Large-scale simulations with particles — From self-gravitating systems to continuum mechanics

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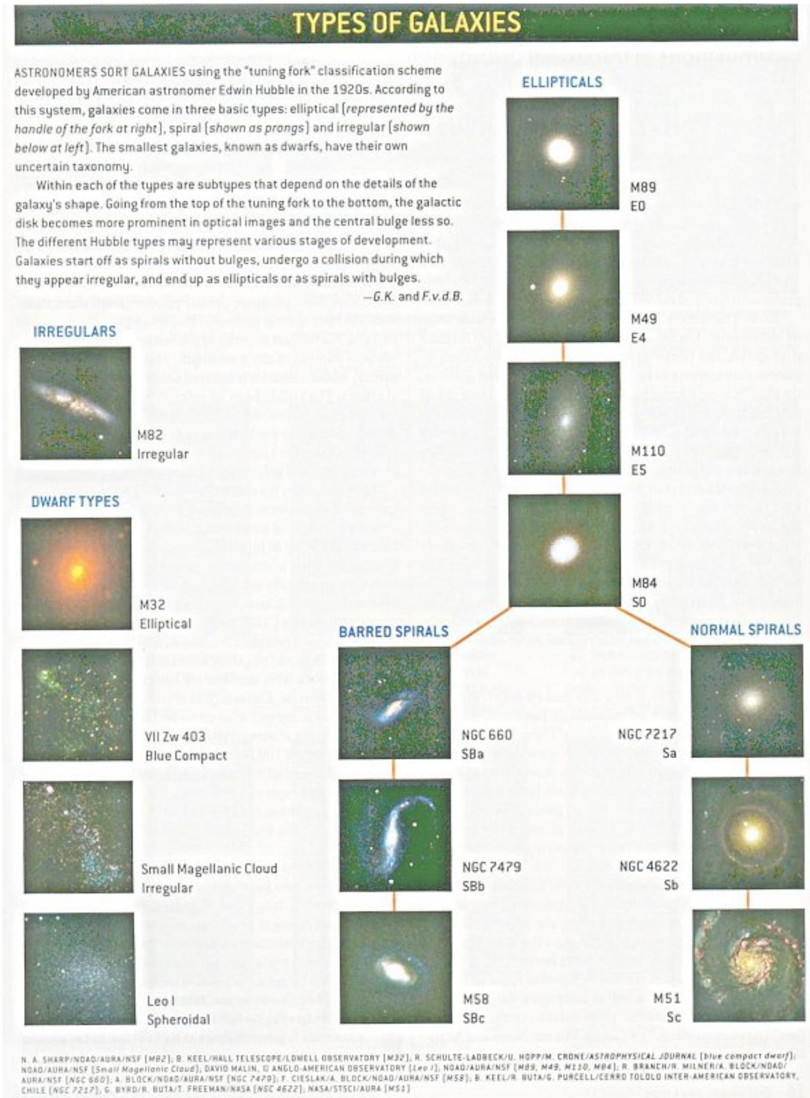
Talk Structure

- **Galaxy formation and the origin of the spiral structure**
- **Numerical Schemes**
  - **Domain Decomposition and Parallelization**
  - **Time Domain**
- **Particle-Based Hydrodynamics (mainly SPH)**
  - **Formulation of "Standard" SPH**
  - **Discontinuity**
  - **Solution**
  - **Other problems**

Simulation of galaxy formation



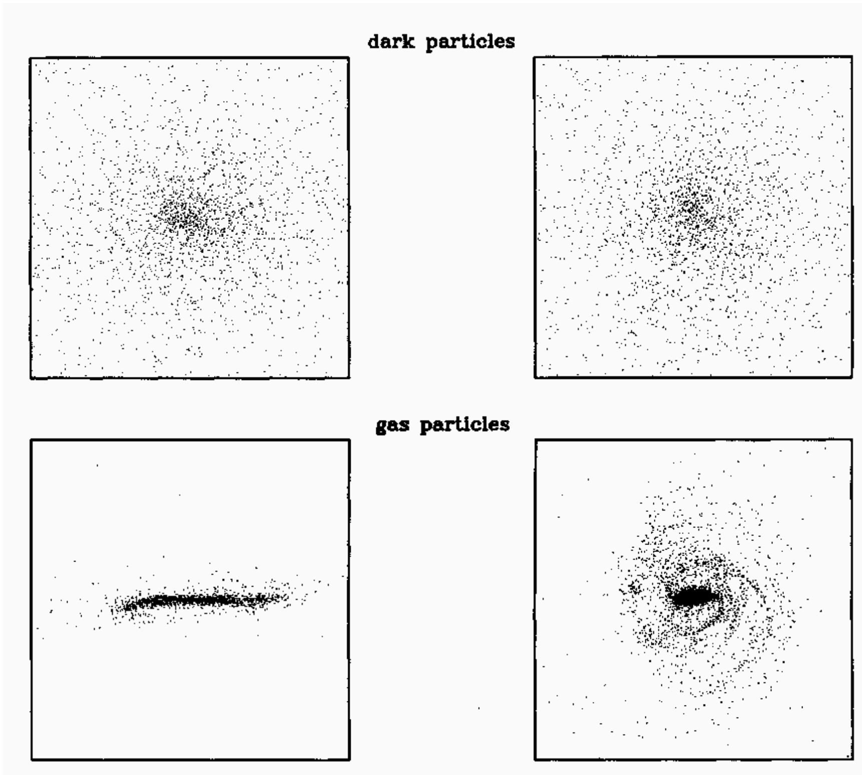
Basic Idea:

- "Holistic" simulation of galaxy, from initial density fluctuation
- To understand the origin of the variety of galaxies

Equations to solve

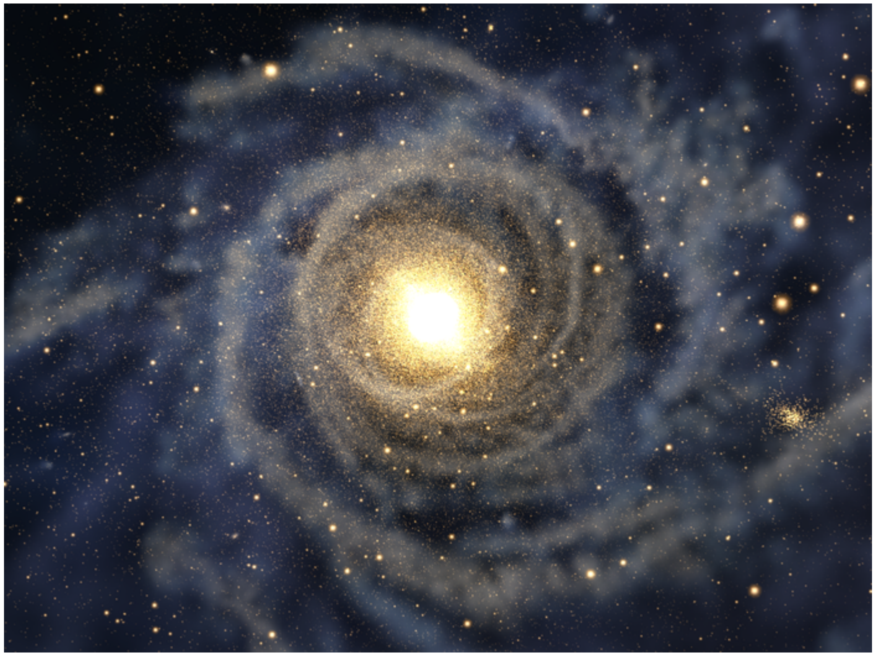
- **Newtonian spacetime + Cosmic expansion (Dark energy)**
- **dark matter particles: Newtonian gravity**
- **gas: hydrodynamics, gravity, radiation (cooling), star formation**
- **stars: gravity, radiation, Supernova explosion**

Katz and Gunn 1992



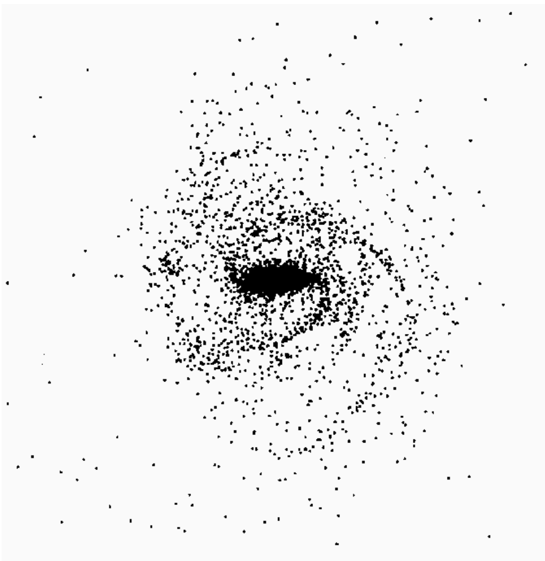
- Dark Matter + gas + stars
- DM, star: particles
  gas :SPH particles
- 10^4 particles, Cray YMP 500-1000 hours
- mass resolution : 10^7 solar mass

Saitoh et al. 2005



- Dark Matter + gas + stars
- DM, stars: particles gas:SPH particles
- 2×10^6 particles, GRAPE-5 $\sim$ 1 year
- mass resolution : 10^4 solar mass

What gain from improved resolution?



- Not much?
- Important things: improved parametrization of “micro-physics”, such as star formation mechanism, energy input from supernovae.

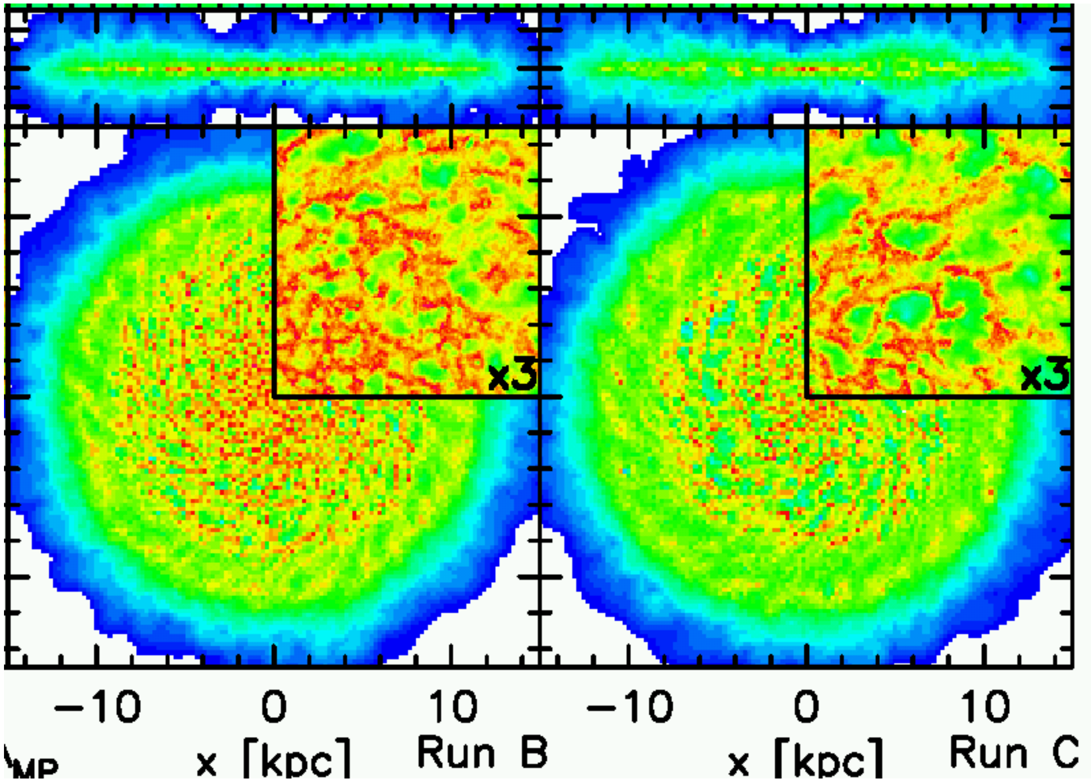
Modeling star formation

- Minimum need for star formation modeling: : 10^{-4} solar mass
- What we can do now: : 10^3 solar mass (10^7 times too large)
- Need some way to form stars
  - Usual model: if interstellar gas is dense and cold enough, part of it will become stars in appropriate timescale.
  - three free parameters
  - The structure of the galaxy depends on these parameters
- Similar problem on supernovae.

What resolution do we need?

- We will know when we reach there....
- If mass of SPH particles is more than that of star-forming clouds, clearly we are not doing things right.
- Theoretically, if we have sufficient resolution, we can just change all mass to stars (that is what the nature does).
- We are approaching there.
- One or two orders of magnitude more?

Saitoh et al. 2007

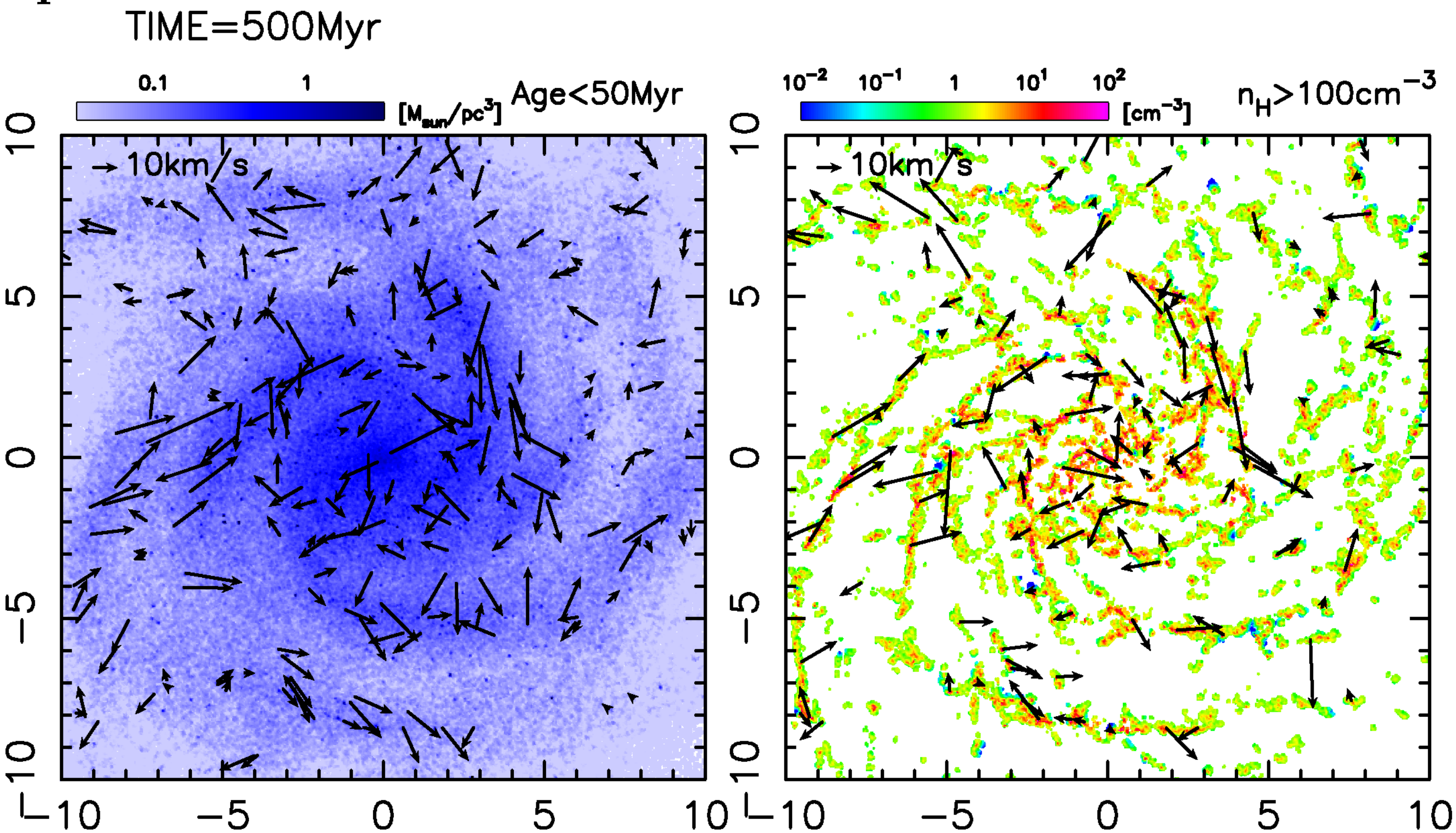


Changed the star formation timescale by a factor of 15
little difference in the result
(In low-resolution calculation, the galaxy would have exploded.)

Galactic disk

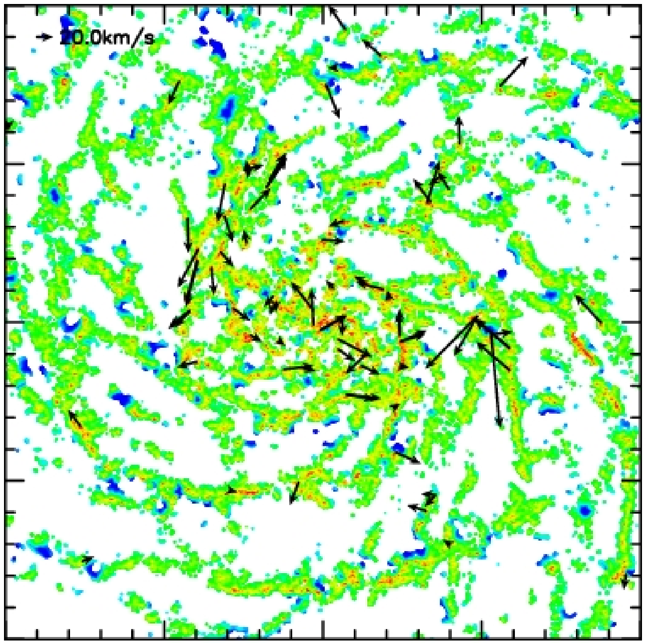
animation (Baba et al 2009) (not available in Web version)

Spiral structure and deviation from the circular motion

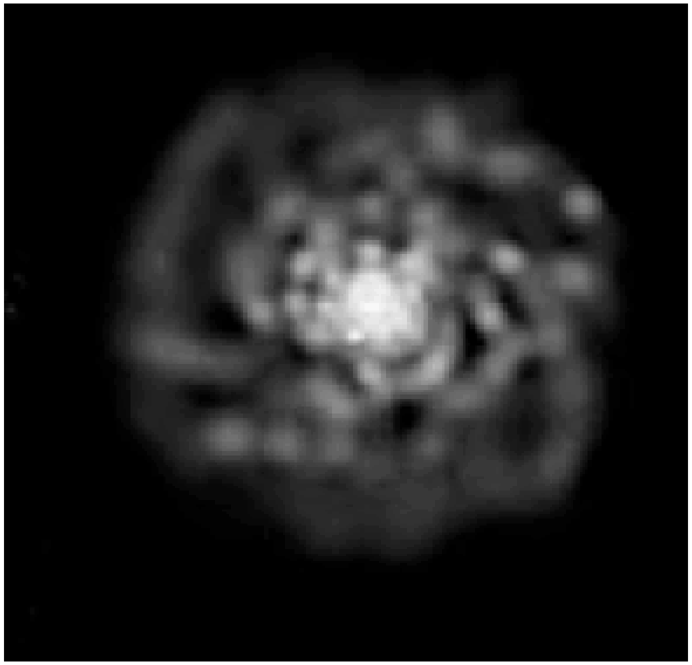


Left: distribution of stars Right: cold gas

High-resolution model and observation



Low-resolution model and observation



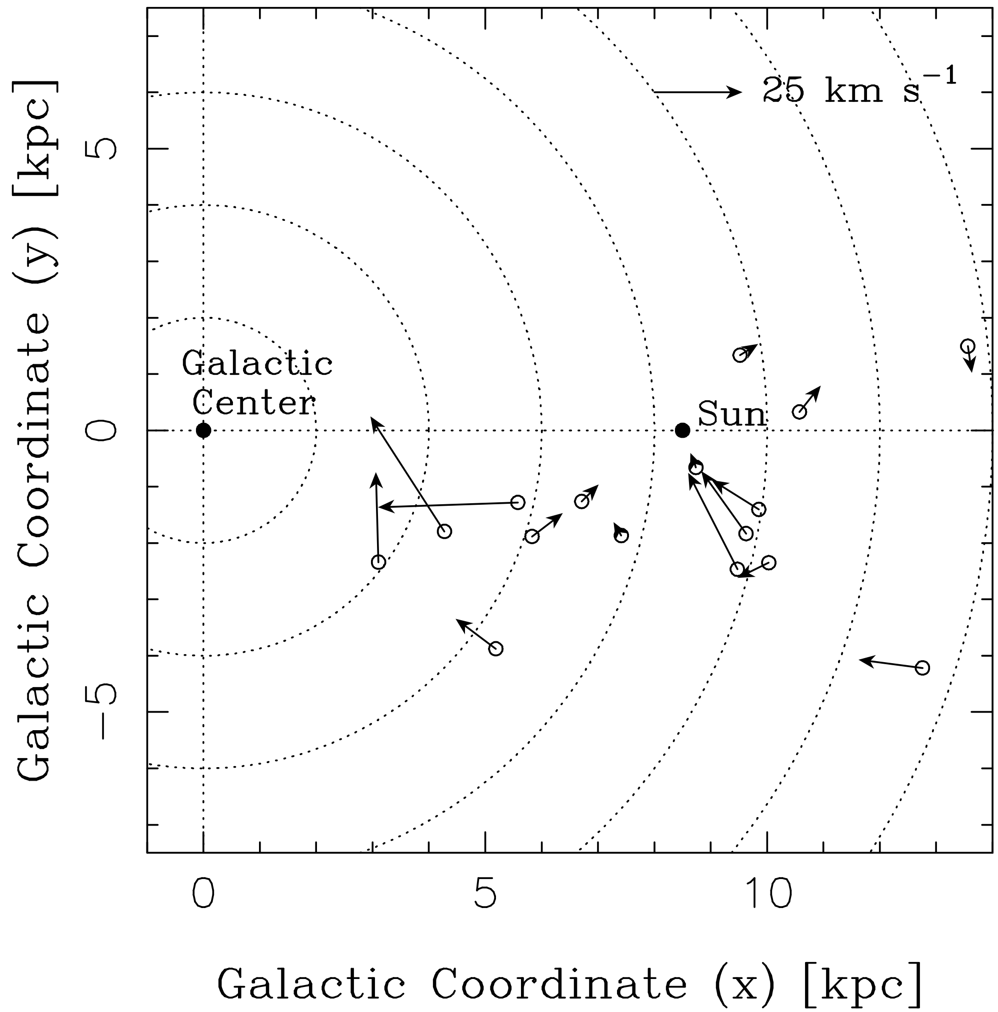
Results from high-resolution simulations

- Star-formation is regulated by large-scale dynamics.
- Observed (multi-arm) spirals can be explained by transient, but recurrent arms.
- These results are robust. Independent of assumption on microphysics such as star-formation timescale.

Observation of Milkyway spiral arms (VLBI)

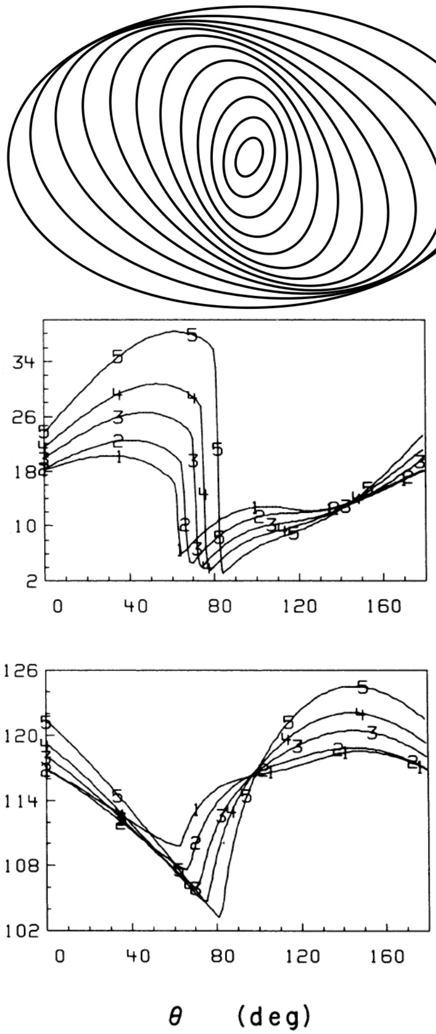
- **Large non-circular motion ($\sim$ 30km/s)**
- **Many data points shows inward motion and counter rotation**
- **Some signs of spacial correlation?**

How these motions are induced?



What you learn from textbooks

Stationary density wave

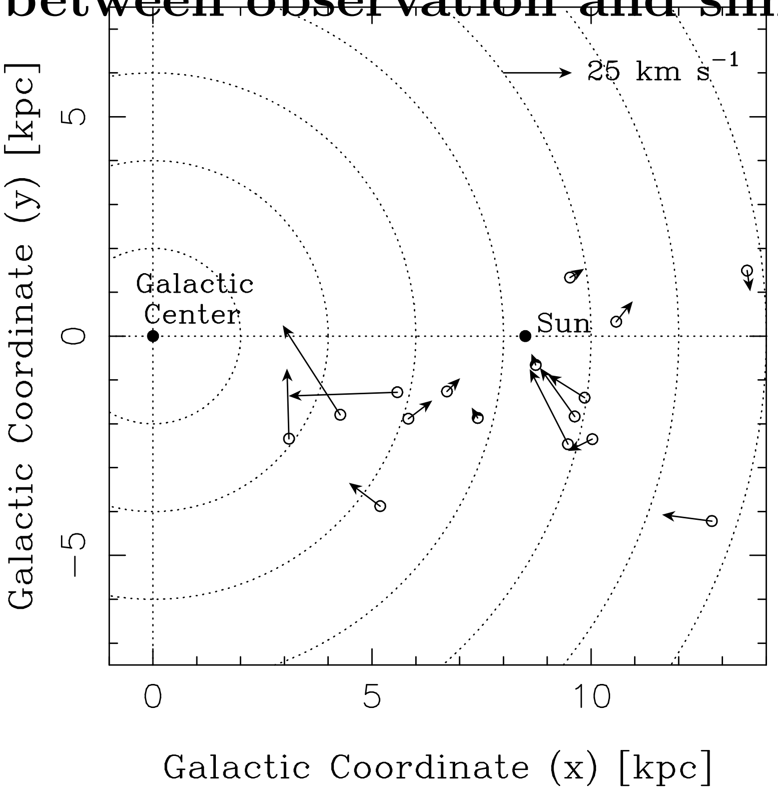


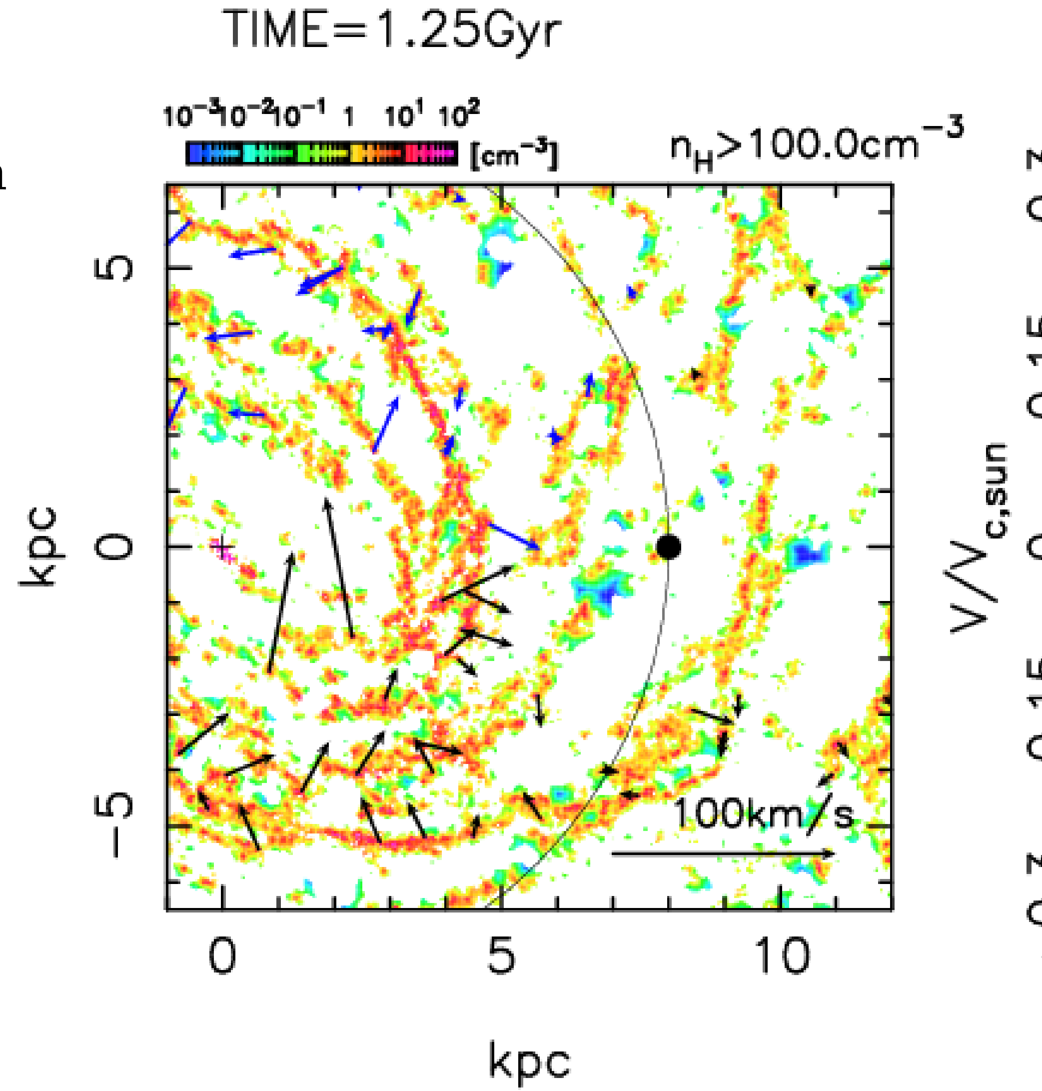
- Spiral arms are not material arms, but density waves
- gas is compressed when it passes through the bottom of the potential well, and form stars there
- It is very difficult to generate non-circular velocity > 10km/s

Quite different from both observation and simulation

Comparison

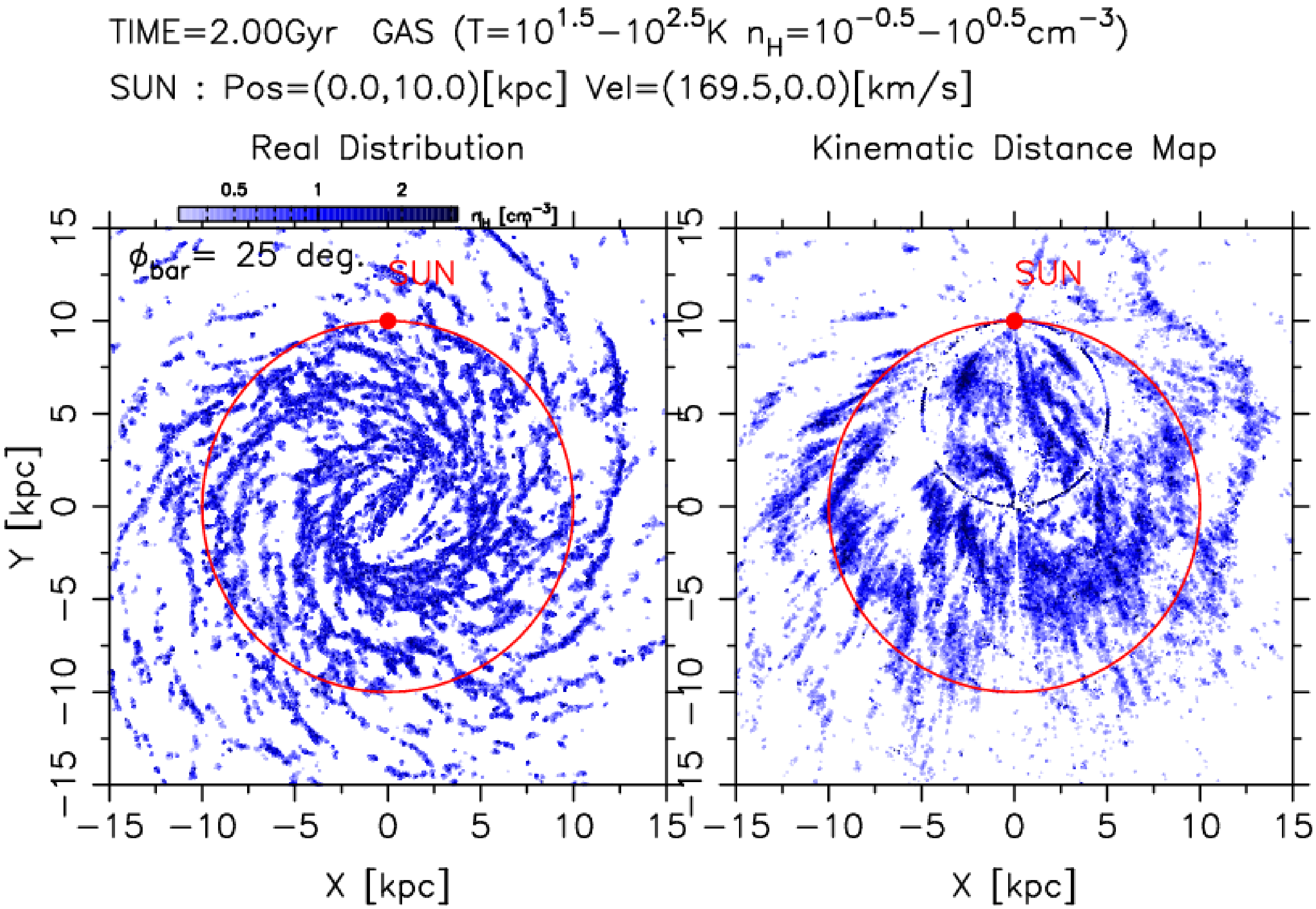
between observation and simulation





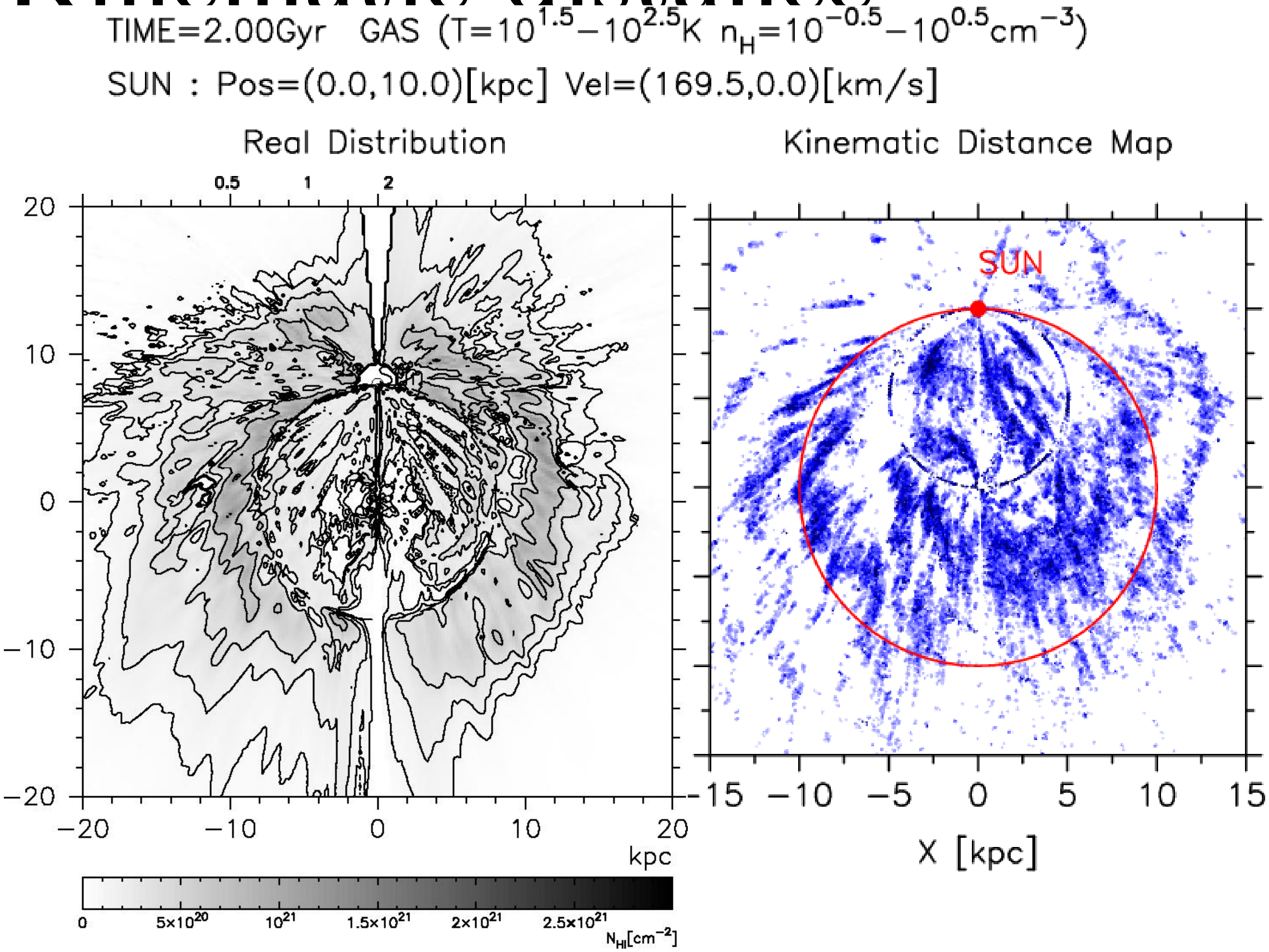
Look sort of similar?

Kinematic distance



Left: Actual distribution Right: Kinematic distance
Quite different...

Kinematic distance

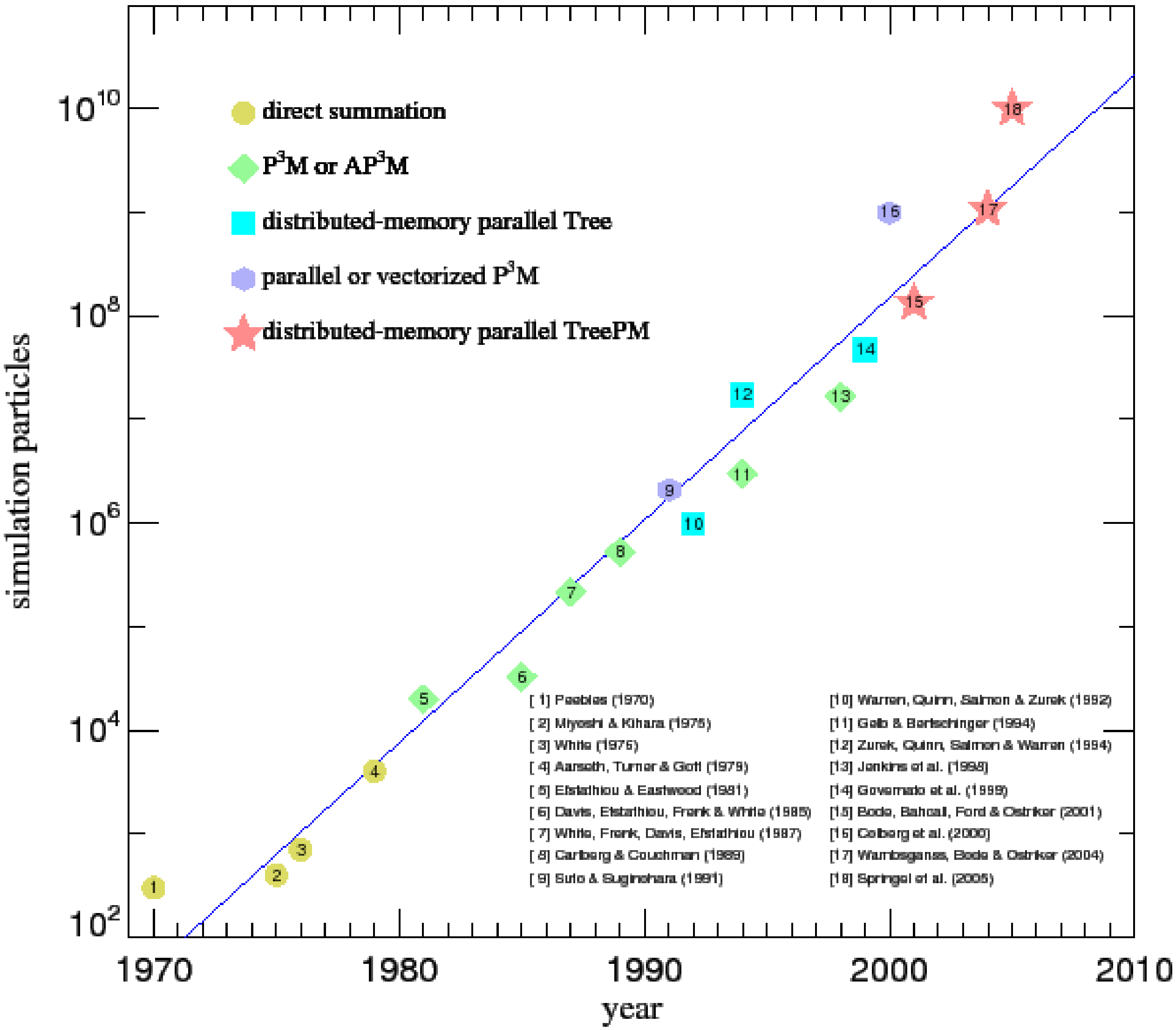


Left : HI observation (Nakanishi and Sofue 2003)
Lots of similar structures

Summary on SPH simulation of spiral arms

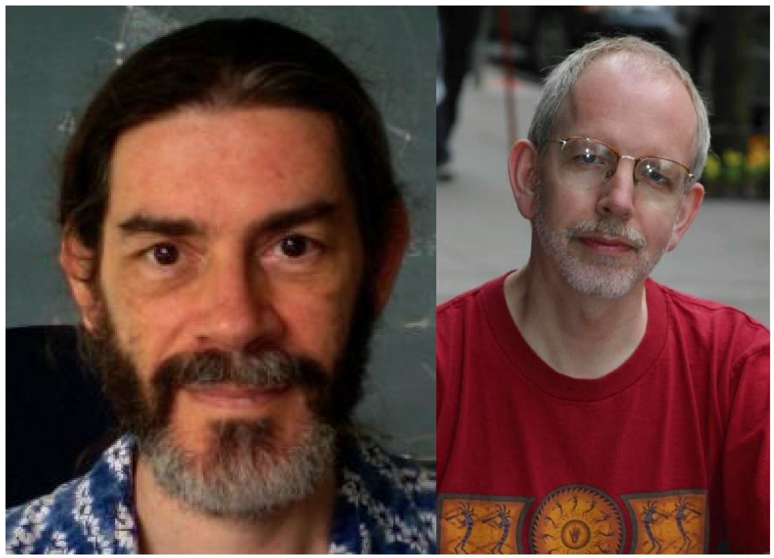
- In high-resolution SPH simulations, spiral arms naturally form
- Spiral arms are not stationary, but transient and recurrent
- "VLBI" and "HI" observations of simulation results look very similar to those of Milky way.

History of the number of particles



How do we calculate gravity?

- A straightforward approach requires $O(N^2)$ operations
- Almost all simulations after 1990 used treecode
- Barnes-Hut tree



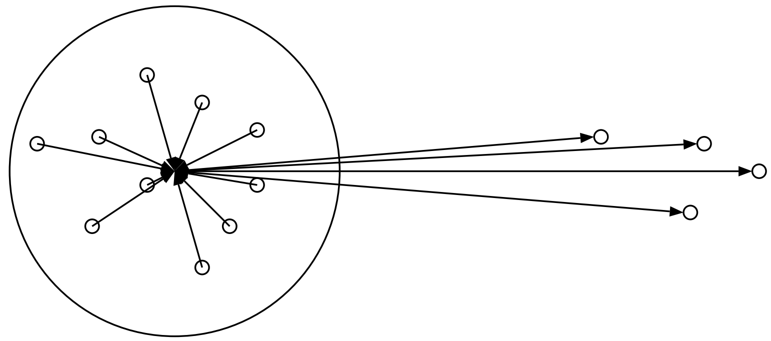
Barnes and Hut

Basic idea for tree method and FMM

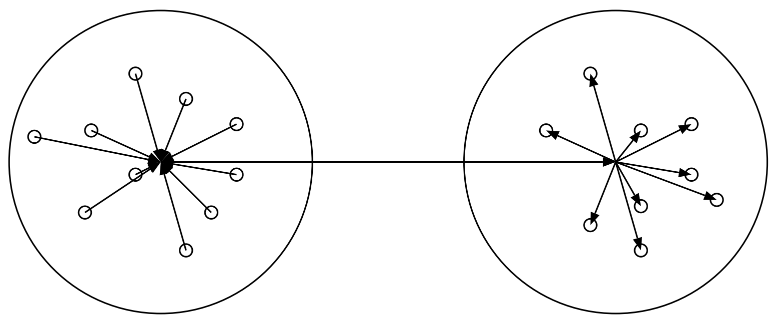
Force from distant particle: Weak

↓

Can't we evaluate many forces at once?



Tree



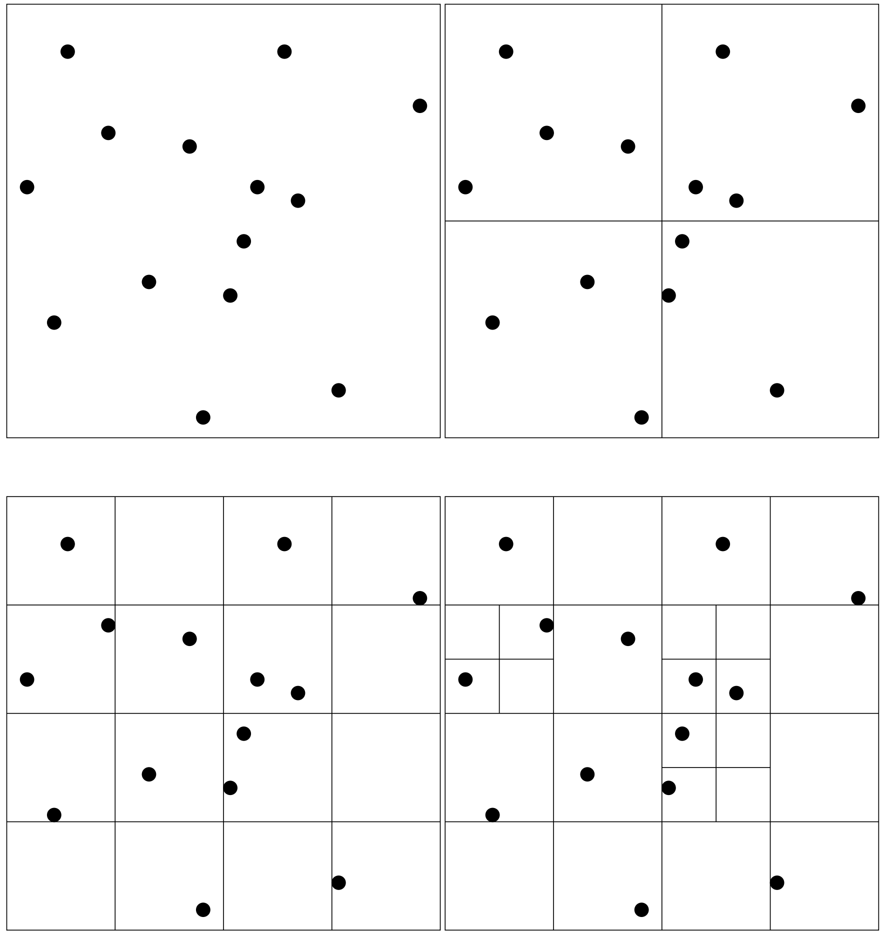
FMM

- Tree: aggregate stars which exert the forces
- FMM: aggregate both side

How do we aggregate — Barnes-Hut tree

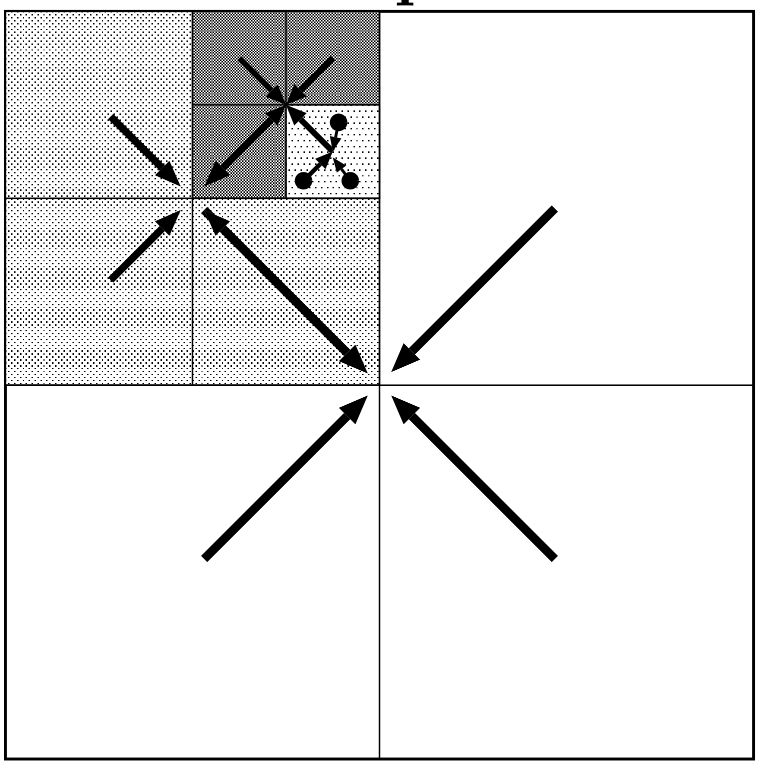
Use tree structure

- First make a cell with all stars in it
- Recursively subdivide the cells to 8 subcells
- Stop if there is small enough stars



Construction of the multipole expansion

Form the expansion for cells.

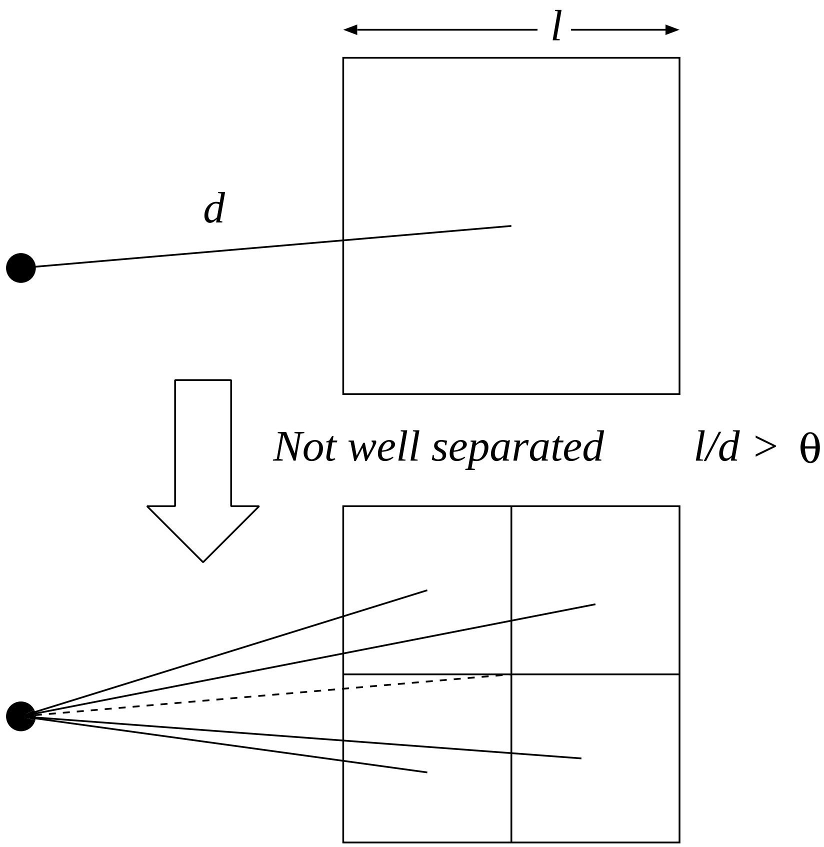


- lowest-level cells: Directly calculate the expansions for stars in it.
- Higher-level cells: Shift and add the expansions for child cells.

Calculate bottom-up.
Calculation cost: $O(Np^4)$ (p: expansion order)

Force calculation in tree method

Recursive expression:



- **Well separated: apply the multipole expansion**
- **not: take summation of the forces from the child cells**

Total force = force from the root cell

The Effect of Tree Method

- Order of the calculation cost reduced from $O(N^2)$ to $O(N \log N)$
- Cray XT1024 1024 cores: 2048^3 particles/ several minutes
- Direct method would take > 1000 years/step
- Calculation cost insensitive to the spacial structure

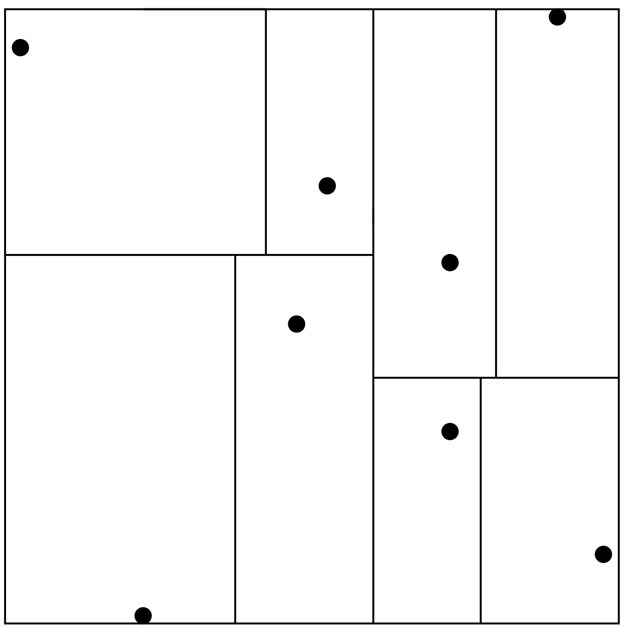
Other fast methods (PME, P^3M) become costly when inhomogeneity develops

Parallelization

Two known and well-studied methods, both first implemented by Salmon and Warren(Caltech Hypercube group)

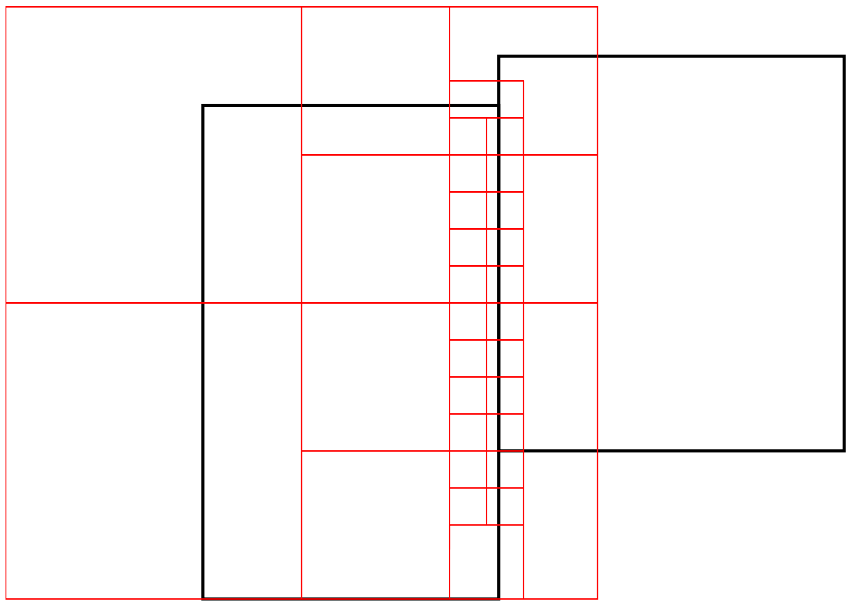
- **Orthogonal Recursive Bysection (ORB)**
- **Hashed Oct Tree (HOT)**

ORB



- **Divide the system by a plane perpendicular to x axis (each has same number of particles)**
- **then do the same thing for y, z, x,... directions, until the number of cells reaches the number of processors**

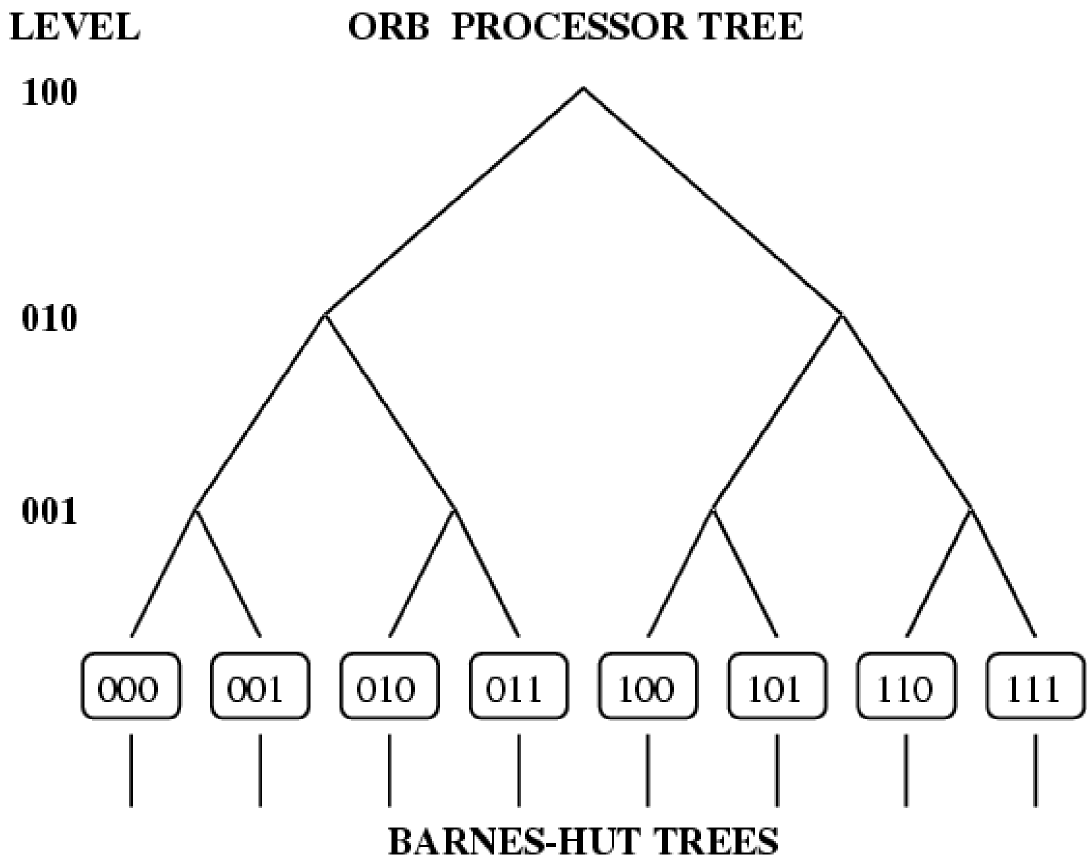
Force from particles in other processors



Get the trees with “unnecessary branches” cut off from other processors (local essential tree, LET) Construct the global tree by combining them with its own tree.

How to combine?

Dubinski: Upper structure is the ORB tree

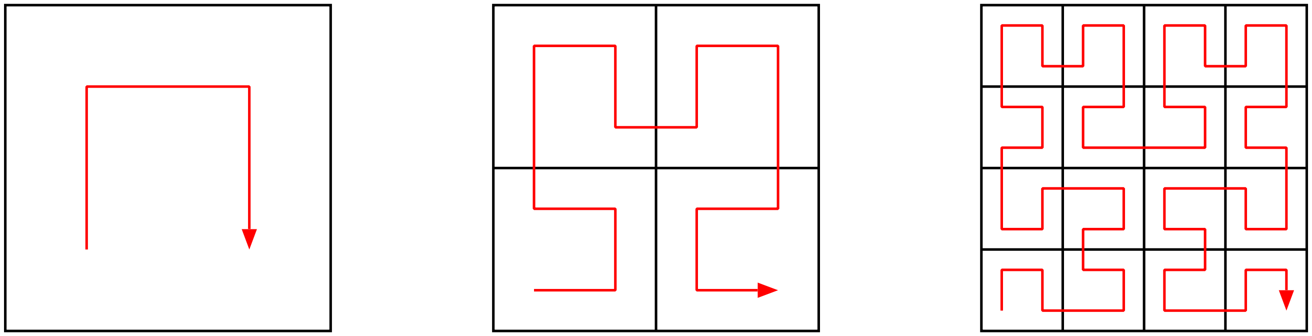


Problems with ORB tree

- Complex implementation
  - Different tree structures for the ORB tree and local tree
  - LET should be transferred maintaining the tree structure
- Poor scalability
  - Communication proportional to the number of processors
- Calculation result depends on the number of processors (within the tree accuracy, but...)

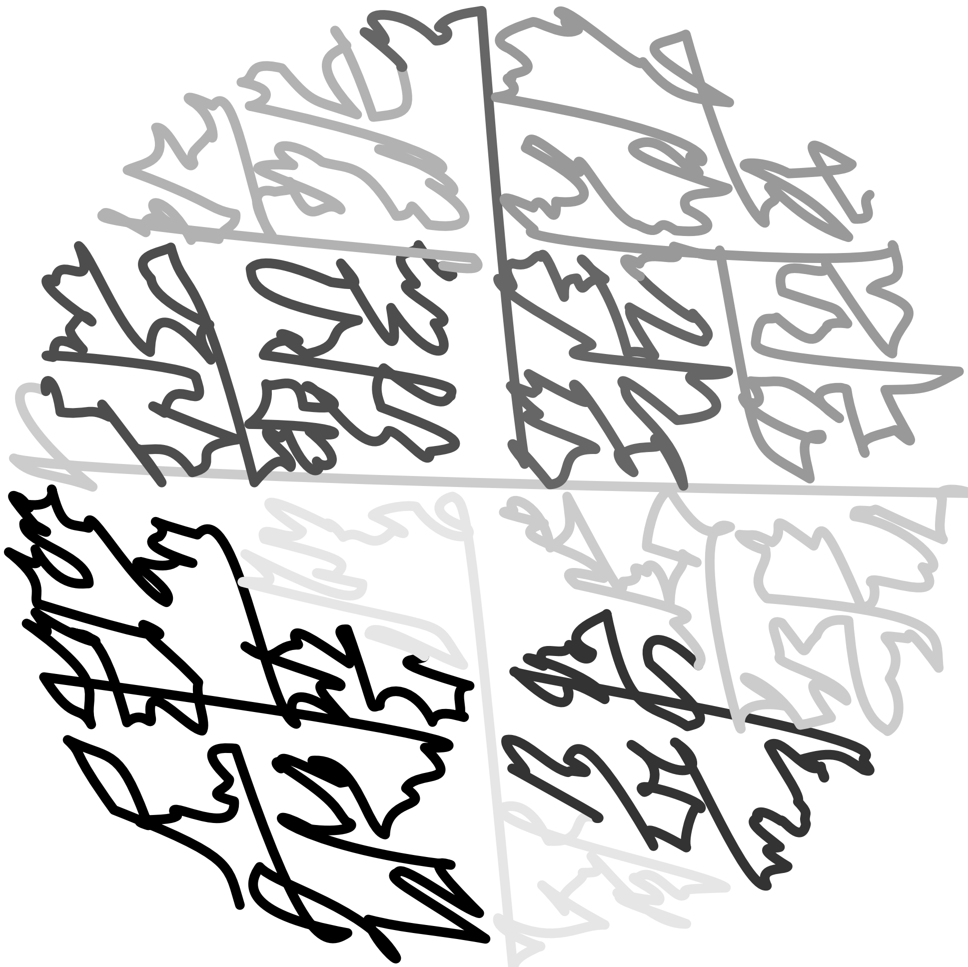
HOT

Peano-Hilbert curve



- **Order particles on the Peano-Hilbert curve**
- **Assign contiguous particles to each processors**

HOT



(This one uses Morton Ordering)

Tree construction and interaction calculation with HOT

Tree construction

- Assign Peano key to each particle
- Perform global parallel sort

Interaction calculation

- On-demand communication: Request necessary data to other processors

Fairly sophisticated message combining, async operation of calculation and communication, delayed evaluation etc...

Our approach

(Makino 2004, Ishiyama et al 2009, 2012)
Modify ORB in two ways

- Limit the depth to three
- Allow divisions to more than two cells

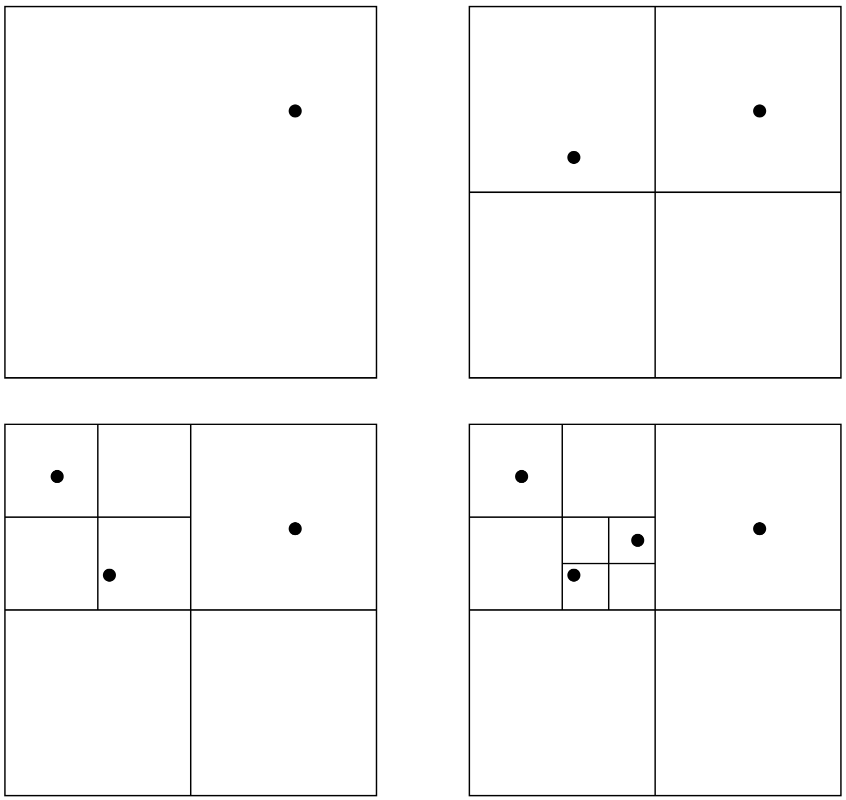
1000 nodes: $10 \times 10 \times 10$. For 2, 4, 8 nodes, The same as traditional ORB.
In principle can be used even on prime numbers of nodes.

Our Implementation

- **Do not send LET. Send only leaf nodes ("particles") of LET**
- **Insert these "particles" to the local tree (JM's code. Ishiyama et al. uses a bit different approach)**

Insertion method: The method used in Barnes' original tree code.

Insertion method for Tree construction



Determine the cell to which the current particle belongs

If there are already child cells, select one of the cells in which the particle belongs

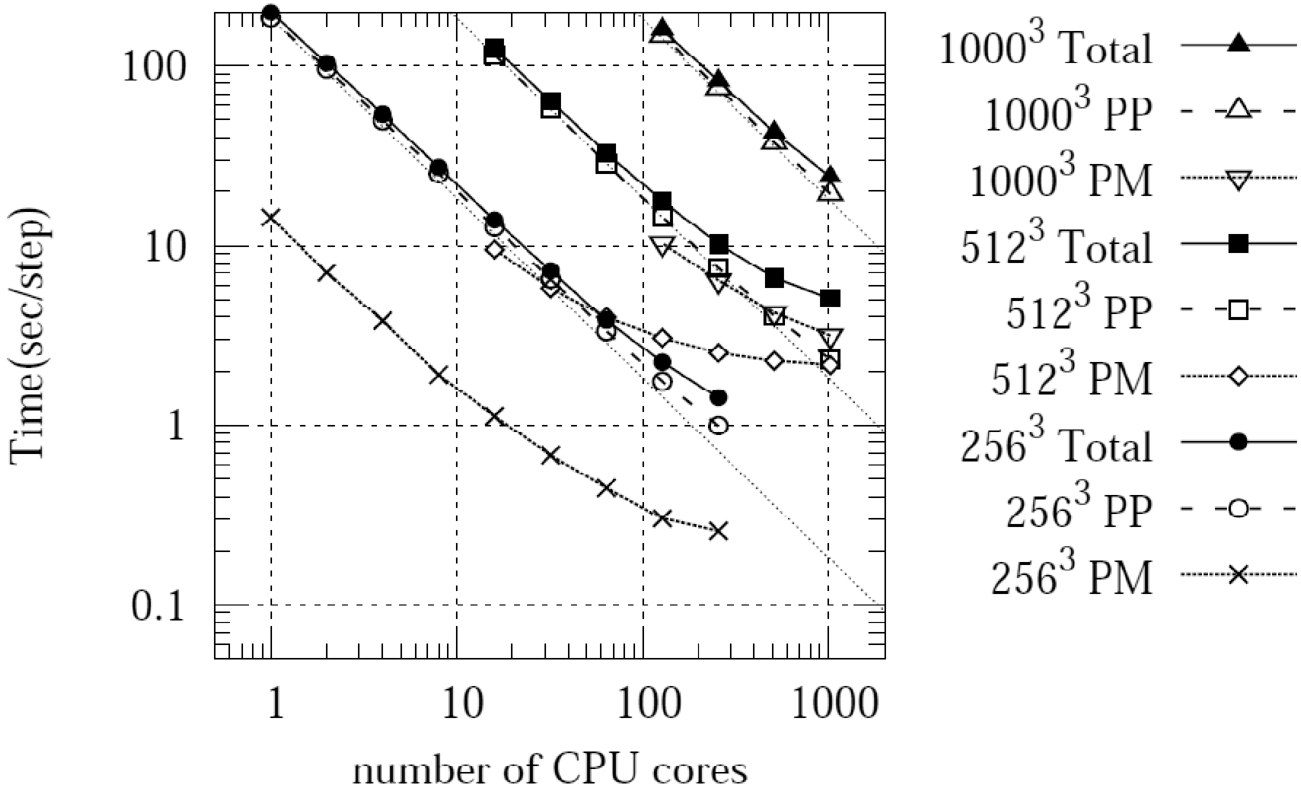
If the cell already contains a particle, divide it

Construction of global tree by insertion

- Simple implementation
- Communication is minimized
- Calculation cost of tree construction is a bit high
- Calculation cost and the result of force calculation does not depend on the number of nodes.

Parallel performance

(Ishiyama et al. 2009, TreePM)



Scaling is OK if we have 10^4-10^5particles/core

An improvement on Particle-Based Hydrodynamics

Advantages of paricle-based method for fluid

- **Naturally adaptive (particles moves to where the mass is there)**
- **Naturally gives Lagrange picture. Useful for low-temperature, high-speed objects**
- **Parallelization fairly easy**

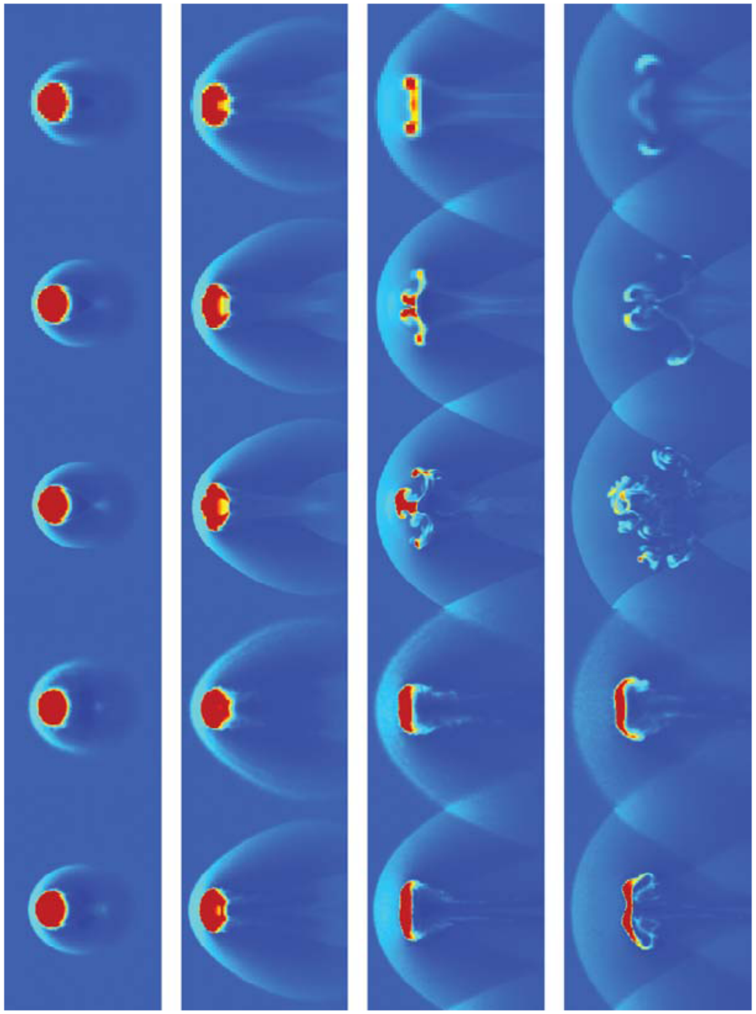
However, there are quite a few problems...

SPH and Contact Discontinuity, KH instability

Agertz et al (MN 2007, 380, 963)

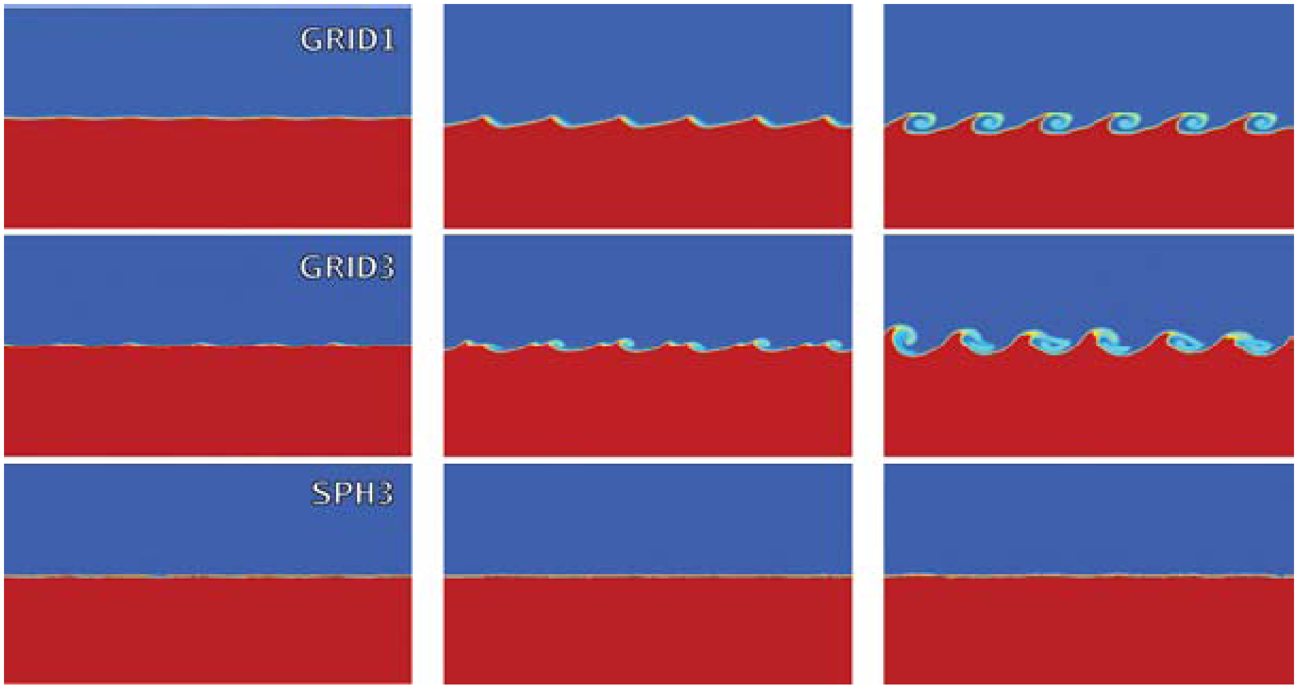
- The result of a simple “Blob test” quite different on SPH Grid
- Kelvin-Helmholtz Instability is not correctly handled with SPH
- Is SPH usable?

Difference (1)



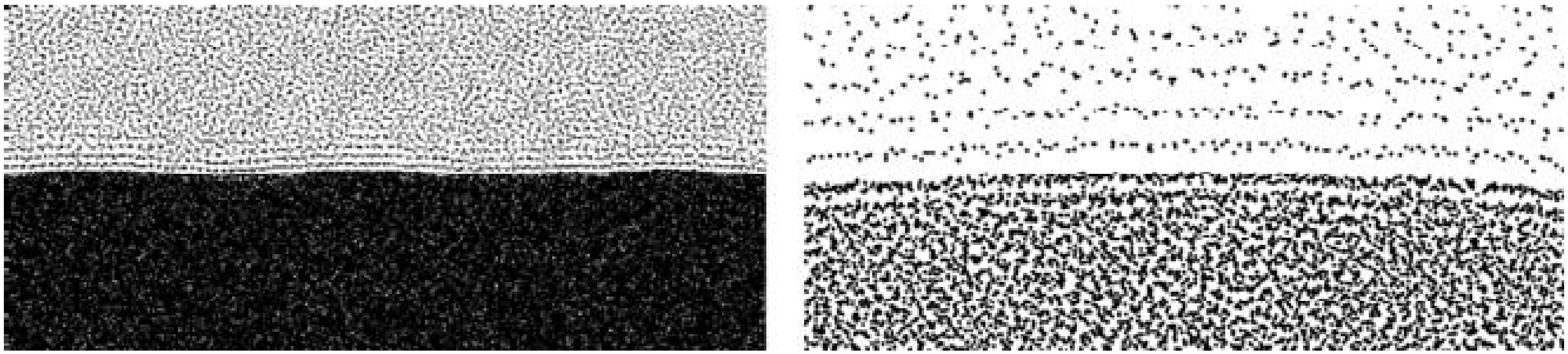
- Let a cold cloud (Temperature 1/10, density 10x) move with a supersonic velocity
- Upper three: Grid
- Lower two: SPH (1 and 10M particles)
- SPH suppresses the KHI at the fluid boundary

How different? (2)



SPH suppress KHI

How different? (3)



Strange-looking gap of particles at the two-fluid boundary.

Why does this happen?

Fundamental problem with SPH approximation

101 of SPH

Density estimate

$$\rho(x) = \sum_j m_j W(x - x_j), \tag{1}$$

Estimate of a quantity f

$$\langle f \rangle(x) = \int f(x') W(x - x') dx'. \tag{2}$$

101 of SPH continued(1)

grad of f: $\langle \nabla f \rangle = \nabla \langle f \rangle$ use the following identity

$$1 = \sum_j m_j \frac{1}{\rho(x)} W(x - x_j). \tag{3}$$

and with a bit more approximation we have

$$\langle \nabla f \rangle(x) \sim \sum_j m_j \frac{f(x_j)}{\rho(x_j)} \nabla W(x - x_j). \tag{4}$$

101 of SPH continued(2)

Equation of motion evaluates $-\frac{1}{\rho}\nabla P$. Use the identity

$$\frac{1}{\rho}\nabla P = \frac{P}{\rho^2}\nabla\rho + \nabla\frac{P}{\rho^2}. \tag{5}$$

and symmetrize. The we have

$$\dot{v}_i = -\sum_j m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2}\right)\frac{\partial}{\partial x_i}W(x_i - x_j), \tag{6}$$

Contact discontinuity

Standard SPH assumes the differentiability of ρ in the following two identities

$$1 = \sum_j m_j \frac{1}{\rho(x)} W(x - x_j). \tag{7}$$

$$\frac{1}{\rho}\nabla P = \frac{P}{\rho^2}\nabla\rho + \nabla\frac{P}{\rho^2}. \tag{8}$$

Density estimated with SPH is smoothed

- **Density in the low- (high-) density side (near CD) is over- (under-)estimated,**
- **Therefore, pressure and its derivatives have $O(1)$ errors, and particles are redistributed.**

Solution?

"Fundamental" reason

ρ is smooth but u contains jump

We could solve the problem by smoothing u. Several proposals

- **Use kernel-estimated u**
- **Let u diffuse (artificial conductivity)**
- **Use density which is continuous at CD.**

Sort of working, but not a "true" solution.

Our proposal: Basic idea

At CD, there is not jump in the pressure or internal energy. Only the density jumps. Why SPH approximation breaks down?

Because we use density to calculate other quantities.

$$\langle f\rangle(x) = \sum_j \frac{m_j f(x_j)}{\rho(x_j)} W(x - x_j). \tag{9}$$

What we do here is to replace volume element dx by $m_j/\rho(x_j)$

In principle, ANY quantity should by okay as far as it gives correct estimate for the volume element, but there seems to be no other quantity used in the literature.

Our proposal: Principle

What should we use instead of the mass density?

An ideal gas is described by the equation of state $PV = nRT$. Here, mass density does not appear. The RHS is the thermal energy.

Can't we use the pressure itself, which is equivalent to the energy density?

Each SPH particle has energy (or entropy). So we can evaluate pressure distribution without using mass density.

Pressure is continuous at CD. So there can be no large error.

Formulation (1)

Define internal energy per particle as

$$U_j = m_j u_j, \tag{10}$$

(u is per unit mass). Define the energy density as

$$q = \sum_j U_j W(x - x_j). \tag{11}$$

Other quantities can be calculated as

$$\langle f \rangle(x) = \sum_j \frac{U_j f(x_j)}{q(x_j)} W(x - x_j), \tag{12}$$

Spacial derivatives are given by

$$\langle \nabla f \rangle(x) = \sum_j \frac{U_j f(x_j)}{q(x_j)} \nabla W(x - x_j). \tag{13}$$

Formulation (2)—Energy Equation

$$\frac{du}{dt} = -\frac{P}{\rho}\nabla \cdot v. \tag{14}$$

The divergence of the velocity is given by

$$\nabla \cdot v = \sum_j (v_i - v_j)\frac{U_j}{q_j}\nabla W(x - x_j). \tag{15}$$

P/ρ is calculated as follows. Using EOS

$$P_i = (\gamma - 1)q_i. \tag{16}$$

Formulation (3)—Energy Equation

The density appears since the LHS is per unit mass. To rewrite this to per-particle form, use

$$\rho_i = \frac{m_i q_i}{U_i}. \tag{17}$$

Then we have

$$\dot{U}_i = \sum_j (\gamma - 1)\frac{U_i U_j}{q_j}(v_i - v_j)\nabla W(x_i - x_j). \tag{18}$$

Formulation (4)—Equation of Motion

From Energy equation we derive EoM using energy conservation. Energy change of two particles, due to the interaction between them are

$$\dot{U}_{ij} + \dot{U}_{ji} = (\gamma - 1) U_i U_j \left(\frac{1}{q_i} + \frac{1}{q_j} \right) (v_i - v_j) \nabla W (x_i - x_j). \quad (19)$$

This should be equal to the change of the kinetic energy

$$\frac{m_i m_j}{m_i + m_j} (v_i - v_j)(\dot{v}_i - \dot{v}_j). \quad (20)$$

Therefore, velocity change is

$$(\dot{v}_i - \dot{v}_j) = -(\gamma - 1) \frac{m_i + m_j}{m_i m_j} U_i U_j \left(\frac{1}{q_i} + \frac{1}{q_j} \right) \nabla W (x_i - x_j), \quad (21)$$

Formulation (5)—Equation of Motion

Using the conservation of the center of mass we have

$$\boldsymbol{m_i \dot{v}_i = -\sum_j (\gamma - 1) U_i U_j \left(\frac{1}{q_i} + \frac{1}{q_j} \right) \nabla W(x_i - x_j).} \quad (22)$$

- **RHS does not depend on mass**
- **This form is symmetric (between i and j particles)**

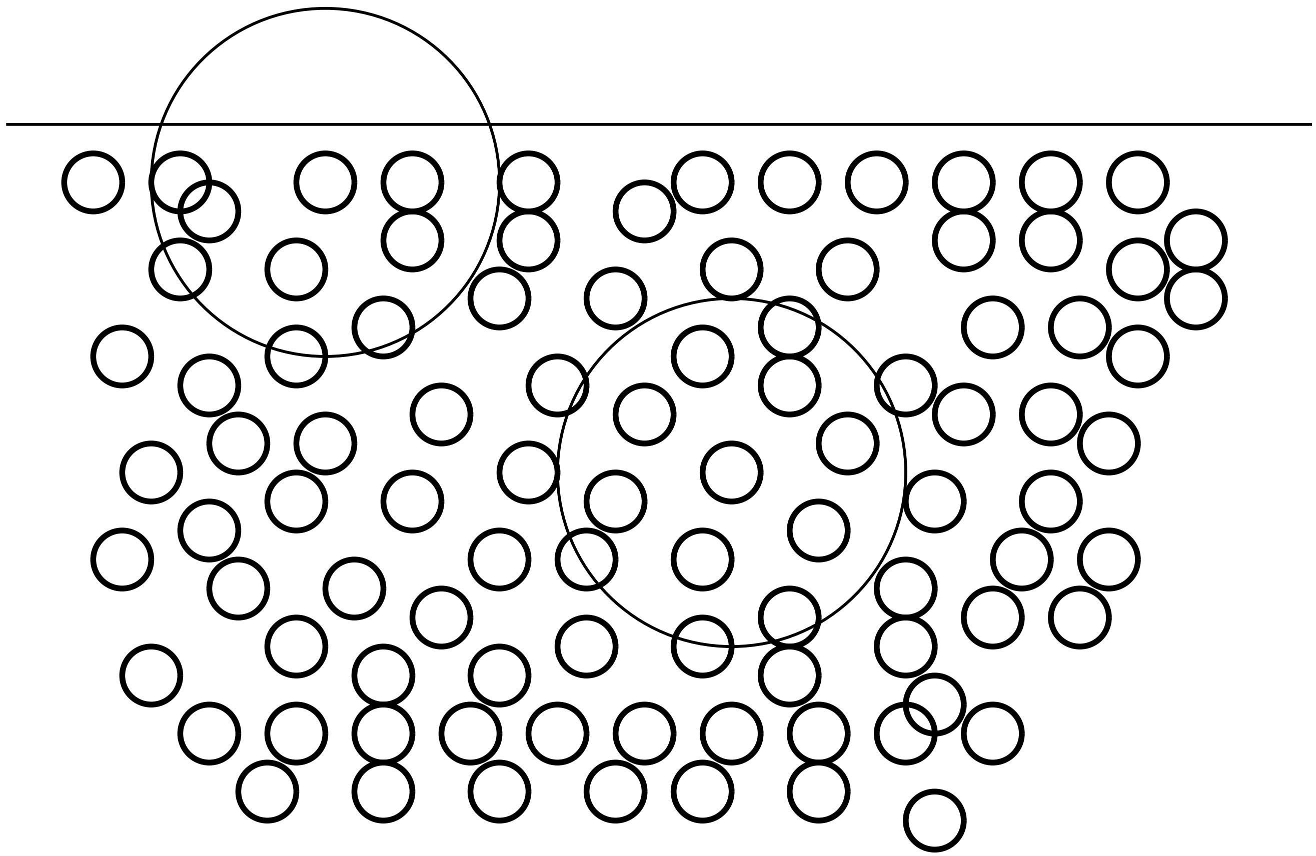
Examples

(not avaible in Web version)

Other (known) problems

- **Free boundary**
- **Numerical viscosity**

Free Boundary



On the particles at the free surface

- **Standard SPH density would be underestimated**
- **Pressure/Internal energy would be overestimated?**

Numerical viscosity

With SPH, votices don't (Prof. Aoki, TiTech)

Sources of viscosity

1. **Artificial viscosity (to capture shocks)**
2. **particle noise**

The contribution of particle noise is not well understood... (cf Lee and Dehnen 2010)

Summary
(for the SPH part of the talk)

- Particle-based hydrodrodynamics is at least potentially useful.
- Known schemes still have many problems with contact discontinuity, free surface, numerical viscausity.
- Improvements have been found to some of them, but not all...