Lattice Boltzmann Method

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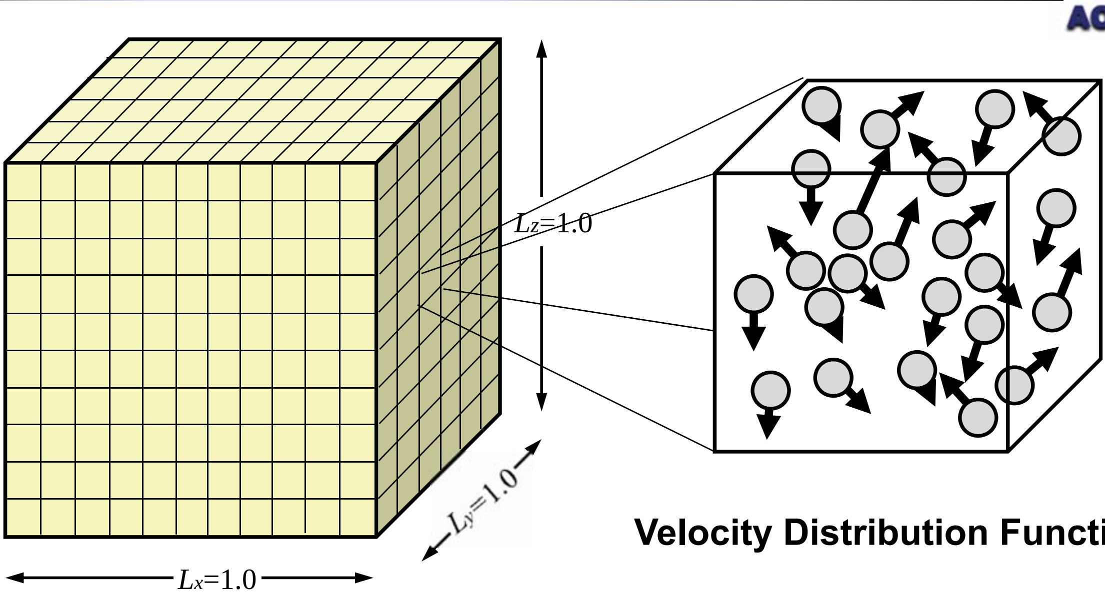
Macroscopic & Microscopic



Density:
Flow Velocity:
Temperature, Pressure:

Velocity Distribution Function:

Number of Particles for
$x_0 < x < x_0 + \Delta x$
$v_0 < v < v_0 + \Delta v$

Knudsen Number : *Kn*

Collision Mean free path: $$\lambda = \frac{1}{\sigma n} = \frac{k_B T}{\sqrt{2}\pi r^2 P}$$

Knudsen Number : $$Kn = \frac{\lambda}{L} = \frac{k_B T}{\sqrt{2}\pi r^2 P} \cdot \frac{1}{L}$$

***Kn* << 1** : **Collision frequency is very high and the velocity distribution function is almost equilibrium. It is possible to apply macroscopic description.**

***Kn* >> 1** : **Low collision frequency and the distribution function is far from the equilibrium one.**

Conservation Law in Phase Space

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial x} + \mathbf{F} \cdot \frac{\partial f}{\partial v} = \left(\frac{\partial f}{\partial t} \right)_c$$

Landau Collision Integral

$$\left(\frac{\partial f}{\partial t} \right)_c = \iint \omega(v, v') f(v) f(v') dv dv'$$

BGK Collision term

$$\left(\frac{\partial f}{\partial t} \right)_c = \frac{f - f^{(0)}}{\tau}$$

Lattice Boltzmann Method

Explicit Time Integration for the particle distribution function

Boltzmann Equation to describe non-equilibrium distribution function

$$\frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i = \left(\frac{\partial f_i}{\partial t}\right)_{coll}$$

Advection term in the phase space

Collision term in the phase space

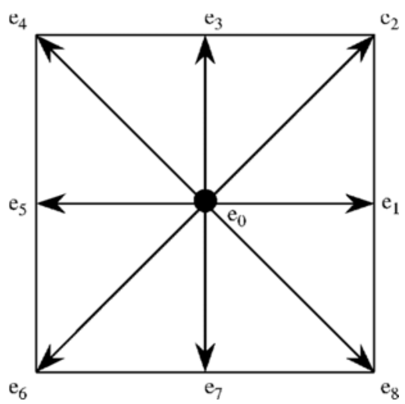
Discretization

Lattice Boltzmann Equation

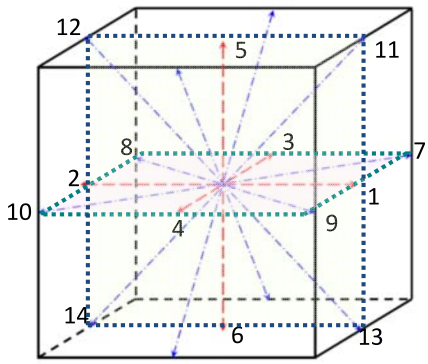
$$f_i(t+\tau, \boldsymbol{r} + \boldsymbol{c}_i \tau) = f_i(t, \boldsymbol{r}) + \Omega_i[f_i(t, \boldsymbol{r})]$$

$\Omega_i[f_i(t, \boldsymbol{r})]$: summation of the particle collisions $\quad \tau$: collision time

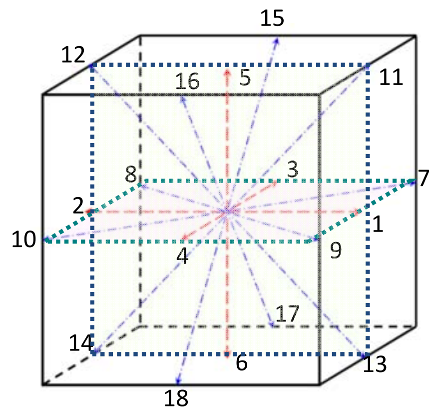
Discretization in Velocity Space



D2Q9 model



D3Q15 model



D3Q19 model

The Components of the velocity distribution function can be understood pseudo particles having the velocity component on the lattice grid and move to the neighbor grid point after the time Δt.

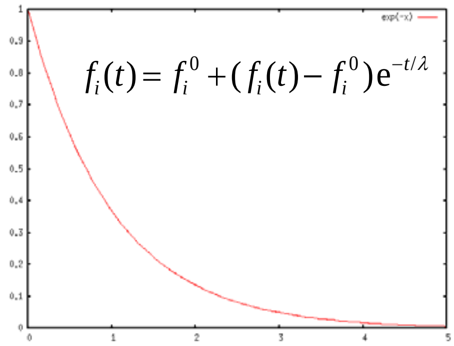
BGK Model

Relaxation to the equilibrium function

$$\left(\frac{\partial f_i}{\partial t}\right)_{coll} = -\frac{f_i - f_i^0}{\lambda}$$

f_i^0 Local equilibrium distribution function

λ Collision time



BGK-Boltzmann Equation

$$\frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i = -\frac{f_i - f_i^0}{\lambda}$$

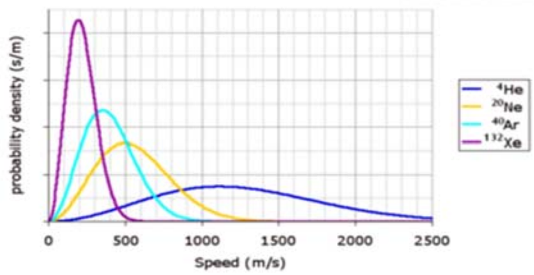
Discretization

BGK (Bhatnagar - Gross - Krook) Equation

$$f_i(t+\tau, \boldsymbol{r} + \boldsymbol{e}_i \tau) = f_i(t, \boldsymbol{r}) - \frac{1}{\lambda}[f_i(t, \boldsymbol{r}) - f_i^{(0)}(t, \boldsymbol{r})]$$

Local Equilibrium Function

Equilibrium Solution of the Boltzmann Equation



Maxwell – Boltzmann Distribution

$$f(v_x, v_y, v_z) = \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(\frac{-m\left(v_x^2 + v_y^2 + v_z^2\right)}{2kT}\right)$$

Low Mach-number expansion,

$$f_i^{(0)}(t, \boldsymbol{r}) = A + B(\boldsymbol{e}_i \cdot \boldsymbol{u}) + C(\boldsymbol{e}_i \cdot \boldsymbol{u})^2 + Du^2$$

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Local Equilibrium Function

Approximation for the function:

$$f_i^{(0)}(t,\boldsymbol{r}) = A + B(\boldsymbol{e}_i\cdot\boldsymbol{u}) + C(\boldsymbol{e}_i\cdot\boldsymbol{u})^2 + Du^2$$

$$\rho = \sum_{i=0}^{N} f_i = \sum_{i=0}^{N} f_i^{(0)}$$

Mass conservation

$$\rho\mathbf{u} = \sum_{i=0}^{N} f_i\boldsymbol{e}_i = \sum_{i=0}^{N} f_i^{(0)}\boldsymbol{e}_i$$

Momentum conservation

$$\frac{1}{2}\rho u^2 + \rho e = \sum_{i=0}^{N}\frac{1}{2} f_i^{(0)} e_i^2$$

Energy Conservation

Three of the 4 coefficients A, B, C, D are determined by the above conditions.

Chapman - Enskog Theorem (1)

Lattice Boltzmann equation:

$$f_i(t+\tau,\boldsymbol{r}+\boldsymbol{e}_i\tau) = f_i(t,\boldsymbol{r}) - \frac{1}{\lambda}[f_i(t,\boldsymbol{r}) - f_i^{(0)}(t,\boldsymbol{r})]$$

Asymptotic expansion

$$f_i = f_i + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} \qquad \frac{\partial}{\partial t} \to \varepsilon\frac{\partial}{\partial t_1} + \varepsilon^2\frac{\partial}{\partial t_2}$$

$$\frac{\partial}{\partial t}\sum_i f_i^{(0)} e_{i\alpha} + \frac{\partial}{\partial r_{1\beta}}\sum_i f_i^{(0)} e_{i\alpha}e_{i\beta} + \left(1-\frac{1}{2\lambda}\right)\frac{\partial}{\partial r_{1\beta}}\sum_i f_i^{(1)} e_{i\alpha}e_{i\beta} = 0$$

Matching condition

$$\frac{\partial}{\partial r_{1\beta}}\sum_i f_i^{(0)} e_{i\alpha}e_{i\beta} = \frac{\partial \rho u_\alpha u_\beta}{\partial r_{1\beta}} + \frac{\partial P}{\partial r_{1\alpha}}$$

Navier-Stokes Equation

$$\frac{\partial \rho u_\alpha}{\partial t} + \frac{\partial \rho u_\alpha u_\beta}{\partial r_\beta} = -\frac{\partial P}{\partial r_\alpha} + \frac{\partial}{\partial r_\beta}\mu\left(\frac{\partial u_\alpha}{\partial r_\beta} + \frac{\partial u_\beta}{\partial r_\alpha}\right) + \frac{\partial}{\partial r_\alpha}\left(\lambda'\frac{\partial u_\alpha}{\partial r_\beta}\right)$$

Chapman - Enskog theorem (2)

$$f_i(t+\tau,\boldsymbol{r}+\boldsymbol{e}_i\tau)=f_i(t,\boldsymbol{r})-\frac{1}{\lambda}[f_i(t,\boldsymbol{r})-f_i^{(0)}(t,\boldsymbol{r})]$$

Asymptotic expansion

$$f_i=f_i+\varepsilon f_i^{(1)}+\varepsilon^2 f_i^{(2)} \qquad \frac{\partial}{\partial t}\to\varepsilon\frac{\partial}{\partial t_1}+\varepsilon^2\frac{\partial}{\partial t_2}$$

Extracting 1st-order and 2nd-order terms,

$$\left(\frac{\partial}{\partial t_1}+\frac{\partial}{\partial t_2}\right)f_i^{(0)}+e_{i\alpha}\frac{\partial f_i^{(0)}}{\partial r_{1\alpha}}+\left(1-\frac{1}{2\lambda}\right)\left[\frac{\partial f_i^{(1)}}{\partial t_1}+e_{i\alpha}\frac{\partial f_i^{(1)}}{\partial t_{1\alpha}}\right]=-\frac{1}{\tau\lambda}\left(f_i^{(1)}+f_i^{(2)}\right)$$

Continuum Equation

$$\frac{\partial\rho}{\partial t}+\frac{\partial\rho u_i}{\partial r_{1i}}=0$$

Chapman - Enskog theorem (3)

$$f_i(t+\tau,\boldsymbol{r}+\boldsymbol{e}_i\tau)=f_i(t,\boldsymbol{r})-\frac{1}{\lambda}[f_i(t,\boldsymbol{r})-f_i^{(0)}(t,\boldsymbol{r})]$$

Asymptotic expansion

$$f_i=f_i+\varepsilon f_i^{(1)}+\varepsilon^2 f_i^{(2)} \qquad \frac{\partial}{\partial t}\to\varepsilon\frac{\partial}{\partial t_1}+\varepsilon^2\frac{\partial}{\partial t_2}$$

Extracting 1st-order and 2nd-order terms for the energy dimension,

$$\frac{\partial}{\partial t}\sum_i\frac{1}{2}f_i^{(0)}e_i^2+\frac{\partial}{\partial r_{1\alpha}}\sum_i\frac{1}{2}f_i^{(0)}e_i^2e_{i\alpha}+\left(1-\frac{1}{2\lambda}\right)\frac{\partial}{\partial r_{1\alpha}}\sum_i\frac{1}{2}f_i^{(1)}e_i^2e_{i\alpha}=0$$

Matching condition

$$\frac{\partial}{\partial r_{1\alpha}}\sum_i\frac{1}{2}f_i^{(0)}e_{ii}^2e_{i\alpha}=\frac{\partial}{\partial r_{1\alpha}}\left(\frac{1}{2}u^2+e+\frac{P}{\rho}\right)\rho u_\alpha$$

Energy Equation

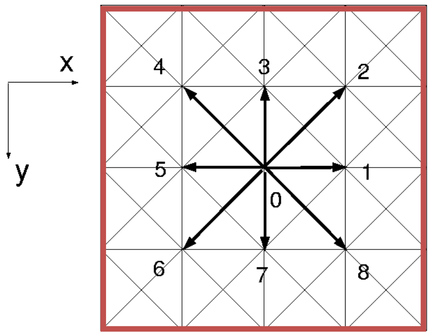
$$\frac{\partial}{\partial t}\rho\left(\frac{1}{2}u^2+e\right)+\frac{\partial}{\partial r_\alpha}\left(\frac{1}{2}u^2+e+\frac{P}{\rho}\right)\rho u_\alpha=\frac{\partial}{\partial r_\alpha}\left(\kappa'\frac{\partial e}{\partial r_\alpha}\right)+\frac{\partial}{\partial r_\alpha}\left[\mu u_\beta\left(\frac{\partial u_\alpha}{\partial r_\beta}+\frac{\partial u_\beta}{\partial r_\alpha}\right)\right]+\frac{\partial}{\partial r_\alpha}\left(\lambda u_\alpha\frac{\partial u_\beta}{\partial r_\beta}\right)$$

D2Q9 Local Equilibrium Function

$$f_0^{eq} = \frac{4}{9}\rho\{1 - \frac{3}{2}\mathbf{u}^2\}$$

$$f_i^{eq} = \frac{1}{9}\rho\{1 + 3(\mathbf{e}_i \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u}^2\} \quad (i=1,3,5,7)$$

$$f_i^{eq} = \frac{1}{36}\rho\{1 + 3(\mathbf{e}_i \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u}^2\} \quad (i=2,4,6,8)$$



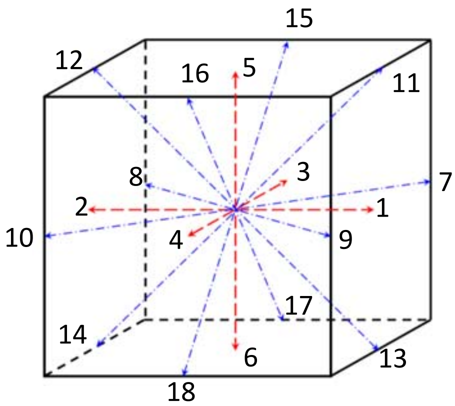
ith	velocity vector $\mathbf{e}_i$	w_i
0	(0,0)	4/9
1,3,5,7	(1,0),(0,1),(-1,0),(0,-1)	1/9
2,4,6,8	(1,1),(-1,1),(-1,-1),(1,-1)	1/36

D3Q19 Local Equilibrium Function

$$f_0^{eq} = \frac{1}{3}\rho\{1 - \frac{3}{2}\mathbf{u}^2\}$$

$$f_i^{eq} = \frac{1}{18}\rho\{1 + 3(\mathbf{e}_i \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u}^2\} \quad (i=1,2,\ldots,6)$$

$$f_i^{eq} = \frac{1}{36}\rho\{1 + 3(\mathbf{e}_i \cdot \mathbf{u}) + \frac{9}{2}(\mathbf{e}_i \cdot \mathbf{u})^2 - \frac{3}{2}\mathbf{u}^2\} \quad (i=7,8,\ldots,18)$$



ith	velocity vector $\mathbf{e}_i$	w_i
0	(0,0)	1/3
1,2,…,6	($\pm$1,0,0), (0,$\pm$1,0), (0,0,$\pm$1)	1/18
7,8,…,18	($\pm$1,$\pm$1,0),($\pm$1,0,$\pm$1),(0,$\pm$1,$\pm$1)	1/36

Computation Procedure

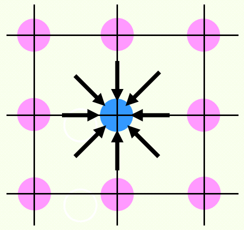
$$f_i(\mathbf{x}+\mathbf{e}_i\delta t, t+\delta t) - f_i(\mathbf{x},t) = -\frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t)\right)$$

$$\tau = \lambda / \delta t$$

LBM code

Collision step:

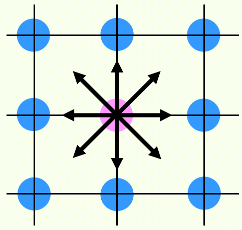
$$\bar{f}_i(\mathbf{x},t) = f_i(\mathbf{x},t) - \frac{1}{\tau}\left(f_i(\mathbf{x},t) - f_i^{eq}(\mathbf{x},t)\right)$$



Purely local !!

Streaming step:

$$f_i(\mathbf{x}+\mathbf{e}_i\delta t, t+\delta t) = \bar{f}_i(\mathbf{x},t)$$

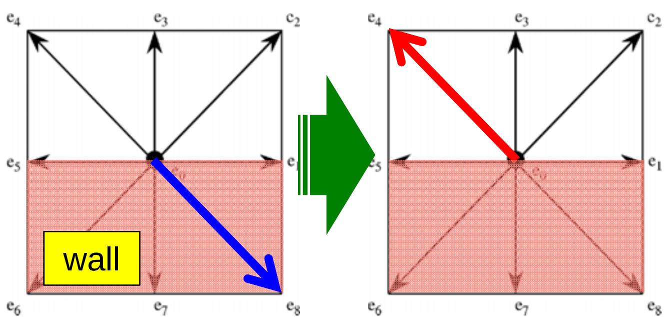


Uniform data shifting
Little computational effort !!

Boundary Condition

Bounce-back condition (D2Q9)

$$f_4(t+\tau,\mathbf{r}) = f_8(t,\mathbf{r})$$
$$f_2(t+\tau,\mathbf{r}) = f_6(t,\mathbf{r})$$
$$f_3(t+\tau,\mathbf{r}) = f_7(t,\mathbf{r})$$

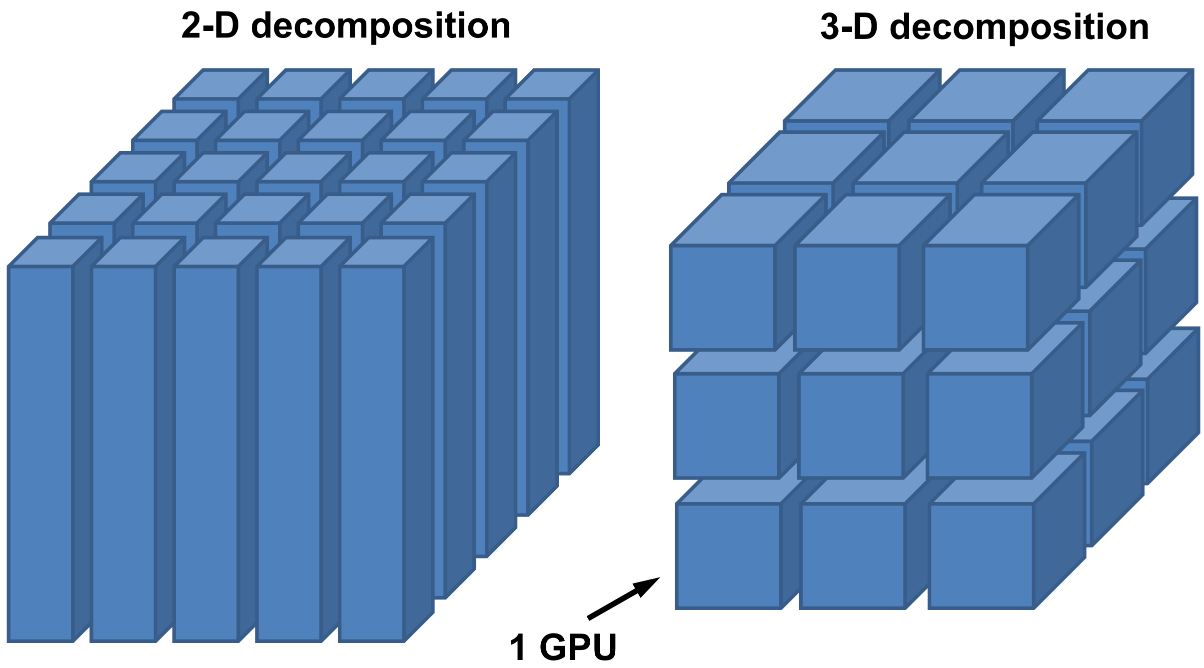


Periodic Boundary condition (D2Q9)

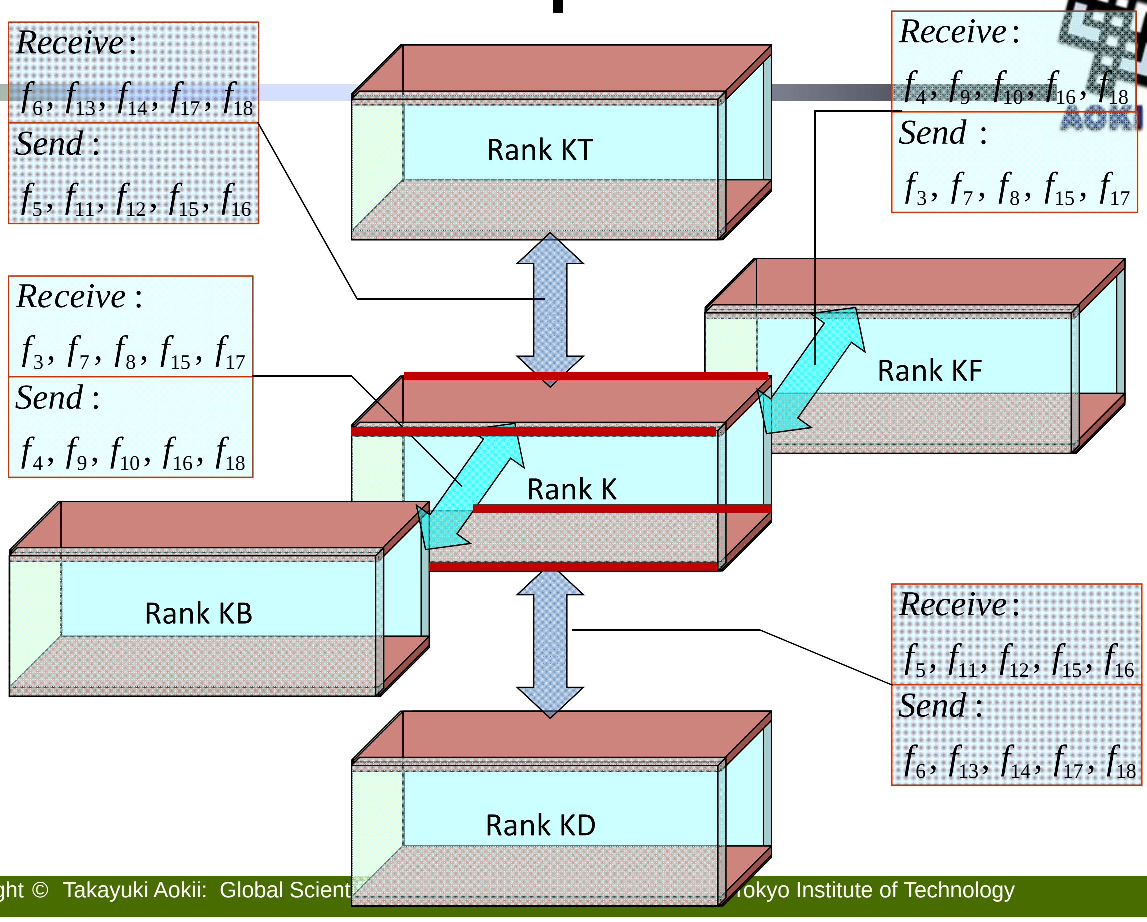
$$f_i(t+\tau,\mathbf{r}_{in}) = f_i(t,\mathbf{r}_{out})$$ i = 2, 1, 8 (右側)

$$f_i(t+\tau,\mathbf{r}_{out}) = f_i(t,\mathbf{r}_{in})$$ i = 4, 5, 6 (左側)

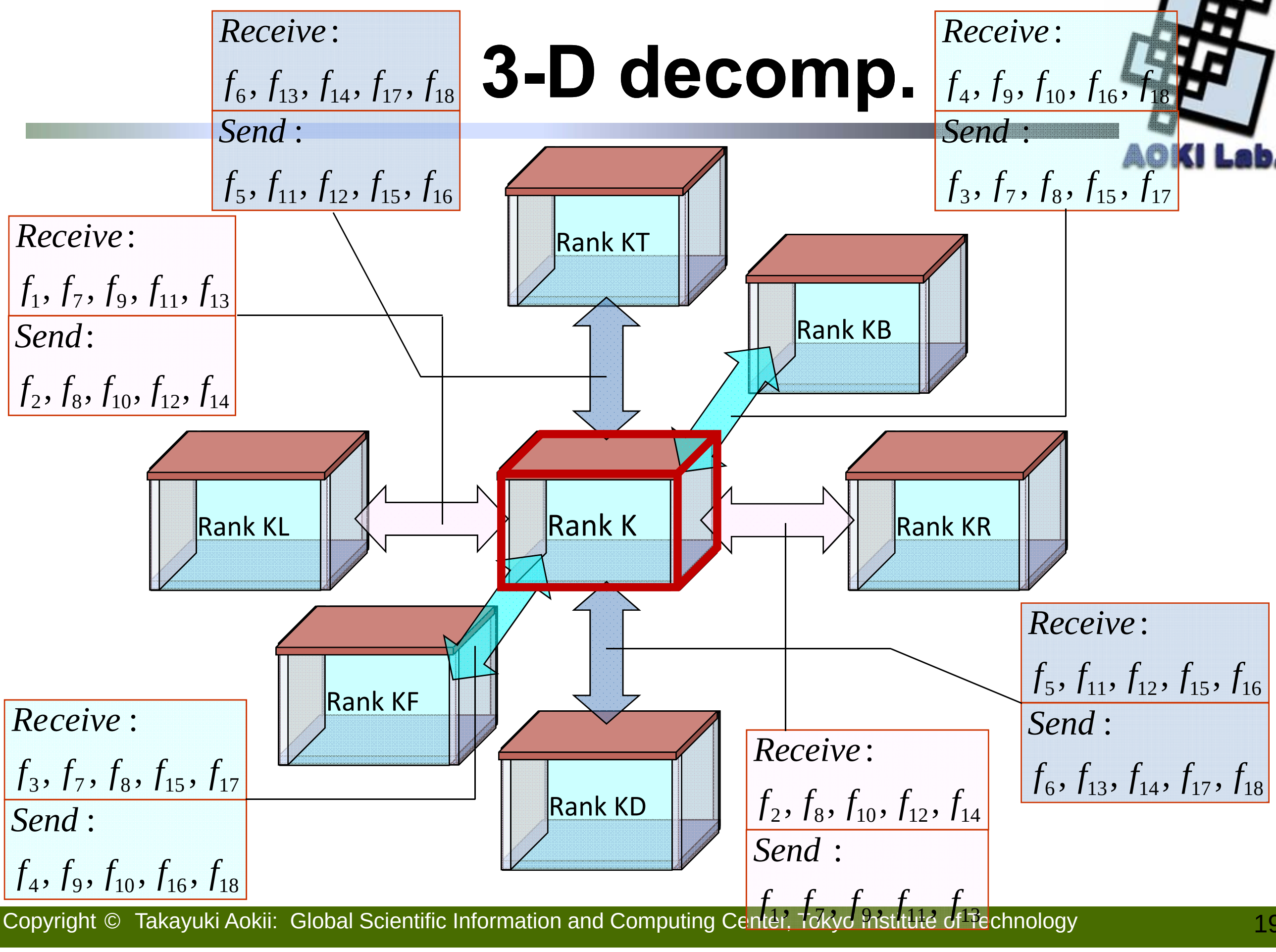
Multi-dimensional Domain Decomposition



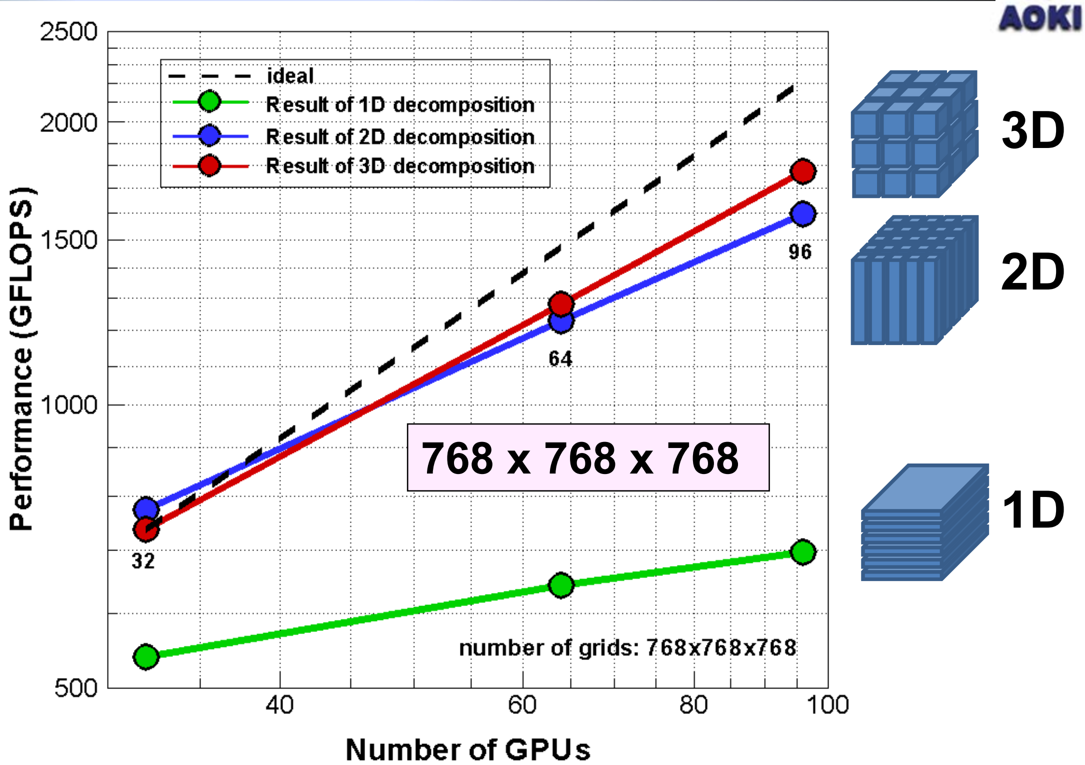
2-D decomposition



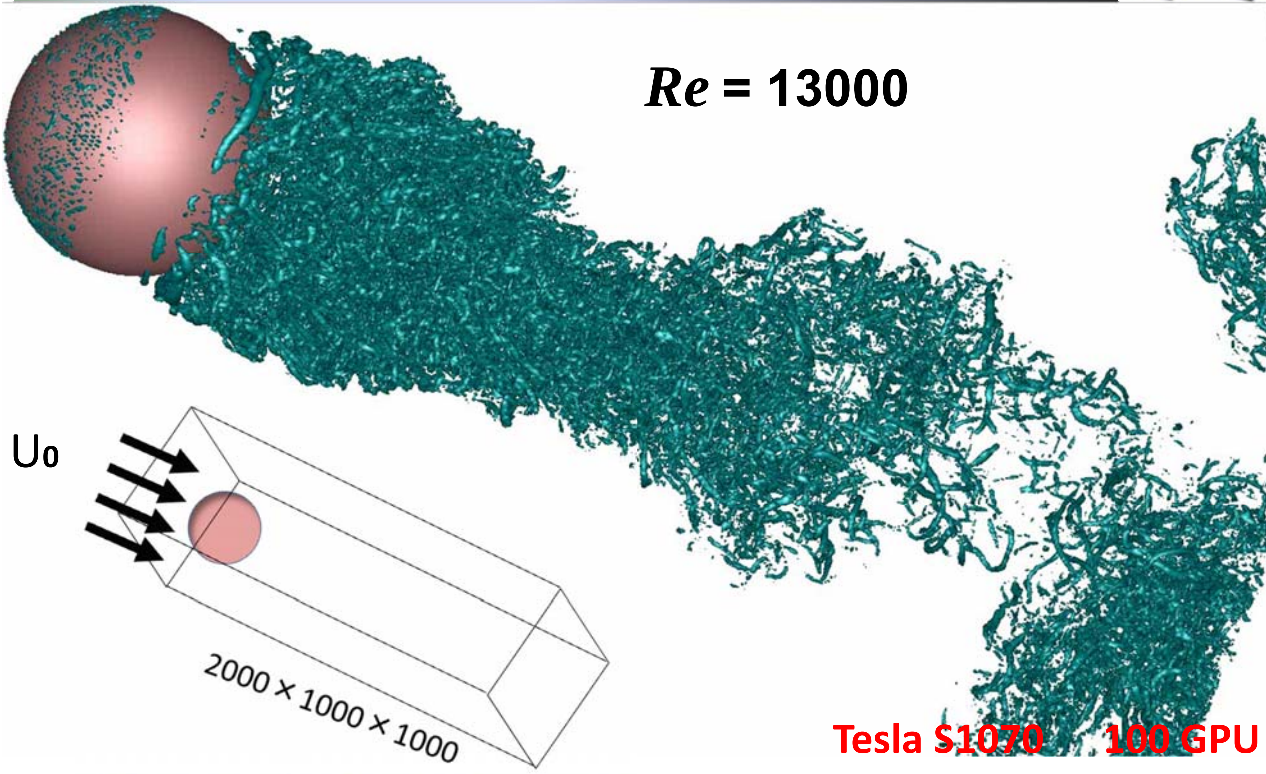
3-D decomp.



Dependency
for Decomposition Direction



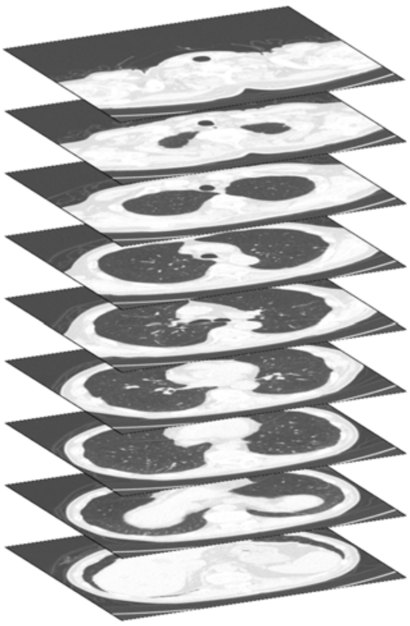
Incompressible Turbulent Flow
behind a spherical body



Pulmonary Airflow Study

Collaboration with Tohoku University

X-Ray CT images
512 × 512 × 512



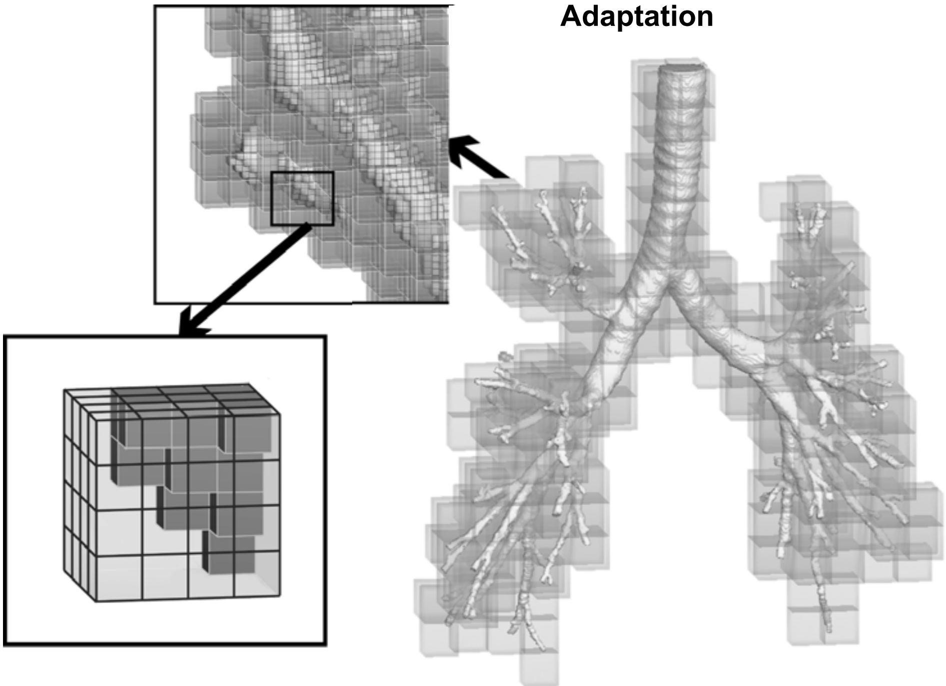
「人体の不思議展」より

Airway structure Extraction

Pulmonary Airflow Study

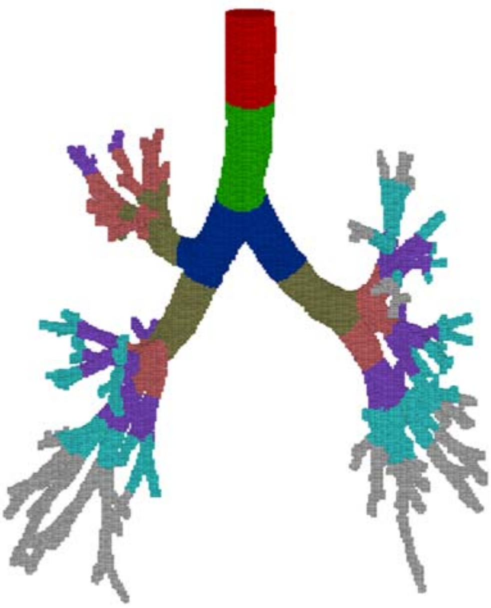
Collaboration with Tohoku University

Level-0 Mesh
Adaptation



Pulmonary Airflow Study

Collaboration with Tohoku University



Assignment to multi-GPU

Real City Atmosphere

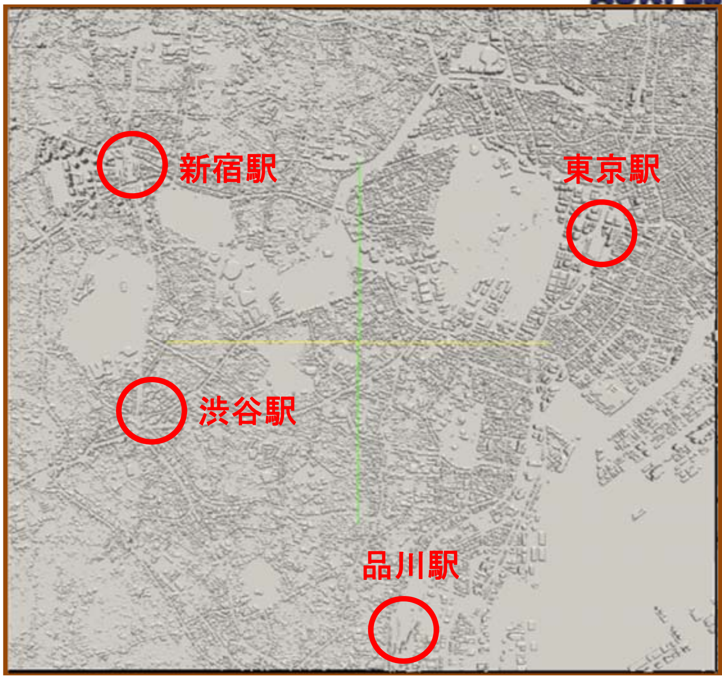
Major part of Tokyo

Including Shnjuku-ku, Chiyoda-ku, Minato-ku, Meguro-ku, Chuou-ku,

10km×10km

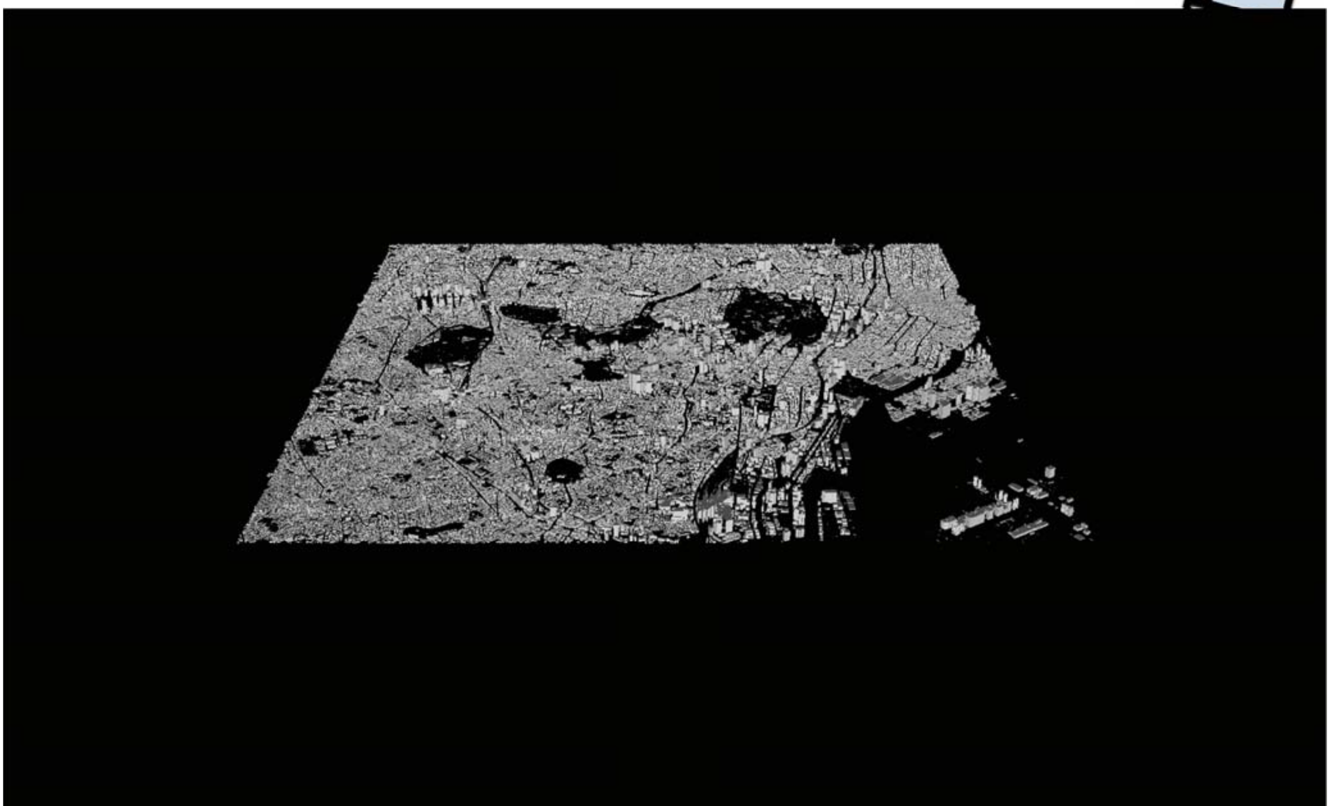
Building Data:

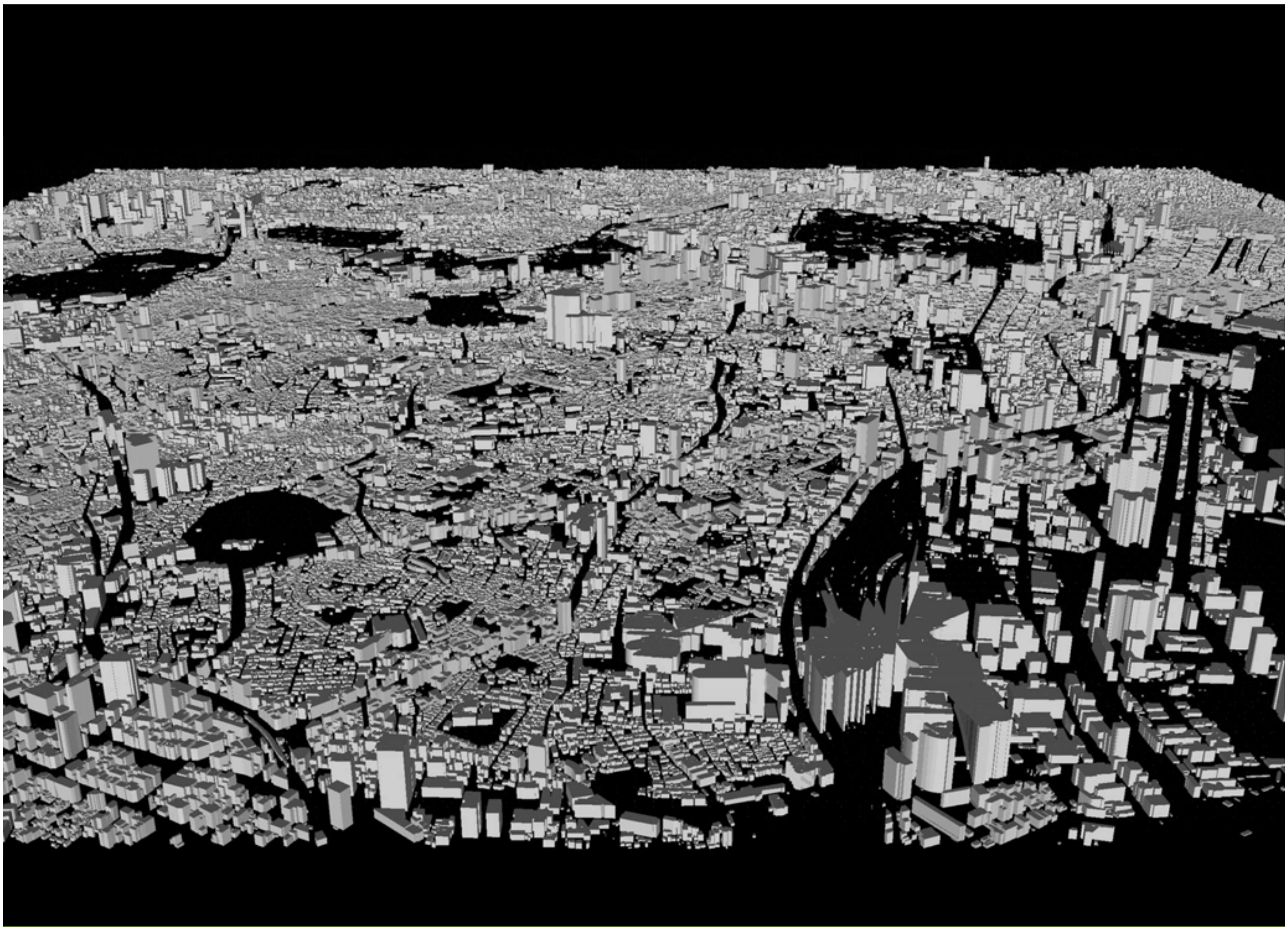
Pasco Co. Ltd.
TDM 3D

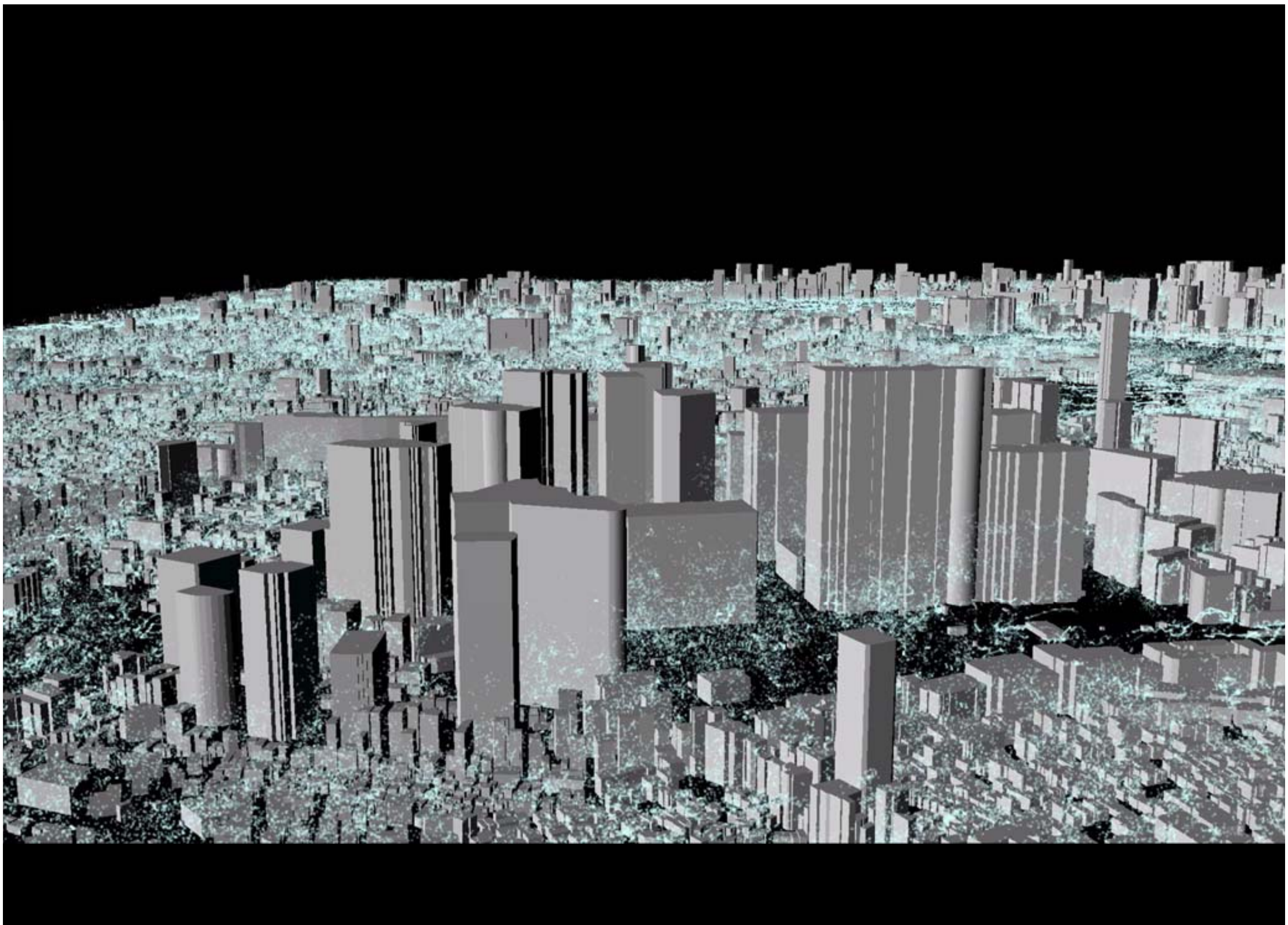


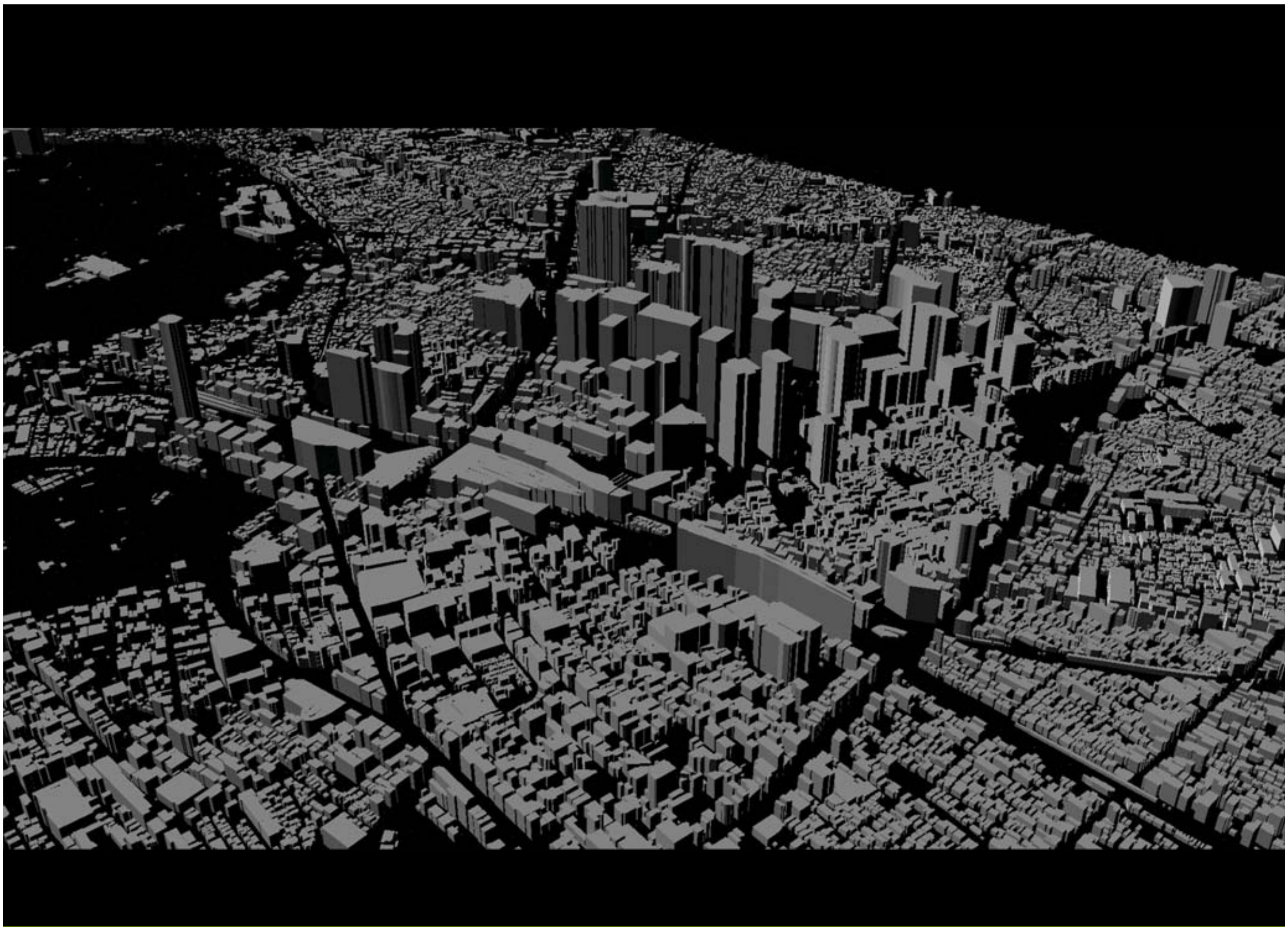
Map ©2012 Google, ZENRIN

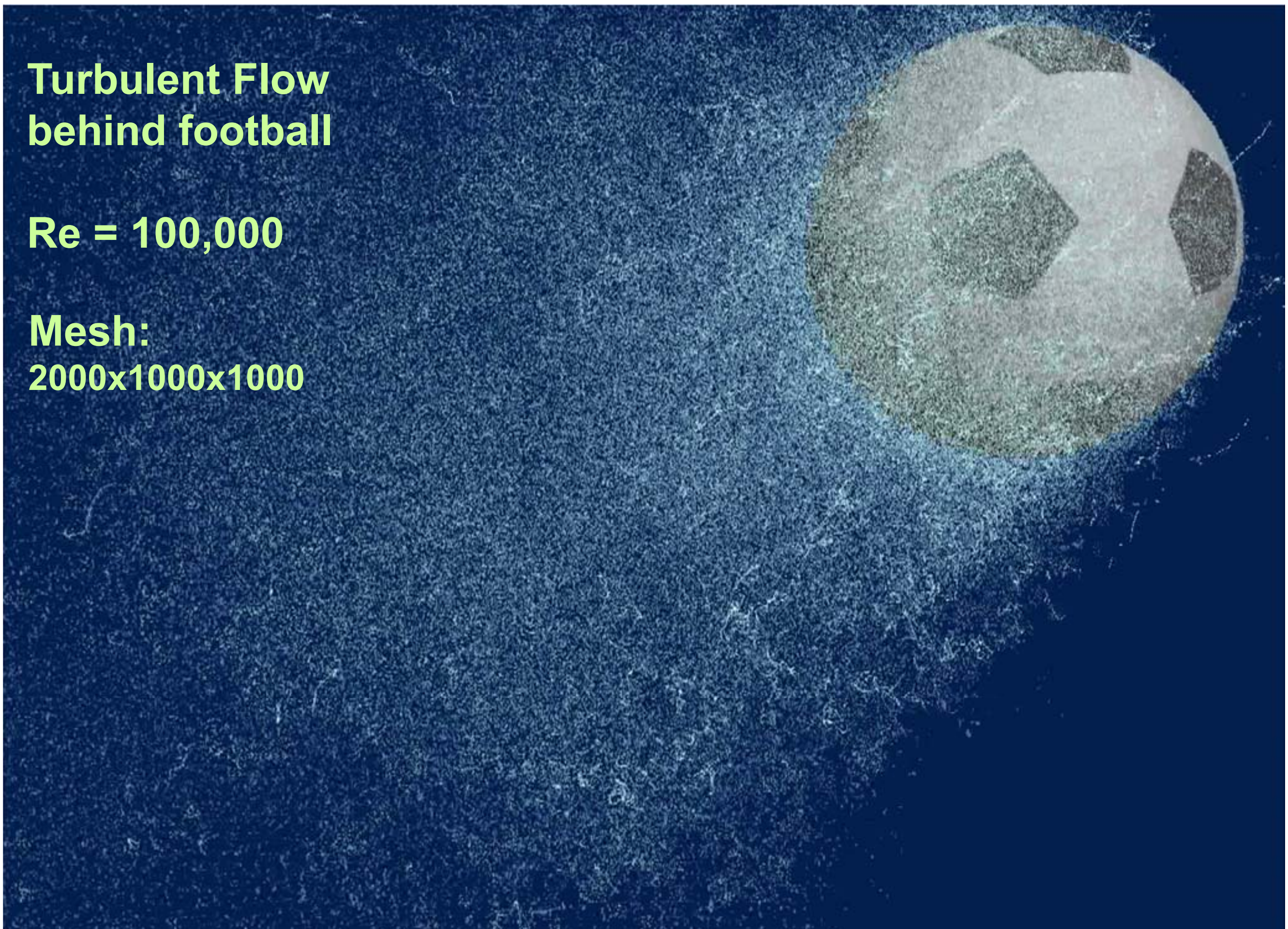
Building Structures



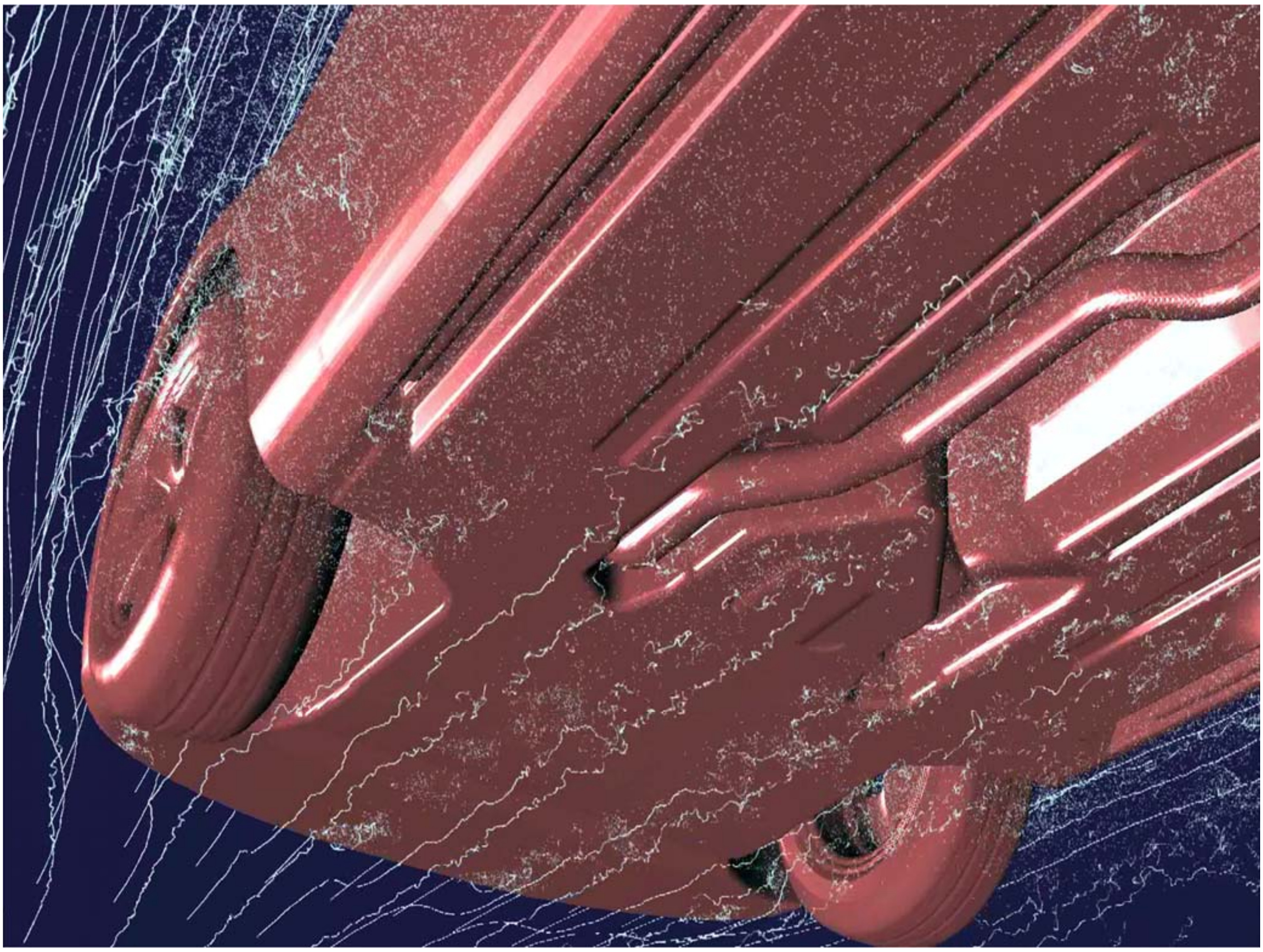







Turbulent Flow
behind football
Re = 100,000
Mesh:
2000x1000x1000


DriVer: BMW-Audi
Lehrstuhl für Aerodynamik und Strömungsmechanik
Technische Universität München



LES (Large-Eddy Simulation)

$$f_i(x + c_i\Delta t, t + \Delta t) = f_i(x,t) - \frac{1}{\tau_*}(f_i(x,t) - f_i^{eq}(x,t)) + F_i$$

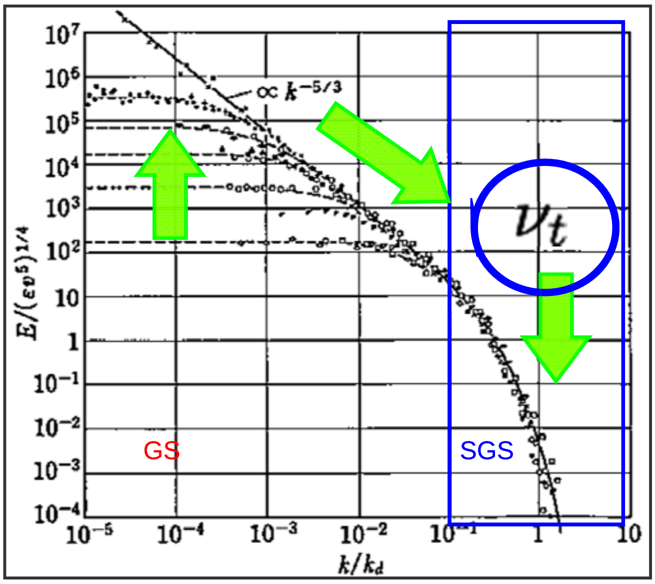
Relaxation time for LES model

$$\tau_* = \frac{1}{2} + \frac{3\nu_*}{c^2\Delta t}$$

$$\nu_* = \nu_0 + \nu_t$$

Molecular viscosity and Eddy viscosity

Energy spectrum



SGS Model

Smagorinsky model

$$\tau_{ij} = -2\nu_{SGS}S_{ij}$$

$$\nu_{SGS} = C\Delta^2|S| \qquad C : const$$

○ Simple
△ inaccurate for the flow with wall boundary
△ emperical tuning for the constant model coefficient

Dynamic Smagorinsky model

$$\nu_{SGS} = C\Delta^2|S|$$

$$C = \frac{< L_{ij}L_{ij} >}{< M_{ij}M_{ij} >} \qquad L_{ij} = \widehat{\bar{u}_i\bar{u}_j} - \hat{\bar{u}}_i\hat{\bar{u}}_j$$

$$M_{ij} = 2\bar{\Delta}^2|\widehat{\bar{S}|\bar{S}_{ij}} - 2\hat{\bar{\Delta}}^2|\hat{\bar{S}}|\hat{\bar{S}}_{ij}$$

○ applicable to wall boundary
△ complicated calculation
△ average process over the wide area
→ not available for complex shaped body
→ not suitable for large-scale problem

Coherent-Structure Smagorinsky model

*H.Kobayashi, Phys. Fluids.17, (2005).

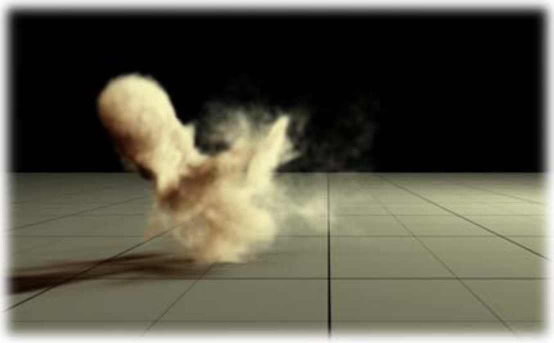
$\nu_{SGS} = C\Delta^2|S|$ → model coefficient determined by the second invariant of the velocity gradient tensor

$$C = C_1|F_{CS}|^{3/2}$$

$$F_{CS} = \frac{Q}{E} \qquad Q = -\frac{1}{2}\frac{\partial \bar{u}_j}{\partial x_i}\frac{\partial \bar{u}_i}{\partial x_j} \qquad E = -\frac{1}{2}\left(\frac{\partial \bar{u}_j}{\partial x_i}\right)^2$$

$$(-1 < F_{CS} < 1)$$

△ model coefficient
○ applicable to wall boundary
○ model coefficient is locally determined.

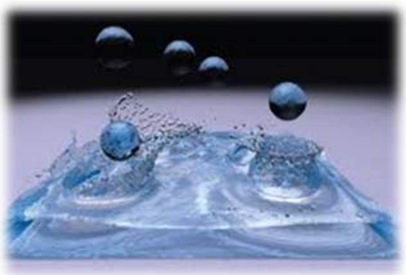


Smoothed Particle Hydrodynamics

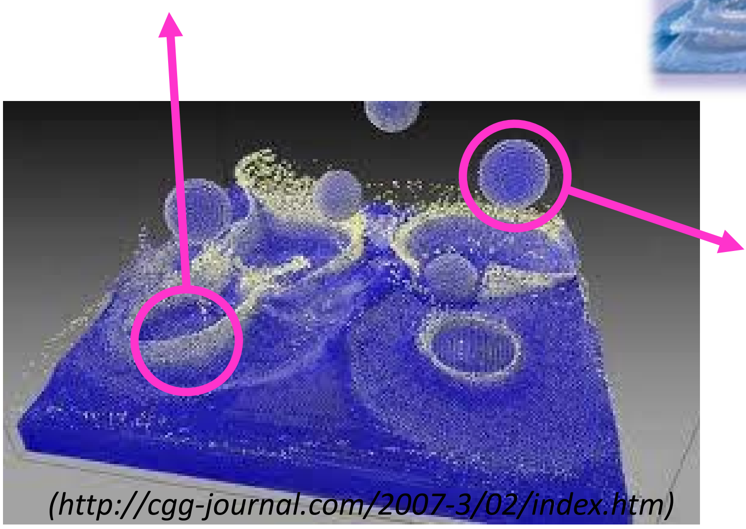
(URL http://labs.aics.riken.jp/makino_j.html)

Smoothed Particle Hydrodynamics

- Compressible and Incompressible Flows represented by particles.



Visualization



Objects are also able to be described by particles.

Solving Navior-Stokes Eq.

Momentum Equation

$$\rho \frac{D\boldsymbol{v}}{Dt} = -\nabla p + \mu \nabla^2 \boldsymbol{v} + \boldsymbol{f} \quad \cdots (1)$$

Pressure gradient — Viscous term — External force

$$\frac{D\boldsymbol{v}}{Dt} = \frac{\partial \phi}{\partial t} + \boldsymbol{v} \cdot \nabla \phi$$

Advection term

In particle methods, the advection term is represented by the particle movement.

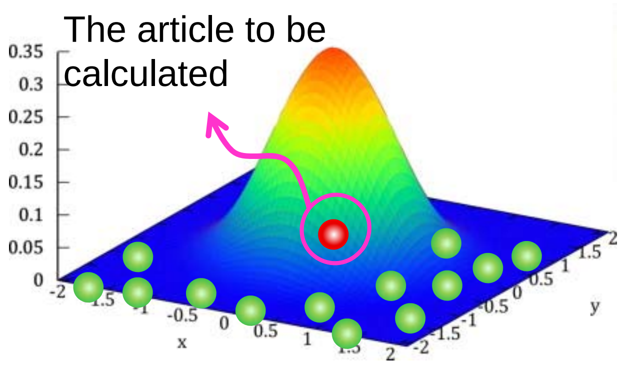
Spatial Profile of Particles

- Each particle has physical properties such as mass, velocity, . . .
- Spatial profile distributing around particles.

$\phi(\boldsymbol{x})$: physical quantity

$$\phi(\boldsymbol{x}) = \int \phi(\boldsymbol{r}) W(\boldsymbol{x} - \boldsymbol{r}) d\boldsymbol{r}$$

Normalization $\int W(\boldsymbol{x} - \boldsymbol{r}) d\boldsymbol{r} = 1$



Kernel Function $W(\boldsymbol{x} - \boldsymbol{r})$

Discretization

$$\phi(\boldsymbol{x}) = \sum_j m_j \frac{\phi_j}{\rho_j} W(\boldsymbol{x} - \boldsymbol{x}_j) \quad \cdots (2)$$

m_j : mass ρ_j : density $m_j = \rho_j \Delta r_j$

Several Expressions (1)

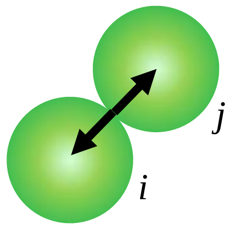
Gradient of Physical Variables

$$\nabla\phi(\boldsymbol{x}) = \int \nabla\phi(\boldsymbol{r})W(\boldsymbol{x}-\boldsymbol{r})d\boldsymbol{r} \quad \longrightarrow \quad \nabla\phi(\boldsymbol{x}) = \int \phi(\boldsymbol{r})\nabla W(\boldsymbol{x}-\boldsymbol{r})d\boldsymbol{r}$$

by applying Gauss law,

$$\nabla\phi(\boldsymbol{x}) = \sum_j m_j \frac{\phi_j}{\rho_j}\nabla W(\boldsymbol{x}-\boldsymbol{x}_j)$$

Pressure Gradient



$$\boldsymbol{f}_i^{press} = -\sum_j m_j \frac{p_j}{\rho_j}\nabla W_{press}(\boldsymbol{x}_i-\boldsymbol{x}_j)$$

$$\longrightarrow \quad -\sum_j m_j \frac{p_i+p_j}{2\rho_j}\nabla W_{press}(\boldsymbol{x}_i-\boldsymbol{x}_j)$$

keeping symmetry

Simple EOS: $p=k(\rho-\rho_0)$

Several Expressions (2)

Viscosity Term

$$\phi_i = \phi_j + \nabla\phi_j \cdot (\boldsymbol{x}_i-\boldsymbol{x}_j) \quad \longrightarrow \quad \nabla\phi_j = (\phi_j-\phi_i)\frac{\boldsymbol{x}_j-\boldsymbol{x}_i}{|\boldsymbol{x}_j-\boldsymbol{x}_i|^2}$$

Taylor expansion

using $\nabla^2\phi = \nabla\cdot(\nabla\phi)$ $\quad \nabla^2\phi_i = \sum_j m_j \frac{\nabla\phi_j}{\rho_j}\nabla W(\boldsymbol{x}_i-\boldsymbol{x}_j)$

$$\nabla^2\phi_i = \sum_j m_j \frac{\phi_j-\phi_i}{\rho_j}\nabla W_{vis}(\boldsymbol{x}_i-\boldsymbol{x}_j)$$

where $\nabla W_{vis}(\boldsymbol{x}_i-\boldsymbol{x}_j) = \frac{\boldsymbol{x}_j-\boldsymbol{x}_i}{|\boldsymbol{x}_j-\boldsymbol{x}_i|^2}\cdot\nabla W(\boldsymbol{x}_i-\boldsymbol{x}_j)$

$$\longrightarrow \quad \sum_j m_j \frac{\boldsymbol{v}_j-\boldsymbol{v}_i}{\rho_j}\nabla W_{vis}(\boldsymbol{x}_i-\boldsymbol{x}_j)$$

Kernel Function

Density: $$W(\boldsymbol{r}) = \begin{cases} \frac{315}{64\pi r_e^9}(r_e^2 - |\boldsymbol{r}|^2)^3 & (0 \le |\boldsymbol{r}| < r_e) \\ 0 & (r_e \le |\boldsymbol{r}|) \end{cases}$$

At the center, the gradient becomes small.

Pressure: $$\nabla W_{press}(\boldsymbol{r}) = -\frac{45}{\pi r_e^6}(r_e - |\boldsymbol{r}|)^2 \frac{\boldsymbol{r}}{|\boldsymbol{r}|}$$

Viscosity: $$\nabla W_{vis}(\boldsymbol{r}) = \frac{45}{\pi r_e^6}(r_e - |\boldsymbol{r}|)$$

Time Integration

Time Integrations for velocity and position:

$$\boldsymbol{v}_i^{t+\Delta t} = \boldsymbol{v}_i^t + \frac{\Delta t}{\rho_i}(\boldsymbol{f}_i^{press} + \boldsymbol{f}_i^{vis} + \boldsymbol{f}_i^g)$$

$$\boldsymbol{x}_i^{t+\Delta t} = \boldsymbol{x}_i^t + \boldsymbol{v}_i^{t+\Delta t}\Delta t$$

Stability conditions:

CFL condition: $$C = \frac{v_{max}\Delta t}{l_0}$$

l_0 : inter-particle distance

v_{max} : maximum particle velocity

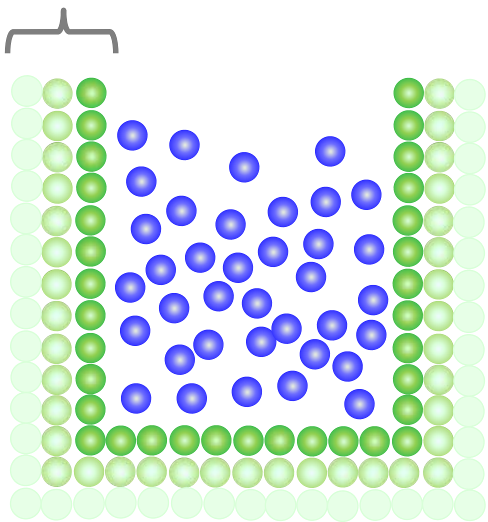
Diffusion stable condition: $$\lambda = \frac{\nu \Delta t}{l_0^2}$$

$\nu = \frac{\mu}{\rho}$: kinetic viscosity coefficient

Boundary Condition

Setting boudary partiles

- Multiple layers are required at the boundary.



- The Surface is 凸凹.