# Lattice Boltzmann Method 

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## Introduction

Lattice Boltzmann Method is a dynamic method that simulates the macroscopic behavior of fluids by using a simple mesoscopic model. It inherited the main principles of Lattice Gas Automaton (LGA) and made improvements. From lattice gas automaton, it is possible to derive the macroscopic Navier-Stokes equations.

## Introduction

Specialty of Lattice Boltzmann Method \& Difference from the traditional macroscopic numerical calculation method:

1. It is based on and starts from Non-equilibrium statistical mechanics and Discrete model
2. It connected dynamic lattice model, whose time, space and velocity phase space are fully discrete, with Boltzmann equation.
3. The implementation of this method can describe the law of fluid motion without Solving Navier-Stokes equations

## Introduction

Achievements of Lattice Boltzmann method from a macroscopic perspective

1. It connected macroscopic and microscopic world;
2. It connected continuous model and discrete model
3. It is an all-new perspective to understand the nature of fluids.

All in all, its successful application reflect a fundamental principle of scientific research. That is, conservation is the most fundamental law in the material world, which guides the movement and development of the material world. There are certain internal links between the macroscopic and microscopic world, which is in fact a dialectical unity.

## PENNSTATE <br> R <br> Introduction

## Compare LBM with CFD

$$
L B M \quad \text { vs. } \quad C F D \text { (traditional) }
$$

CFD(traditional): Computational Fluid Dynamics, including NavierStokes equations, Euler equation, Burnett equation.

LBM: Lattice-Boltzmann method

## Introduction

The extent of gas rarefaction refers to the ratio of the average firee path of gas molecule to the characteristic length.

The Knudsen number ( $k \downarrow n$ ) represents: $k \downarrow n=\lambda / L$
$\lambda$ is the average free path of gas molecule;
L is the characteristic length.

The following figure will show that different CFD equations could be applied to different ranges of $k \downarrow n$.

## Introduction

## Boltzmann equation



## Introduction

Navier-Stokes equation
$\rho\left(\frac{\partial \mathrm{u}}{\partial t}+(\mathbf{u} \cdot \nabla) \mathbf{u}\right)=-\nabla p+\mu \nabla^{2} \mathbf{u}$
second-order PDE
need to treat the non-linear convective term $u \cdot \nabla u$
need to solve Poisson equation for the pressure $p$

## Lattice Boltzmann equation

$$
\frac{\partial f}{\partial t}+\mathrm{e} \cdot \nabla f=-\frac{1}{\tau}\left(f-f^{\mathrm{EQ}}\right)
$$

first-order PDE avoids convective term, convection becomes simple advection pressure $p$ is obtained from equation of state

Table 1: Comparison between Navier-Stokes equation and lattice Boltzmann equation.

## Introduction

Compared with traditional computational fluid dynamics methods, Lattice-Boltzmann method has the following advantages:
(1) Its algorithm is simple, which can simulate various complicated nonlinear macroscopic phenomena;
(2) It can handle complicated boundary conditions
(3) The values of pressure in the lattice Boltzmann method can be directly solved by the state equation;
(4) It is easy to program, and the processing before and after calculation is also very simple
(5) It is easy to process and complete the parallel tasks based LBM;
(6) It can directly simulate connected-domain flow fields with complex geometric boundaries, such as porous media.

## Historical Perspective



Ludwig Eduard Boltzmann (February 20, 1844 - September 5, 1906) was an Austrian physicist and philosopher whose greatest achievement was in the development of statistical mechanics, which explains and predicts how the properties of atoms (such as mass, charge, and structure) determine the physical properties of matter (such as viscosity, thermal conductivity, and diffusion).

## Historical Perspective

## Boltzmann Equation(1872):

Describe the dynamics of an ideal gas.

$$
\frac{\partial f}{\partial t}+v \frac{\partial f}{\partial x}+\frac{F}{m} \frac{\partial f}{\partial v}=\left.\frac{\partial f}{\partial t}\right|_{\text {collision }}
$$

Where, $f$ represents the distribution of single-particle position and momentum.

## Lattice Boltzmann Equation:

$$
f\left(x+\xi \delta_{t}, \xi, t+\delta_{t}\right)=e^{-\frac{\delta_{t}}{\lambda}} f(x, \xi, t)+\frac{1}{\lambda} e^{-\delta_{t} / \lambda} \times \int_{0}^{\delta_{t}} e^{t^{\prime}} g\left(x+\xi t^{\prime}, \xi, t+t^{\prime}\right) d t^{\prime}
$$

## PENNSTATE <br> LBM Derivation

Novier-stokes equation
Engineer

Boltzmann equation
physics

Newton
Lattice Gas automata

## Historical Perspective

The Lattice gas model meaning:
> to establish a simple model as far as possible to be able to simulate a system consisting of a large number of particles;
> reflecting the true collision of granules, so that we can get the fluid Macro features for a long time.

## Historical Perspective

J•Hardy, Y•Pomeau and O•Pazzis (1973)-HPP Model

## Only Four Direction!!



U•Frish, Y•Pomeau and B•HassIacher (1986)-FHP Model
Non-Galilean invariance!!


McNamara and Zanetti(1988)-LB Model
Still improving !!


## Historical Perspective

Lattice Gas Automata (LGA,1992):

- Type of cellular automation used to simulate fluid flow
- Precursor to the Lattice Boltzmann Methods

Disadvantages:

- Lack of Galilean invariance
- Statistical noise
- Difficulty in expanding the model to handle three dimensional problems


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## Why Lattice Boltzmann method?

## Simplicity and efficiency

$\checkmark$ When solving compressible Navier-Stokes equations, LBM resembles a pseudo-compressible method, increasing its simplicity and extensibility through artificial compressibility.
$\checkmark$ Similar pseudo-compression method, LBM does not involve Poisson equation
$\checkmark$ Most of the calculations in LBM are local and more suitable for parallel
$>$ LBM requires a lot of memory to store the distribution function, which is also the main bottleneck of LBM
> The nature of LBM is time-dependent, so calculating steady flow is not particularly efficient

## Why Lattice Boltzmann method?

## Geometry

$\checkmark$ LBM is well suited for mass-conservative fluid simulation of complex boundaries (e.g. porous media)
$\checkmark$ LBM can well realize mass-conserving mobile boundary problems and it is very attractive for soft material simulation

## Thermal effect

$\checkmark$ Thermal disturbances originate from the microscopic and average macroscopic, LBM includes them in the mesoscopic description
> Simulation of energy conservation in LBM is not straightforward

## Sound generation

> LBM is not suitable for direct simulation of long-distance acoustic transmission under real adhesion
> LBM does not adapt to strong compressible (eg ultrasonic and transonic) fluids

## Why Lattice Boltzmann method?

## Multiphase flow and multicomponent flow

$\checkmark$ Many methods for solving multiphase flow and multicomponent flow using LBM
$\checkmark$ LBM is suitable for simulation of multi-phase flow and multi-component flow in complex boundary
> The lattice-based method has the existence of spurious currents between fluid-fluid interface
> The current multiphase flow and multicomponent flow methods of LBM do not make good use of the kinetics principle.
> In the simulation of multi-phase flow and multi-component flow, the values of viscosity and density are limited.

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## General Principles

Continuum( Macroscopic scale), finite difference, finite volume, finite element, etc),
Navier-Stokes Equations


Lattice Boltzmann Method (Mesoscopic scale),

Boltzmann Equation


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## General Principles

## Lattice Gas Automata (LGA)



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## PENNSTATE <br> General Principles

## Lattice Gas Automata (LGA)

## LGA



Single-Particle Distribution Function
(Boolean Variables)


Averaged Particle Distribution (Mesoscopic Variables)

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## General Principles

## Lattice Arrangement



## DnQm


$\omega i=1 / 4$

$\omega i=2 / 6,1 / 6^{*} 4$


D3Q15

## PENNSTATE <br> General Principles

## Bounce Back

Good For Porous Media



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## Governing Equation

## Boltzmann Transport Equation

$$
d f / d t=\text { 回 }(f)
$$



$$
\begin{gathered}
\frac{\partial f}{\partial t}+\frac{\partial f}{\partial r} \cdot c+\frac{F}{m} \cdot \frac{\partial f}{\partial c}=\Omega \\
\frac{\partial f}{\partial t}+c \cdot \nabla f=\Omega
\end{gathered}
$$

## Governing Equation

The Bhatnagar, Gross, Krook and Welander (BGKW) Approximation

$$
\begin{gathered}
\Omega=\omega\left(f^{\mathrm{eq}}-f\right)=\frac{1}{\tau}\left(f^{\mathrm{eq}}-f\right) \\
\omega=1 / \tau \\
\frac{\partial f}{\partial t}+c \cdot \nabla f=\frac{1}{\tau}\left(f^{\mathrm{eq}}-f\right)
\end{gathered}
$$

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## Governing Equation

Streaming

## Collision

$$
\frac{\partial f_{i}}{\partial t}+c_{i} \nabla f_{i}=\frac{1}{\tau}\left(f_{i}^{\mathrm{eq}}-f_{i}\right)
$$

LBM Equation

$$
f_{i}\left(r+c_{i} \Delta t, t+\Delta t\right)=f_{i}(r, t)+\frac{\Delta t}{\tau}\left[f_{i}^{\mathrm{eq}}(r, t)-f_{i}(r, t)\right]
$$

After discretizing

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Governing Equation

## Chapman-Enskog Expansion

$$
\begin{aligned}
& \frac{\partial T(x, t)}{\partial t}=\Gamma \frac{\partial^{2} T(x, t)}{\partial x^{2}} \\
& \frac{\partial T(x, t)}{\partial t}=\Gamma \frac{\epsilon^{\epsilon^{2} \partial^{2} T(x, t)}}{\partial x^{2}} \\
& T(x, t)=\sum_{i=1}^{i=2} f_{i}(x, t)=f_{1}(x, t)+f_{2}(x, t) \\
& f_{i}^{\text {eq }}=w_{i} T(x, t) \\
& \sum_{i=1}^{i=2} w_{i}=1 \\
& f(x+c i \Delta t, t+\Delta t)=f(x, t)+\epsilon \frac{\partial f_{f}}{\alpha} \Delta t+\epsilon \frac{\partial f_{i}}{\tilde{c} \cdot \Delta \Delta t}
\end{aligned}
$$

$$
\begin{aligned}
& f_{i}\left(x+c_{i} \Delta t, t+\Delta t\right)=f_{i}(x, t)+\frac{\Delta t}{\tau}\left[f_{i}^{0}(x, t)-f_{i}(x, t)\right]
\end{aligned}
$$

## Governing Equation

## Relative to Macroscopic View

$$
\begin{gathered}
\rho(r, t)=\int m f(r, c, t) \mathrm{d} c \\
\rho(r, t) u(r, t)=\int m c f(r, c, t) \mathrm{d} c \\
\rho(r, t) e(r, t)=\frac{1}{2} \int m u_{a}^{2} f(r, c, t) \mathrm{d} c
\end{gathered}
$$

## Hand-Calculation Example

## Model \& Example Introduction

1. Our calculation example is a long pipeline of oil, whose initial pressure is zero $(\mathrm{t}=0 ; \mathrm{P}=0)$.
2. The pressure of the pipeline's left boundary changes to one $(\mathrm{P}=1)$ when time goes by ( $\mathbf{t}>0$ ).
3.This example is aimed to simulate the pressure variations of the whole pipeline as time goes by.
3. This example is based on this assumption that the surroundings outside the pipeline have no influences on the pipeline's pressure changes.

## PENNSTATE <br> Hand-Calculation Example

## Model \& Example Introduction

Our example could be processed and regarded as D1Q3 model

1. For this example, it would obey this following equation : $\partial P / \partial t=\alpha \partial \nmid 2 P / \partial x 12$

In addition, it is feasible to set that :
$\alpha=A k \downarrow f / \mu \downarrow g c \downarrow g V \downarrow b C \downarrow t=1 / 3$

## Hand-Calculation Example

## Model \& Example Introduction



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For this D1Q3 model, it has following character and definition:

1. In this model, each element has corresponding distribution functions, the weight factors corresponding to the distribution function $f \downarrow 0, f \downarrow 1, f \downarrow 2$ are showed below:

$$
w \downarrow o=4 / 6 ; \quad w \downarrow 1=1 / 6 ; \quad w \downarrow 2=1 / 6
$$

2. The velocity vectors are defined as follow:
$\boldsymbol{C l 0}=\mathbf{0} ; \quad \boldsymbol{C} \mathbf{1}=1 ; \quad C \downarrow \mathbf{2}=-1$
3. The displacement and time interval are defined as follow:
$\Delta t=1 ; \quad \Delta x=1$

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## Hand-Calculation Example

The flow chart of hand-calculation


## Hand-Calculation Example

## Initialization

1. Initialize macroscopic properties:

As assumed before, when time goes by, the pressure of the left boundary is one ( $\mathrm{P}_{\text {Boundary }}=1$ )
2.Start the iteration calculation with suitable initialization of distribution function:

For this case, distribution function $f \downarrow i$ is set as $w \downarrow i$ in first element, and in the second and third elements distribution function $f \downarrow i$ set as $c \downarrow i$ initially.

## Hand-Calculation Example

## Initialization Calculation------Equilibrium Distribution Function Calculation

As initialization:
$f \downarrow 0(1,0)=4 / 6 ; f \downarrow 1(1,0)=1 / 6 ; f \downarrow 2(1,0)=1 / 6$;
Because,
$P(x, t)=\sum i=1 \uparrow 3 .{ }_{n} f \downarrow(x, t)$
So,

$$
P(1,0)=f \downarrow 0(1,0)+f \downarrow 1(1,0)+f \downarrow 2(1,0)=1 ;
$$

In addition, the same as the process above:

$$
\begin{aligned}
& f \downarrow 0(2,0)=0 ; f \downarrow 1(2,0)=1 ; f \downarrow 2(2,0)=-1 ; \\
& f \downarrow 0(3,0)=0 ; f \downarrow 1(3,0)=1 ; f \downarrow 2(3,0)=-1 ;
\end{aligned}
$$

Therefore:

$$
P(2,0)=0 ; P(3,0)=0
$$

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## Hand-Calculation Example

Initialization Calculation------Equilibrium Distribution Function Calculation
Because,
$f \downarrow \boldsymbol{i} \uparrow e q(x, t)=w \downarrow i P(x, t)$
So,

$$
f \downarrow 0 \text { 个eq }(1,0)=w \downarrow 1 \times P(1,0)=4 / 6 \times 1=4 / 6 ;
$$

In the same way, the following the result values of equilibrium distribution function could be obtained:

$$
\begin{gathered}
f \downarrow 1 \uparrow e q(1,0)=1 / 6 ; f \downarrow 2 \uparrow e q(1,0)=1 / 6 ; \\
f \downarrow 0 \uparrow e q(2,0)=f \downarrow 1 \uparrow e q(2,0)=f \downarrow 2 \uparrow e q(2,0)=0 ; \\
f \downarrow 0 \uparrow e q(3,0)=f l 1 \uparrow e q(3,0)=f l 2 \uparrow e q(3,0)=0 ;
\end{gathered}
$$

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## Hand-Calculation Example

## Collisions Calculations

1. When calculate collisions, the following equation is obeyed:

$$
f \downarrow i \uparrow *(x, t)=(1-\omega) f \downarrow i(x, t)+w f \downarrow i \uparrow e q(x, t)
$$

This model uses BGK Approximation for the collision calculation .
For this example,
$\because \alpha=\tau-\Delta t / 2=1 / 3 ; \Delta t=1 ; \omega=\Delta t / \tau$;
$\therefore \omega=6 / 5$
Therefore,
$f \downarrow 0 \uparrow *(1,0)=(1-6 / 5) \times \mathbf{4} / \mathbf{6}+6 / 5 \times \mathbf{4} / \mathbf{6}=2 / 3$;
$f \downarrow 1 \uparrow *(1,0)=(1-6 / 5) \times \mathbf{1} / \mathbf{6}+6 / 5 \times \mathbf{1} / \mathbf{6}=1 / 6$;
$f \downarrow 2 \uparrow *(1,0)=(1-6 / 5) \times \mathbf{1} / 6+6 / 5 \times \mathbf{1} / 6=1 / 6$;

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## Hand-Calculation Example

## Collisions Calculations

In the same way, the following values could be calculated:
$f \downarrow 0 \uparrow *(2,0)=(1-6 / 5) \times 0+6 / 5 \times 0=0$;
$f \downarrow 1 \uparrow *(2,0)=(1-6 / 5) \times 1+6 / 5 \times 0=-1 / 5$;
$f \downarrow 2 \uparrow *(2,0)=(1-6 / 5) \times-1+6 / 5 \times 0=1 / 5$;
And,
$f \downarrow 0 \uparrow *(3,0)=(1-6 / 5) \times 0+6 / 5 \times 0=0$;
$f \downarrow 1 \uparrow *(3,0)=(1-6 / 5) \times 1+6 / 5 \times 0=-1 / 5$;
$f \downarrow 2 \uparrow *(3,0)=(1-6 / 5) \times-1+6 / 5 \times 0=1 / 5$;

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## Hand-Calculation Example

## Streaming Calculations

When calculate streaming, the following equation is obeyed:
$f \downarrow i(x+c \downarrow i \Delta t, t+\Delta t)=f \downarrow i \uparrow *(x, t)$
$C \downarrow 0=0 ; \quad C \downarrow 1=1 ; \quad C \downarrow 2=-1$

Therefore,
$f \downarrow 0(1,1)=f \downarrow 0 \uparrow *(1,0)=2 / 3$;
$f \downarrow 0(2,1)=f \downarrow 0 \uparrow *(2,0)=0$;
$f \downarrow 0(3,1)=f \downarrow 0 \uparrow *(3,0)=0$;
Similarly,
$f \downarrow 1(3,1)=f \downarrow 1 \uparrow *(2,0)=-1 / 5$;
$f \downarrow 1(2,1)=f \downarrow 1 \uparrow *(1,0)=1 / 6$;

$$
f \downarrow 1(1,1)=f \downarrow 1 \uparrow *(1,0)=1 / 6 \text {; (Boundary Condition) }
$$

## PENNSTATE <br> Hand-Calculation Example

## Streaming Calculations

$f \downarrow 2(3,1)=f \downarrow 2 \uparrow *(3,0)=1 / 5$;

$$
f \downarrow 2(2,1)=f \downarrow 2 \uparrow *(3,0)=1 / 5 ;
$$

$f \downarrow 2(1,1)=f \downarrow 2 \uparrow *(1,0)=1 / 6$; (Boundary Condition)

Because they are under boundary condition:
$f \downarrow 1(1,1)=f \downarrow 1 \uparrow *(1,0)=1 / 6$; (Boundary Condition)
$f \downarrow 2(1,1)=f \downarrow 2 \uparrow *(1,0)=1 / 6$; (Boundary Condition)

## Hand-Calculation Example

## Re-Calculation of Macroscopic Properties

As presented above:
$P(x, t)=\sum i=1 \uparrow 3 \#_{\text {\# }} f \downarrow i(x, t)$
Submit the latest value of $f \downarrow i(x, t)$ into this equation,
Therefore,

$$
\begin{aligned}
& P(1,1)=f \downarrow 0(1,1)+f \downarrow 1(1,1)+f \downarrow 2(1,1)=2 / 3+1 / 6+1 / 6=1 ; \\
& P(2,1)=f \downarrow 0(2,1)+f \downarrow 1(2,1)+f \downarrow 2(2,1)=0+0+1 / 5=1 / 5 ; \\
& P(3,1)=f \downarrow 0(3,1)+f \downarrow 1(3,1)+f \downarrow 2(3,1)=0-1 / 5+1 / 5=0 ;
\end{aligned}
$$

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## Hand－Calculation Example

## Re－Calculation－－－－－－Equilibrium Distribution Function Calculation

As presented above：
$f \downarrow \boldsymbol{i} \uparrow e q(x, t)=w \downarrow i P(x, t)$
$w \downarrow o=4 / 6 ; \quad w \downarrow 1=1 / 6 ; \quad w \downarrow 2=1 / 6$
Submit the latest value of $\boldsymbol{P}(\boldsymbol{x}, \boldsymbol{t})$ into this equation，therefore：
$f \downarrow 0$ 个eq $(1,1)=w \downarrow 0 P(1,1)=4 / 6 \times 1=4 / 6$
$f \downarrow 1$ 个eq $(1,1)=w \downarrow 1 P(1,1)=1 / 6 \times 1=1 / 6$
$f \downarrow 2$ 个eq $(1,1)=w \downarrow 2 P(1,1)=1 / 6 \times 1=1 / 6$
Similarly：
$f \downarrow 0$ 个eq $(2,1)=w \downarrow 0 P(2,1)=4 / 6 \times 1 / 5=2 / 15$
$f \downarrow 1$ 个eq $(2,1)=w \downarrow 1 P(2,1)=1 / 6 \times 1 / 5=1 / 30$
$f \downarrow 2$ 个eq $(2,1)=w \downarrow 2 P(2,1)=1 / 6 \times 1 / 5=1 / 30$

## Hand-Calculation Example

Re-Calculation------Equilibrium Distribution Function Calculation
And similarly:
flîeq $(x, t)=w l i P(x, t)$
$f \downarrow 0$ 个eq $(3,1)=w \downarrow 0 P(3,1)=4 / 6 \times 0=0$
$f \downarrow 1$ Teq $(3,1)=w \downarrow 1 P(3,1)=1 / 6 \times 0=0$
$f \downarrow 2$ 个eq $(3,1)=w \downarrow 2 P(3,1)=1 / 6 \times 0=0$

That is a whole process of one iteration, aiming to obtain the final result, more iterations are needed, here is just an example. When the latest macroscopic properties are pretty closed to the previous macroscopic result, get out of the iterations and output the final result.

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## Matlab Implementation



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## Matlab Implementation



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## Matlab Implementation



## PENNSTATE

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Matlab Implementation


## PENNSTATE

## Matlab Implementation



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## Matlab Implementation



```
% MICROSCOPIC BOUNDARY CONDITIONS
for i=1:9
    % Left boundary
    fOut(i,1,col) = fEq(i,1,col) + ...
    18*t(i)*cx(i)*cy(i)* ( fIn(8,1,col) - ...
    fIn(7,1,col)-fEq(8,1,col)+fEq(7,1,col) );
    % Right boundary
    fOut(i,lx,col) = fEq(i,lx,col) + ...
    18*t(i)*cx(i)*cy(i)* ( fIn(6,lx,col) - ...
    fIn(9,lx,col)-fEq(6,lx,col)+fEq(9,lx,col) );
    % Bounce back region
    fOut(i,bbRegion) = fIn(opp(i),bbRegion);
end
```


## PENNSTATE

## Matlab Implementation



```
% STREAMING STEP
for i=1:9
    fIn(i,:,:) = ...
    circshift(fOut(i,:,:), [0,cx(i),cy(i)]);
end
% VISUALIZATION
if (mod(cycle,tPlot)==0)
    u = reshape(sqrt(ux.^2+uy.^2),lx,ly);
    u(bbRegion) = nan;
    imagesc(u');
    axis equal off; drawnow
end
end
% end main loop
```


## 4 <br> Other simulation



## Flow around moving boundary



## PENNSTATE <br> Field Application

- Stimulate Material crystal condensation and diffusion
- Application of urban development planning


## Stimulation Changing Process



Simulate rules of the surface growth process, the probability cellular automata rules of the model forest fire, and the sand pile rules, even simulating the basic accumulation and collapse of particles like sand grains.

This method has been widely used in studying the recrystallization of metallic materials and dendritic growth of metal solidification process .

## PENNSTATE <br> N <br> 855 <br> Field Application

The lattice Boltzmann method is based on the same idea of cellular automata.

Application of Lattice-Boltzmann method:

1. Land-cover variations
2. Human-land relationships
3. Urban development planning

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## Field Application



Fig. Numerical simulation of the different forms of the rock cranny


Fig. Simulation result on things of one kind come together

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Thank You!

## Further information and resources

> Palabos: open-source code and lattice Boltzmann documentation:
www.palabos.org.
> Master's and PhD theses around the lattice Boltzmann method: wiki.palabos.org/literature:theses
ح Forum for questions and discussions around lattice Boltzmann: palabos.org/forum/

## Additional simulation examples

- Industrial applications of multi-phase flow:
www.flowkit.com/showcases/multi-phase-rotors-and-pumps.
- Calculation of mixing quality in static fluid mixers:
www.flowkit.com/showcases/static-mixers

