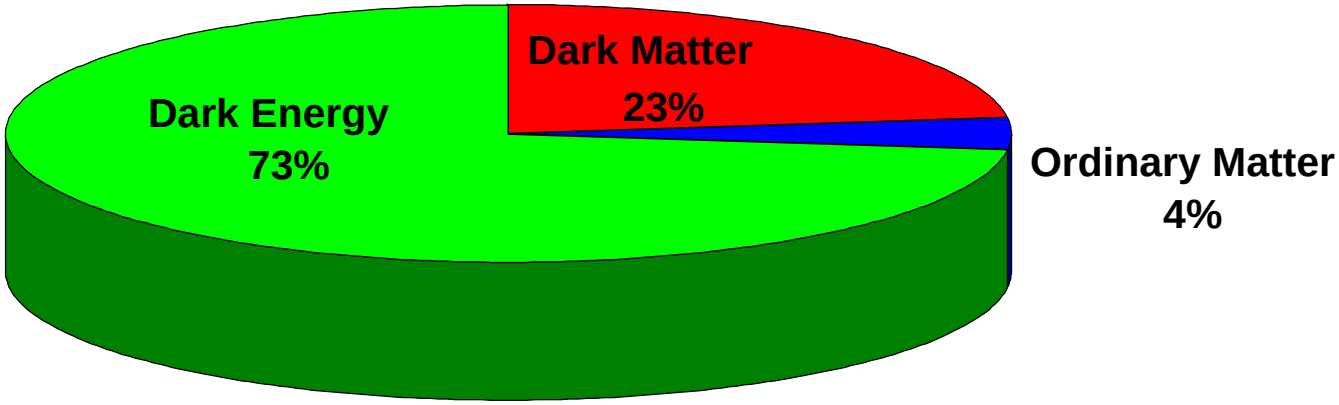
Cosological Simulations

Klaus Dolag

Max-Planck-Institut für Astrophysik

Introduction I

Composition of the Universe



Ordinary Matter

Ordinary Matter makes up only 4% of the Universe !

Dark Matter

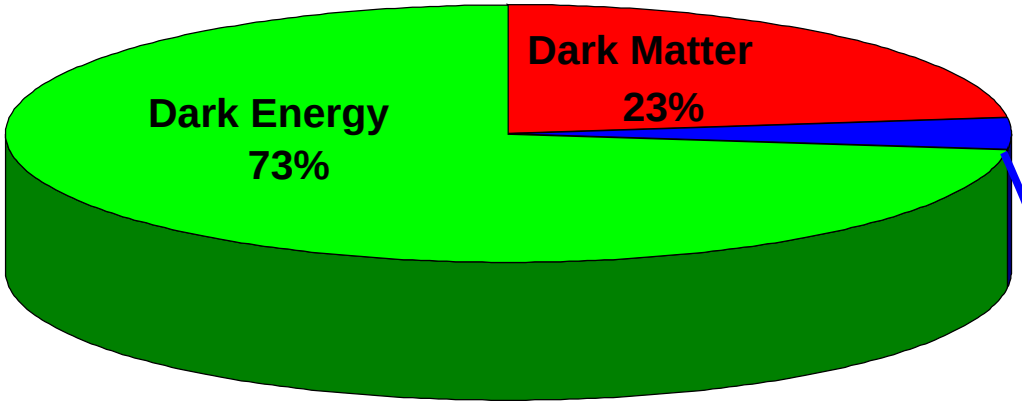
Galaxies and galaxy cluster are embedded in an invisible structure, the so called dark matter !

Dark Energy

The universe is dominated by an even more exotic component, called Dark Energy !

Introduction I

Composition of the Universe



Ordinary Matter

Ordinary Matter makes up only 4% of the Universe !

Dark Matter

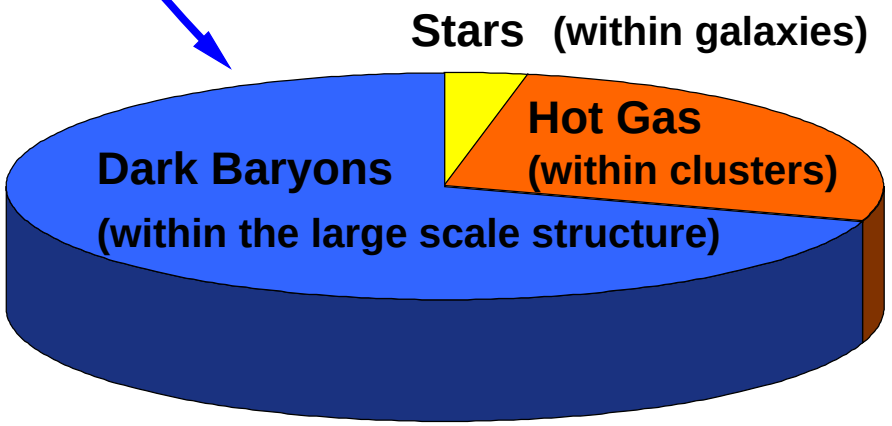
Galaxies and galaxy cluster are embedded in an invisible structure, the so called dark matter !

Dark Energy

The universe is dominated by an even more exotic component, called Dark Energy !

Dark Baryons

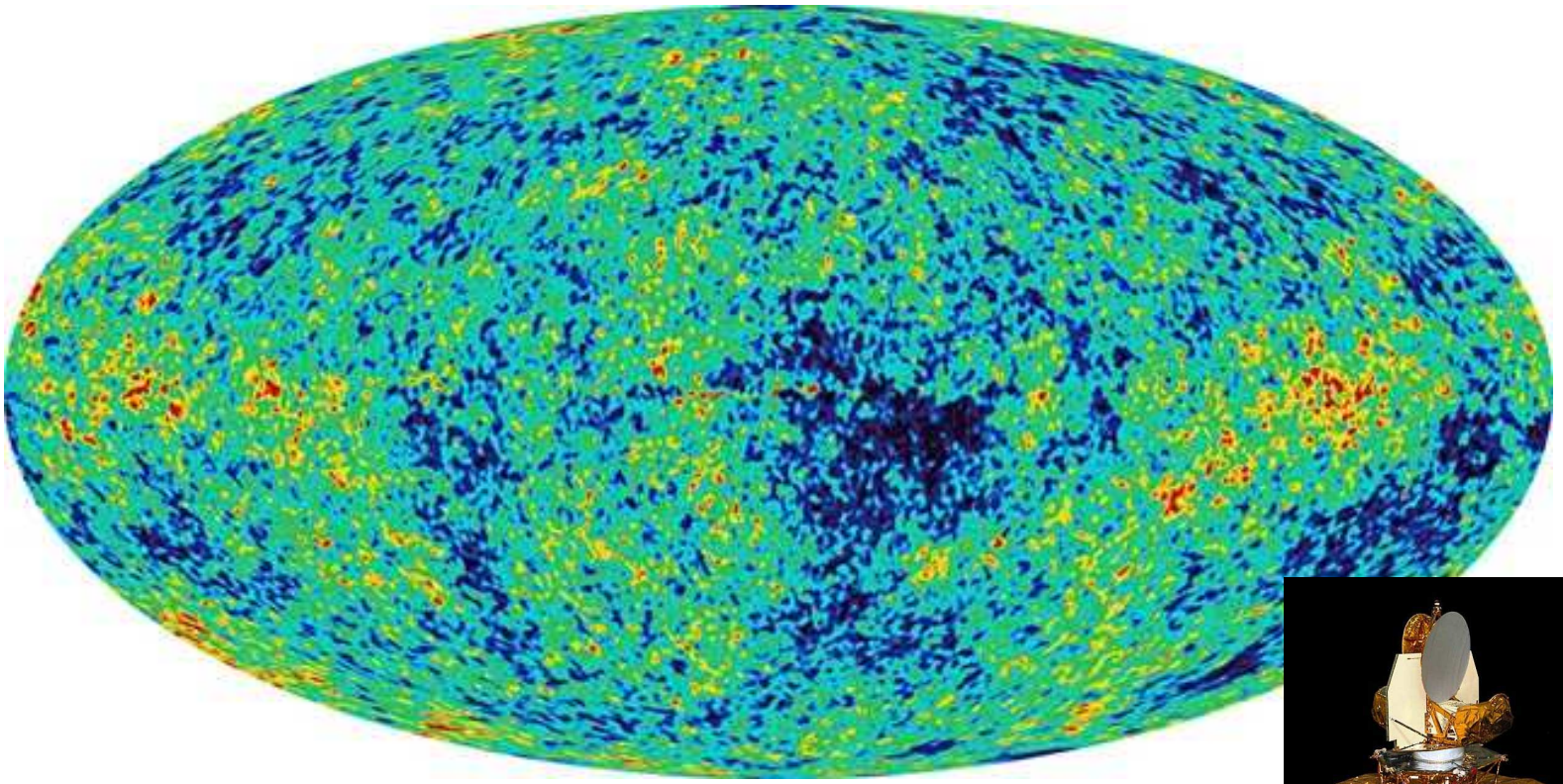
60% − 80% of the Baryons are also 'dark' !



Introduction II

Evolution of the structures in the Universe

t = 0.38 Myr

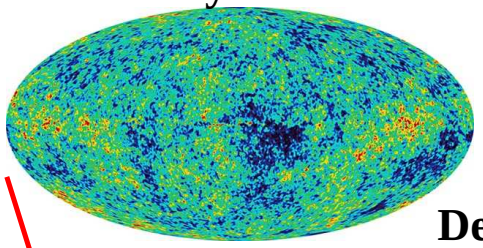


Cosmic Microwave Background, early picture of the structure in the Universe.

Introduction II

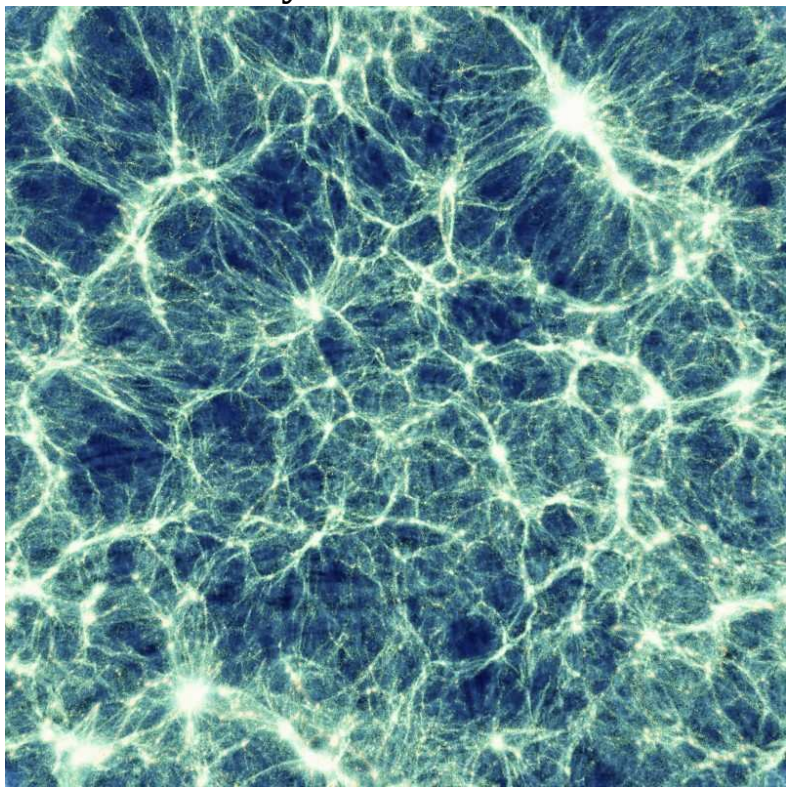
Evolution of the structures in the Universe

t = 0.38 Myr

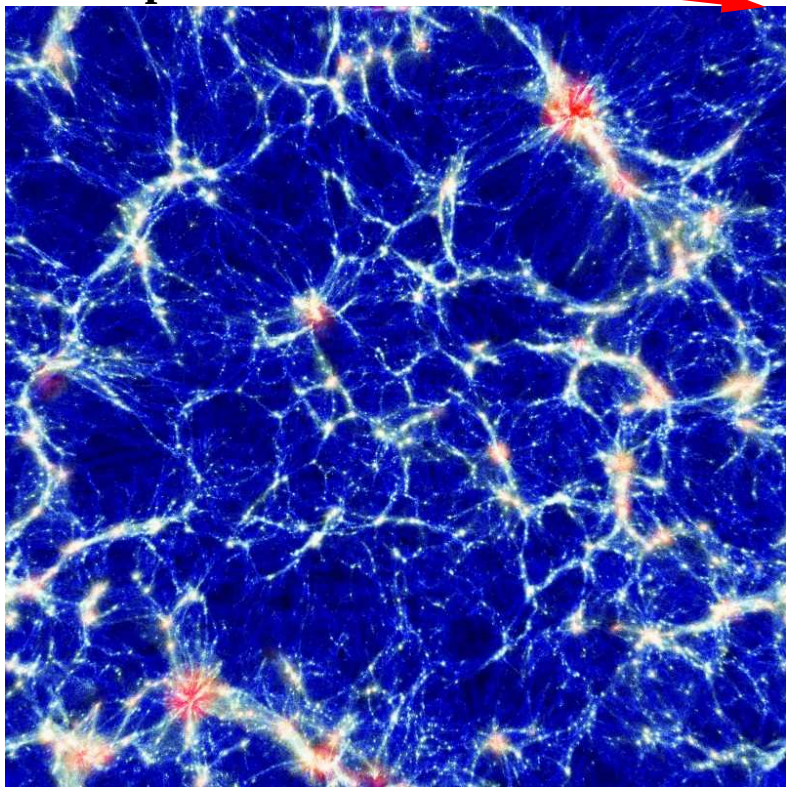


Cosmic structure today (T = 13.7 Gyr)

Density



Temperature



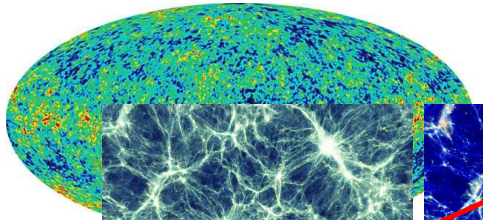
Cosmological Simulation
CINECA Keyproject 2002

275 Mpc

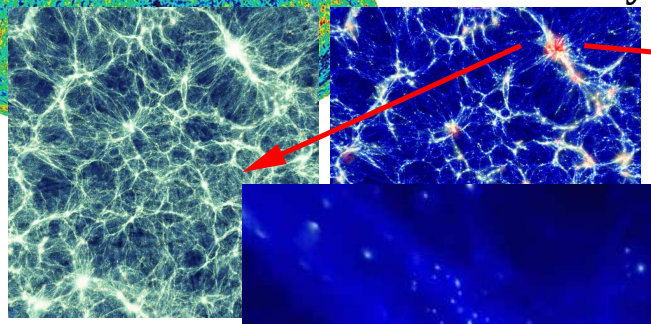
Introduction II

Evolution of the structures in the Universe

t = 0.38 Myr



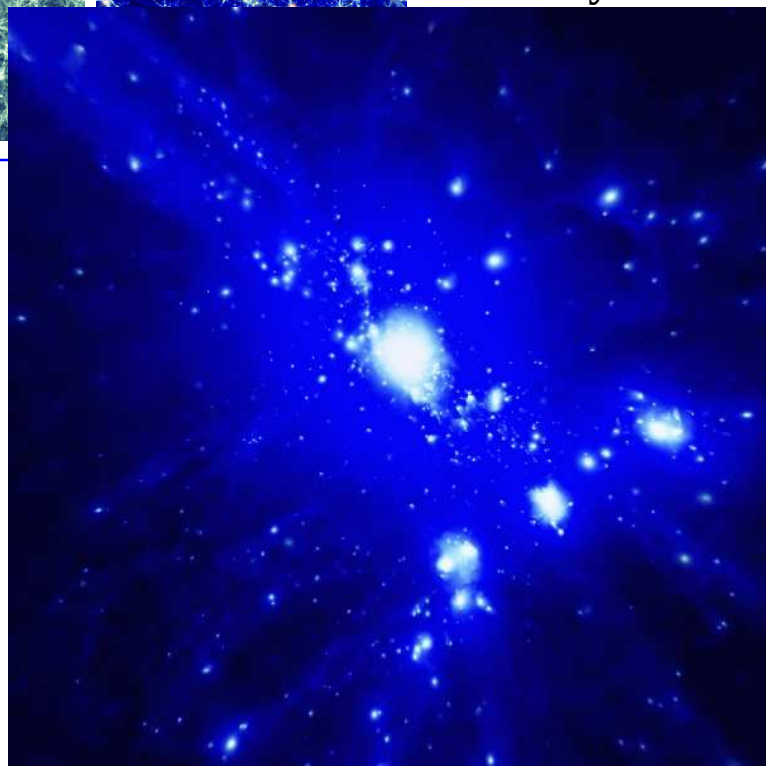
T = 13.7 Gyr



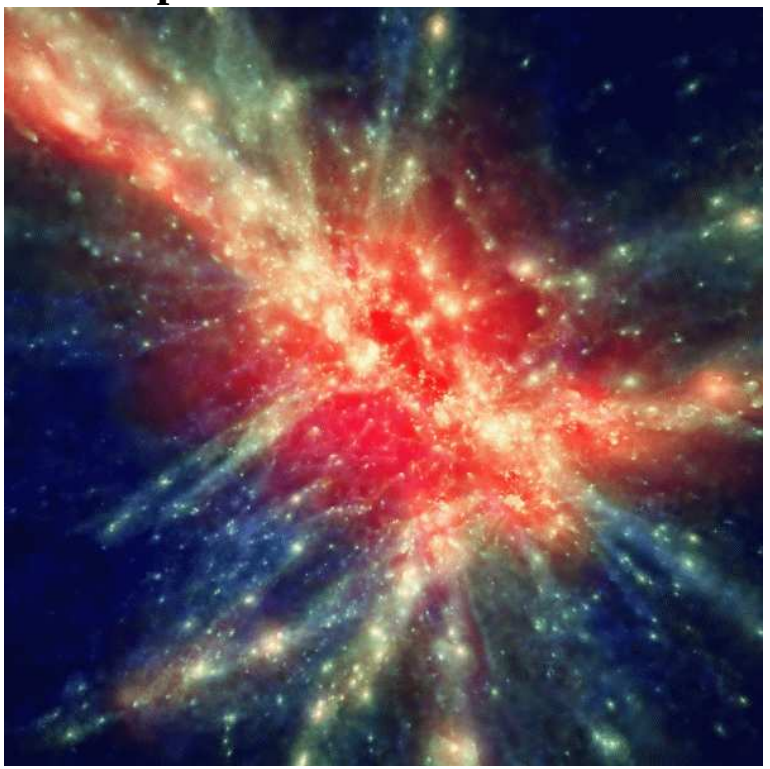
275 Mpc

"Zoomed" Simulation of a galaxy cluster

Density



Temperature



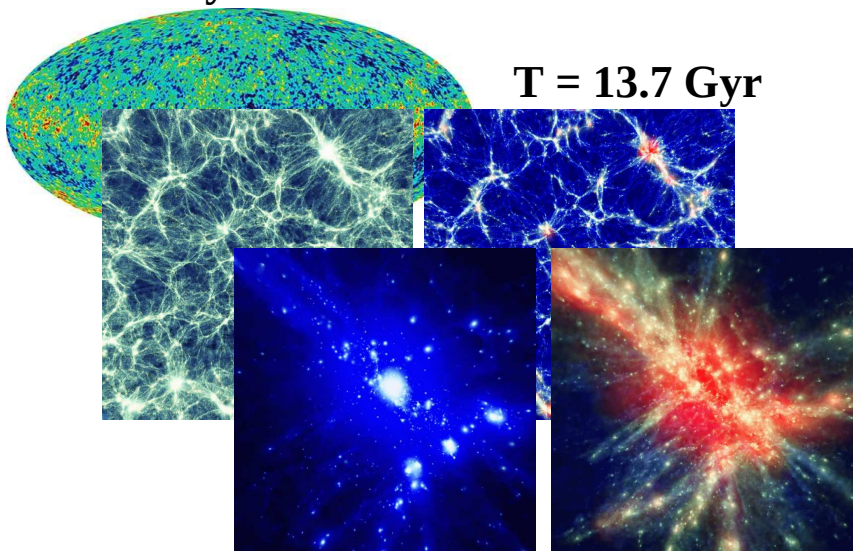
40 Mpc

Simulation
galaxy cluster g1

Introduction II

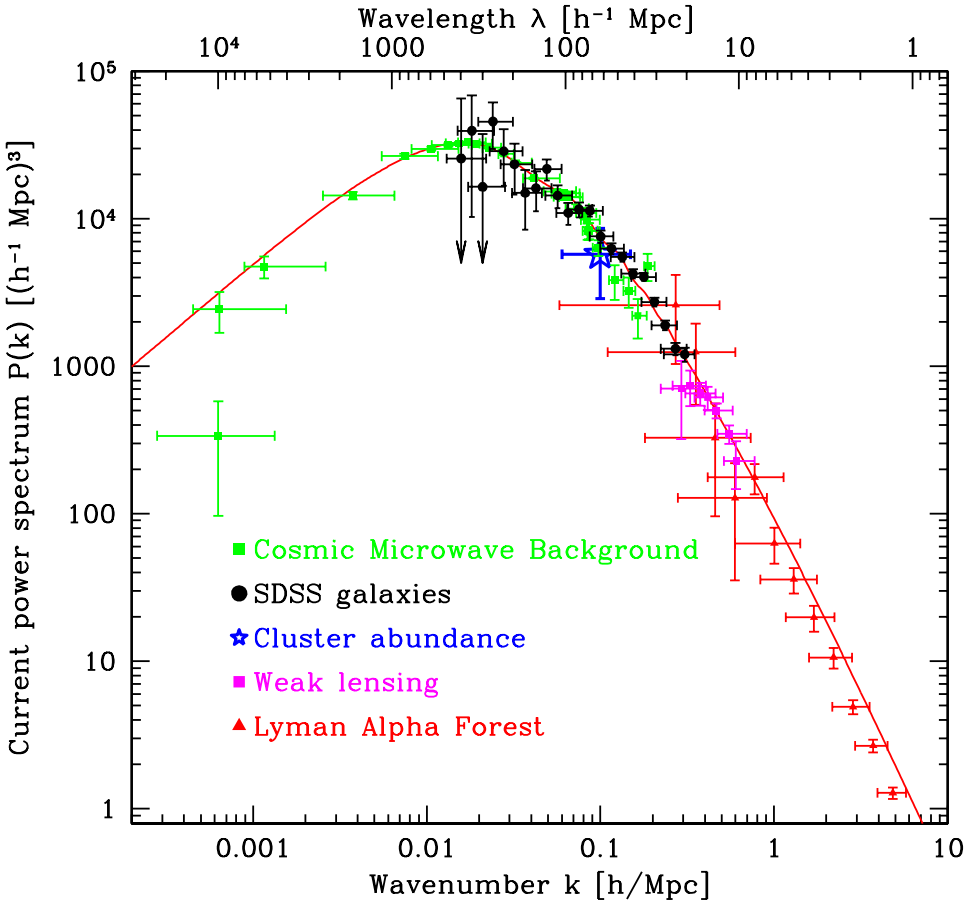
Evolution of the structures in the Universe

t = 0.38 Myr



T = 13.7 Gyr

Measured power−spectra of density fluctuations

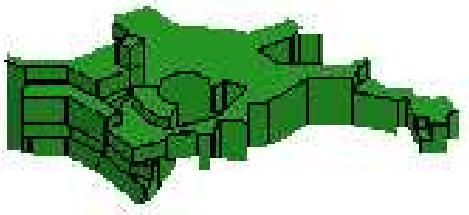


Taken from Tegmark et al. 2003

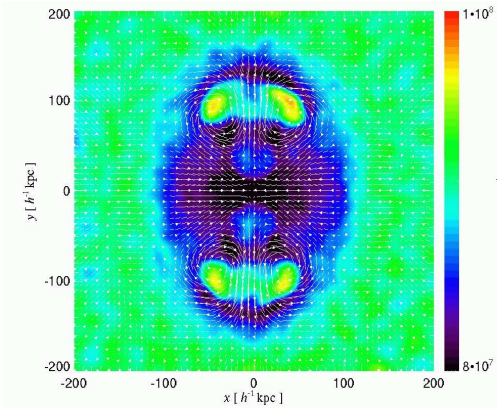
For precisely measuring the cosmological parameter we need a detailed understanding of the relevant astronomical objects and all relevant physical processes within.

Introduction II

Recent developments



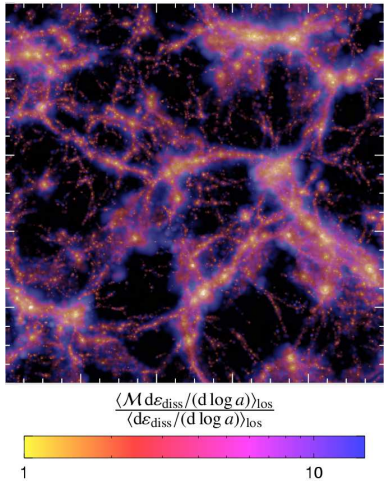
Max Planck Institute for Astrophysics



Sijacki & Springel 2006

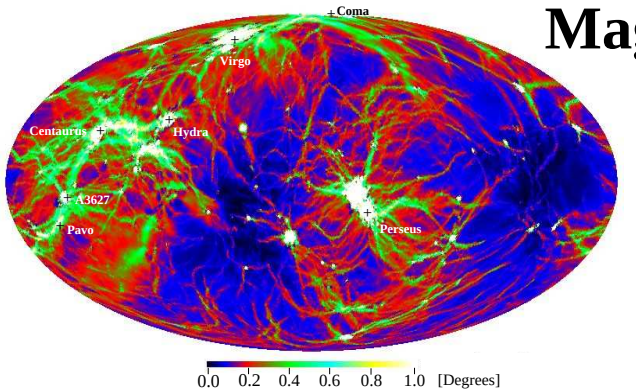
AGN − Cluster interaction

Shocks & Cosmic Rays



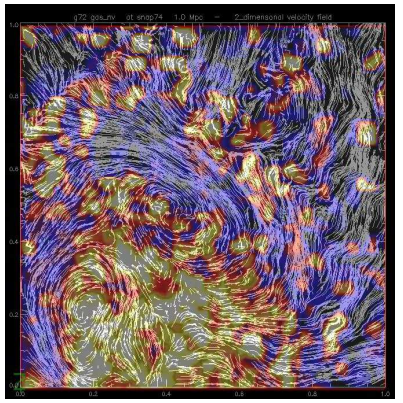
Pfrommer, Springel, Ensslin & Jubelgas 2006

Magnetic Fields



Dolag et al. 2005

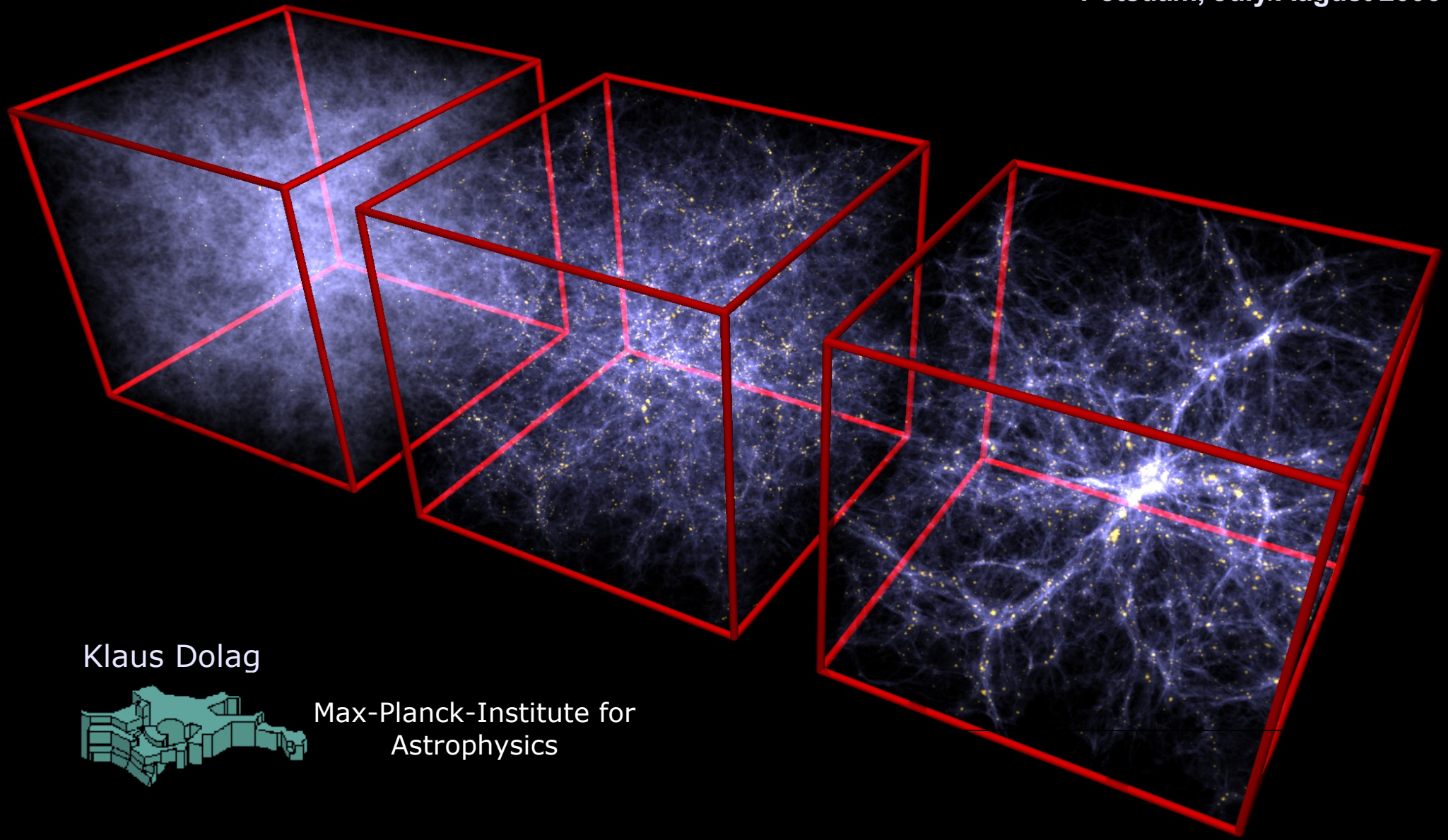
Turbulence



Dolag et al. 2005

Lecture slides kindly provided by **Volker Springel** from the Summer school on cosmological numerical simulations

Helmholtz School of Astrophysics
Potsdam, July/August 2006



Klaus Dolag

Max-Planck-Institute for Astrophysics

The N-body method uses a finite set of particles to sample the underlying distribution function

"MONTE-CARLO" APPROACH TO COLLISIONLESS DYNAMICS

We discretize in terms of N particles, which approximately move along characteristics of the underlying system.

$$\ddot{\mathbf{x}}_i = -\nabla_i \Phi(\mathbf{x}_i)$$

$$\Phi(\mathbf{x}) = -G \sum_{j=1}^{N} \frac{m_j}{[(\mathbf{x} - \mathbf{x}_j)^2 + \epsilon^2]}$$

The need for **gravitational softening**:

- Prevent large-angle particle scatterings and the formation of bound particle pairs.
- Ensure that the two-body relexation time is sufficiently large.

} Needed for faithful collisionless behaviour

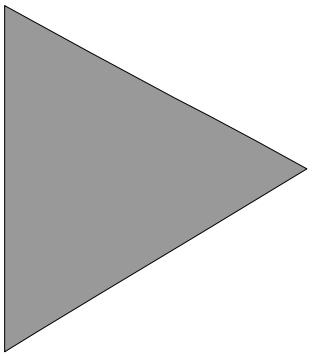
- Allows the system to be integrated with low-order intergations schemes.

Two conflicting requirements complicate the study of **hierarchical** structure formation

DYNAMIC RANGE PROBLEM FACED BY COSMOLOGICAL SIMULATIONS

Want **small particle mass** to resolve internal structure of halos

Want **large volume** to obtain respresentative sample of universe



need large N

where N is the particle number

Problems due to a small box size:

- Fundamental mode goes non-linear soon after the first halos form. ⇨ Simulation cannot be meaningfully continued beyond this point.
- No rare objects (the first halo, **rich** galaxy clusters, etc.)

Problems due to a large particle mass:

- Physics cannot be resolved.
- Small galaxies are missed.

At any given time, halos exist on a large range of mass-scales !

Several questions come up when we try to use the N-body approach for cosmological simulations

- How do we compute the gravitational forces efficiently and accurately?
- How do we integrate the orbital equations in time?
- How do we generate appropriate initial conditions?

$$\ddot{\mathbf{x}}_i = -\nabla_i \Phi(\mathbf{x}_i)$$

$$\Phi(\mathbf{x}) = -G \sum_{j=1}^{N} \frac{m_j}{[(\mathbf{x} - \mathbf{x}_j)^2 + \epsilon^2]}$$

Note: The naïve computation of the forces is an N^2 - task.

The particle mesh (PM) force calculation

The particle-mesh method

Poisson's equation can be solved in real-space by a convolution of the density field with a Green's function.

$$\Phi(\mathbf{x}) = \int g(\mathbf{x}-\mathbf{x}')\,\rho(\mathbf{x})\,\mathrm{d}\mathbf{x}'$$

Example for vacuum boundaries:

$$\Phi(\mathbf{x}) = -G\int \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{x}'|}\,\mathrm{d}\mathbf{x}' \qquad g(\mathbf{x}) = -\frac{G}{|\mathbf{x}|}$$

In Fourier-space, the convolution becomes a simple multiplication!

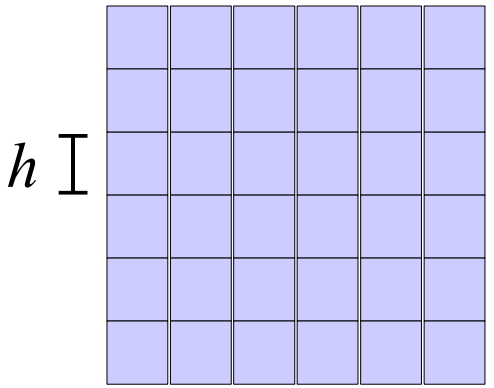
$$\hat{\Phi}(\mathbf{k}) = \hat{g}(\mathbf{k}) \cdot \hat{\rho}(\mathbf{k})$$

→ **Solve the potential in these steps:**

(1) FFT forward of the density field
(2) Multiplication with the Green's function
(3) FFT backwards to obtain potential

The four steps of the PM algorithm
(a) Density assignment
(b) Computation of the potential
(c) Determination of the force field
(d) Assignment of forces to particles

Density assignment



$\{\mathbf{x}_m\}$ set of discrete mesh centres

Give particles a „shape‰ S(x). Then to each mesh cell, we assign the fraction of mass that falls into this cell. The overlap for a cell is given by:

$$W(\mathbf{x_m} - \mathbf{x}_i) = \int_{\mathbf{x_m}-\frac{h}{2}}^{\mathbf{x_m}+\frac{h}{2}} S(\mathbf{x}' - \mathbf{x}_i)\,\mathrm{d}\mathbf{x}' = \int \Pi\left(\frac{\mathbf{x}' - \mathbf{x_m}}{h}\right) S(\mathbf{x}' - \mathbf{x}_i)\,\mathrm{d}\mathbf{x}'$$

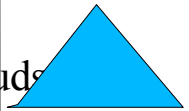
The assignment function is hence the convolution:

$$W(\mathbf{x}) = \Pi\left(\frac{\mathbf{x}}{h}\right) \star S(\mathbf{x}) \qquad \text{where} \qquad \Pi(x) = \begin{cases} 1 & \text{for } |x| \le \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

The density on the mesh is then a sum over the contributions of each particle as given by the assignment function:

$$\rho(\mathbf{x_m}) = \frac{1}{h^3} \sum_{i=1}^{N} m_i\, W(\mathbf{x}_i - \mathbf{x_m})$$

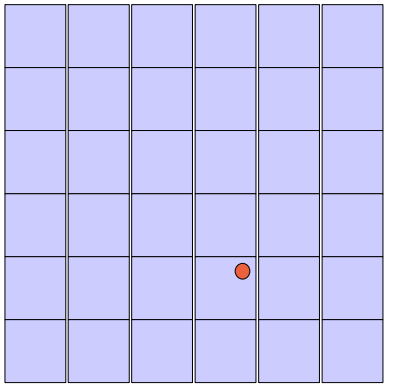
Commenly used particle shape functions and assignment schemes

Name	Shape function S(x)	# of cells involved	Properties of force
NGP Nearest grid point	 $\delta(\mathbf{x})$	$1^3 = 1$	piecewise constant in cells
CIC Clouds in cells	 $\frac{1}{h^3}\Pi\left(\frac{\mathbf{x}}{h}\right) \star \delta(\mathbf{x})$	$2^3 = 8$	piecewise linear, continuous
TSC Triangular shaped clouds	 $\frac{1}{h^3}\Pi\left(\frac{\mathbf{x}}{h}\right) \star \frac{1}{h^3}\Pi\left(\frac{\mathbf{x}}{h}\right)$	$3^3 = 27$	continuous first derivative

Note: For interpolation of the grid to obtain the forces, the same assignment function needs to be used to ensure momentum conservation. (In the CIC case, this is identical to tri-linear interpolation.)

Finite differencing of the potential to get the force field

Approximate the force field $\mathbf{f} = -\nabla\Phi$ with finite differencing



2nd order accurate scheme:

$$f^{(x)}_{i,j,k} = -\frac{\Phi_{i+1,j,k} - \Phi_{i-1,j,k}}{2h}$$

4th order accurate scheme:

$$f^{(x)}_{i,j,k} = -\frac{4}{3}\frac{\Phi_{i+1,j,k} - \Phi_{i-1,j,k}}{2h} + \frac{1}{3}\frac{\Phi_{i+2,j,k} - \Phi_{i-2,j,k}}{4h}$$

Interpolating the mesh-forces to the particle locations

$$F(\mathbf{x}_i) = \sum_{\mathbf{m}} W(\mathbf{x}_i - \mathbf{x}_\mathbf{m})\, f_\mathbf{m}$$

The interpolation kernel needs to be the same one used for mass-assignment to ensure force anti-symmetry.

Advantages and disadvantages of the PM-scheme

Pros: **SPEED** and simplicity

Cons:

- Spatial force resolution limited to mesh size.
- Force errors somewhat anisotropic on the scale of the cell size

→ *serious problem:*

cosmological simulations cluster strongly and have a very large dynamic range

cannot make the PM-mesh fine enough and resolve internal structure of halos as well as large cosmological scales

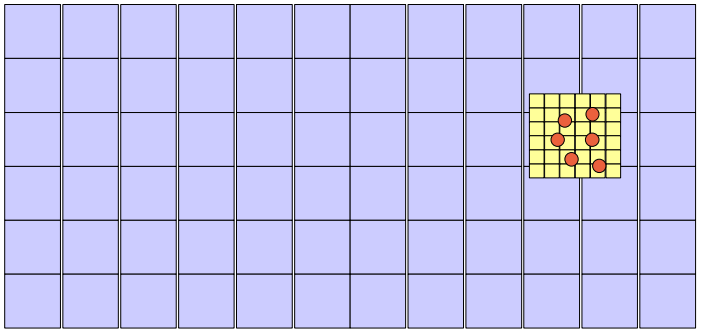
→ we need a method to increase the **dynamic range** available in the force calculation

Particle-Particle PM schemes (P^3M)

Idea: Supplement the PM force with a direct summation short-range force at the scale of the mesh cells. The particles in cells are linked together by a chaining list.

Offers much higher dynamic range, but becomes slow when clustering sets in.

In AP^3M, mesh-refinements are placed on clustered regions



Can avoid clustering slow-down, but has higher complexity and ambiguities in mesh placement

Codes that use AP^3M: **HYDRA** (Couchman)

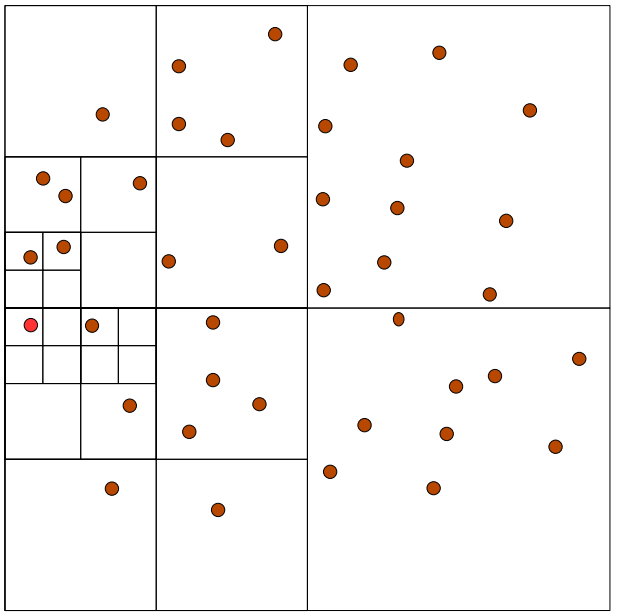
TREE algorithms

Gravity is the driving force for structure formation in the universe

HIERARCHICAL TREE ALGORITHMS

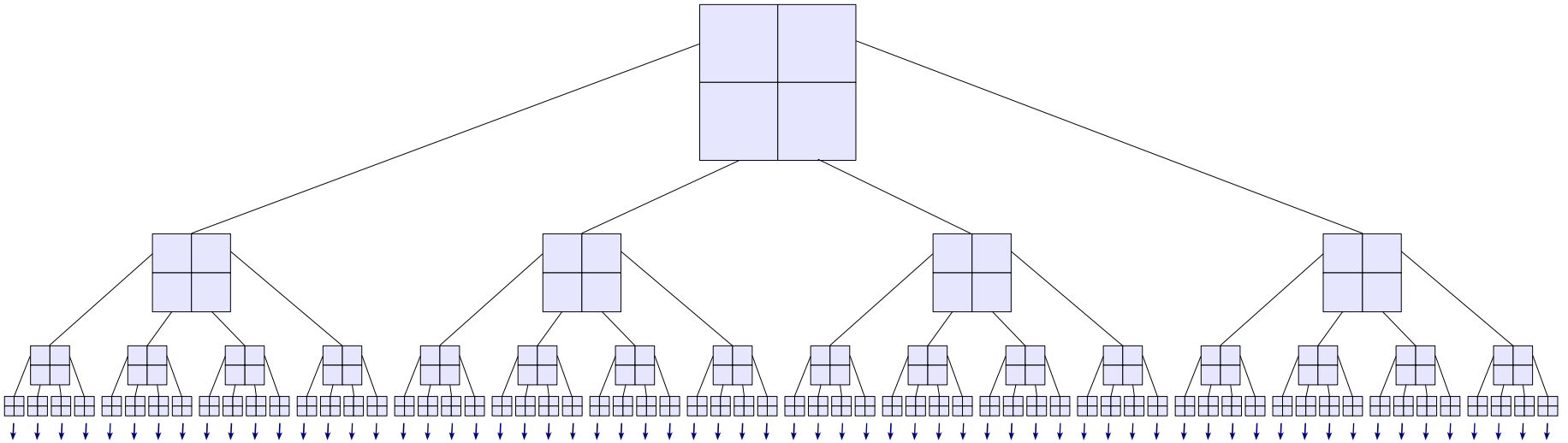
The N^2 - scaling of direct summation puts serious limitations on N...

But we want N ~ 10^6-10^{10} for collisionless dynamics of dark matter !

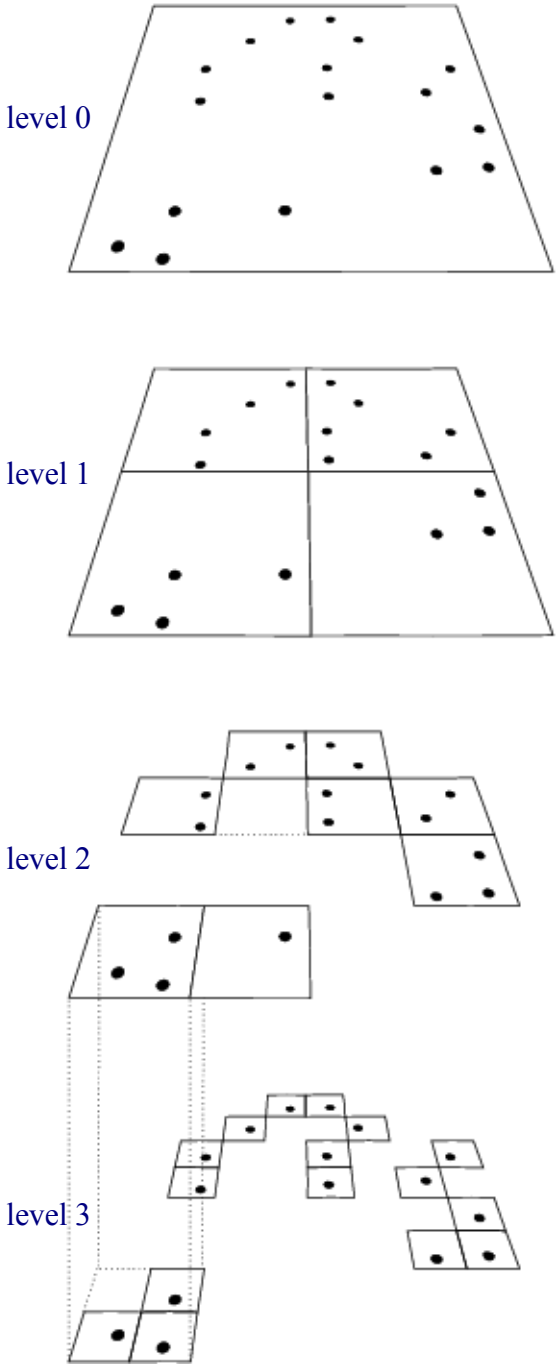


Idea: Group distant particles together, and use their multipole expansion.

→ Only ~ log(N) force terms per particle.



Oct-tree in two dimensions



Tree algorithms

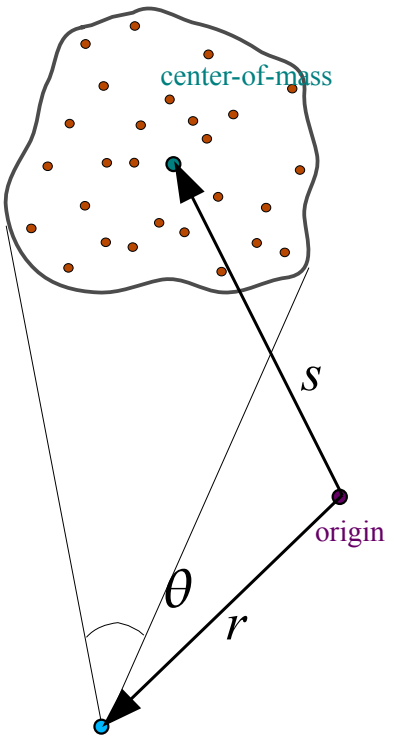
Idea: Use hierarchical multipole expansion to account for distant particle groups

$$\Phi(\mathbf{r}) = -G\sum_i \frac{m_i}{|\mathbf{r}-\mathbf{x}_i|}$$

We expand:

$$\frac{1}{|\mathbf{r}-\mathbf{x}_i|} = \frac{1}{|(\mathbf{r}-\mathbf{s})-(\mathbf{x}_i-\mathbf{s})|}$$

for $|\mathbf{x}_i-\mathbf{s}| \ll |\mathbf{r}-\mathbf{s}|$ $\mathbf{y} \equiv \mathbf{r}-\mathbf{s}$



and obtain:

$$\frac{1}{|\mathbf{y}+\mathbf{s}-\mathbf{x}_i|} = \frac{1}{|\mathbf{y}|} - \frac{\mathbf{y}\cdot(\mathbf{s}-\mathbf{x}_i)}{|\mathbf{y}|^3} + \frac{1}{2}\frac{\mathbf{y}^T\left[3(\mathbf{s}-\mathbf{x}_i)(\mathbf{s}-\mathbf{x}_i)^T - \mathbf{I}(\mathbf{s}-\mathbf{x}_i)^2\right]\mathbf{y}}{|\mathbf{y}|^5} + \cdots$$

the dipole term vanishes when summed over all particles in the group

The multipole moments are computed for each node of the tree

Monpole moment:

$$M = \sum_i m_i$$

Quadrupole tensor:

$$Q_{ij} = \sum_k m_k \left[3(\mathbf{x}_k - \mathbf{s})_i (\mathbf{x}_k - \mathbf{s})_j - \delta_{ij} (\mathbf{x}_k - \mathbf{s})^2 \right]$$

Resulting potential/force approximation:

$$\Phi(\mathbf{r}) = -G \left[\frac{M}{|\mathbf{y}|} + \frac{1}{2} \frac{\mathbf{y}^T \mathbf{Q}\, \mathbf{y}}{|\mathbf{y}|^5} \right]$$

For a single force evaluation, not *N* single-particle forces need to be computed, but **only of order *log(N)* multipoles**, depending on opening angle.

- The tree algorithm has no intrinsic restrictions for its dynamic range
- force accuracy can be conveniently adjusted to desired level
- the speed does depend only very weakly on clustering state
- geometrically flexible, allowing arbitrary geometries

TreePM force calculation algorithm

Particularly at high redshift, it is expensive to obtain accurate forces with the tree-algorithm

THE TREE-PM FORCE SPLIT

Periodic peculiar potential

$$\nabla^2\phi(\mathbf{x}) = 4\pi G[\rho(\mathbf{x}) - \overline{\rho}] = 4\pi G \sum_{\mathbf{n}} \sum_i m_i \left[\tilde{\delta}(\mathbf{x} - \mathbf{x}_i - \mathbf{n}L) - \frac{1}{L^3}\right]$$

Idea: Split the potential (of a single particle) in Fourier space into a long-range and a short-range part, and compute them separately with PM and TREE algorithms, respectively.

Poisson equation in Fourier space:

$$\phi_{\mathbf{k}} = -\frac{4\pi G}{\mathbf{k}^2}\rho_{\mathbf{k}} \qquad (\mathbf{k} \neq 0)$$

$$\phi_{\mathbf{k}}^{\text{long}} = \phi_{\mathbf{k}} \exp(-\mathbf{k}^2 r_s^2)$$

Solve with PM-method

- CIC mass assignment
- FFT
- multiply with kernel
- FFT backwards
- Compute force with 4-point finite difference operator
- Interpolate forces to particle positions

$$\phi_{\mathbf{k}}^{\text{short}} = \phi_{\mathbf{k}} \left[1 - \exp(-\mathbf{k}^2 r_s^2)\right]$$

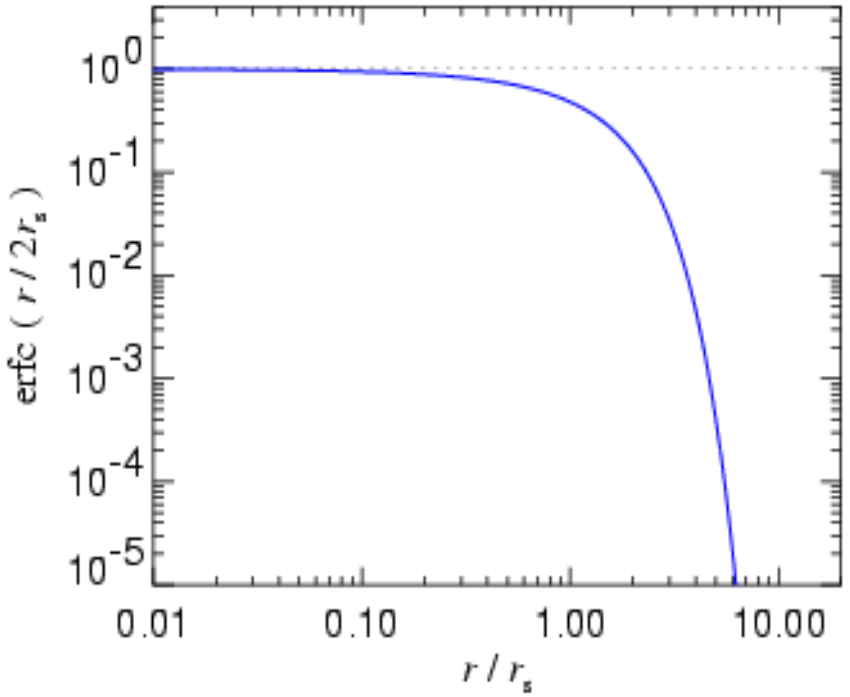
FFT to real space $\quad \phi(r) = -\frac{Gm}{r}\,\text{erfc}\left(\frac{r}{2r_s}\right)$

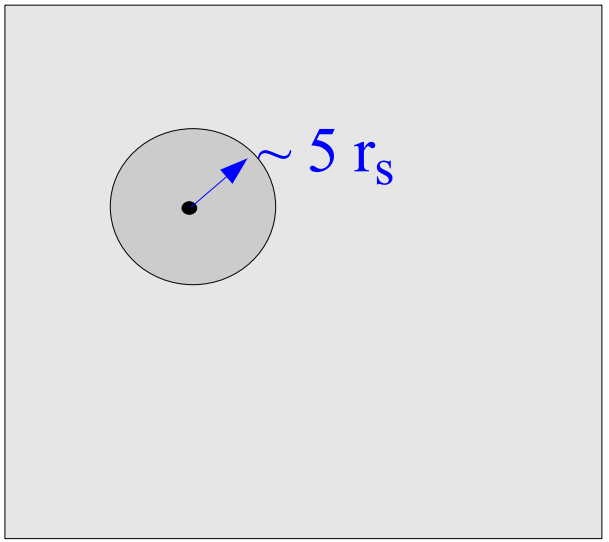
Solve in real space with TREE

In the TreePM algorithm, the tree has to be walked locally only

PERFORMANCE GAIN DUE TO LOCAL TREE WALK

$$\phi(r) = -\frac{Gm}{r}\,\mathrm{erfc}\left(\frac{r}{2r_s}\right)$$





Advantages of TreePM include:

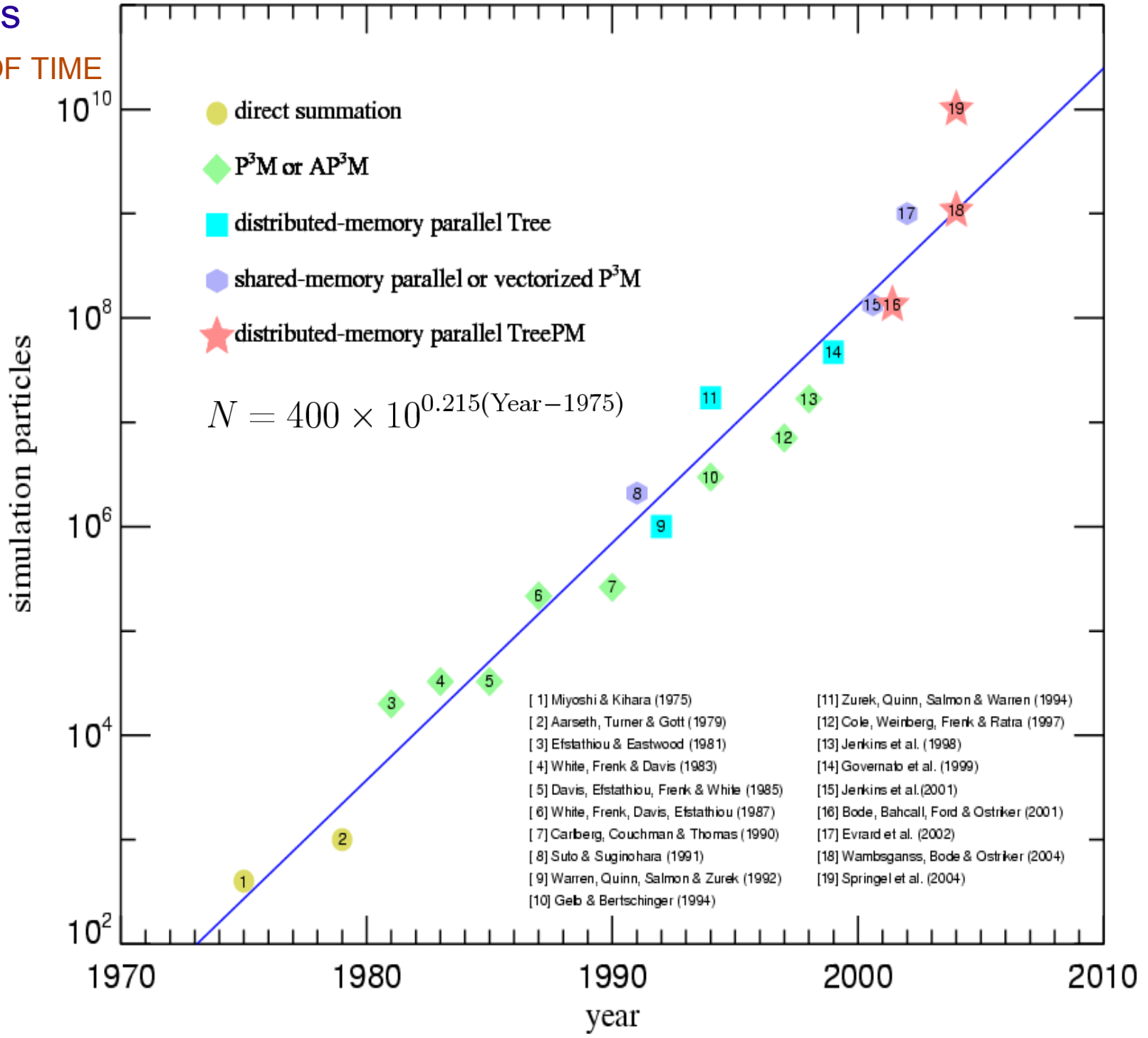
- Accurate and fast long-range force
- No force anisotropy
- Speed is largely insensitive to clustering (as for tree algorithm)
- No Ewald correction necessary for periodic boundary conditions

Using zero-padding and a different Greens-Function, the long-range force can also be computed for vaccuum boundaries using the FFT.
(Implemented in Gadget-2)

Cosmological N-body simulations have grown rapidly in size over the last three decades

"**N**" AS A FUNCTION OF TIME

- Computers double their speed every 18 months (Moore's law)
- N-body simulations have doubled their size every 16-17 months
- Recently, growth has accelerated further.
  The Millennium Run should have become possible in 2010 · we have done it in 2004 !



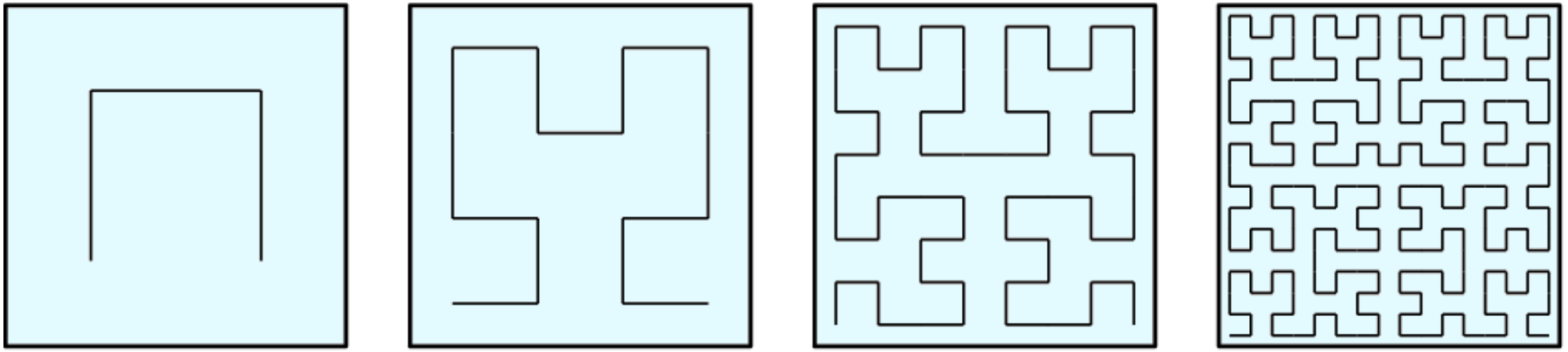
Organization of tree and domain decomposition

The tree-algorithm of Gadget-2 has been optimized for providing better memory locality

REDUCTION OF CACHE MISSES AND DOMAIN DECOMPOSITION

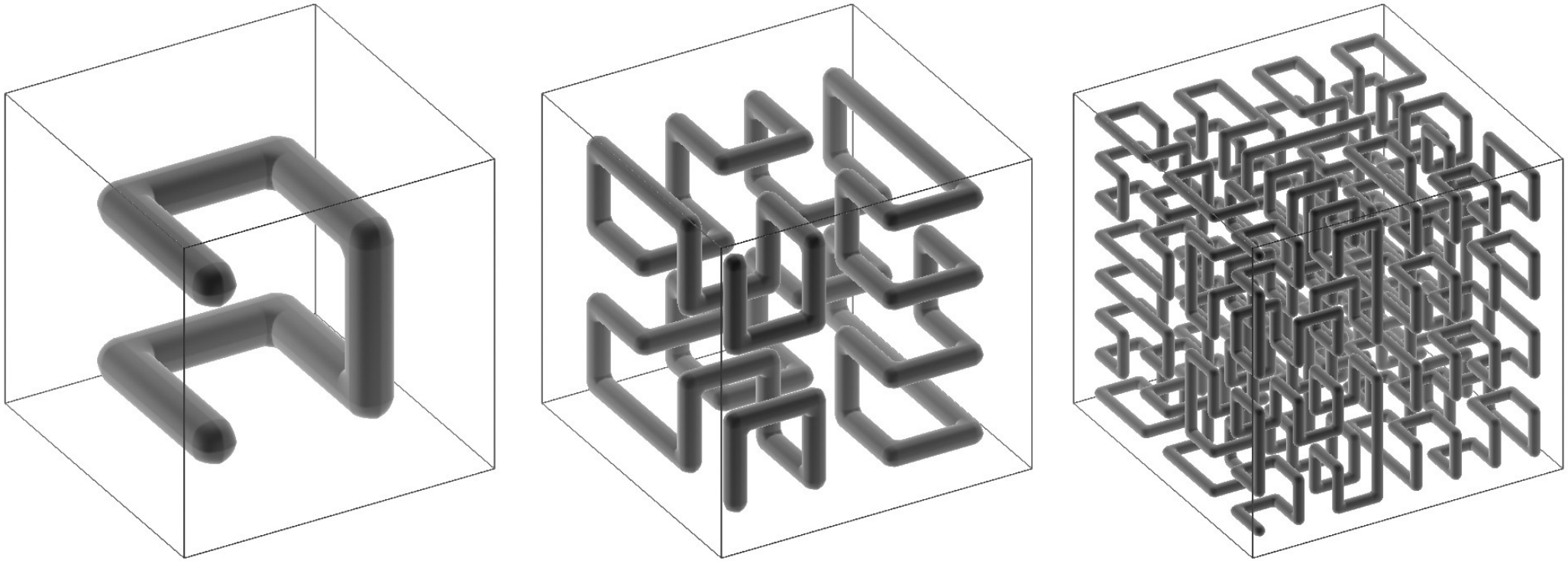
Idea: Order the particles along a space-filling curve

Hilbert's curve: A fractal that fills the square



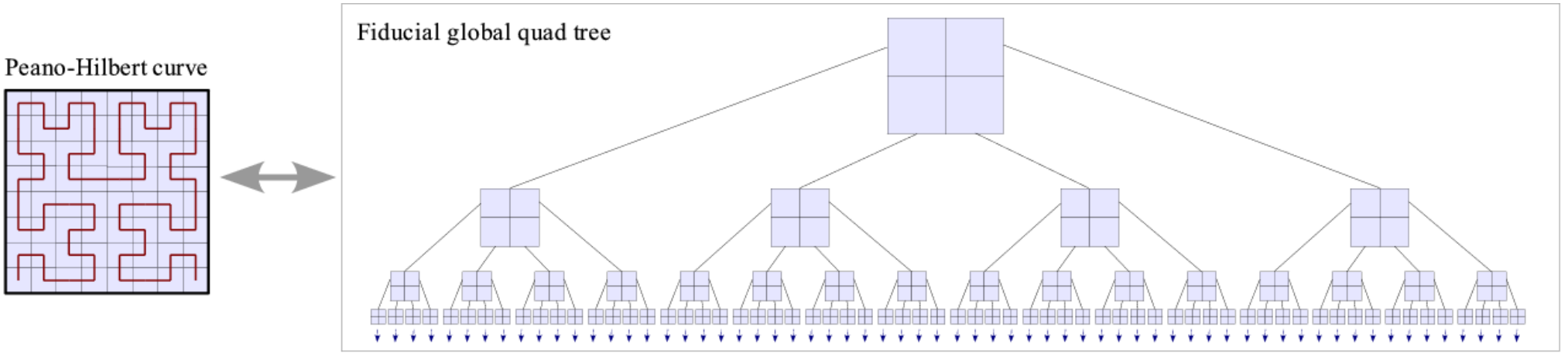
The space-filling Hilbert curve can be readily generalized to 3D

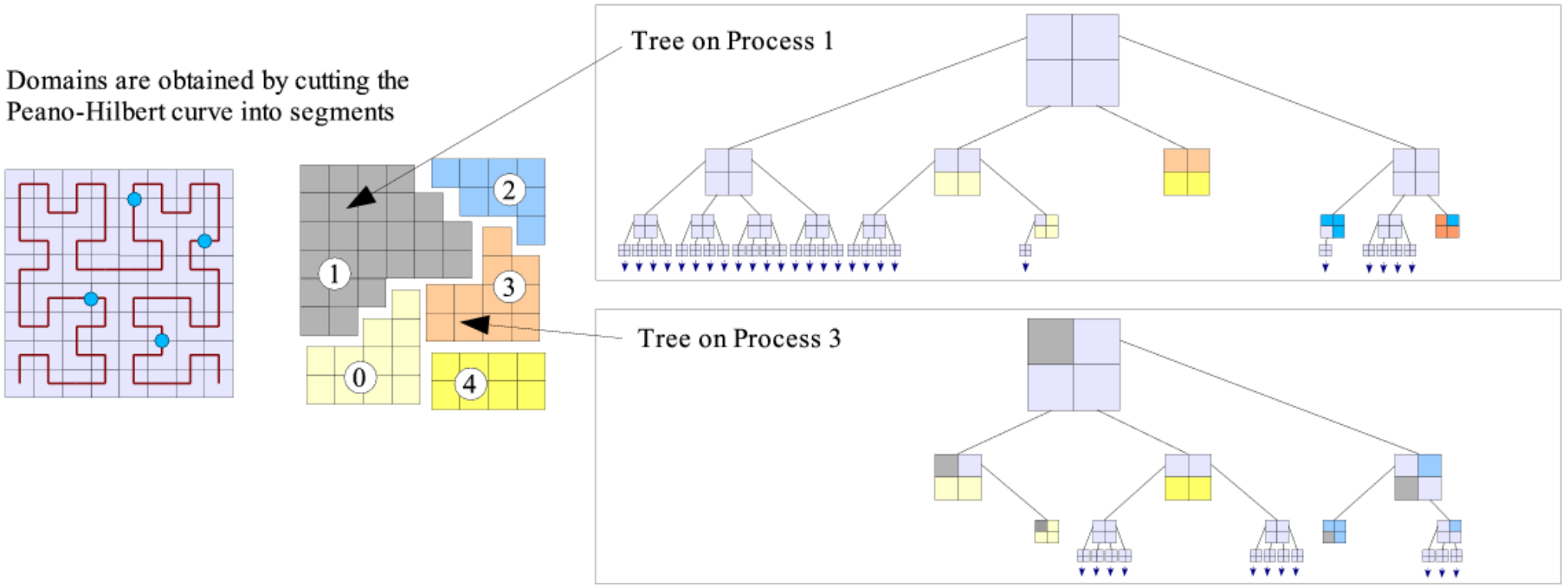
THE PEANO-HILBERT CURVE



A space-filling Peano-Hilbert curve is used in GADGET-2 for a novel domain-decomposition concept

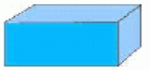
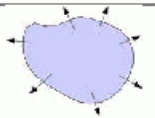
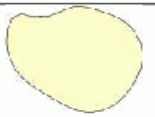
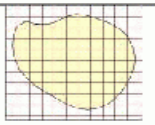
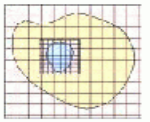
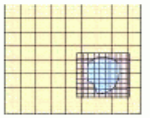
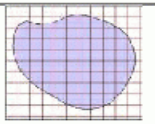
HIERARCHICAL TREE ALGORITHMS





GADGET2 supports different types of simulation set-ups

OVERVIEW OF TYPES OF SIMULATIONS POSSIBLE WITH GADGET

	Type of Simulation		Computational methods	Remarks
1	**Newtonian space**		Gravity: Tree, SPH (optional), vacuum boundary conditions	OmegaLambda should be set to zero
2	**Periodic long box**		No gravity, only SPH, periodic boundary conditions	NOGRAVITY needs to be set, LONG_X/Y/Z may be set to scale the dimensions of the box
3	**Cosmological, physical coordinates**		Gravity: Tree, SPH, vacuum boundaries	ComovingIntegrationOn set to zero
4	**Cosmological, comoving coordinates**		Gravity: Tree, SPH, vacuum boundaries	ComovingIntegrationOn set to one
5	**Cosmological, comoving periodic box**		Gravity: Tree with Ewald-correction, SPH, periodic boundaries	PERIODIC needs to be set
6	**Cosmological, comoving coordinates, TreePM**		Gravity: Tree with long range PM, SPH, vacuum boundaries	PMGRID needs to be set
7	**Cosmological, comoving periodic box, TreePM**		Gravity: Tree with long range PM, SPH, periodic boundaries	PERIODIC and PMGRID need to be set
8	**Cosmological, comoving coordinates, TreePM, Zoom**		Gravity: Tree with long-range and intermediate-range PM, SPH, vacuum boundaries	PMGRID and PLACEHIGHRESREGION need to be set
9	**Cosmological, periodic comoving box, TreePM, Zoom**		Gravity: Tree with long-range and intermediate-range PM, SPH, periodic boundaries	PERIODIC, PMGRID and PLACEHIGHRESREGION need to be set
10	**Newtonian space, TreePM**		Gravity: Tree with long-range PM, SPH, vacuum boundaries	PMGRID needs to be set

In a parallel code, numerous sources of performance losses can limit scalability to large processor numbers

TROUBLING ASPECTS OF PARALLELIZATION

- **Incomplete parallelization**
  The residual serial part in an application limits the theoretical speed-up one can achieve with an arbitrarily large number of CPUs ('Ahmdahl's Law'), e.g. 5% serial code left, then parallel speed-up is at most a factor 20.

- **Parallelization overhead**
  The bookkeeping code necessary for non-trivial communication algorithms increases the total cost compared to a serial algorithm. Sometimes this extra cost increases with the number of processors used.

- **Communication times**
  The time spent in waiting for messages to be transmitted across the network (bandwith) and the time required for starting a communication request (latency).

- **Wait times**
  Work-load imbalances will force the fastest CPU to idly wait for the slowest one.

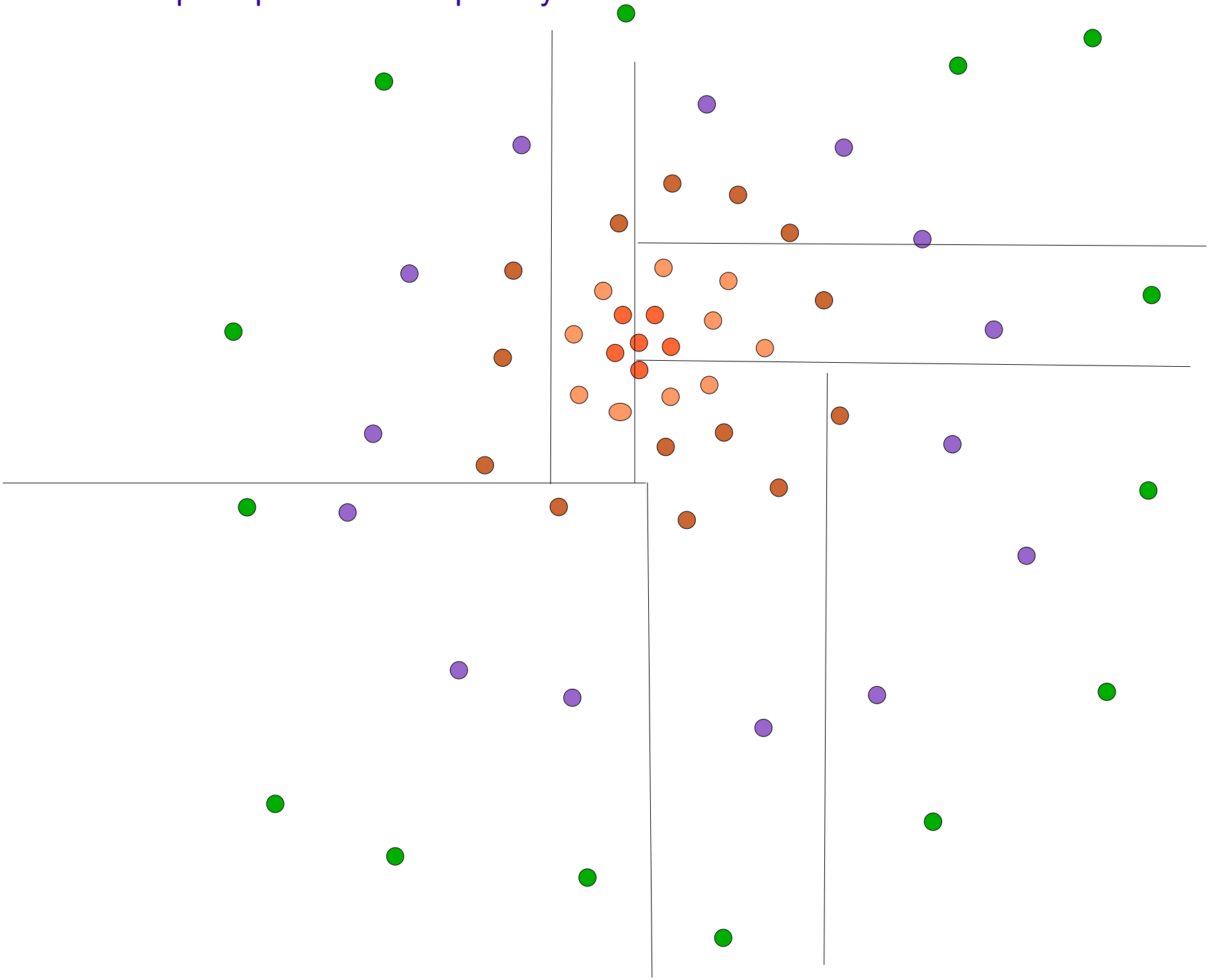
Strong scaling: Keep problem size fixed, but increase number of CPUs

Weak scaling: When number of CPUs is increased, also increase the problem size

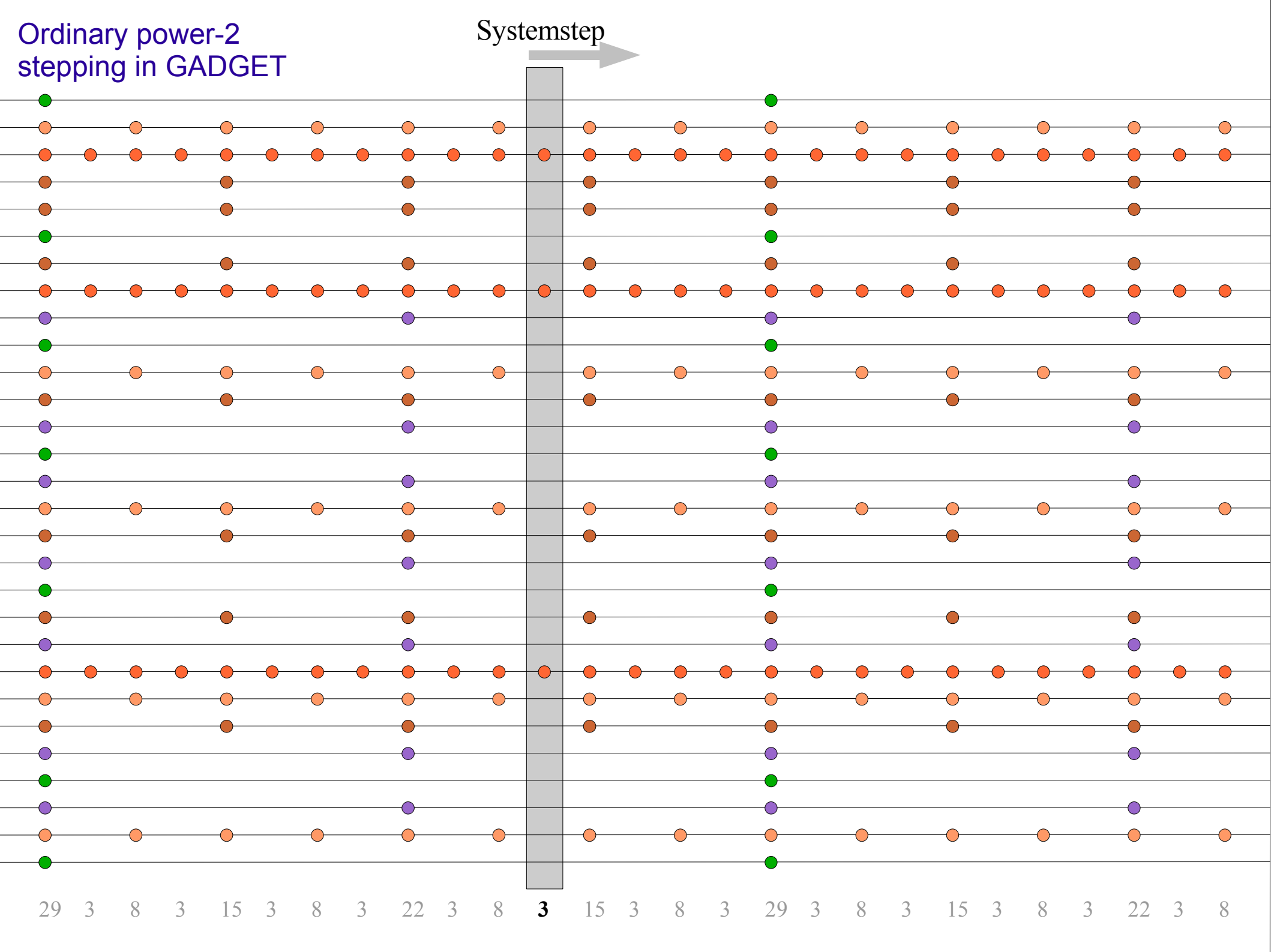
As a rule, scalability can be more easily retained in the weak scaling regime.

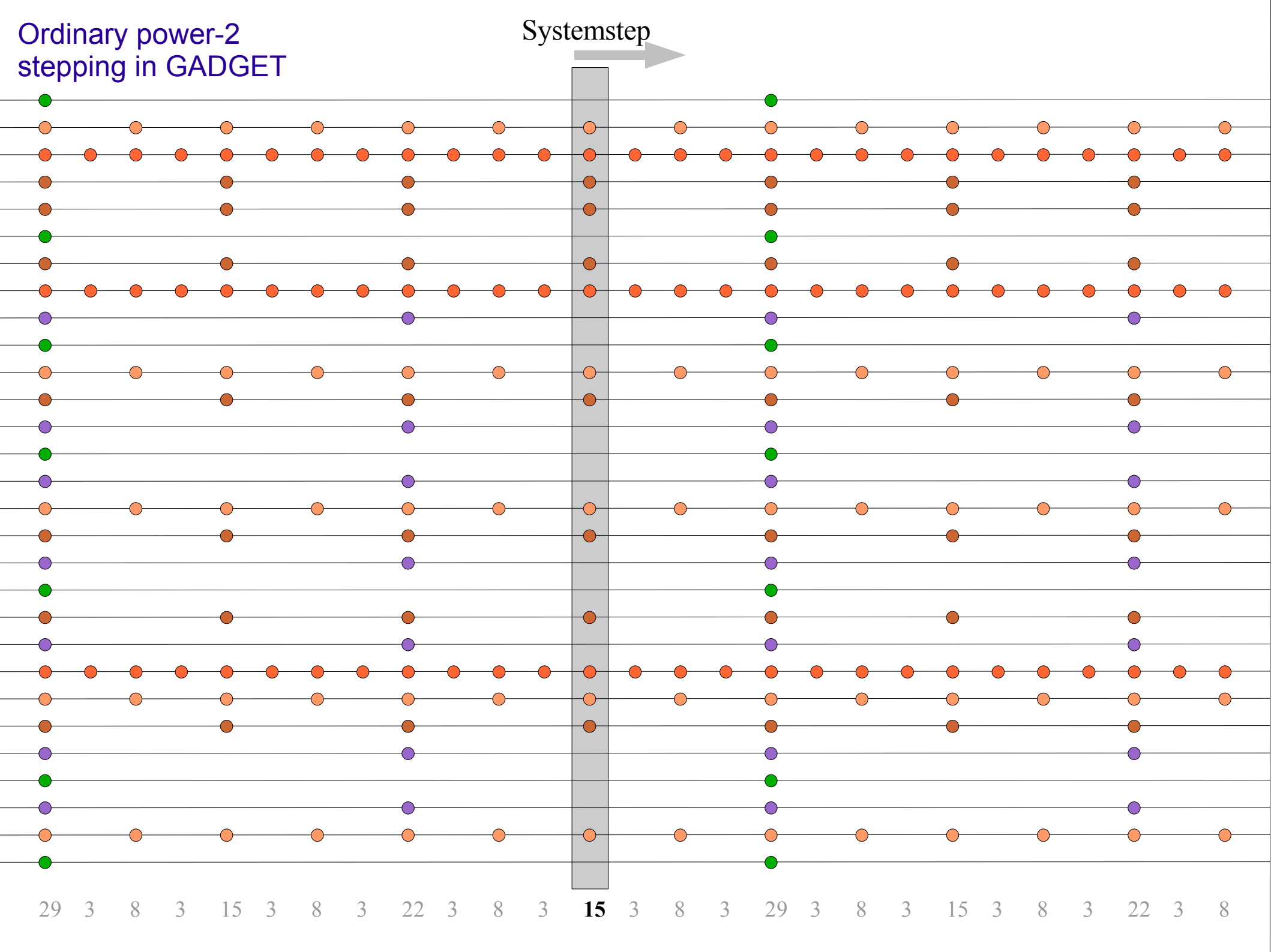
→ **In practice, it usually doesn't make sense to use a large number of processors for a (too) small problem size !**

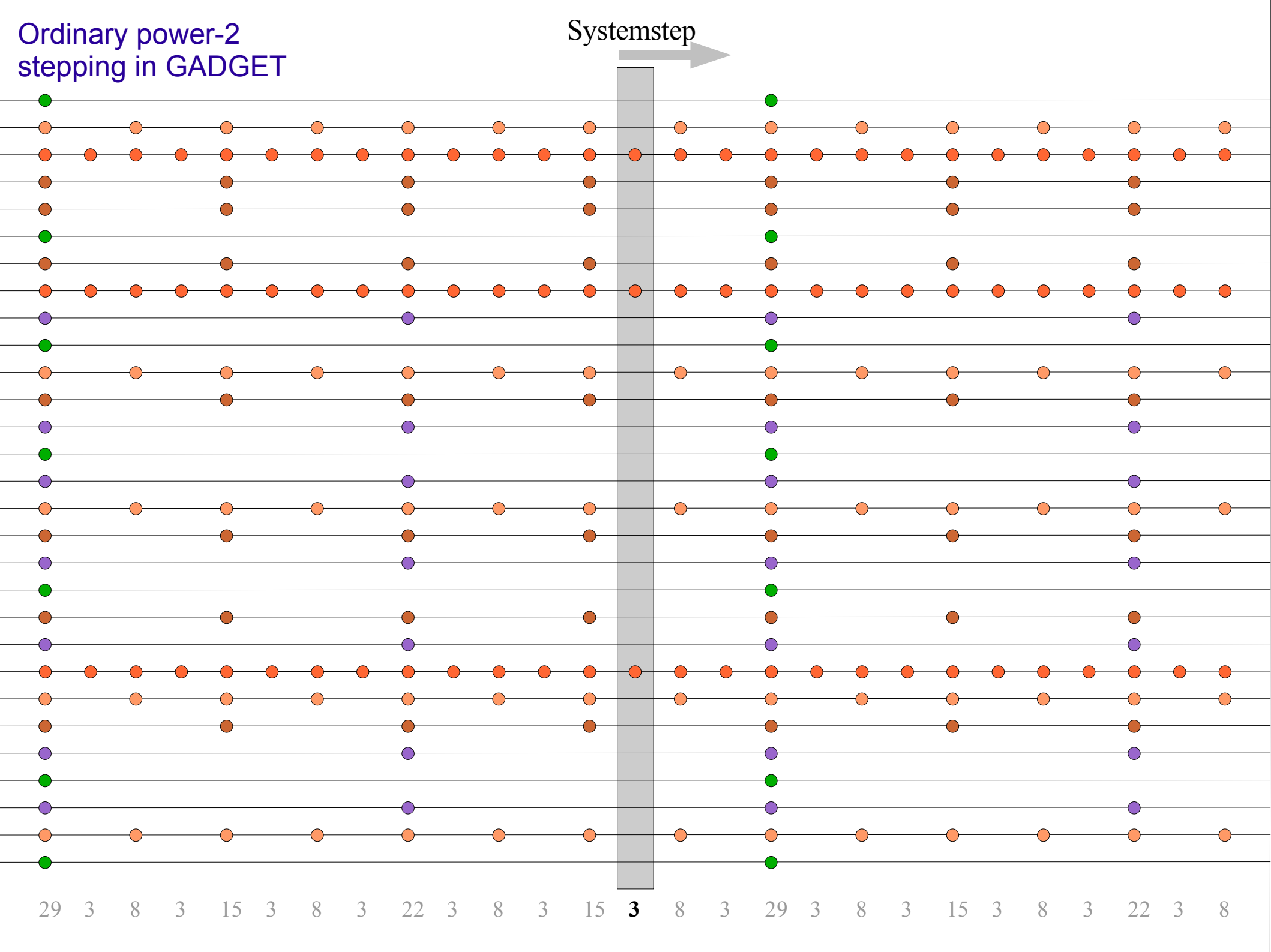
The time-steps of particles are spatially correlated

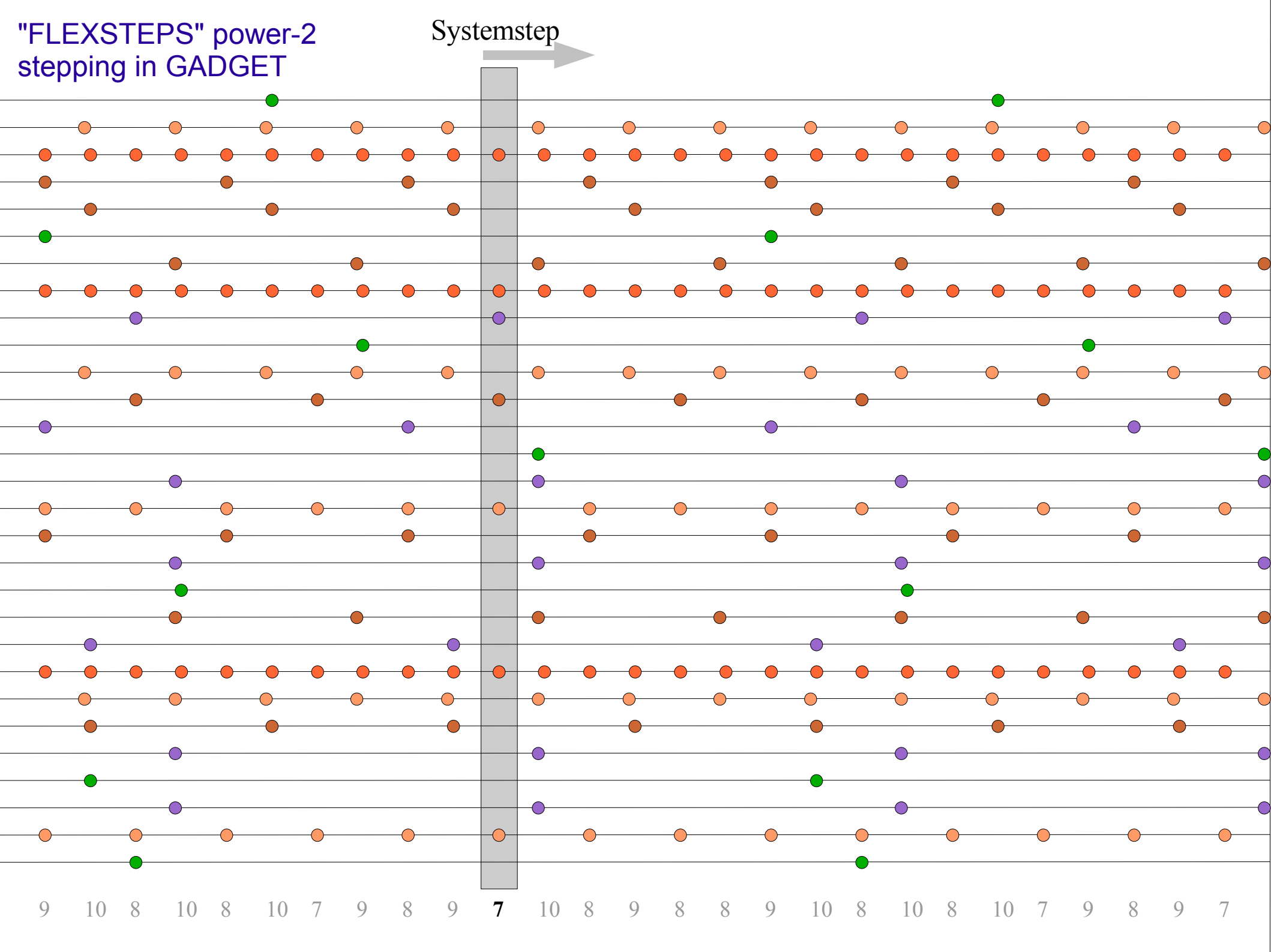



Ordinary power-2
stepping in GADGET
Systemstep
29 3 8 3 15 3 8 3 22 3 8 3 15 3 8 3 29 3 8 3 15 3 8 3 22 3 8


Ordinary power-2
stepping in GADGET
Systemstep
29 3 8 3 15 3 8 3 22 3 8 3 15 3 8 3 29 3 8 3 15 3 8 3 22 3 8

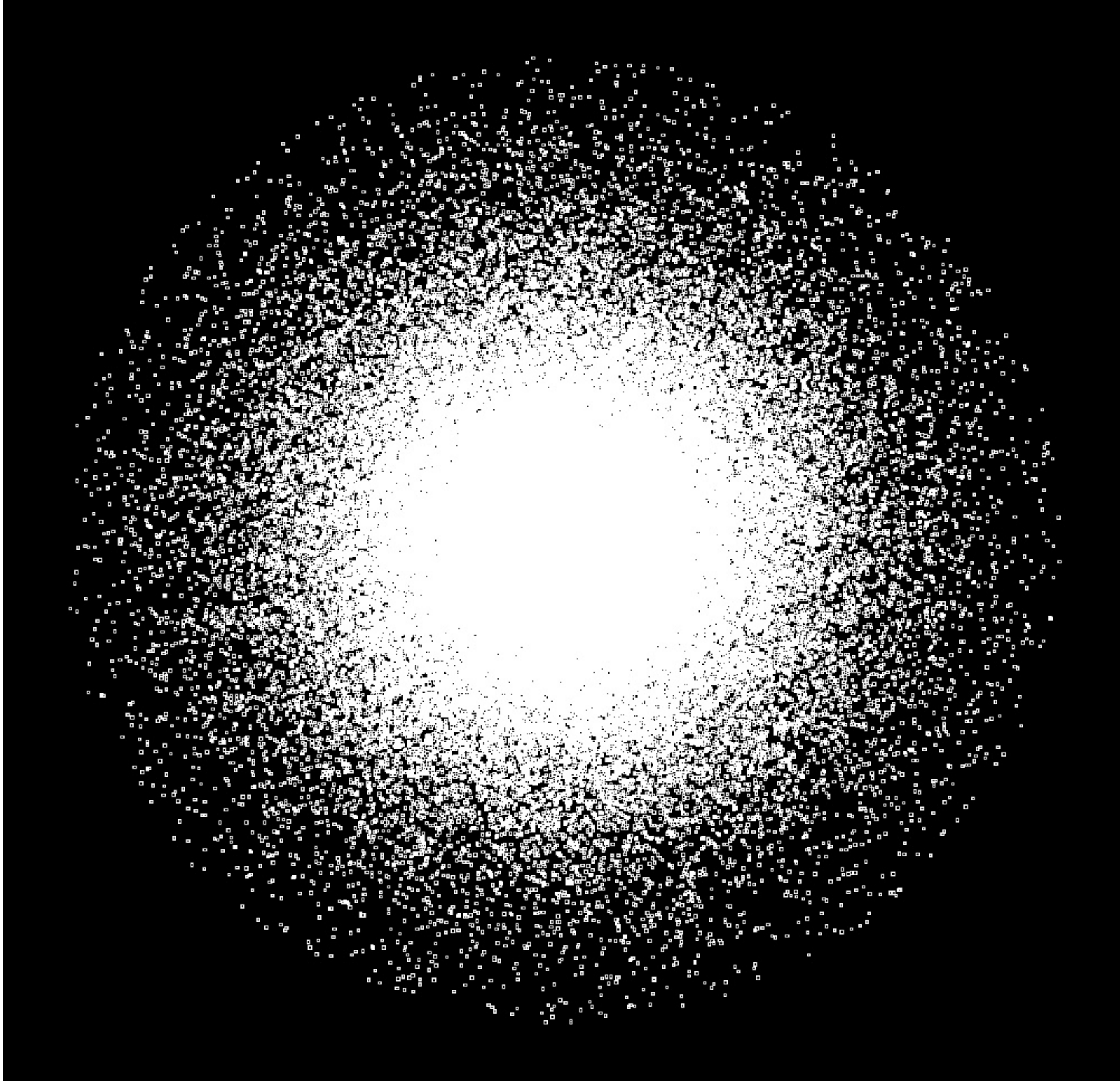

Ordinary power-2
stepping in GADGET
Systemstep
29 3 8 3 15 3 8 3 22 3 8 3 15 3 8 3 29 3 8 3 15 3 8 3 22 3 8


Ordinary power-2
stepping in GADGET
Systemstep
29 3 8 3 15 3 8 3 22 3 8 3 15 3 8 3 29 3 8 3 15 3 8 3 22 3 8


"FLEXSTEPS" power-2
stepping in GADGET
Systemstep
9 10 8 10 8 10 7 9 8 9 7 10 8 9 8 8 9 10 8 10 8 10 7 9 8 9 7

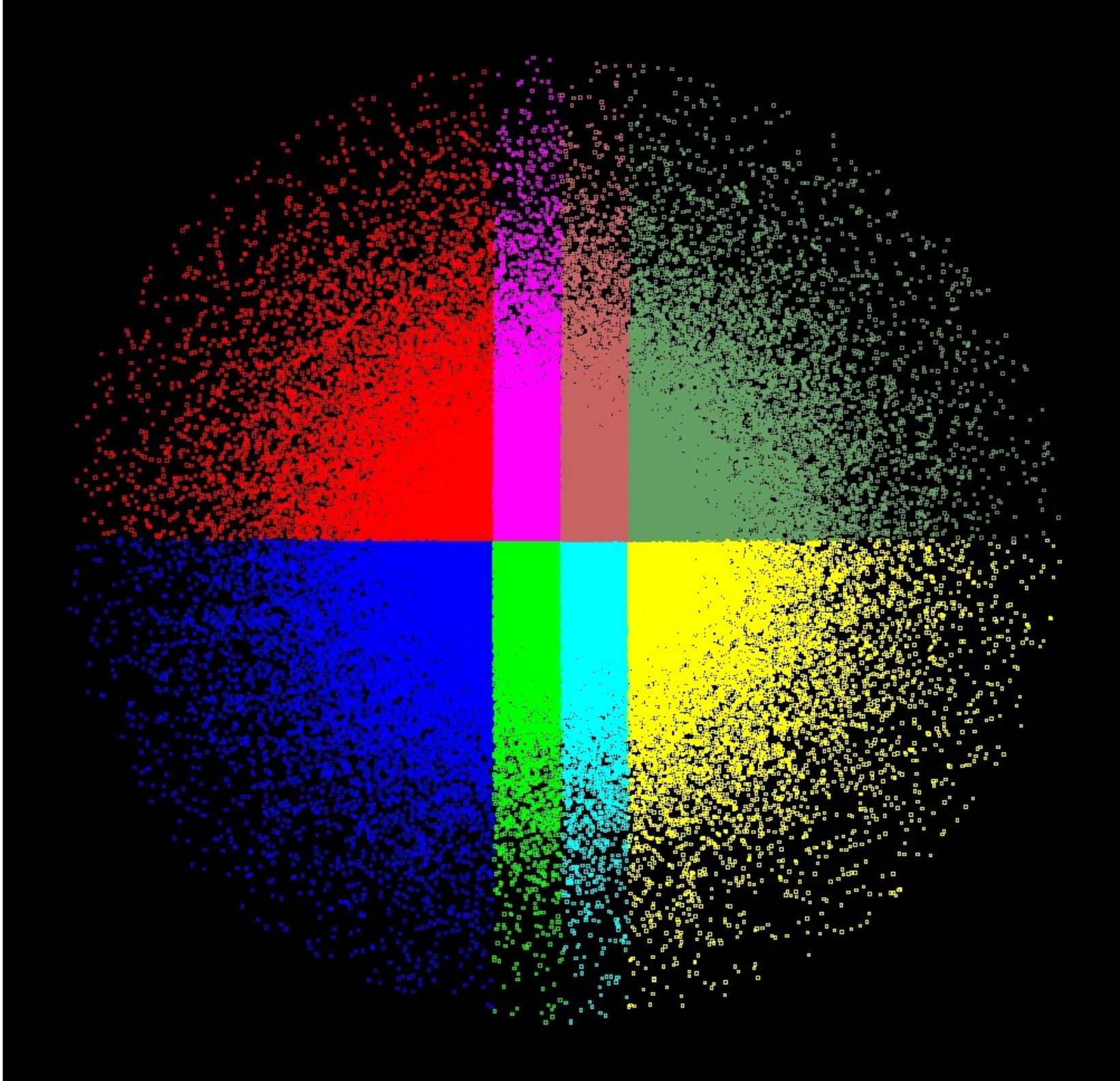
The inhomogeneous particle distribution and the different timesteps as a function of density make it challenging to find an optimum domain decomposition that balances work-load (and ideally memory-load)

PARTICLE DISTRIBUTION IN AN EXPONENTIAL DISK



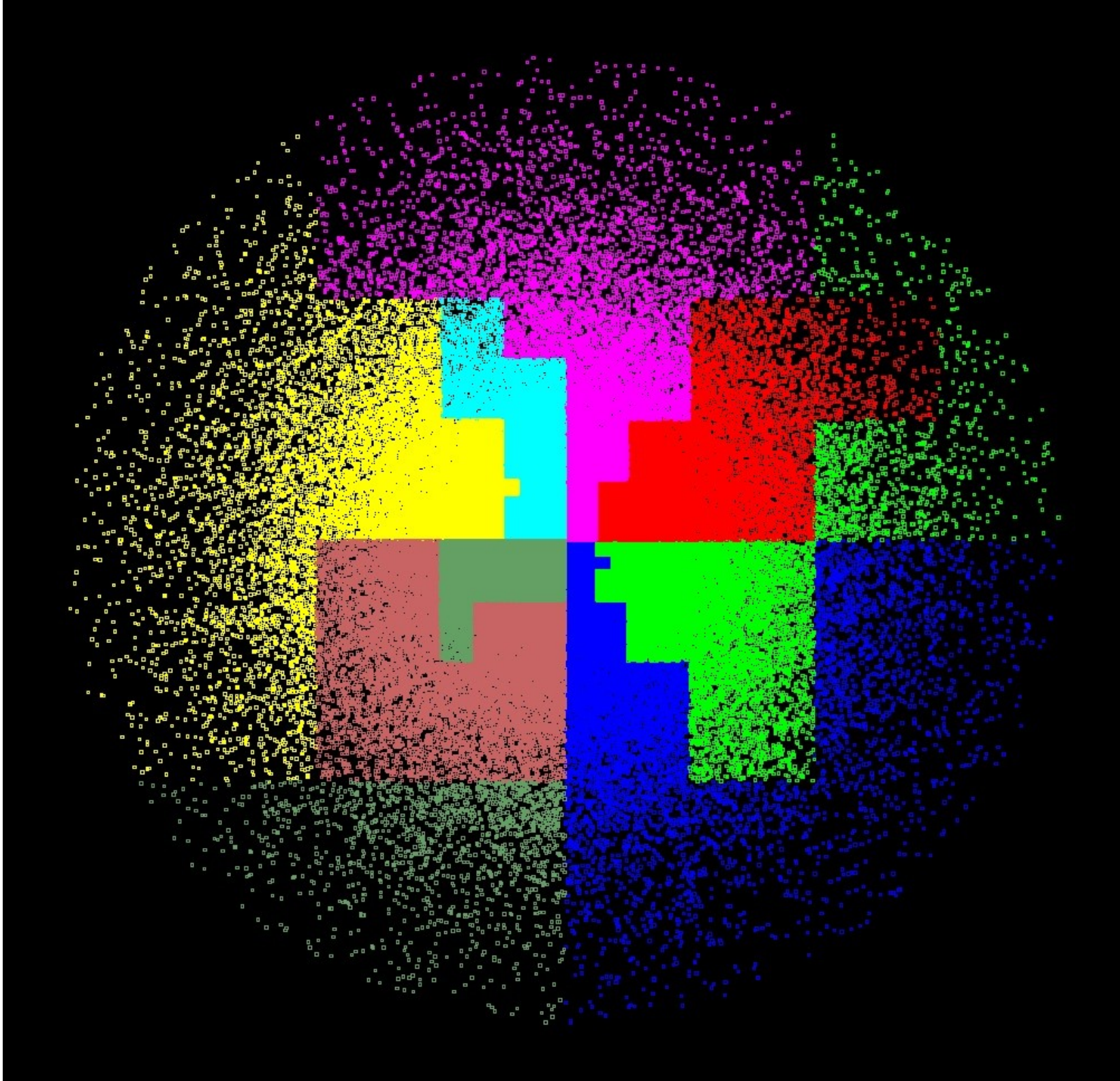
GADGET-1 used a simple orthogonal recursive bisection

EXAMPLE OF DOMAIN DECOMPOSITION IN GADGET-1



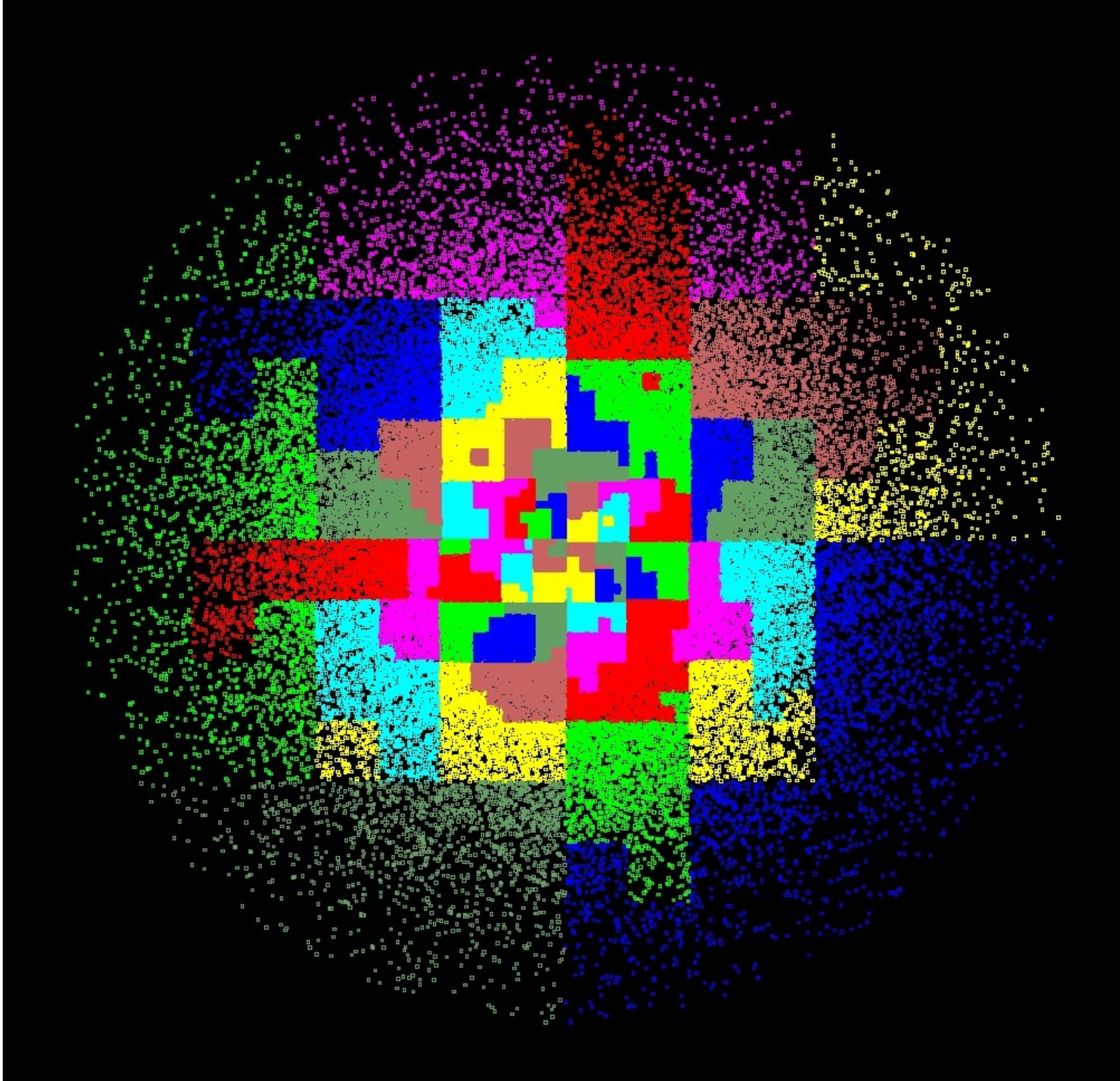
GADGET-2 uses a more flexible space-filling Peano-Hilbert curve

EXAMPLE OF DOMAIN DECOMPOSITION IN GADGET-2



GADGET-3 uses a space-filling Peano-Hilbert curve which is more flexible

EXAMPLE OF DOMAIN DECOMPOSITION IN GADGET-3



Basics of SPH

The baryons in the universe can be modelled as an *ideal* gas

BASIC HYDRODYNAMICAL EQUATIONS

Euler equation:

$$\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\frac{\nabla P}{\rho} - \nabla\Phi$$

Continuity equation:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho\nabla\cdot\mathbf{v} = 0$$

First law of thermodynamics:

$$\frac{\mathrm{d}u}{\mathrm{d}t} = -\frac{P}{\rho}\nabla\cdot\mathbf{v} - \frac{\Lambda(u,\rho)}{\rho}$$

Equation of state of ideal monoatomic gas:

$$P = (\gamma - 1)\rho u\ , \qquad \gamma = 5/3$$

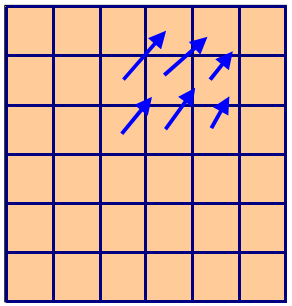
What is smoothed particle hydrodynamics?

DIFFERENT METHODS TO DISCRETIZE A FLUID

Eulerian

discretize space

representation on a mesh
(volume elements)



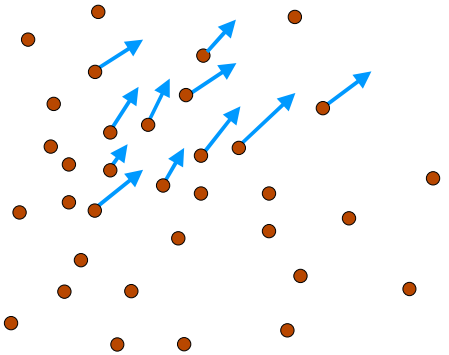
principle advantage:

high accuracy (shock capturing), low numerical viscosity

Lagrangian

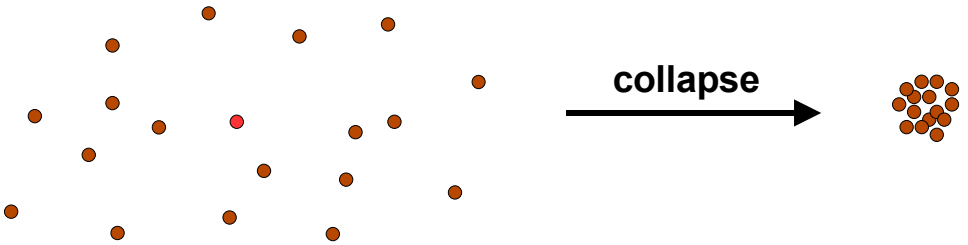
discretize mass

representation by fluid elements
(particles)



principle advantage:

resolutions adjusts automatically to the flow

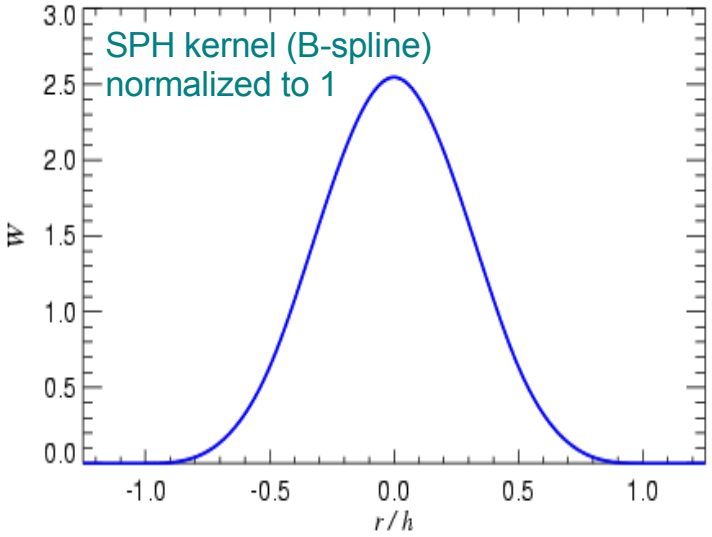


Kernel interpolation is used in smoothed particle hydrodynamics (SPH) to build continous fluid quantities from discrete tracer particles

DENSITY ESTIMATION IN SPH BY MEANS OF ADAPTIVE KERNEL ESTIMATION

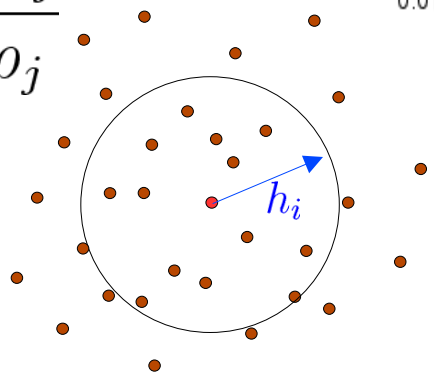
Kernel interpolant of an arbitrary function:

$$\langle A(\mathbf{r})\rangle = \int W(\mathbf{r}-\mathbf{r}', h)\, A(\mathbf{r}')\, \mathrm{d}^3 r'$$



If the function is only known at a set of discrete points, we approximate th integral as a sum, using the replacement:

$$\mathrm{d}^3 r' \mapsto \frac{m_j}{\rho_j}$$



$$\langle A_i\rangle = \sum_{j=1}^{N} \frac{m_j}{\rho_j}\, A_j\, W(\mathbf{r}_{ij}; h_i)$$

This leads to the SPH density estimate, for $A_i = \rho_i$

$$\rho_i = \sum_{j=1}^{N} m_j W(|\mathbf{r}_{ij}|, h_i)$$

→ **This can be differentiated !**

Kernel interpolants allow the construction of derivatives from a set of discrete tracer points

EXAMPLES FOR ESTIMATING THE VELOCITY DIVERGENCE

Smoothed estimate for the velocity field:

$$\langle \mathbf{v}_i \rangle = \sum_j \frac{m_j}{\rho_j} \mathbf{v}_j W(\mathbf{r}_i - \mathbf{r}_j)$$

Velocity divergence can now be readily estimated:

$$\nabla \cdot \mathbf{v} = \nabla \cdot \langle \mathbf{v}_i \rangle = \sum_j \frac{m_j}{\rho_j} \mathbf{v}_j \nabla_i W(\mathbf{r}_i - \mathbf{r}_j)$$

But alternative (and better) estimates are possible also:

Invoking the identity

$$\rho \nabla \cdot \mathbf{v} = \nabla \cdot (\rho \mathbf{v}) - \mathbf{v} \cdot \nabla \rho$$

one gets a „pair-wise‰ formula:

$$\rho_i (\nabla \cdot \mathbf{v})_i = \sum_j m_j (\mathbf{v}_j - \mathbf{v}_i) \nabla_i W(\mathbf{r}_i - \mathbf{r}_j)$$

What is smoothed particle hydrodynamics?

BASIC EQUATIONS OF SMOOTHED PARTICLE HYDRODYNAMICS

Each particle carries either the energy or the entropy per unit mass as independent variable

Density estimate

$$\rho_i = \sum_{j=1}^{N} m_j W(|\mathbf{r}_{ij}|, h_i)$$

→ **Continuity equation automatically fulfilled.**

$$\rightarrow P_i = (\gamma - 1)\rho_i u_i$$

Euler equation

$$\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = -\sum_{j=1}^{N} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij} \right) \nabla_i \overline{W}_{ij}$$

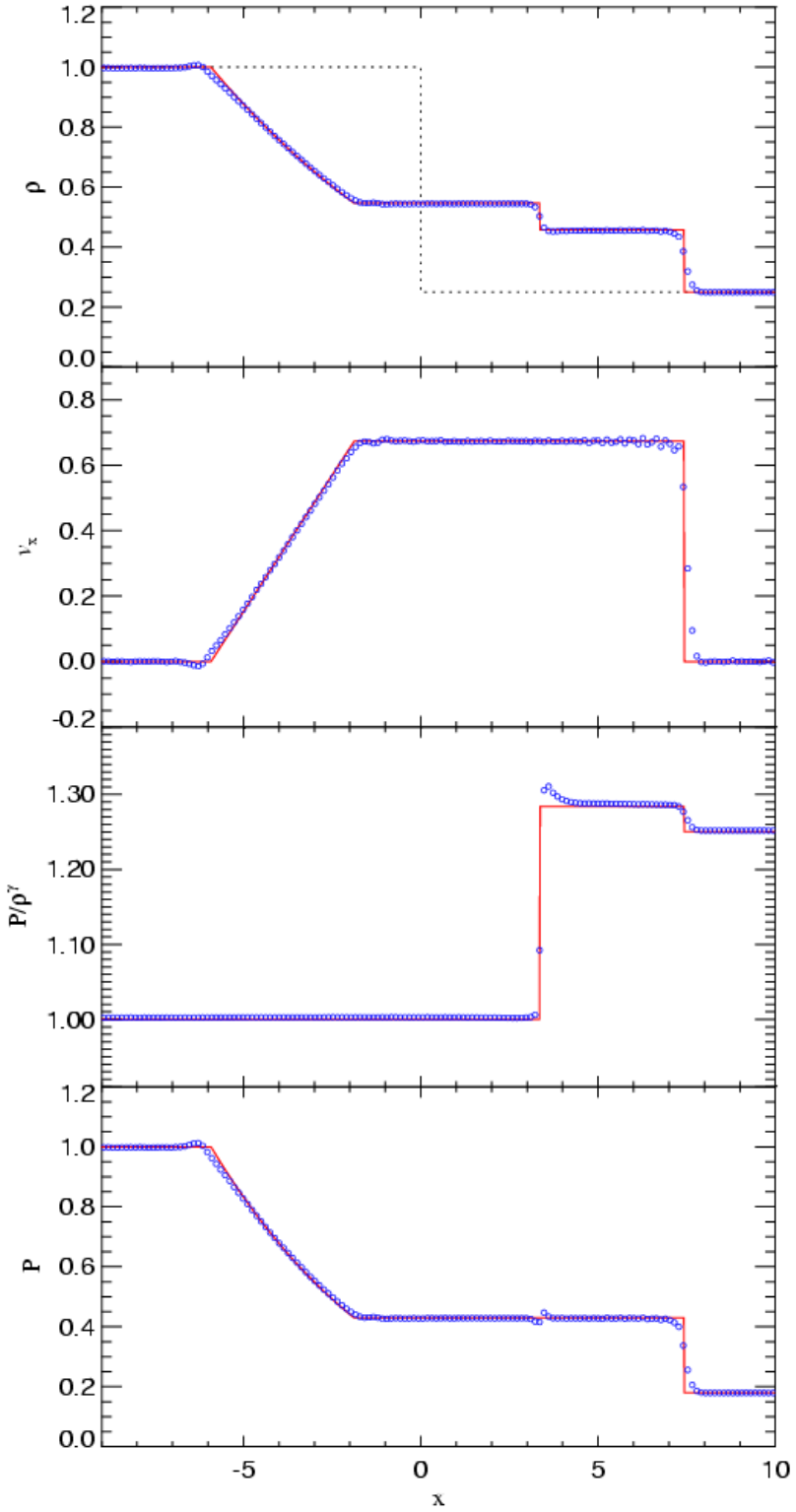
$+\Pi_{ij}$ **Artificial viscosity**

First law of thermodynamics

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \frac{1}{2} \sum_{j=1}^{N} m_j \left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2} + \Pi_{ij} \right) \mathbf{v}_{ij} \cdot \nabla_i \overline{W}_{ij}$$

$+\Pi_{ij}$

Viscosity and shock capturing



An artificial viscosity needs to be introduced to capture shocks

SHOCK TUBE PROBLEM AND VISCOSITY

viscous force:

$$\left.\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t}\right|_{\mathrm{visc}} = -\sum_{j=1}^{N} m_j \Pi_{ij} \nabla_i \overline{W}_{ij}$$

parameterization of the artificial viscosity:

$$\Pi_{ij} = \begin{cases} -\frac{\alpha}{2}\frac{[c_i + c_j - 3w_{ij}]w_{ij}}{\rho_{ij}} & \text{if } \mathbf{v}_{ij}\cdot\mathbf{r}_{ij} < 0 \\ 0 & \text{otherwise} \end{cases}$$

$$v_{ij}^{\mathrm{sig}} = c_i + c_j - 3w_{ij},$$

$$w_{ij} = \mathbf{v}_{ij}\cdot\mathbf{r}_{ij}/|\mathbf{r}_{ij}|$$

heat production rate:

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} = \frac{1}{2}\sum_{j=1}^{N} m_j \Pi_{ij}\mathbf{v}_{ij}\cdot\nabla_i \overline{W}_{ij}$$

Variational derivation of SPH

The traditional way to derive the SPH equations leaves room for many different formulations

SYMMETRIZATION CHOICES

Symmetrized kernel:

$$\overline{W}_{ij} = W(|\mathbf{r}_{ij}|, [h_i + h_j]/2)$$

$$\overline{W}_{ij} = \frac{1}{2}\left[W(|\mathbf{r}_{ij}|, h_i) + W(|\mathbf{r}_{ij}|, h_j)\right]$$

Symmetrization of pressure terms:

Using $\nabla P = 2\sqrt{P}\nabla\sqrt{P}$

$$\frac{1}{2}\left(\frac{P_i}{\rho_i^2} + \frac{P_j}{\rho_j^2}\right) \iff \sqrt{\frac{P_i\, P_j}{\rho_i^2\, \rho_j^2}}$$

Is there a best choice?

For an adiabatic flow, temperature can be derived from the specific entropy

ENTROPY FORMALISM

Definition of an **entropic function**:

$$P_i = A_i \, \rho_i^{\gamma}$$

for an adiabtic flow:

$$A_i = A_i(s_i) = \text{const.}$$

don't intergrate the temperature, but infer it from:

$$u_i = \frac{A_i}{\gamma - 1} \rho^{\gamma - 1}$$

Use an artificial viscosity to generate entropy in shocks:

$$\frac{\mathrm{d}A_i}{\mathrm{d}t} = \frac{1}{2} \frac{\gamma - 1}{\rho_i^{\gamma - 1}} \sum_{j=1}^{N} m_j \Pi_{ij} \mathbf{v}_{ij} \cdot \nabla_i \overline{W}_{ij}$$

None of the adaptive SPH schemes conserves energy and entropy simultaneously

CONSERVATION LAW TROUBLES

Hernquist (1993):

> If the **thermal energy** is **integrated**, **entropy** conservation can be **violated**...
>
> If the **entropy** is **integrated**, total **energy** is **not** necessarily **conserved**...

The trouble is caused by varying smoothing lengths... ∇h-terms

Do we have to worry about this? **YES**

Can we do better? **YES**

A fully conservative formulation of SPH

DERIVATION

Springel & Hernquist (2002)

Lagrangian:

$$L(\mathbf{q},\dot{\mathbf{q}}) = \frac{1}{2}\sum_{i=1}^{N} m_i \dot{\mathbf{r}}_i^2 - \frac{1}{\gamma-1}\sum_{i=1}^{N} m_i A_i \rho_i^{\gamma-1}$$

$$\mathbf{q} = (\mathbf{r}_1, \ldots, \mathbf{r}_N, h_1, \ldots, h_N)$$

Constraints:

$$\phi_i(\mathbf{q}) \equiv \frac{4\pi}{3} h_i^3 \rho_i - M_{\rm sph} = 0$$

Equations of motion:

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = \sum_{j=1}^{N} \lambda_j \frac{\partial \phi_j}{\partial q_i}$$

$$\frac{\mathrm{d}\mathbf{v}_i}{\mathrm{d}t} = -\sum_{j=1}^{N} m_j \left[f_i \frac{P_i}{\rho_i^2} \nabla_i W_{ij}(h_i) + f_j \frac{P_j}{\rho_j^2} \nabla_i W_{ij}(h_j) \right]$$

$$f_i = \left[1 + \frac{h_i}{3\rho_i} \frac{\partial \rho_i}{\partial h_i} \right]^{-1}$$

Movies

- Millennium Simulation, zoom in, flight through.
- Shock hits cloud test.
- Colliding Galaxies with Black Hole
- Fly though gas in galaxy cluster static, evolving.
- Substructure of galaxy clusters.
- Formation of a galaxy clusters (gas,stars).