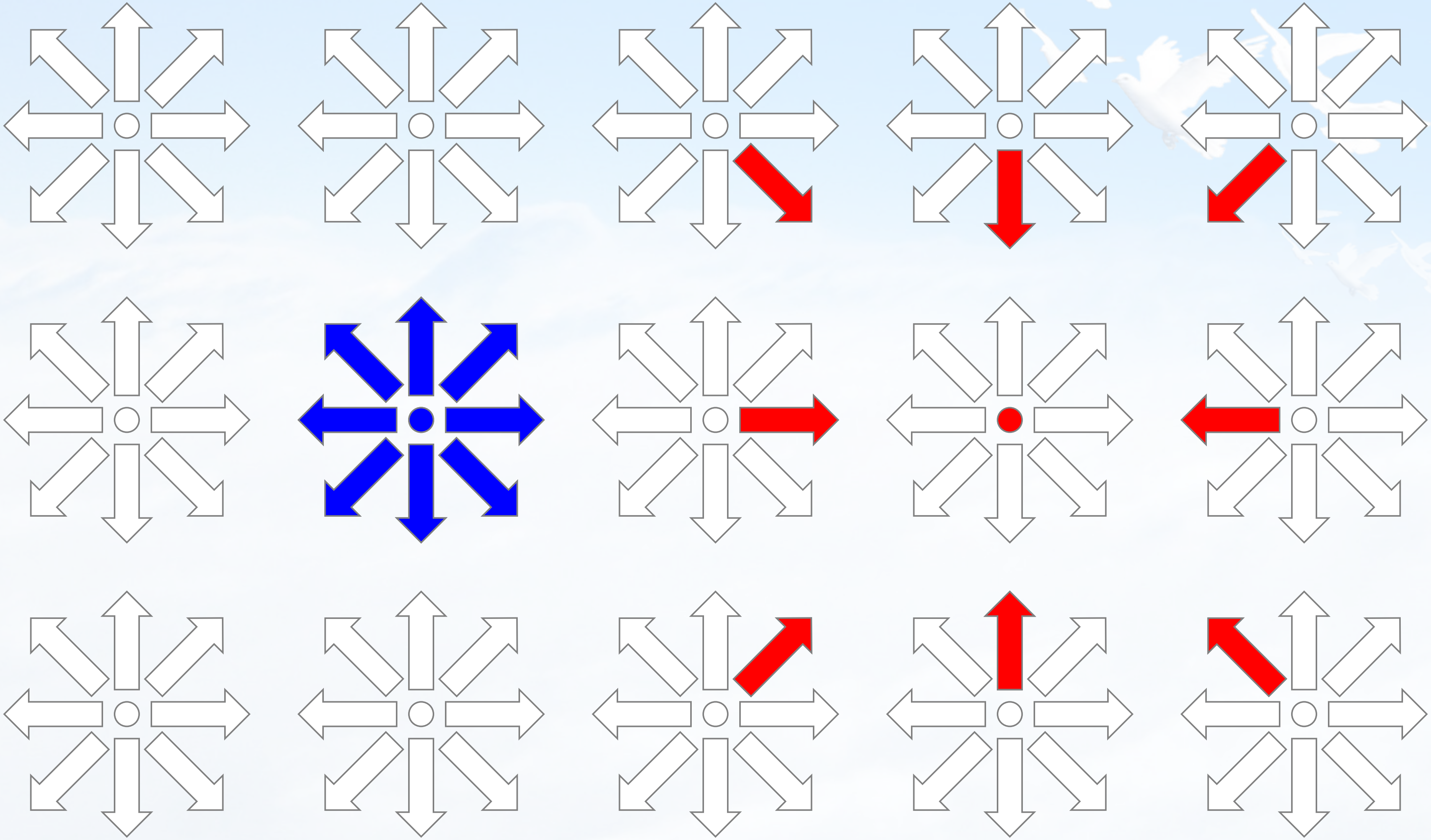
Directional densities f_i

Macroscopic velocity $\mathbf{u} = \frac{1}{\rho}\sum_i \mathbf{e}_i f_i$

Macroscopic density $\rho = \sum_i f_i$

Streaming step

$$f_i\left(\boldsymbol{x}+\mathbf{e}_i\delta_t,\,t+\delta_t\right)=f_i^*\left(\boldsymbol{x},\,t\right)$$

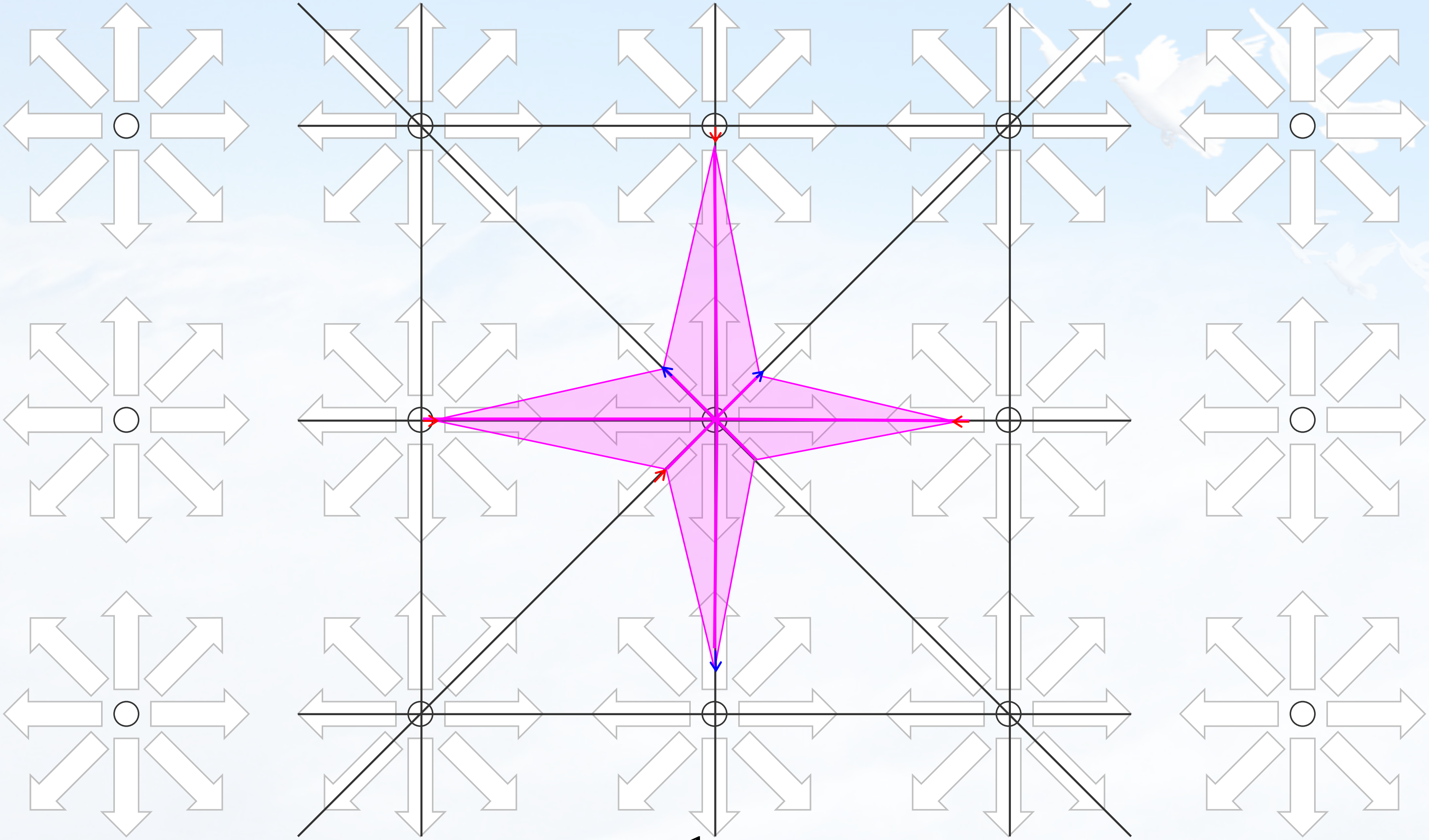


（a） From the node to its neighboring nodes

（b） From the neighboring nodes to local node

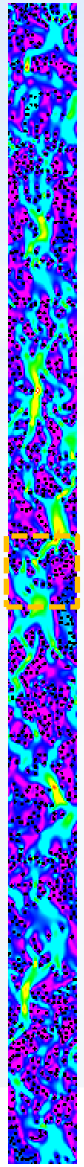
Collision step

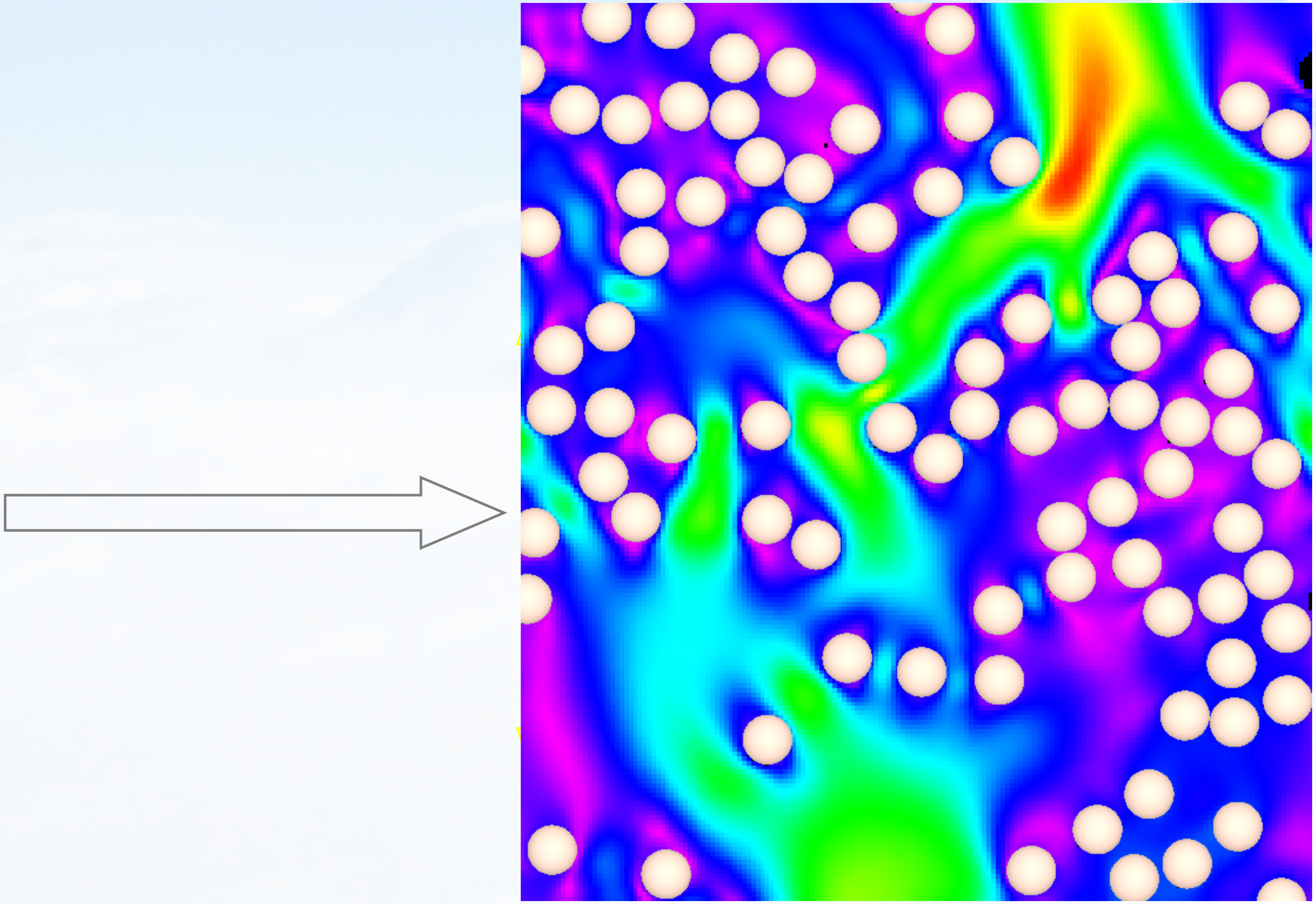
$$f_i^*(x,t) = f_i(x,t) + \frac{1}{\tau}\left[f_i^{eq}(x,t) - f_i(x,t)\right]$$



Calculate f f^{eq} $\frac{1}{\tau}\left[f_i^{eq}(\mathbf{x},t) - f_i(\mathbf{x},t)\right]$

Computation’s Speedup 3000x





Traditional algorithm: 1024 particles, 1024CPU takes one month

New algorithm: 1400 particles, single CPU takes 7 days!

Strategy 2
IBM

Immersed Boundary Method

$$f_i\left(\mathbf{x}+\mathbf{e}_i\Delta t,t+\Delta t\right)=f_i\left(\mathbf{x},t\right)+\frac{1}{\tau}\left(1-\beta\left(\varepsilon_s,\tau\right)\right)\left(f_i^{eq}\left(\rho,\mathbf{v}\right)-f_i\left(\mathbf{x},t\right)\right)+\beta\left(\varepsilon_s,\tau\right)\Omega_i^s$$

Weighting function

Additional collision term

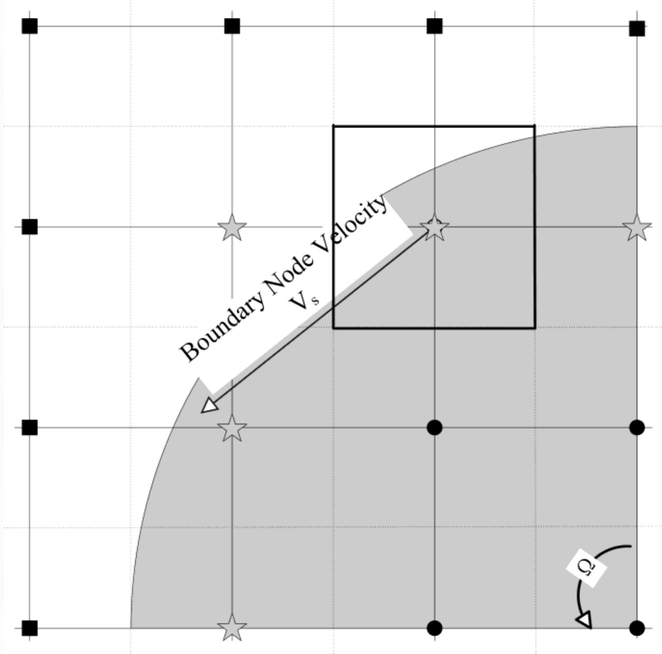
Weighting function

$$\beta\left(\varepsilon_s,\tau\right)=\frac{\varepsilon_s\left(\tau-0.5\right)}{\left(1-\varepsilon_s\right)+\left(\tau-0.5\right)}$$

Additional collision term

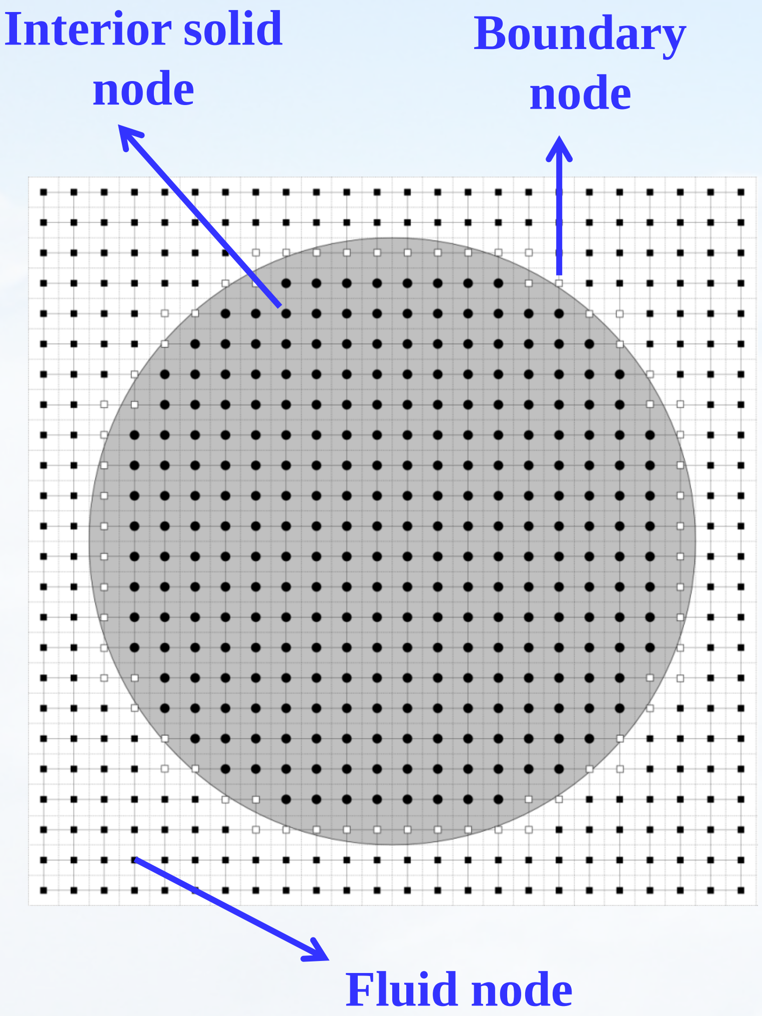
$$\Omega_i^s=f_{-i}\left(\mathbf{x},t\right)-f_i\left(\mathbf{x},t\right)+f_i^{eq}\left(\rho,\mathbf{V}_s\right)-f_{-i}^{eq}\left(\rho,\mathbf{v}\right)$$

Solid volume fraction $\varepsilon_s=\dfrac{V_{solid}}{V_{cell}}$



Noble D R, Torczynski J R. *Int. J. Mod. Phys. C*, 1998. 9:1189-1201

Fluid-structure Interactions



Force acting on particle:

$$\mathbf{F}_{f\to p}=\frac{h^2}{\Delta t}\sum_{j=1}^{n}\left(\beta_j\sum_{i=1}^{8}\Omega_i^s\mathbf{e}_i\right)$$

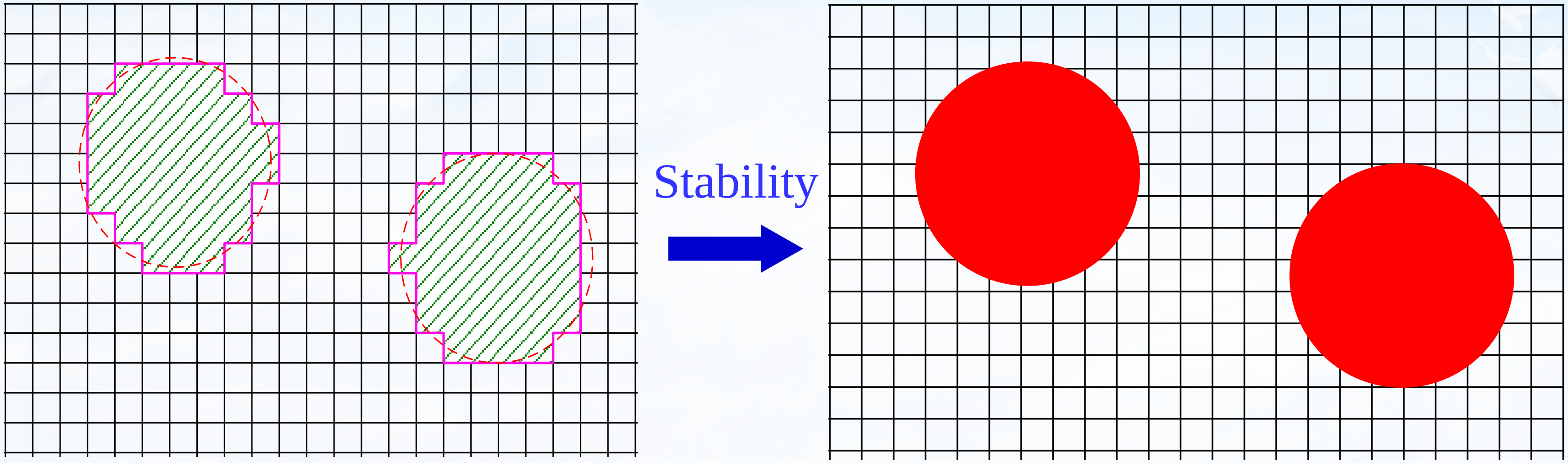
Fluid-induced torque:

$$\mathbf{T}_{f\to p}=\frac{h^2}{\Delta t}\sum_{j=1}^{n}\left(\left(\mathbf{x}_j-\mathbf{x}_c\right)\times\beta_j\sum_{i=1}^{8}\Omega_i^s\mathbf{e}_i\right)$$

Enhance Stability of Parallel Algorithm

Traditional link-based LBM method
(Ladd A.J.C., J. Fluid Mech. 1994,271:311-339)

Our proposed LBM-DEM method



Gas-solid **$\Delta t<10^{-8}$s**

$\Delta t \sim 10^{-6}$s

Time step by 100 times

Wang Limin*, Zhou Guofeng, Wang Xiaowei, Xiong Qingang, Ge Wei. ***Particuology*,** 2010, 8(4): 379-382.
Zhou Guofeng, **Wang Limin*,** Wang Xiaowei, Ge Wei*. ***Phys. Rev. E***, 2011, 84(6): 066701.

Strategy 3
GPU

Large-scale GPU Parallel Computing

Mole-8.5 (born on April 24) 2P

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Institute of Process Engineering, Chinese Academy of Sciences

is ranked

9th

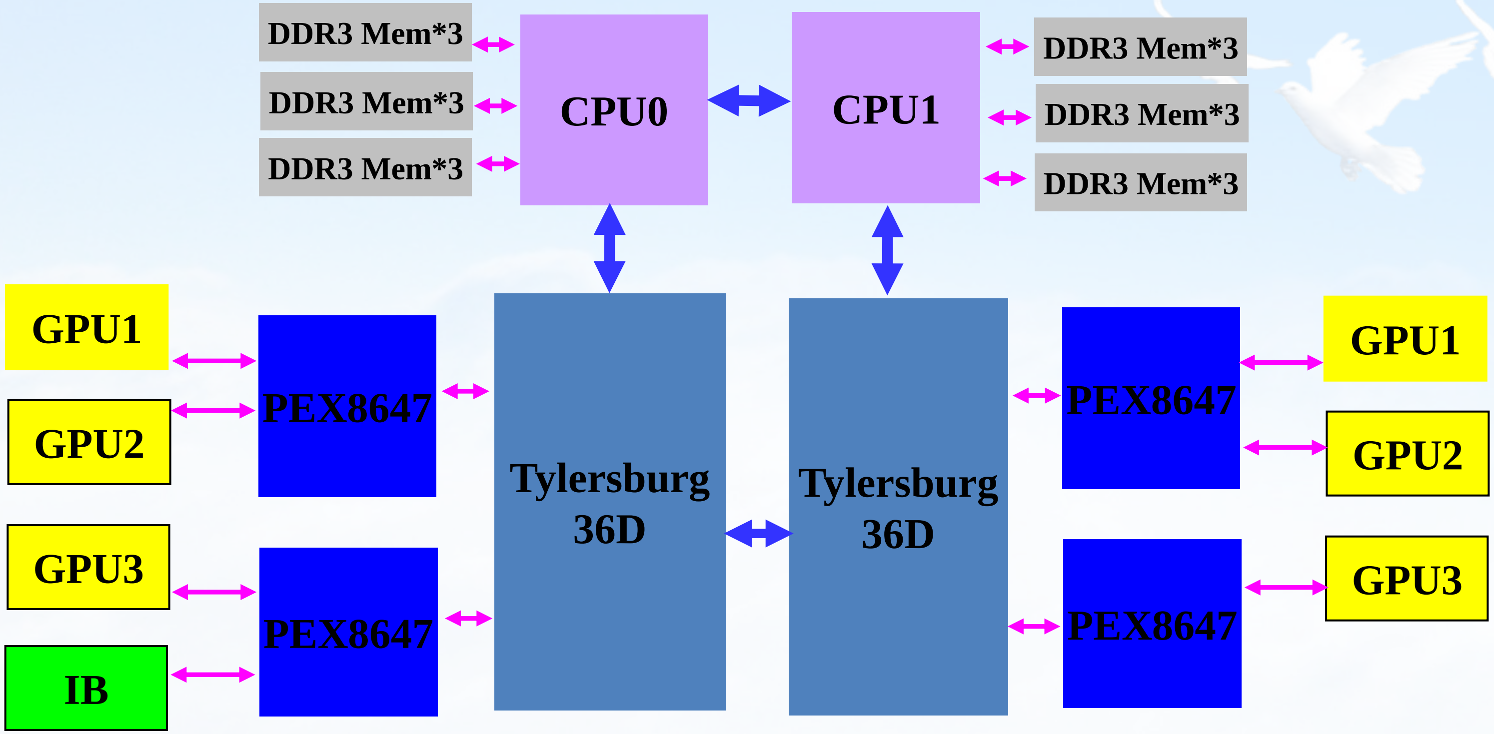
on the world's Green500 List of computer systems as of

November 2011

Wu-chun Feng, Co-Chair
Kirk Cameron, Co-Chair

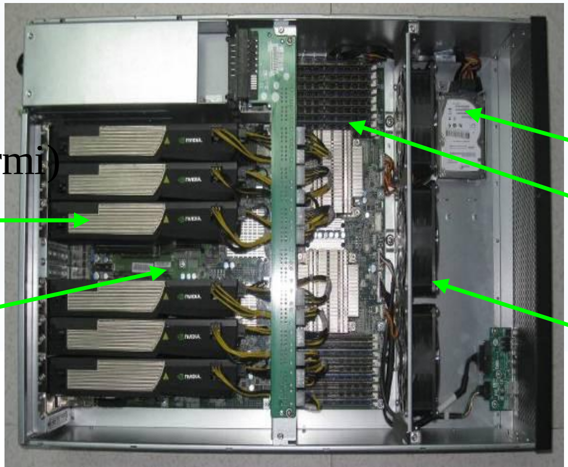
(19th, June 2010, Top500) (9th, Nov 2011, Green500)

Node layout of Mole-8.5



DDR3 Mem*3
DDR3 Mem*3
DDR3 Mem*3
CPU0
CPU1
DDR3 Mem*3
DDR3 Mem*3
DDR3 Mem*3

GPU1
GPU2
GPU3
IB
PEX8647
PEX8647
Tylersburg 36D
Tylersburg 36D
PEX8647
PEX8647
GPU1
GPU2
GPU3



6xC2050 (Fermi)

QDR IB
Tyan S7015

HD
Mem
2xE5520/70
Fan

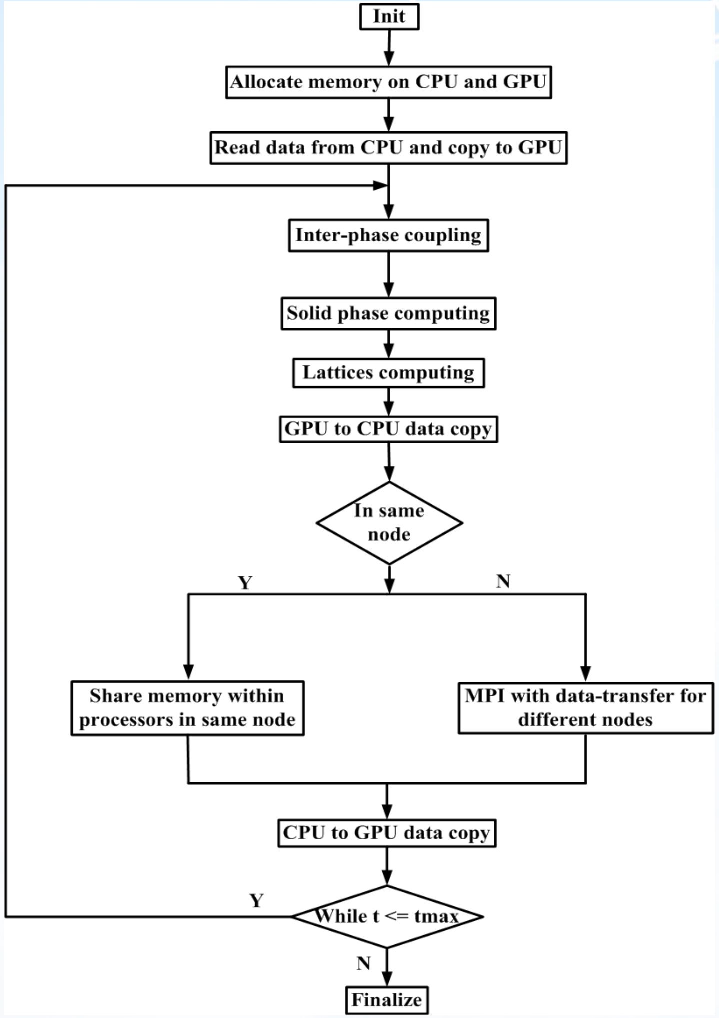
GPU Parallel Implementation

CPU

Center Processing Unit

GPU

Graphic Processing Unit



Flow Chart of GPU implementation

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Performance of GPU vs. CPU

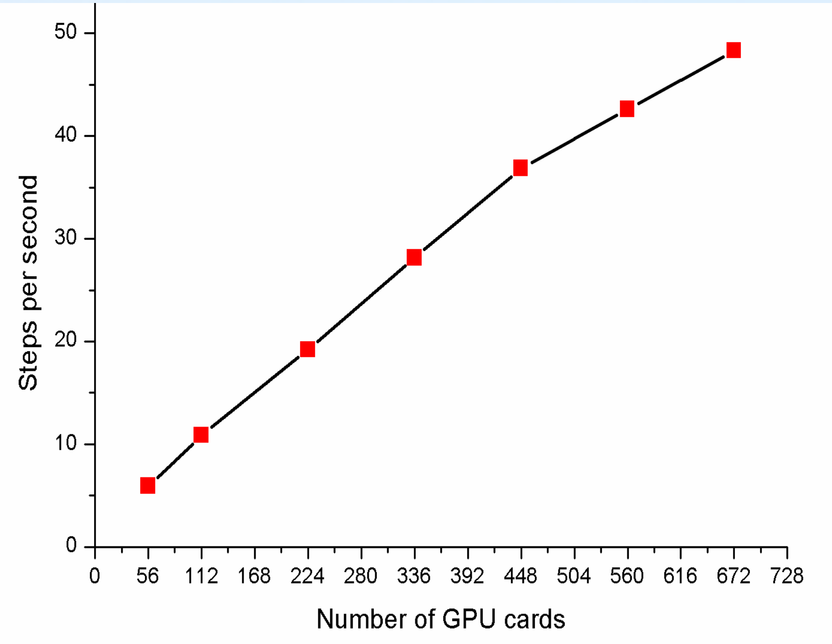
(Single GPU)

D3Q19 LBM-DEM

Domain size (W×H×L)	Steps per second (Fermi GPU)	Steps per second (Intel E5520)	**Speedup**	Perf. (MLUPS) (double precision)
32×64×32	1784.1	65.71	**27.1**	**116.8**
64×64×64	458.6	16.44	**27.9**	**120.2**
64×128×64	237.5	8.167	**29.1**	**124.5**
128×128×128	60.4	2.043	**29.6**	**126.6**
128×256×128	33.3	1.056	**31.5**	**139.8**

***MLUPS: mega-lattice-updates-per-second**

Performance of Large-scale Simulation



D3Q19 TDHS-LBM

(Multi GPUs)

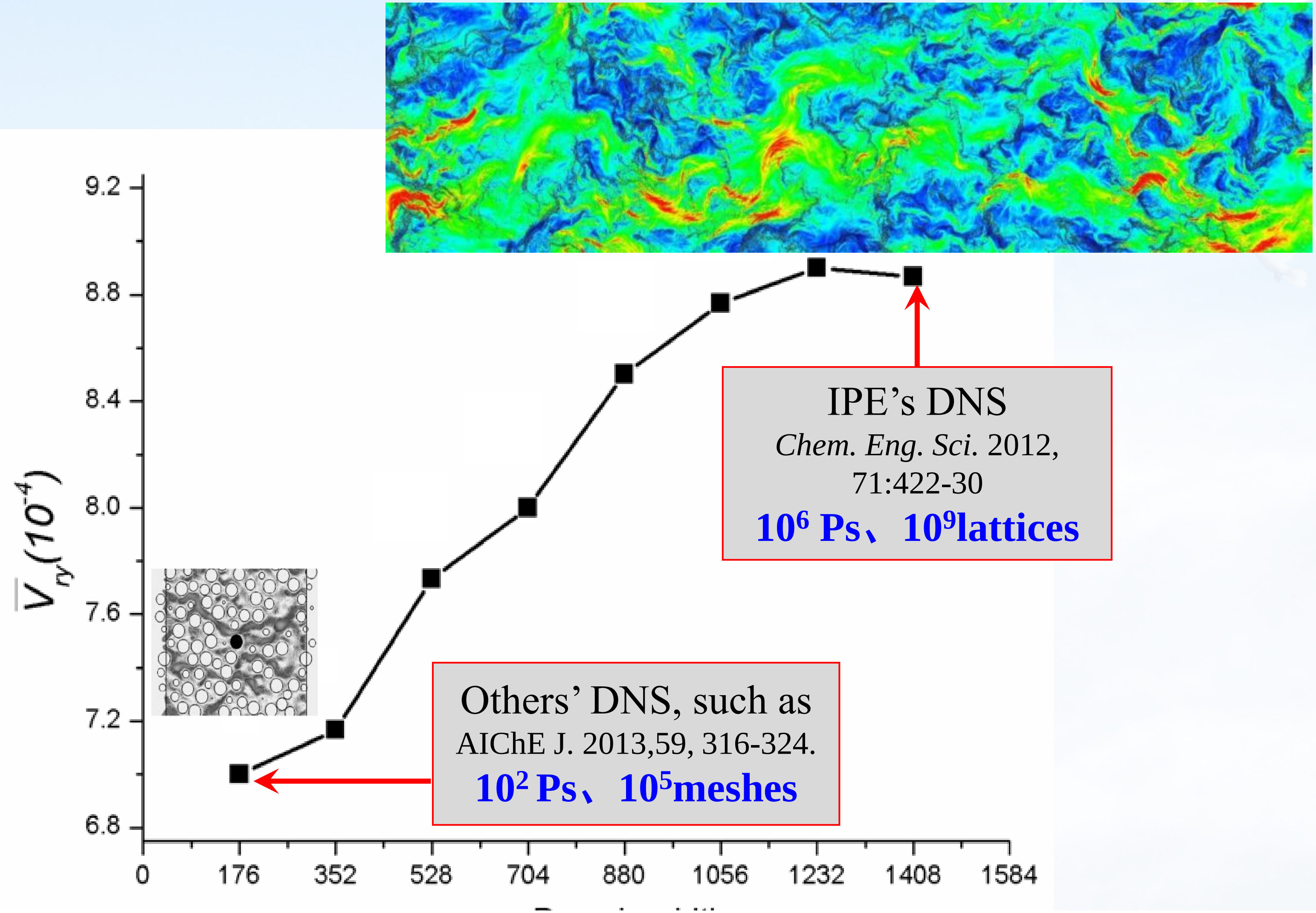
Strong scaling for large-scale gas-solid simulations on Mole-8.5

Case	Lattice	GPU	Steps	Time	Perf. (MLUPS)	Perf./GPU	Gflops
1	1024×1152×1024	8×8×8	2000	100.2	24111	47.1	10558
2	1536×1728×1536	12×12×12	2000	106.2	76741	44.4	33611

The number of float operations per step of case1: 529 Gflop, case2: 1785.6 Gflop

Largest Scale DNS of Gas-solid Suspensions

1M solid particles & 1G fluid lattices @ 576 GPUs



IPE's DNS

Chem. Eng. Sci. 2012, 71:422-30

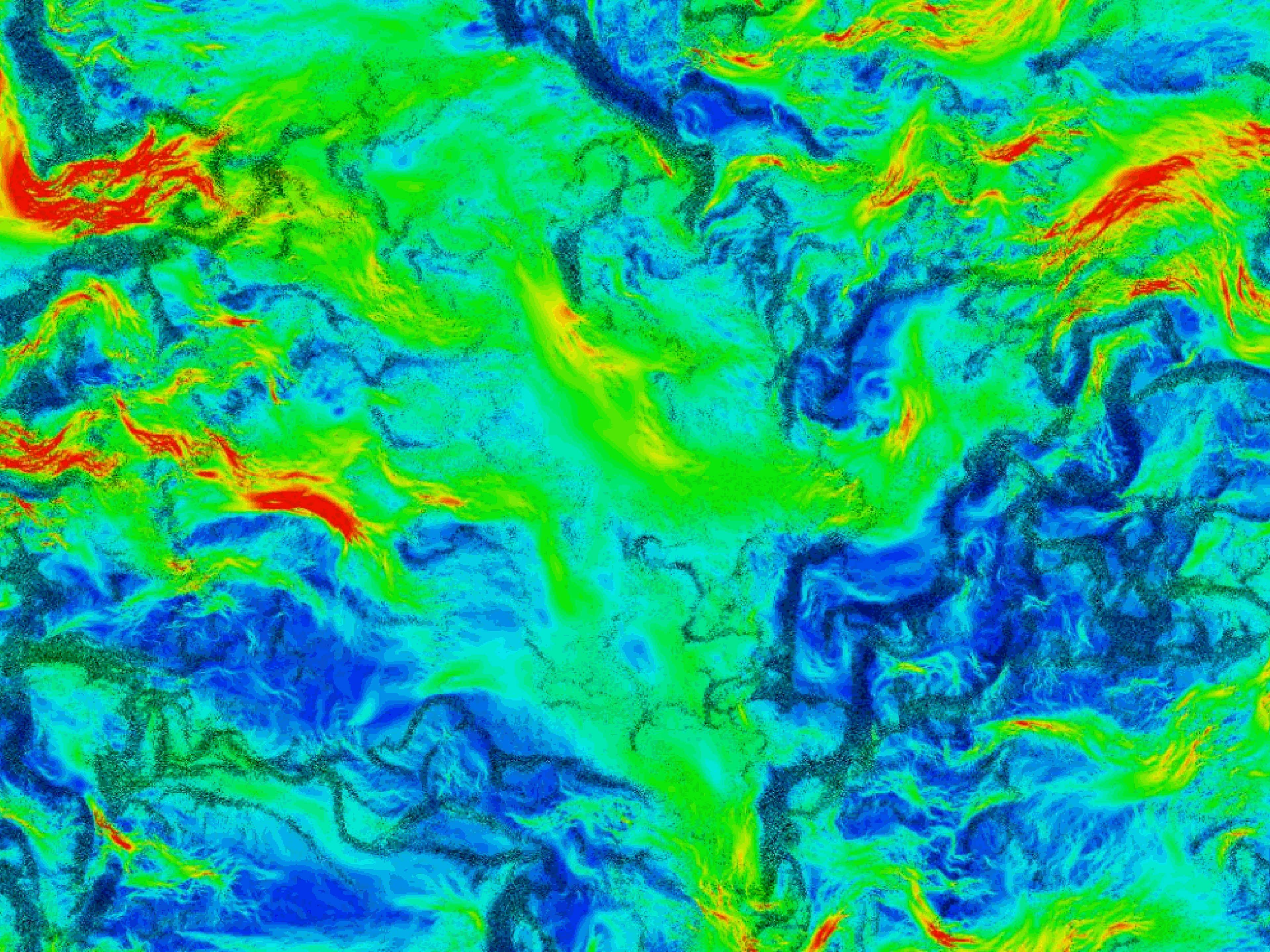
10^6 Ps、10^9lattices

Others' DNS, such as

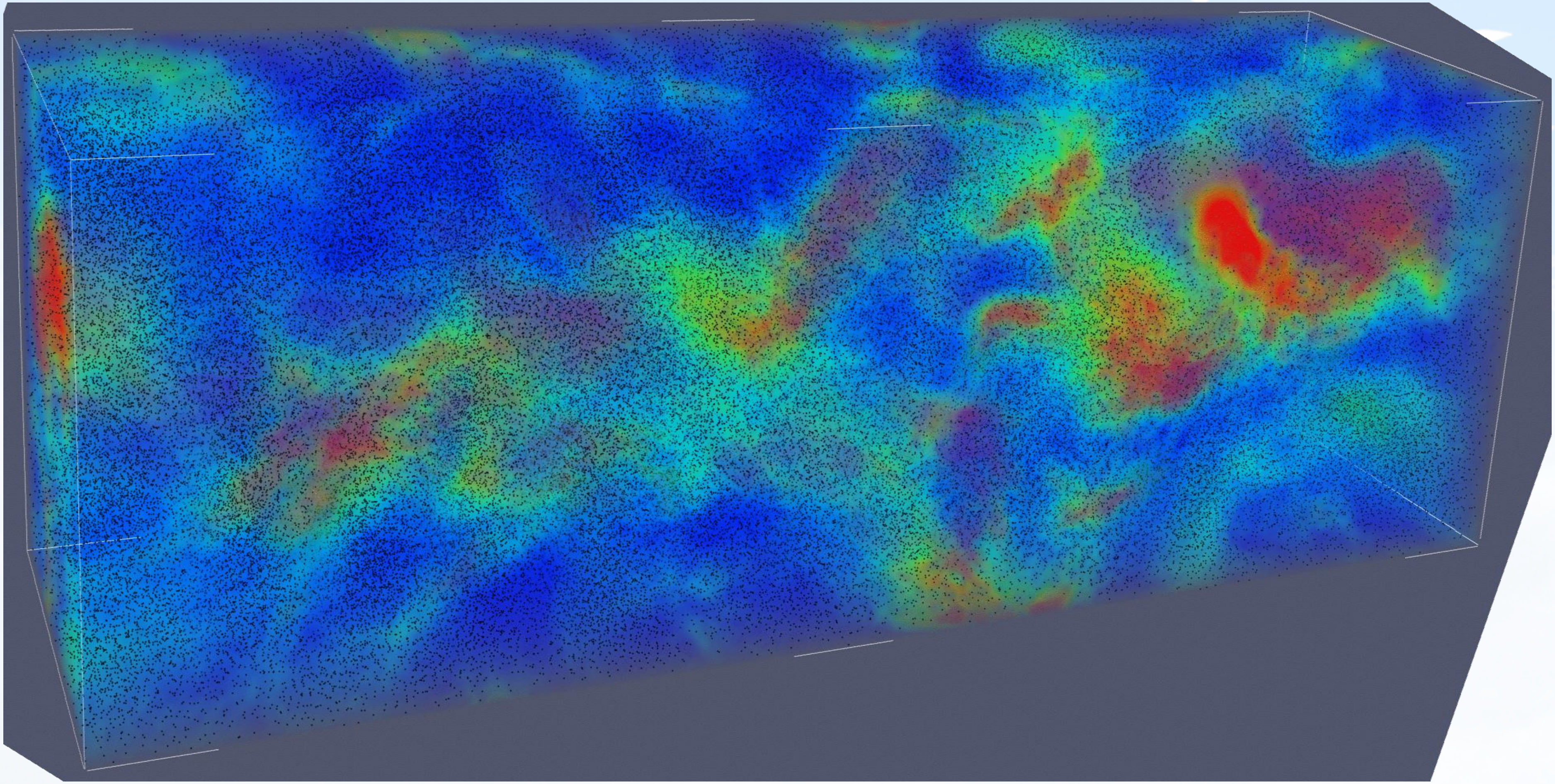
AIChE J. 2013,59, 316-324.

10^2 Ps、10^5meshes

Chem. Eng. Sci., 2011, 66: 4426-4458; ***Chin. Sci. Bull***., 2012, 57:707–715.



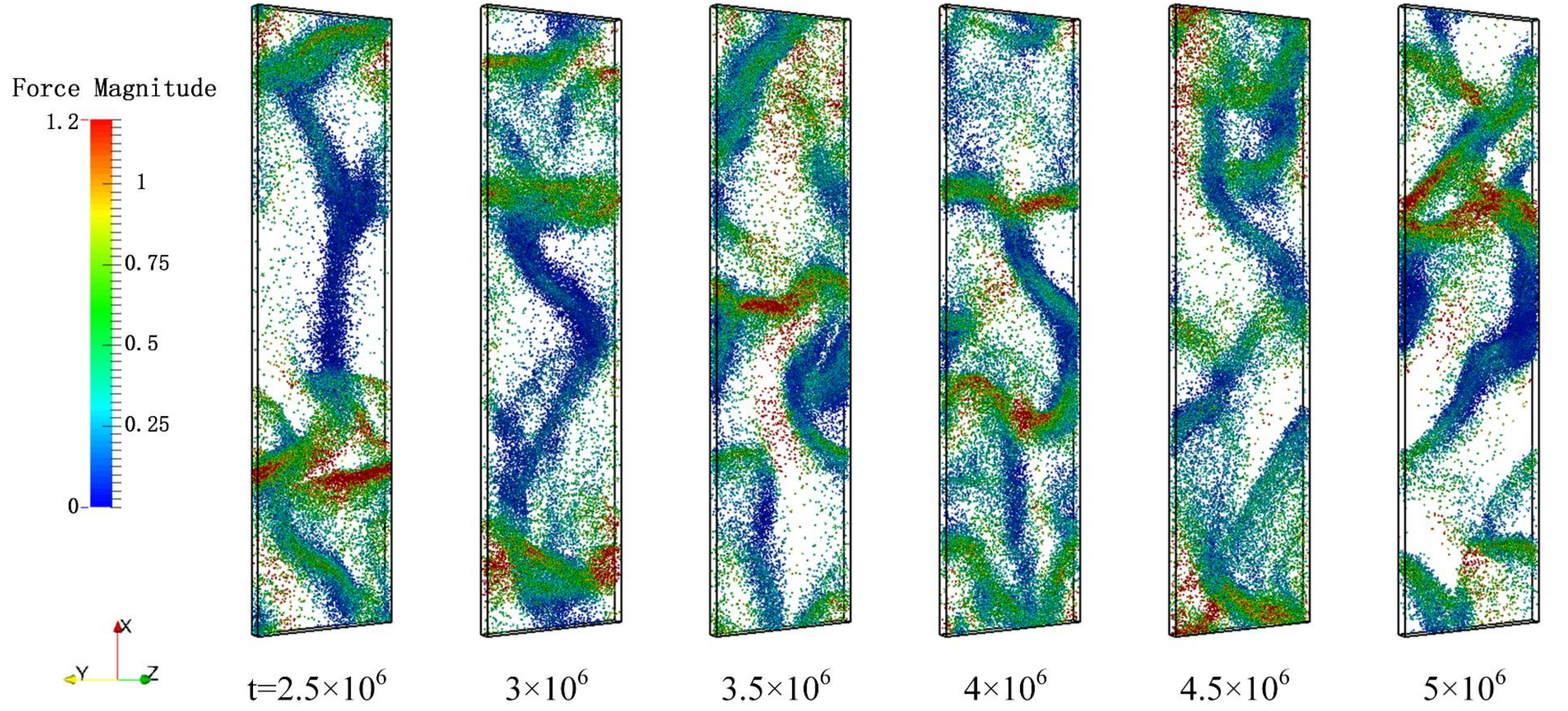
130K solid particles in 3D @ 224 GPUs



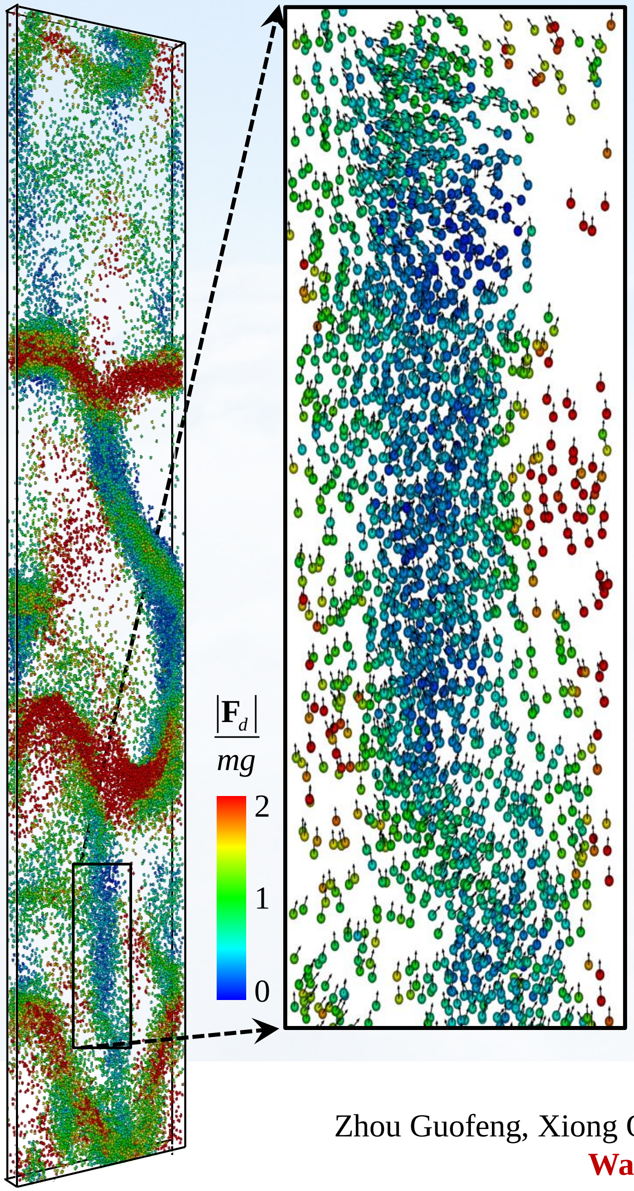
3D: 0.384cm x 1.536cm x 0.384cm, 130000 particles (512 X 2560 X 512)

Xiong et al., 2012, *Chem. Eng. Sci.*, 67:422-430

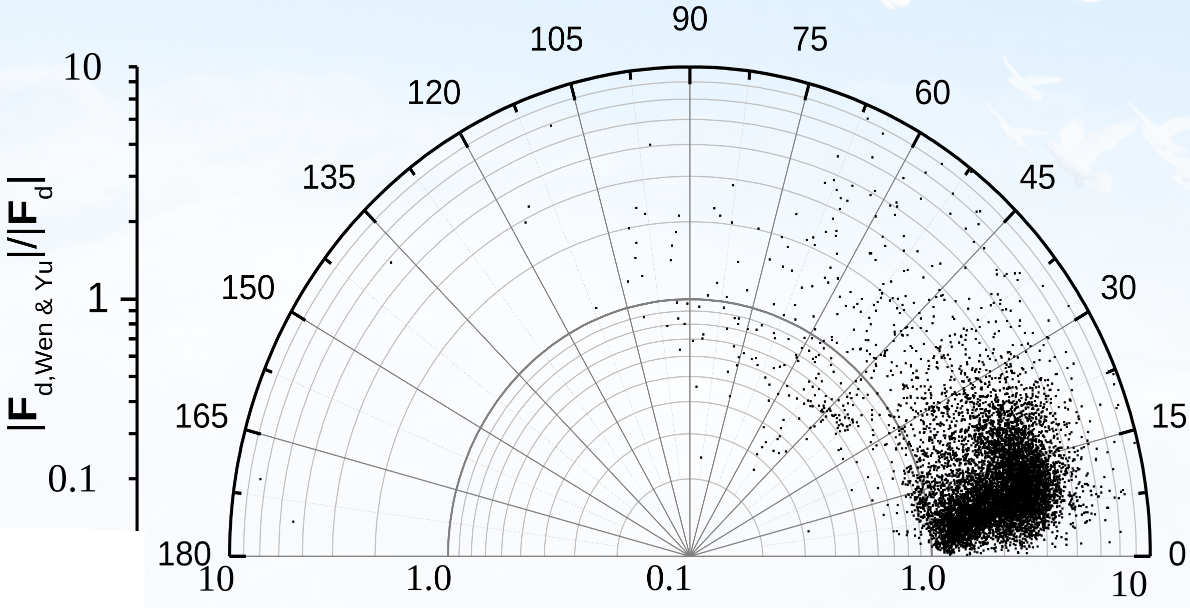
Snapshots for 3D DNS and Drag Distribution



Effect of Mesoscale Structure on Drag



$$\mathbf{F}_{g\leftrightarrow s,i} = \boldsymbol{\beta}\cdot\left(\mathbf{u}_g - \mathbf{u}_s\right)$$

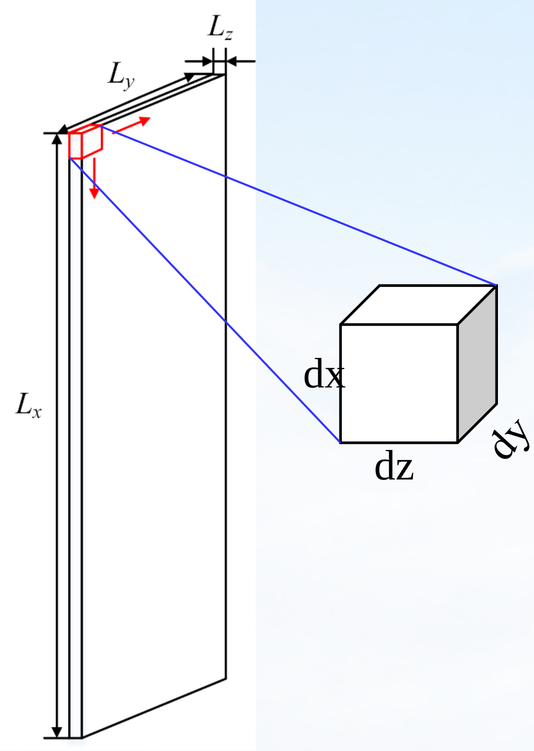


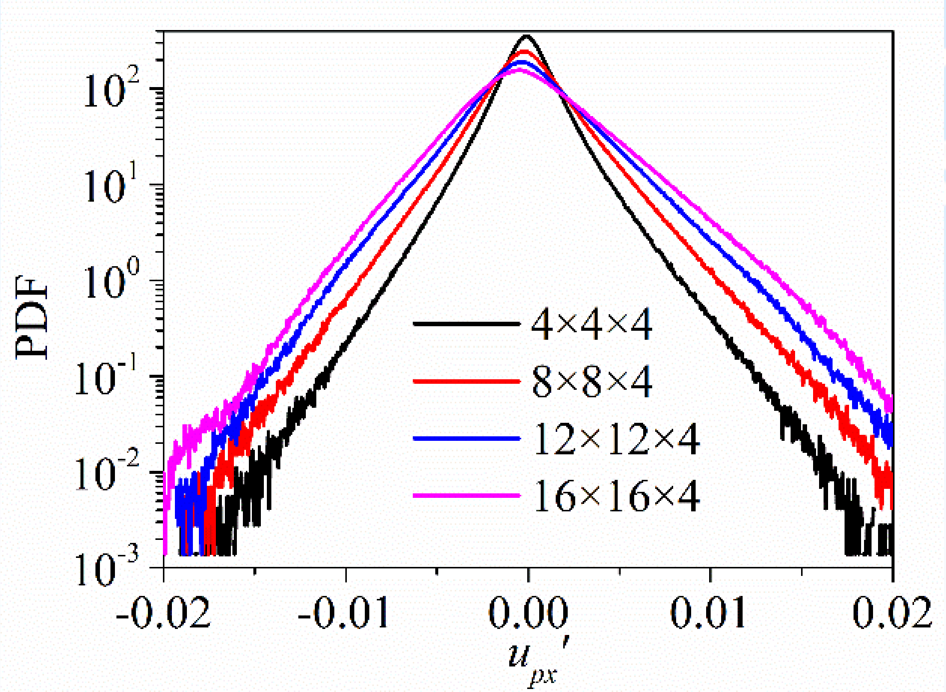
$$\boldsymbol{\beta}\cdot\left(\mathbf{u}_g - \mathbf{u}_s\right) \approx \beta\mathbf{I}\cdot\left(\mathbf{u}_g - \mathbf{u}_s\right) = \beta\left(\mathbf{u}_g - \mathbf{u}_s\right)$$

Zhou Guofeng, Xiong Qingang, **Wang Limin*,** Wang Xiaowei, Ren Xinxin, Ge Wei*. ***Chem. Eng. Sci.,*** 2014,116: 9–22
Wang Limin*, Zhang Bo, Wang Xiaowei, Ge Wei, Li Jinghai. ***Chem. Eng. Sci.***, 2013, 101:228–239.

Scale-dependence of Domain Size

External force field





Fluctuating velocity distribution

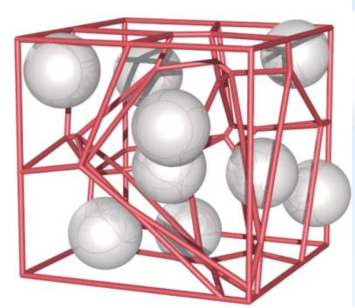
Granular Temperature

Sampling box	Θ_x	Θ_y	Θ_z	Θ
4×4×4	3.21×10^{-6}	2.61×10^{-6}	1.68×10^{-6}	2.50×10^{-6}
8×8×4	5.85×10^{-6}	4.23×10^{-6}	1.74×10^{-6}	3.94×10^{-6}
12×12×4	8.96×10^{-6}	5.98×10^{-6}	1.76×10^{-6}	5.57×10^{-6}
16×16×4	1.25×10^{-5}	7.56×10^{-6}	1.77×10^{-6}	7.28×10^{-6}

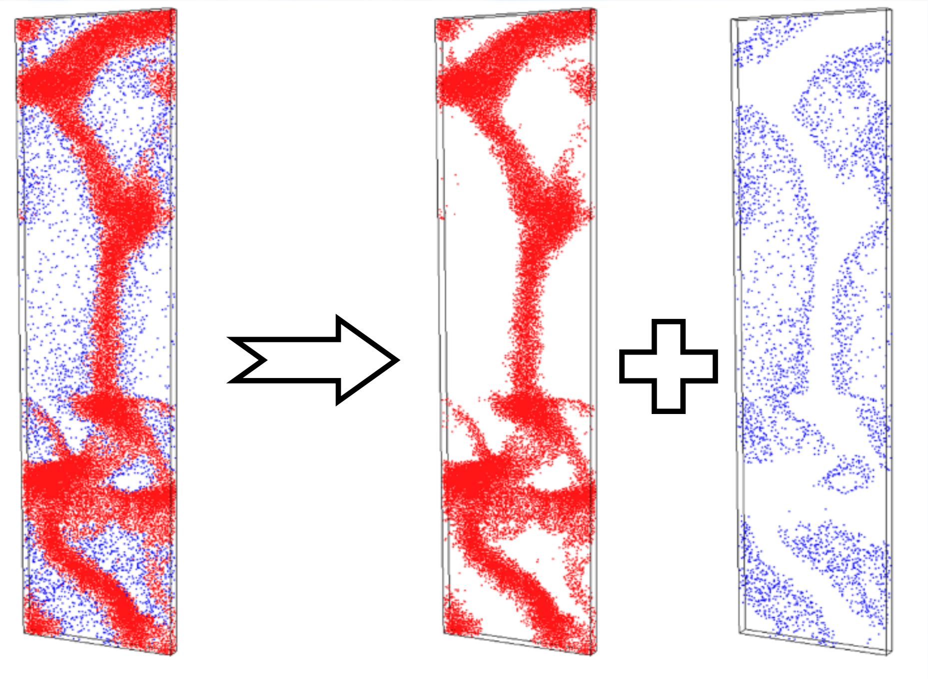
Effect of Mesoscale Structure on Statistical Properties of Particles

Fluctuating velocity of particle *i* at *j* direction

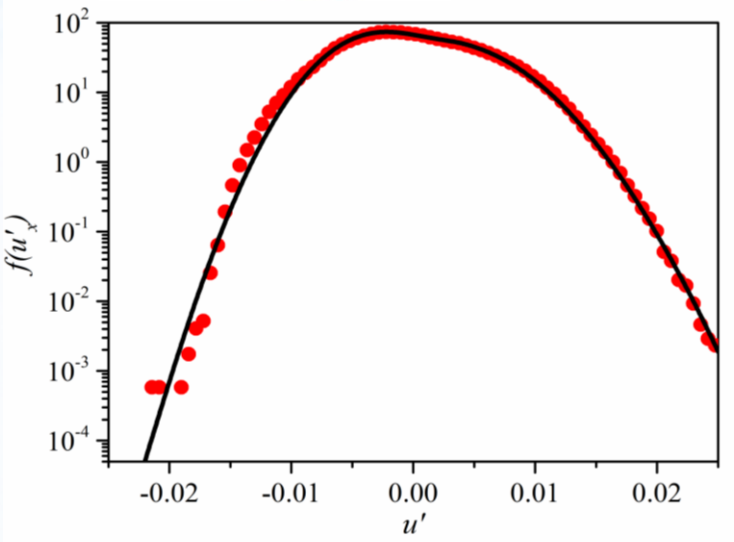
$$u'_{i,j}\begin{cases} u_{i,j}-\overline{u_{dilute,j}} \\ u_{i,j}-\overline{u_{dense,j}} \end{cases}$$



Voronoi tessellation



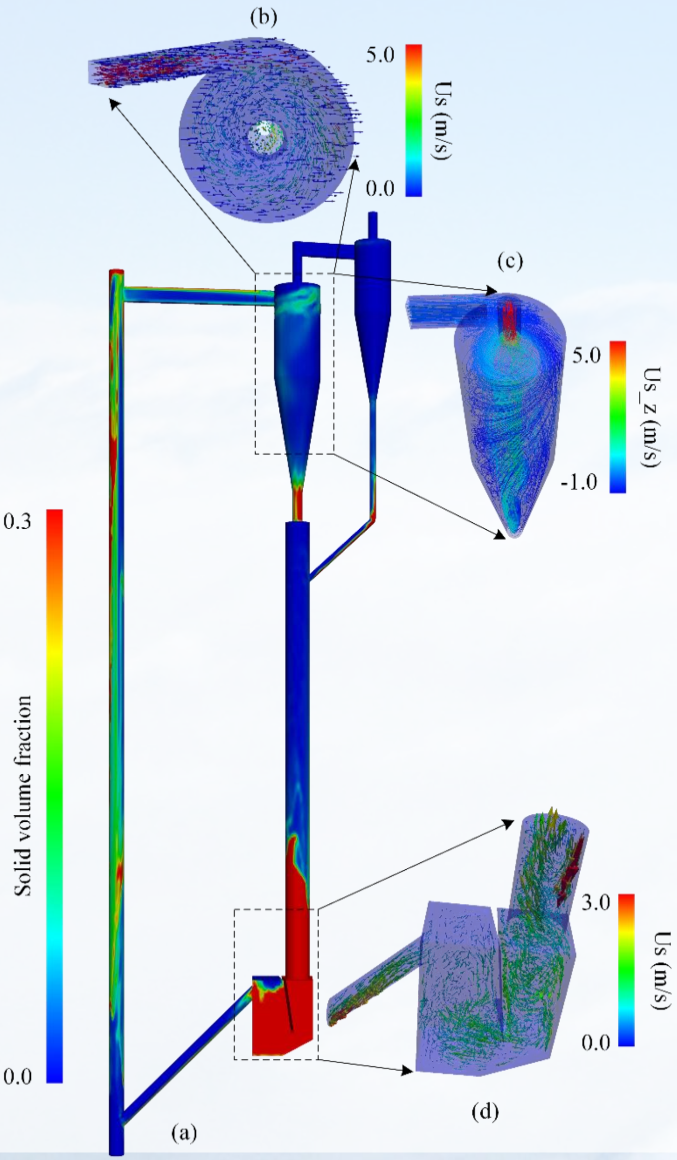
Dense phase Dilute phase



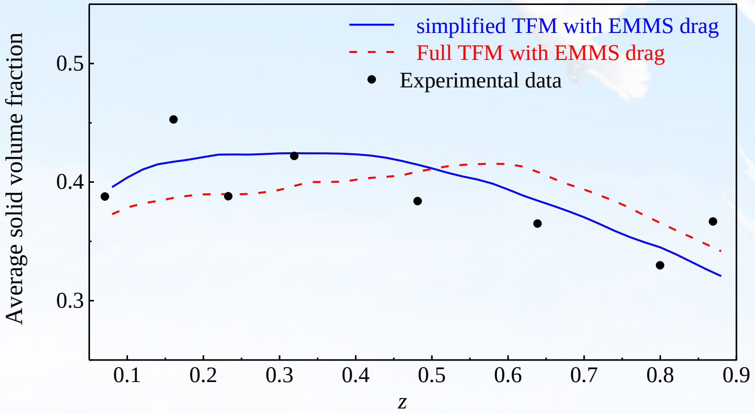
$$f(u'_x)=A_1\exp\left(-\left|\frac{(u'_x-b_1)}{\sqrt{\overline{u'^2_{dilute,x}}}}\right|^{1.8}\right)+A_2\exp\left(-\left|\frac{(u'_x-b_2)}{\sqrt{\overline{u'^2_{dense,x}}}}\right|^{2}\right)$$

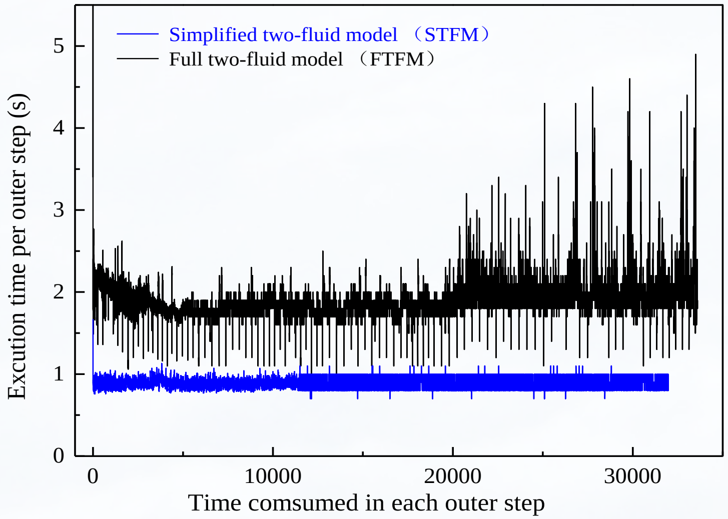
Liu Xiaowen, Wang Limin, Ge Wei. ***AIChE Journal***, 2017, 63:3-14.

Simplified TFM with EMMS Drag



Prediction of STFM coupled with EMMS drag also agrees with experimental data.





Simplified TFM is 2.14 times faster than full TFM!

Qiu Xiaoping, **Wang Limin*,** Yang Ning, Li Jinghai. ***Powder Technology***, 2017, 314:299-314.

Outline

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- Enabling Large-scale DNS
- Numerical Results
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Conclusions

Presented gas-solid statistical analysis of where we have used three strategies for enabling large-scale DNS including:

- **A LBM-based DNS algorithm is proposed to simulate gas-solid flow**
- **LBM-DEM algorithm is feasible to be implemented on GPU**
- **Large-scale DNS of gas-solid flow has been efficiently run on GPU cluster**
- **The effects of mesoscale structure on both drag and statistical properties of particles were explored**

Further investigations needed in constitutive laws (drag, solid stress, transfer of heat and mass, chemical reactions)

Better ways to link resolved models to coarse-grid simulation

Acknowledgements

Xiaowei Wang， Qingang Xiong, Guofeng Zhou, Xiaowen Liu

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Thank you for your attention!