Lattice Boltzmann for flow and transport phenomena

1. Introduction to the lattice Boltzmann method

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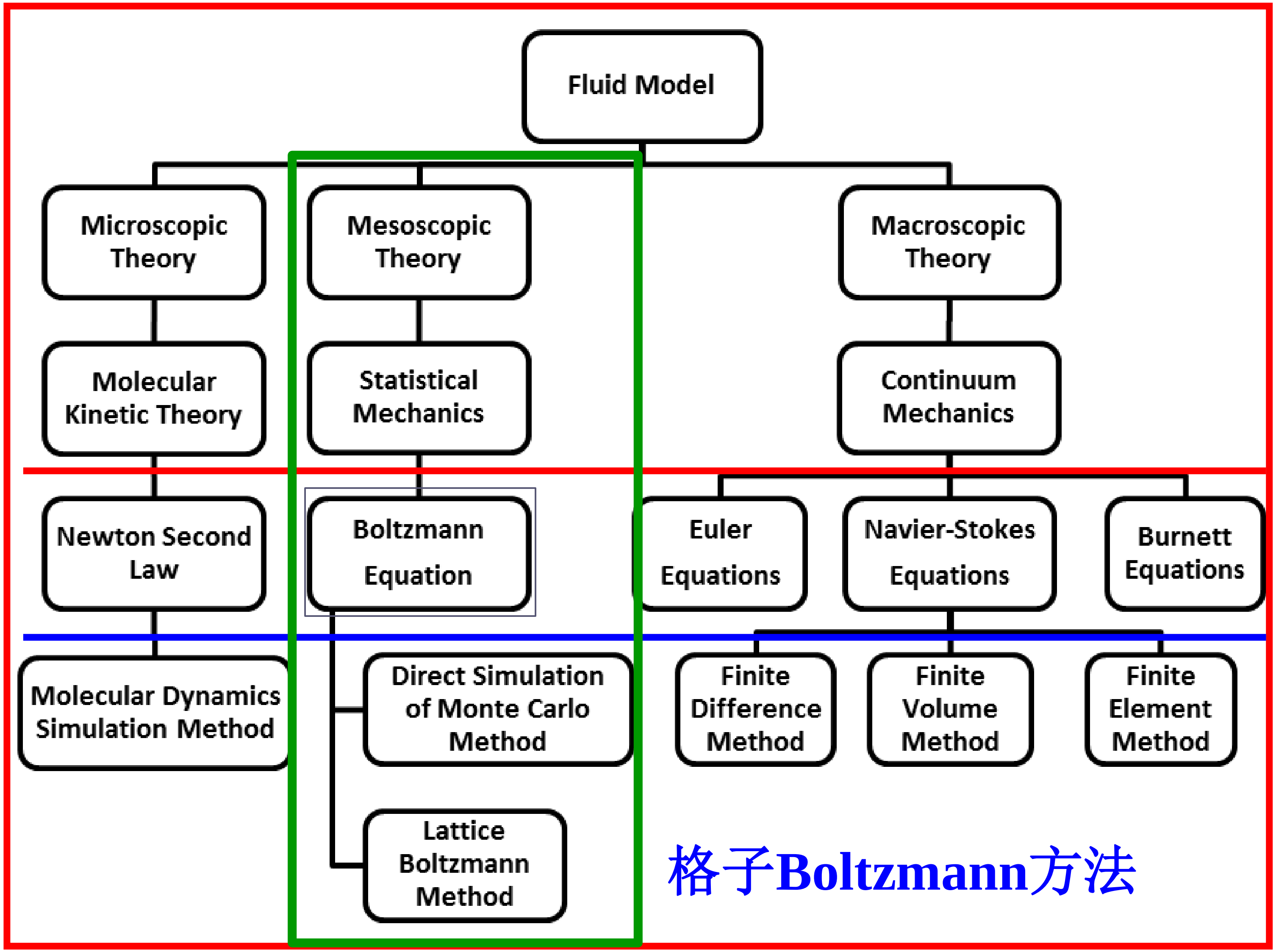
Content

1.1 Background



Micro, meso and macroscopic models and equations

1.1 Background

Microscopic models require huge computational resources.

(1mol, $6.02*10^{23}$)

Macroscopic models cannot provide underlying details.

Chang-Lin Tien (Microscale Thermophysical Engineering: 1997, 1: 71~84)

(1935-2002, 7th president of UC Berkeley, 1990-1997)

Many physical phenomena and engineering problems may have their origins at molecular scales, although they need to interface with the macroscopic or "human" scales. The difficulty arises in bridging the results of these models across the span of length and time scales. The lattice Boltzmann method attempts to bridge this gap.（联系微观和宏观的桥梁）

Mesoscopic scale (介尺度）

What is mesoscopic（介观的） scale （Mesoscale) ?

The scale between microscale and macroscale.

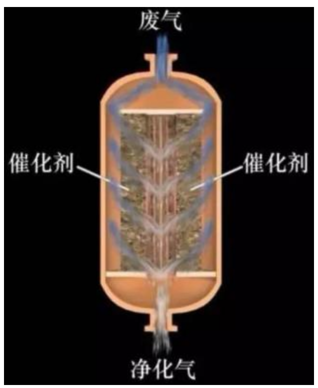
介于微观和宏观的状态

Proposed by Van Kampen 1981.

The size of this scale is comparable to the macroscale, yet lots of transport phenomena which we thought only take place at the microscale also can be observed at this scale.

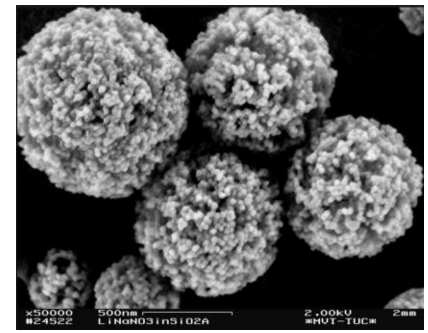
Serve as a bridge between the gas of microscale and macroscale!

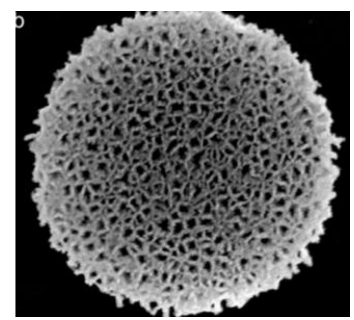
Macroscale



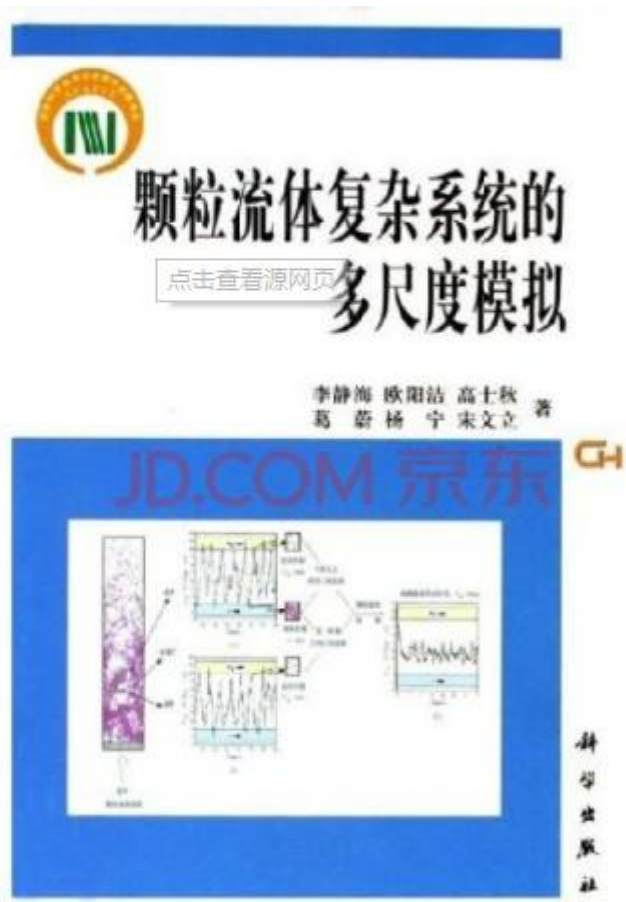
Mesoscale

Microscale





《颗粒流体复杂系统的多尺度模拟》
李静海，科学出版社，2005



对物质转化过程的认识，可分为如图 1-1 所示的三个层次：①分子与超分子层次，包括原子、分子、分子簇、自组织结构和催化剂颗粒，化学和物理主要研究这一层次。②反应器层次，包括化学工程研究的单颗粒、聚团、设备单元和不同设备构成的反应系统，一个化工多相反应系统，在系统尺度上存在物料、温度、压力、流速等参数的分布；在设备内各反应物及产物可能存在复杂的轴向和径向分布；在更小的尺度上则存在颗粒聚团和反应器局部浓度、温度梯度；在聚

团内部的介观尺度上颗粒浓度以及反应物、产物浓度会与聚团外有很大的不同；而颗粒本身则有可能是由具有高度自组织微观结构的微小单元组成。过程工程主要在这一层次上开展工作。③生态环境层次，包括工厂、环境生态、大气等，系统生态学主要研究这一层次。目前，

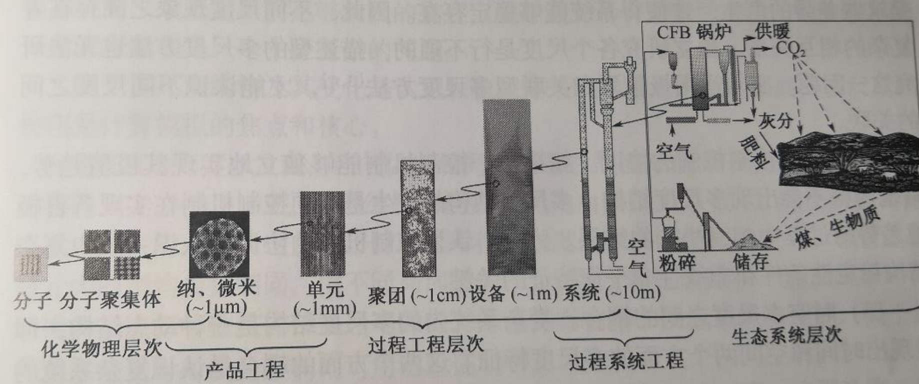
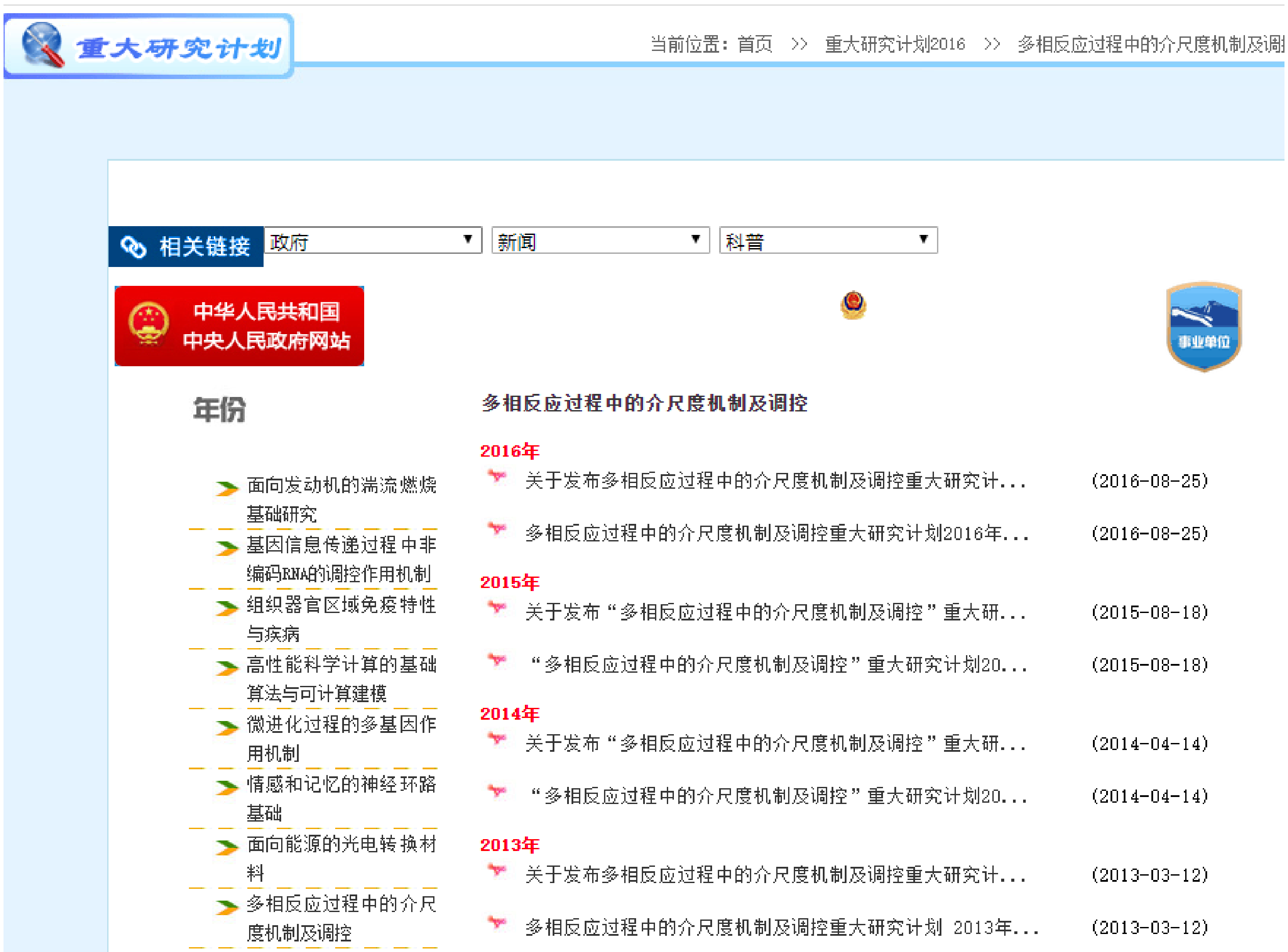


图 1-1 物质转化多层次的时空多尺度结构

自然科学基金委：多相反应过程中的介尺度机制及调控



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多相反应过程中的介尺度机制及调控

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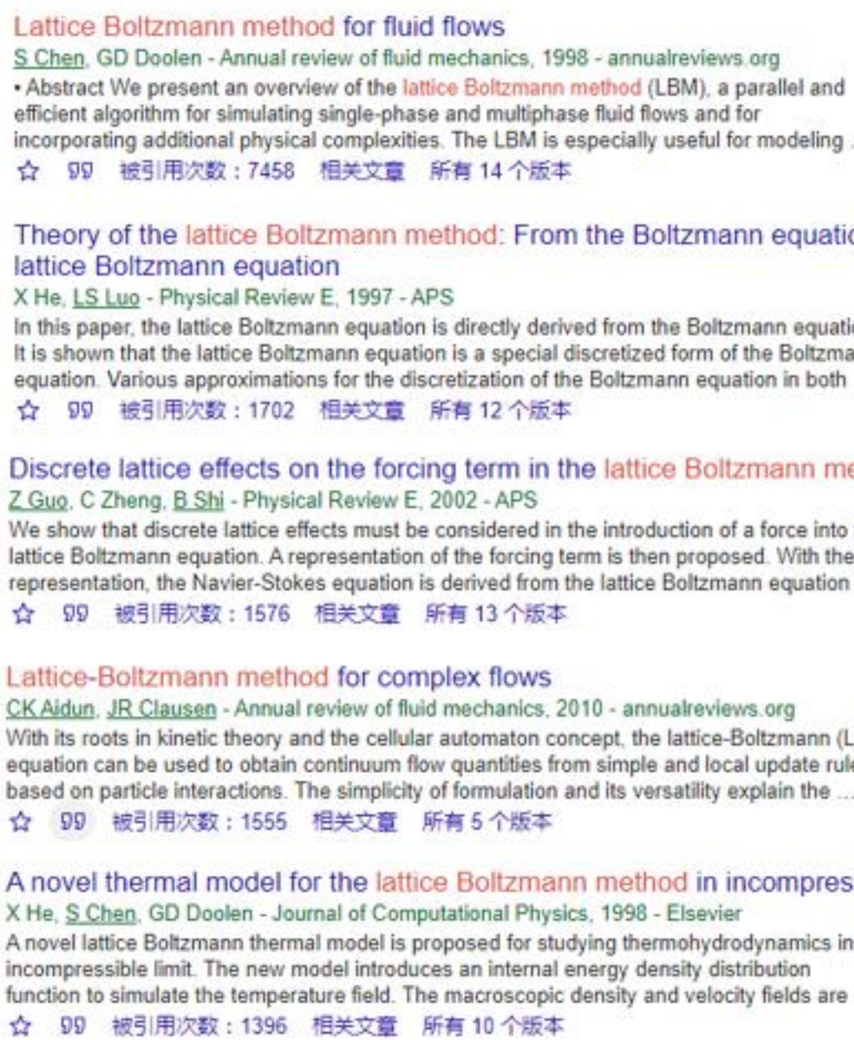
华人的贡献

❖在LBM近30年的发展历史中，华人科学家做出了重要的贡献。LBM被他引次数最高的文献中华人的参与非常高。

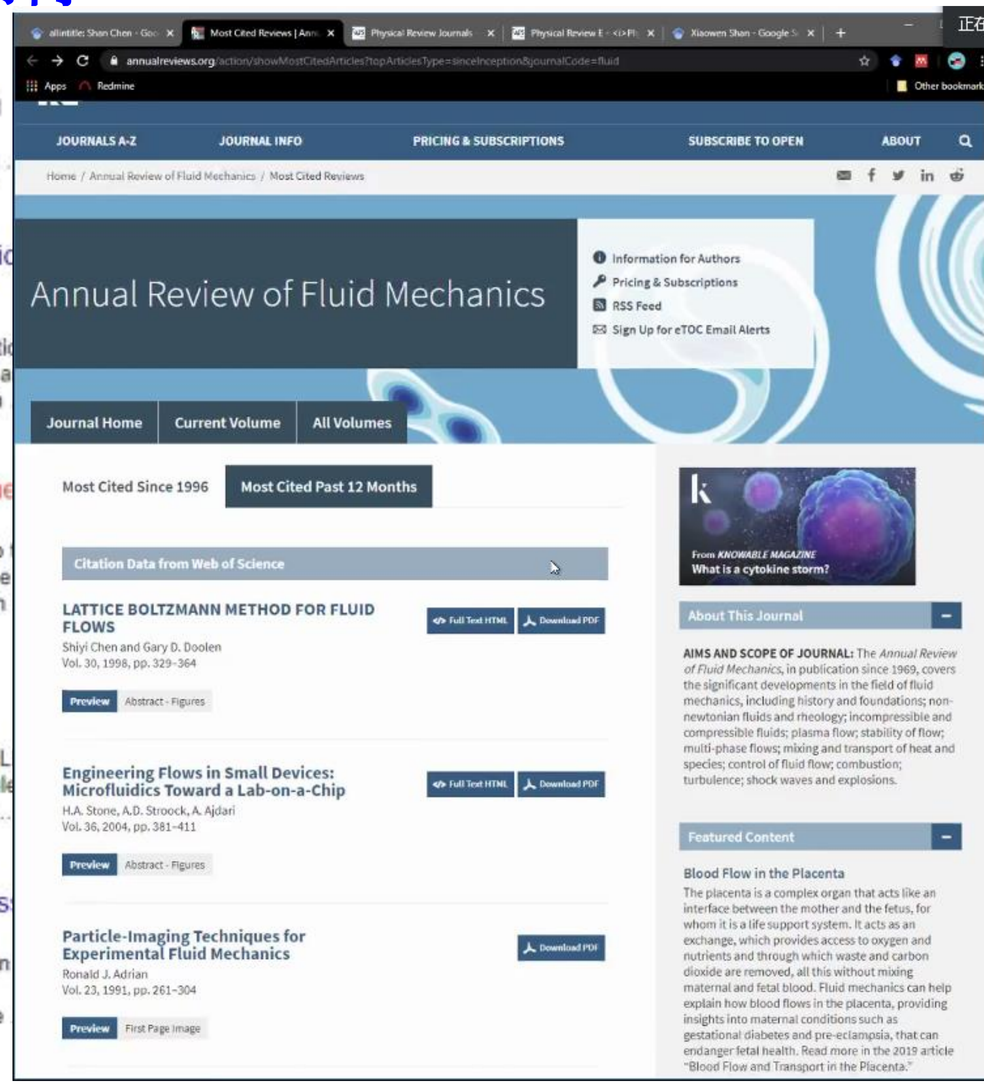

Lattice Boltzmann method for fluid flows
S Chen, GD Doolen - Annual review of fluid mechanics, 1998 - annualreviews.org
• Abstract We present an overview of the lattice Boltzmann method (LBM), a parallel and efficient algorithm for simulating single-phase and multiphase fluid flows and for incorporating additional physical complexities. The LBM is especially useful for modeling
☆ 99 被引用次数：7458 相关文章 所有 14 个版本

Theory of the lattice Boltzmann method: From the Boltzmann equatio… lattice Boltzmann equation
X He, LS Luo - Physical Review E, 1997 - APS
In this paper, the lattice Boltzmann equation is directly derived from the Boltzmann equati… It is shown that the lattice Boltzmann equation is a special discretized form of the Boltzma… equation. Various approximations for the discretization of the Boltzmann equation in both
☆ 99 被引用次数：1702 相关文章 所有 12 个版本

Discrete lattice effects on the forcing term in the lattice Boltzmann me…
Z Guo, C Zheng, B Shi - Physical Review E, 2002 - APS
We show that discrete lattice effects must be considered in the introduction of a force into… lattice Boltzmann equation. A representation of the forcing term is then proposed. With the… representation, the Navier-Stokes equation is derived from the lattice Boltzmann equation
☆ 99 被引用次数：1576 相关文章 所有 13 个版本

Lattice-Boltzmann method for complex flows
CK Aidun, JR Clausen - Annual review of fluid mechanics, 2010 - annualreviews.org
With its roots in kinetic theory and the cellular automaton concept, the lattice-Boltzmann (L… equation can be used to obtain continuum flow quantities from simple and local update rule… based on particle interactions. The simplicity of formulation and its versatility explain the …
☆ 99 被引用次数：1555 相关文章 所有 5 个版本

A novel thermal model for the lattice Boltzmann method in incompres…
X He, S Chen, GD Doolen - Journal of Computational Physics, 1998 - Elsevier
A novel lattice Boltzmann thermal model is proposed for studying thermohydrodynamics in… incompressible limit. The new model introduces an internal energy density distribution function to simulate the temperature field. The macroscopic density and velocity fields are
☆ 99 被引用次数：1396 相关文章 所有 10 个版本



Lattice Boltzmann model for simulating flows with multiple phases and components X Shan, H Chen Physical review E 47 (3), 1815	3047	1993
Simulation of nonideal gases and liquid-gas phase transitions by the lattice Boltzmann equation X Shan, H Chen Physical Review E 49 (4), 2941	1228	1994
Kinetic theory representation of hydrodynamics: a way beyond the Navier–Stokes equation X Shan, XF Yuan, H Chen Journal of Fluid Mechanics 550, 413-441	771	2006
Simulation of Rayleigh-Bénard convection using a lattice Boltzmann method X Shan Physical Review E 55 (3), 2780	599	1997
Discrete Boltzmann equation model for nonideal gases X He, X Shan, GD Doolen Physical Review E 57 (1), R13	596	1998
Multicomponent lattice-Boltzmann model with interparticle interaction X Shan, G Doolen Journal of Statistical Physics 81 (1-2), 379-393	565	1995
Discretization of the velocity space in the solution of the Boltzmann equation X Shan, X He Physical Review Letters 80 (1), 65	423	1998

Equations of state in a lattice Boltzmann model

P Yuan, L Schaefer - Physics of Fluids, 2006 - aip.scitation.org

In this paper we consider the incorporation of various equations of state into the single-component multiphase lattice Boltzmann model. Several cubic equations of state, including the van der Waals, Redlich-Kwong, and Peng-Robinson, as well as a noncubic equation of ...

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西安交通大学热流科学与工程与教育部重点实验室在微纳米尺度传热传质、非牛顿流体、可压缩流、两相流、反应输运、多孔介质流动等方面也做出了贡献。

Lattice Boltzmann method for gaseous microflows using kinetic theory boundary conditions GH Tang, WQ Tao, YL He Physics of Fluids 17 (5), 058101	171	2005
Thermal boundary condition for the thermal lattice Boltzmann equation GH Tang, WQ Tao, YL He Physical Review E 72 (1), 016703	126	2005
Electroosmotic flow of non-Newtonian fluid in microchannels GH Tang, XF Li, YL He, WQ Tao Journal of Non-Newtonian Fluid Mechanics 157 (1-2), 133-137	145	2009
Lattice Boltzmann modeling of microchannel flows in the transition flow regime Q Li, YL He, GH Tang, WQ Tao Microfluidics and nanofluidics 10 (3), 607-618	125	2011
Nanoscale simulation of shale transport properties using the lattice Boltzmann method: permeability and diffusivity L Chen, L Zhang, Q Kang, HS Viswanathan, J Yao, W Tao Scientific reports 5 (1), 1-8	239	2015
Pore-scale flow and mass transport in gas diffusion layer of proton exchange membrane fuel cell with interdigitated flow fields L Chen, HB Luan, YL He, WQ Tao International Journal of Thermal Sciences 51, 132-144	185	2012
Pore-scale modeling of multiphase reactive transport with phase transitions and dissolution-precipitation processes in closed systems L Chen, Q Kang, BA Robinson, YL He, WQ Tao Physical Review E 87 (4), 043306	111	2013
A critical review of the pseudopotential multiphase lattice Boltzmann model: Methods and applications L Chen, Q Kang, Y Mu, YL He, WQ Tao International journal of heat and mass transfer 76, 210-236	452	2014

Review

Content

1.2 Boltzmann equation

Velocity distribution function

$$f\,(x,\xi,t)$$

Number of molecules is *fdxdξ* in control volume *dx* with velocity in the range of (ξ , ξ +dξ) at time *t*.

Thus, the total molecules in the control volume *dx* is

$$\int f d\xi = n$$

Correspondingly, the total mass, momentum and energy are

$$\int m f d\xi = \rho$$

$$\int m\xi f d\xi = \rho u$$

$$\int m\frac{\xi^2}{2} f d\xi = \rho E = \rho e + \frac{1}{2}\rho u^2$$

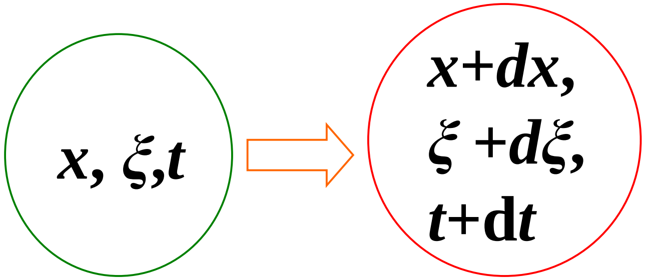
1.2 Boltzmann equation

For a certain molecular, if during the time *dt*, it does not collision with other molecules, its position and velocity will change as follows

$$\boldsymbol{x} + \xi dt, \quad \xi + \boldsymbol{a}dt$$

Therefore, at time *t*+*dt*, those molecules in (*x*, *ξ*) at time *t* will move to (*x*+*dx*, *ξ* +*dξ*)

$$f(\mathbf{x} + d\mathbf{x}, \boldsymbol{\xi} + \boldsymbol{a}dt, t + dt)d\mathbf{x}d\boldsymbol{\xi} = f(\mathbf{x}, \boldsymbol{\xi}, t)d\mathbf{x}d\boldsymbol{\xi}$$



1.2 Boltzmann equation

$$f(\boldsymbol{x}+d\boldsymbol{x},\xi+adt,t+dt)d\boldsymbol{x}d\xi = f(\boldsymbol{x},\xi,t)d\boldsymbol{x}d\xi$$

Taylor expansion

$$\frac{\partial f}{\partial t}+\xi\cdot\frac{\partial f}{\partial \boldsymbol{x}}+a\cdot\frac{\partial f}{\partial \xi}=0$$

The above equation is the Boltzmann equation without collision. It describes the conservation of velocity distribution function.

However, collision between molecules also change the velocity of molecules, thus a collision term should be added

1.2 Boltzmann equation

Collision between molecules also change the velocity of molecules, thus a collision term should be added

$$(\frac{\partial f}{\partial t})_{\text{collision}}$$

$$\frac{\partial f}{\partial t}+\xi\frac{\partial f}{\partial \boldsymbol{x}}+a\cdot\frac{\partial f}{\partial \xi}=(\frac{\partial f}{\partial t})_{\text{collision}}=\Omega(f)$$

Collision between molecules are complex. Even if we assume two-molecule collision, velocities are uncorrelated pre-collision, at during the short time of collision, external force does not play a role

$$(\frac{\partial f}{\partial t})_{\text{collision}}=\int\int(f'f_1'-ff_1)d_D^2|g|\cos\theta d\Omega d\xi_1$$

1.2 Boltzmann equation

Boltzmann equation

$$\frac{\partial f}{\partial t}+\xi\frac{\partial f}{\partial \boldsymbol{x}}+a\cdot\frac{\partial f}{\partial \xi}=\int\int(f'f_1'-ff_1)d_D{}^2|g|\cos\theta d\Omega d\xi_1$$

Devised by Ludwig Boltzmann in 1872.

The collision term is a integral-differential term. Thus, it is really hard to solve Boltzmann equation due to this complex term.

Simplify the collision term: Boltzmann *H* theorem

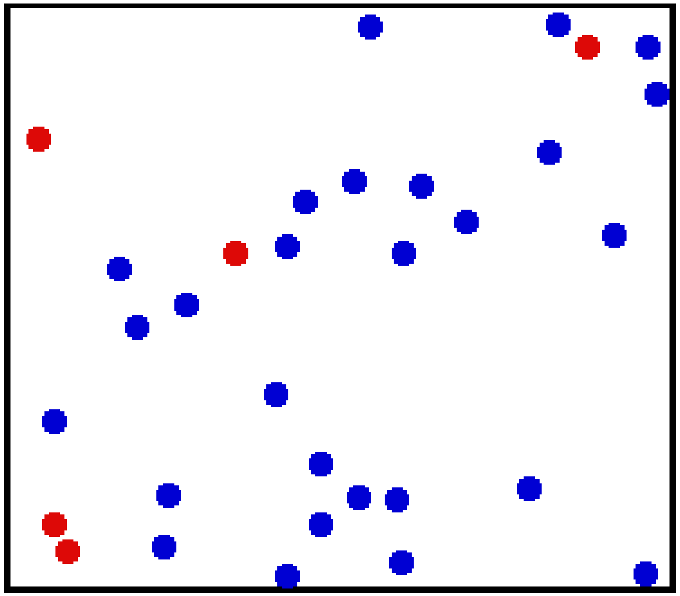
$$H=\overline{\ln f}=\frac{\int f\ln f\,\mathrm{d}\xi}{\int f\,\mathrm{d}\xi}=\frac{1}{n}\int f\ln f\,\mathrm{d}\xi$$

1.2 Boltzmann equation

Boltzmann *H* theorem

$$\partial H / \partial t \le 0$$

Indicating that *H* of a system decreases with the time. The final state means the equilibrium system. The corresponding *f* is equilibrium distribution function. Maxwell distribution is a solution



$$f^{eq} = \frac{1}{(2\pi RT)^{3/2}} \exp\left(-\frac{(\xi - \mathrm{u})^2}{2RT}\right)$$

In this mechanical model of a gas, the motion of the molecules appears very disorderly. Boltzmann showed that, assuming each collision configuration in a gas is truly random and independent, the gas converges to the Maxwell speed distribution even if it did not start out that way.

1.2 Boltzmann equation

BGK collision term: In 1954, **B**hatnagar, **G**ross and **K**rook proposed the BGK collision model（SRT)

$$-\frac{1}{\tau}(f-f^{\mathrm{eq}})$$

where τ is the relaxation time, f^{eq} is the equilibrium distribution function.

1) Approximate that the effect of collision is to force the non-equilibrium distribution back to Maxwell equilibrium distribution

2) The collision term should maintain the conservation of mass, momentum and energy.

$$\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\frac{\partial f}{\partial \mathbf{x}}+a\cdot\frac{\partial f}{\partial \boldsymbol{\xi}}=-\frac{1}{\tau}(f-f^{\mathrm{eq}})$$

1.2 Boltzmann equation

Velocity distribution function

$$f(x,\xi,t)$$

Boltzmann Equation

$$\frac{\partial f}{\partial t}+\xi\cdot\frac{\partial f}{\partial \mathbf{x}}+a\cdot\frac{\partial f}{\partial \xi}=-\frac{1}{\tau}(f-f^{\mathrm{eq}})$$

BGK (SRT) collision term

Equilibrium distribution function

$$f^{\mathrm{eq}}=\frac{1}{(2\pi RT)^{3/2}}\exp\left(-\frac{(\xi-\mathrm{u})^2}{2RT}\right)$$

Content

1.3 Lattice Boltzmann method

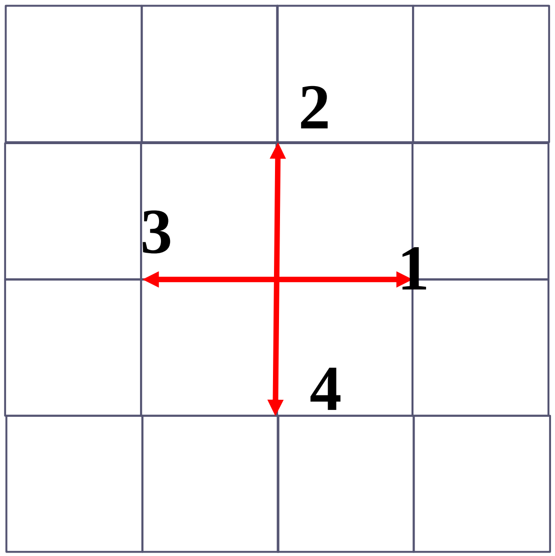
Lattice Boltzmann method

From lattice gas automata
1973-1988
HPP
FHP

Discretization of
Boltzmann equation
1997~1998

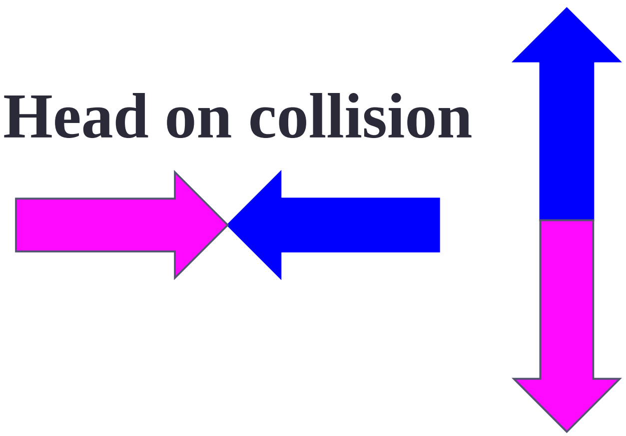
1.3.1 Lattice Gas Automata

Hardy, de Pazzls, Pomeau, 1973 HPP



$C_1=(1,0)$
$C_2=(0,1)$
$C_3=(-1,0)$
$C_4=(0,-1)$

Head on collision



1. **Pauli incompatible principle**

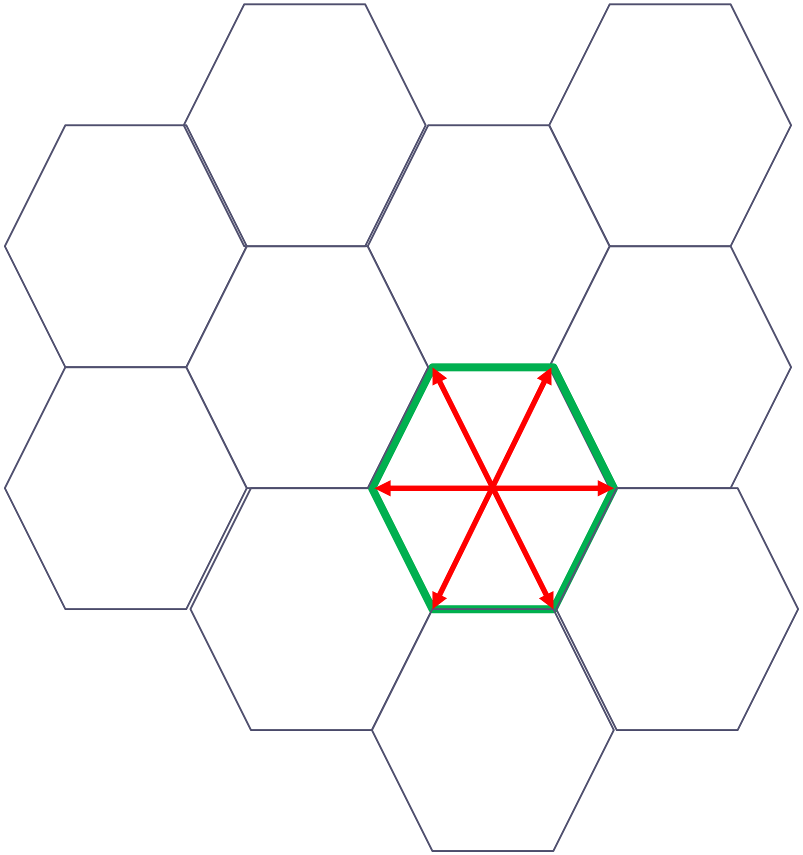
   $$n(x,t)=n_1n_2n_3n_4$$

$$c_i(n)=n_{i\oplus 1}n_{i\oplus 3}(1-n_i)(1-n_{i\oplus 2})-(1-n_{i\oplus 1})(1-n_{i\oplus 3})n_in_{i\oplus 2}$$

2. **Collision and streaming**

1.3.1 Lattice Gas Automata

Frisch, Hasslacher, Pomeau, 1986 FHP



NS equation can be recovered.

Because of Boolean number, statistic noise is huge.

The collision operator is complex.

1988: McNamara and Zanetti proposed to use real numbers rather than Boolean value "0" and "1" (PRL, 1999)

- **Avoid statistic noise**
- **Becomes complicated with multiple particles collision at one site.**

1989: Higuere and Jinenes developed the linear collision term. (Europhys. Lett)

1991-1992: several groups simultaneously proposed the BGK collision term or SRT collision term.
The purpose of collision to approach equilibrium state. (S. Chen et al. PRL, 1991; Y. Qian et al. Europhys. Lett 1992)

20210323 Review

Velocity distribution function

$$f(x,\xi,t)$$

Boltzmann equation with SRT (BGK) collision term:

$$\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\frac{\partial f}{\partial \mathbf{x}}+a\cdot\frac{\partial f}{\partial \boldsymbol{\xi}}=-\frac{1}{\tau}(f-f^{\mathrm{eq}})$$

Equilibrium distribution function

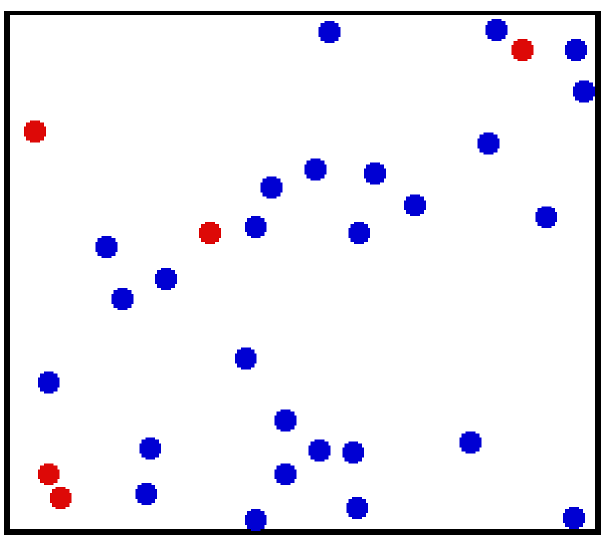
$$f^{\mathrm{eq}}=\frac{1}{(2\pi RT)^{3/2}}\exp\left(-\frac{(\xi-\mathrm{u})^2}{2RT}\right)$$

1.3.2 Discretization of Boltzmann equation

Discretization of velocity, space and time of Boltzmann equation

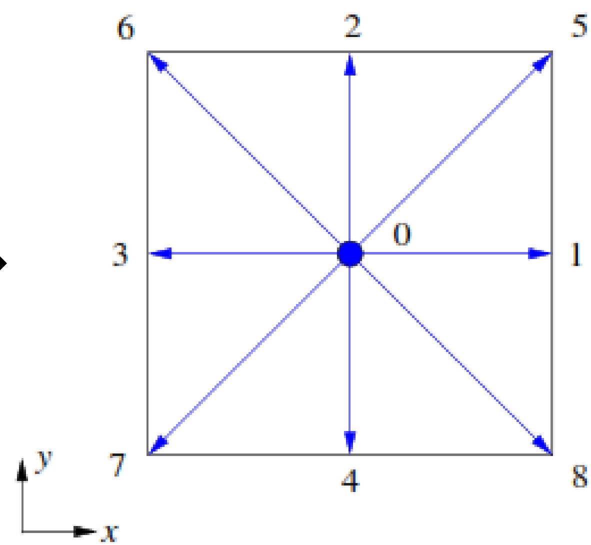
Velocity is continuous, however it is impossible to consider all the PDF in all velocity directions.

The velocity is discretized. The most famous model is DnQm lattice model. n denotes dimension, and m is the number of velocity directions. (Q: Yuehong Qian, 钱跃竑老师).



Infinity to just 9

$$f \rightarrow f_i$$

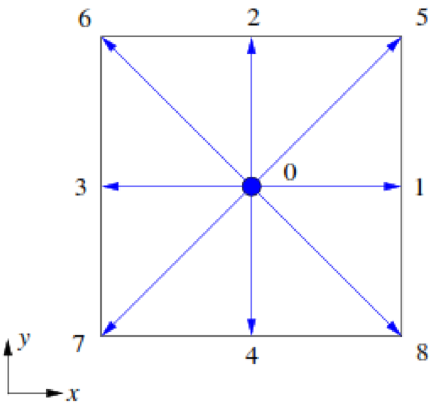


1.3.2 Discretization of Boltzmann equation

$$\mathbf{c}_0 = \mathbf{0} \quad ,$$

$$\mathbf{c}_i = \left(\cos\frac{i-1}{2}\pi, \sin\frac{i-1}{2}\pi\right)\frac{\Delta x}{\Delta t} \quad , \quad i = 1-4 \quad ,$$

$$\mathbf{c}_i = \sqrt{2}\left(\cos\frac{2i-9}{4}\pi, \sin\frac{2i-9}{4}\pi\right)\frac{\Delta x}{\Delta t} \quad , \quad i = 5-8$$



$$f^{\text{eq}} = \frac{\rho}{(2\pi RT)^{3/2}}\exp\left(-\frac{(\xi-\mathrm{u})^2}{2RT}\right)$$

$$e^x = \sum_{n=0}^{\infty}\frac{x^n}{n!} = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots \quad \text{for all } x$$

Expanded around *u*:

$$f^{\text{eq}} = \frac{\rho}{(2\pi RT)^{3/2}}\exp\left(-\frac{\xi^2}{2RT}\right)\left(1 + \frac{\xi u}{2RT} + \frac{(\xi u)^2}{2(RT)^2} - \frac{(u)^2}{2(RT)^2}\right)$$

1.3.2 Discretization of Boltzmann equation

Equilibrium distribution function

$$f_i^{\mathrm{eq}} = \rho w_i \left[1 + \frac{\mathbf{u}\cdot\mathbf{c}_i}{c_s^2} + \frac{1}{2}\left(\frac{\mathbf{u}\cdot\mathbf{c}_i}{c_s^2}\right)^2 - \frac{\mathbf{u}\cdot\mathbf{u}}{2c_s^2} \right]$$

$$\sum f_i^{\mathrm{eq}} = \sum f^{\mathrm{eq}} = \rho$$

$$\sum f_i^{\mathrm{eq}}\mathbf{c}_i = \sum f^{\mathrm{eq}}\boldsymbol{\xi} = \rho\mathbf{u}$$

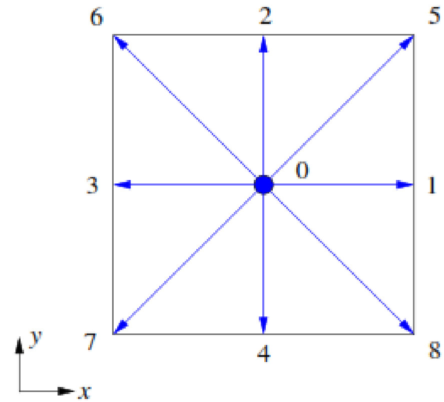
$$\sum f_i^{\mathrm{eq}}\mathbf{c}_i\mathbf{c}_i = \sum f^{\mathrm{eq}}\boldsymbol{\xi}\boldsymbol{\xi} = \rho\mathbf{u}\mathbf{u} + p\mathbf{I}$$

$$\sum_{i=1}^{4}\mathbf{c}_{i\alpha} = 0 \qquad \sum_{i=5}^{8}\mathbf{c}_{i\alpha} = 0 \qquad \sum_{i=1}^{4}\mathbf{c}_{i\alpha}\mathbf{c}_{i\beta}\mathbf{c}_{i\gamma} = 0 \qquad \sum_{i=5}^{8}\mathbf{c}_{i\alpha}\mathbf{c}_{i\beta}\mathbf{c}_{i\gamma} = 0$$

$$\sum_{i=1}^{4}\mathbf{c}_{i\alpha}\mathbf{c}_{i\beta} = 2\delta_{\alpha\beta} \qquad \sum_{i=5}^{8}\mathbf{c}_{i\alpha}\mathbf{c}_{i\beta} = 4\delta_{\alpha\beta} \qquad \sum_{i=1}^{4}\mathbf{c}_{i\alpha}\mathbf{c}_{i\beta}\mathbf{c}_{i\gamma}\mathbf{c}_{i\chi} = 2\delta_{\alpha\beta\gamma\chi} \qquad \sum_{i=5}^{8}\mathbf{c}_{i\alpha}\mathbf{c}_{i\beta}\mathbf{c}_{i\gamma}\mathbf{c}_{i\chi} = 4\Delta_{\alpha\beta\gamma\chi} - 8\delta_{\alpha\beta\gamma\chi}$$

$$\Delta_{\alpha\beta\gamma\chi} = \delta_{\alpha\beta}\delta_{\gamma\chi} + \delta_{\alpha\gamma}\delta_{\beta\chi} + \delta_{\alpha\chi}\delta_{\beta\gamma}$$

$$\sum_{i=1}^{4}\mathbf{c}_{i\alpha}=0 \qquad \sum_{i=5}^{8}\mathbf{c}_{i\alpha}=0$$



***i* is the *i*th lattice velocity, and α is the coordinate.**

$$c_{1x}+c_{2x}+c_{3x}+c_{4x}=1+0+(-1)+0=0$$

$$c_{1y}+c_{2y}+c_{3y}+c_{4y}=0+1+0+(-1)=0$$

$$\sum_{i=1}^{4}\mathbf{c}_{i\alpha}\mathbf{c}_{i\beta}=2\delta_{\alpha\beta} \qquad \sum_{i=5}^{8}\mathbf{c}_{i\alpha}\mathbf{c}_{i\beta}=4\delta_{\alpha\beta}$$

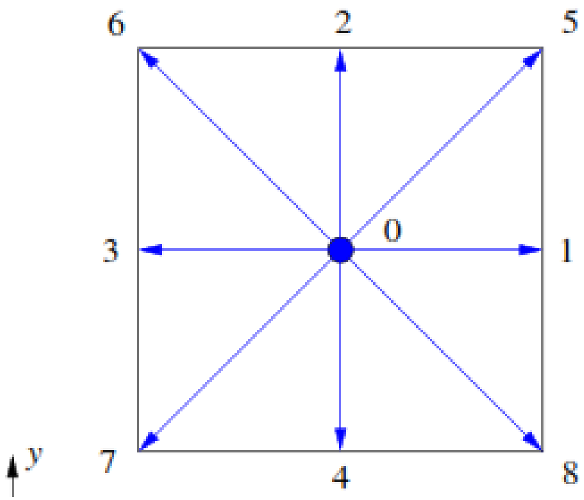
$$c_{1x}c_{1x}+c_{2x}c_{2x}+c_{3x}c_{3x}+c_{4x}c_{4x}=1\wedge 2+0+(-1)\wedge 2+0=2$$

$$c_{1x}c_{1y}+c_{2x}c_{2y}+c_{3x}c_{3y}+c_{4x}c_{4y}=1*0+0*1+(-1)\ *0+0*1=0$$

$$c_{1y}c_{1y}+c_{2y}c_{2y}+c_{3y}c_{3y}+c_{4y}c_{4y}=0+1\wedge 2+0+(-1)\wedge 2+=2$$

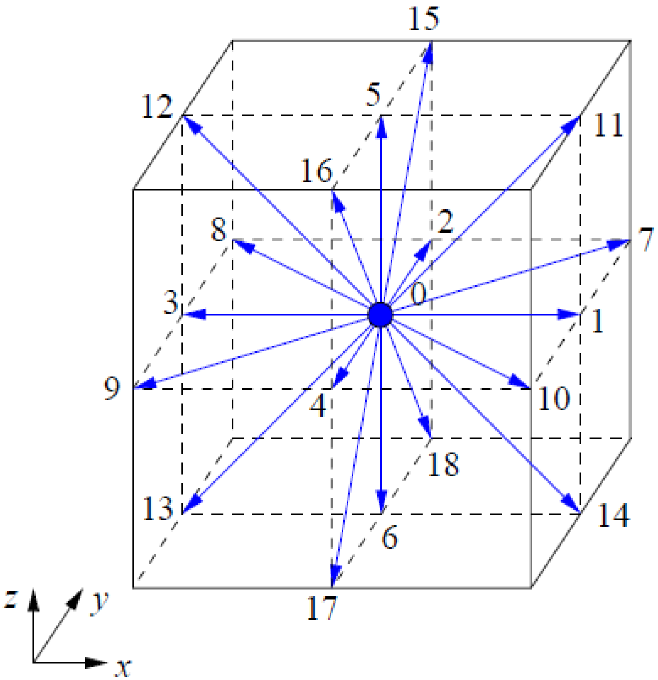
1.3.2 Discretization of Boltzmann equation

D2Q9



$$w_0 = 4/9$$
$$w_{1-4} = 1/9$$
$$w_{5-8} = 1/36$$

D3Q19



$$w_0 = 1/3$$
$$w_{1-6} = 1/18$$
$$w_{7-18} = 1/36$$

1.3.2 Discretization of Boltzmann equation

$$\frac{\partial f}{\partial t}+\xi\cdot\frac{\partial f}{\partial \mathbf{x}}+a\cdot\frac{\partial f}{\partial \xi}=-\frac{1}{\tau}(f-f^{\mathrm{eq}})$$

$$\frac{\partial f_i}{\partial t}+\xi\cdot\frac{\partial f_i}{\partial \mathbf{x}}+a\cdot\frac{\partial f_i}{\partial \xi}=-\frac{1}{\tau}(f_i-f_i^{\mathrm{eq}})$$

Evolution equation for the LBM

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t,t+\Delta t)-f_i(\mathbf{x},t)=-\frac{1}{\tau}(f_i(\mathbf{x},t)-f_i^{\mathrm{eq}}(\mathbf{x},t))$$

3 key components

- **Evolution equation**
- **Lattice model**
- **Equilibrium distribution function** f^{eq}

1.3.3 From LBM to NS equation

Fundamentally, the NS equation can be derived from the Boltzmann equation.

Champan-Ensokog expansion: **C-E expansion denotes such derivation from Boltzmann equation to NS equation as well as transport coefficient from Boltzmann equation (Chapman and Enskog between 1910 and 1920)**

ε Small expansion parameter

$$f_i = f_i^{(0)} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)}$$

$$\partial_{x_\alpha} = \varepsilon \partial_{x_\alpha}^{(1)}$$

$$\partial_t = \varepsilon \partial_t^{(1)} + \varepsilon^2 \partial_t^{(2)}$$

1.3.3 From LBM to NS equation

Taylor expansion

$$f_i(\boldsymbol{x}+\boldsymbol{c}_i\Delta t, t+\Delta t) = f_i(\boldsymbol{x}, t) + \Delta t D_{i\alpha} f_i(\boldsymbol{x}, t) + \frac{(\Delta t)^2}{2} D_{i\alpha}^2 f_i(\boldsymbol{x}, t) + O\left[(\Delta t)^3\right]$$

$$D_{i\alpha} = \partial_t + c_i \partial_{x_\alpha}$$

$$\varepsilon D_{i\alpha}^{(1)} f^{(0)} + \varepsilon^2 \left[D_{i\alpha}^{(1)} f_i^{(1)} + \partial_t^{(2)} f_i^{(0)}\right] + \varepsilon^2 \frac{\Delta t}{2}\left[D_{i\alpha}^{(1)}\right]^2 f_i^{(0)} = -\frac{1}{\Delta t \tau_f}\left(f_i^{(0)} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} - f_i^{(eq)}\right) + O\left[(\Delta t)^3\right]$$

1.3.3 From LBM to NS equation

$$\varepsilon^0: f_i^{(0)} = f_i^{(eq)}$$

$$\varepsilon^1: f_i^{(1)} = -\Delta t \tau_f D_{i\alpha}^{(1)} f_i^{(0)} + O\left[(\Delta t)^2\right]$$

$$\varepsilon^2: f_i^{(2)} = -\Delta t \tau_f \left[D_{i\alpha}^{(1)} f_i^{(1)} + \partial_t^{(2)} f_i^{(0)}\right] - \tau_f \frac{(\Delta t)^2}{2}\left[D_{i\alpha}^{(1)}\right]^2 f_i^{(0)} + O\left[(\Delta t)^3\right]$$

$$\varepsilon^1: \partial_t^{(1)} \rho + \partial_{x_\alpha}^{(1)}(\rho u_\alpha) + O[(\Delta t)^2] = 0$$

$$\partial_t^{(1)}(\rho u_\alpha) + \partial_{x_\beta}^{(1)}(\rho u_\alpha u_\beta + p\delta_{\alpha\beta}) + O[(\Delta t)^2] = 0$$

$$\varepsilon^2: \partial_t^{(2)} \rho + O\left[(\Delta t)^3\right] = 0$$

$$\partial_t^{(2)}(\rho u_\alpha) - \nu \partial_{x_\beta}^{(1)}\left\{\rho\left[\partial_{x_\alpha}^{(1)} u_\beta + \partial_{x_\beta}^{(1)} u_\alpha\right]\right\} + O\left[(\Delta t)^3\right] = 0$$

1.3.3 From LBM to NS equation

$$f_i^{(0)} = f_i^{(eq)}$$

$$f_i^{(1)} = -\tau_f \Delta t \left[U_{i\alpha} f_i^{(0)} \frac{1}{\rho} \partial_{x_\alpha}^{(1)} \rho + U_{i\alpha} U_{i\beta} f_i^{(0)} \frac{1}{c_s^2} \partial_{x_\alpha}^{(1)} u_\beta - U_{i\alpha} f_i^{(0)} \frac{1}{\rho c_s^2} \partial_{x_\alpha}^{(1)} p \right]$$

$$= -\tau_f \Delta t U_{i\alpha} U_{i\beta} f_i^{(0)} c_s^{-2} \partial_{x_\alpha}^{(1)} u_\beta$$

$$f_i^{(2)} = -\Delta t \tau_f \nu U_{i\beta} f_i^{(0)} c_s^{-2} \left[\frac{1}{\rho} \partial_{x_\alpha}^{(1)} \rho \left(\partial_{x_\alpha}^{(1)} u_\beta + \partial_{x_\beta}^{(1)} u_\alpha \right) + \left(\partial_{x_\alpha}^{(1)} \right)^2 u_\beta \right]$$

$$= -\Delta t \tau_f \nu U_{i\beta} f_i^{(0)} c_s^{-2} \left[\frac{1}{\rho} S_{\alpha\beta}^{(1)} \partial_{x_\alpha}^{(1)} \rho + \left(\partial_{x_\alpha}^{(1)} \right)^2 u_\beta \right]$$

$$S_{\alpha\beta} = \partial_{x_\beta} u_\alpha + \partial_{x_\alpha} u_\beta$$

1.3.3 From LBM to NS equation

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) - f_i(\mathbf{x},t) = -\frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)\right)$$

$$\upsilon = \frac{1}{3}\left(\tau - \frac{1}{2}\right)\frac{\Delta x^2}{\Delta t}$$

$$p = \rho c_s^{\,2}$$

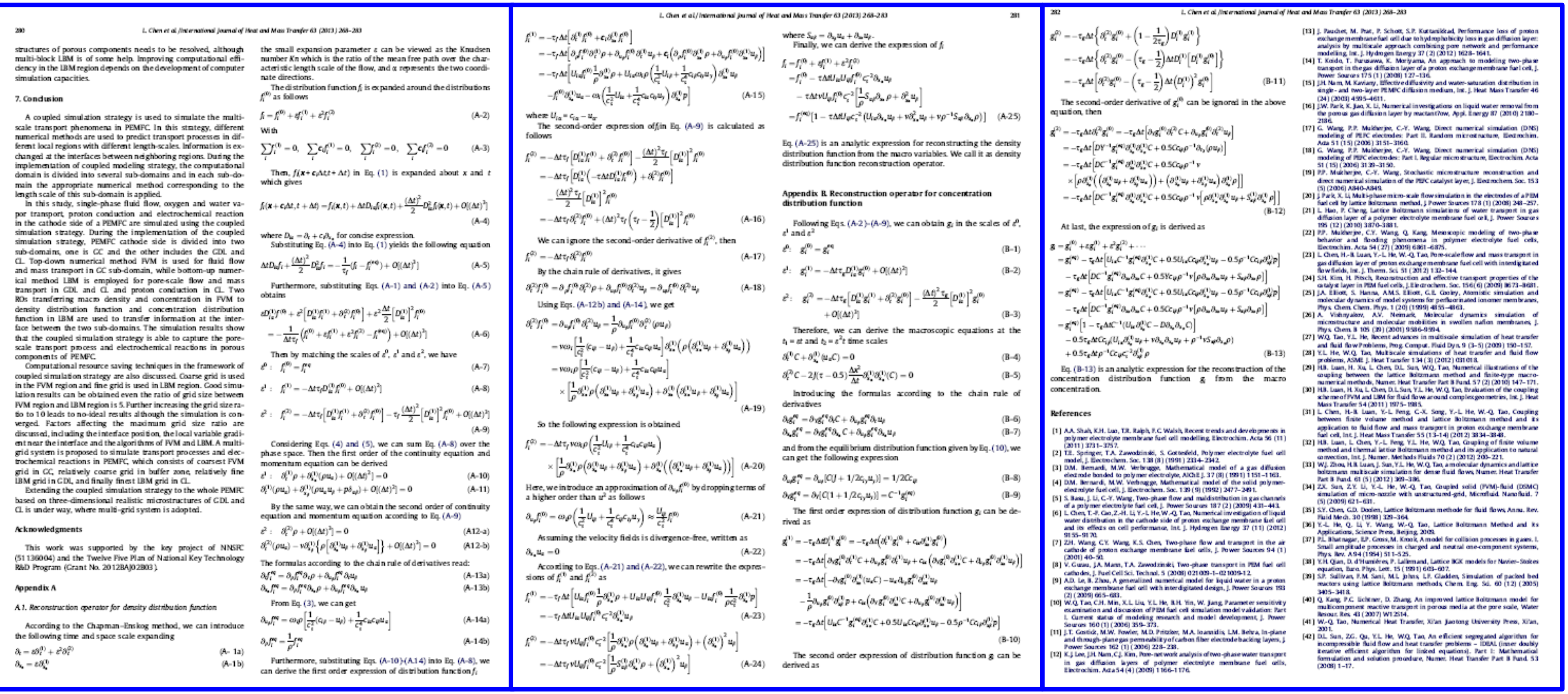
$$\rho = \sum_{i=0} f_i, \qquad \rho\mathbf{u} = \sum_{i=0} f_i \mathbf{e}_i .$$

⇩

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0$$

$$\frac{\partial \rho\mathbf{u}}{\partial t} + \nabla\cdot(\rho\mathbf{u}\mathbf{u}) = -\nabla p + \nabla\cdot\left[\rho\upsilon(\nabla\mathbf{u}+\nabla\mathbf{u}^{\mathrm{T}}) - \frac{v}{cs^2}\nabla\cdot(\rho\mathbf{u}\mathbf{u})\right]$$

1.3.3 From LBM to NS equation



采用前述的平衡态分布函数，可以证明NS方程是LBM的二阶近似。

求解LBM，实际上就是求解NS方程。

1.3.3 From LBM to NS equation

徐辉博士，栾辉宝博士，陈黎博士

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) - f_i(\mathbf{x},t) = -\frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)\right)$$

Collision （碰撞）

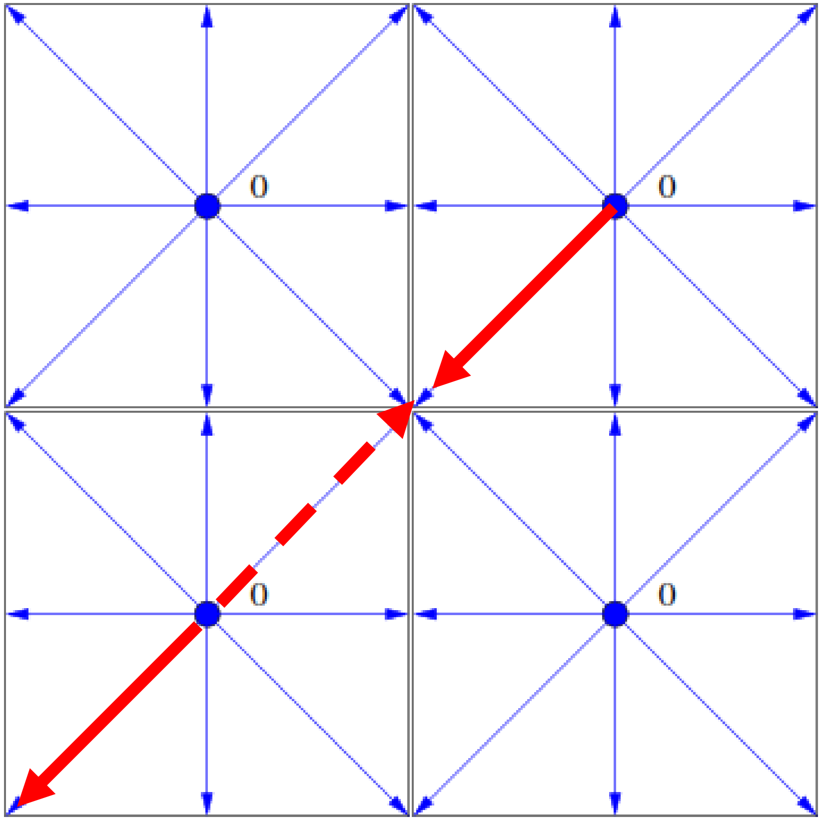
$$f_i^{'}(\mathbf{x},t) = -\frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)\right)$$

Streaming （迁移)

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) = f_i^{'}(\mathbf{x},t)$$

Macroscopic variables calculation

$$\rho = \sum_{i=0} f_i, \qquad \rho\mathbf{u} = \sum_{i=0} f_i \mathbf{e}_i .$$



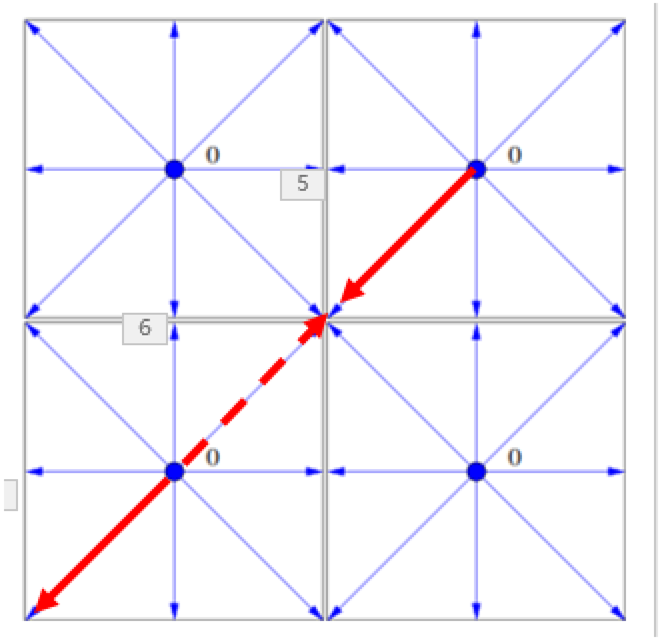
Collision （碰撞）

$$f_i^{'}(\mathbf{x},t) = -\frac{1}{\tau}(f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t))$$

Totally local and linear.

Streaming （迁移)

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) = f_i^{'}(\mathbf{x},t)$$



Only requires the information of the closest neighbors.

$$f_0(\mathbf{x}+\mathbf{c}_0\Delta t, t+\Delta t) = f_0^{'}(\mathbf{x},t) \Rightarrow f_0(x,y,t+\Delta t) = f_0^{'}(x,y,t)$$

$$f_1(\mathbf{x}+\mathbf{c}_1\Delta t, t+\Delta t) = f_1^{'}(\mathbf{x},t) \Rightarrow f_1(x+\Delta x,y,t+\Delta t) = f_1^{'}(x,y,t)$$

$$f_8(\mathbf{x}+\mathbf{c}_8\Delta t, t+\Delta t) = f_8^{'}(\mathbf{x},t) \Rightarrow f_8(x+\Delta x,y-\Delta y,t+\Delta t) = f_8^{'}(x,y,t)$$

Content

1.4 Boundary condition of the LBM

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) - f_i(\mathbf{x},t) = -\frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)\right)$$

Collision

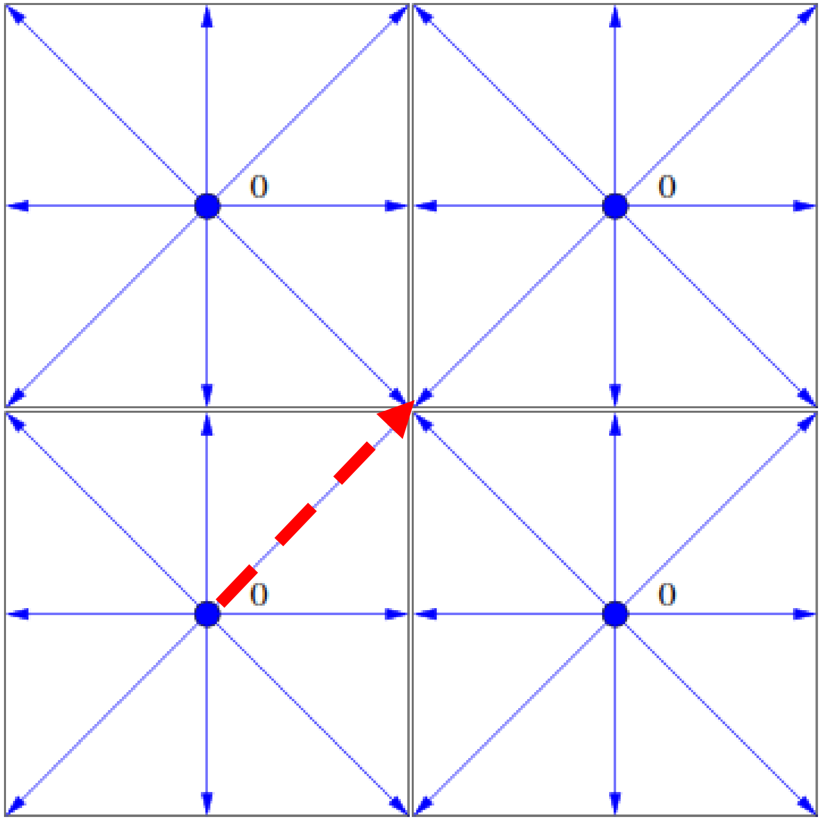
$$f_i^{'}(\mathbf{x},t) = -\frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)\right)$$

Streaming

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) = f_i^{'}(\mathbf{x},t)$$

Macroscopic variables calculation

$$\rho = \sum_{i=0} f_i, \qquad \rho\mathbf{u} = \sum_{i=0} f_i \mathbf{e}_i .$$



1.4 Boundary condition of the LBM

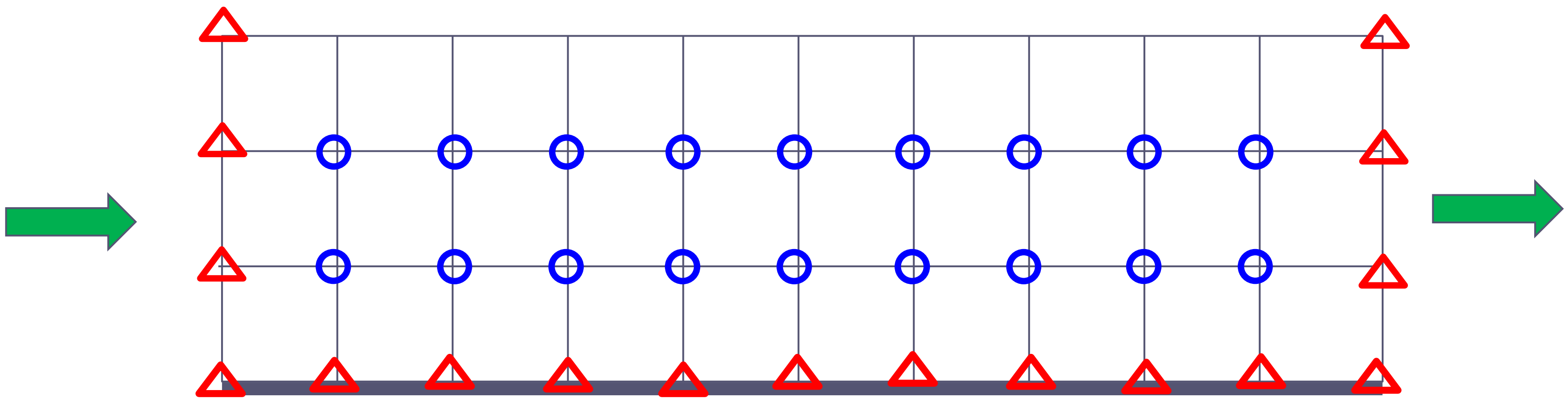
Unlike traditional CFD methods such as FVM, FEM, and FDM, in the LBM the basic variable is particle distribution function (PDF)

Boundary condition is to give values to these PDF whose values are unknown after streaming step.

Since most of the parts in the LBM are standard, such as f^{eq}, streaming, calculation, macroscopic variables calculation, successfully conducting LBM simulation is highly depended on boundary condition implementation.

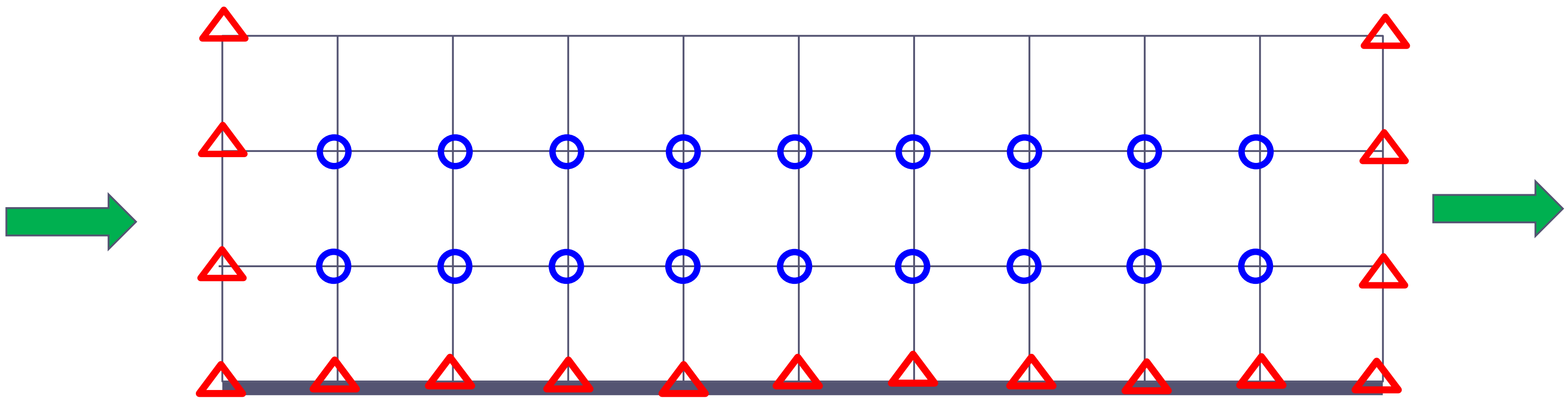
BC is important for accuracy, stability and efficiency of the LBM.

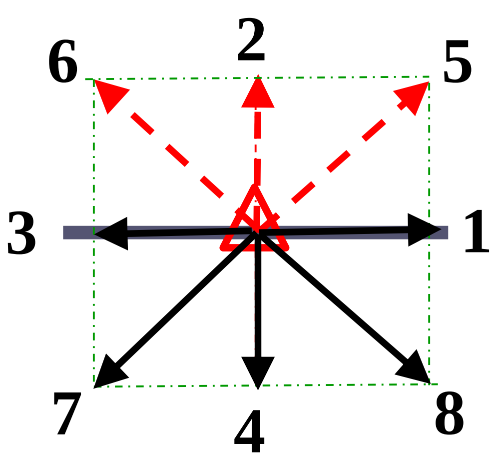
1.4 Boundary condition of the LBM



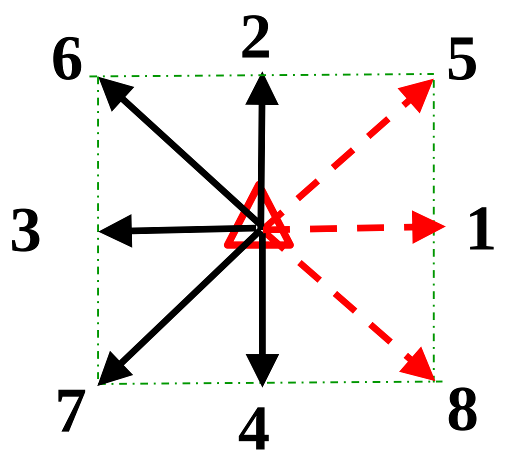
- Heuristic BC: periodic BC, symmetrical BC, full developed BC, bounce-back BC, specular reflection BC
- Kinetic BC: Zou-He BC, counter-slip BC
- Extrapolation scheme
- BC for curved boundary

1.4 Boundary condition of the LBM

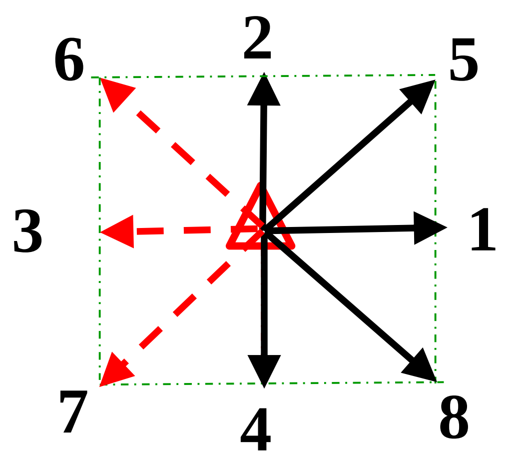




Bottom boundary



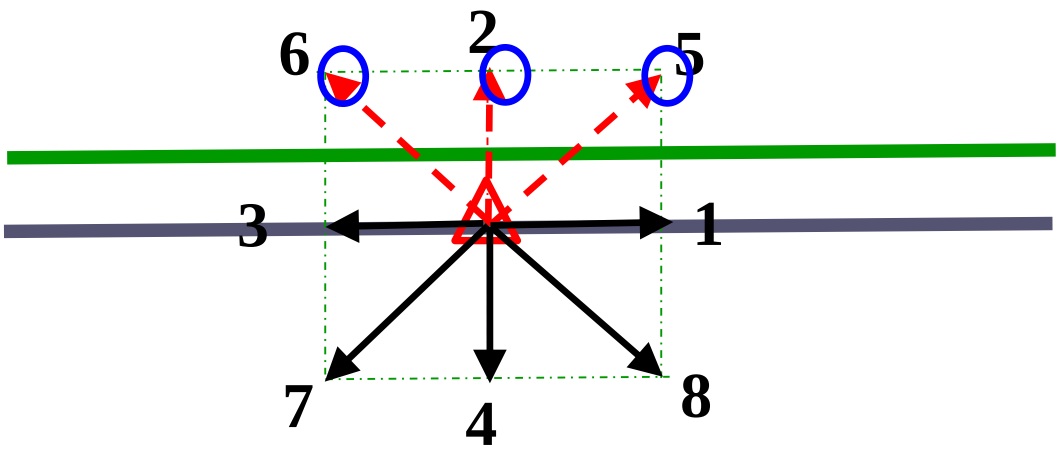
Left boundary



Right boundary

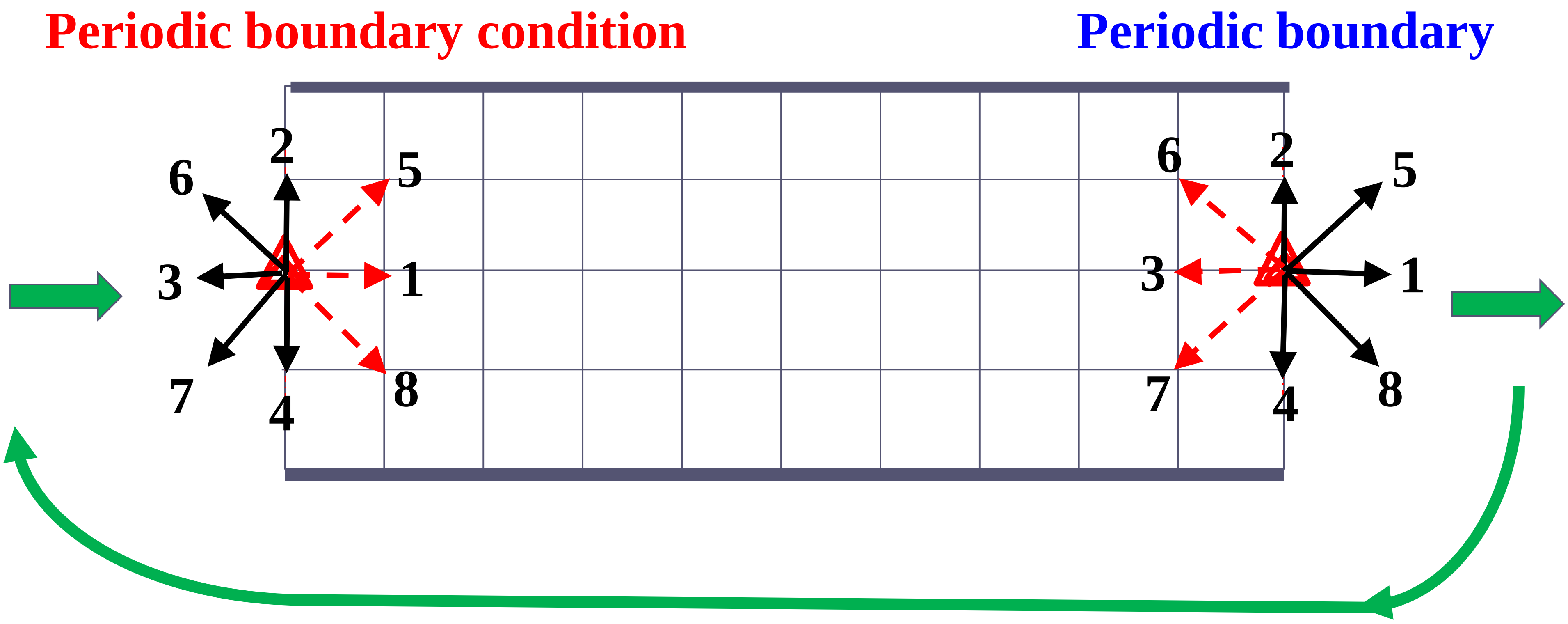
1.4 Boundary condition of the LBM

Bounce back **Non-slip boundary**



Standard bounce back	$f_{2,5,6}(i,j,t) = f_{4,7,8}(i,j,t)$	**1 order**
Modified bounce back	$f'_{2,5,6}(i,j,t) = f_{4,7,8}(i,j,t)$	**2 order**
Half-way bounce back	$f_{2,5,6}(i,j,t) = f_{4,7,8}(i,j,t)$	**2 order**

1.4 Boundary condition of the LBM

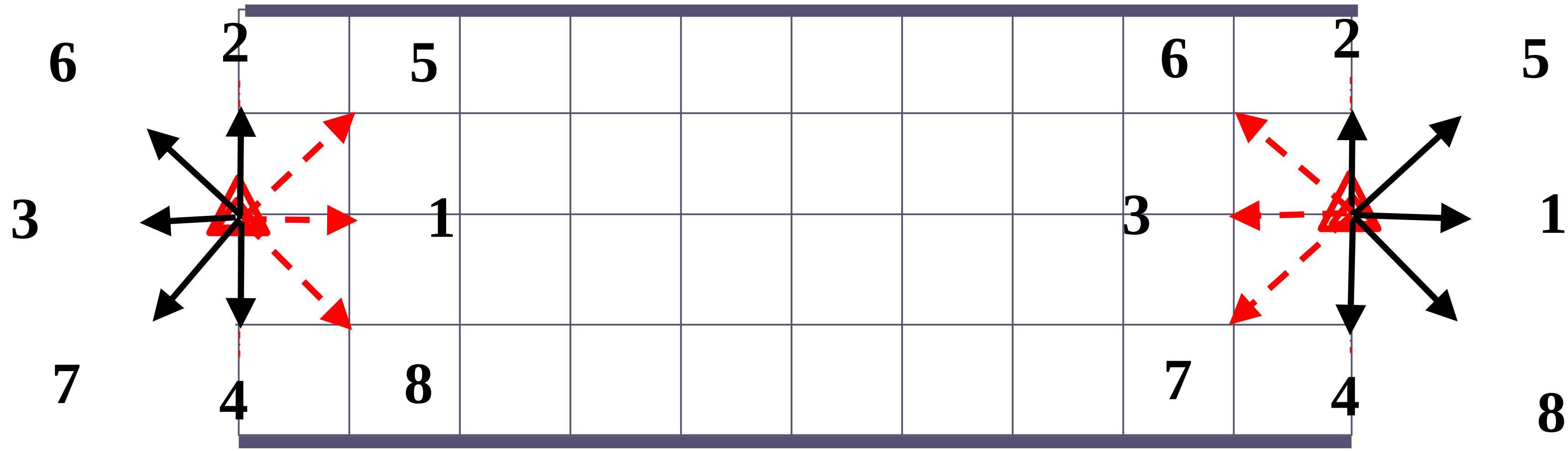


$$f_{1,5,8}(1, j, t) = f_{1,5,8}(\mathrm{nx}, j, t)$$

$$f_{3,6,7}(\mathrm{nx}, j, t) = f_{3,6,7}(1, j, t)$$

1.4 Boundary condition of the LBM

Zou-He boundary condition **Velocity or pressure is known**



$$f_1 + f_5 + f_8 - f_3 - f_6 - f_7 = u_x$$

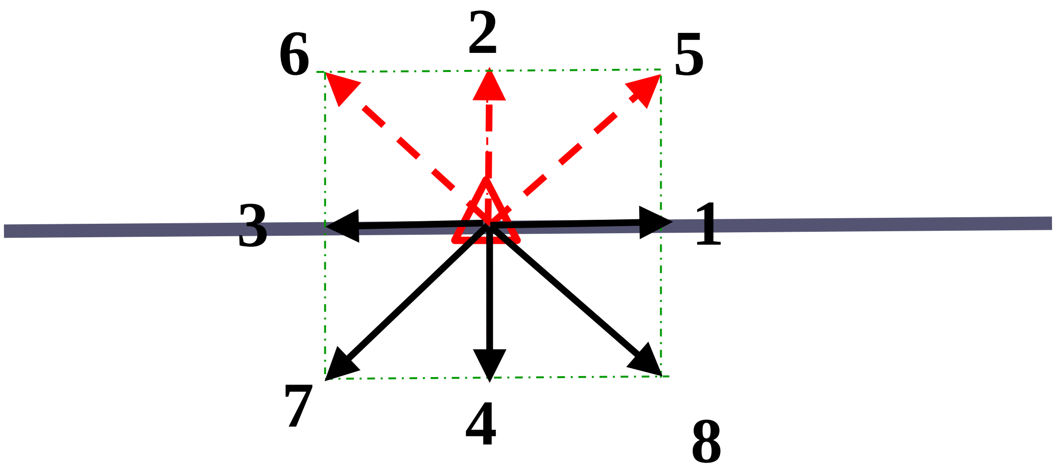
$$\rho \mathbf{u} = \sum_{i=0} f_i \mathbf{e}_i .$$

$$f_2 + f_5 + f_6 - f_4 - f_7 - f_8 = u_y$$

$$f_1 - f_1^{eq} = f_3 - f_3^{eq}$$

1.4 Boundary condition of the LBM

Extrapolation



$$f_2(\mathrm{i},1) = f_2^{\mathrm{eq}}(\mathrm{i},1)\left(\rho(i,2),\mathrm{u}(\mathrm{i},1)\right) + f_2(i,2) - f_2^{\mathrm{eq}}(i,2)$$

$$f_2(\mathrm{i},1) = f_2^{\mathrm{eq}}(\mathrm{i},1)\left(\rho(i,1),\mathrm{u}(\mathrm{i},2)\right) + f_2(i,2) - f_2^{\mathrm{eq}}(i,2)$$

Content

1.5 External force implementation

He-Shan-Doolen model

$$\frac{\partial f}{\partial t}+\boldsymbol{\xi}\cdot\frac{\partial f}{\partial \mathbf{x}}+\mathbf{a}\cdot\frac{\partial f}{\partial \boldsymbol{\xi}}=-\frac{1}{\tau}(f-f^{\mathrm{eq}})$$

$$\mathbf{a}\cdot\frac{\partial f}{\partial \boldsymbol{\xi}}\approx \mathbf{a}\cdot\frac{\partial f^{\mathrm{eq}}}{\partial \boldsymbol{\xi}}$$

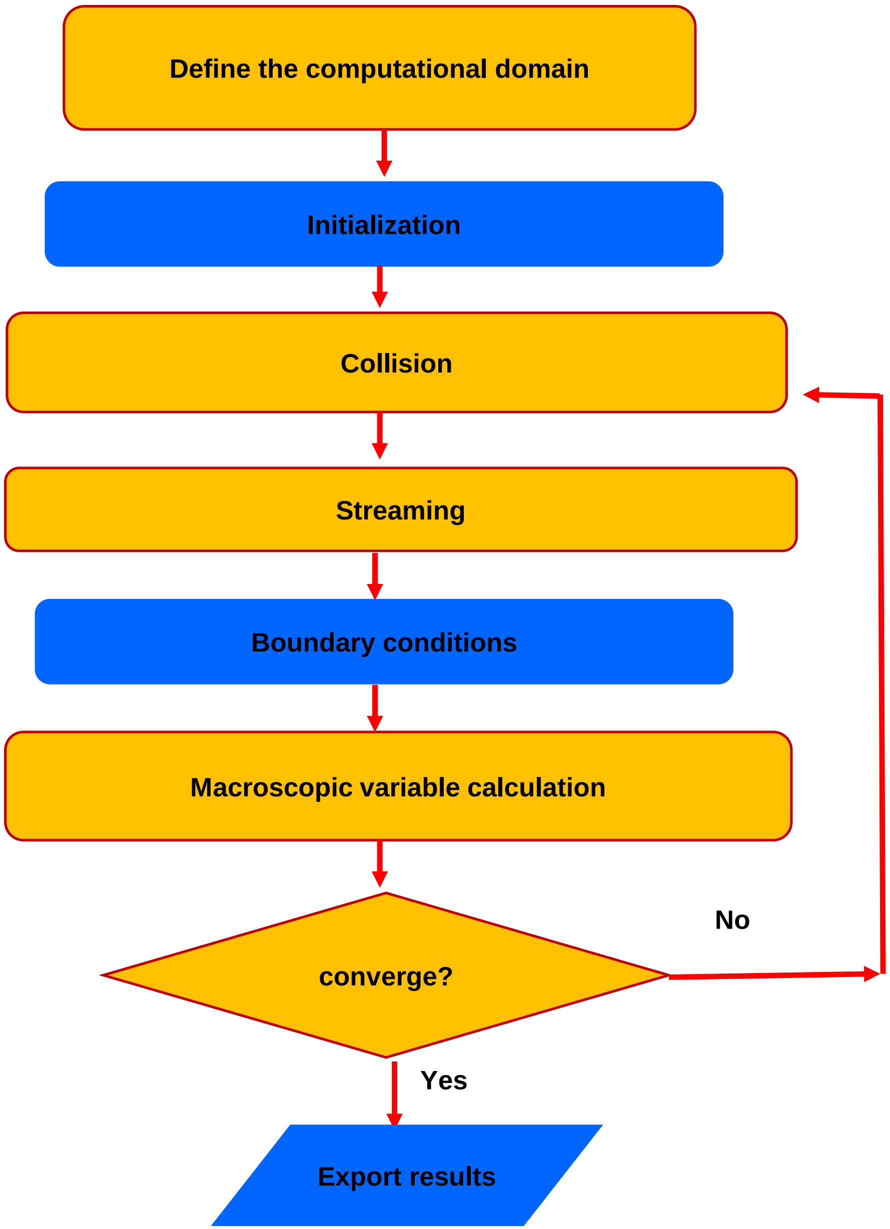
$$=\mathbf{a}\cdot\frac{\partial}{\partial \boldsymbol{\xi}}\left(\frac{1}{(2\pi RT)^{3/2}}\exp\left(-\frac{(\boldsymbol{\xi}-\mathbf{u})^2}{2RT}\right)\right)$$

$$=-\frac{(\boldsymbol{\xi}-\mathbf{u})\cdot\mathbf{a}}{RT}f^{\mathrm{eq}}$$

$$\rho\mathbf{u}=\sum_i \mathbf{c}_i f_i+\frac{1}{2}\mathbf{F}\delta t$$

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t,t+\Delta t)-f_i(\mathbf{x},t)=-\frac{1}{\tau}(f_i(\mathbf{x},t)-f_i^{\mathrm{eq}}(\mathbf{x},t))+\left(1-\frac{1}{2\tau}\right)\frac{(\mathbf{c}_i-\mathbf{u})\cdot\mathbf{a}}{c_s^{\,2}}f^{\mathrm{eq}}$$

1.6 LBM program structure



$$f \to f^{\mathrm{eq}}$$

$$f' \to f - \frac{1}{\tau}(f - f^{\mathrm{eq}})$$

$$f_i(\mathbf{x} + \mathbf{c}_i \Delta t, t + \Delta t) = f'$$

$$\rho = \sum_{i=0} f_i, \quad \rho\mathbf{u} = \sum_{i=0} f_i \mathbf{e}_i .$$

1.6 LBM program structure

1. 物理概念清晰

2. 程序简单

3. 天然并行性

4. 动理学特性 (Kinetic theory)

特别适用于复杂结构输运过程和多相流过程

If you wants to use the LBM, just week is enough; If you want to understand the LBM, one year may be not sufficient.

Low compressible model （弱可压）

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) - f_i(\mathbf{x},t) = -\frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)\right)$$

$$\upsilon = \frac{1}{3}\left(\tau - \frac{1}{2}\right)\frac{\Delta x^2}{\Delta t}$$

$$p = \rho c_s^{\ 2}$$

$$\rho = \sum_{i=0} f_i, \qquad \rho\mathbf{u} = \sum_{i=0} f_i \mathbf{e}_i .$$

⇩

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0$$

$$\frac{\partial \rho\mathbf{u}}{\partial t} + \nabla\cdot(\rho\mathbf{u}\mathbf{u}) = -\nabla p + \nabla\cdot\left[\rho\upsilon(\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}) - \frac{v}{cs^2}\nabla\cdot(\rho\mathbf{u}\mathbf{u})\right]$$

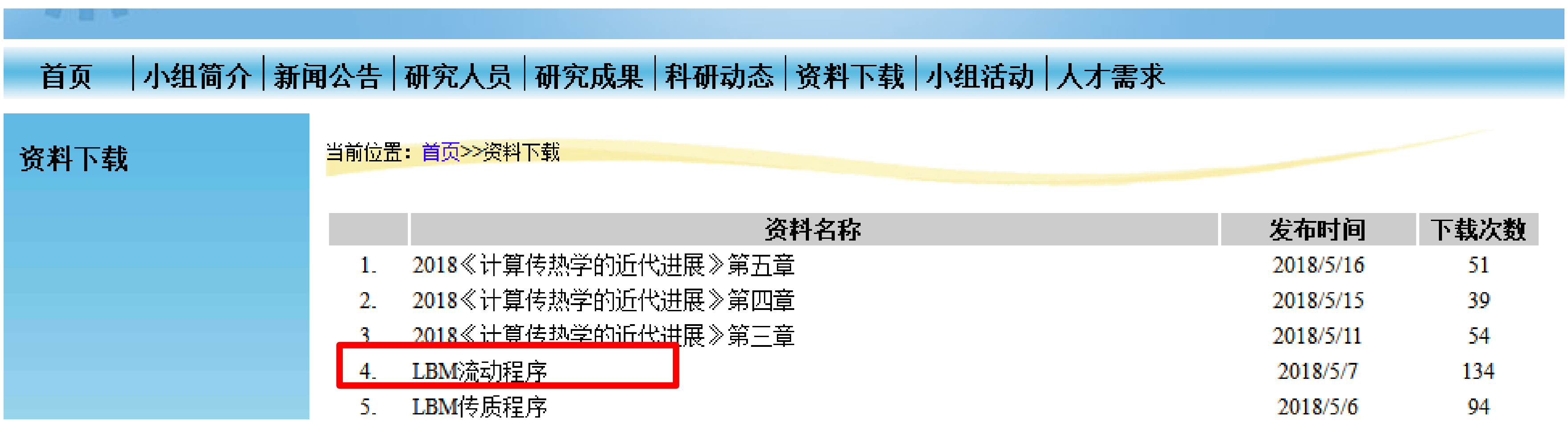
标准的格子模型是弱可压的。

1.6 LBM program structure

The LB model adopted is the imcompressible model developed by Prof. Zhaoli Guo in 2000.

Lattice BGK Model for Incompressible Navier–Stokes Equation, Journal of Computational Physics, 165(1), 2000, Pages 288-306.

The code can be downloaded at: http://nht.xjtu.edu.cn/down.asp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3.	2018《计算传热学的近代进展》第三章	2018/5/11	54
4.	LBM流动程序	2018/5/7	134
5.	LBM传质程序	2018/5/6	94

Imcompressible model

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) - f_i(\mathbf{x},t) = -\frac{1}{\tau_\upsilon}\left(f_i(\mathbf{x},t) - f_i^{\mathrm{eq}}(\mathbf{x},t)\right)$$

$$f_i^{eq} = \begin{cases} -4\sigma\dfrac{p}{c^2} + s_i(\mathbf{u}) & (i=0) \\ \lambda\dfrac{p}{c^2} + s_i(\mathbf{u}) & (i=1-4) \\ \gamma\dfrac{p}{c^2} + s_i(\mathbf{u}) & (i=5-8) \end{cases}$$

$$\begin{cases} \lambda + \gamma = \sigma \\ \lambda + 2\gamma = \dfrac{1}{2} \end{cases}$$

$$s_i(\mathbf{u}) = \omega_i\left[3\frac{\mathbf{e}_i\cdot\mathbf{u}}{c} + 4.5\frac{(\mathbf{e}_i\cdot\mathbf{u})^2}{c^2} - 1.5\frac{\mathbf{u}\cdot\mathbf{u}}{c^2}\right]$$

$$\mathbf{u} = \sum_{i=1}^{8}\mathbf{e}_i f_i \qquad \frac{p}{\rho} = \frac{c^2}{4\sigma}\left[\sum_{i=1}^{8} f_i + s_0(u)\right]$$

Imcompressible LB model for fluid flow

```
!============================================================================
!    This code was written by Li Chen at Xi'an Jiaotong University.
!    This code was for single-phase in a 2D channel.
!    Pressures are known at the left inlet and right outlet,
!    and non_slip conditions at the top and bottom walls.
!    One can refer to the following papers for more details:
!    Li Chen et al., Water Resources Research Volume: 50(12): 9343-9365, 2014
!    Li Chen: lichennht08@mail.xjtu.edu.cn.
!============================================================================
```

The program is used only for the teaching purpose. No part of it may be published. You may use it as a frame to re-develop your own code for research purpose.

```
!========================================================
MODULE START_L
   PARAMETER (nx=21,ny=81)
   integer::I,J,K,LAST,ITER
   double precision,PARAMETER::XL=20.E-5,YL=80.E-5
   double precision,dimension(nx)::X
   double precision,dimension(ny)::Y
   double precision,dimension(0:nx+1,0:ny+1)::U,V,PRE
!--------------------------------------------------
   double precision::DX,DY,DT
   double precision,PARAMETER::C=1.d0,CS2=1.d0/3.d0
   integer,dimension(0:8)::FCX=(/0,1,0,-1,0,1,-1,-1,1/)
   integer,dimension(0:8)::FCY=(/0,0,1,0,-1,1,1,-1,-1/)
   double precision,dimension(0:8)::wi
   double precision,dimension(0:2)::lambda
   !--------------------------------------------------------------
   double precision,dimension(0:8,0:nx+1,0:ny+1)::f1,ff1
   double precision::ftao,vmu_phy,vmu_lat,preleft,preright,feq1
!---------------------------------------------------------------
   integer,dimension(0:nx+1,0:ny+1)::ls
   logical,dimension(0:nx+1,0:ny+1)::walls
   double precision::delta
   double precision::sumc_last,sumu
 END MODULE
!========================================================
```

Velocity and pressure

Lattice velocity and sound speed

DnQm model

Parameters in LB model

PDF

Define of solid structure

Main program

```
!=============================================================================
PROGRAM MAIN
USE START_L

    CALL SOLID_STRUCTURE
    CALL INITIALIZATION

    DO iter=1,last
        CALL COLLISIONF
        CALL STREAMF
        CALL BOUNDARYF
        CALL MACROF
        if(mod(iter,1000).eq.0) CALL OUTPUT
    ENDDO

END PROGRAM
!=============================================================================
```

Structure

```
!=================================================================-=
SUBROUTINE SOLID_STRUCTURE
USE START_L
   ! ls represents the porous structure: 0 denotes nodes of void space, 1 denotes solid node.
   ls=0
   ls(:,ny:ny+1)=1
   ls(:,0:1)=1
   walls=.false.
   do j=0,ny+1
   do i=0,nx+1
      if(ls(i,j).eq.1) then
         walls(i,j)=.true.
      endif
   enddo
   enddo
RETURN
END SUBROUTINE
!===================================================================
```

Here, you can input the solid structures you want to simulate!
Input the structure date. A 2D matrix with 0 for fluid and 1 for solid.

See Slides for porous flow!

Initialization

```
!=======================================================
SUBROUTINE INITIALIZATION
USE START_L
double precision::z1,z2

    dx=xl/float(nx-1)
    dy=dx
    last=500000
    delta=1.d0
    lambda(0)=-5.d0/3.d0
    lambda(1)=1.0d0/3.d0
    lambda(2)=1.d0/12.d0
    wi(0)=4.d0/9.d0
    wi(1:4)=1.d0/9.d0
    wi(5:8)=1.d0/36.d0
    vmu_phy=20.e-6
    ftao=1.d0
    vmu_lat=(ftao-0.5d0)/3.d0
    scale=vmu_phy/vmu_lat
    dt=dx**2./scale
    preleft=1.0002d0
    preright=1.d0

    do j=1,ny
    do i=1,nx
       pre(i,j)=preleft-float(i-1)/float(nx-1)*(preleft-preright)
       u(i,j)=0.d0
       v(i,j)=0.d0
    enddo
    enddo
```

Physical length of a lattice

Parameters in LB model.

Viscosity in physical units

Relaxation time

Viscosity in lattice units

Physical of one lattice iteration step.

Pressure difference between inlet and outlet.

Velocity and pressure initialization

$$f_i^{eq} = \begin{cases} -4\sigma \dfrac{p}{c^2} + s_i(\mathbf{u}) & (i=0) \\ \lambda \dfrac{p}{c^2} + s_i(\mathbf{u}) & (i=1-4) \\ \gamma \dfrac{p}{c^2} + s_i(\mathbf{u}) & (i=5-8) \end{cases}$$

$\sigma=5/12$

$\lambda=1/3$

$\gamma=1/12$

Initialization

```
  do j=1,ny
  do i=1,nx
     z2=u(i,j)**2.d0+v(i,j)**2.d0
     do k=0,8
        z1=fcx(k)*u(i,j)+fcy(k)*v(i,j)
        if(k.eq.0) then
           feq1=lambda(0)*pre(i,j)+wi(k)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)
        elseif(k.le.4.and.k.ge.1) then
           feq1=lambda(1)*pre(i,j)+wi(k)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)
        elseif(k.le.8.and.k.ge.5) then
           feq1=lambda(2)*pre(i,j)+wi(k)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)
        endif
        f1(k,i,j)=feq1
        ff1(k,i,j)=feq1
     enddo
  enddo
  enddo

RETURN
END SUBROUTINE
!=============================================================
```

$$f_i^{eq}=\begin{cases}-4\sigma\dfrac{p}{c^2}+s_i(\mathbf{u}) & (i=0)\\ \lambda\dfrac{p}{c^2}+s_i(\mathbf{u}) & (i=1-4)\\ \gamma\dfrac{p}{c^2}+s_i(\mathbf{u}) & (i=5-8)\end{cases}$$

$$s_i(\mathbf{u})=\omega_i\left[3\frac{\mathbf{c}_i\cdot\mathbf{u}}{c}+4.5\frac{(\mathbf{c}_i\cdot\mathbf{u})^2}{c^2}-1.5\frac{\mathbf{u}\cdot\mathbf{u}}{c^2}\right]$$

Distribution function initialization!

Collision

```
!==============================================================
SUBROUTINE COLLISIONF
USE START_L
double precision::z1,z2

   do j=1,ny
   do i=1,nx
      if(.not.walls(i,j)) then
      z2=u(i,j)**2.+v(i,j)**2.
      do k=0,8
         z1=fcx(k)*u(i,j)+fcy(k)*v(i,j)
         if(k.eq.0) then
            feq1=lambda(0)*pre(i,j)+wi(k)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)
         elseif(k.le.4.and.k.ge.1) then
            feq1=lambda(1)*pre(i,j)+wi(k)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)
         elseif(k.le.8.and.k.ge.5) then
            feq1=lambda(2)*pre(i,j)+wi(k)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)
         endif
         ff1(k,i,j)=f1(k,i,j)-1.d0/ftao*(f1(k,i,j)-feq1)
     enddo
    endif
   enddo
   enddo

RETURN
END SUBROUTINE
!==============================================================
```

$$f' \to f - \frac{1}{\tau}(f - f^{\mathrm{eq}})$$

Stream

```
!=========================================
SUBROUTINE STREAMF
USE START_L

!------------------periodic boundary along y---------------
    do j=1,ny
    do i=1,nx
    do k=0,8
        f1(k,i,j)=ff1(k,i-int(fcx(k)),j-int(fcy(k)))
    enddo
    enddo
    enddo

RETURN
END SUBROUTINE
!=========================================
```

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) = f\,'$$

Boundary condition

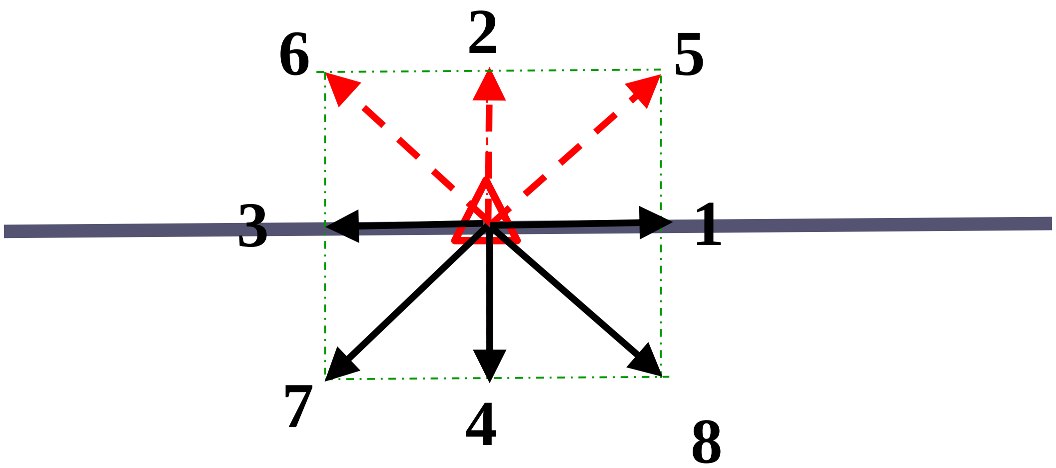
```
!=======================================================================
SUBROUTINE BOUNDARYF
USE START_L

   do j=1,ny
   do i=1,nx
      if(walls(i,j)) then
        ff1(1,i,j)=f1(3,i,j)
        ff1(3,i,j)=f1(1,i,j)
        ff1(2,i,j)=f1(4,i,j)
        ff1(4,i,j)=f1(2,i,j)
        ff1(5,i,j)=f1(7,i,j)
        ff1(7,i,j)=f1(5,i,j)
        ff1(6,i,j)=f1(8,i,j)
        ff1(8,i,j)=f1(6,i,j)
     endif
   enddo
   enddo

   do j=1,ny
      z1=fcx(1)*u(2,j)+fcy(1)*v(2,j)
      z2=u(2,j)**2.d0+v(2,j)**2.d0
      feq1=lambda(1)*pre(2,j)+wi(1)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)
      f1(1,1,j)=lambda(1)*pre(1,j)+wi(1)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2) +F1(1,2,J)-FEQ1
      z1=fcx(5)*u(2,j)+fcy(5)*v(2,j)
      feq1=lambda(2)*pre(2,j)+wi(5)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)
      f1(5,1,j)=lambda(2)*pre(1,j)+wi(5)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)+F1(5,2,J)-FEQ1
      z1=fcx(8)*u(2,j)+fcy(8)*v(2,j)
      feq1=lambda(2)*pre(2,j)+wi(8)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)
      f1(8,1,J)=lambda(2)*pre(1,j)+wi(8)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)+F1(8,2,J)-FEQ1
  enddo
```

非平衡外推！

Non-equilibrium extrapolation method for velocity and pressure boundary conditions in the lattice Boltzmann method
ZL Guo, CG Zheng, BC Shi
Chinese Physics 11 (4), 366

Boundary condition of the LBM

Extrapolation



$$f_2(\mathrm{i},1) = f_2^{\mathrm{eq}}(\mathrm{i},1)\left(\rho(i,2),\mathrm{u}(\mathrm{i},1)\right) + f_2(i,2) - f_2^{\mathrm{eq}}(i,2)$$

$$f_2(\mathrm{i},1) = f_2^{\mathrm{eq}}(\mathrm{i},1)\left(\rho(i,1),\mathrm{u}(\mathrm{i},2)\right) + f_2(i,2) - f_2^{\mathrm{eq}}(i,2)$$

```
do j=1,ny
    z1=fcx(3)*u(nx-1,J)+fcy(3)*v(nx-1,j)
    z2=u(nx-1,j)**2.d0+v(nx-1,j)**2.d0
    feq1=lambda(1)*pre(nx-1,j)+wi(3)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)
    f1(3,nx,j)=lambda(1)*pre(nx,j)+wi(3)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2) +F1(3,nx-1,J)-FEQ1
    z1=fcx(6)*u(nx-1,j)+fcy(6)*v(nx-1,j)
    feq1=lambda(2)*pre(nx-1,j)+wi(6)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)
    f1(6,nx,j)=lambda(2)*pre(nx,j)+wi(6)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2) +F1(6,nx-1,J)-FEQ1
    z1=fcx(7)*u(nx-1,j)+fcy(7)*v(nx-1,j)
    feq1=lambda(2)*pre(nx-1,j)+wi(7)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2)
    f1(7,nx,j)=lambda(2)*pre(nx,j)+wi(7)*(3.d0*z1+4.5d0*z1**2.-1.5d0*z2) +F1(7,nx-1,J)-FEQ1
 enddo

RETURN
END SUBROUTINE
!=========================================================================
```

```
!=================================================
SUBROUTINE MACROF
USE START_L

   do j=1,ny
   do i=1,nx
      IF(.not.walls(i,j)) THEN
         temppre=0.0d0
         tempu=0.0d0
         tempv=0.0d0
         do k=1,8
            temppre=temppre+f1(k,i,j)
            tempu=tempu+f1(k,i,j)*fcx(k)
            tempv=tempv+f1(k,i,j)*fcy(k)
         enddo
         u(i,j)=tempu
         v(i,j)=tempv
         temp1=u(i,j)**2.d0+v(i,j)**2.d0
         pre(i,j)=(temppre-2.d0/3.d0*temp1)/(-lambda(0))
      elseif(walls(i,j))then
         u(i,j)=0.d0
         v(i,j)=0.d0
         pre(i,j)=0.d0
      endif
   enddo
   enddo

   do j=1,ny
       pre(1,j)=preleft
       pre(nx,j)=preright
   enddo

RETURN
END SUBROUTINE
```

$$\mathbf{u}=\sum_{i=1}^{8}\mathbf{c}_i f_i,\quad \frac{p}{\rho}=\frac{c^2}{4\sigma}\left[\sum_{i=1}^{8} f_i+s_0(\mathbf{u})\right]$$

$$s_i(\mathbf{u})=\omega_i\left[3\frac{\mathbf{c}_i\cdot\mathbf{u}}{c}+4.5\frac{(\mathbf{c}_i\cdot\mathbf{u})^2}{c^2}-1.5\frac{\mathbf{u}\cdot\mathbf{u}}{c^2}\right]$$

$$S_0(u)$$

```
!=======================================================================
SUBROUTINE OUTPUT
USE START_L

    sumu_last=sumu
    sumu=0.d0
    do j=1,ny
    do i=1,nx
        if(.not.walls(i,j)) sumu=sumu+u(i,j)
    enddo
    enddo
    delta=abs(sumu_last-sumu)/abs(sumu)
    write(*,*) iter,u(nx-10,ny/2),delta

    open(10,file="velocity_pressure.dat")
    write(10,*)'VARIABLES= X,Y,u,v,pre'
    WRITE(10,*)'ZONE I=',nx,',J=',ny,',T=TT'
    do j=1,ny
    do i=1,nx
        write(10,*) i,j,u(i,j),v(i,j),pre(i,j)
    enddo
    enddo
    close(10)

    if(delta.le.1.e-8) stop

RETURN
END SUBROUTINE
!=======================================================================
```

Reference

Chen, S. Y., and G. D. Doolen (1998), Lattice Boltzmann methode for fluid flows, Annual Review of Fluid Mechanics, 30, 329-364.

Succi, S. (2001), The lattice Boltzmann equation: for fluid dynamics and beyond, Oxford University Press, OXford.

Sukop, M. C., and D. T. J. Thorne (2006), Lattice Boltzmann Modeling: An Introduction for Geoscientists and Engineers, Springer Publishing Company, New York.

郭照立，郑楚光，格子**Boltzmann**方法的原理及应用，科学出版社，**2009**

何雅玲，王勇，李庆，格子Boltzmann方法的理论及应用，科学出版社，2009

Inception phase: 1988-1992 (孕育期）

The predecessor of LBM is LGA (lattice gas automata，格子气自动机)

1988: McNamara and Zanetti proposed to use real numbers rather than Boolean value "0" and "1" (PRL, 1988)

- **Avoid statistic noise**
- **Becomes complicated with multiple particles collision at one site.**

1989: Higuere and Jinenes developed the linear collision term（线性碰撞项）(Europhys. Lett, 1989)

1991-1992: several groups simultaneously proposed the BGK collision term or SRT (single relaxation time) collision term. The purpose of collision is to approach equilibrium state.

(S. Chen et al. PRL, 1991; Y. Qian et al. Europhys. Lett 1992)

Development Phase: 1988-1998 （发展期)

Several groups proved that LBM can be rigorously derived from Boltzmann equation

(T. Abe. JCP 1997; X. He and L-S Luo 1997 PRE; X. Shan and X. He. PRL, 1998)

Heat Transfer:

- **Double distribution** (X. Shan 1997 PRE, X. He, S. Chen, G. D. Doolen. JCP 1998)
- **Multi-speed model**

Multiphase and multicomponent flow (多组分多相流）

- **Pseudopotential model (X. Shan, H. Chen, PRE, 1993)**
- **Color model (A. K. Gunstensen, et al., PRA, 1991)**
- **Free energy model (Swift et al. PRL, 1995)**

Particle flow:

(A. J. C. Ladd, PRL, 1993, JFM 1994, JSP, 1995)

Reaction:

S. P. Dawson et al. J. Chem. Phys. 1993

S. Succi, G. Bella and F. Papetti, J. Sci. Comput. 1997

Other complex flow:

Non-newtonian fluid flow, magnetic fluid, blood flow, polymeric flow……

Boundary condition

Porous media flow （渗流）

Rapid Development Phase: 1999- present (快速发展期)

It has been paid great attention both on theory development and Engineering application. High *Re* flow, multiphase flow with large density and viscosity ratio, turbulent flow, combustion, three-phase flow, phase change heat transfer (boiling, condensation, melting, solidification), multicomponent reactive transport, slip flow, electro osmotic flow, MRT LB model…..

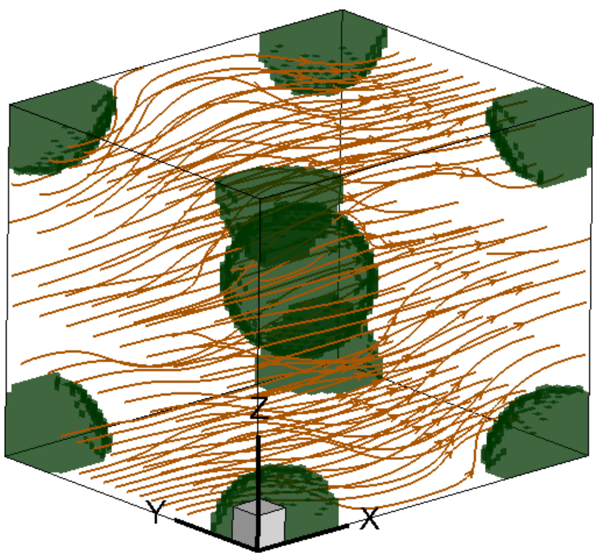
Commercial software is developed, such as Power Flow

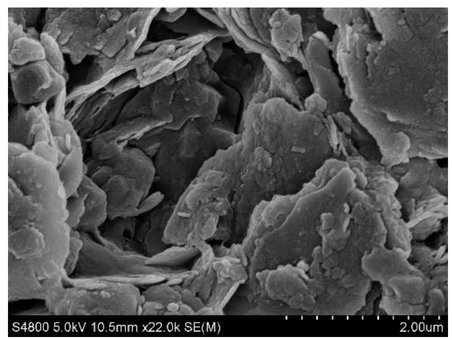
Now it has been developed as an powerful alternative tool for flow and transport process, especially for that in complex structures and multiphase flow.

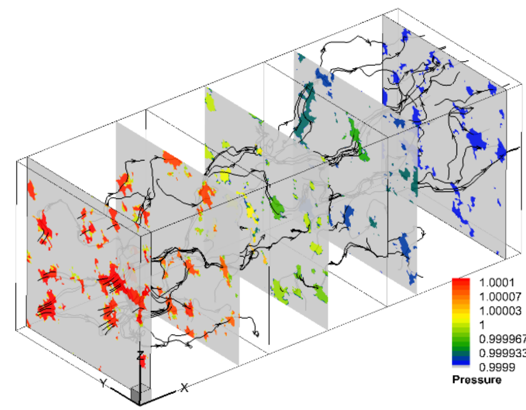
应用案例

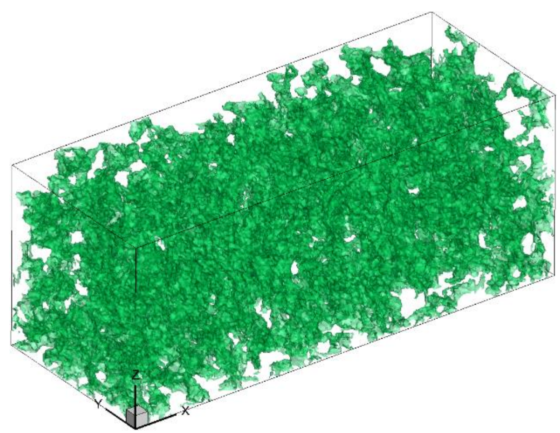
The LBM has been adopted for flow and transport phenomena in a wide range of scientific and engineering problem, especially for porous media flow and multiphase flow.

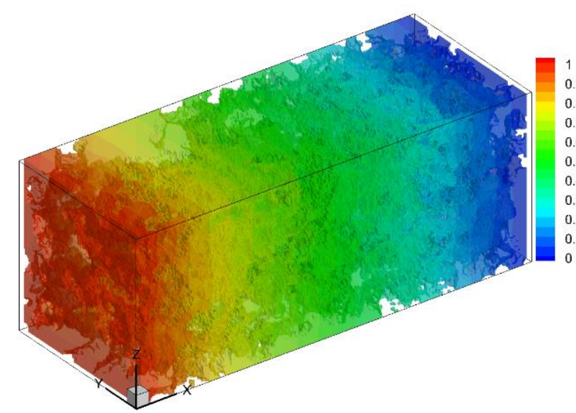
- 多孔介质流动





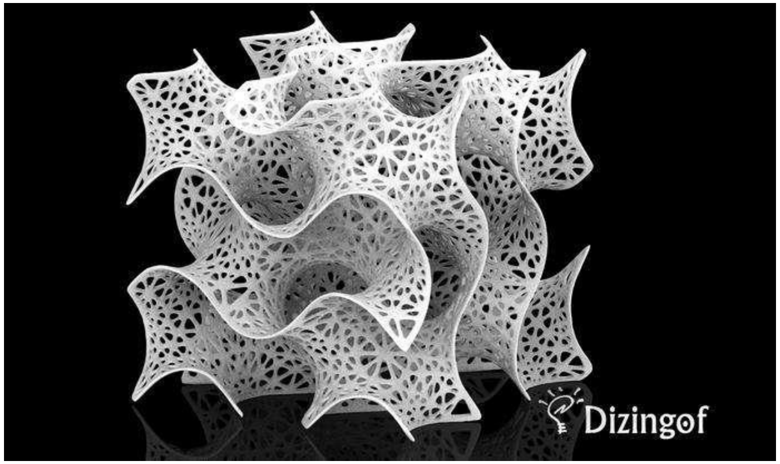


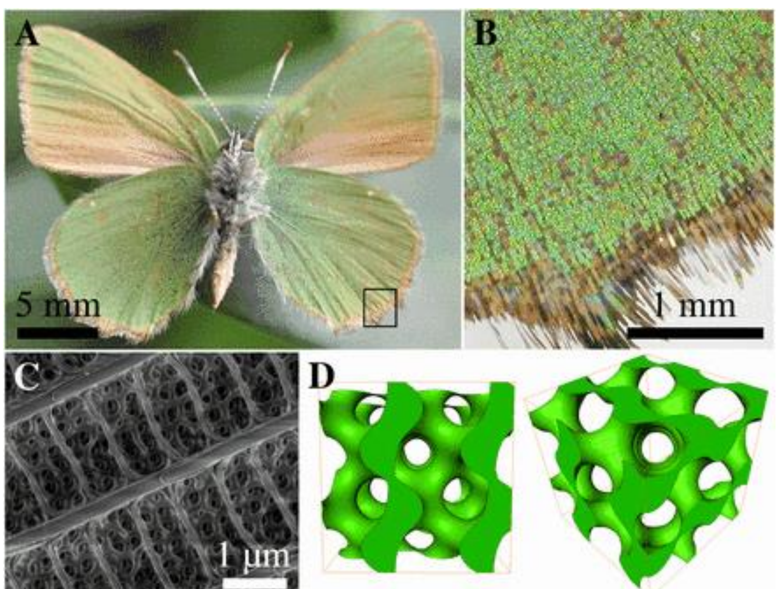


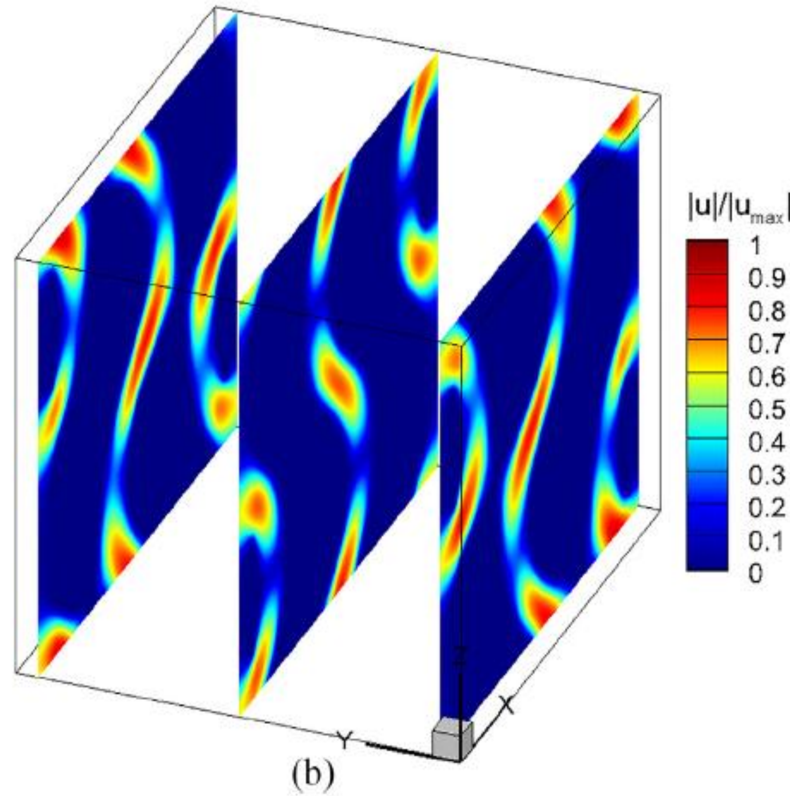


Li Chen, et al, Scientific reports,2015; Hui Wang, Li Chen, et al, Applied Energy, 2020.

多孔介质单相流动

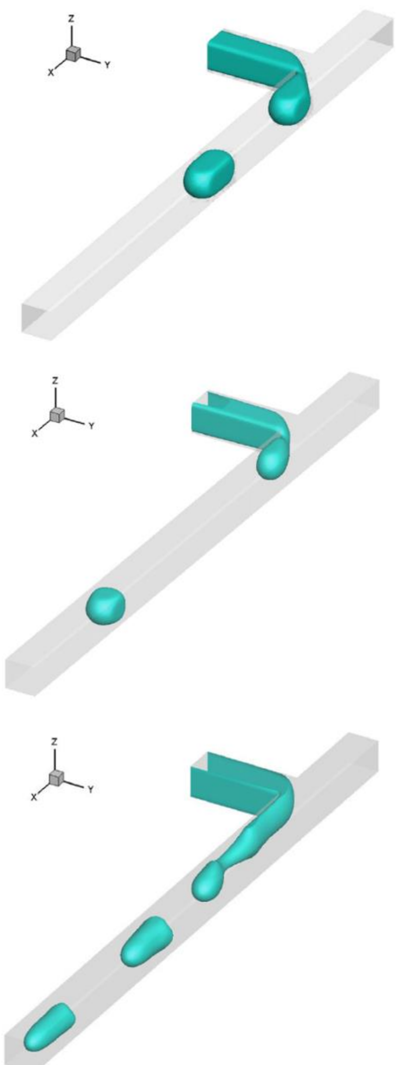


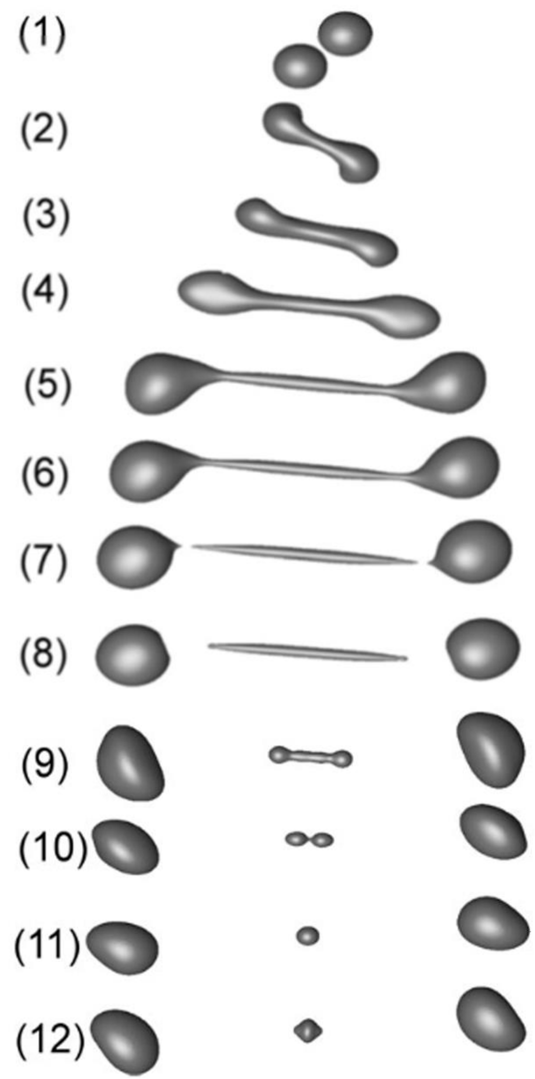


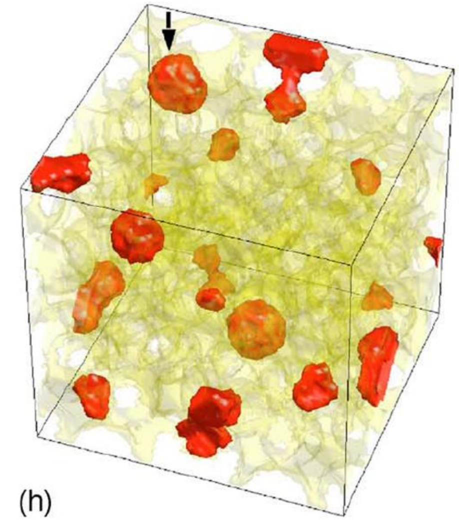


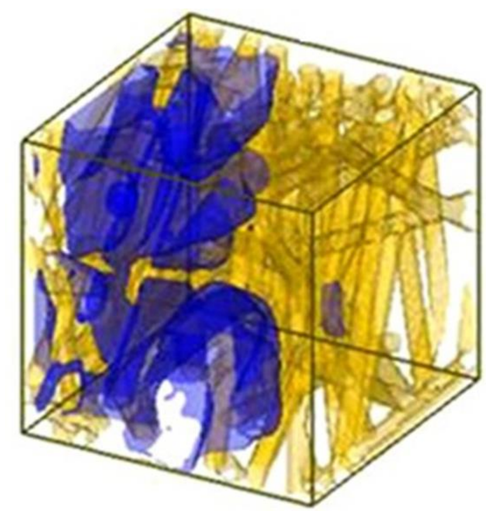
Jiwang Luo, et al., 2020, IJHMT

多相流



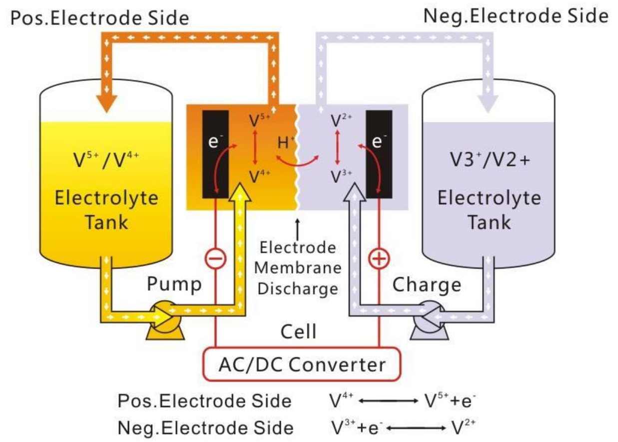


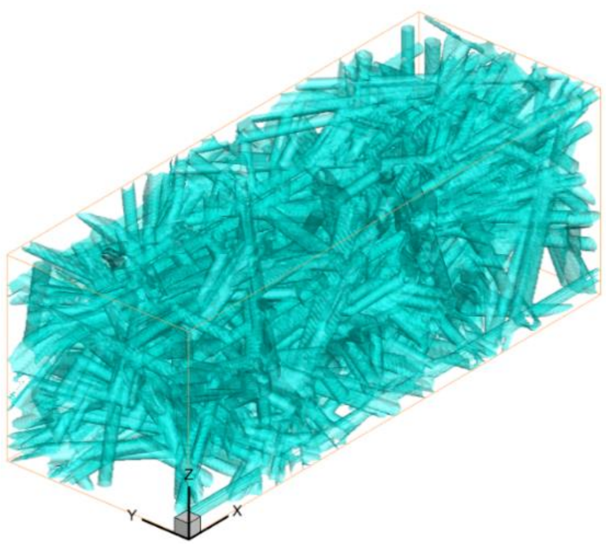


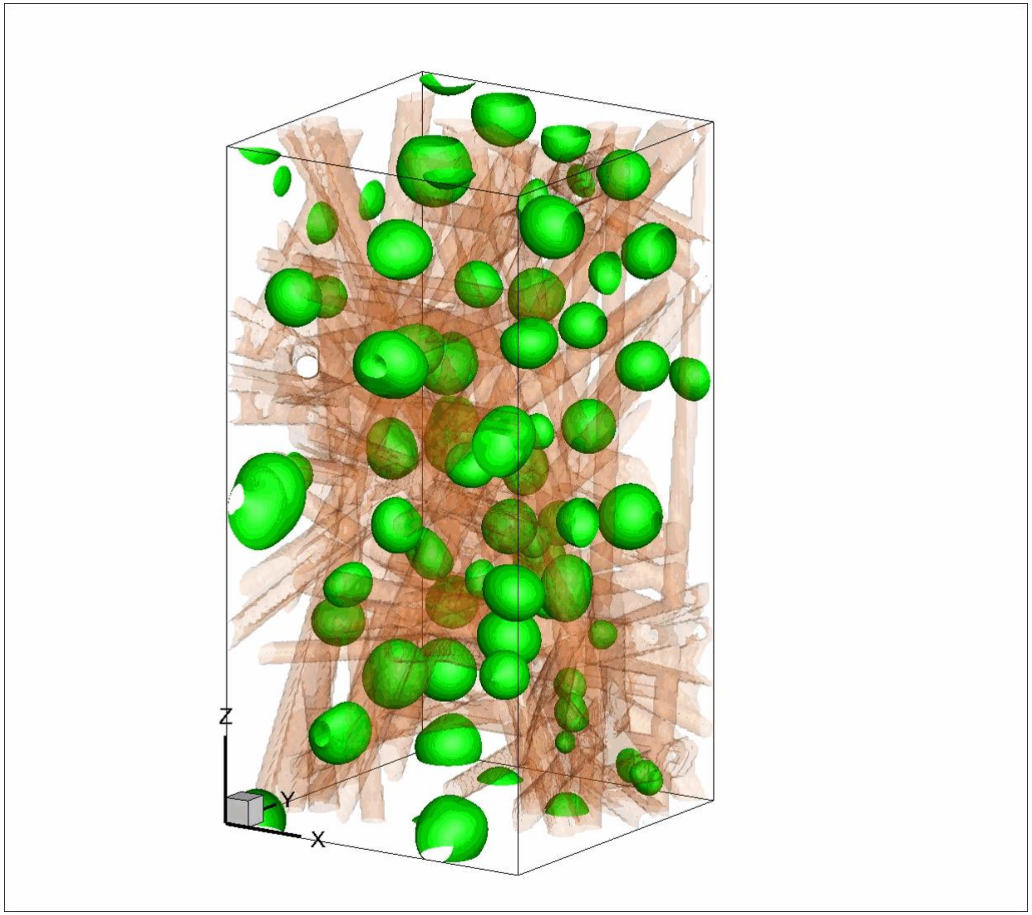


Li Chen, et al, IJHMT, 2014

全钒流电池内寄生氢气动态演变过程

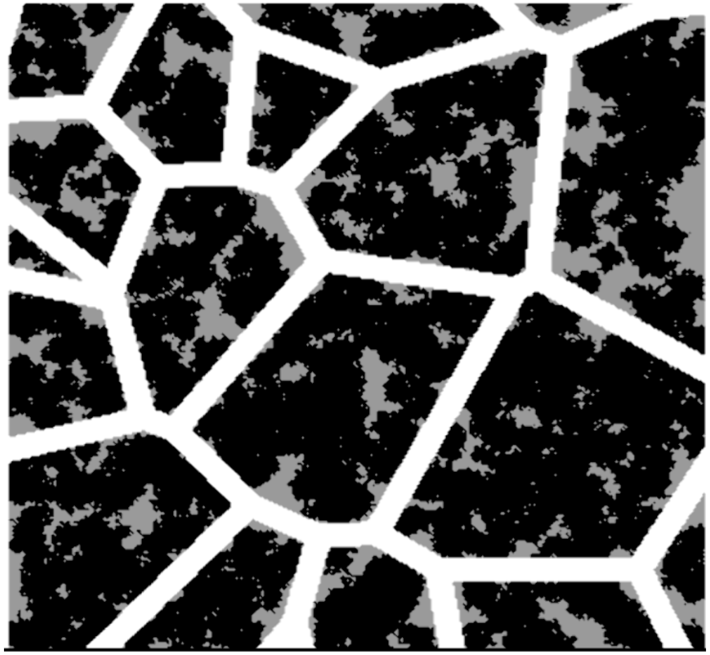


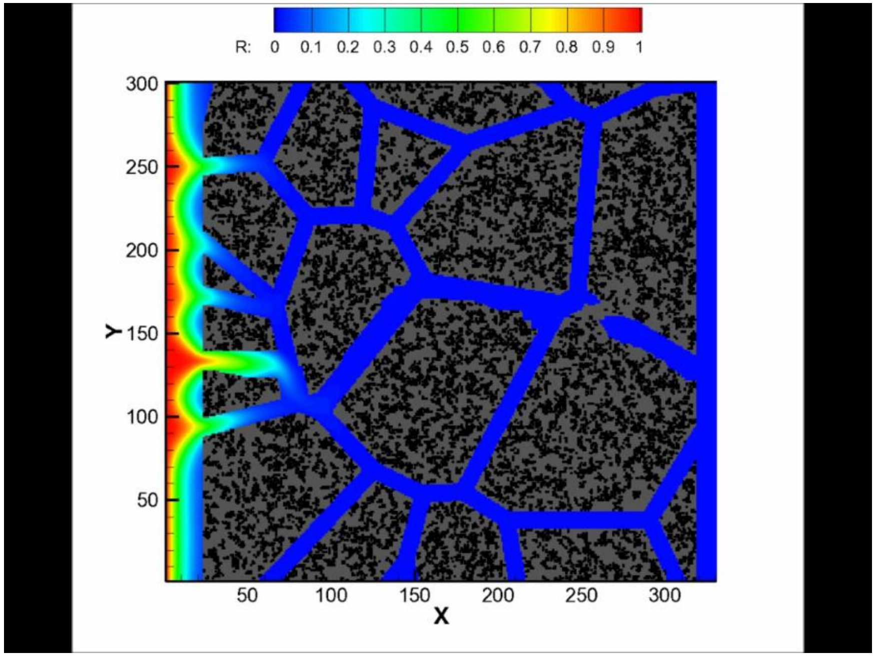




Li Chen, et al. Electrochimica Acta, 2017.

反应输运过程（温室气体埋存、石油增产）

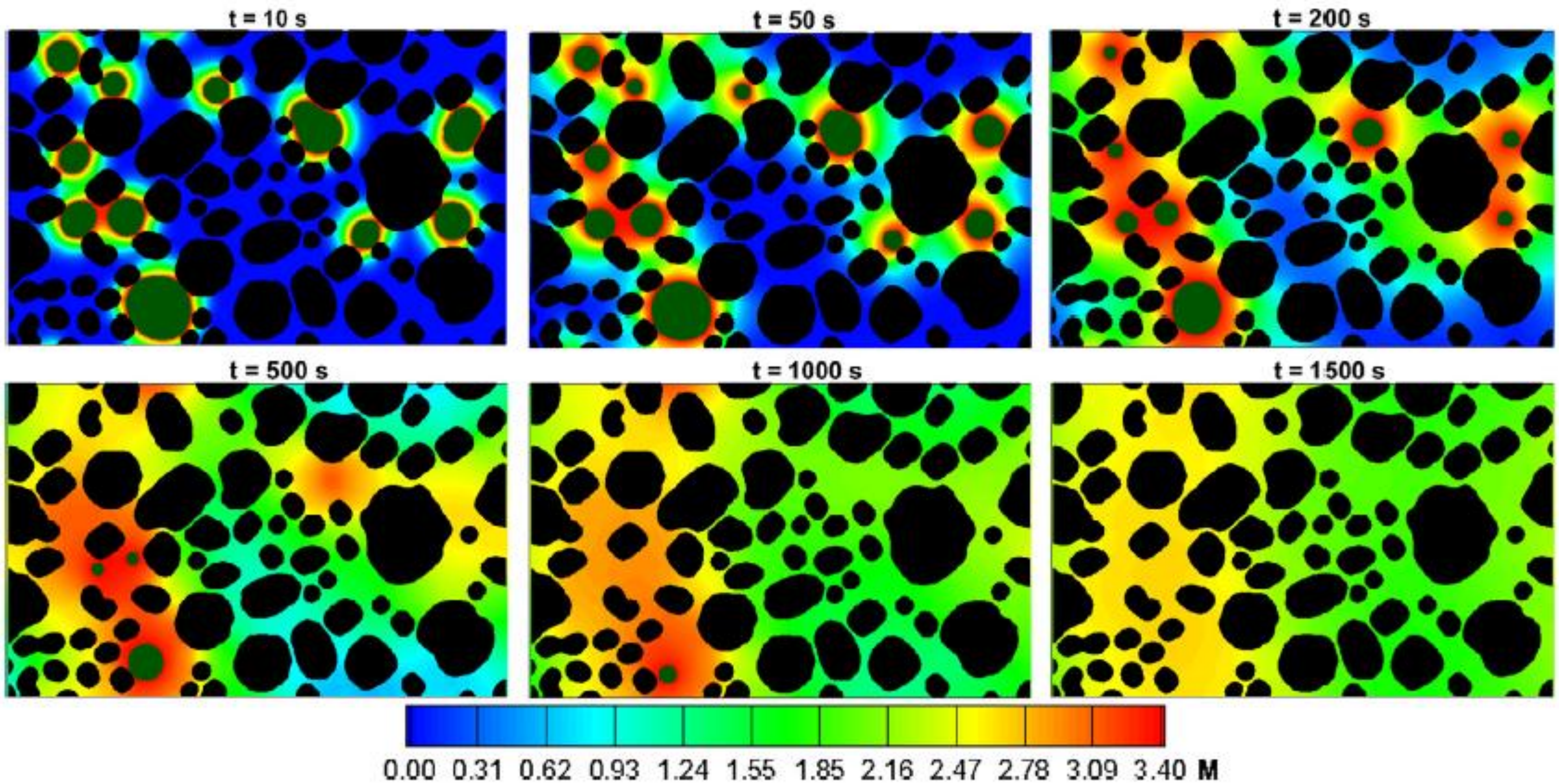




Li Chen, et al, IJHE, 2012

Li Chen, et al, WRR, 2014；Langmuir, 2012

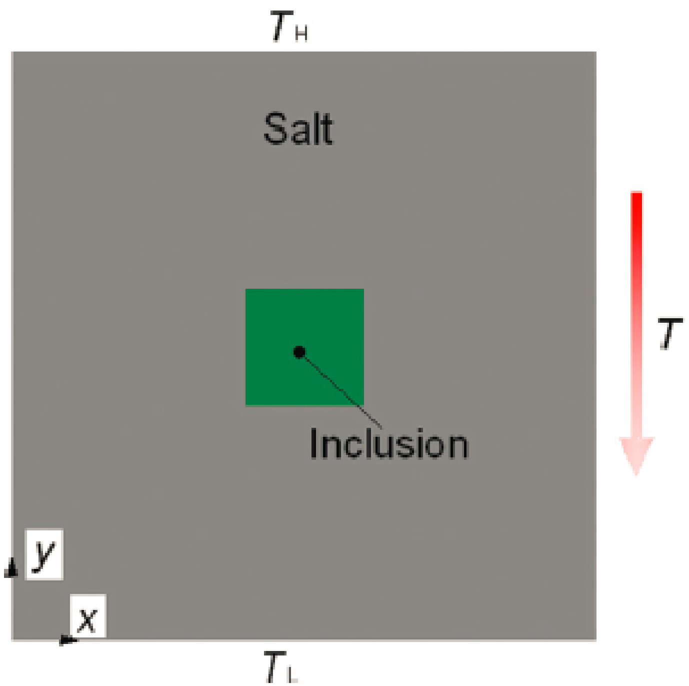
反应输运过程（温室气体埋存、石油增产）

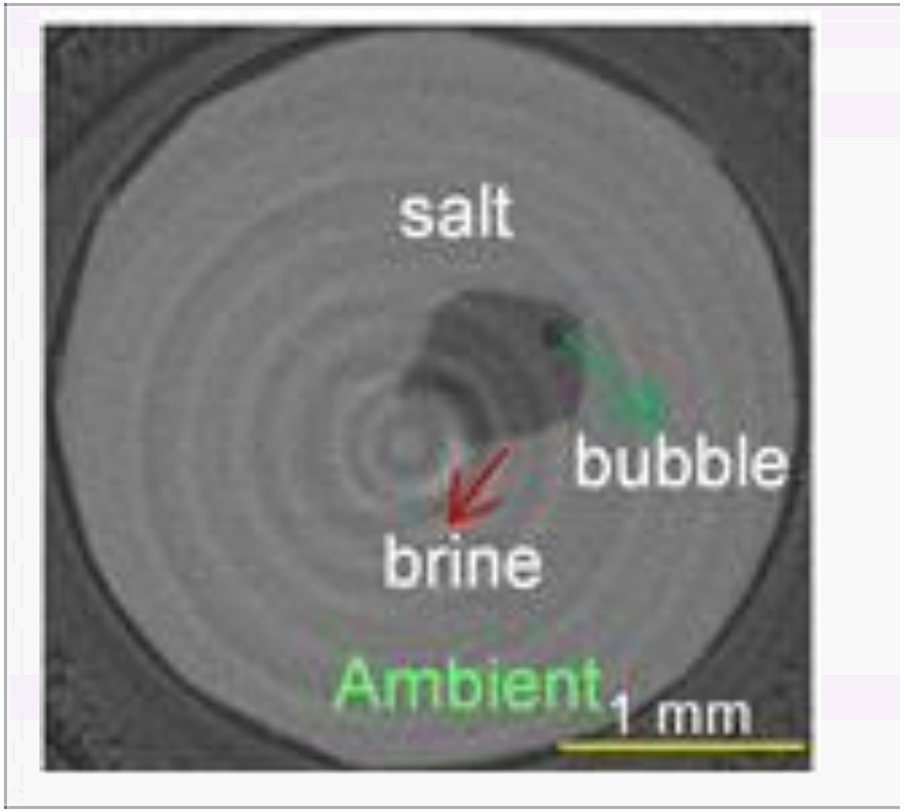


L Chen, M Wang, Q Kang, W Tao, 2018, Advances in Water Resources 116, 208-218

多相流传质反应过程：核废料封存

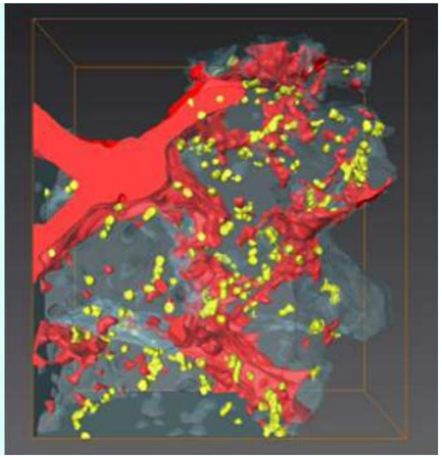
核废料



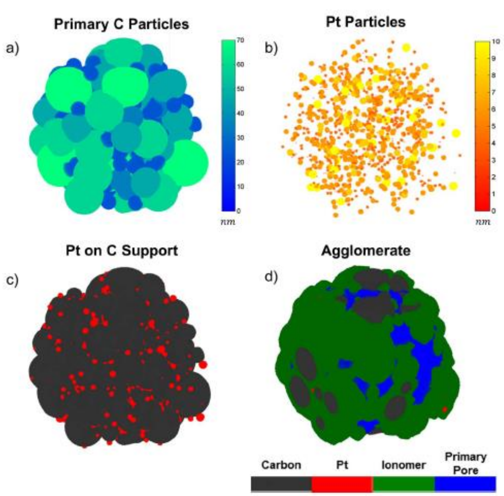


L Chen et al. 2013, PRE.

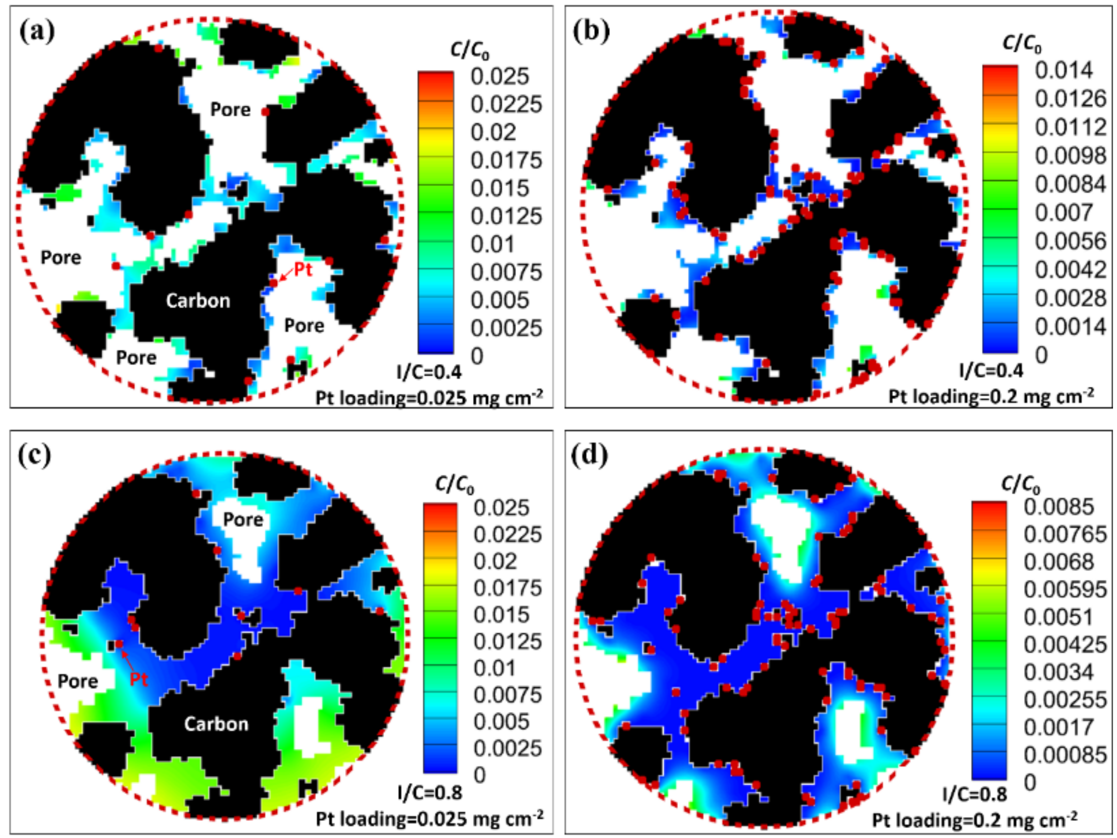
氢燃料电池“气-水-热-电”反应输运过程



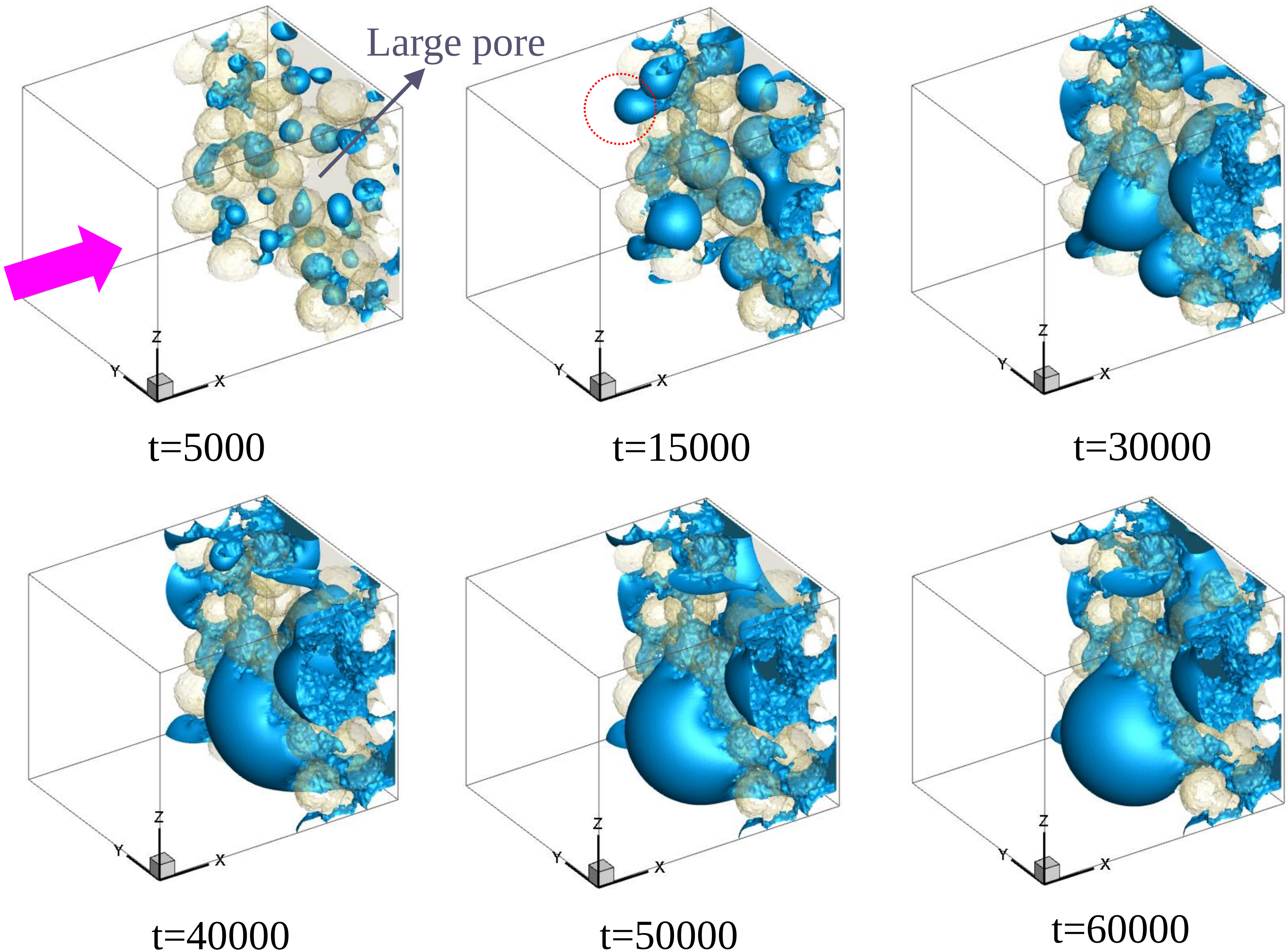
日本东立公司



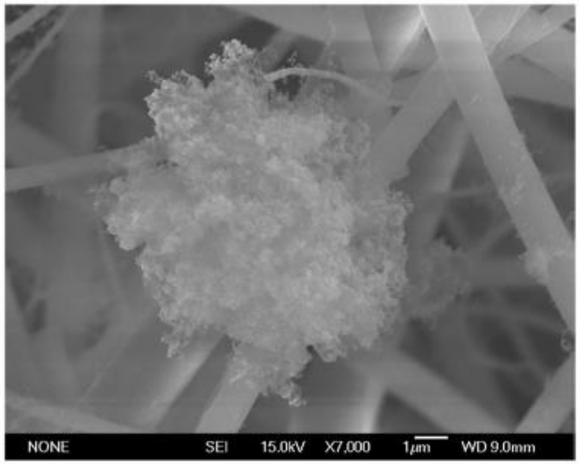
美国阿贡国家实验室

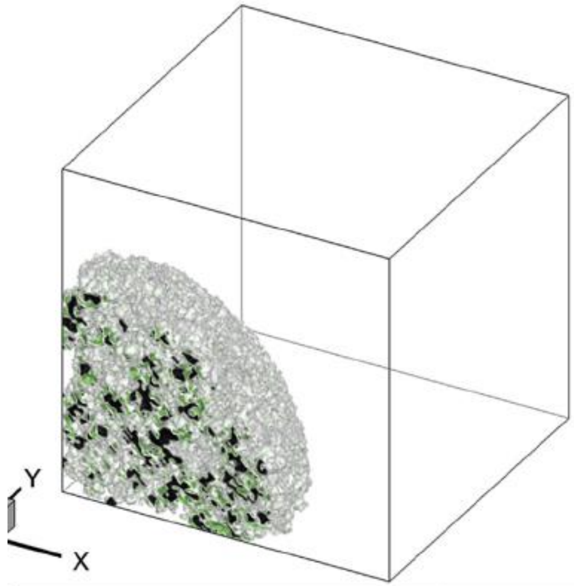


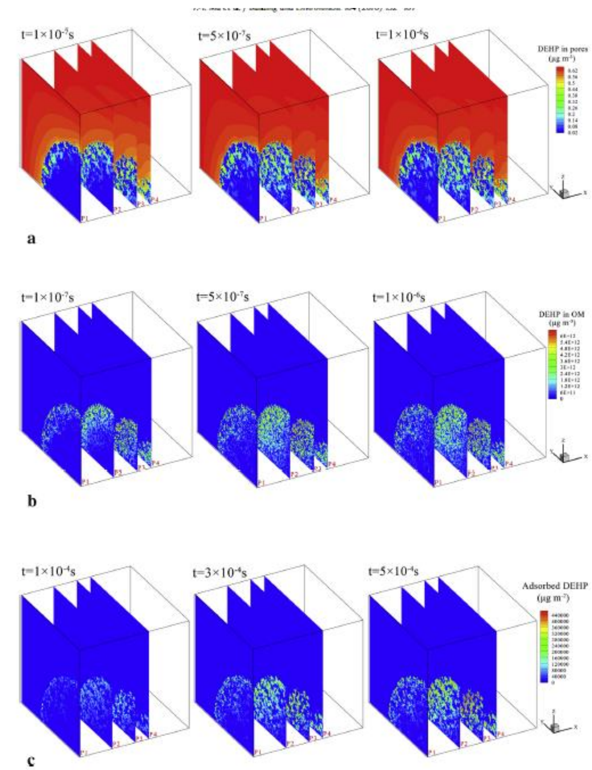
L. Chen, Wen-Quan Tao., 2018, Journal of Power Sources;
L. Chen, Wen-Quan Tao., 2019, Electrochimica Acta;
L. Chen, Wen-Quan Tao., 2019, CEJ;

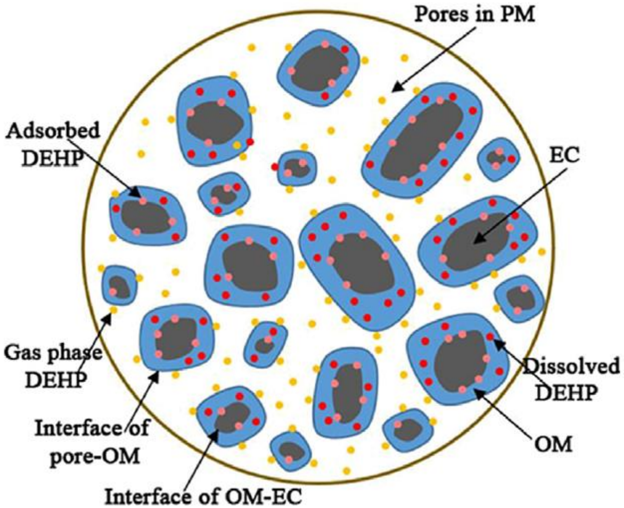

Large pore
Z
Y
X
t=5000
t=15000
t=30000
t=40000
t=50000
t=60000

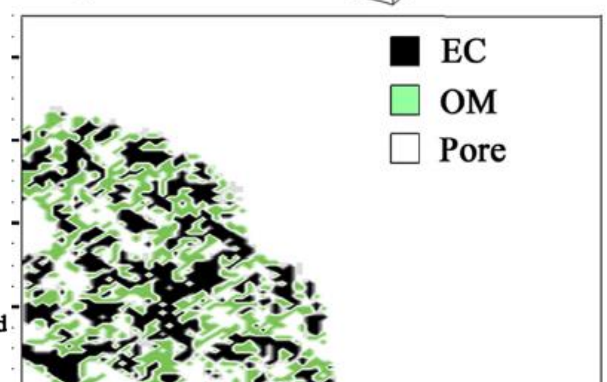
PM2.5 内 VOC 吸附过程





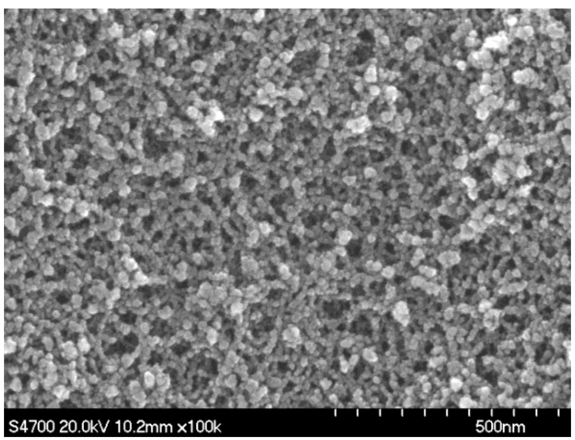


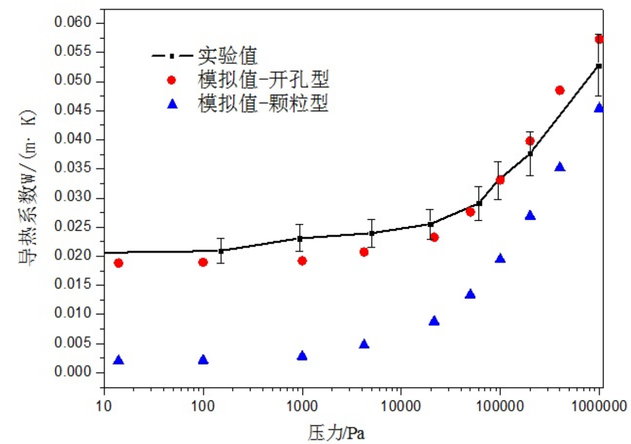




微纳米尺度传热

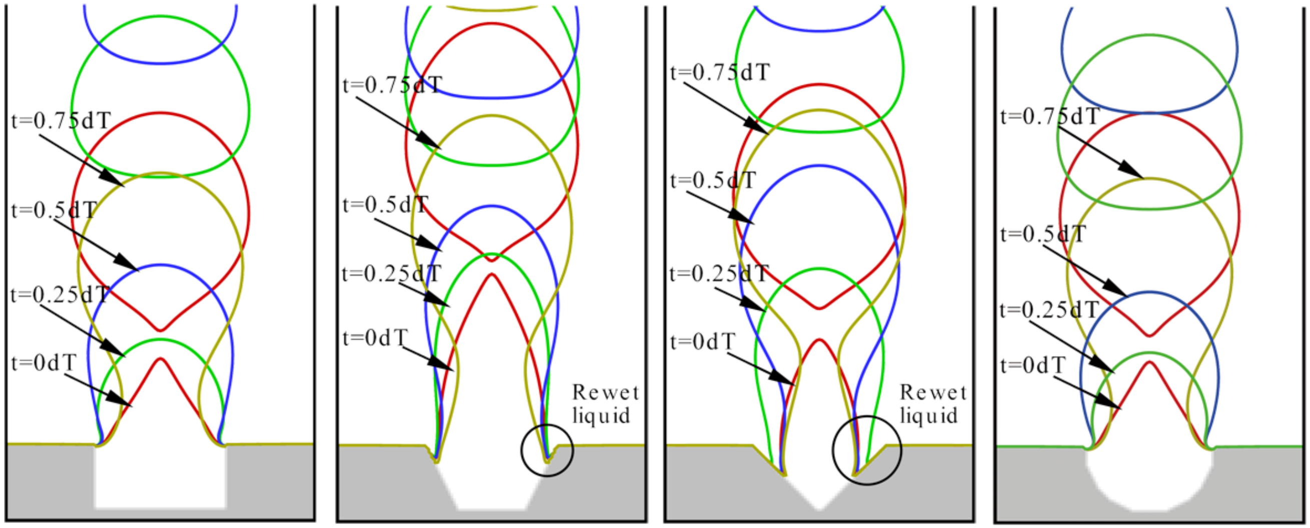
二氧化硅气凝胶有效导热系数

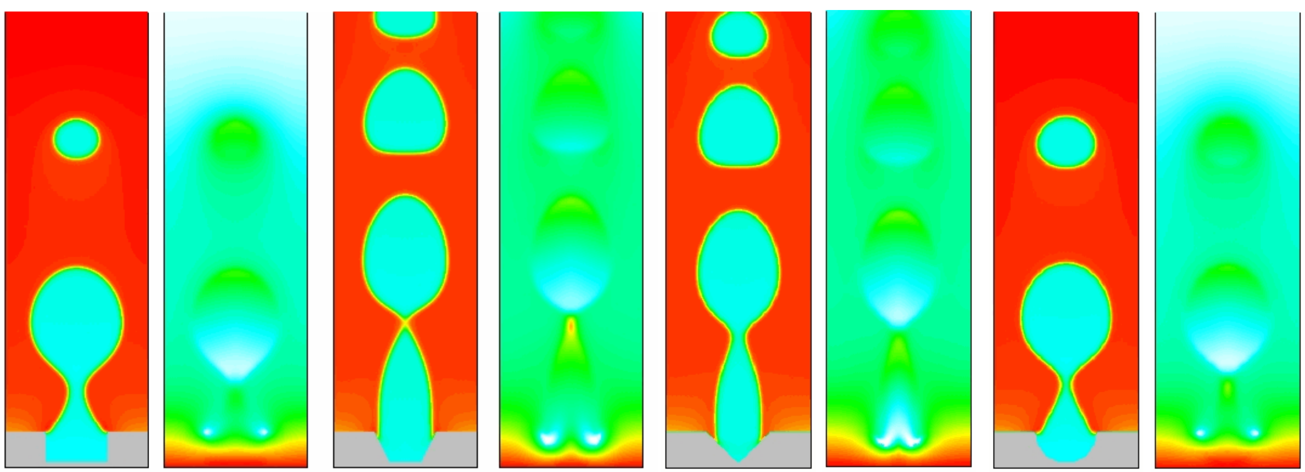




2015 WZ Fang, et al., IJHMT

沸腾传热

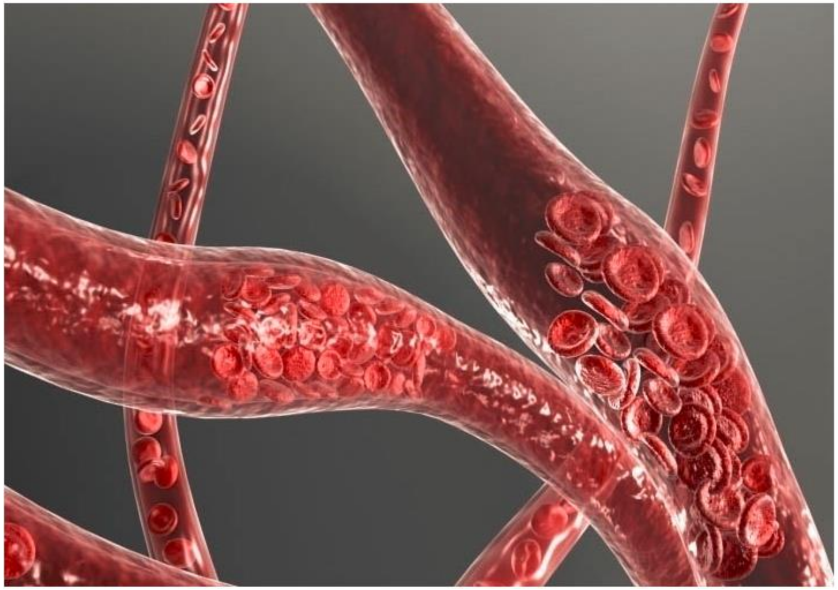


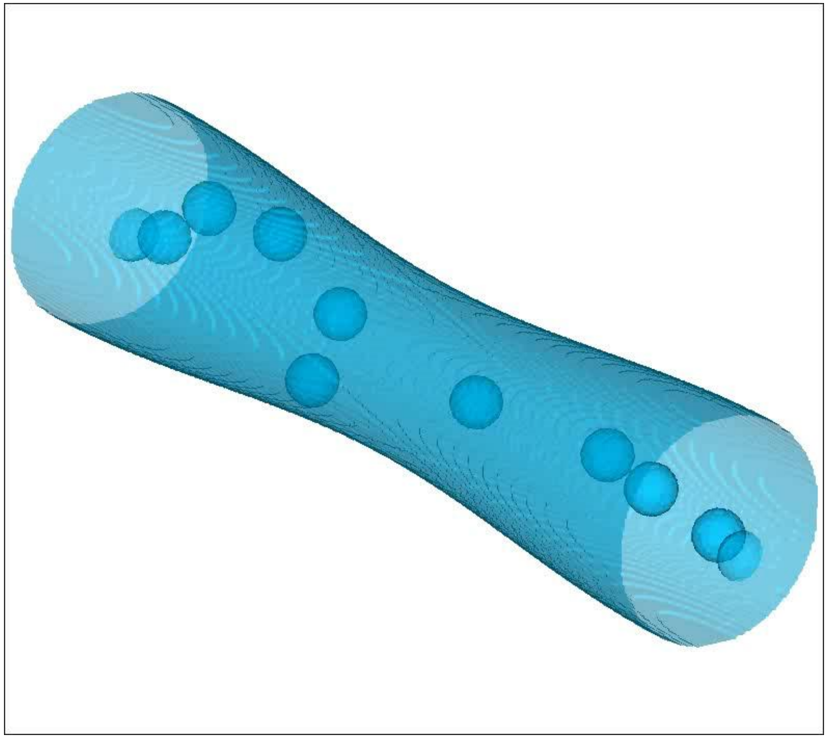


Density (left) and temperature (right) distribution

2016 Yutong Mu, et al., IJHMT

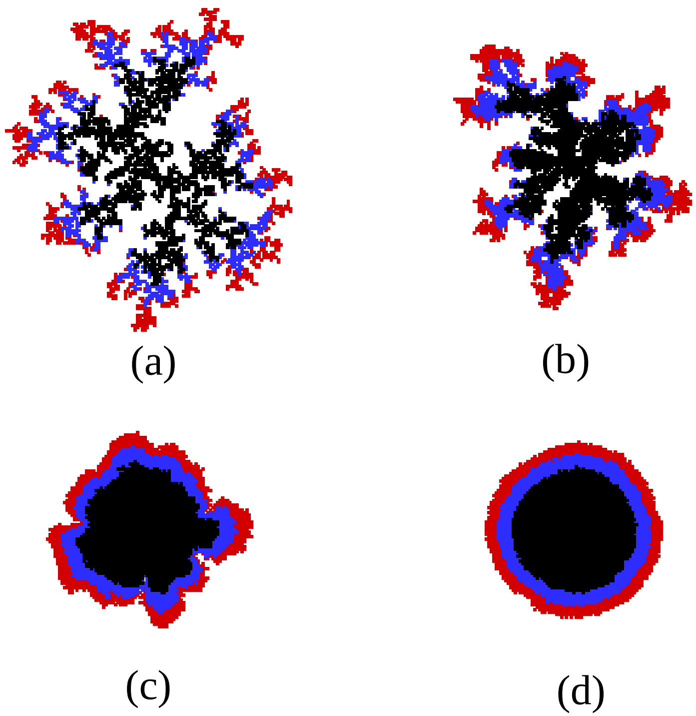
颗粒流

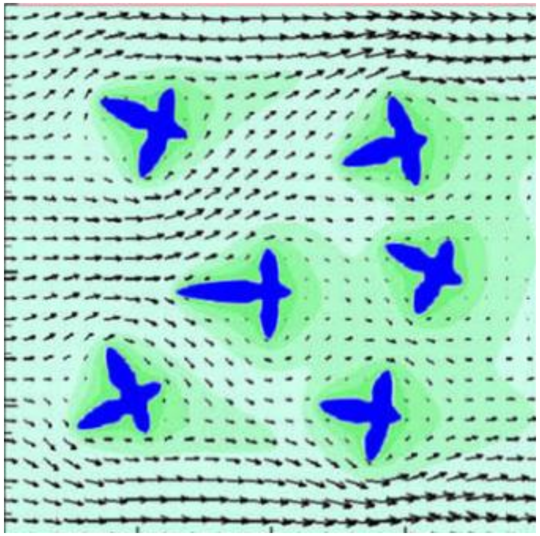


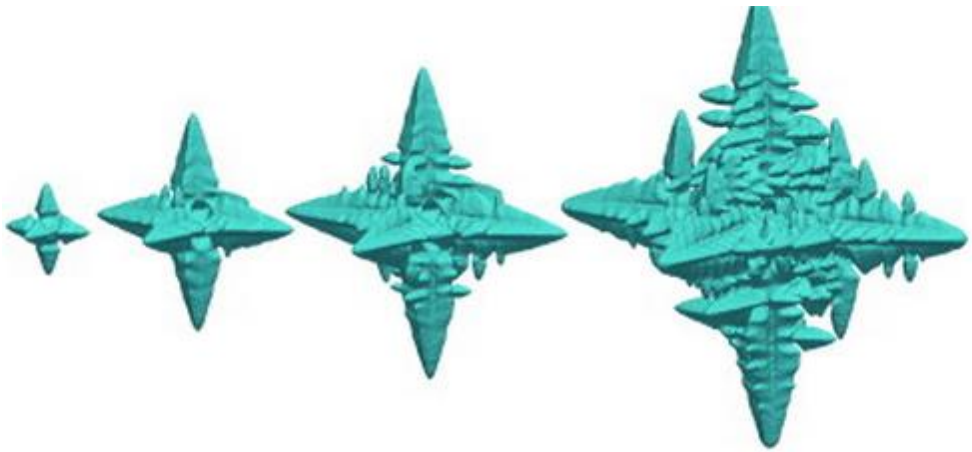


K. Connington, et al., Physics of Fluids, 21(5) (2009) 053301

晶体生长

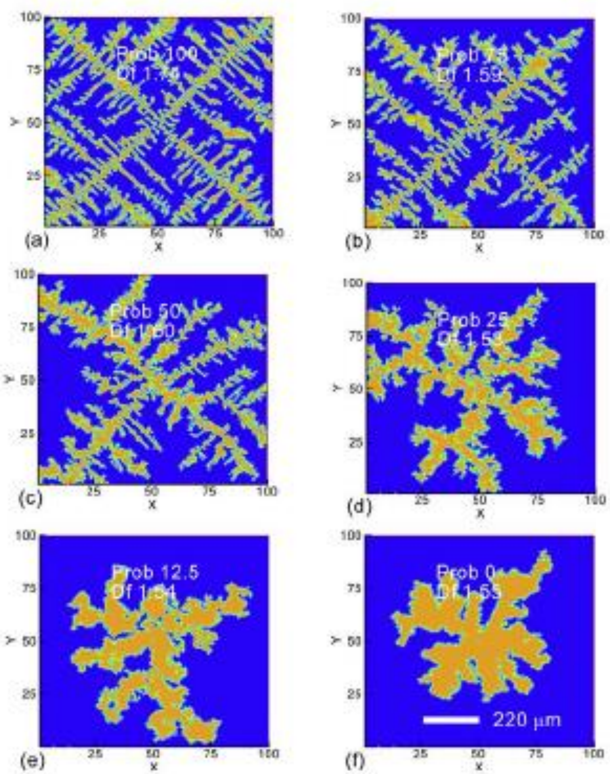






Q. Kang, D. Zhang, P.C. Lichtner, I.N. Tsimpanogiannis, Lattice Boltzmann model for crystal growth from supersaturated solution, Geophysical research letters, 31 (2004) L21604.

雪花生长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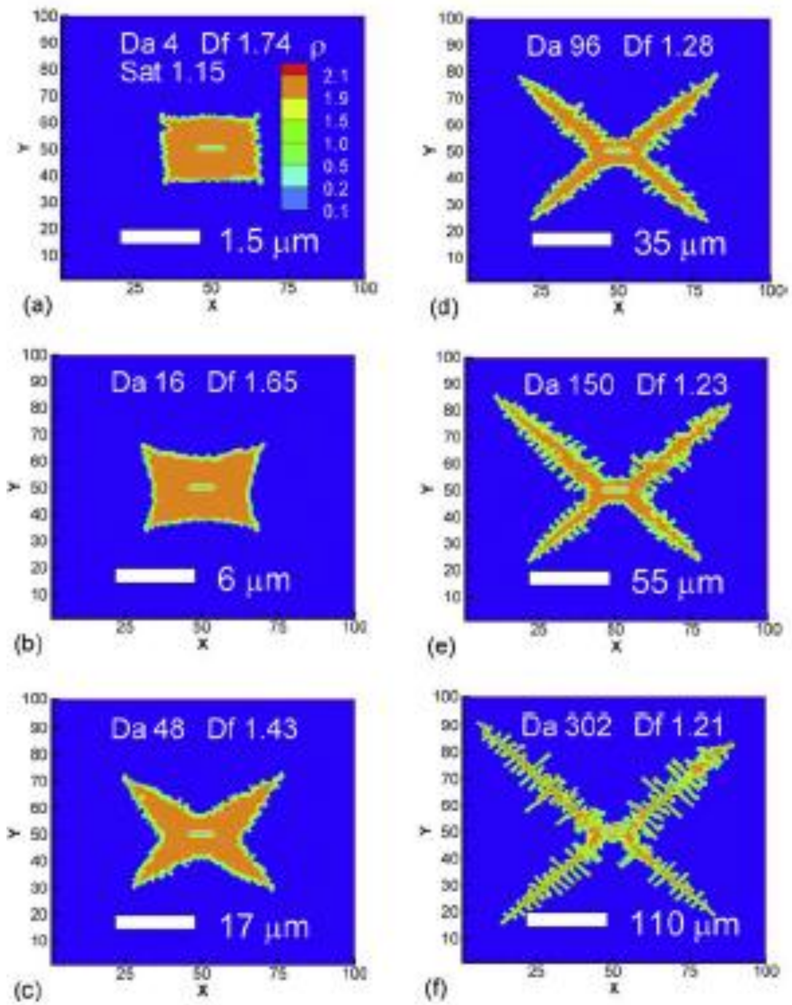
Df 1.79
Prob 75
Df 1.59
Prob 50
Df 1.60
Prob 25
Df 1.53
Prob 12.5
Df 1.54
Prob 0
Df 1.55
220 μm
(a)
(b)
(c)
(d)
(e)
(f)


Da 4 Df 1.74
Sat 1.15
ρ
2.1
1.9
1.5
1.0
0.5
0.2
0.1
1.5 μm
Da 16 Df 1.65
6 μm
Da 48 Df 1.43
17 μm
Da 96 Df 1.28
35 μm
Da 150 Df 1.23
55 μm
Da 302 Df 1.21
110 μm
(a)
(b)
(c)
(d)
(e)
(f)

三相流