Avogadro Challenge Project

Climate 2009: The 11th International Specialist Meeting
The Next Generation Models on Climate Change and Sustainability for Advanced High-Performance Computing
ORNL USA, Mar. 17th, 2009

Toward Exaflops Applications: Molecular Dynamics Simulation of Liquid-Gas Transition

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THE UNIVERSITY OF TOKYO

collaboration with

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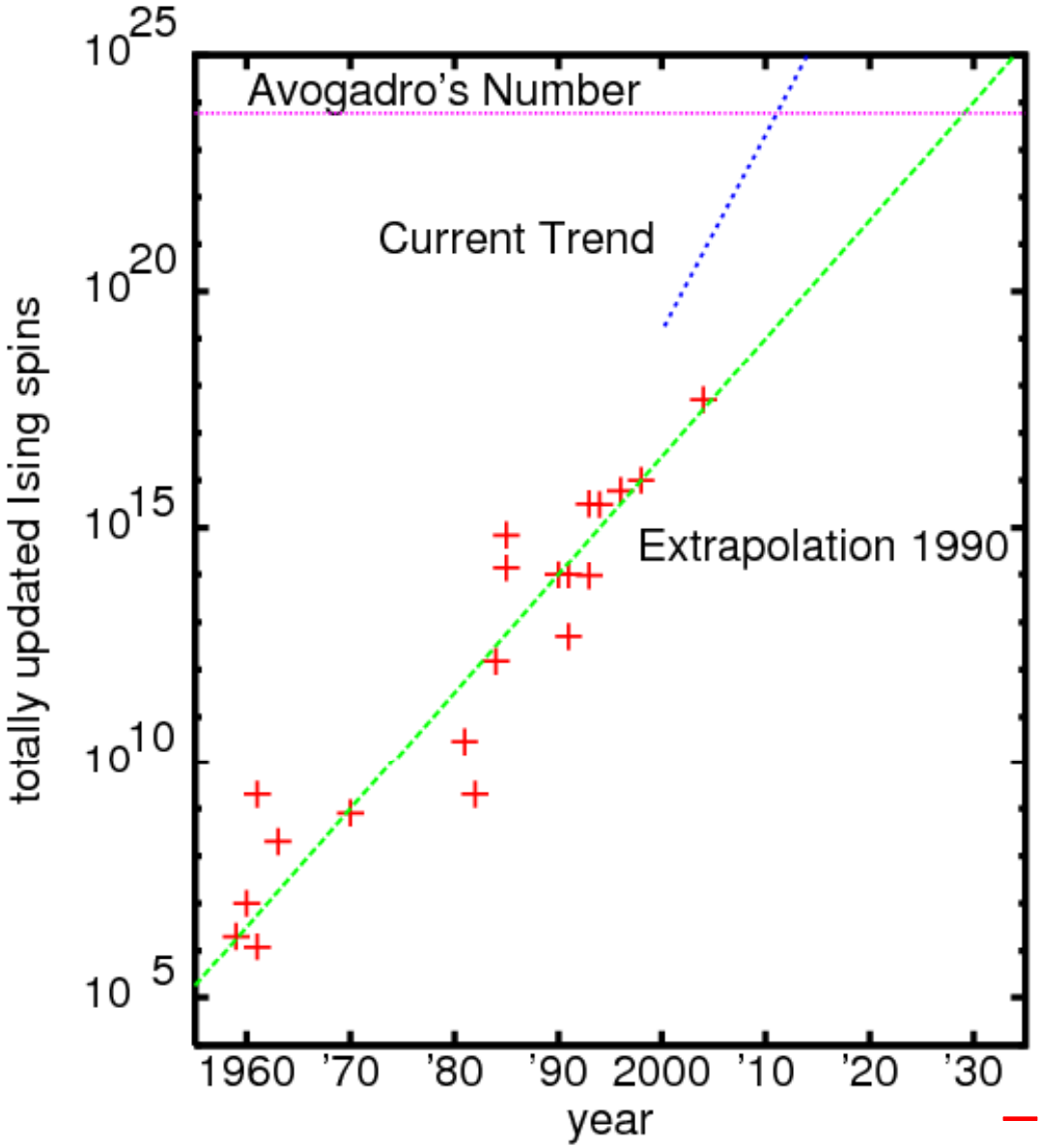
Nagoya University

OSAKA UNIVERSITY

partly supported by: JSPS Grants-in-Aid for Scientific Research <KAKENHI> King Abdullah University of Science and Technology KAUST Global Research Partnership

Perspective of computer power
Scale-up History of Ising Simulation
(revised from N. Ito, 1991)



10 times larger at every 4 years.

cf. CPU speed: x2 every 18 months
G. E. Moore, Electronics 38(1965) 8

disk: x2 every 12 months,
network bandwidth: x2 every 9 months
I. Foster, Phys. Today 55(2002) 35

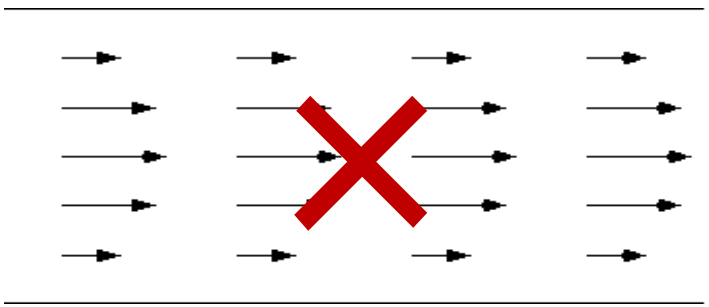
Accelerated in this century.

We will reach to
the Avogadoro Number
in 2010s.

— THE AVOGADRO CHALLENGE —

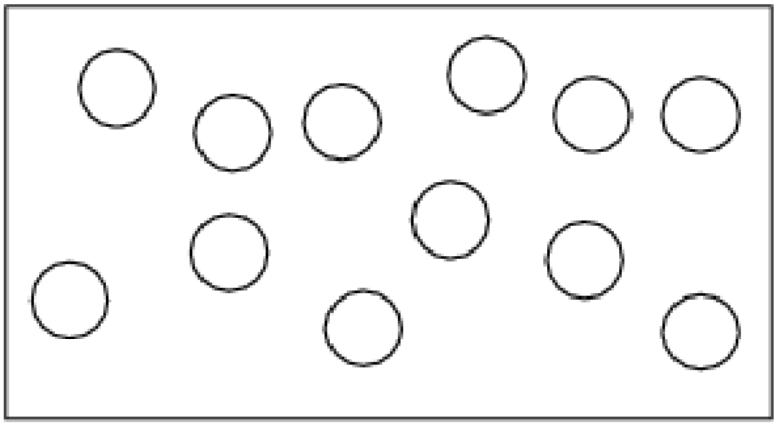
What is the ACP?

Water is not flowing,
water molecules are moving!



Navier-Stokes Equation

$$\frac{\partial v}{\partial t} + (v \cdot \nabla)v = -\nabla(\frac{p}{\rho_0}) + \nu \nabla^2 v + f$$

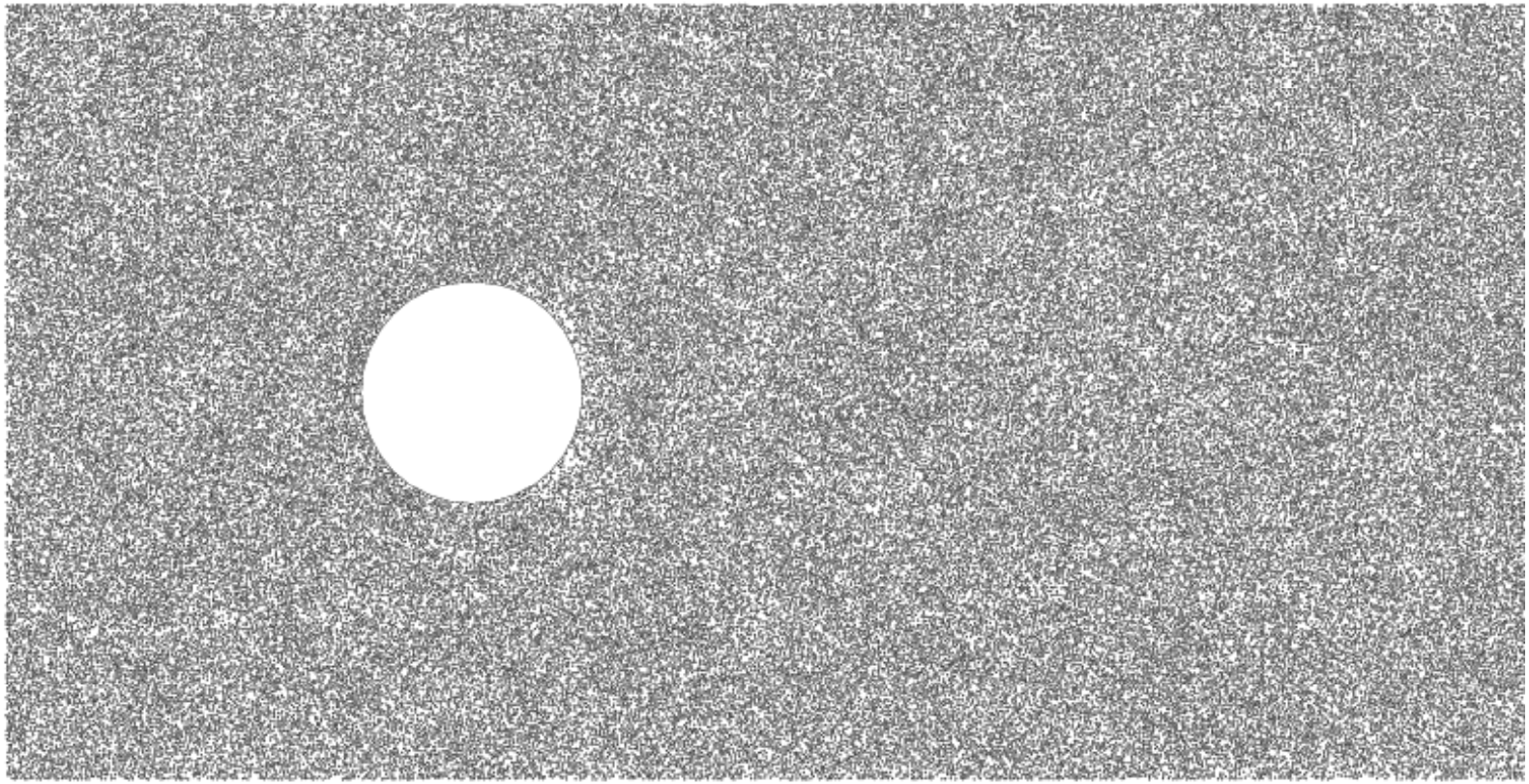


Newtonean Equation of Motion

$$\boldsymbol{F} = m\,\boldsymbol{a}$$

Avogadro Challenge Project

370,000 hard-disks



Avogadro Challenge Project

Result for Re = 110

Avogadro Challenge Project

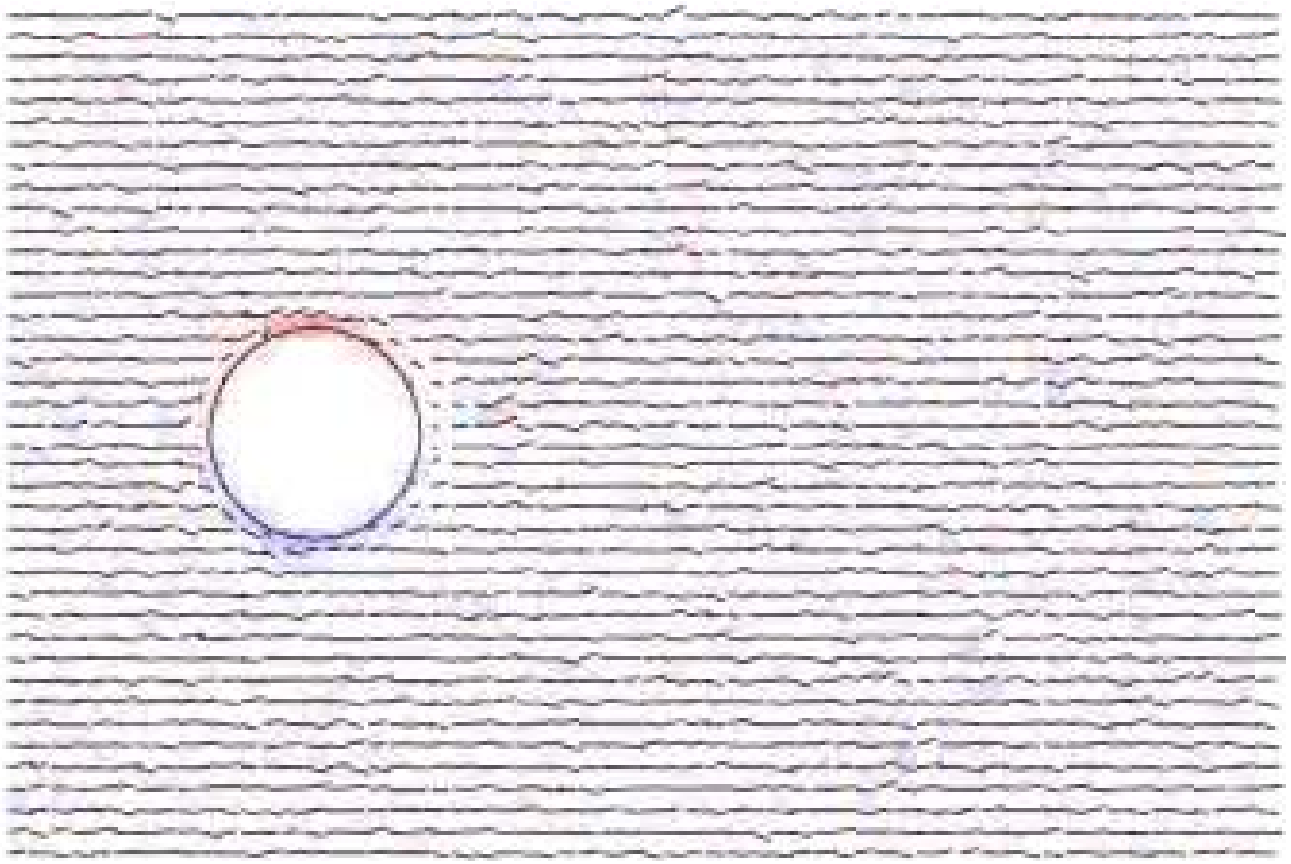
370,000 particles

system 1200x800

diameter of cylinder 200

(diameter of particle is 1)

color shows vorticity

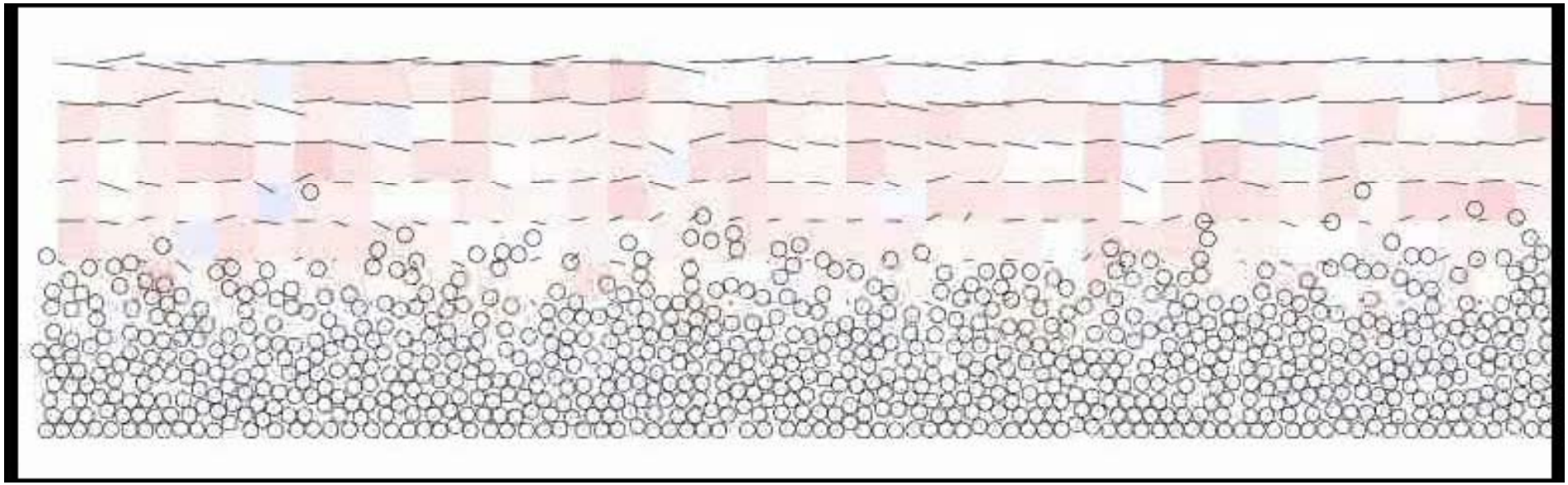


T. Ishiwata, T. Murakami, S. Yukawa and N. Ito, Intern. J. Mod. Phys. C15 No.10 (2004).

GRAIN TRANSPORT BY FLOW

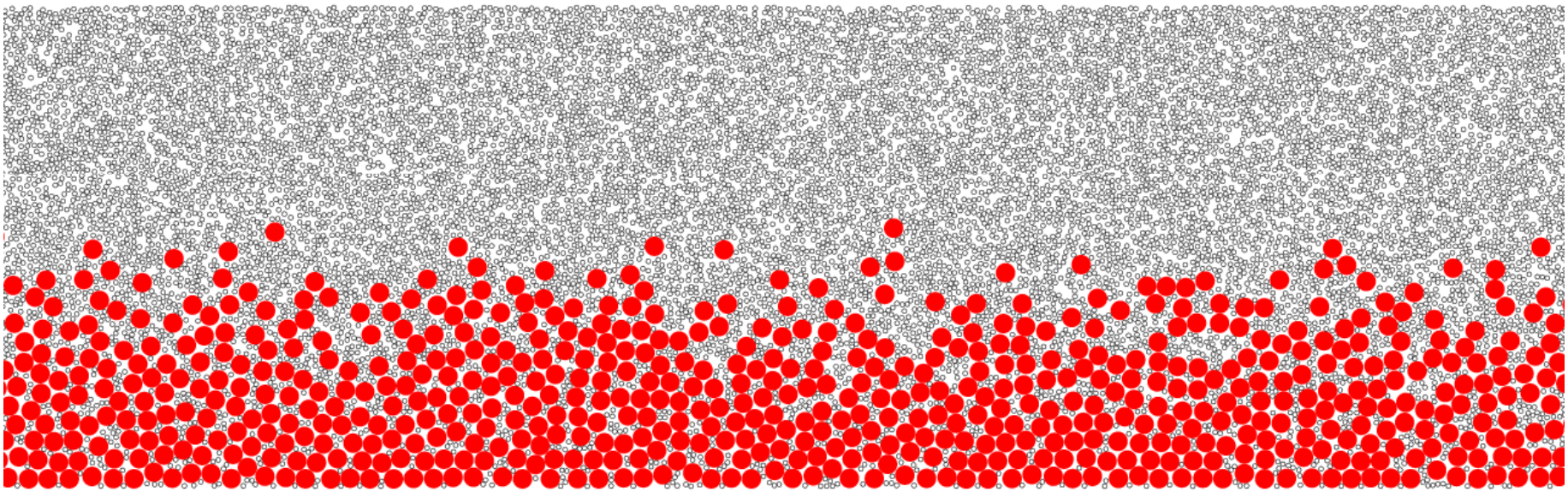
T. Ishiwata, Mater Thesis
(Univ. Tokyo, 2003).

FLOW →



Avogadro Challenge Project

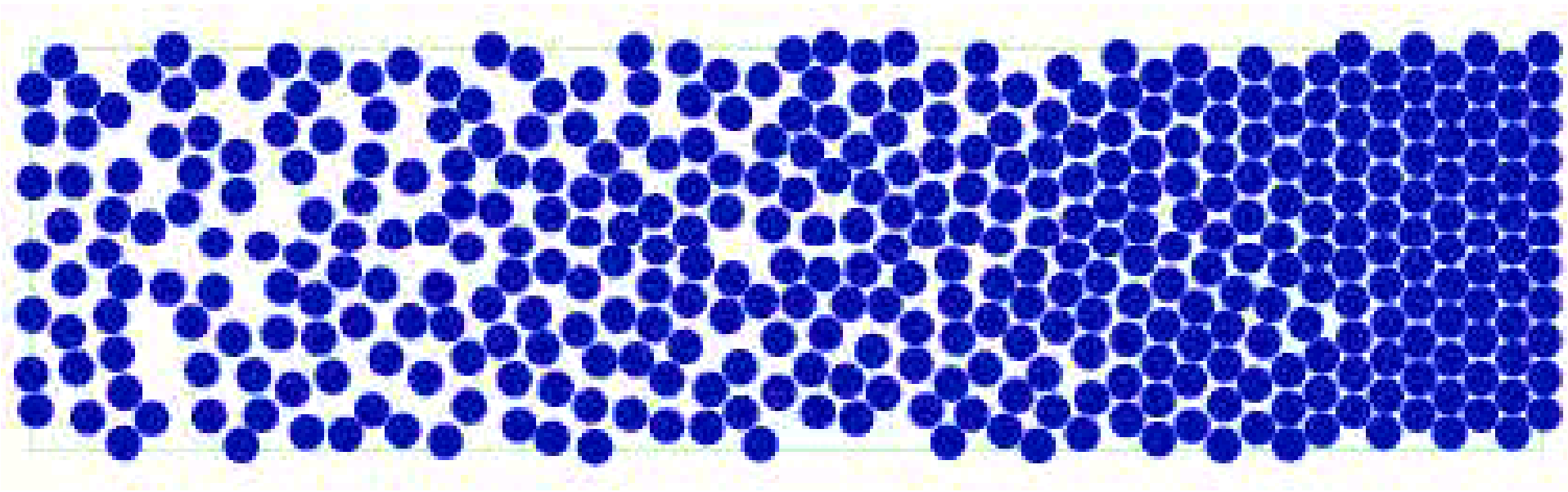
An application



Nonequilibrium Steady State
— temperature gradient —

energy flux(heat conduction)

Hight T → Low T

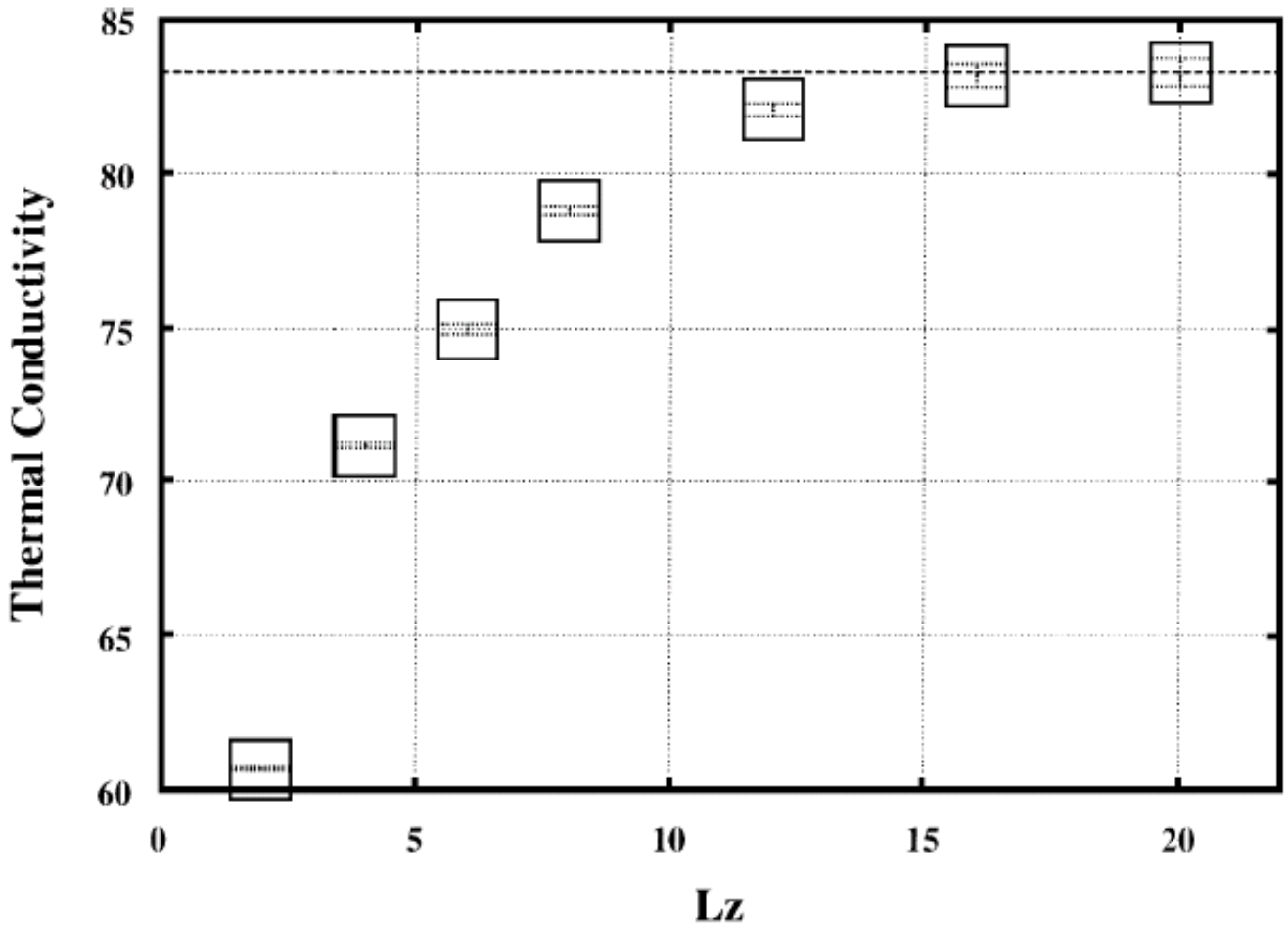


FLUID PHASE SOLID PHASE

Avogadro Challenge Project

T. Shimada, T. Murakami, S. Yukawa, K. Saito and N. Ito,
J. Phys. Soc. Jpn. 69 (2000) 3150.

System Length Dependence of Heat Conductivity
3D Hard Sphere Fluid



System Length

T. Shimada, T. Murakami, S. Yukawa, K. Saito and N. Ito,
J. Phys. Soc. Jpn. 69 (2000) 3150.

Avogadro Challenge Project

How does energy flow in nonequilirium steady state?

$$J_x^{-2/3} \mathrm{e}^{-\alpha J_x^{2/3}} \quad \mathrm{e}^{-\lambda J}$$

linear response theoretical sense, perturbation

↑ equilibrium distribution

↑transport nonequilibrium distribution

True distorsion of the distribution function with transport

$$\Delta P(J) = P(J) - P_{\mathrm{eq.}}(J)$$

How does it look like?

Confirms above distribution?

cf. R. Kubo, M. Yokota and S. Nakajima, J. Phys. Soc. Jpn. vol. 12 (1957) 1203.

$$e^{-(\beta+\delta\beta) H - \alpha J}$$

An outcome

“Discovery of a new distribution in heat conduction”

in Feb. 20th, 2009 issue of Science News(in Japanese)

The Science News 科学新聞 2009年(平成21年) 2月20日(金曜日) 第3252号

科学新聞

週刊

放医研の高橋氏ら

妬む感情が強い人ほど他人の不幸を喜びがち

fMRIで脳科学的に証明

蛋白質分子内小分子移動

定常的な熱伝導状態 新たな分布法測 発見

大阪大の瀬川淳教授ら

な発光色

み明らかに

氏ら成果

へ貢献期待

緑色光～赤色光 (530–640 nm)

自民党 科学技術創造立国推進調査会

科学技術力強化へ向けて さらなる予算獲得を

化学

One lesson in nonequilibrium statistical physics

Energy flux distribution

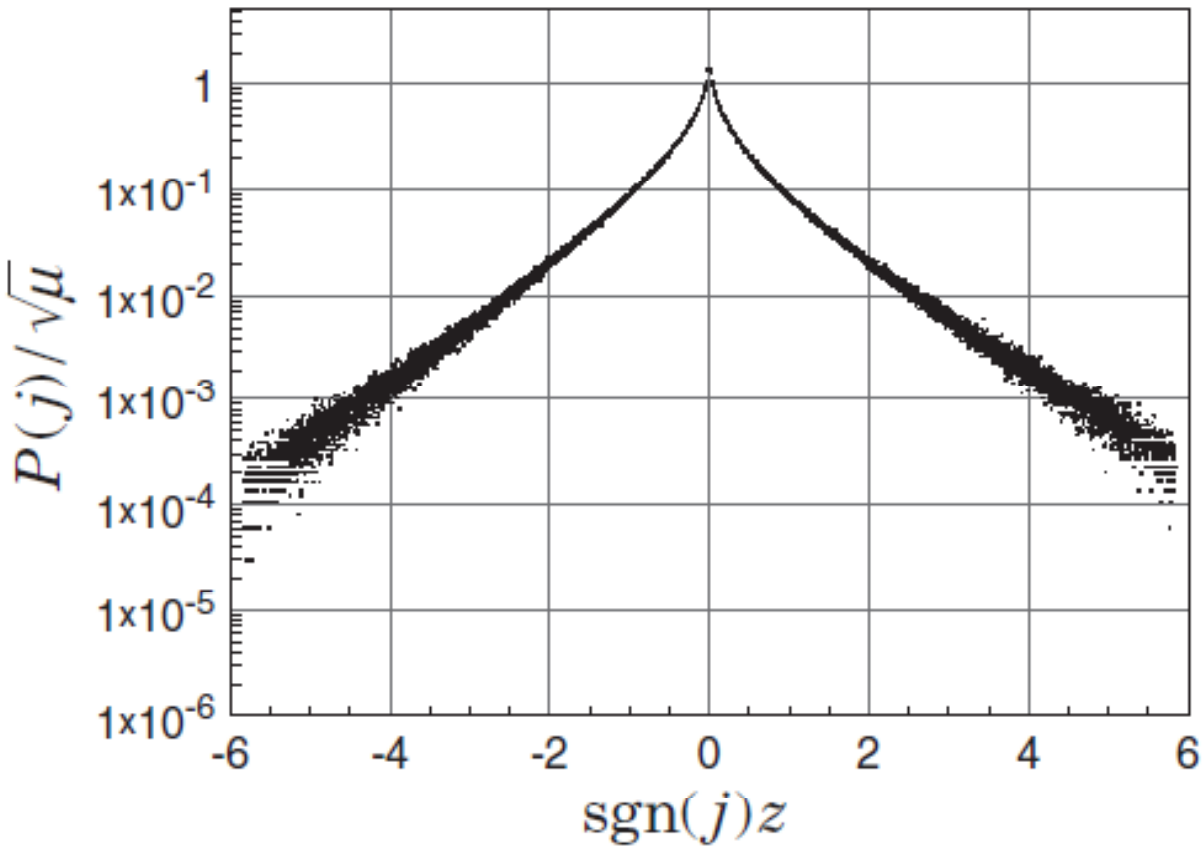


Fig. 2. Distribution of j_K^x, which is a parallel component of the thermal gradient: The horizontal axis represents $\mathrm{sgn}(j)z$ and the vertical axis represents $\ln[P(j)/\sqrt{\mu}]$, where z and μ are identical to definitions used in the equilibrium distribution eq. (2). Three different thermal gradient cases are superposed.

Energy Flux Distribution in Equilibrium

- ideal gas -

K

$\bigcirc \longrightarrow \vec{p}$

energy flux: $\vec{J} = \frac{1}{m} K \cdot \vec{p}, K = \frac{\vec{p}^2}{2m}$

equilibrium distribution: $P_{\mathrm{eq.}}(\vec{p})\mathrm{d}\vec{p} \sim \mathrm{e}^{-\beta K}\mathrm{d}\vec{p}$

$$\longrightarrow \quad P_{\mathrm{eq.}}(J_x)\mathrm{d}J_x \sim J_x^{-2/3}\mathrm{e}^{-\alpha J_x^{2/3}}\mathrm{d}J_x, \alpha = \frac{\beta}{(2m)^{1/3}}$$

$$P(j) = N' j^{\frac{d-3}{3}} \exp\left\{-\left(\frac{m}{2}\right)^{\frac{1}{3}} \beta\, j^{\frac{2}{3}}\right\}$$

stretched exponential form

T. Shimada, F. Ogushi and N. Ito, J. Phys. Soc. Jpn. 76 No. 7 (2007) 075001

Anisotropic Temperature

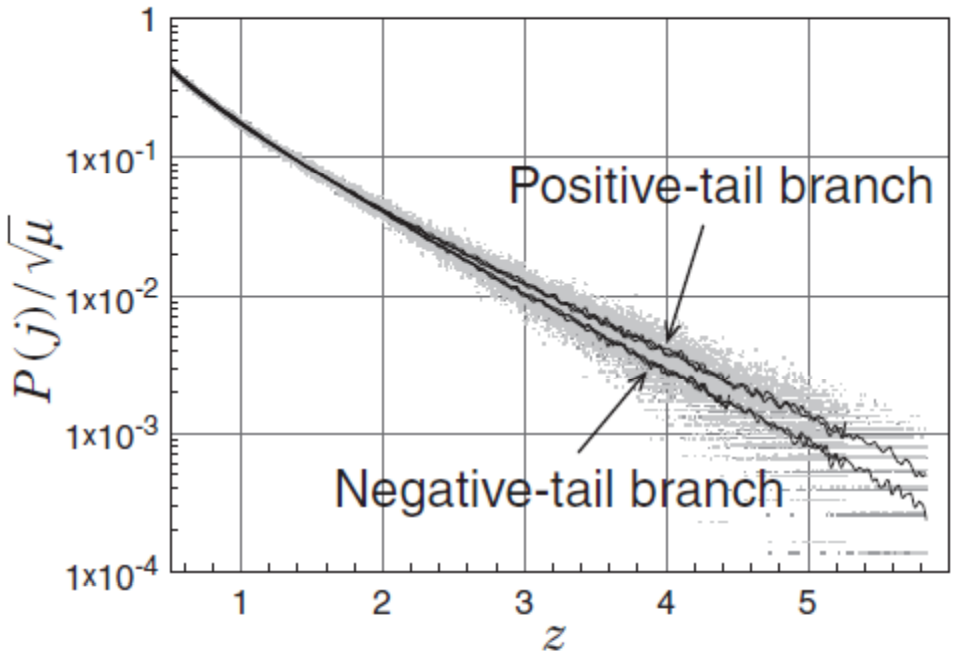


Fig. 3. Negative tails are flipped at $z = 0$ and superposed tails: Gray scattered dots are original data and black lines over several bins for each data point of three different grad we observe two branches for negative and positive current

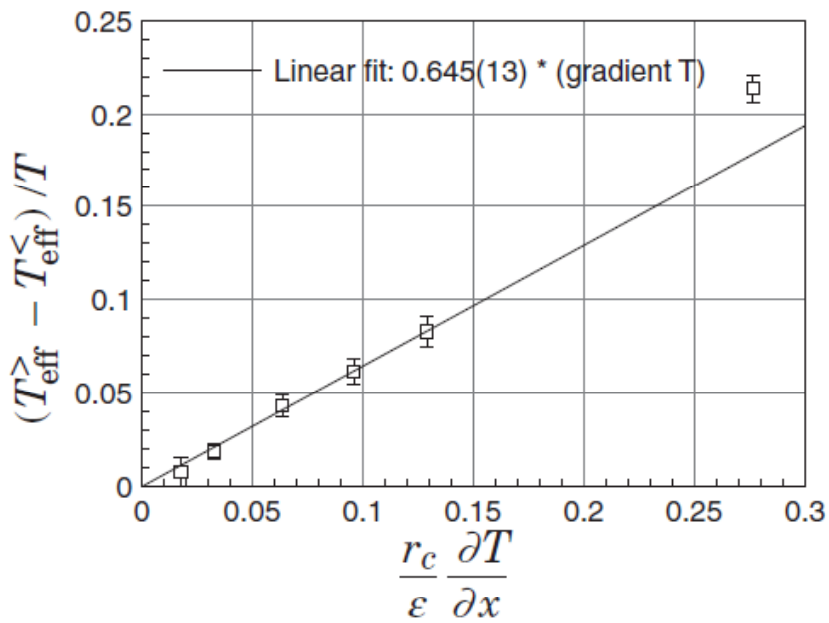


Fig. 5. Difference in effective kinetic temperature between both tails normalized by the local kinetic temperature plotted against the local temperature gradient for the Lennard-Jones particle system.

S. Yukawa, T. Shimada, F. Ogushi and N. Ito,
J. Phys. Soc. Jpn. 78 (2009) 023002,

Awarded the Editor's Choice Prize

Open Choice(Free Access) Article
Visit http://www.ipap.jp/

Summary of nonequilibrium heat-flux distribution
― the simplest phenomenology ―

$$e^{-(\beta-\delta\beta)H} \qquad for\ J_x>0$$

$$e^{-(\beta+\delta\beta)H} \qquad for\ J_x>0$$

for example

$$\exp\left[-\left(\beta+\alpha\,\frac{\vec{p}}{|\vec{p}|}\cdot\mathrm{grad}\ T\right)\ H\right]$$

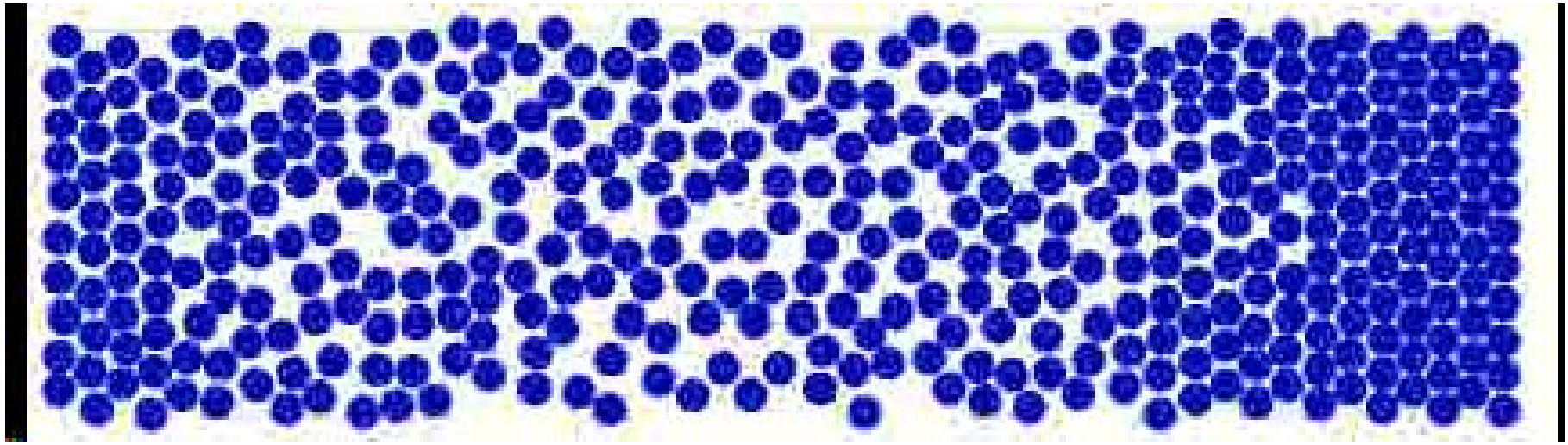
※ smooth connection at J=0?

Nonequilibrium Steady State
− temperature gradient and hyrdodynamic shear −

energy flux(heat conduction)

Hight T → Low T

↑ v_y

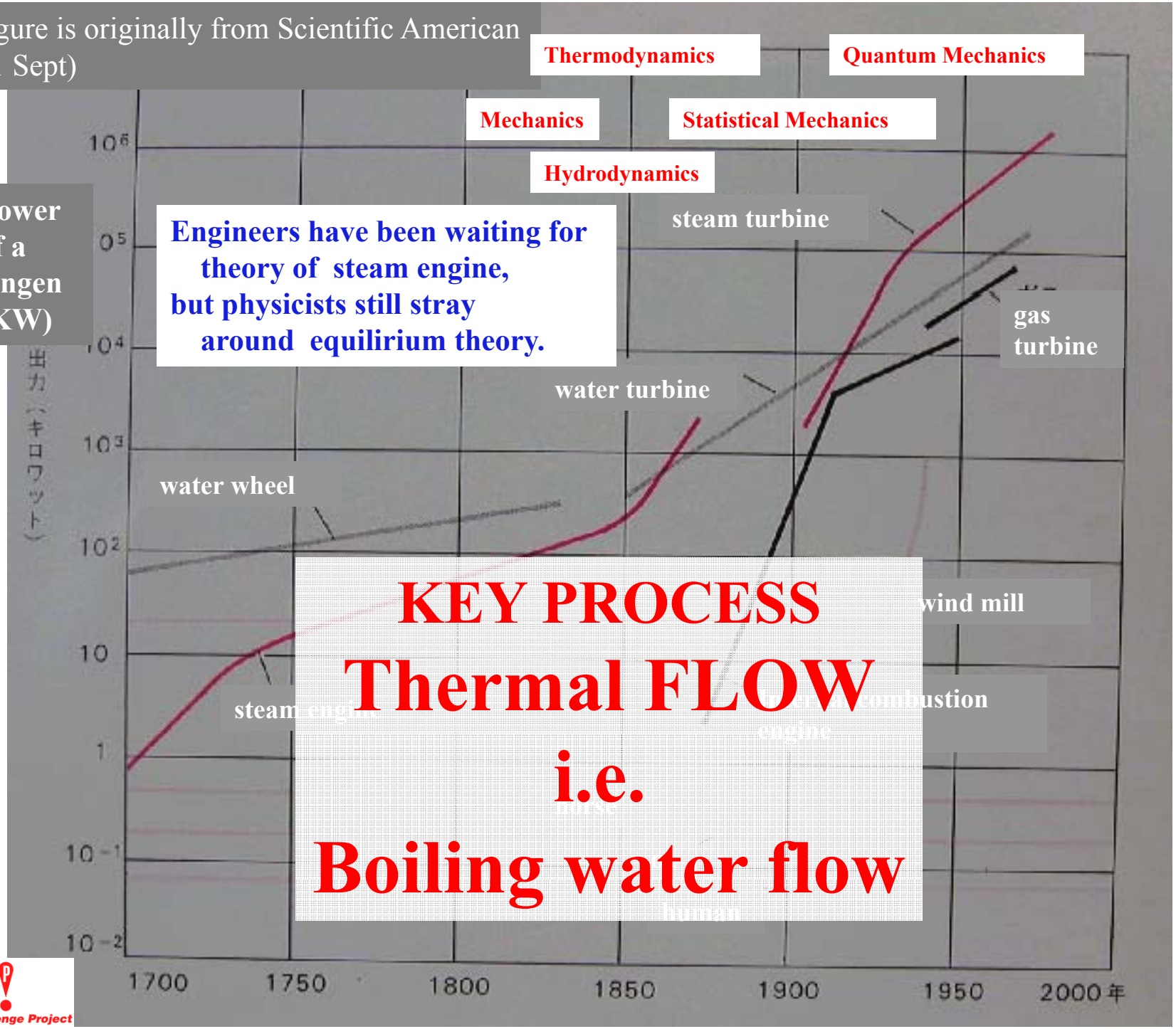


SOLID FLUID SOLID

Shear Induced Freezing

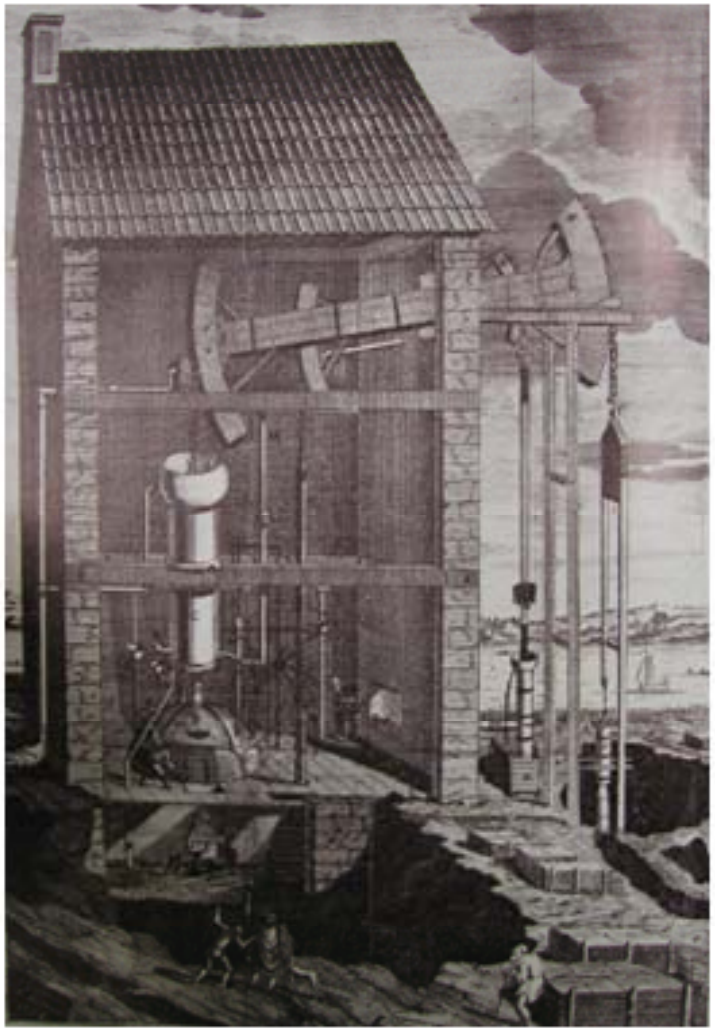
Avogadro Challenge Project

This figure is originally from Scientific American (1971 Sept)

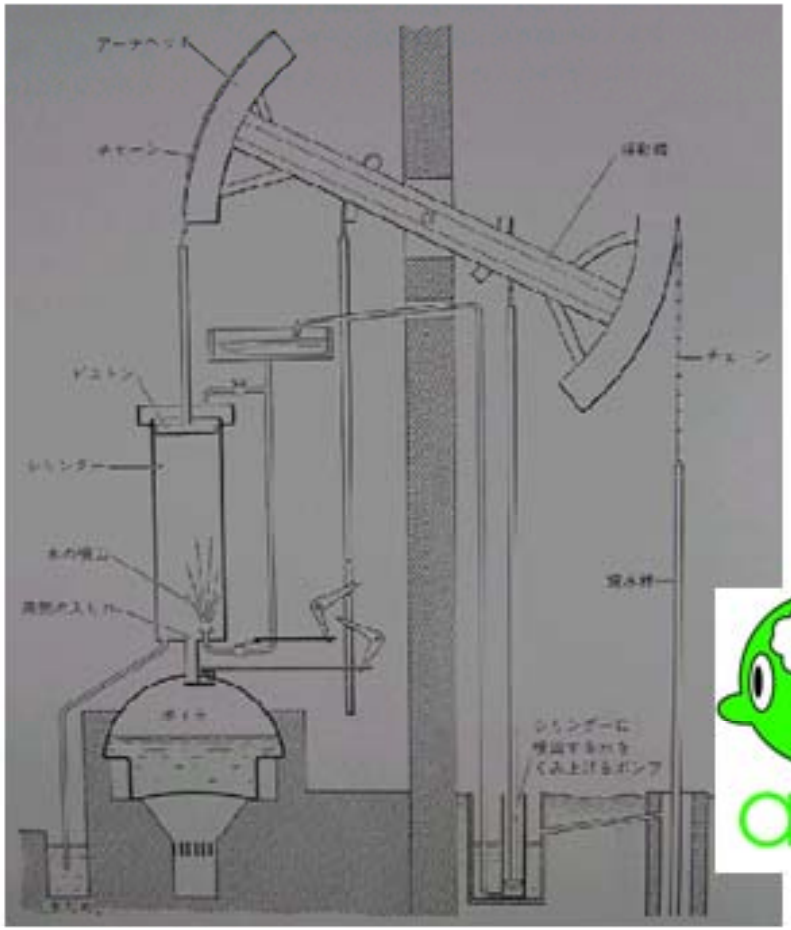


Avogadro Challenge Project

Modern world began with steam engines.



KAUST King Abdullah University of Science and Technology

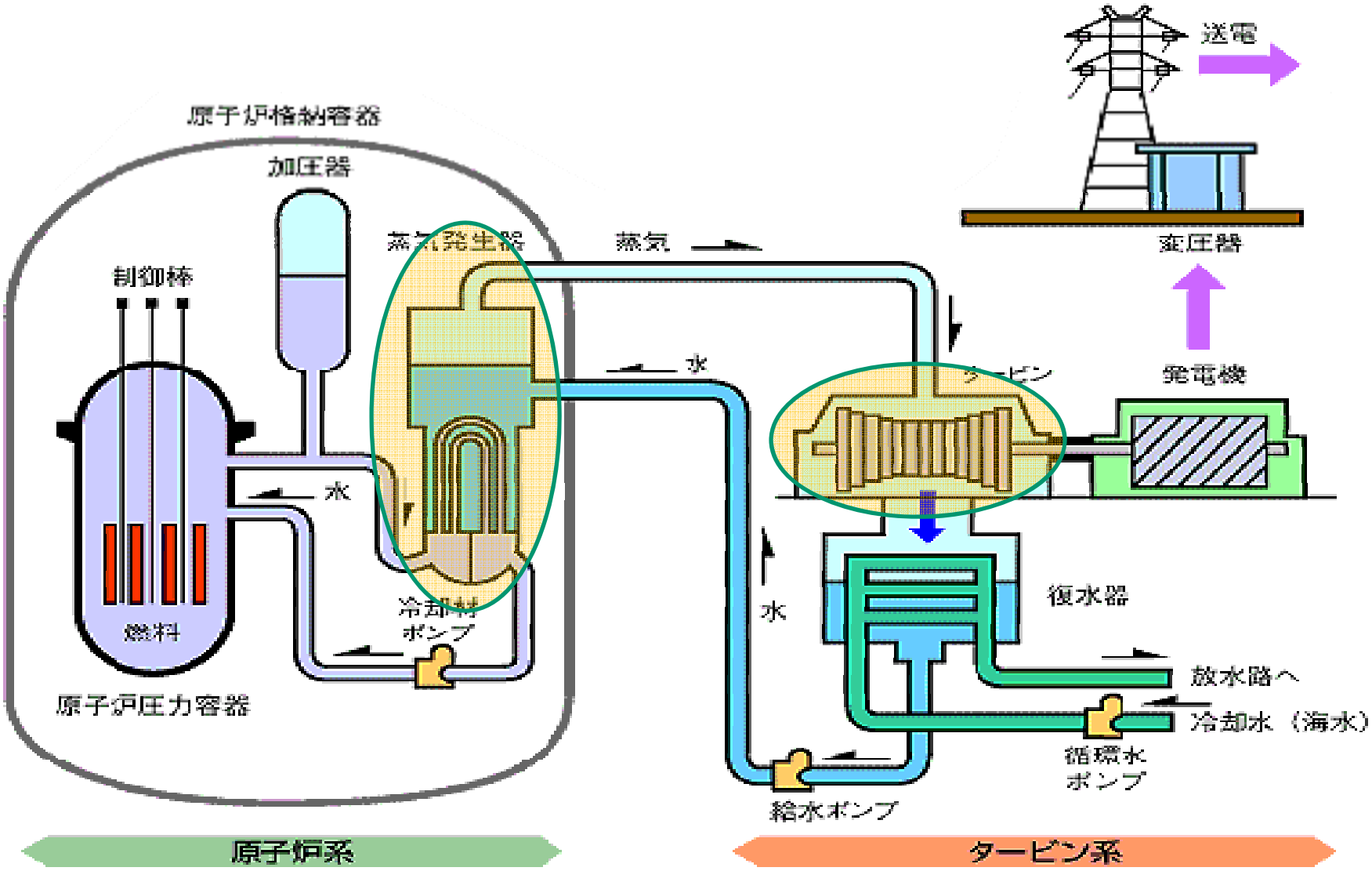


A Newcomen engine in the beginning of 18th century
from Scientific American (1964 Jan)

… and we reached GW systems:

The Target

A typical energy system: nuclear plant

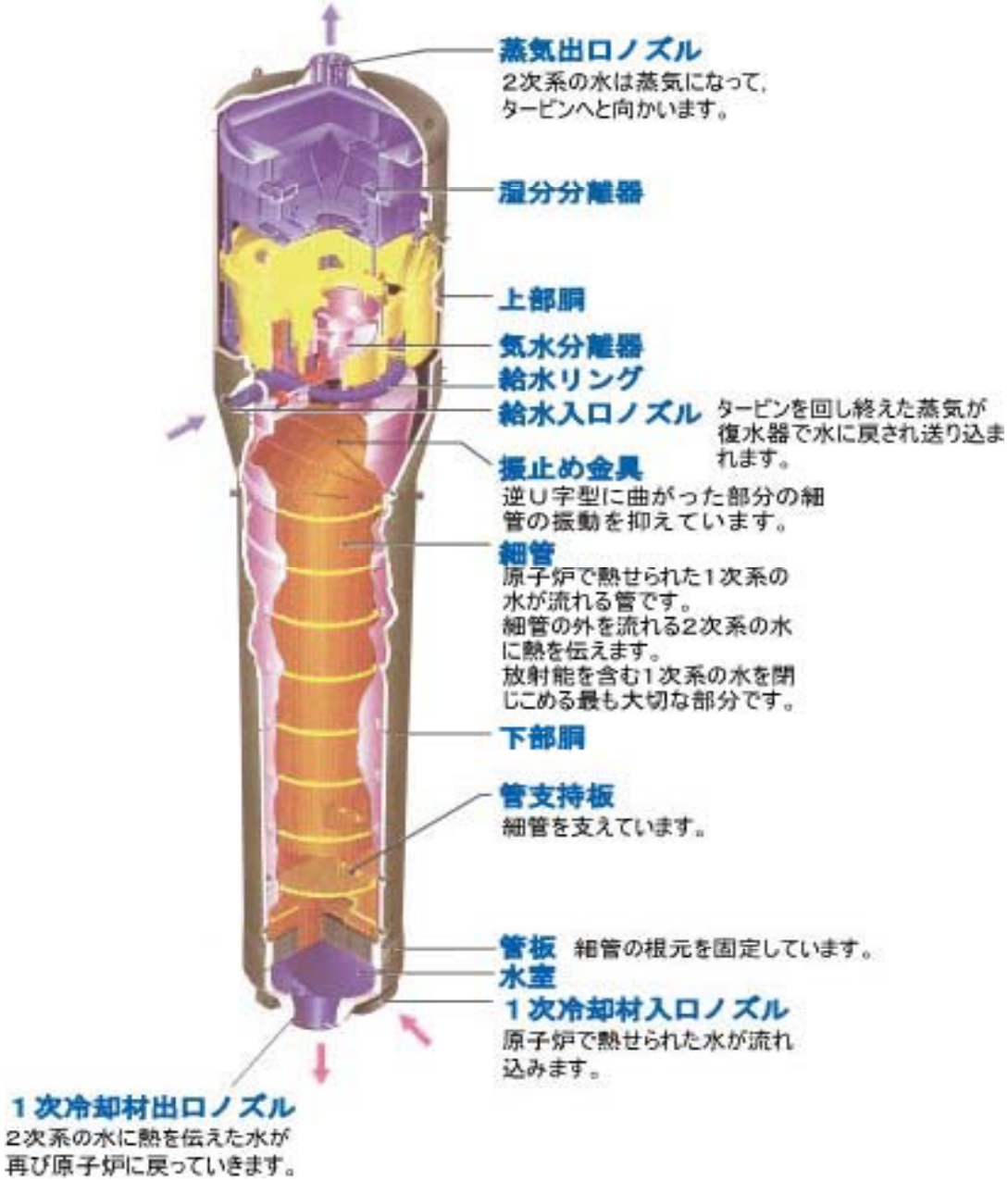


From Hitachi Nuclear Power HP:

http://www.pi.hitachi.co.jp/Div/power/moreinfo/s_power/waterway/index.html

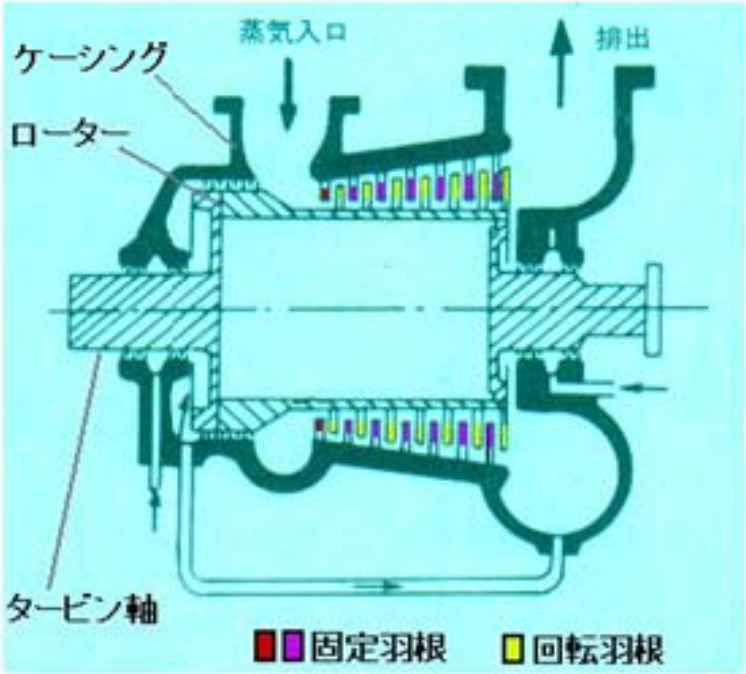
Steam Generator

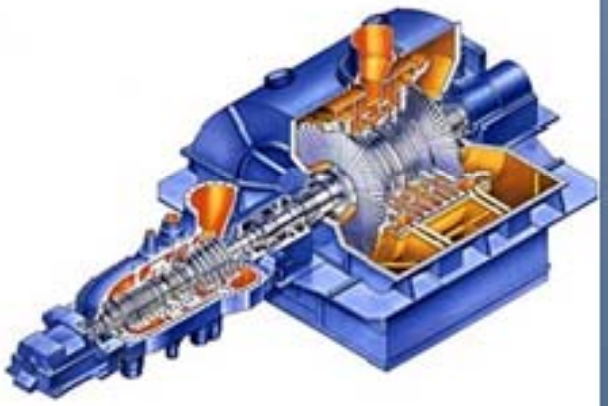
320t
Height 21m
Diameter 4.5m max
3,382 pipe
Steam output ~1GW

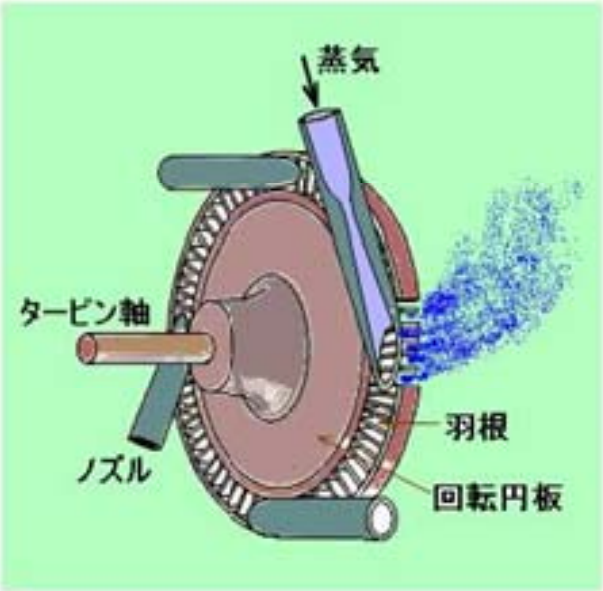


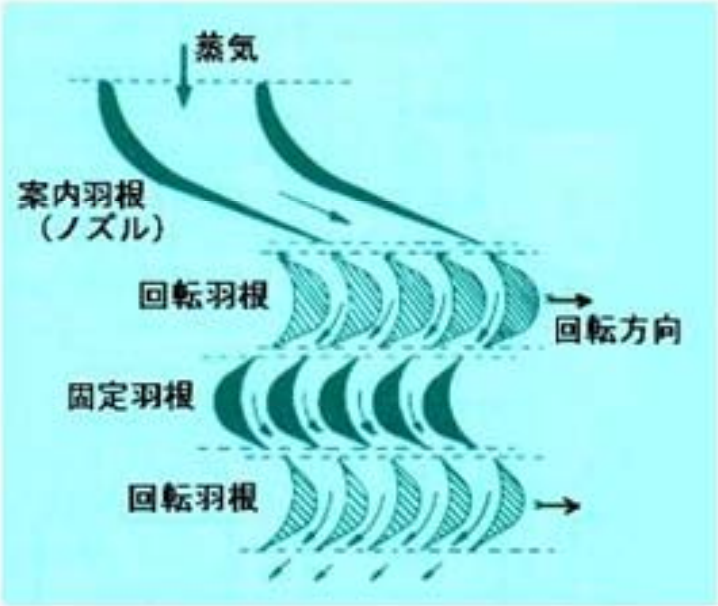
SG of Genkai the third plant manufactored by Mitsubishi Heavy Industory Corporation
From HP of Kyushu Electoric Power Corporation: http://www.kyuden.co.jp/genkai_history_b.html

Steam Turbine





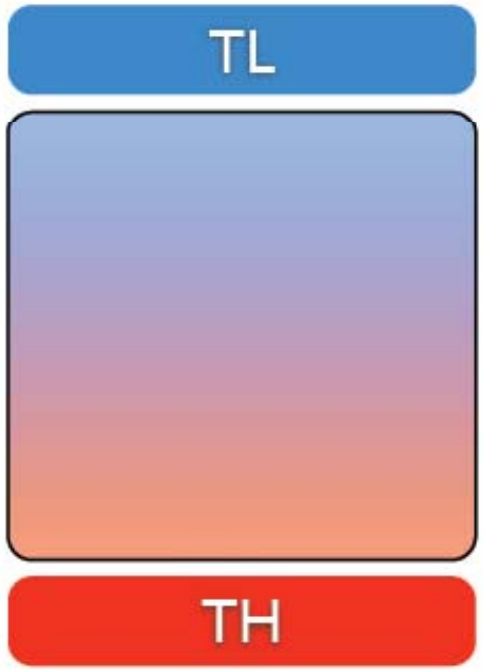


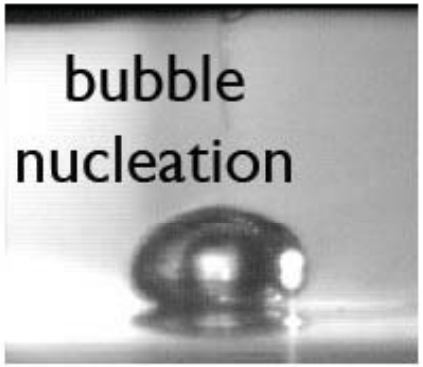


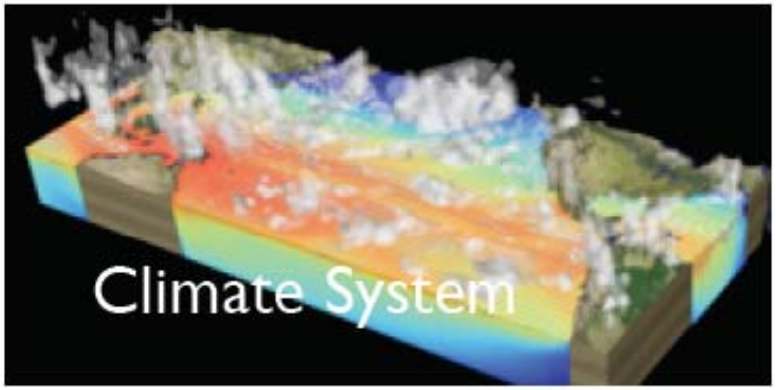
Target Phenomena

Avogadro Challenge Project

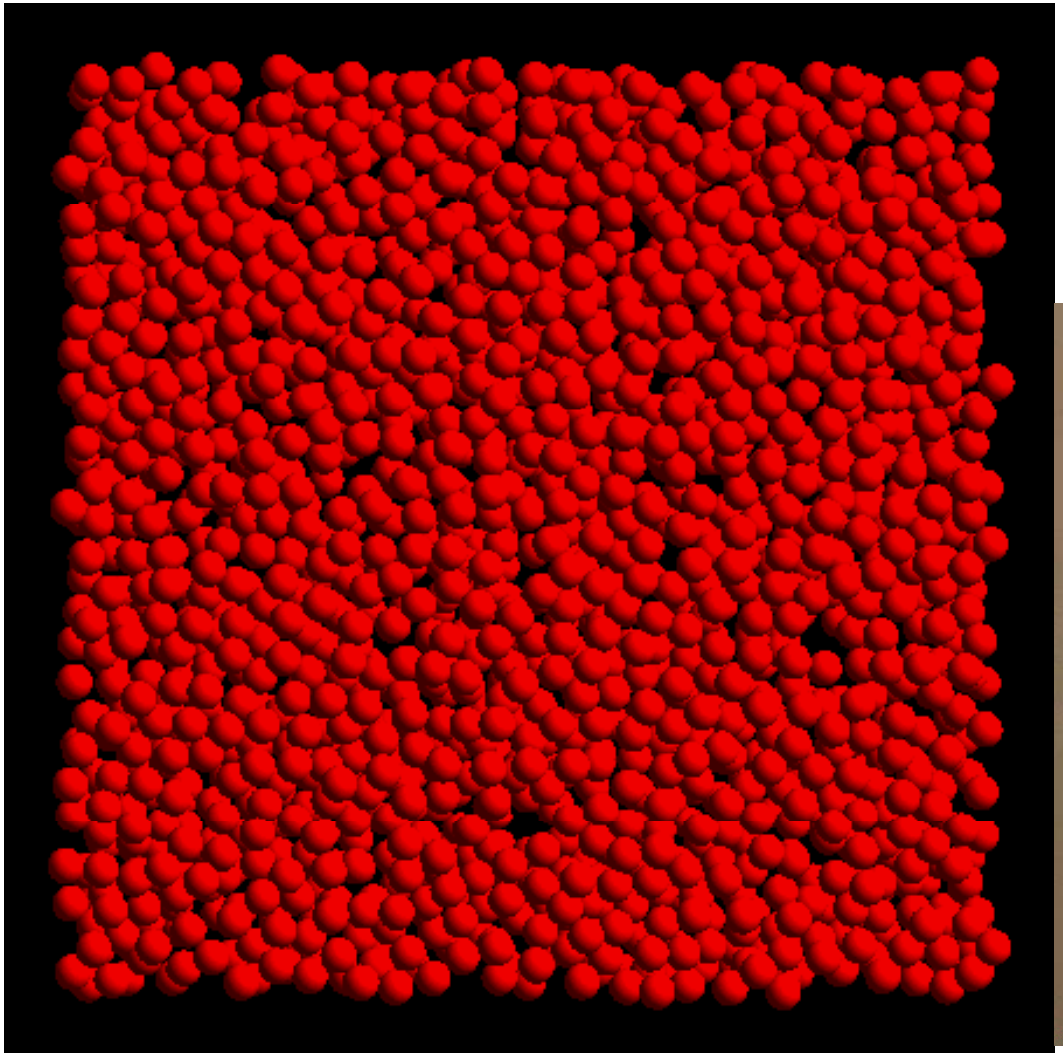
- heat in our life -



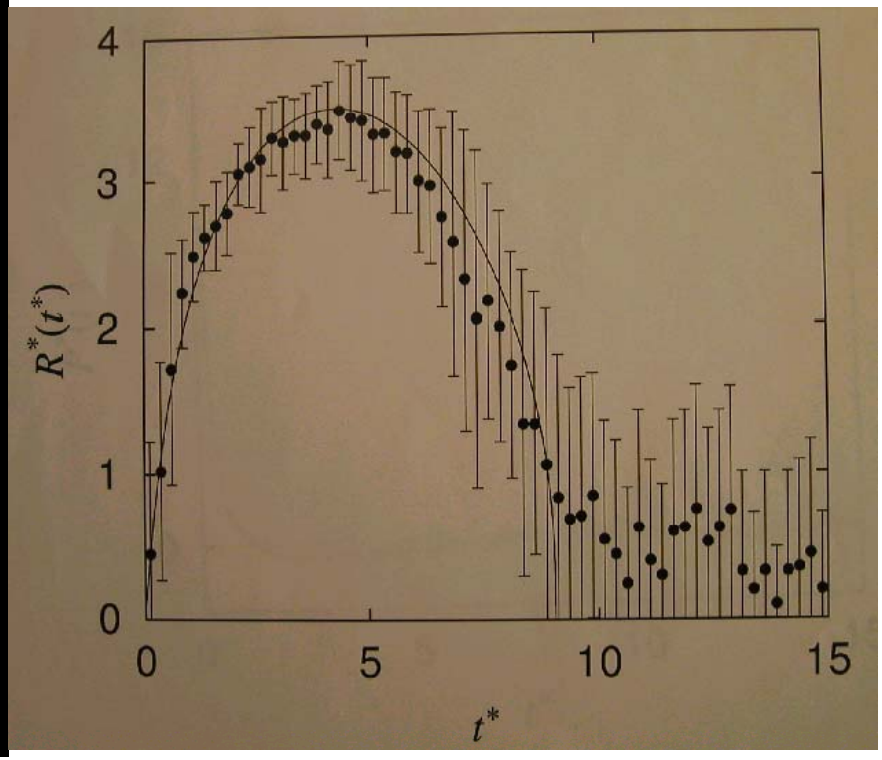




Nano-vapor Dynamics



with Lennard-Jones particles
quasi-EPN-ensemble



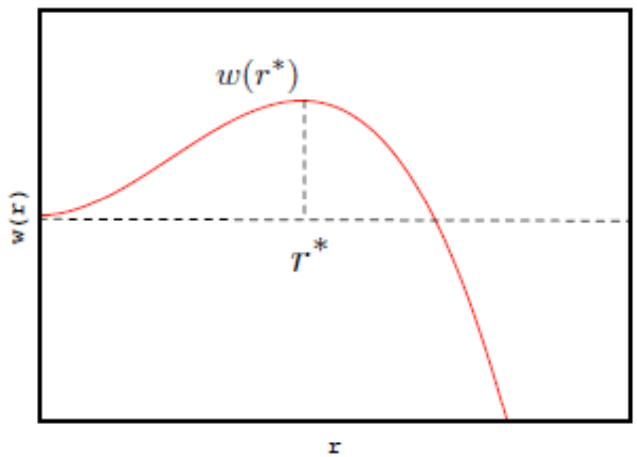
Η. Οκυμυρα ανδ Ν. Ιτο, Πηψσ. Ρεϖ. Ε (2003) Ε67 (2003) 045301

nucleation theory

Avogadro Challenge Project

nucleation theory

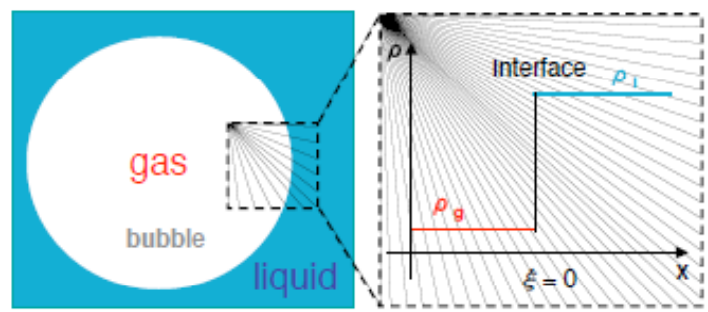
$$w(r) = 4\pi r^2 \gamma - \frac{4}{3}\pi r^3 \rho \Delta\mu$$



$$r^* = \frac{2\gamma}{\rho \Delta\mu}$$

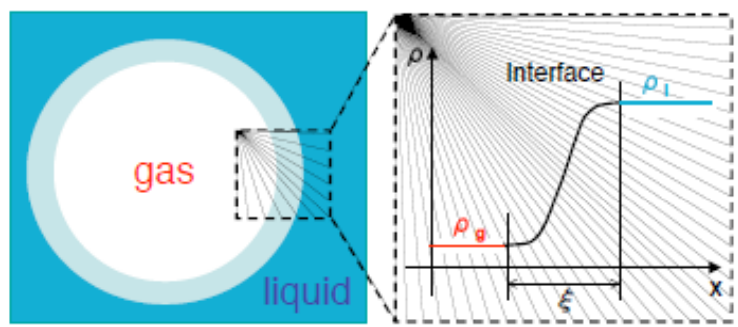
$$\Delta\mu = k_B T \ln S$$

Classical Nucleation Theory (CNT)



Ignoring the thickness of the interface

Density Functional Theory

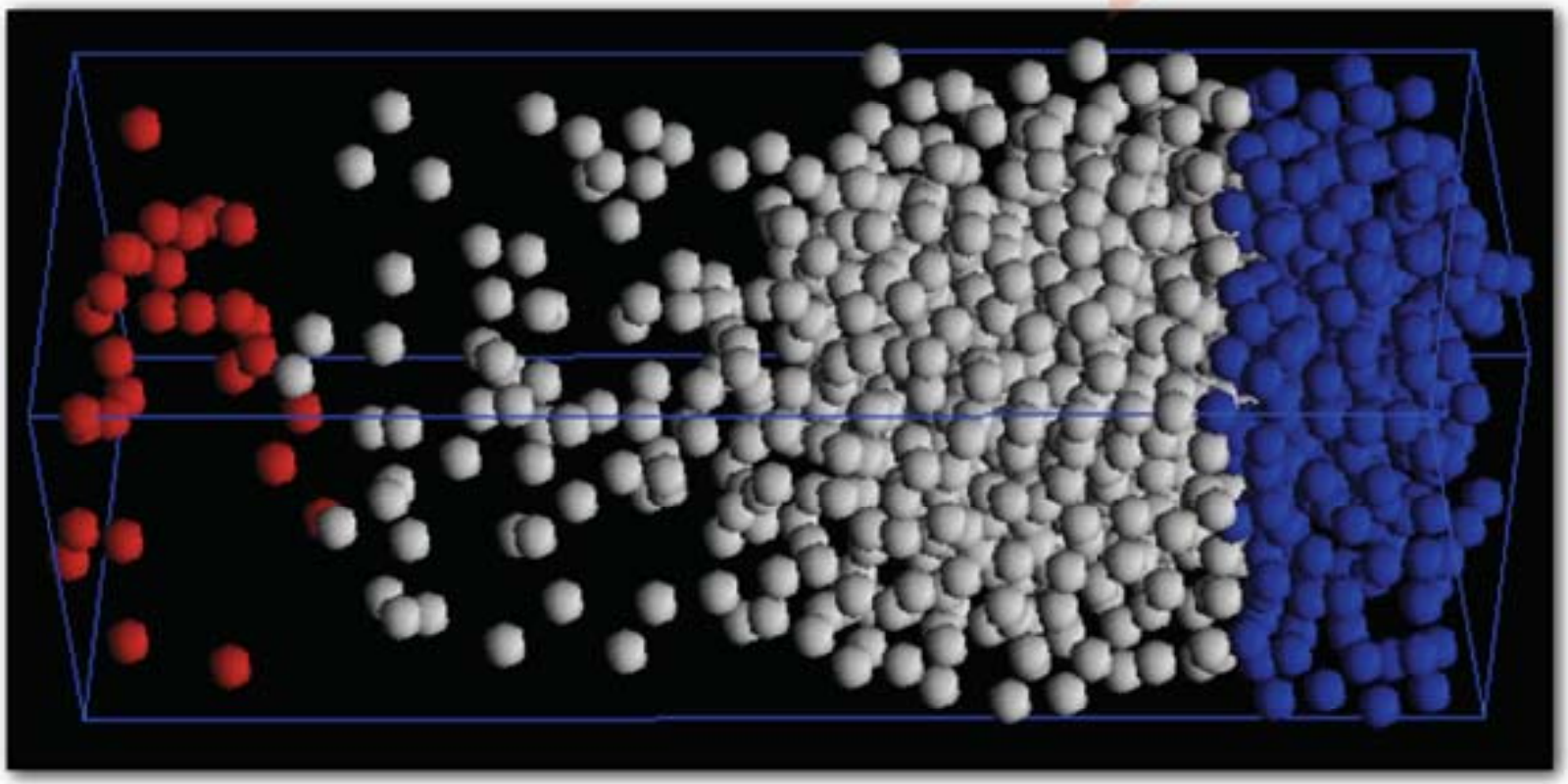


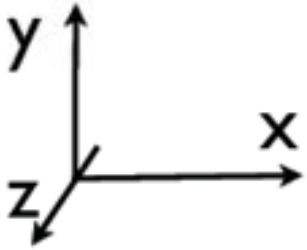
Finite thickness

heat bath
T_H

heat flux

heat bath
T_L

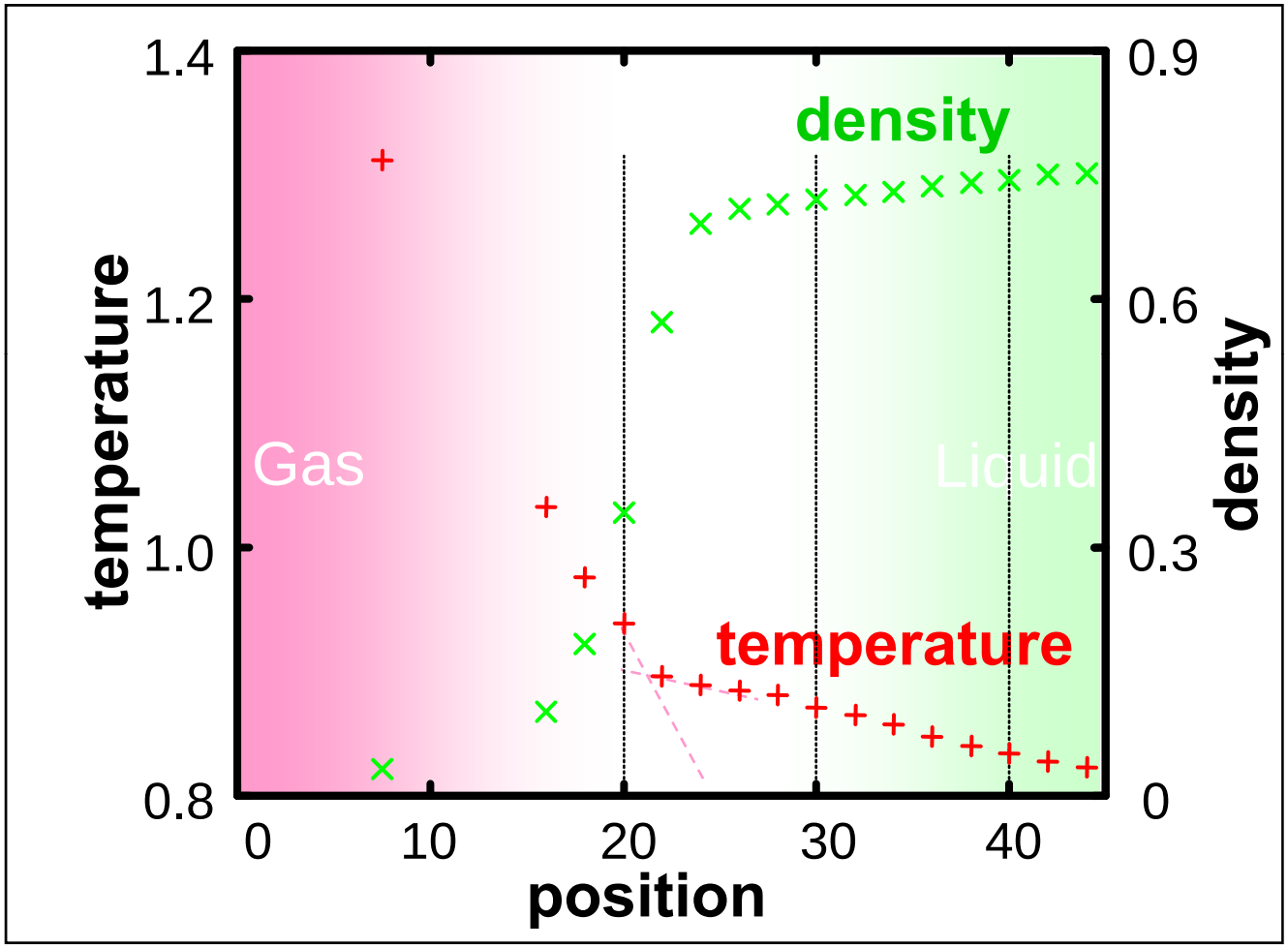




3D system $L_x \times L_y \times L_z$
Nosé-Hoover heat bath
local cell

Avogadro Challenge Project

Temperature and Density

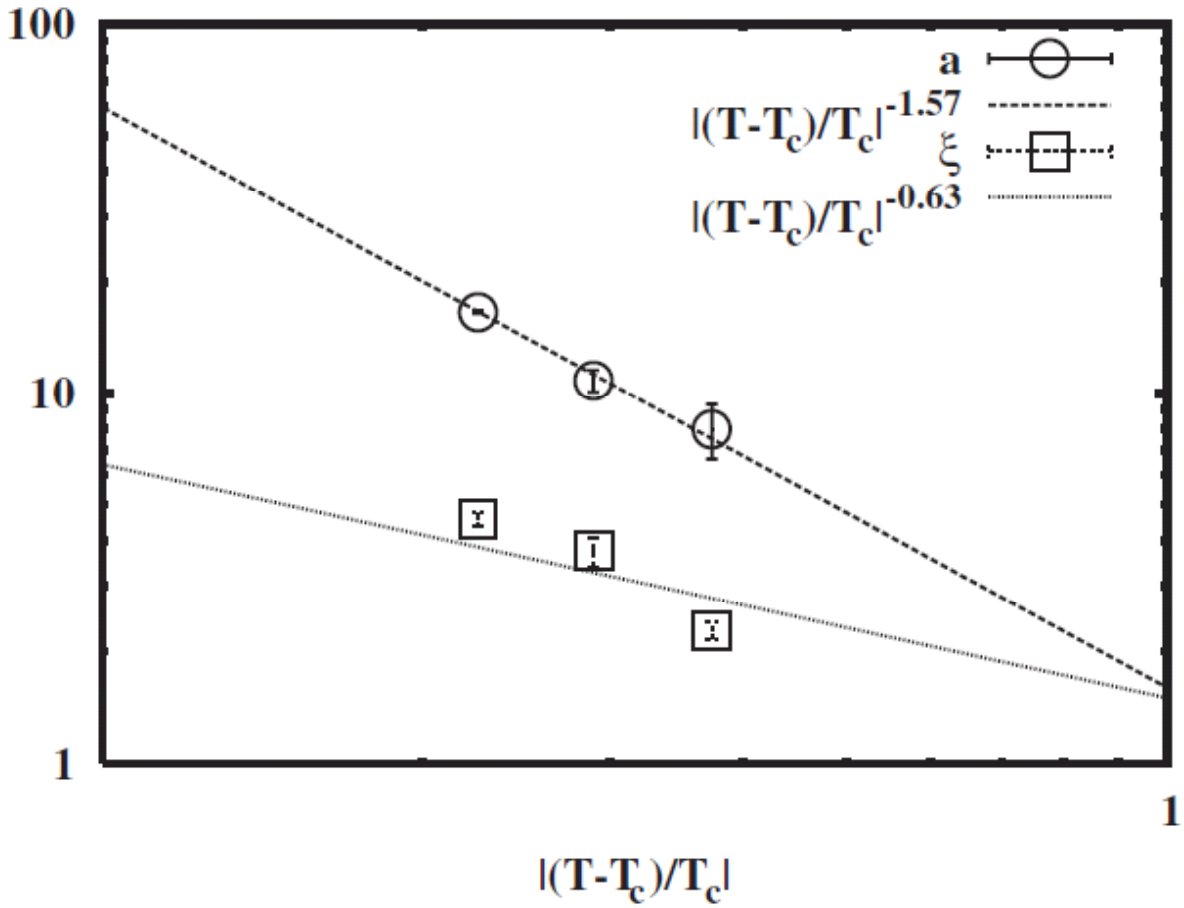


ρ0.323
L_x 60
T_L 1.32
T_H 0.8

F. Ogushi, S. Yukawa and N. Ito, J. Phys. Soc. Jpn. 75 (2006) 073001.

Avogadro Challenge Project

Critical behavior



$$\xi \sim |(T - T_c)/T_c|^{-\nu}$$

$$a \sim |(T - T_c)/T_c|^{-(3\nu-\beta)}$$

Ising universality class

F. Ogushi, S. Yukawa and N. Ito, J. Phys. Soc. Jpn. 75 (2006) 073001.

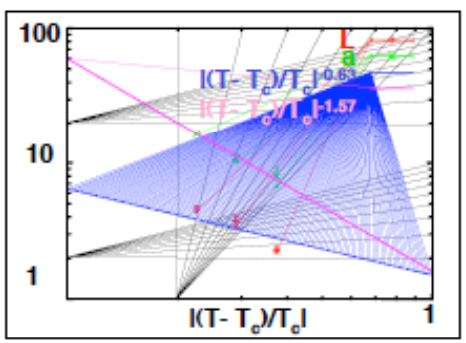
nucleation theory

classical nucleation theory

density functional theory

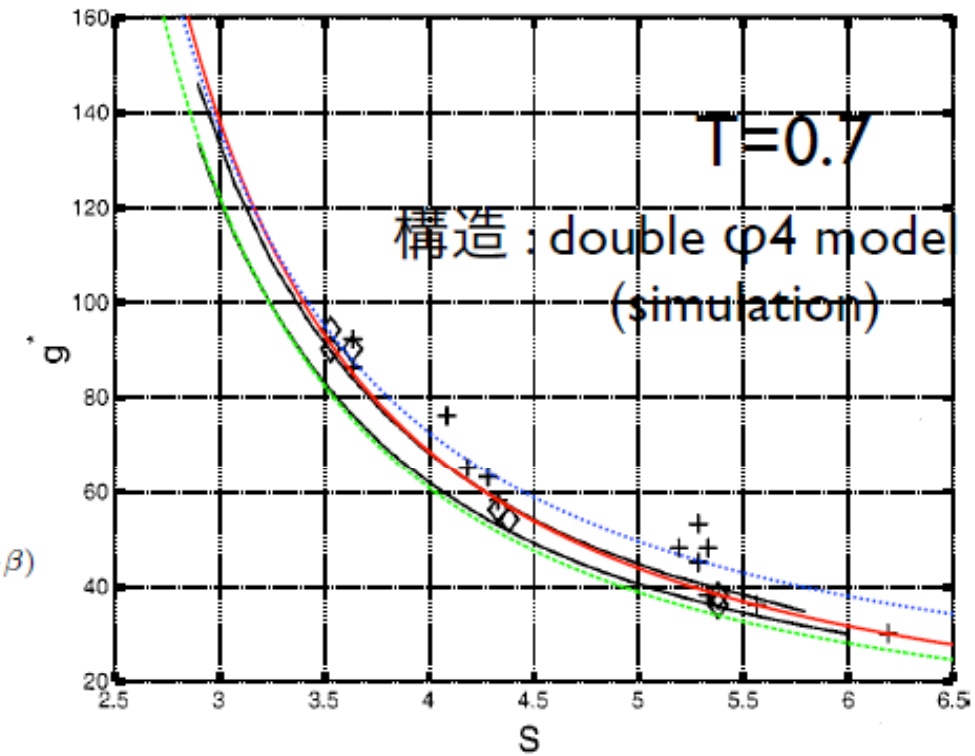
double φ4 model

$$f_{g,l}[\rho] = \frac{1}{2}\frac{\Delta\rho}{\xi}\left\{1-\left(\frac{\rho-\rho_0}{\Delta\rho}\frac{\xi}{\xi_{g,l}}\right)^2\right\}^2$$



$$\xi \sim \left|\frac{T-T_c}{T_c}\right|^{-\nu}$$

$$a \sim \left|\frac{T-T_c}{T_c}\right|^{-(3\nu-\beta)}$$



g^*: number of particles in critical nucleus

2,592,000 LJ particles

$T_h = 1.1$

(around the critical temperature)

$T_l = 0.7$

(low temperature within the lipuid phase)

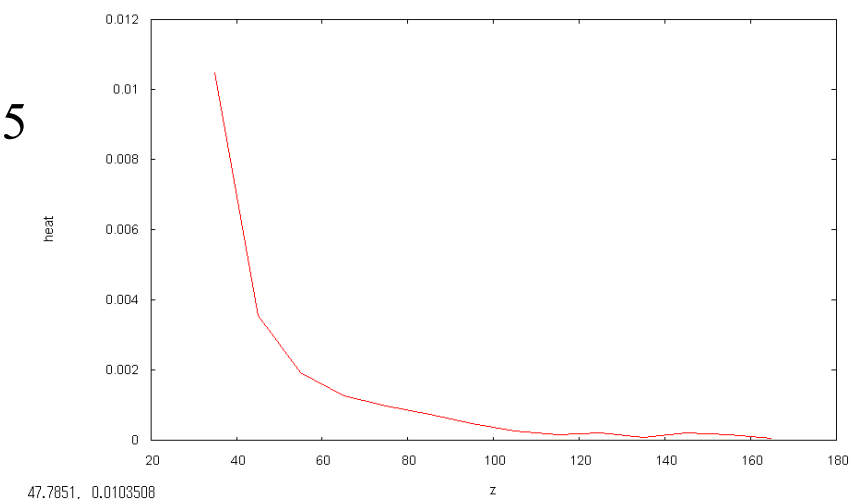
average density

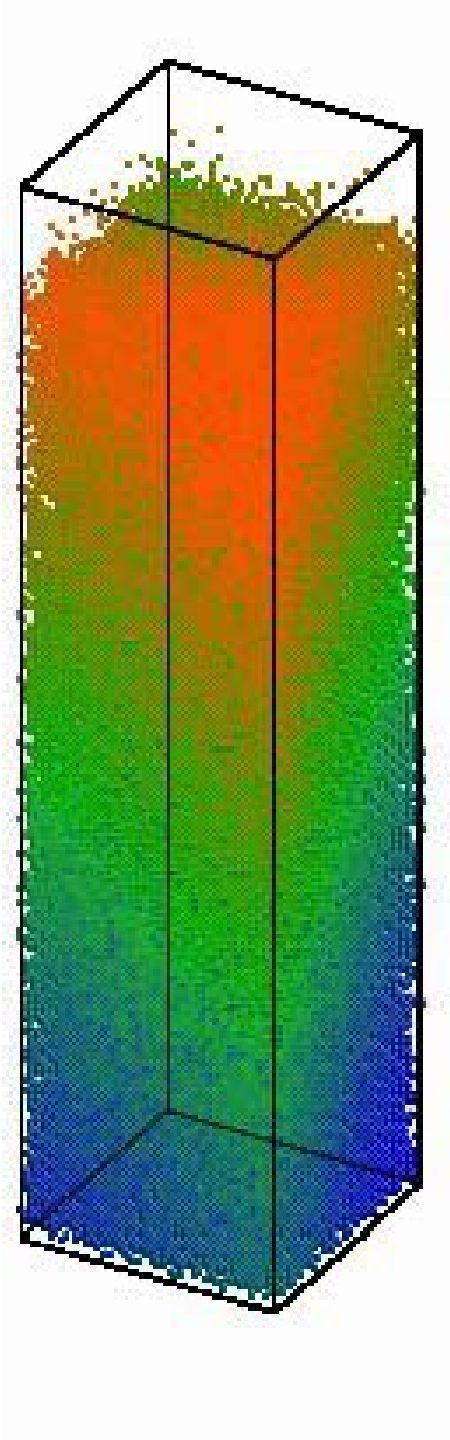
$\rho = 0.35 \sim \rho = 0.4$

aspect ratio

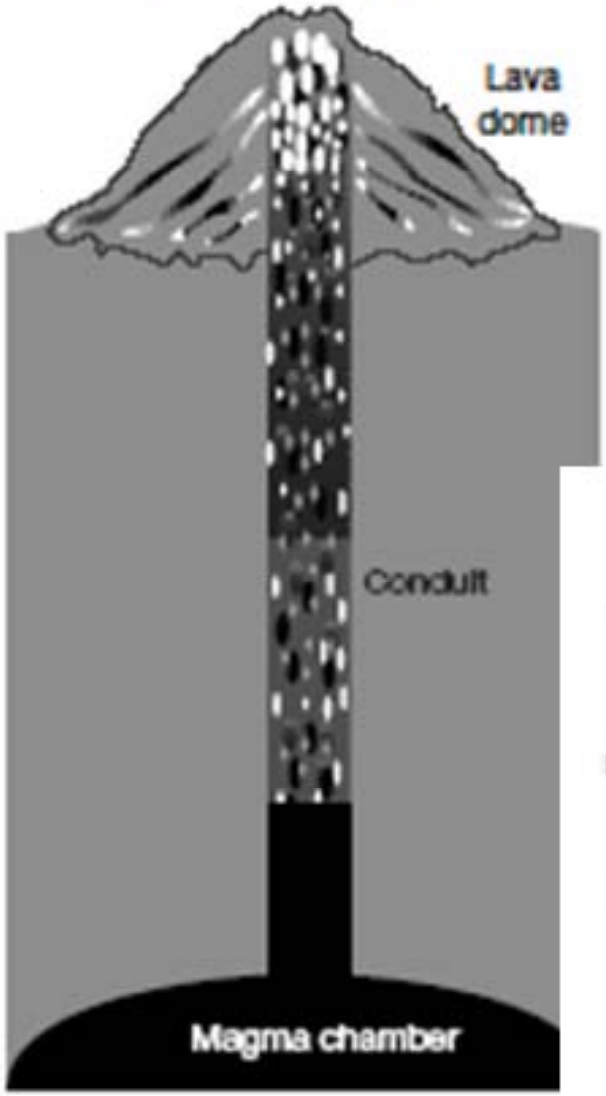
$L_z / L_x = 4 \sim L_z / L_x = 5$

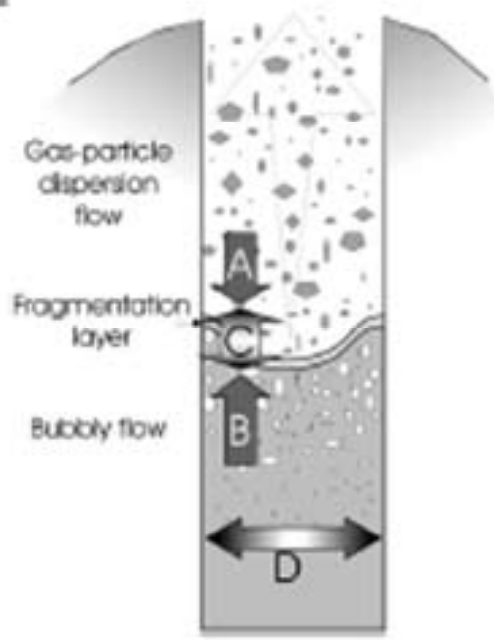
Heat transfer from the wall





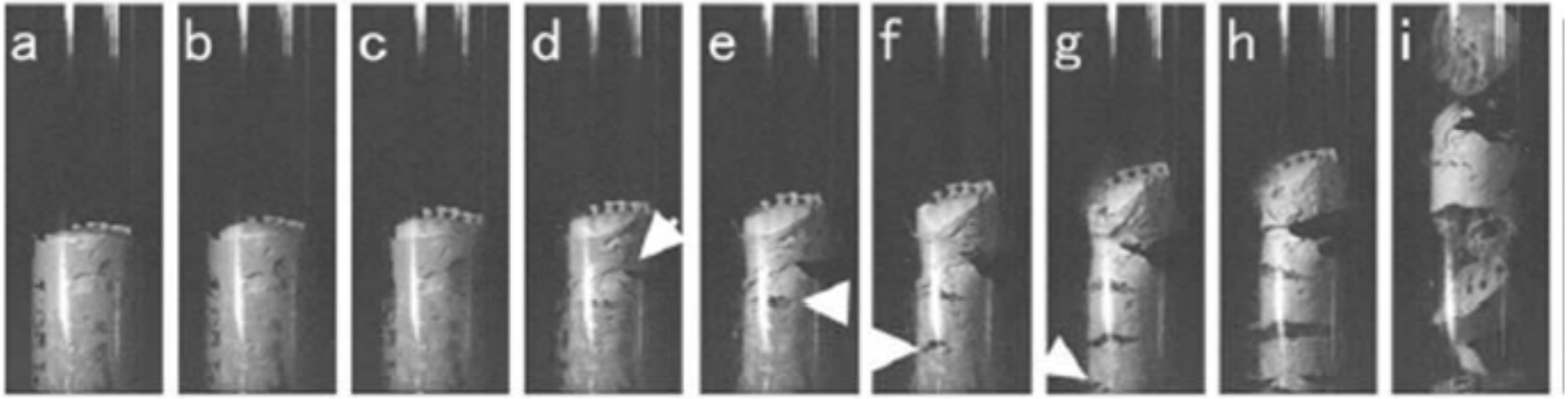
Another example:
Eruption dynamics of volcano



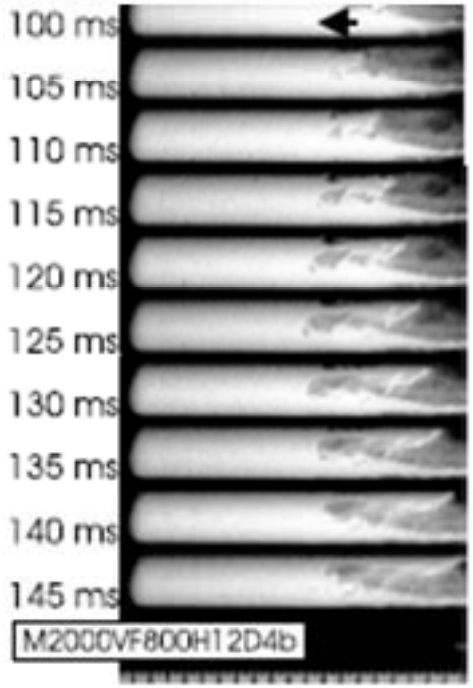


Vulcanian eruption

Experiment with shock tube

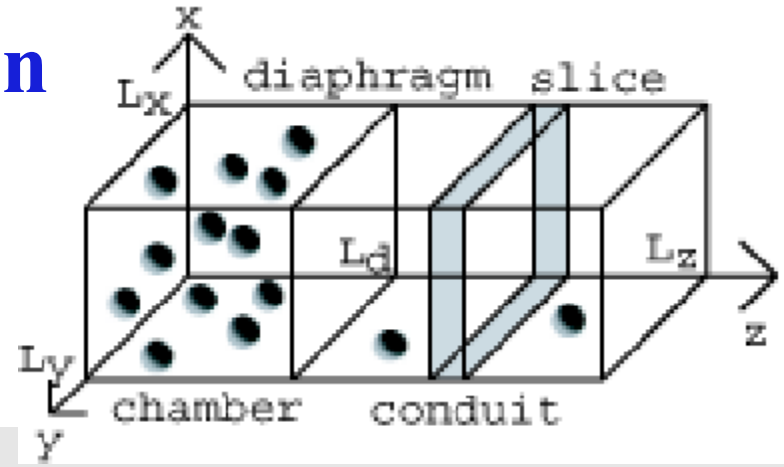


粘弾性体

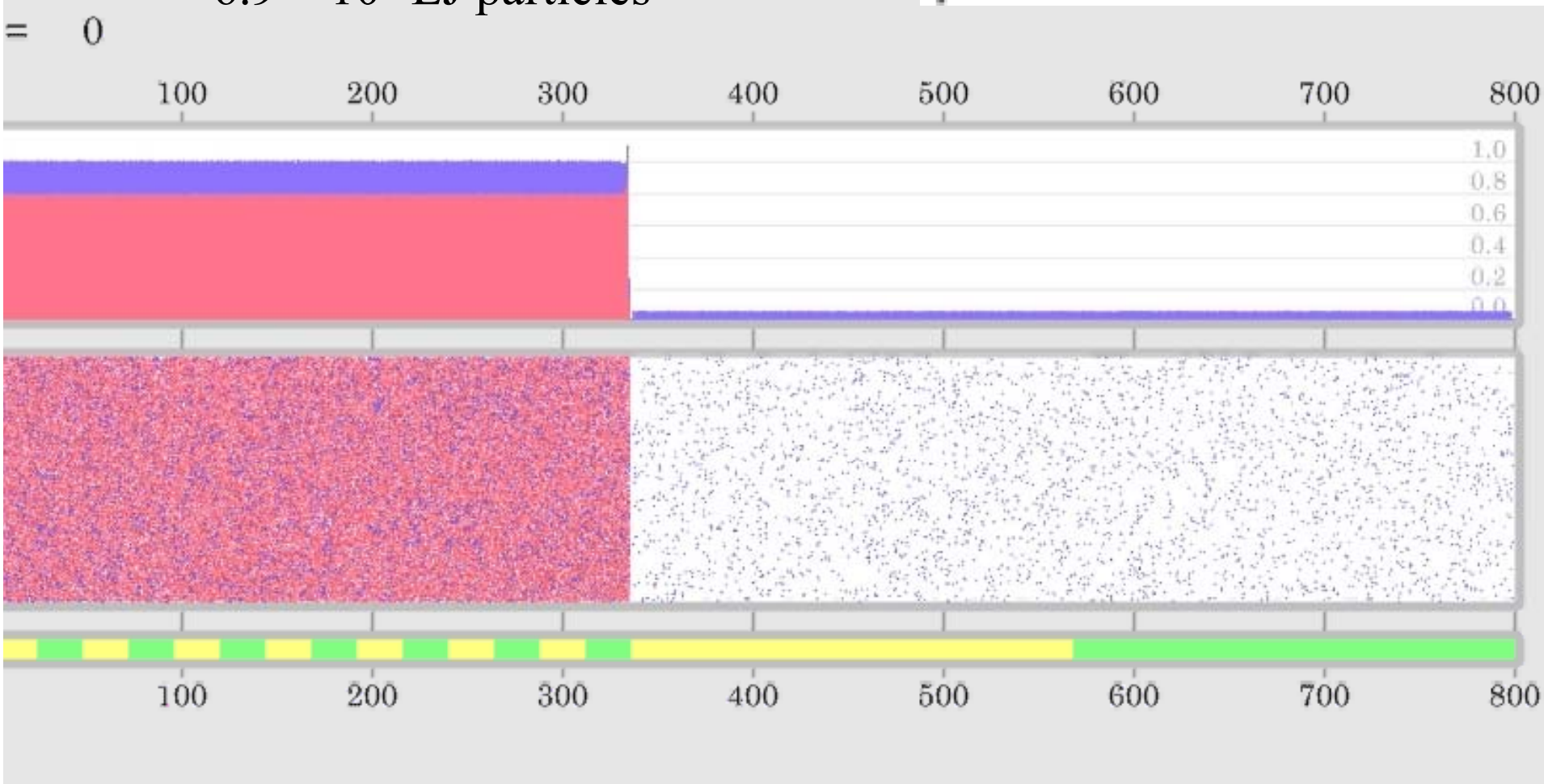


粉体

Molecular dynamics simulation of eruption

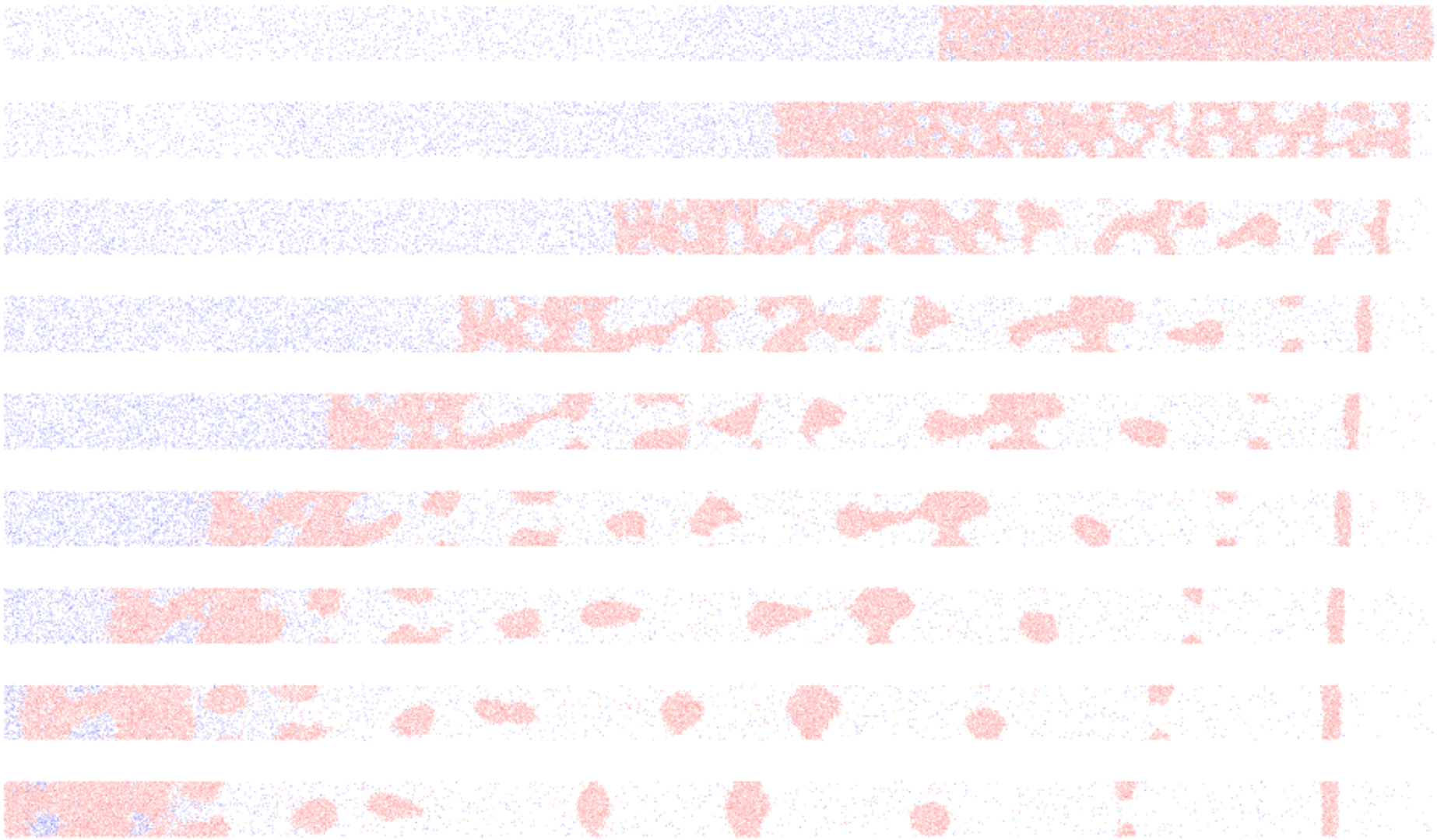


6.9×10^6 LJ particles

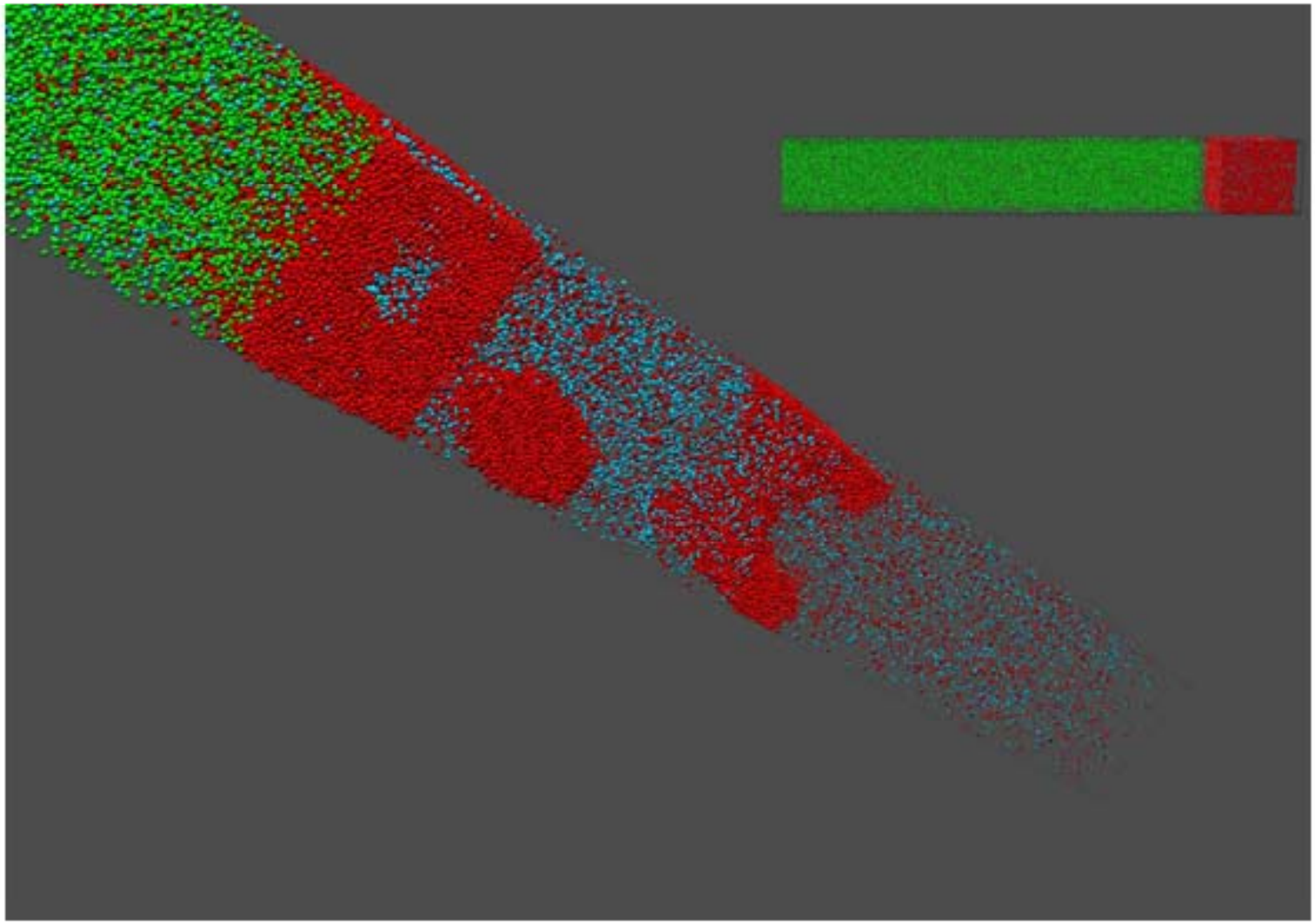


One slice

system size 40x40x1024(magma chamber 40x40x240)
totally 509,440 particles(chamber 384,000 including 10% gas particles, vent 125,440)
temperature: 2 in chamber, 0.8 in vent

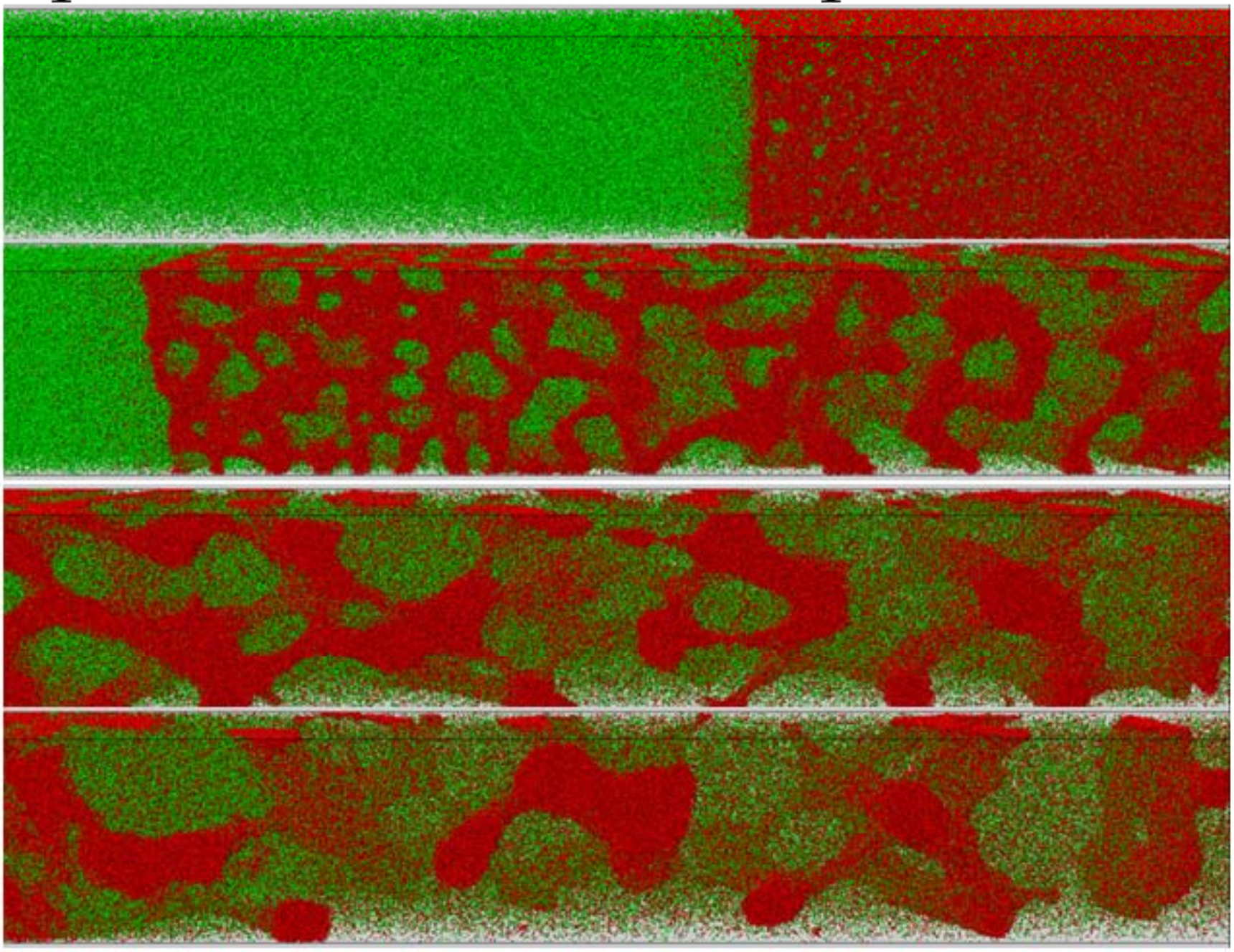


Eruption with 1.8×10^5 particles



大きさ 40x40x704(40) 57600マグマ粒子(赤)＋6400ガス粒子(青)＋112000ガス粒子(緑)
初期数密度：1, 0.1、初期温度：2, 0.8

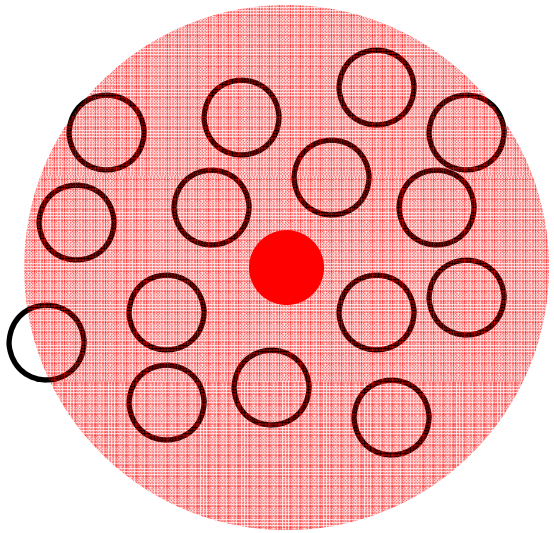
Eruption with ~4,800,000 particles



3D Lennard-Jones MD

Force Calculation

- 50% Cost of the whole computation
- 30 to 40 operations for 1 pair
- Density 0.5, Cutoff 2.5 sigma gives
  30 interacting par / particle
- 1000 to 1500 operations / particle updates

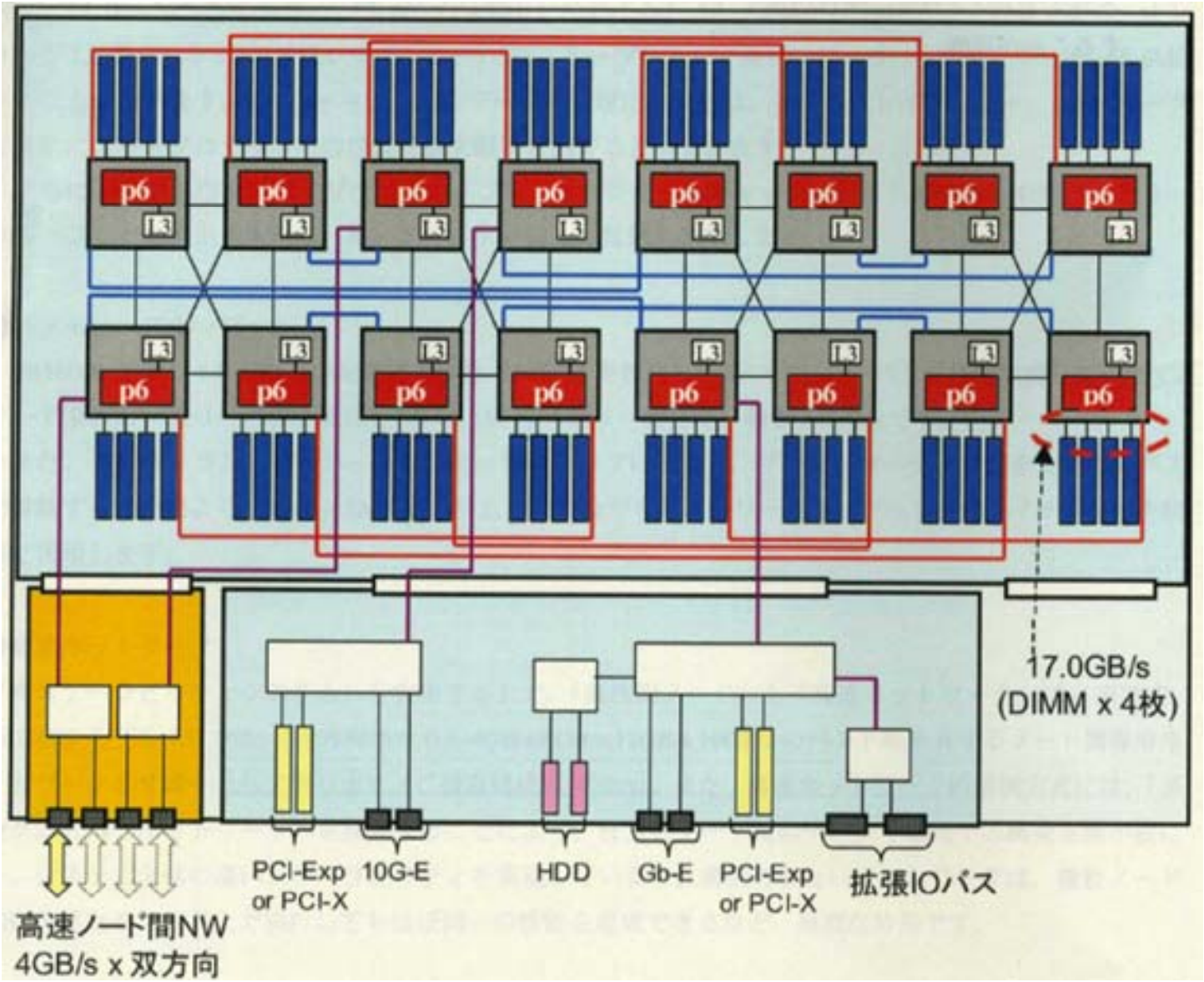


Construct Pair list

- 50% Cost

→ 1500 to 2000 operations / particle

Each node of ACP1(SR16000/POWER 575)



Theoretical Peak Performance

If we have X GFLOPS machine,

X / 2000 gives about 0.5 MUPS

MUPS (Million Particle Update Per Second)

Examples

0.5G ($793^3 \sim 1\mu m^3$) Particles Update Per Second on 1 TFLOPS

0.5T ($7937^3 \sim 10\mu m^3$) Particles Update Per Second on 1 PFLOPS

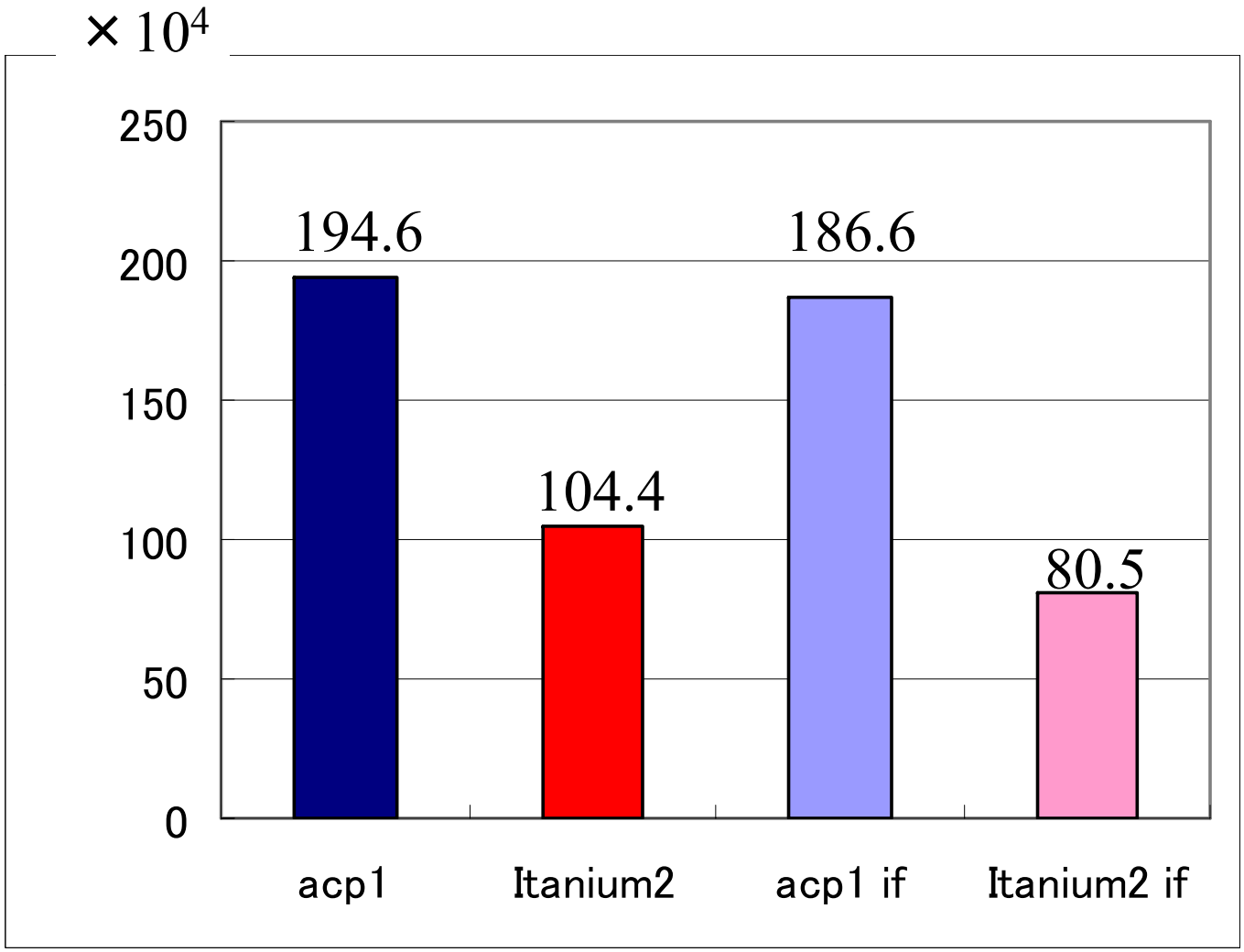
memory-core balance:

assumption

1 particle ～100 byte, 10 update per second

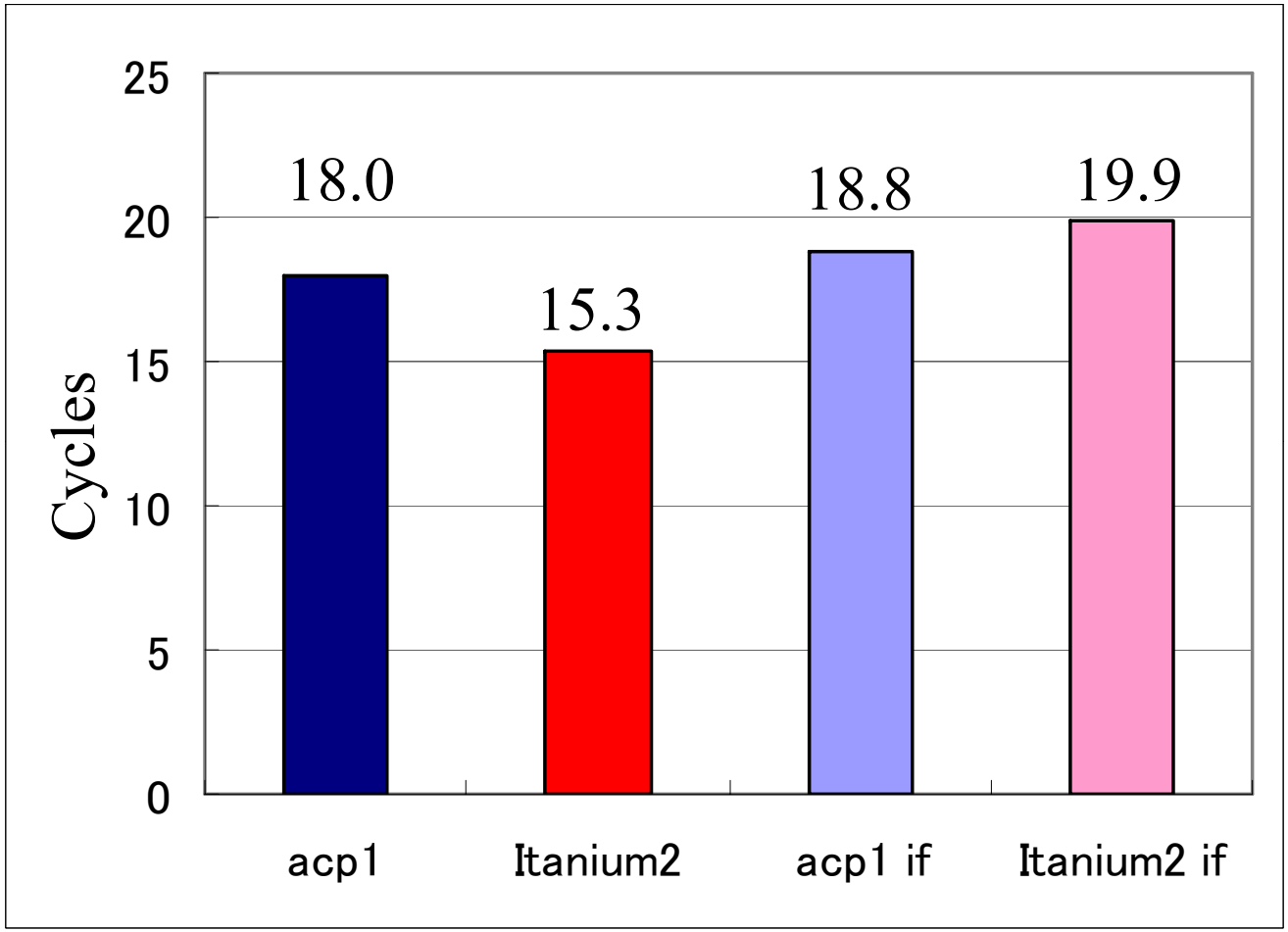
→ 100 B × 0.5 MUPS/GFLOPS /10 = 5 MB /GFLOPS

Result (with optimization)



Performance is proportional to frequency

Result (with optimization)



Add/Sub 12 + Mul 14 + Div 1 = 27

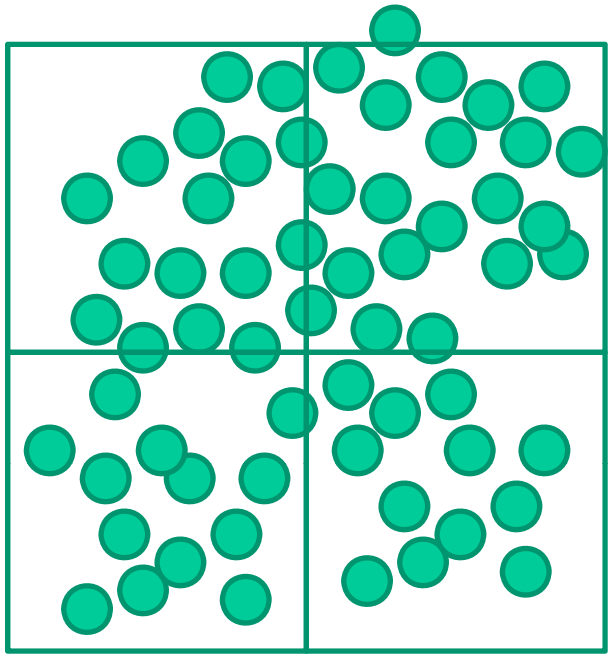
27 / (18*4) = 0.375

37.5% to its Peak Performance

Parallelized MD (1/2)

Multi-thread MD

Space division strategy
Generally, the cost for communication is almost negligible with high enough density.



Two kinds of communication

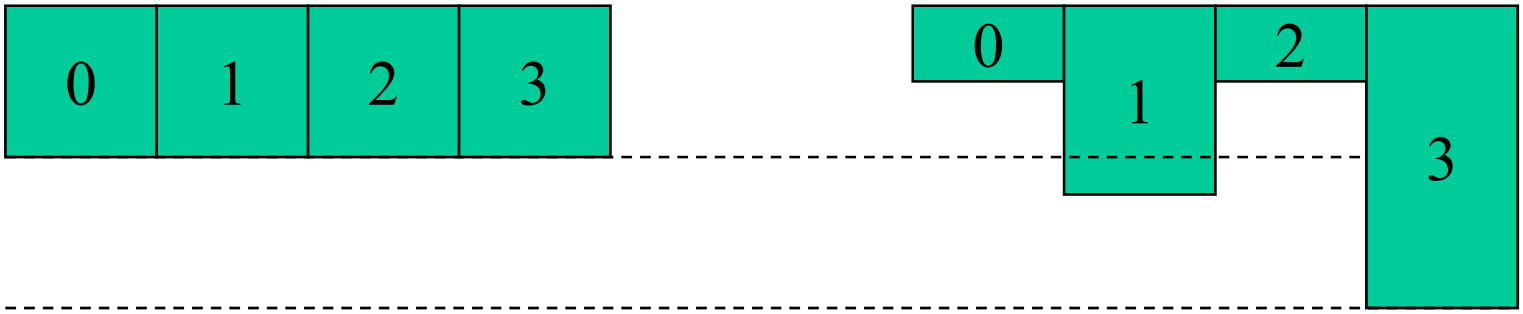
Exchanging particles

Exchanging information of particles on edges.

Load balance (1/2)

Simple division may cause unbalance load.

Computational time for each threads



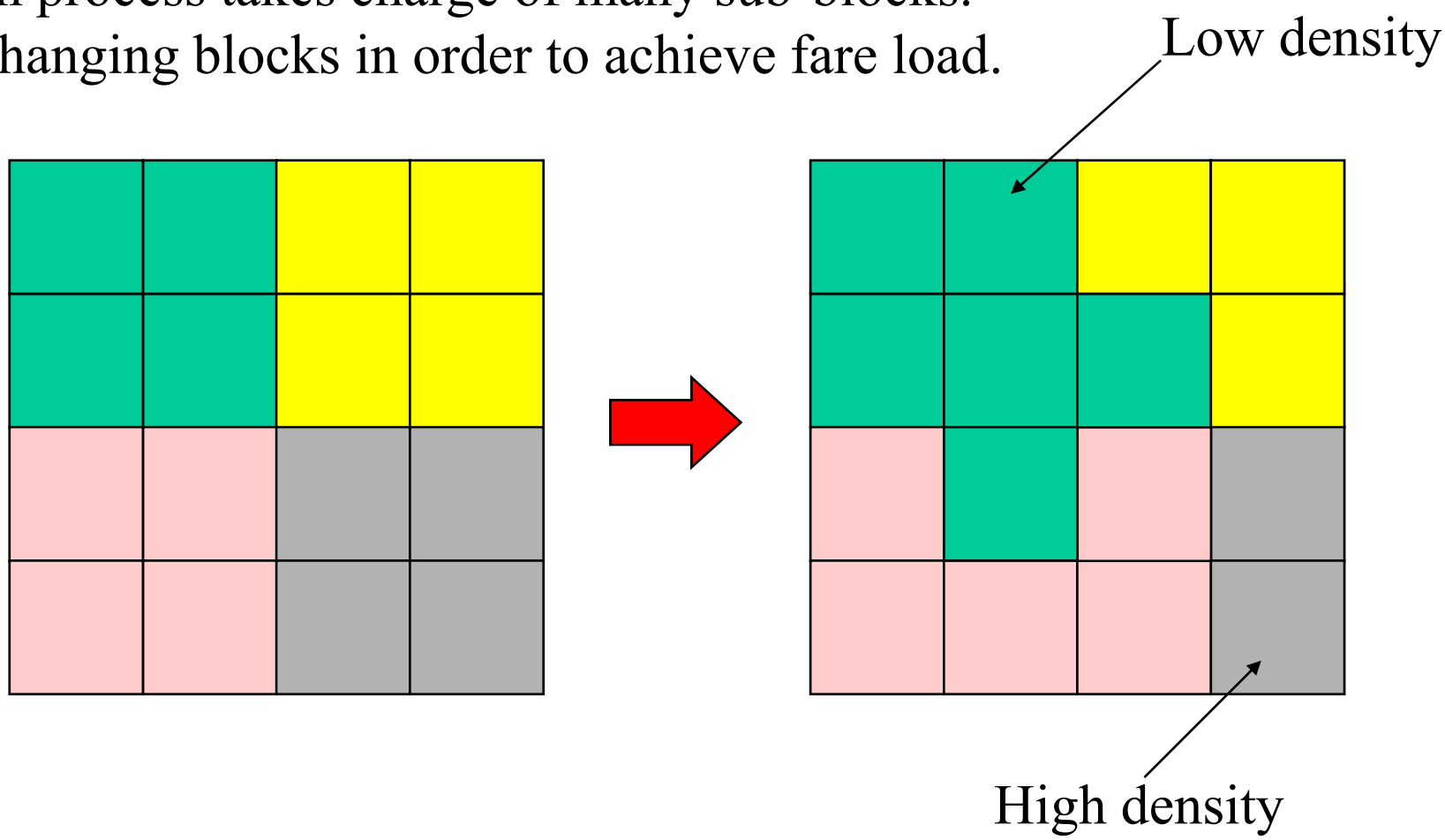
The slowest process determines the total speed.

Optimization for load balance is necessary

Load balance (1/2)

Sub-block division

Each process takes charge of many sub-blocks.
Exchanging blocks in order to achieve fare load.



Toward EFLOPS
(10^{18} arithmetics per second)

Macroscopic constraints:

maximum 1024 nodes → 1PFLOPS per node

1 node contains at most 32 boards → 32TFLOPS per board

1 board contains at most 256～1024 cores

→ 32～128GFLOPS per CPU

Millions of cores!

From demand for system reliability and latency,

minimize the number of chips

Statistical mechanics modellings fit very well!

Architecture of EFLOPS computer in 2015～2020

― *a proposal* ―

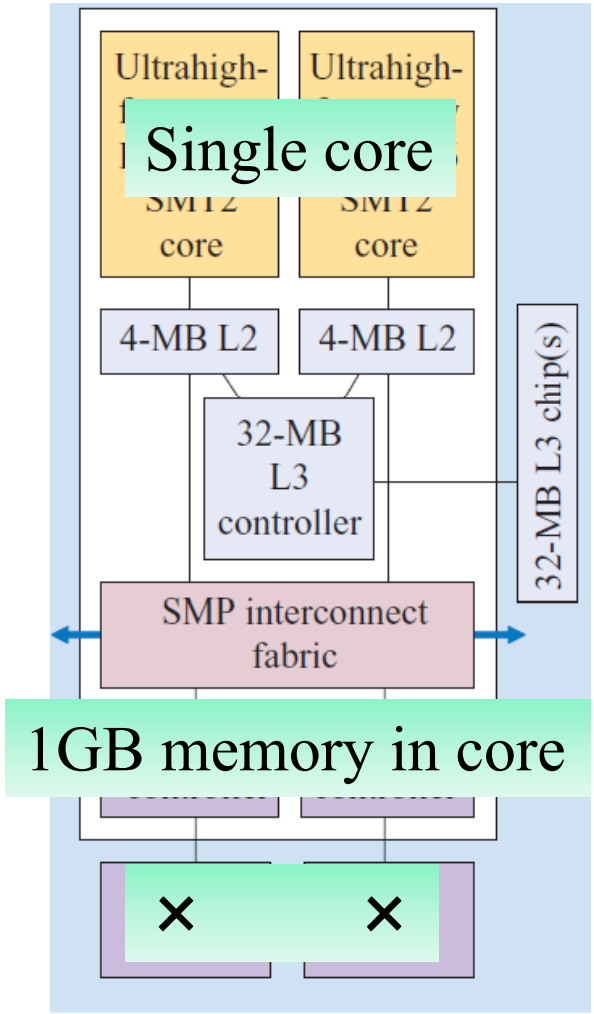
Present(2007)

billion gates, 5GHz

40GFLOPS with two cores

→ tens billiongates,10GHz

1TFLOPS with 16 cores



severe bottleneck

in memory bandwidth and latency

and cooling

instead,

One 64GFLOPS core

with 1GB memory on chip

and CDM architecture

von Neumann Bottleneck, again and again …

- Bottleneck is data bandwidth between CPU core and memory.
- Memory-FLOPS balance(simple PD simulation)

5 MB /GFLOPS

1 particle(50B) per KFLOPS

or 1.5GB per 32GFLOPS core

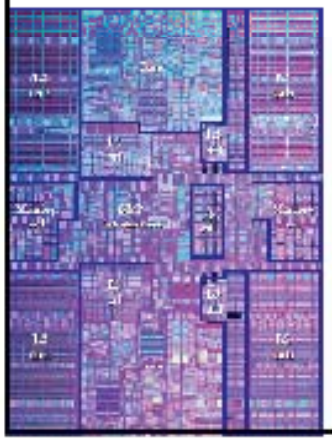
→ ***Put core(64GFLOPS) in memory(as L1 cache, 320MB)***

CDM(Core dilution in memory-cell) Architecture

- **high memory bandwidth**
- **high reliability**
- **less heat per die area(less cooling load)**

CDM
core dilution in memory

2015～2020：
64GFLOPS core in 1GB memory
with CDM architecture



Let's celebrate bicentenary!

- [Poisson bracket(1809)]
- Avogadro's law (1811)

  [Jean Baptiste Perrin (1909)]

il Conte Lorenzo Romano Amedeo Carlo Avogadro di Quaregna e Cerreto (1776 Aug. 9 – 1856 July 9) the first mathematical physics professor in Italia

- Fourier's law (1812)

Jean Baptiste Joseph Fourier, Baron de (1768 Mar. 21 – 1830 May 16)

Avogadro Challenge Project