High performance computing and numerical modeling

Volker Springel

Plan for my lectures

Lecture 1: Collisional and collisionless N-body dynamics

Lecture 2: Gravitational force calculation

Lecture 3: Basic gas dynamics

Lecture 4: Smoothed particle hydrodynamics

Lecture 5: Eulerian hydrodynamics

Lecture 6: Moving-mesh techniques

Lecture 7: Towards high dynamic range

Lecture 8: Parallelization techniques and current computing trends

Heidelberg Institute for Theoretical Studies
HITS

Universität Heidelberg

43rd Saas Fee Course
Villars-Sur-Ollon, March 2013

Calculating gravitational forces

Direct summation calculates the gravitational field **exactly**

FORCE ACCURACY IN COLLISIONLESS SIMULATIONS

Direct summation approch:

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

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

N^2 complexity

Are ***approximate*** force calculations sufficient?

Yes, provided the force errors are random and small enough.

Since the N-body force field is noisy anyway, small random errors will only insignificantly reduce the relaxation time.

Systematic errors in the force, or error correlations are however very problematic.

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:

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

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

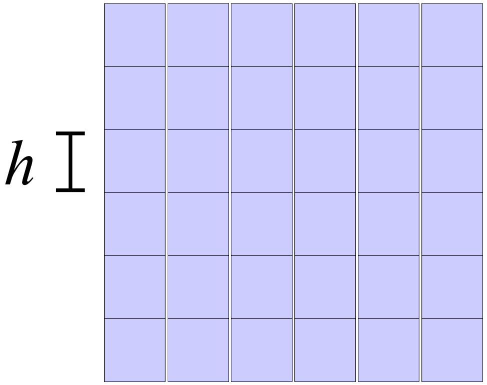
$$\hat{\Phi}(\mathbf{k}) = \hat{g}(\mathbf{k})\cdot\hat{\rho}(\mathbf{k})$$

→ **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:

$$W(\mathbf{x}) = \Pi\left(\frac{\mathbf{x}}{h}\right) \star S(\mathbf{x})$$

where

$$\Pi(x) = \begin{cases} 1 & \text{for } |x| \leq \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$$

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

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

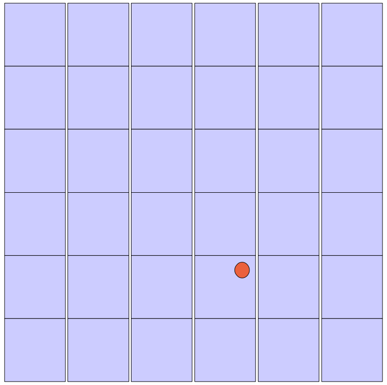
Commenly used particle shape functions and assignment schemes

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 $\mathbf{f} = -\nabla\Phi$ by 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

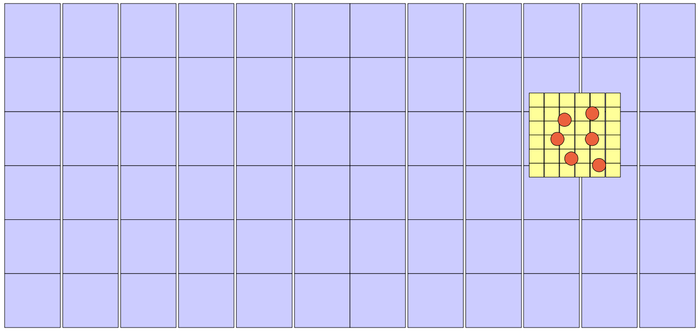
→ we need a method to increase the **dynamic range** available in the force calculation

Particle-Particle PM schemes (P^{3}M)

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^{3}M, 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^{3}M: **HYDRA** (Couchman)

Iterative Poisson solvers can determine the potential directly on a (hierarchical) grid

Idea: Start with a trial potential and then iteratively relax the solution by updating with a finite difference approximation to the Laplacian.

$$\Phi'_{i,j,k} = \frac{1}{6}\left(\Phi_{i+1,j,k} + \Phi_{i-1,j,k} + \Phi_{i,j+1,k} + \Phi_{i,j-1,k} + \Phi_{i,j,k+1} + \Phi_{i,j,k-1} - 4\pi G h^2 \rho_{i,j,k}\right)$$

This updating eliminates errors on the scale of a few grid cells rapidly, but longer-range fluctuations die out much more slowly.

In **multigrid methods**, a hierarchy of meshes is used to speed up convergence, resulting in a fast method that allows for locally varying resolution.

Examples for codes that use a real-space Poisson solver:

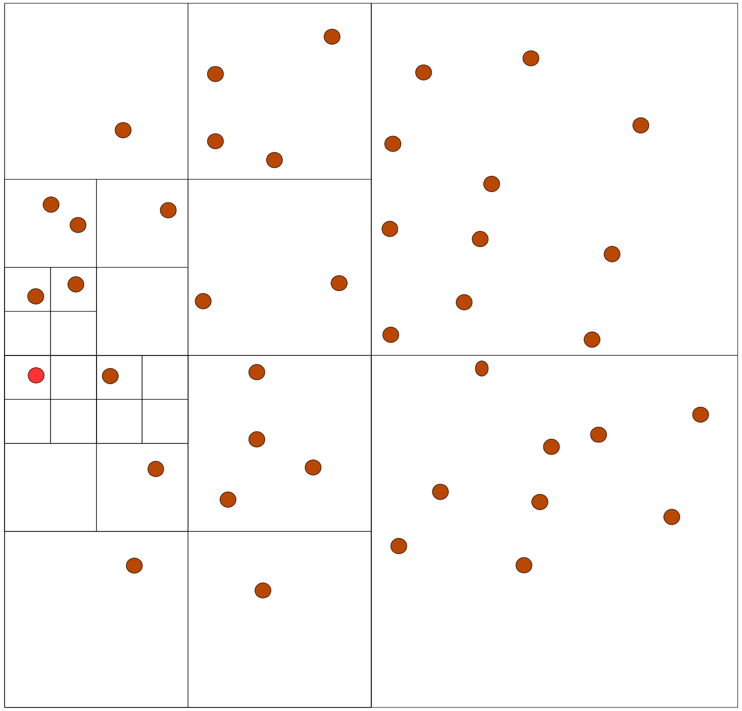
RAMSES	(Teyssier)
ART	(Kravtsov)
MLAPM	(Knebe)

On adaptive meshes, sometimes a combination of Fourier techniques and real-space solvers is used.

TREE algorithms

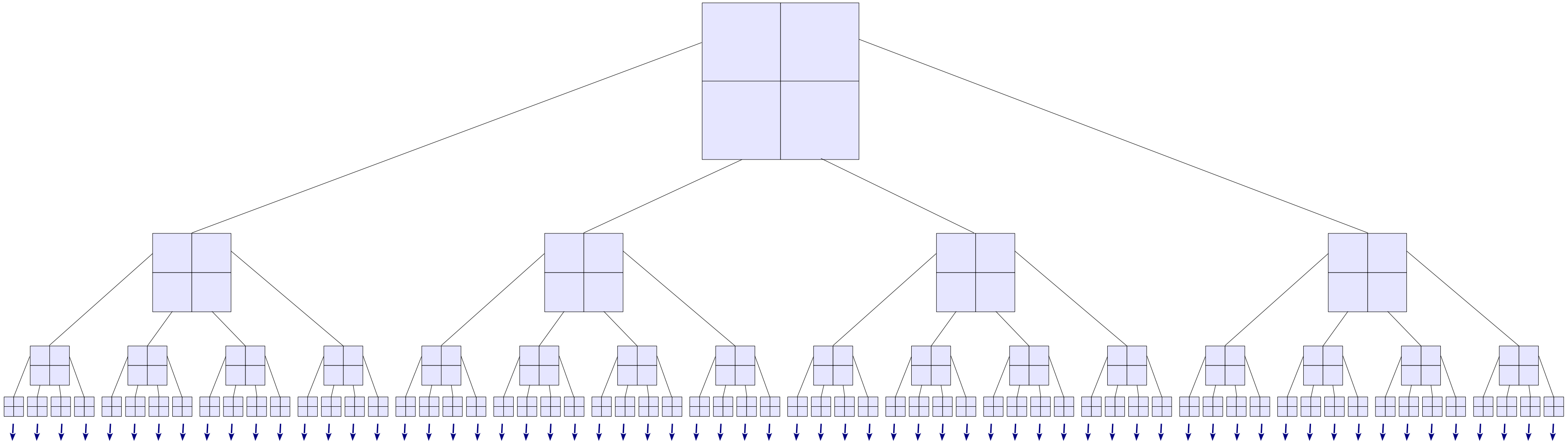
Tree algorithms approximate the force on a point with a multipole expansion

HIERARCHICAL TREE ALGORITHMS



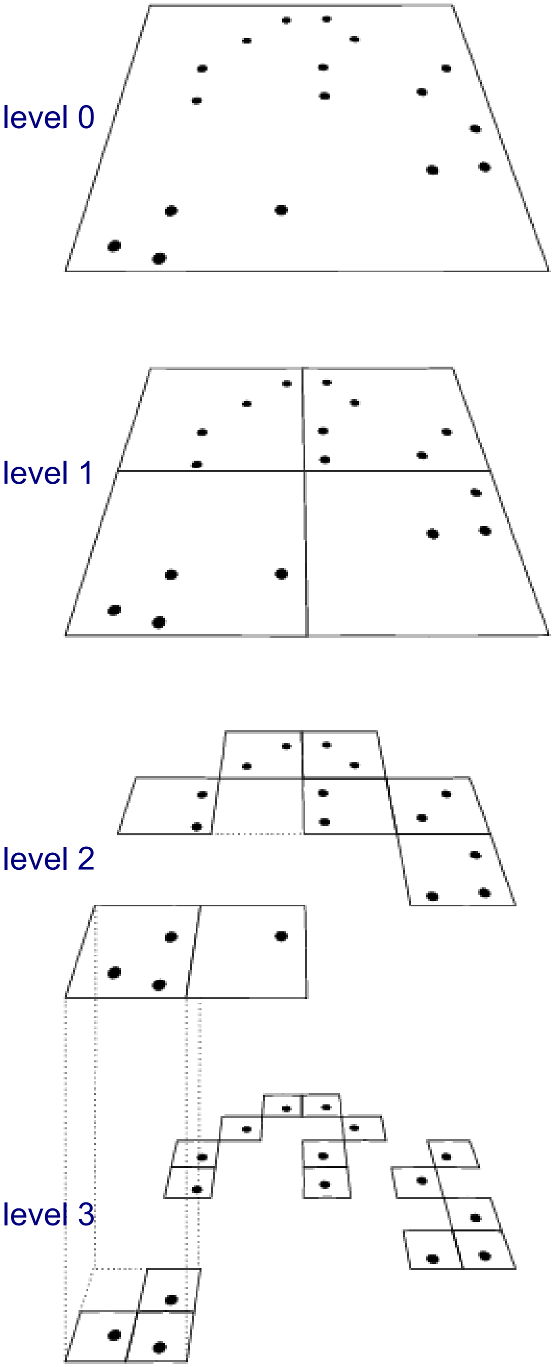
Idea: Group distant particles together, and use their multipole expansion.

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



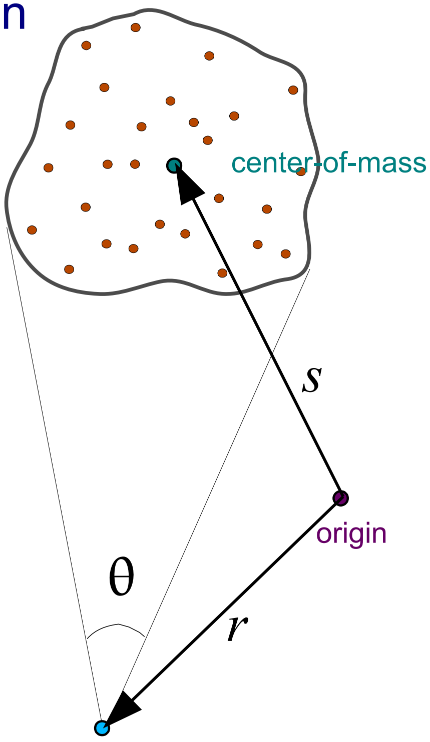
Tree algorithms

Oct-tree in two dimensions



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

and obtain:

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

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: Mass and center-of-mass

$$M = \sum_i m_i$$

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:

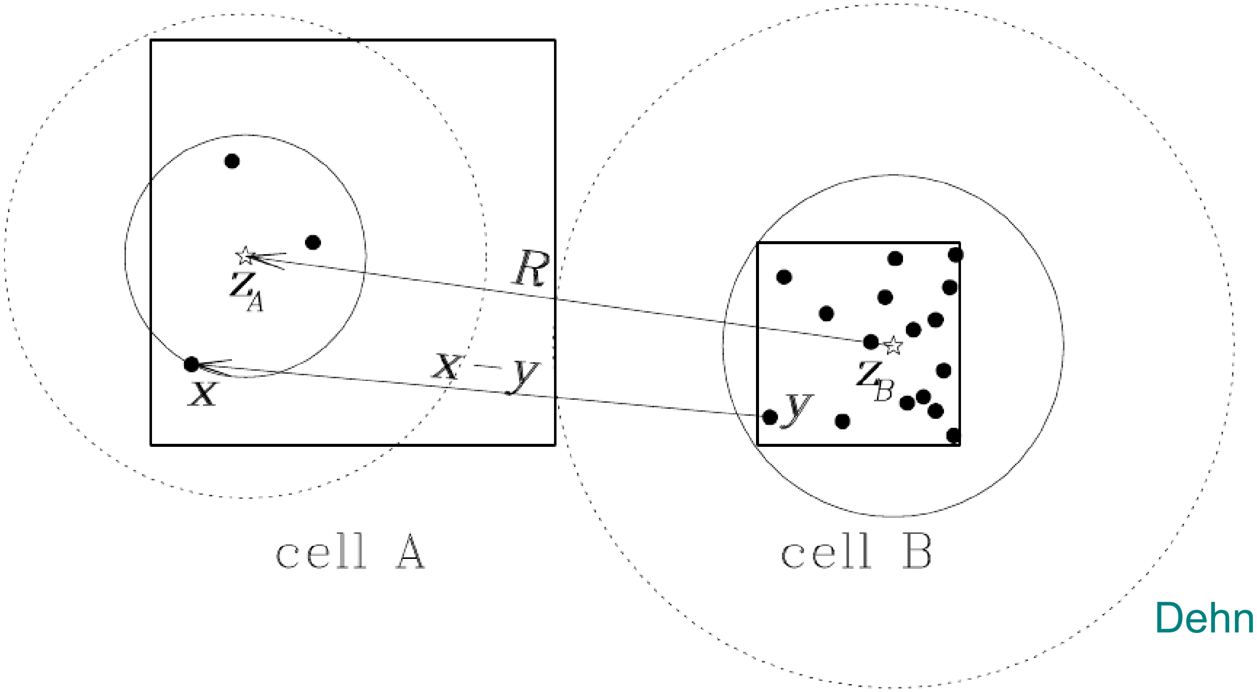
$$\Phi(\mathbf{r}) = -G \left[\frac{M}{|\mathbf{y}|} + \frac{1}{2} \frac{\mathbf{y}^T \mathbf{Q}\, \mathbf{y}}{|\mathbf{y}|^5} \right]$$

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

The fast multipole method (FFM) generalizes the tree algorithm and expands the field symmetrically for each pair of interacting cells

Two interacting cells:



Dehnen (2002)

- Very fast
- Manifest momentum conservation

But:

- Doesn't work well with individual timesteps
- Difficult to parallelize for distributed memory machines

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:

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

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

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

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

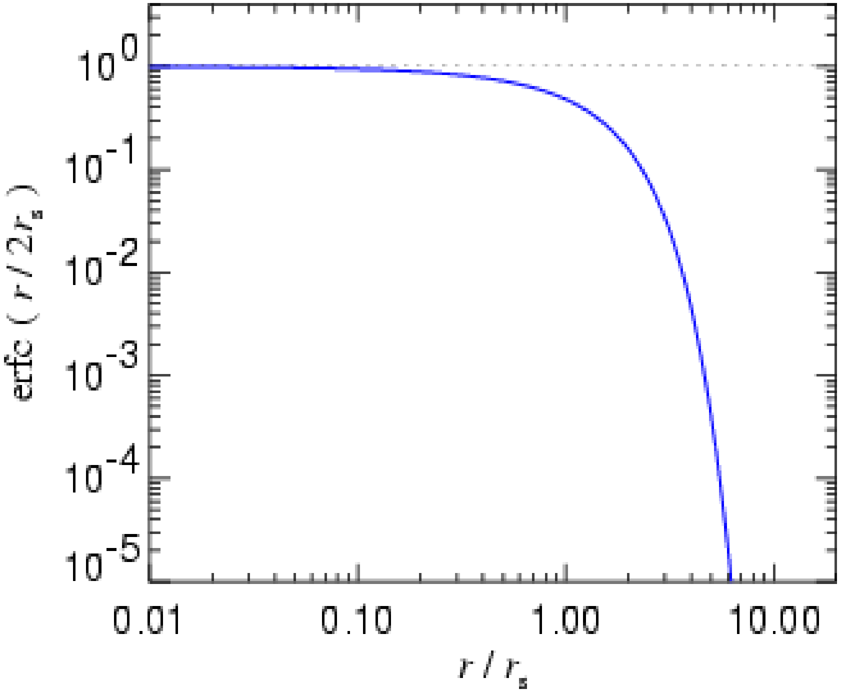
FFT to real space $\phi(r) = -\frac{Gm}{r}\,\mathrm{erfc}\left(\frac{r}{2r_s}\right)$

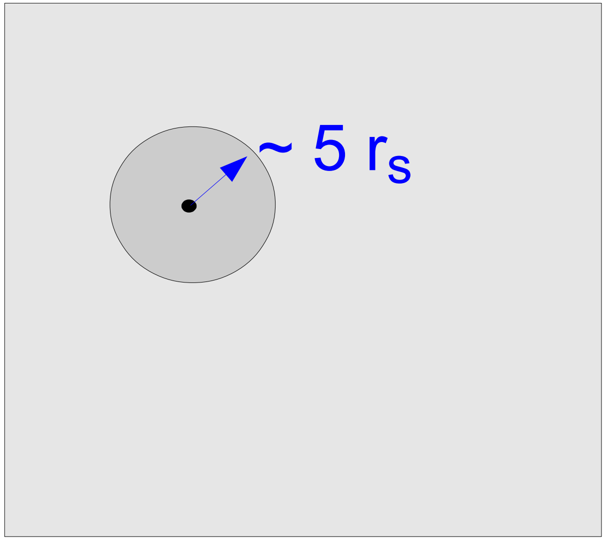
Solve in real space with TREE

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

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)

Brief digression back to time integration

The force-split can be used to construct a symplectic integrator where long- and short-range forces are treated independently

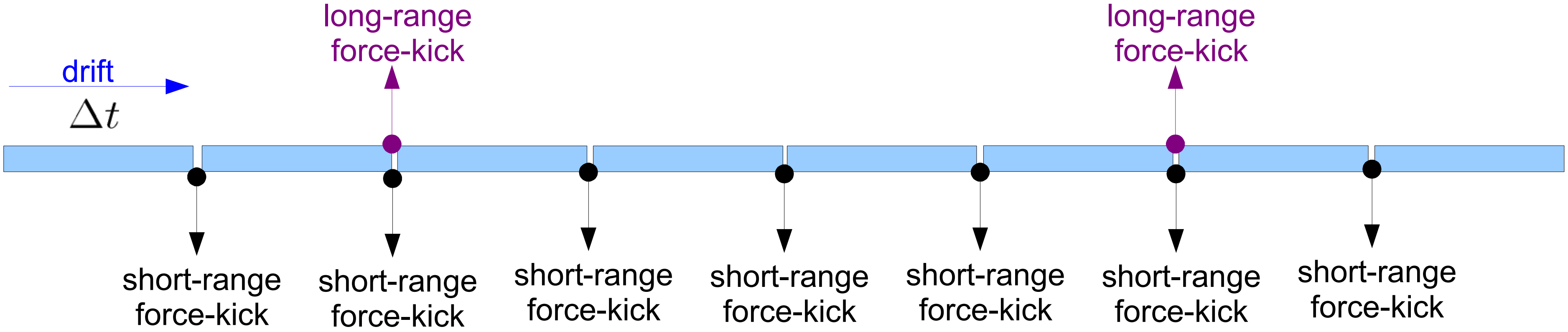
TIME INTEGRATION FOR LONG AND SHORT-RANGE FORCES

Separate the potential into a long-range and a short-range part:

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m_i a(t)^2} + \frac{1}{2}\sum_{ij} \frac{m_i m_j\, \varphi_{\rm sr}(\mathbf{x}_i - \mathbf{x}_j)}{a(t)} + \frac{1}{2}\sum_{ij} \frac{m_i m_j\, \varphi_{\rm lr}(\mathbf{x}_j - \mathbf{x}_j)}{a(t)}$$

The short-range force can then be evolved in a symplectic way on a smaller timestep than the long range force:

$$\tilde{\mathbf{U}}(\Delta t) = \mathbf{K}_{\rm lr}\left(\frac{\Delta t}{2}\right)\left[\mathbf{K}_{\rm sr}\left(\frac{\Delta t}{2m}\right)\mathbf{D}\left(\frac{\Delta t}{m}\right)\mathbf{K}_{\rm sr}\left(\frac{\Delta t}{2m}\right)\right]^m \mathbf{K}_{\rm lr}\left(\frac{\Delta t}{2}\right)$$



drift

Δt

long-range force-kick

long-range force-kick

short-range force-kick

short-range force-kick

short-range force-kick

short-range force-kick

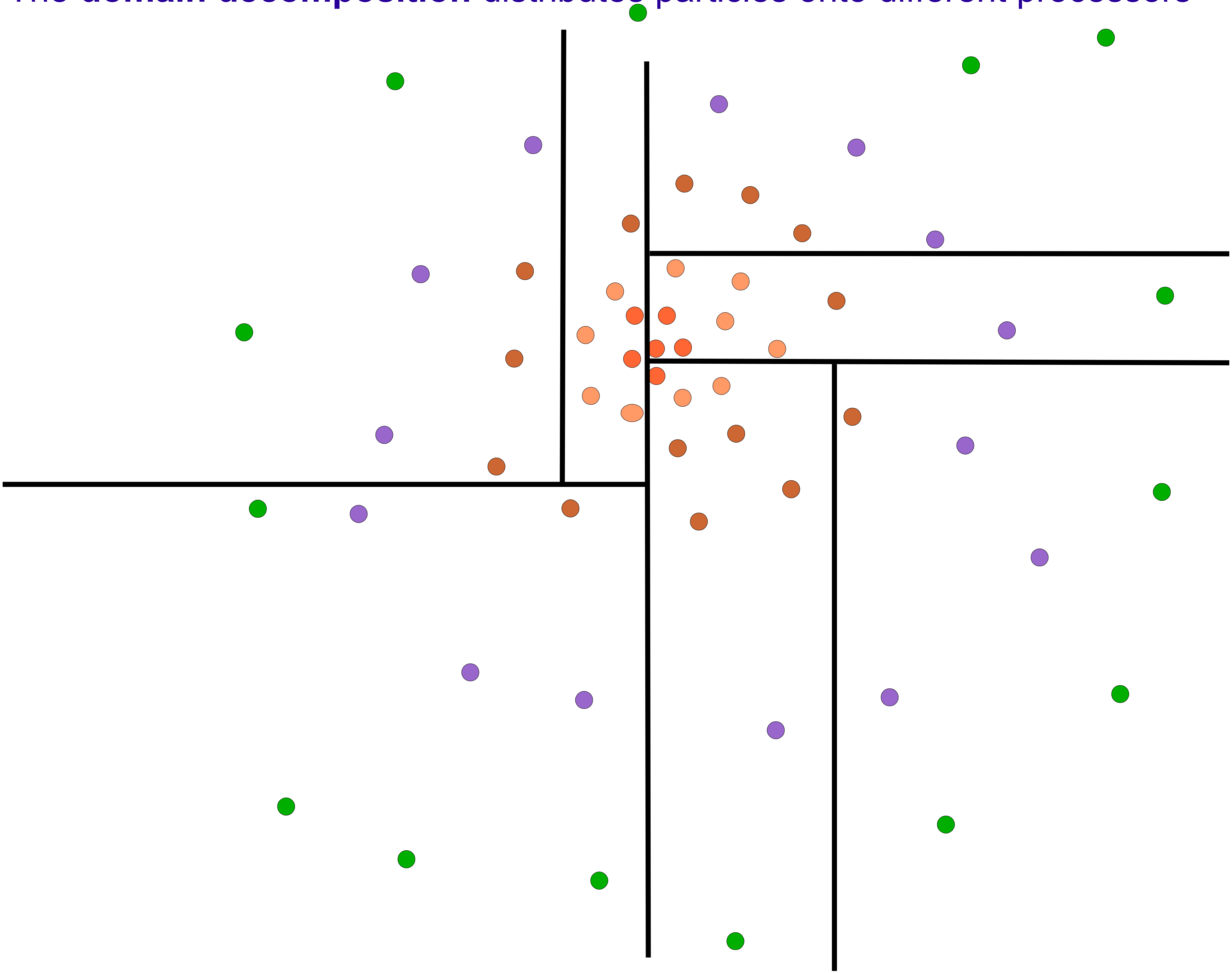
short-range force-kick

short-range force-kick

short-range force-kick

Parallelization:
Domain decomposition

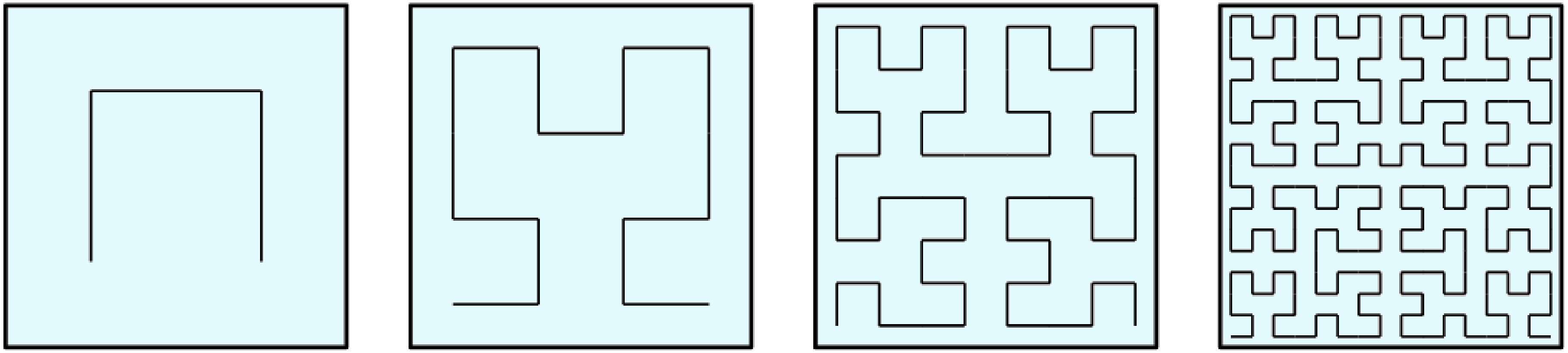
The **domain decomposition** distributes particles onto different processors

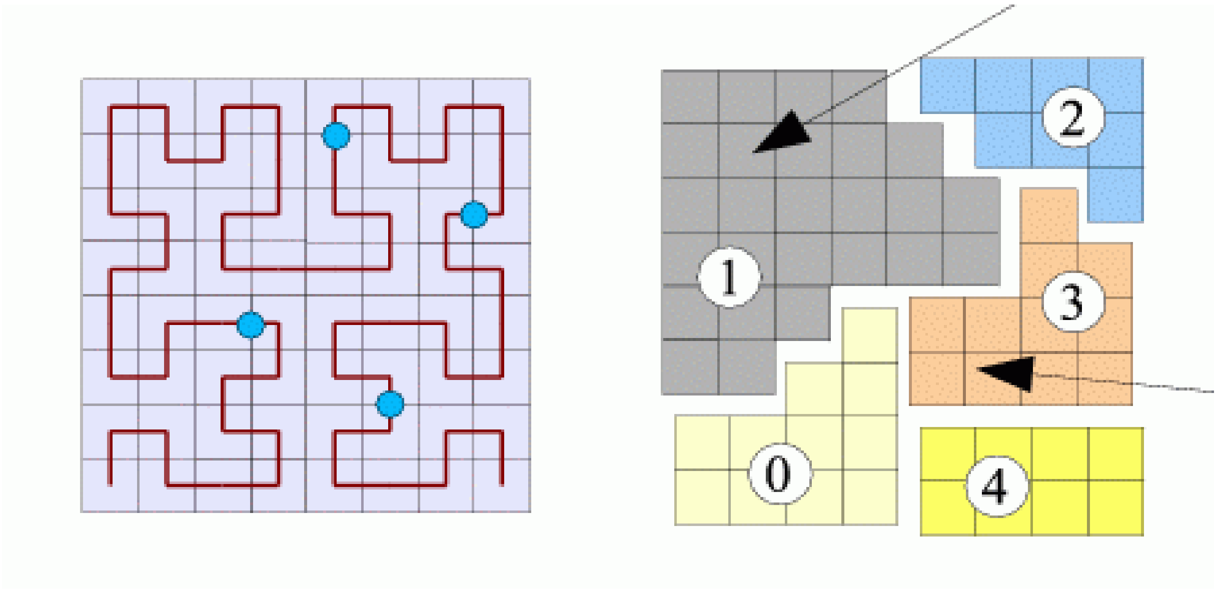


The space-filling Hilbert curve is a fractal that fills the square

CONSTRUCTION OF A FLEXIBLE DOMAIN DECOMPOSITION WITH CACHE BENEFITS

Idea: Order the particles along a space-filling curve



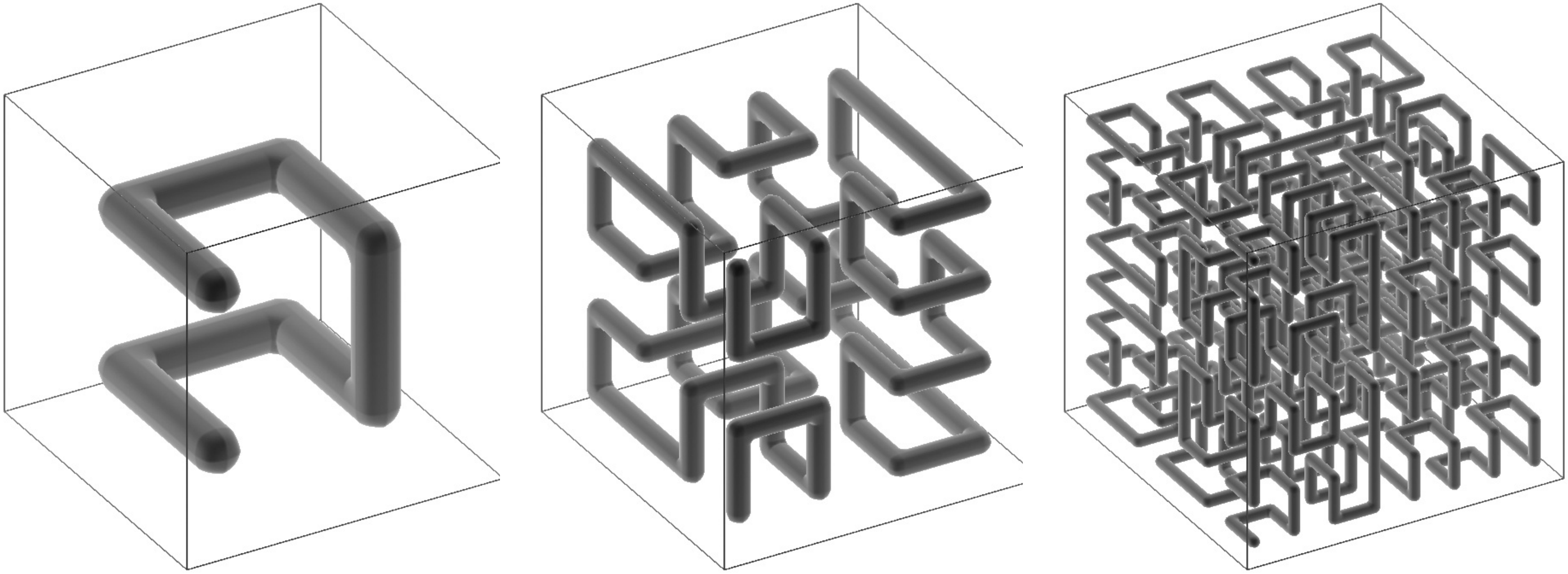


Mapped to CPU 1

Mapped to CPU 3

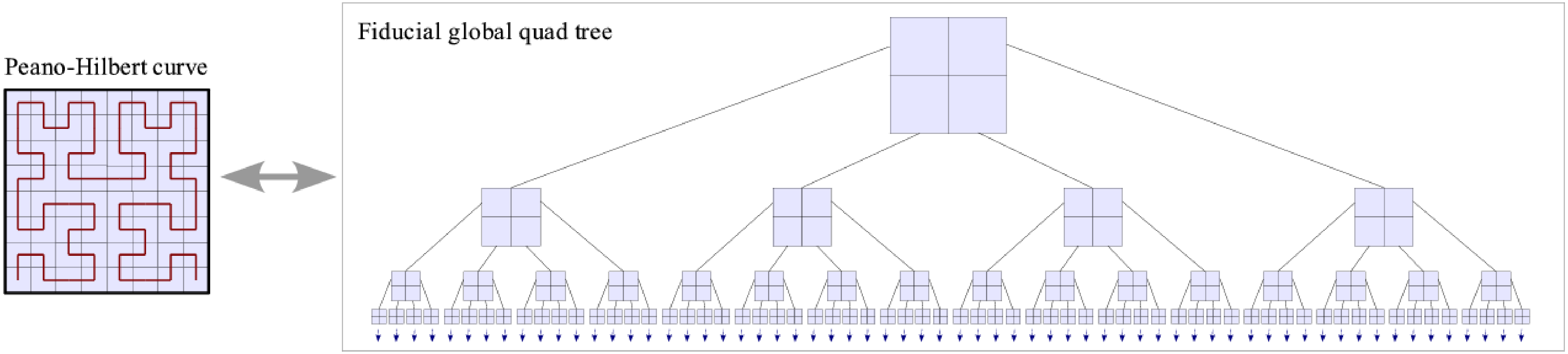
The space-filling Hilbert curve can be readily generalized to 3D

THE PEANO-HILBERT CURVE

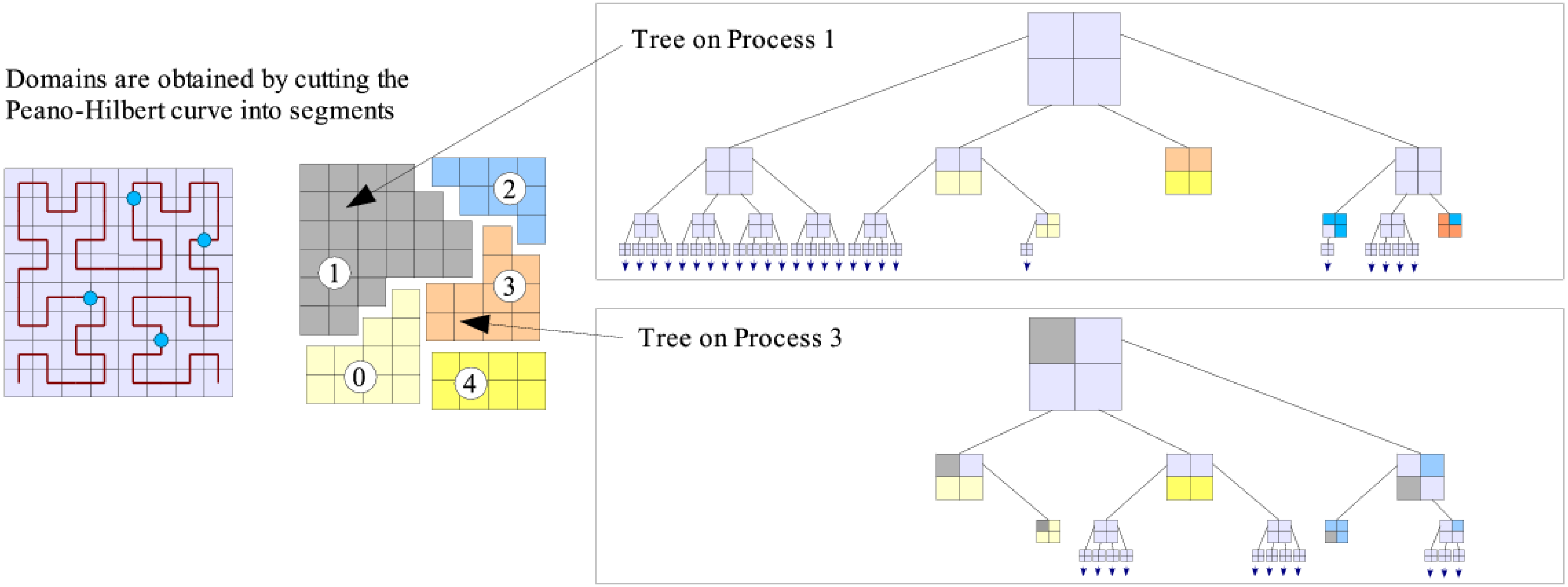


The space-filling Peano-Hilbert is used in GADGET and other codes for the domain-decomposition

SPLITTING UP THE TREE FOR DIFFERENT PROCESSORS



Domains are obtained by cutting the Peano-Hilbert curve into segments



Initial conditions generation

- Prefabricated galaxies / halos / disks
- Cosmological initial conditions

In special cases, the distribution function for static solutions of the CBE can be constructed analytically

An integral of motion $I = I(\mathbf{x}(t), \mathbf{v}(t))$ is constant along orbits, i.e.: $\frac{\mathrm{d}I}{\mathrm{d}t} = 0$

→ Then I is a solution of the CBE.

Jeans theorem: Steady-state solutions of the CBE only depend on integrals of motion.

For a spherical mass distribution, a DF that only depends on energy can be constructed with **Eddington's formula**.

Example:

Hernquist halo:

$$\rho(r) = \frac{M}{2\pi}\frac{a}{r(r+a)^3}$$

$$f(E) = \frac{1}{\sqrt{2}(2\pi)^3(GMa)^{3/2}}\frac{\sqrt{e}}{(1-e)^2}\left[(1-2e)(8e^2-8e-3)+\frac{3\sin^{-1}(\sqrt{e})}{\sqrt{e(1-e)}}\right]$$

where: $e = -\frac{aE}{GM}$ $\quad E = \frac{\mathbf{v}^2}{2} + \Phi$

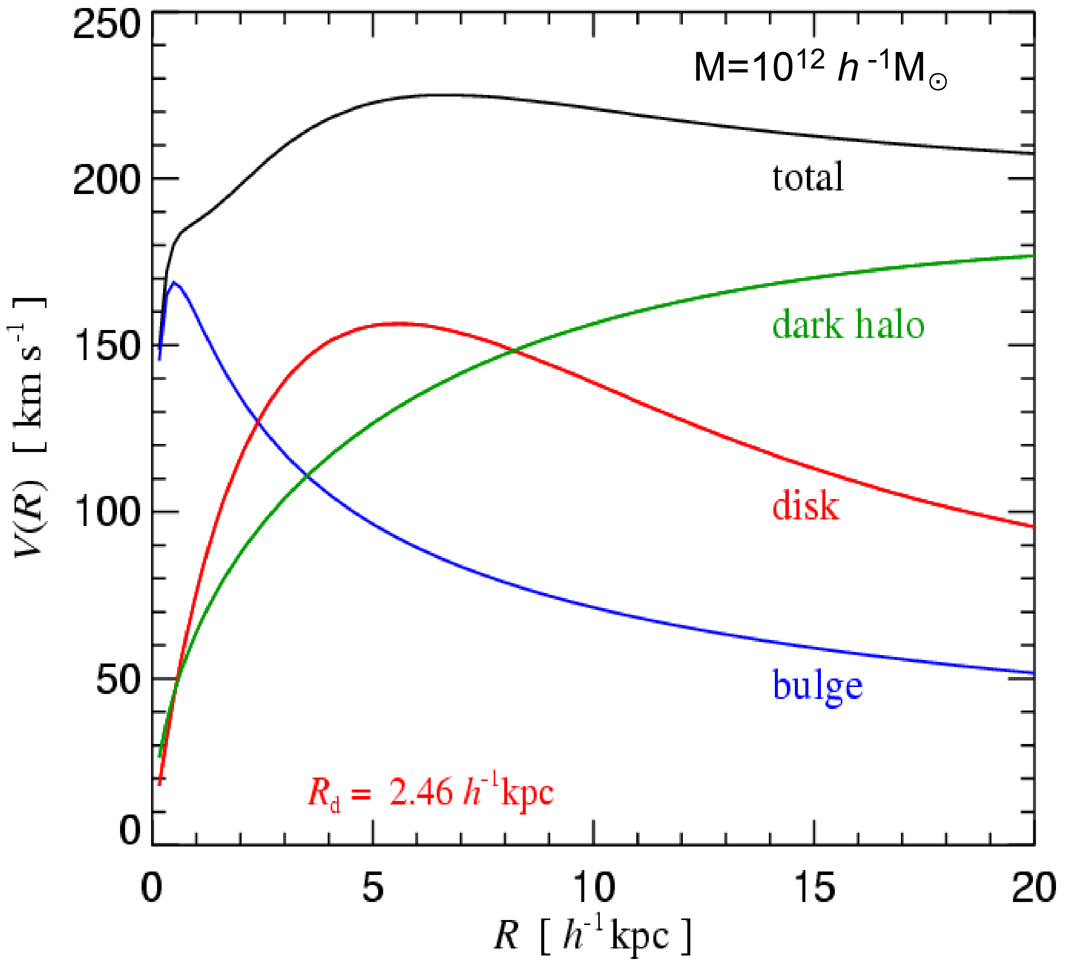
Construction of compound disk galaxies that are in dynamical equilibrium

STRUCTURAL PROPERTIES OF MODEL GALAXIES

Components:

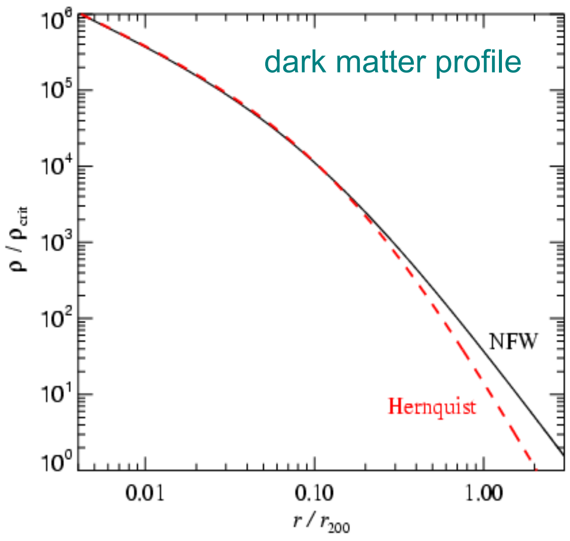
- Dark halo (Hernquist profile matched to NFW halo)
- Stellar disk (exponential)
- Stellar bulge
- Gaseous disk (exponential)
- Central supermassive black hole

One approach: Compute the exact gravitational potential for the axisymmetric mass distribution and solve the **Jeans equations**



The first step in constructing an isolated galaxy model is the specification of the density structure of all mass components

DENSITY DISTRIBUTIONS OF DARK MATTER AND STARS IN BULGE AND DISK



Dark matter:

$$\rho_{\rm dm}(r) = \frac{M_{\rm dm}}{2\pi}\,\frac{a}{r(r+a)^3}$$

Hernquist or NFW profile

Stars in the disk:

$$\Sigma_\star(r) = \frac{M_\star}{2\pi h^2}\,\exp(-r/h)$$

“Isothermal sheet” with exponential profile

$$\rho_\star(R,z) = \frac{M_\star}{4\pi z_0\, h^2}\,{\rm sech}^2\left(\frac{z}{2\,z_0}\right)\exp\left(-\frac{R}{h}\right)$$

Disk scale length ***h*** determined by spin parameter of halo.

Stars in the bulge:

$$\rho_{\rm b}(r) = \frac{M_{\rm b}}{2\pi}\,\frac{b}{r(r+b)^3}$$

Bulge scale length ***b*** can be set to a fraction of the disk scale-length ***h.***

Gas in the disk:

$$\Sigma_{\rm gas}(r) = \frac{M_{\rm gas}}{2\pi h^2}\,\exp(-r/h)$$

Vertical structure given by hydrostatic equilibrium. Depends on the equation of state of the gas.

$$-\frac{1}{\rho_{\rm g}}\frac{\partial P}{\partial z} - \frac{\partial \Phi}{\partial z} = 0$$

Solving the Jeans equations allows the construction of dynamically stable disk galaxy models

MOMENT EQUATIONS FOR THE VELOCITY STRUCTURE

We assume that the **velocity distribution function** of dark matter and stars can be approximated everywhere by a **triaxial Gaussian.**

Further, we assume axisymmetry, and that the distribution function depends only on ***E*** and ***L_z***

Then cross-moments vanish:

$$\langle v_R v_z \rangle = \langle v_z v_\phi \rangle = \langle v_R v_\phi \rangle = 0$$

$$\langle v_R \rangle = \langle v_z \rangle = 0$$

The radial and vertical moments are given by:

$$\left\langle v_z^2 \right\rangle = \left\langle v_R^2 \right\rangle = \frac{1}{\rho} \int_z^\infty \rho(z', R) \frac{\partial \Phi}{\partial z'} \, \mathrm{d}z'$$

The azimuthal dispersion fulfills a separate equation:

$$\left\langle v_\phi^2 \right\rangle = \left\langle v_R^2 \right\rangle + \frac{R}{\rho} \frac{\partial \left(\rho \left\langle v_R^2 \right\rangle\right)}{\partial R} + v_c^2$$

Circular velocity: $v_c^2 \equiv R \dfrac{\partial \Phi}{\partial R}$

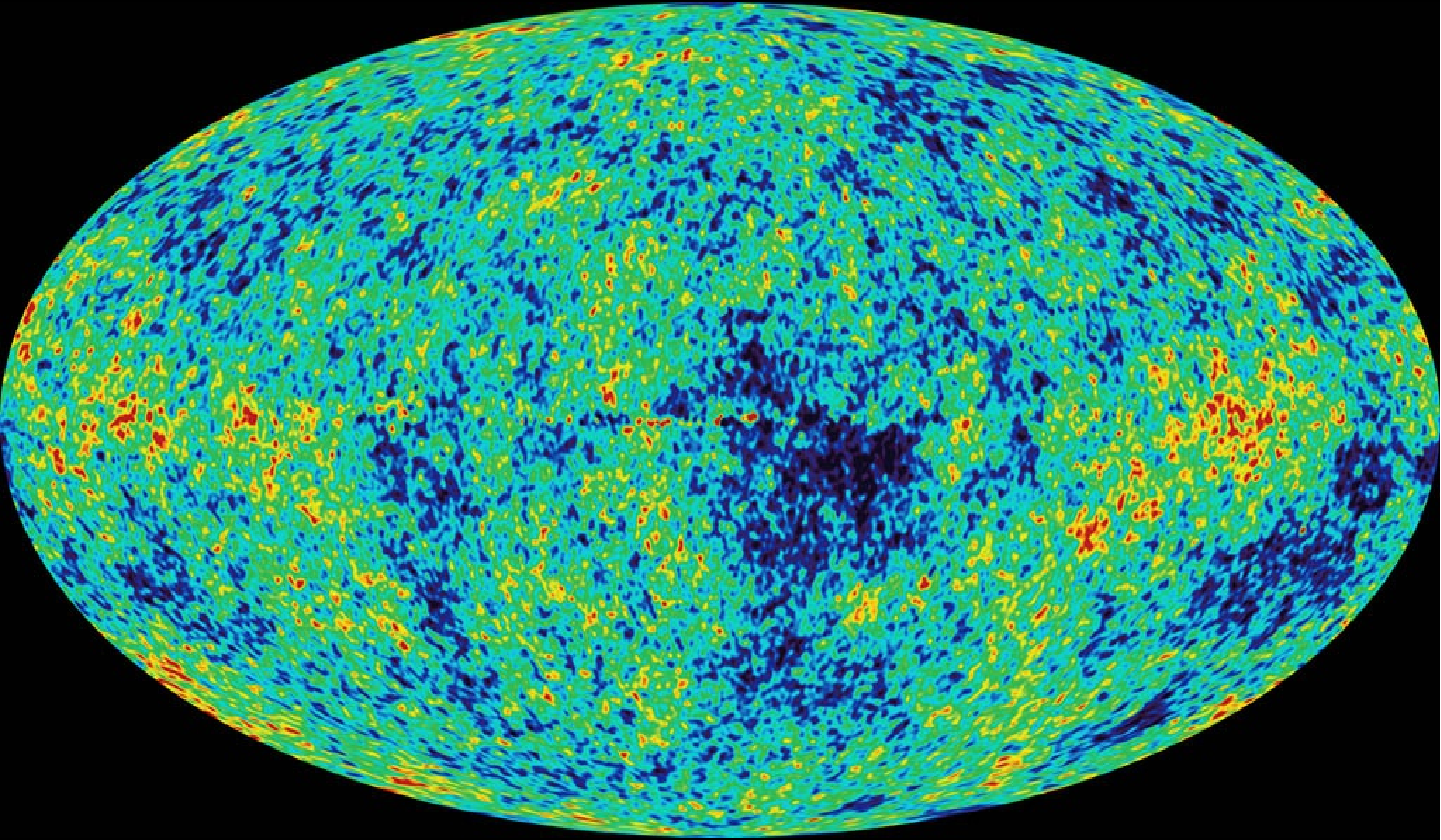
A remaining freedom lies in the azimuthal streaming $\langle v_\phi \rangle$, which is not determined by the above assumptions. For the dark matter, it can be set to zero, or to a value corresponding to a prescribed spin.

$$\sigma_\phi^2 = \left\langle v_\phi^2 \right\rangle - \langle v_\phi \rangle^2$$

Note: For the stellar disk, we instead use the epicycle theory to relate radial and vertical dispersions.

The initial conditions for cosmic structure formation are directly observable

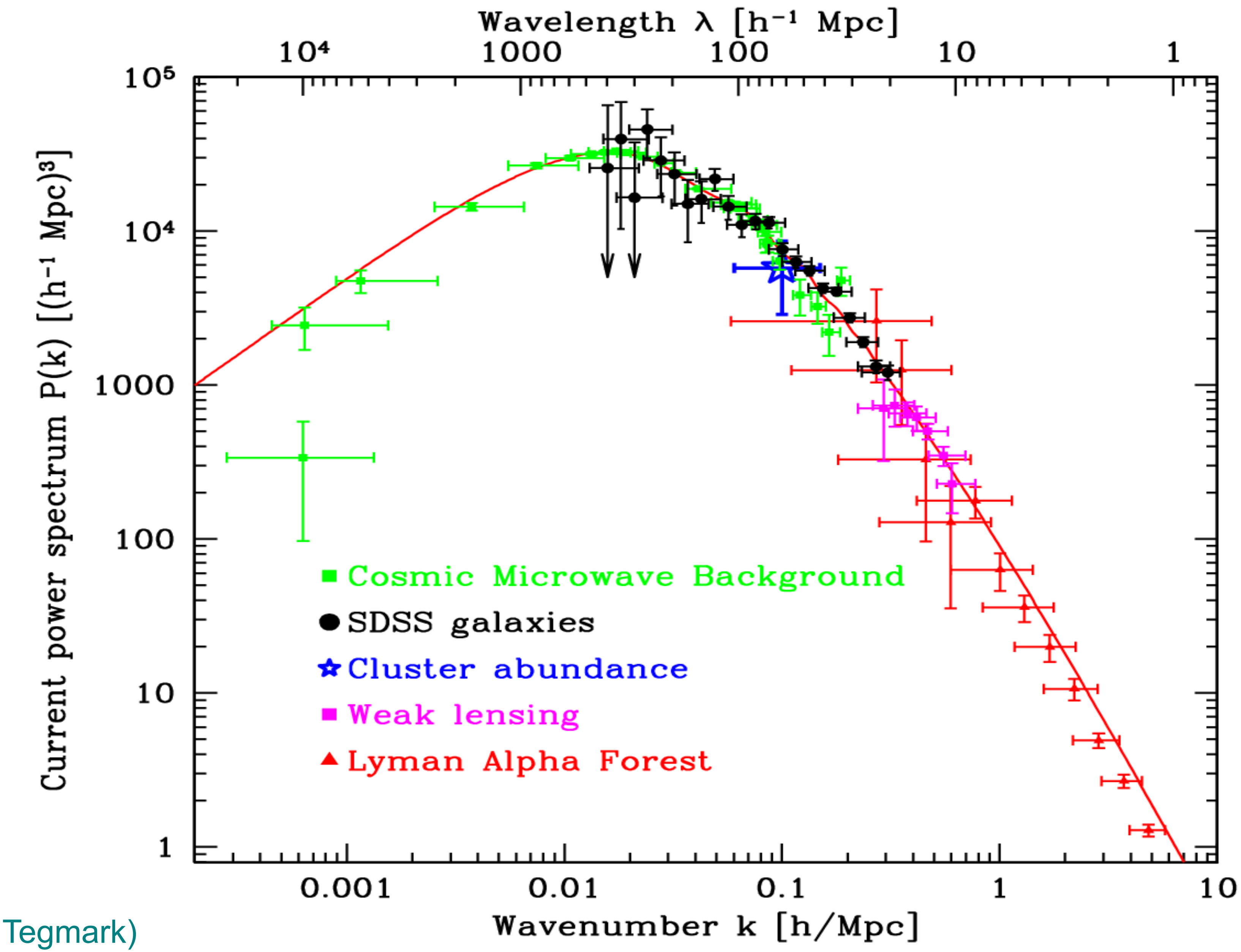
THE MICROWAVE SKY



WMAP Science Team (2003, 2006, 2008)

If the initial fluctuations are a Gaussian random field, we only need to know the power spectrum and the cosmological parameters to describe the ICs

DIFFERENT PROBES OF THE MASS POWER SPECTRUM



(figure from Max Tegmark)

To determine the power spectrum amplitude, we normalize the spectrum to observations of clustering (usually galaxy clusters)

FILTERED DENSITY FIELD AND THE NORMALIZATION OF THE POWER SPECTRUM

The filtered density field:

$$\sigma^2(M,z) = D^2(z)\int_0^\infty \frac{\mathrm{d}k}{2\pi^2} k^2 P(k)\left[\frac{3j_1(kR)}{kR}\right]^2$$

Observational input:

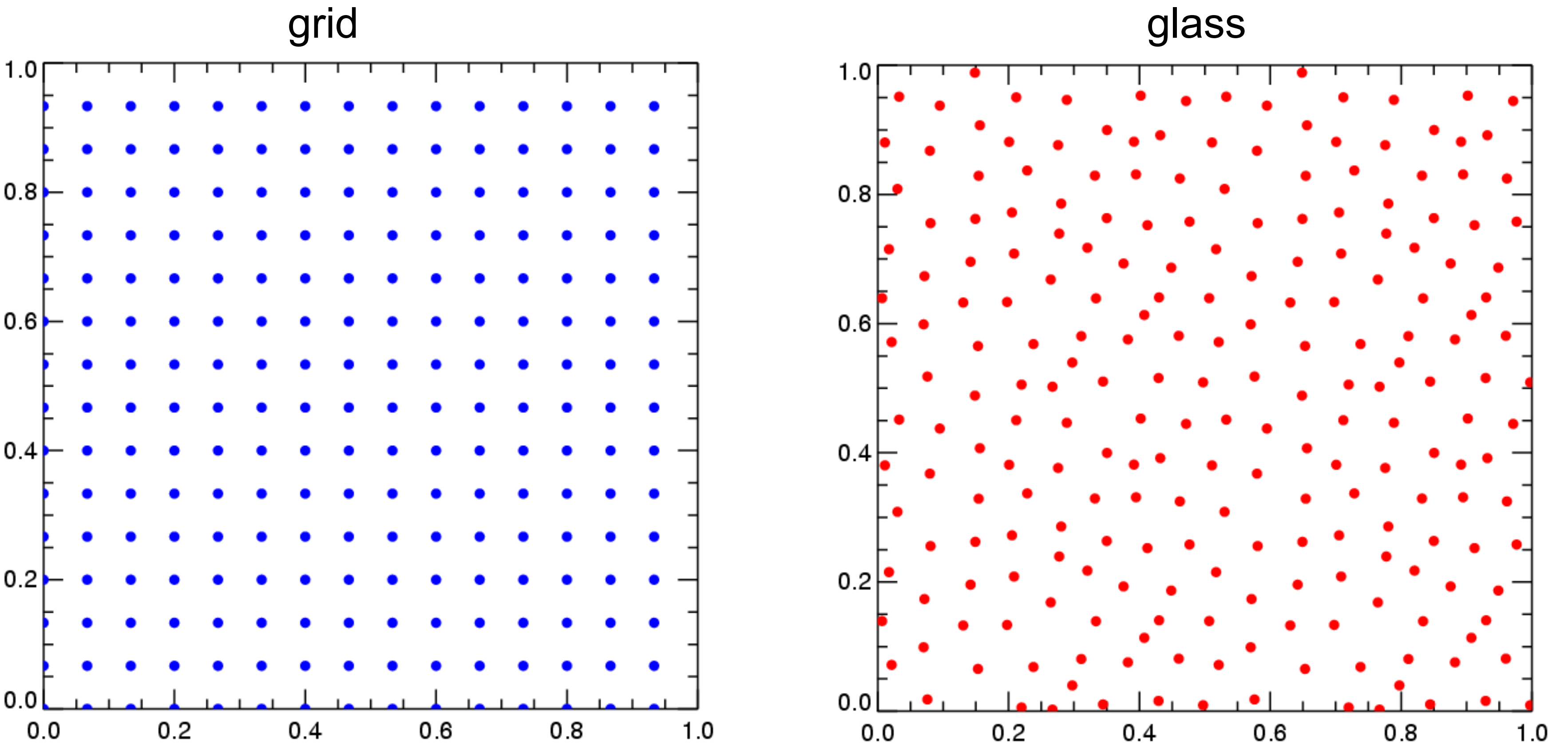
$$\sigma_8 = 0.74 - 0.9 \qquad R = 8\,h^{-1}\mathrm{Mpc}$$

Extrapolate back to the starting redshift with the growth factor D(z)
This depends on cosmology.

→ fluctuation spectrum of initial conditions fully specified.

To create a realization of the perturbation spectrum, a model for an unperturbed density field is needed

GLASS OR CARTESIAN GRID



For CDM, the initial velocity dispersion is negligibly small.

But there is a mean streaming velocity, which we need to imprint in initial conditions.

Using the Zeldovich approximation, density fluctuations are converted to displacements of the unperturbed particle load

SETTING INITIAL DISPLACEMENTS AND VELOCITIES

Particle displacements:

$$\mathbf{d}_i(t) = \mathbf{x}_i(t) - \mathbf{q}_i$$

Density change due to displacements:

$$\rho(\mathbf{x}) = \frac{\rho_0}{\left|\frac{\partial \mathbf{x}}{\partial \mathbf{q}}\right|} = \frac{\rho_0}{\left|\delta_{ij} + \frac{\partial \mathbf{d}}{\partial \mathbf{q}}\right|}$$

For small displacements:

$$\left|\delta_{ij} + \frac{\partial \mathbf{d}}{\partial \mathbf{q}}\right| \simeq 1 + \nabla_{\mathbf{q}} \cdot \mathbf{d}$$

Resulting density contrast:

$$\delta(\mathbf{x}) = \frac{\rho(\mathbf{x}) - \rho_0}{\rho} = -\nabla_{\mathbf{q}} \cdot \mathbf{d}$$

During linear growth:

$$\delta(t) = D(t)\delta_0$$

$$\mathbf{d}(t) = D(t)\mathbf{d}_0$$

$$\Longrightarrow$$

$$\dot{\mathbf{x}} = \dot{\mathbf{d}} = \dot{a}\frac{\mathrm{d}D}{\mathrm{d}a}\mathbf{d}_0 = \frac{\dot{a}}{a}\frac{a}{D}\frac{\mathrm{d}D}{\mathrm{d}a}\mathbf{d}$$

Particle velocities:

$$\boxed{\dot{\mathbf{x}} = H(a) f(\Omega)\mathbf{d} \qquad f(\Omega) = \frac{\mathrm{d}\ln D}{\mathrm{d}\ln a} \simeq \Omega^{0.6}}$$

Note: Particles move on straight lines in the Zeldovich approximation.

Displacement field:

$$\nabla^2\phi = \delta \qquad \mathbf{d} = -\nabla\phi$$

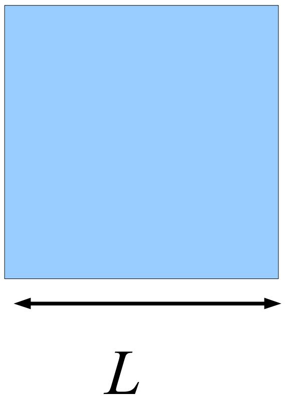
Fourier realization:

$$\phi_{\mathbf{k}} = -\frac{1}{k^2}\delta_{\mathbf{k}} \qquad \mathbf{d}_{\mathbf{k}} = -i\mathbf{k}\phi_{\mathbf{k}} = \frac{i\mathbf{k}}{k^2}\delta_{\mathbf{k}} \qquad \mathbf{d}_{\mathbf{k}} = -\nabla\phi = \sum_{\mathbf{k}} \frac{i\mathbf{k}\delta_{\mathbf{k}}}{k^2}\exp(i\mathbf{k}\mathbf{x})$$

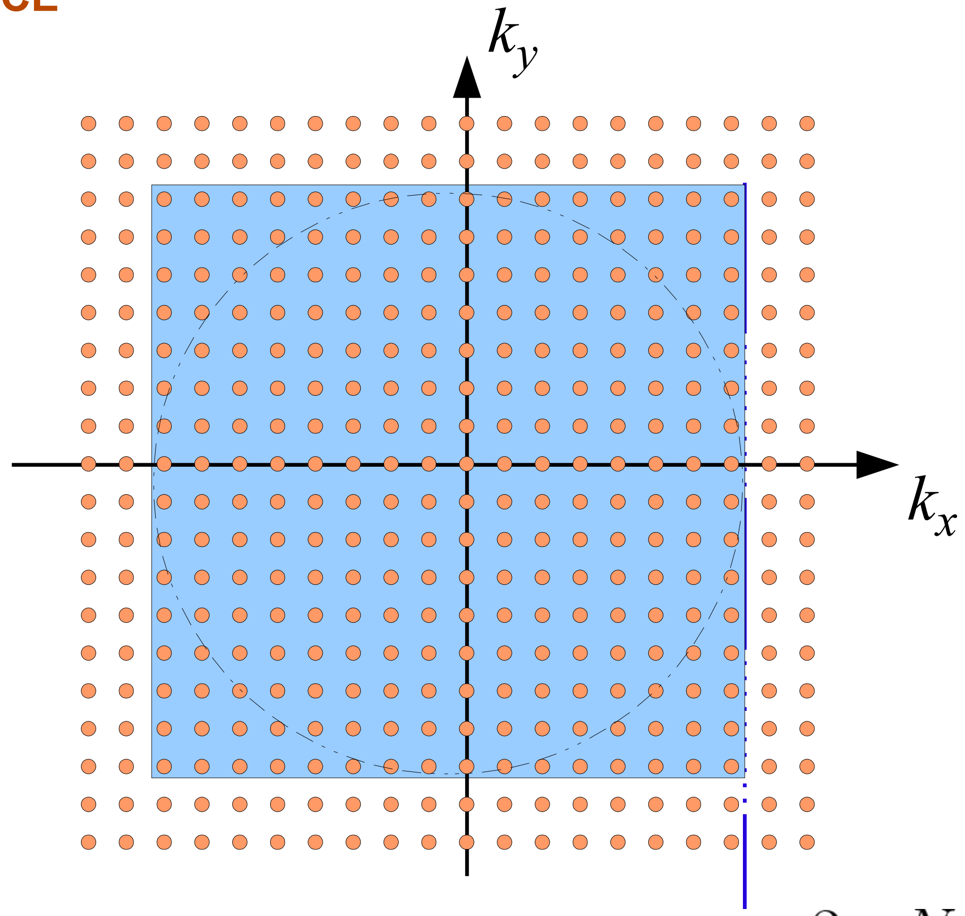
One can assign random amplitudes and phases for individual modes in Fourier space

GENERATING THE FLUCTUATIONS IN K-SPACE

Simulation box



sampled with
N^2 points



$$k_{\mathrm{Nyquist}} = \frac{2\pi}{L}\,\frac{N}{2}$$

$$\delta_{\mathbf{k}} = B_{\mathbf{k}} \exp^{\mathrm{i}\,\phi_{\mathbf{k}}}$$

For each mode, draw a random phase, and an amplitude from a Rayleigh distribution.

$$\left\langle \delta_{\mathbf{k}}^2 \right\rangle = P(k)$$