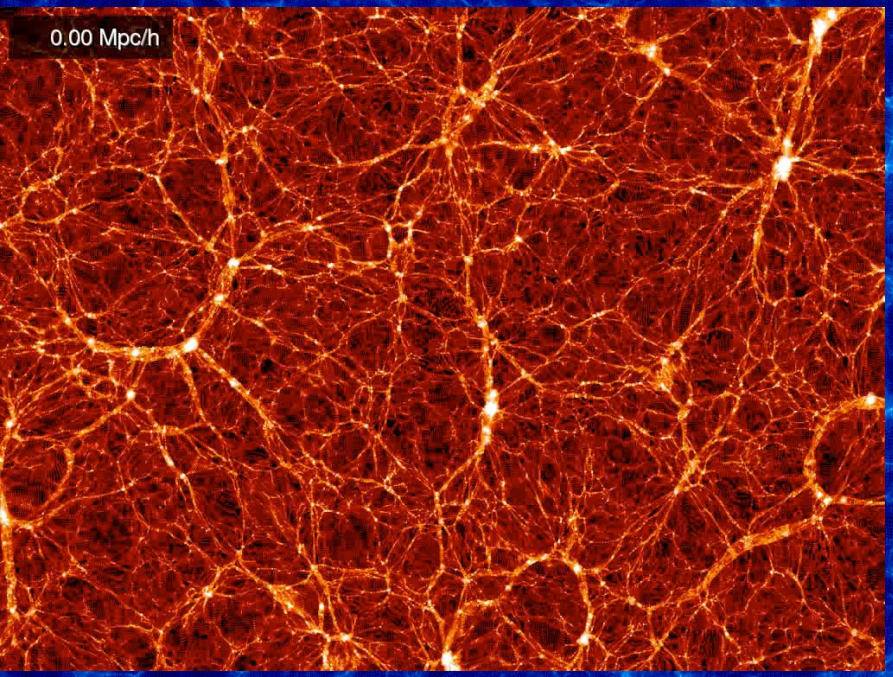

Cosmological N-body Simulations

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Non linear gravitational evolution

- Structure formation in the Universe can be studied using Linear Perturbation theory when $\delta\rho < 1$.
- Lagrangian Perturbation Theory (1LPT, 2LPT) can be used to study the quasi-linear regime $\delta\rho \gtrsim 1$)
- But for the strong non-linear regimen when $\delta\rho >> 1$, there is no analytical approximations for the gravitational evolution of density perturbations…

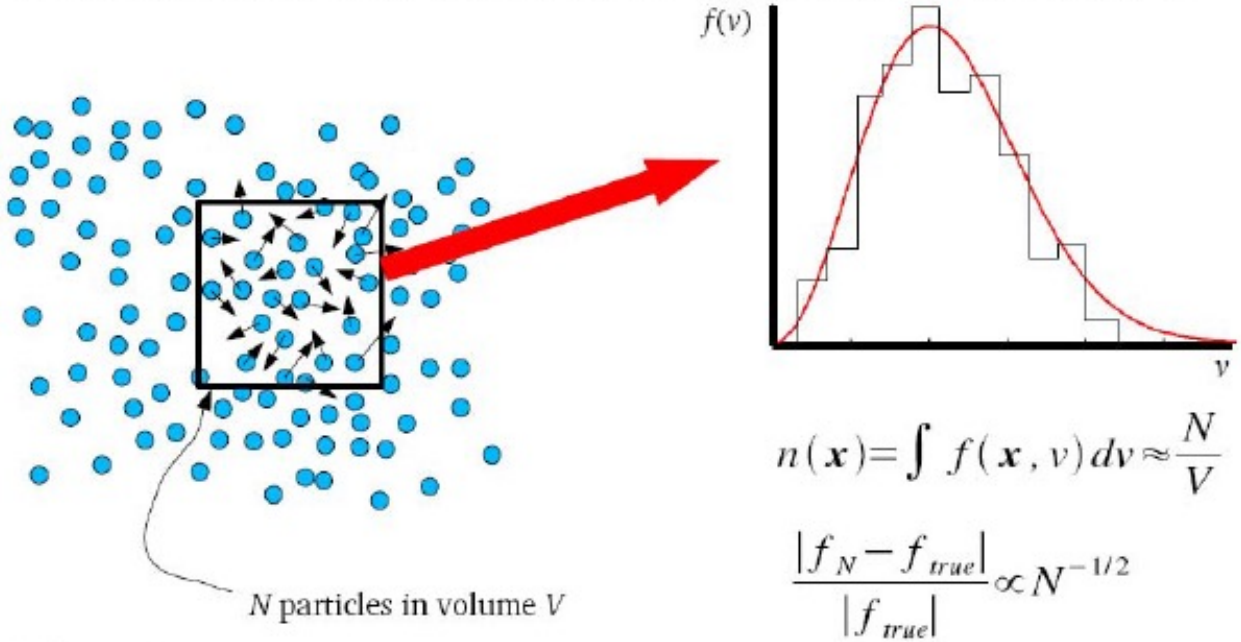
Non linear gravitational evolution

- Therefore…
- One has to resort to numerically integrate the equations governing the dynamical evolution of self gravitating systems.
- Since they are made of a large number elements (stars, or dark matter particles) one can treat them as statistical mechanical systems that are described by a **distribution function in phase space.**

Basic Equations

Particle representations

- Direct representation of objects (galaxies, stars, planets)
- Monte Carlo sampling of particle distribution function (gas, dust, dark matter)



$$n(\boldsymbol{x}) = \int f(\boldsymbol{x}, v)\, dv \approx \frac{N}{V}$$

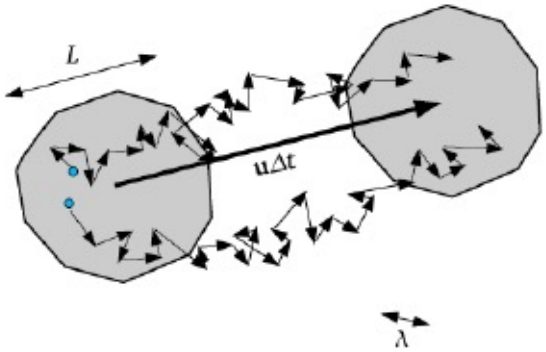
$$\frac{|f_N - f_{true}|}{|f_{true}|} \propto N^{-1/2}$$

Basic requirements:

- As $N \to \infty$, error ("shot noise") in approximate distribution function f_N goes to 0
- As $N \to \infty$, equation describing evolution of f_N becomes the Boltzmann equation

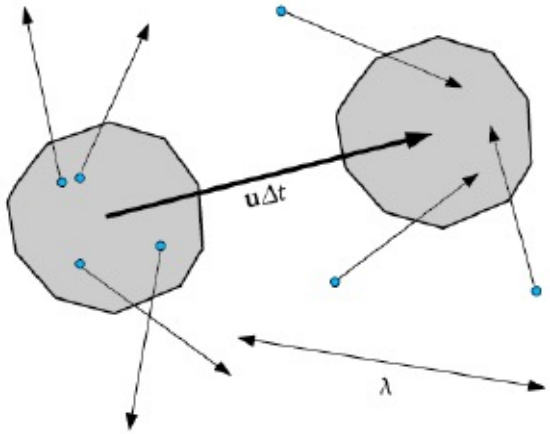
Basic Equations

Collisionality of a gas



Collisional gas (fluid): Kn → 0

- Mean free path $\lambda \ll$ typical scale L
- Random motions do not carry particles far from mean trajectory
- Solve moment equations for motion of fluid elements



Collisionless gas: Kn → ∞

- Mean free path $\lambda \gg$ typical scale L
- Random motions carry particles far from mean trajectory
- Solve kinetic equations for motion of particles (or distribution)

Knudsen number $\mathrm{Kn} \equiv \lambda/L$

Basic Equations

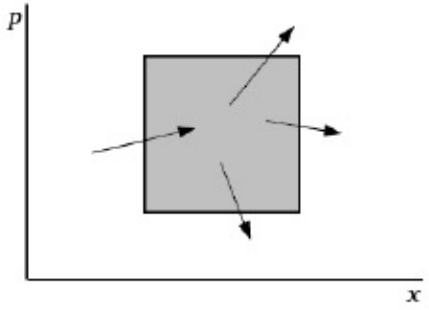
Boltzmann equation

Write single-particle Hamiltonian as

$$H(\mathbf{x},\mathbf{p}) = H_{\text{smooth}}(\mathbf{x},\mathbf{p}) + H_{\text{irregular}}(\mathbf{x},\mathbf{p})$$

Use classical mechanics for H_{smooth}; treat $H_{\text{irregular}}$ statistically

Single-particle distribution function is $f(\mathbf{x},\mathbf{p},t)$
Number of particles in differential volume element is $f(\mathbf{x},\mathbf{p},t)\ d^3x\ d^3p$



Net flux in x-direction

$$f\,\dot{x} = f\,\frac{\partial H_{sm}}{\partial p}$$

Net flux in p-direction

$$f\,\dot{p} = -f\,\frac{\partial H_{sm}}{\partial x}$$

Basic Equations

The Boltzmann equation is then

$$\frac{\partial f}{\partial t}+\nabla_x f\cdot\nabla_p H_{sm}-\nabla_p f\cdot\nabla_x H_{sm}=\left(\frac{\delta f}{\delta t}\right)_c$$

or, for $H_{sm}=\frac{p^2}{2\mathrm{m}}+\Phi(x)$

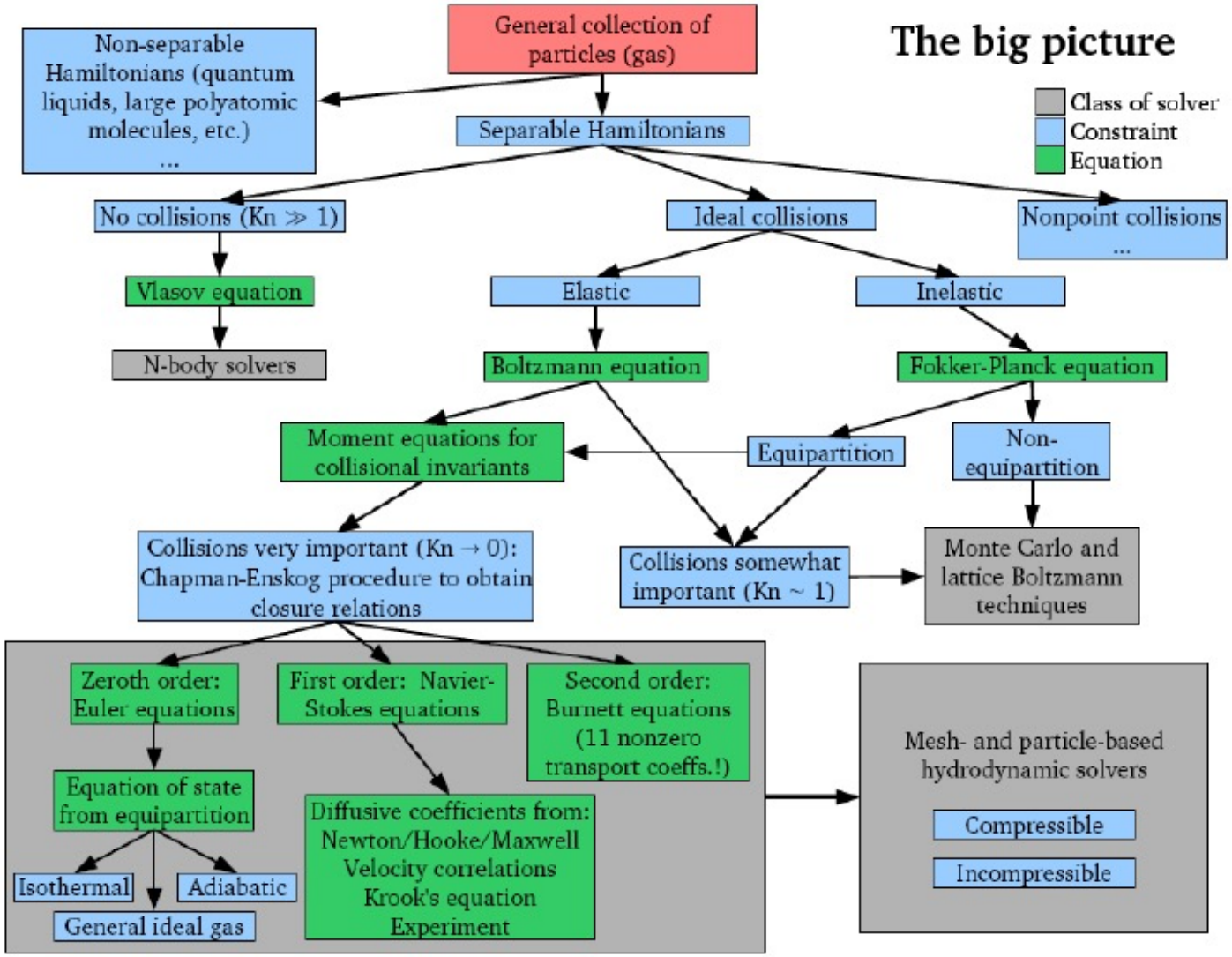
$$\frac{\partial f}{\partial t}+\frac{p}{m}\cdot\nabla_x f-\nabla_x\Phi\cdot\nabla_p f=\left(\frac{\delta f}{\delta t}\right)_c$$

For self-gravity as a potential source we have

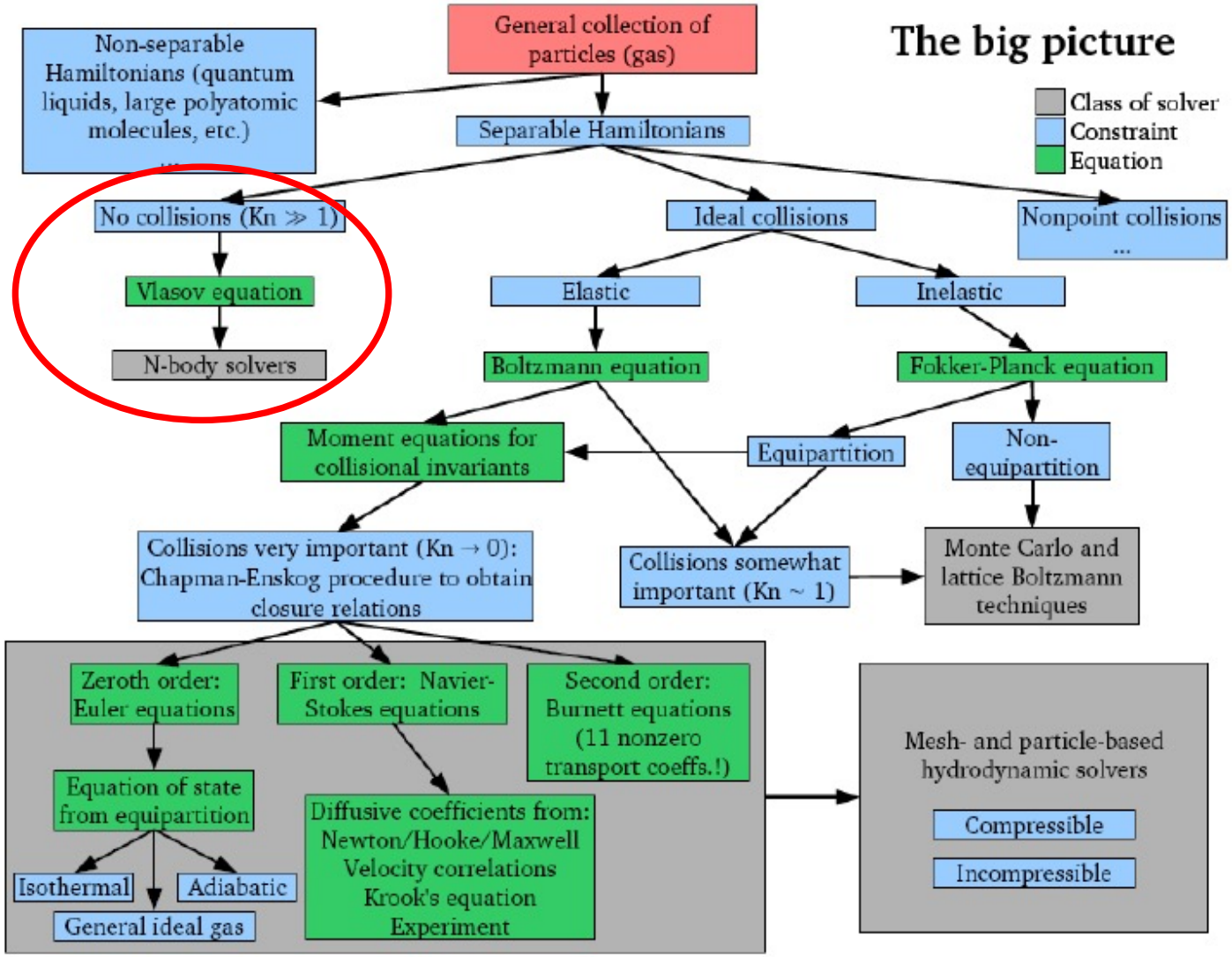
$$\nabla^2\phi=4\pi G\rho$$

where ρ = space density.

$$\rho(\mathbf{x})=\int f(\mathbf{x},\mathbf{p})d^3p$$



•Credit P. Ricker



•Credit P. Ricker

The Vlasov-Poisson Equation

- For pure collisionless gravitational systems

$$\left.\frac{\delta f}{\delta t}\right|_c = 0$$

..and the equation to integrate is the integro-differential Vlasov-Poisson equations:

$$\frac{\partial f}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla_x f - \nabla_x \phi \cdot \nabla_p f = 0$$

$$\nabla^2 \phi = 4\pi G \int f(x, p, t) d^3 p$$

The N-body method

- How can we solve de collisionless Bolzmann (Vlasov) equation?.
- **Method of the characteristics**: f(x,p,t) is constant along the characteristics.
- Discretize the f(x,p,t) in N phase space volume elements (pseudo particles).
- For systems where f(x,p,t) only depens on positions, the N tracers of the distribution function can be just subvolumes of 3D space variables such $\sum_{i=1}^{N} m_i = \int_V \rho(x) d^3x$

The N-body method

- If f(x,p) has a dependence on momentum, (eg. Neutrinos, or other relativistic particles following Fermi-Dirac statistics, there must be a sampling of the velocity distribution for each subvolume of the space variables.
- The equations of the characteristics of each of these pseudo-particles representing one phase space element will be just the equations of motion of N bodies subject to their mutual gravity forces.

The N-body method

Therefore: Solution of the Vlasov equation is equivalent to solving the coupled system of 6N first order ordinary differential equations:

$$\frac{d\mathbf{x}_i}{dt} = \frac{\mathbf{p}_i}{m_i}$$

$$\frac{d\mathbf{p}_i}{dt} = -m_i \nabla \phi$$

$$\phi(\mathbf{r}) = -G \sum_{i=1}^{N} \frac{m_i}{\left(|\mathbf{r}-\mathbf{r_i}|^2+\epsilon_i^2\right)^{1/2}}$$

The N-body method

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$$\frac{d\mathbf{p}_i}{dt} = -m_i \nabla_i \phi(\mathbf{x}_i)$$

$$\phi(\mathbf{x}) = -G \sum_{i=1}^{N} \frac{m_i}{\left(|\mathbf{x}-\mathbf{x_i}|^2+\epsilon_i^2\right)^{1/2}}$$

ε_i is the gravitational softening parameter to avoid large angle two body scattering and prevent formation of bound particle. This ensures the collisionless nature of the fluid

The N-body method

$$\frac{d\mathbf{x}_i}{dt} = \frac{\mathbf{p}_i}{m_i}$$

$$\frac{d\mathbf{p}_i}{dt} = -m_i \nabla_i \phi(\mathbf{x}_i)$$

$$\phi(\mathbf{x}) = -G \sum_{i=1}^{N} \frac{m_i}{\left(|\mathbf{x}-\mathbf{x_i}|^2+\epsilon_i^2\right)^{1/2}}$$

- Major problem: The $O(N^2)$ scaling due to the computation of the gravitational potential $\phi(\mathbf{x})$
- In cosmology, one requires large volumes and small masses per particles to resolve nternal structure of halos hosting the galaxias.
  - SO N is pretty large : $N \sim 10^{12}$

The N-body method in Cosmology

For cosmological problems, space coordinates depend on time through the Friedman equations.

Therefore, it is better to work in comoving coordinates: $\mathbf{r} = a(t)\,\mathbf{x}$;

$$\mathbf{u} = \dot{\mathbf{r}} = \dot{a}\mathbf{x} + a\dot{\mathbf{x}} = H(t)\mathbf{r} + \mathbf{v}$$

In addition, we also transform t -> a(t)

$$\frac{d\mathbf{x}}{da} = \frac{\mathbf{p}}{a^3 H}, \quad \frac{d\mathbf{p}}{da} = -\frac{\nabla\phi}{aH}, \quad \mathbf{p} \equiv \mathbf{a^2\dot{x}}$$

$$\nabla^2\phi = \frac{3}{2}\frac{H_0^2\Omega_0\delta_{\rm dm}}{a}, \qquad \Phi(\mathbf{x}) = -G\sum_{j=1}^{N}\frac{m_j}{[(\mathbf{x}-\mathbf{x}_j)^2+\epsilon^2]^{1/2}}$$

$$H^2 = H_0^2\left(\frac{\Omega_0}{a^3} + \Omega_{\Lambda,0}\right), \quad \Omega_0 + \Omega_{\Lambda,0} = 1.$$

Numerical Methods

- PARTICLE-BASED
  - Particle-particle
  - Tree codes
- GRID-BASED
  - Particle-Mesh
  - ART (Adaptive Refinement Mesh tree)
- HYBRID
  - Particle-Particle-Particle-Mesh (P3M)
  - Tree + PM

PARTICLE BASED METHODS

Particle-Particle (PP)

- Easiest of all methods. Numerically integrate the 3N differencial equations.

- Particles are considered extended objects of size ϵ (Plummer softening)

$$\mathbf{F}_{ij} = Gm^2 \frac{\mathbf{x}_i - \mathbf{x}_j}{(\epsilon^2 + |\mathbf{x}_i - \mathbf{x}_j|^2)^{3/2}}$$

- First method used to study growth of cosmological fluctuations in expanding Universe (Aarshet, Gott, Turner, 1979; Doroshkevich et al 1980).

- Advatages:

  - ⊕ Arbitrary boundary conditions
  - ⊕ Very accurate computation of forces.
  - ⊕ Highly parallelizable. Well suited for Massively parallel computers and GPU or FPGA

TREE METHODS

Do not used any mesh at all.

Compute only particle-particle forces in a hierchical decomposition using recursive splitting of space domain.

Easy to implement boundary conditions.

Store particles in a tree data structure. Particles are at leaves of tree; parent nodes store total mass of children.

When the force on a particle is needed, we traverse the tree, starting at the root.

If a node is terminal (leaf node), directly sum the force from the particle at that node.

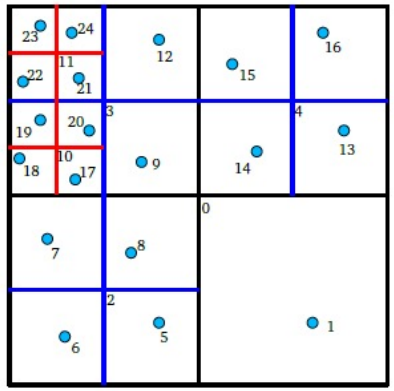
If not, ask: is the monopole (or quadrupole, ...) of the node an adequate approximation to the force from the child particles?

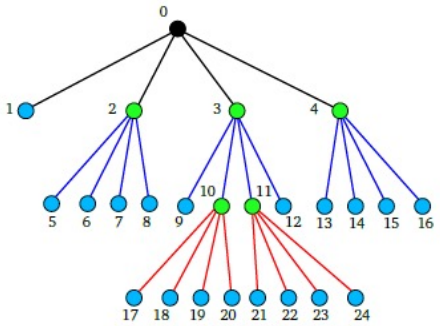
- **(i) If yes, use the approximate force and stop traversing this branch.**
- **If no, traverse to the children.**

- **Scaling as O (N log(N)).**

Periodic Boundary conditions can be implemented using Ewald summation of infinite replicas of the simulations box

Treecodes – 2





Advantages:

- No grid to limit resolution! (Must introduce force softening explicitly...)
- Scales as $N \ln N$! (However, must tighten MAC as $N \to \infty$)
- Parallelizes extremely well
- Isolated boundaries are natural

Disadvantages:

- Error properties harder to analyze than mesh-based methods
- Periodic boundaries must be introduced via Ewald summation

- Example of Tree codes
- TREECODE (Barns-Hut Oct-tree)
- PKDGRAV (K-D tree)+ Multipoles)
- GADGET (Oct-tree)+
- 2HOT (Oct-tree)
- CHANGA (Oct tree + Hexadecapoles)

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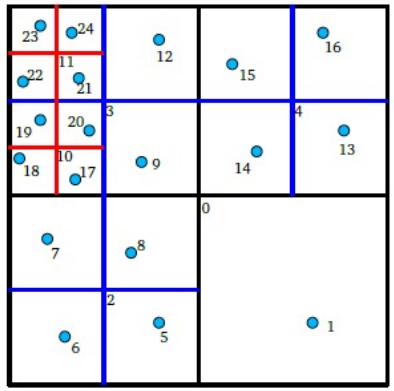

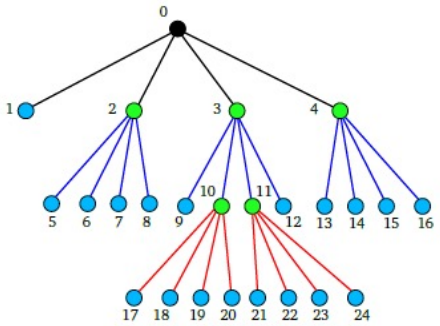

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- Public available Tree codes
- PKDGRAV3 (Potter+ 16)
- http://www.pkdgrav.com
- GADGET (Springel 20)

https://wwwmpa.mpa-garching.mpg.de/gadget4/

- ChaNGa (Quinn+15)

https://github.com/N-BodyShop/changa/

GRID BASED METHODS

Grid based numerical methods

Particle-Mesh (PM)

Basic reference $\Longrightarrow$Hockney and Eastwood's *Computer simulations using particles* book

- Use a eulerian regular mesh in comoving space to compute density from particles by interpolation.
- Solve Poisson equation in the mesh by convolution of density with Green's functions in Fourier space.
- Fourier transformation is done by Fast Fourier Transform algorithm $\Longrightarrow$ $O(N\log(N))$. Much faster than PP !
- Periodic Boundary conditions. Adequate for cosmological simulations.
- First application to cosmology (in 3D): Klypin & Shandarin, 1983; White et al 1983. Many codes have been developed since then.
- Can treat more particles than any other method.

Basic steps of the PM algorithm

1. Assign *charge* to the mesh points $(\mathbf{q_l})$ from particle positions $(\mathbf{x_l})$.

   - $\rho(\mathbf{q_l}) = \frac{M^3}{N} \sum_{j=1}^{N} W(\mathbf{x_j} - \mathbf{q_l})$
   - Momentum conserving schemes: (W)
     - ⋆ No interpolation. *Nearest-Grid-Point* NGP
     - ⋆ Multilinear interpolation. *Clouds-in-Cell.* (CIC) *Particle-in-Cell* (PIC)
     - ⋆ Multiquadratic interpolation. *Triangular-Shaped-Clouds* (TSC)

2. Solve Poisson equation in the mesh.

   $$\phi(\mathbf{q}) = \frac{1}{M^3} \sum_{\mathbf{q'}} \mathcal{G}(\mathbf{q} - \mathbf{q'}) \rho(\mathbf{q'})$$

   - In Fourier space: Convolution $\Longrightarrow$ Product

   $$\hat{\phi}(l,m,n) = \sum_{p,q,r} \hat{\mathcal{G}}(p,q,r) \hat{\rho}(p,q,r) \exp\left(\frac{2\pi}{M}(p*l + q*m + r*n)\right)$$

   - Fast-Fourier-Transform (FFT) is $O(N \log(N))$
   - Different types of Green's Functions to reduce GRID NOISE (eg. EDFW 95)

- Simplest assumption: Greens F. for a 7-point finite difference Laplacian:

$$\hat{\mathcal{G}}(i,j,k) = \frac{-1}{\pi(i^2+j^2+k^2)}$$

3. Find force from potential in the mesh.

$$\mathbf{F}(\mathbf{q}) = -\frac{1}{N}\vec{D}\phi(\mathbf{q})$$

$\vec{D}$: 10-point differencing operator:

$$D_x(i,j,k)\phi = \tfrac{1}{6}(\phi_{i-1,j,k} - \phi_{i+1,j,k}) + \tfrac{1}{12}(\phi_{i-1,j+1,k} - \phi_{i+1,j+1,k} + \phi_{i-1,j-1,k} - \phi_{i+1,j-1,k} + \phi_{i-1,j,k+1} - \phi_{i+1,j,k+1} + \phi_{i-1,j,k-1} - \phi_{i+1,j,k-1})$$

4. Interpolate force from mesh to particles

$$\mathbf{F}(\mathbf{x}_\mathbf{l}) = \frac{M^3}{N}\sum_{\mathbf{q}} W(\mathbf{x}_\mathbf{l} - \mathbf{q})\mathbf{F}(\mathbf{q})$$

5. Move particles

$$\frac{d\mathbf{p}_\mathbf{l}}{da} = -\frac{\mathbf{F}(\mathbf{x}_\mathbf{l})}{\dot{a}} \quad ; \quad \frac{d\mathbf{x}_\mathbf{l}}{da} = \frac{\mathbf{p}_\mathbf{l}}{a^2\dot{a}}$$

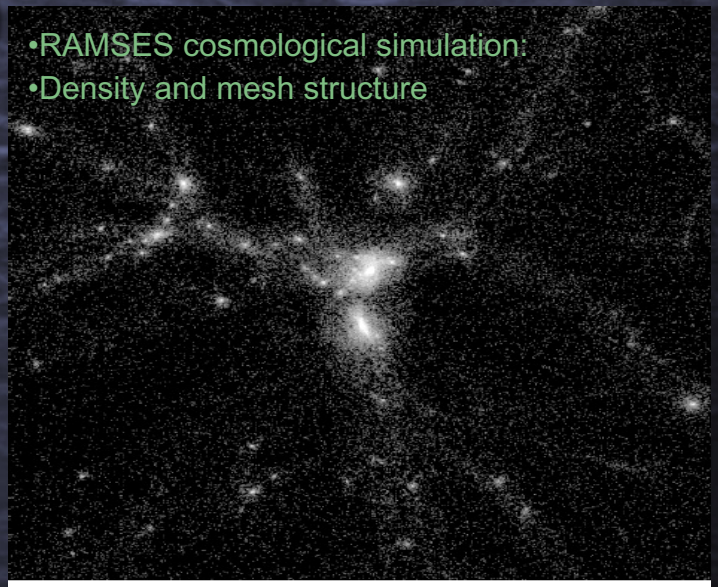
- Usual numerical techniques to integrate oridnary diff. equations:

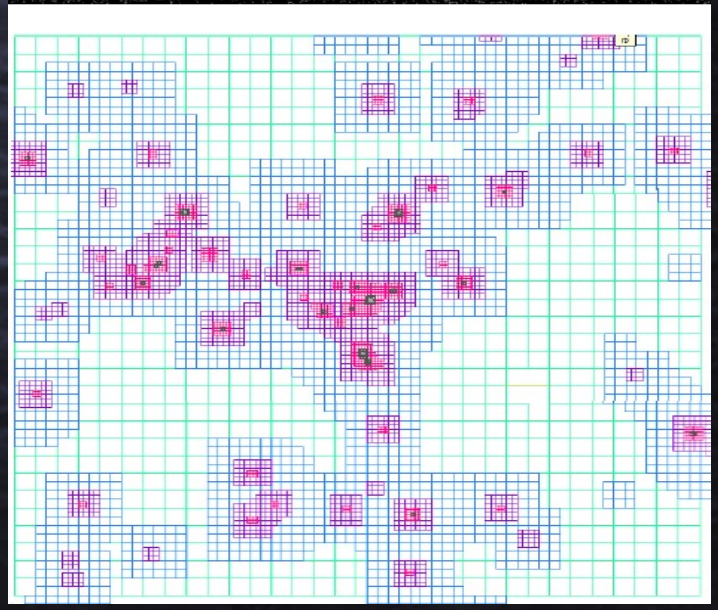
PM method

- Advantages of PM method:
  - easy to implement
  - Well suited for cosmological applications in which the mass is volume-filling,
  - Good scaling (O(N ln N). Easy to parallelize.
  - Natural implementation of periodic conditions.
  - No problema with 2 body relaxation. Particles do not see each other.
- Disadvantages of PM method:
  - Force approximation is anisotropic on the grid.
  - Newtonian force resolution ~2 mesh sizes.
  - Resolution depends on the mesh size.
- Some public parallel PM codes (+ IC generators)
  - FASTPM (Feng+16 https://github.com/fastpm/fastpm
  - PMFAST (Merz+ 05 https://www.cita.utoronto.ca/~merz/pmfast/

ADAPTIVE MESH REFINEMENT (AMR)

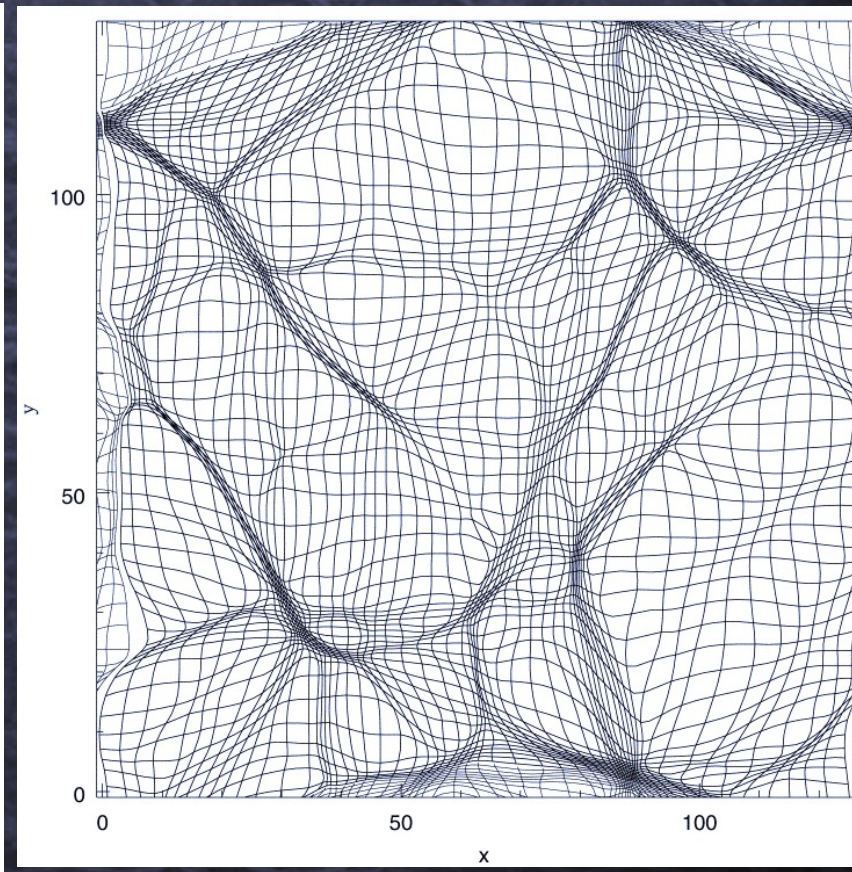
- Use staggered meshes to compute poisson's equation in different levels: PM is used at level 0 and then cells are refined depending on density. Typically each cell is recursively refined if the number of particle per cell exceed some threshold (around 10 particles).
- Use relaxation methods to solve Poisson equation in deeper levels can be cross talk with upper levels.
- Main problem is the bookkeeping of the mesh structure.
  - ENZO (Bryan & Norman 97)
  - https://enzo-project.org/
  - ART (Kravtsov & Klypin 96)
  - RAMSES (Teyssier 2002)
  - https://www.ics.uzh.ch/~teyssier/ramses/
  - AMIGA (former MLAPM) (Knebe+01)
  - http://popia.ft.uam.es/AMIGA/





Moving Mesh methods

- Gnedin 1995, Pen 1995.
- Full Lagrangian approach. The meash points move with the fluid.
- Same number of points. Resolution increases in high density and decreases elsewhere.
- Solves Poisson equation in the Lagrangian space.
- Do not use particles.
- Mesh distortions may introduce severe anisotropies in the force calculation (Gnedin & Bertschinger 1996)

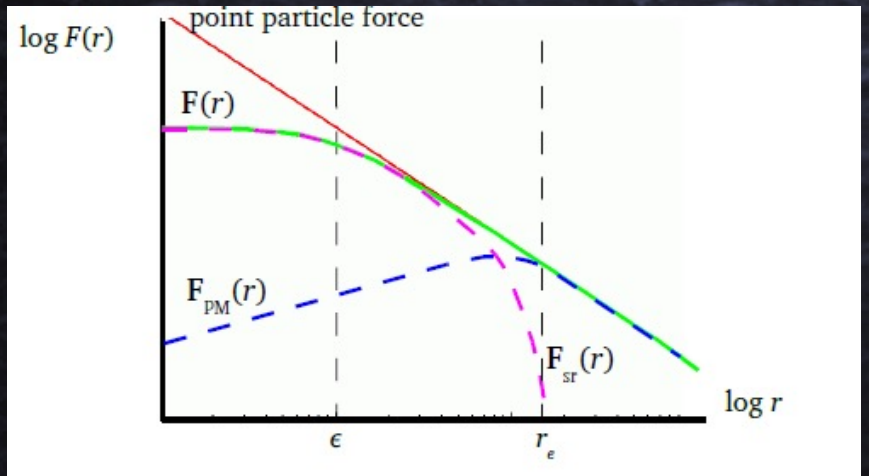


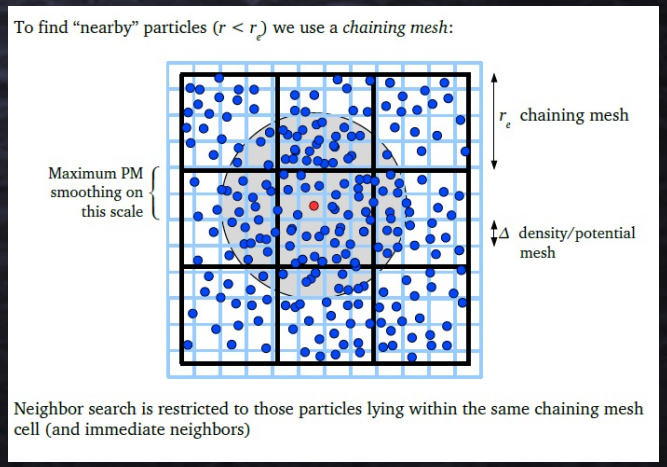
•MMH-code, Pen, 1995, ApJS,115,19

HYBRID N-BODY METHODS

Particle-Particle-Particle-Mesh (P^3M):

- PM force accuracy only for scales > 2-3 cell size.
- Gravitational clustering produces large density gradients: poor resolution when system becomes too small compared with mesh discreetness.
- Possible Solution:
  - Increase the number of cells.
  - Divide the net force in Short-range (P-P) + Long-range (PM). Neighbor search can be very expensive

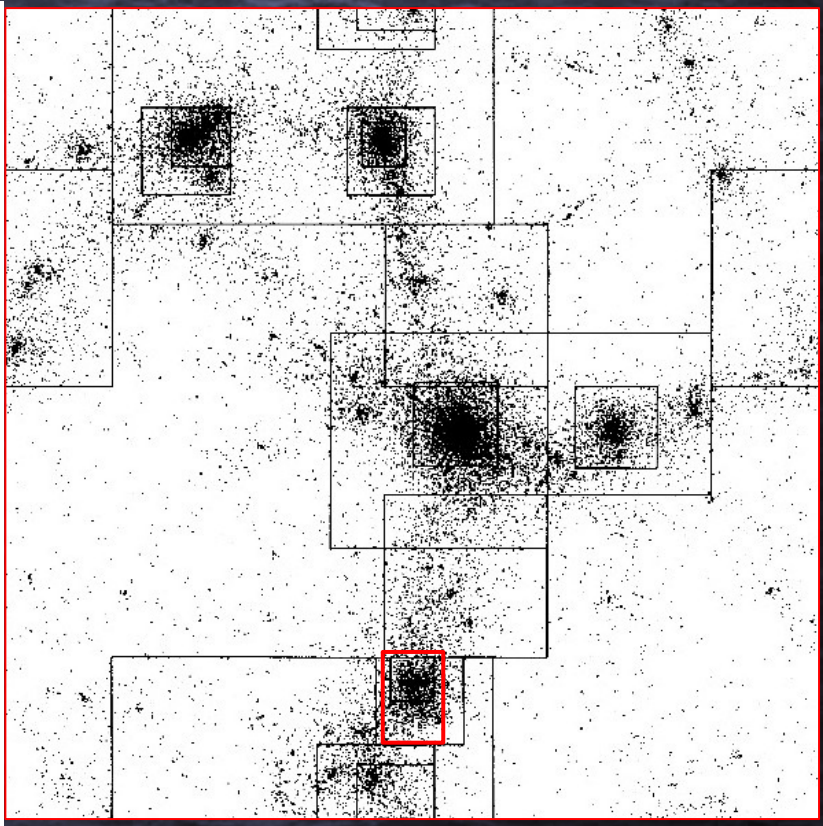




Adaptive P^3M (AP^3M):

- ♡ Use of subgrids in areas of high clustering regime
- ♡ Basic Procedure:
  1. Identify regions for refinement.
  2. PM forces in the main grid
  3. PP-force for particles excepts those in high density areas
  4. P^3M calculation in areas of 1. PP forces are calculated.
  5. Allow for further refinement in these new grids.
- ♡ Dramatic speed up factors with respect to P^3M.
- ♡ One of the first implementations of adaptive mesh refinement (AMR) methods
- ♡ One of the FIRST cosmological codes to be in PUBLIC. domain.!.

(Thanks to Hugh Couchmann.)



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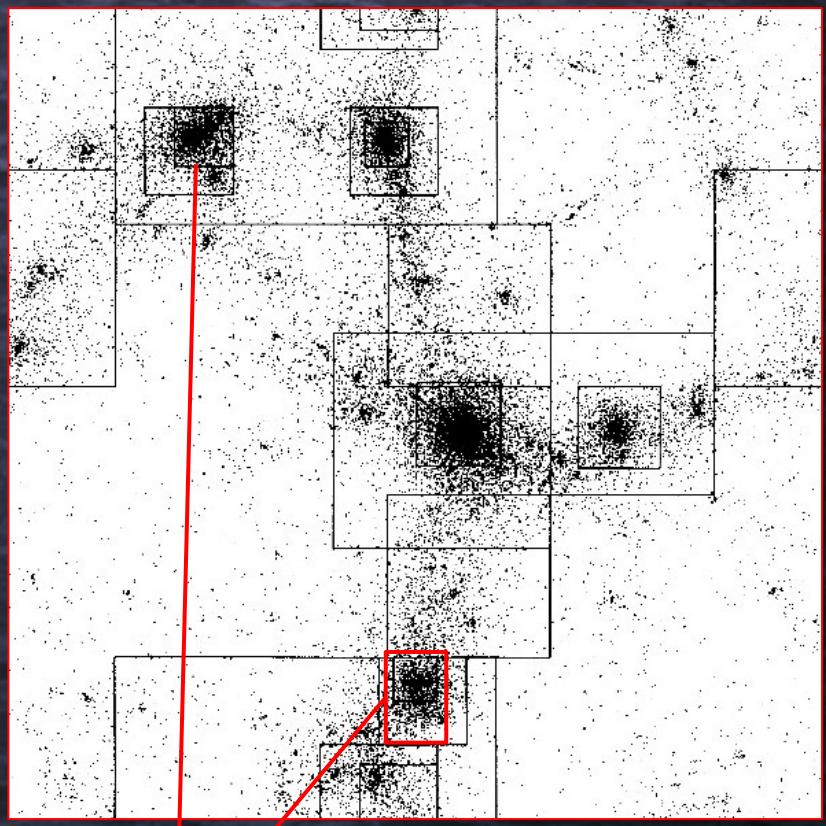


Individual P3M calculation with isolated boundary conditions

•Hydra: Couchmann+96
https://hydra.mcmaster.ca

•HACC: Habib+14
•https://arxiv.org/abs/1410.2805

•CUBEP3M (Harnois-Deraps+ 13)
•https://github.com/jharno/cubep3m

TREE + PM

- Another method to account for the short –long range gravitational forces is to combine a PM method to account for long range with a TREE code to speed up the short scale force
- The potential is split into two parts in Fourier space (Xu 97, Bagla 2002, Dubinski 2004, Springel 2005)

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:

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

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

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

Solve in real space with TREE

credit V. Springel

TREEPM CODES

GADGET4 (Springel 20)
https://gitlab.mpcdf.mpg.de/vrs/gadget4

GREEM (Ishiyama09)

GOTPM (Dubinski+ 04)

GIZMO (Hopkins, 15)
http://www.tapir.caltech.edu/~phopkins/Site/GIZMO.html

TIME INTEGRATION

- Once the gravitational forces are calculated for every particle, the equations of orbital motions fhas to be integrated in time.
- Different time integrators can be used to integrate a second order ODE (e.g. Runge-Kutta 4^{th} order, or LeapFrog)
- The most often used method in N-body problems is Leap-frog scheme:
  - Velocities and positions are shifted by half time interval.
  - There are two versions of the Leapfrog, depending on whether one starts first by shifting velocities at half timestep using forces at the present timestep (kick) and then update positions to the full time step (drift) and recomputing forces with new positions and update velocities to full step (Kick)… or viceversa.

TIME INTEGRATION

$$\frac{\mathbf{dv}}{\mathbf{dt}} = \mathbf{f}(\mathbf{x}); \quad \frac{\mathbf{dx}}{\mathbf{dt}} = \mathbf{v}(\mathbf{t})$$

The DRIFT-KICK-DRIFT (DKD)

$$\mathbf{x}_{n+1/2} = \mathbf{x}_n + \mathbf{v}_n \Delta t/2$$

$$\mathbf{v}_{n+1} = \mathbf{v}_n + \mathbf{f}(\mathbf{x}_{n+1/2}) \Delta t$$

$$\mathbf{x}_{n+1} = \mathbf{x}_{n+1/2} + \mathbf{v}_{n+1} \Delta t/2.$$

The KICK-DRIFT-KICK (KDK)

$$\mathbf{v}_{n+1/2} = \mathbf{v}_n + \mathbf{f}(\mathbf{x}_n) \Delta t/2$$

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \mathbf{v}_{n+1/2} \Delta t$$

$$\mathbf{v}_{n+1} = \mathbf{v}_{n+1/2} + \mathbf{f}(\mathbf{x}_{n+1}) \Delta t/2$$

LEAP FROG

- KDK and DKD are second order time accuracy ($O(\Delta t^2)$).
- Contrary to Runge-Kutta, they are symplectic time integrators
  - Symplectic: D & K operators conserves the Hamiltonian structure of the dynamical system
  - The time evolution is a continuous canonical transformation generated by the Hamiltonian of the system

$$H(\mathbf{p}_1, \ldots, \mathbf{p}_n, \mathbf{x}_1, \ldots, \mathbf{x}_n) = \sum_i \frac{\mathbf{p}_i^2}{2m_i} + \frac{1}{2}\sum_{ij} m_i m_j \phi(\mathbf{x}_i - \mathbf{x}_j)$$

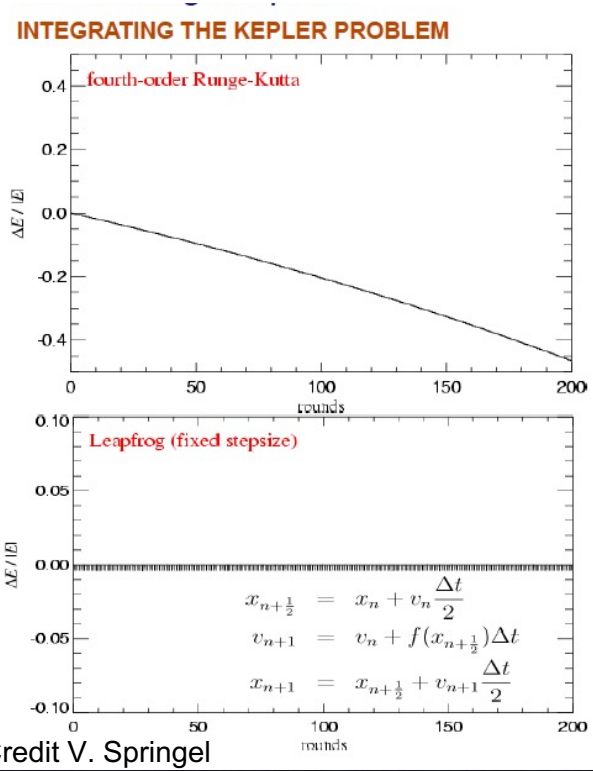
  - Time-reversible integrators

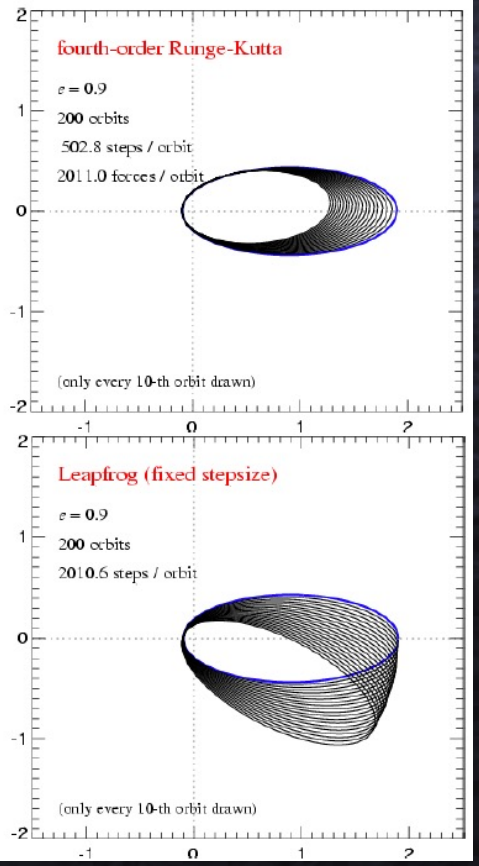
LEAP FROG

Exercise: Integrate the 2-body Kepler problem using Leap-Frog (KDK and DKD) and RK4 .

Test the total energy conservation as function of orbital periods.

Despite the lower accuracy, Leapfrog behaves much better than RK4



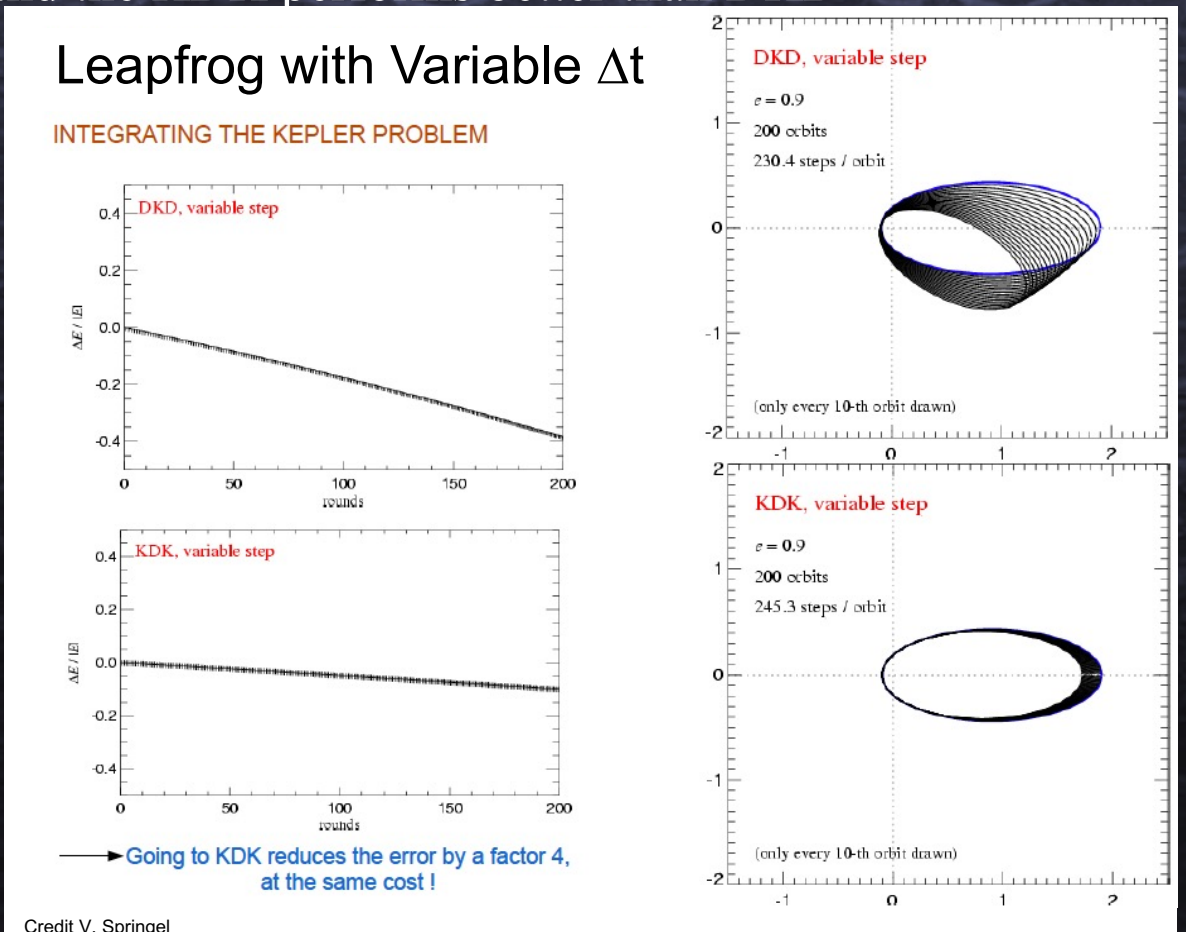


Credit V. Springel

LEAP FROG

Exercise: Integrate the 2-body Kepler problem

If variable Δt is used during time integration, the energu conservation is worse and the KDK performs better than DKD



Credit V. Springel

LEAP FROG

Variable timesteps is a must for simulations with large N, so, KDK is mostly used in cosmological codes.

Time step selection criteria:

Cosmological criterion: Δt *must be much smaller than the age of the Universe* : $\Delta t << \frac{1}{H}$

Acceleration/velocity criterion: ***Particles should not move faster than some preselected threshold ε, of order of the force resolution***

$$\Delta t \le \sqrt{\frac{\varepsilon}{a_{\max}}} \qquad \Delta t \le \frac{\varepsilon}{v_{\max}}$$

Timesteps can be individually assigned to each particle following the above criteria such that $a_{max} = a_i$ (particle acceleration)

(e.g. GADGET and PKDGRAV3 codes)

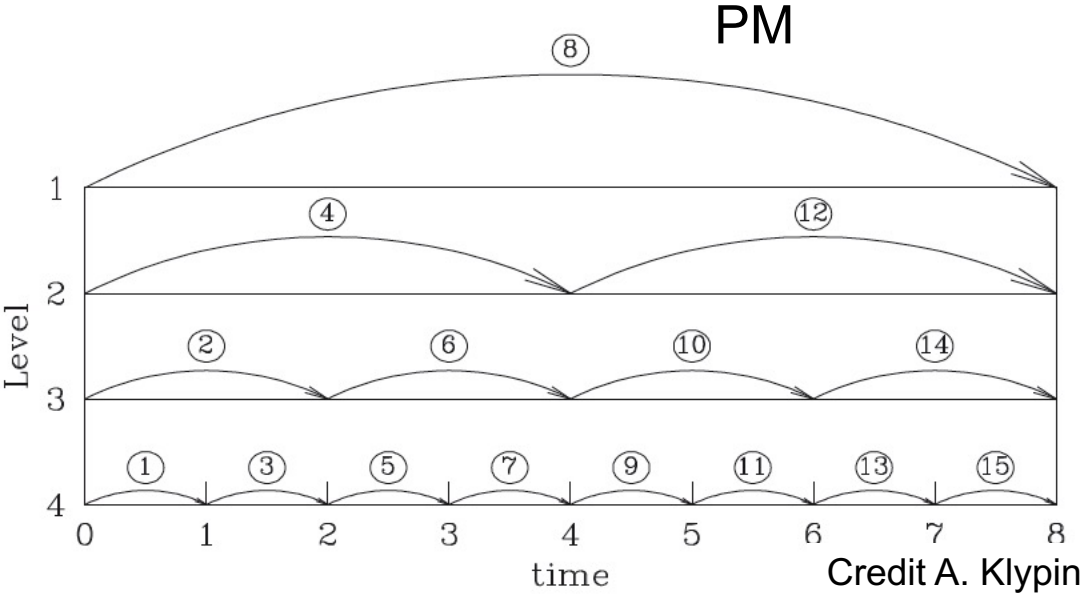
LEAP FROG

- For grid based codes (e.g. PM), constant timesteps are used.
- For AMR codes (e.g. ART and RAMSES), time step is reduced a factor 2 for each refinemet level.

Time step is scaling as
$\Delta t \propto \rho^{-1/3}$.

Zemp+07 suggest
$\Delta t \propto \rho^{-1/2}$

(2.8 reduction of Δt per level)



DOMAIN DECOMPOSITION

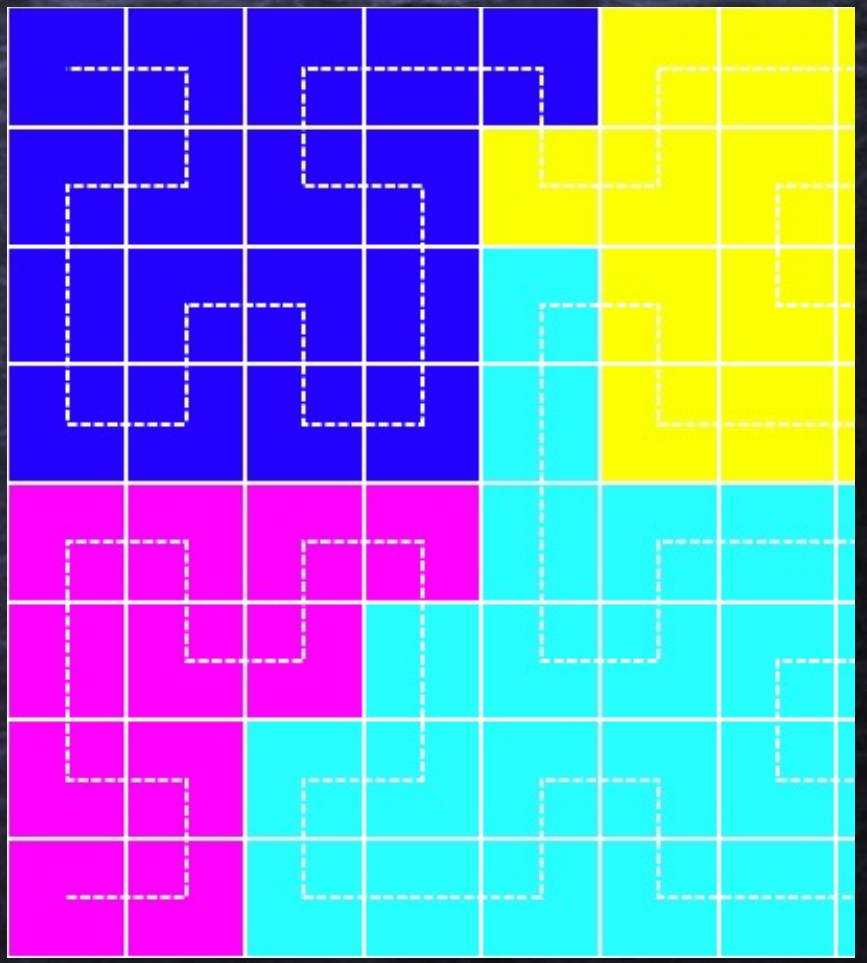
- Modern cosmological N-body codes must have some degree of parallelism to be able to run in HPC infrastructures. All of them use MPI Library to communicate among the different nodes, some also have OpenMP directives to speed up in-node computations.
- The computational domain (e.g. particles, or particles + grids) has to be decompose into smaller pieces that will be distributed among the available compute nodes.

DOMAIN DECOMPOSITION

- The domain decomposition algorithm is one the most important ingredients of a N-body code because it controls the load-balancing of the computations.
- Domain decomposition has to minimize exchange of information, so they must conserve locality of particle positions and account for work load in each node.

HILBERT CURVE DECOMPOSITION

- All particles are ordered according to a 1D index that preserves locality in 3D.
- The Hilbert curve is chuncked in as many pieces as processors with the same number particles or same work load (weighting by FLOPS/particle)
- For very clustered situations, more domains than available CPUS can be considered (e.g. `MULTIPLEDOMAINS` options in GADGET4)

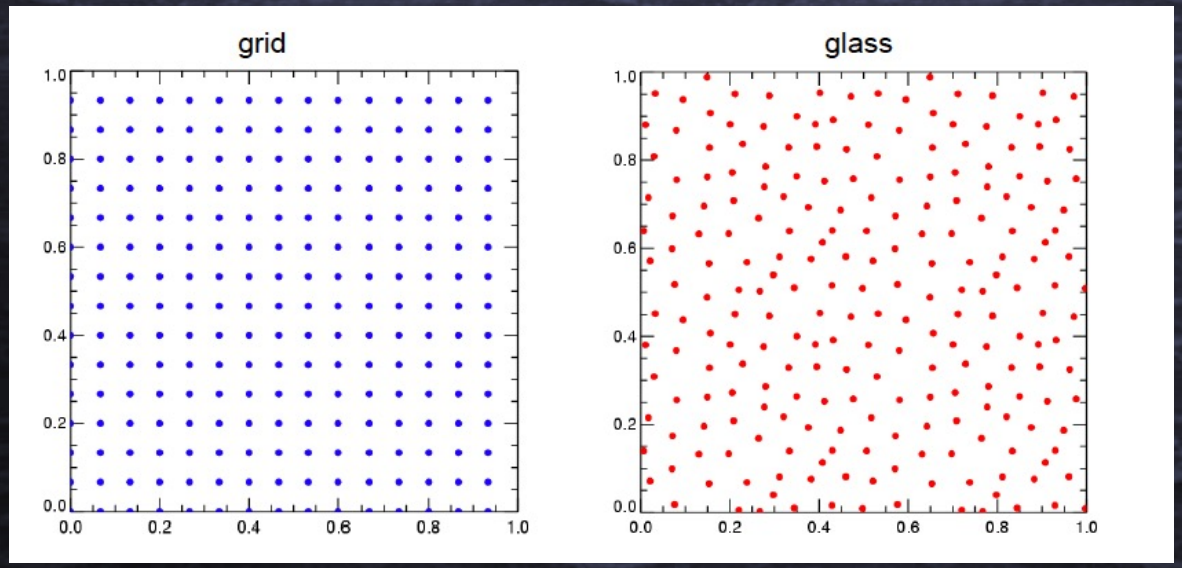


INITIAL CONDITIONS GENERATORS

- Cosmological N-BODY simulations are used to follow the gravitational evolution of density perturbations beyond linear theory.
- Therefore, the initial conditions for N-body have to be in agreement with the results from linear perturbation calculations.
- Lagrangian Perturbation Theory (LPT) can follow the distribution o particles in 3D comoving volume to the quasi-linear regime.
- So, it is natural to use the first or 2^{nd} order LPT to set up Ics for N-BODY.

INITIAL CONDITIONS GENERATORS

- **FIRST STEP**: generate a realization of the linear density gaussian fluctuation $\delta\rho(x, t_{init}) = FFT\ (\ P^{1/2}_{lin}(k)\ e^{i\theta})$



R and C Gauss (0,1)

- $\delta\rho(\mathbf{x}, t_{init}) = D^{+}(t_{init})\sum_{k_{min}}^{k_{max}}(\sqrt{P_{lin}}(k)(R_k + iC_k)\ e^{-\boldsymbol{ikx}}$
- $k_{min} = \frac{2\pi}{L}$ $k_{max}\ \frac{2\pi}{L}\ \frac{N^{1/3}}{2}$ (Nyquist Frequency)

INITIAL CONDITIONS GENERATORS

- Second Step: Compute the displacement field

$d_i(t) = x_i(t) - q_i$ and velocities $\dot{x} = H(a)f(\Omega)d$

From 1LPT, Zeldovich or 2LPT approximations.

$$\nabla^2\phi = \delta \qquad \mathbf{d} = -\nabla\phi \qquad \text{1LPT}$$

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

- Move particles from lagrangian positions q_i using the displacement field **d** and assign velocities.
- Phase space for the N particles is ready. Start the N-body integration using your prefer code.
- Some IC codes available:

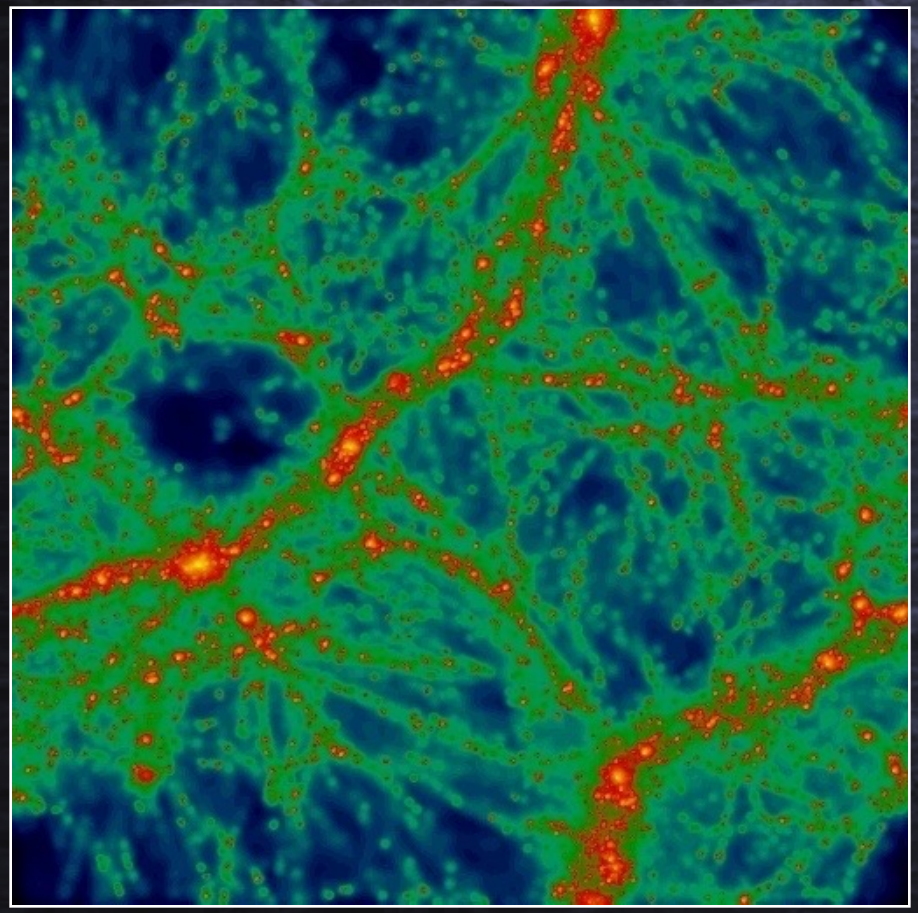
UNIGRID:

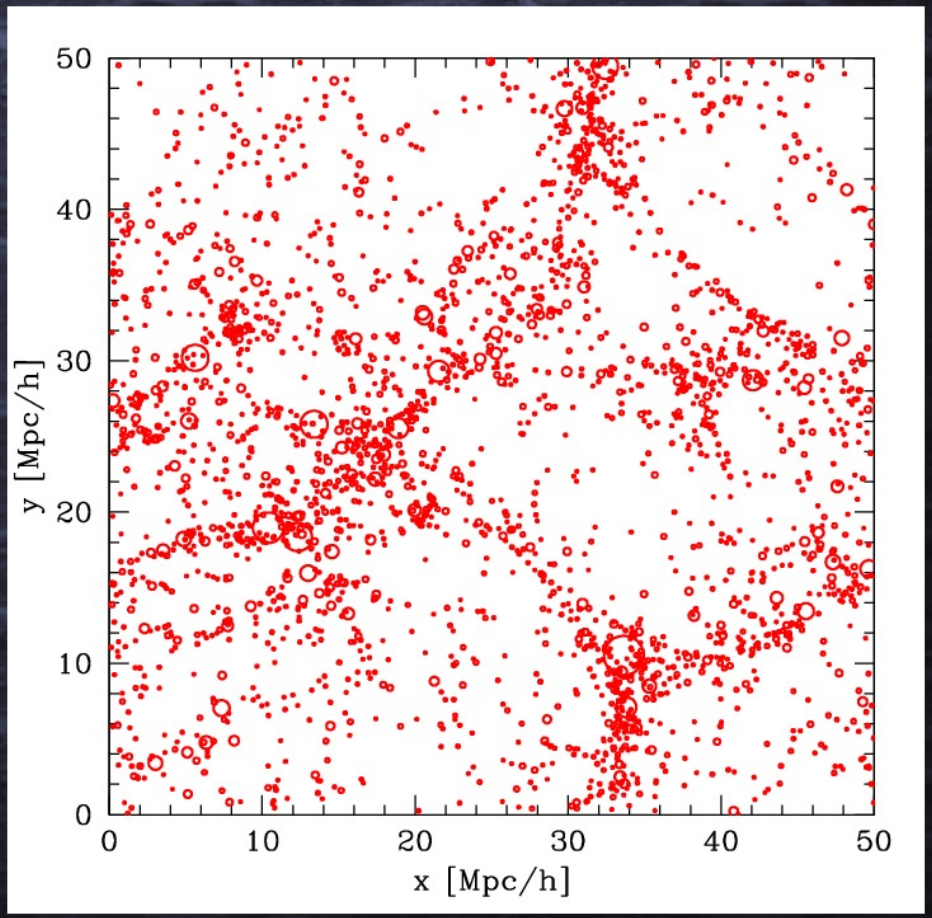
- 2LPTIC (https://cosmo.nyu.edu/roman/2LPT/)
- FASTPM (https://github.com/fastpm/fastpm
- N-GENICS (comes with GADGET4 code)
- PANPHASIA (http://icc.dur.ac.uk/Panphasia.php

MULTIGRID (valid for zoom simulations or single box)

- MUSIC (multiscale ics, valid for zooms,) https://www-n.oca.eu/ohahn/MUSIC
- Mpgrapfic (included in RAMSES) , PMSTARTM (ART, http://astro.nmsu.edu/~aklypin/PM/pmcode
- GINNUNGAGAP (MPI + OpenMP) https://github.com/ginnungagapgroup/ginnungagap

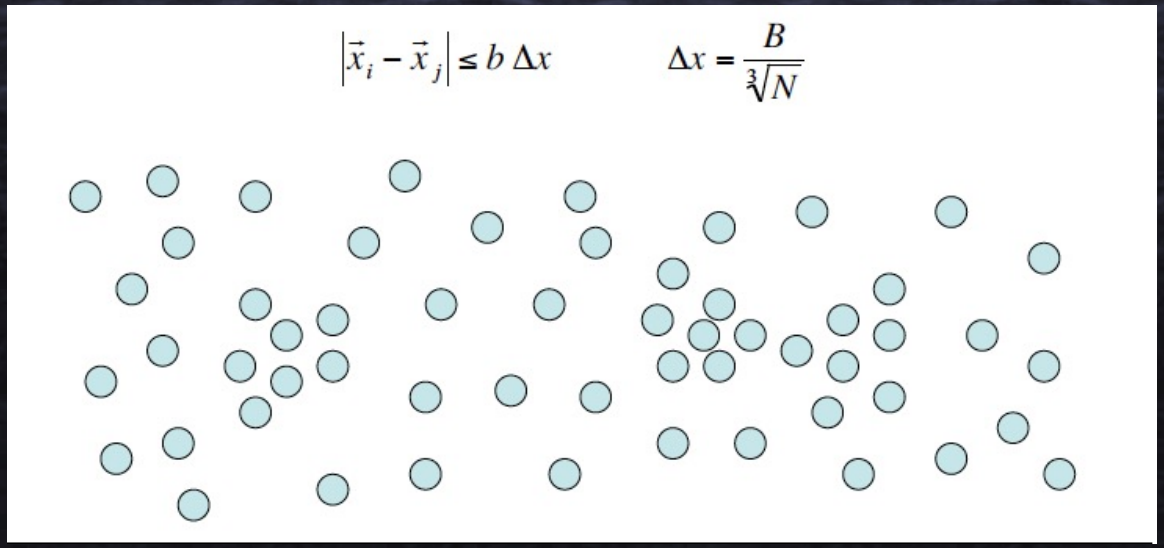
Halo Finders





Halo finders

- Different possibilities:
  - 3D configuration space (x,y,z)
    - Friend Of Friends (FoF).
      - Percolation algorithm.
      - Group particles that are spatially closer than a given distance b= linking length



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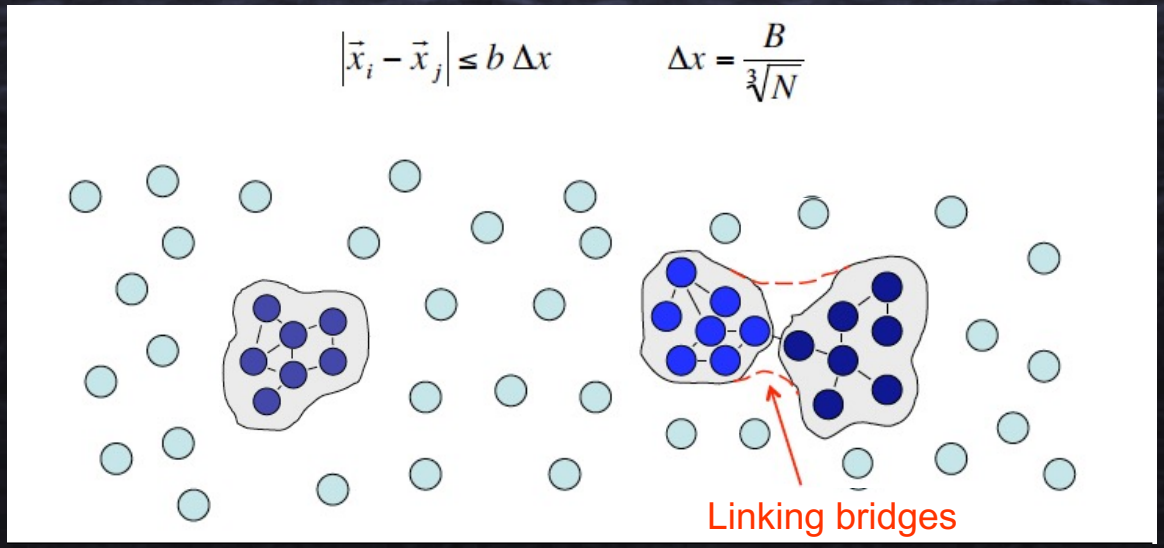

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    - FoF halos have arbitrary shape.
    - Not capable of finding subhalos by itself. Can be recursively applied with smaller linking lengths. Hierachical FOF (Gottloeber+ 99).
    - Problems with linking bridges….

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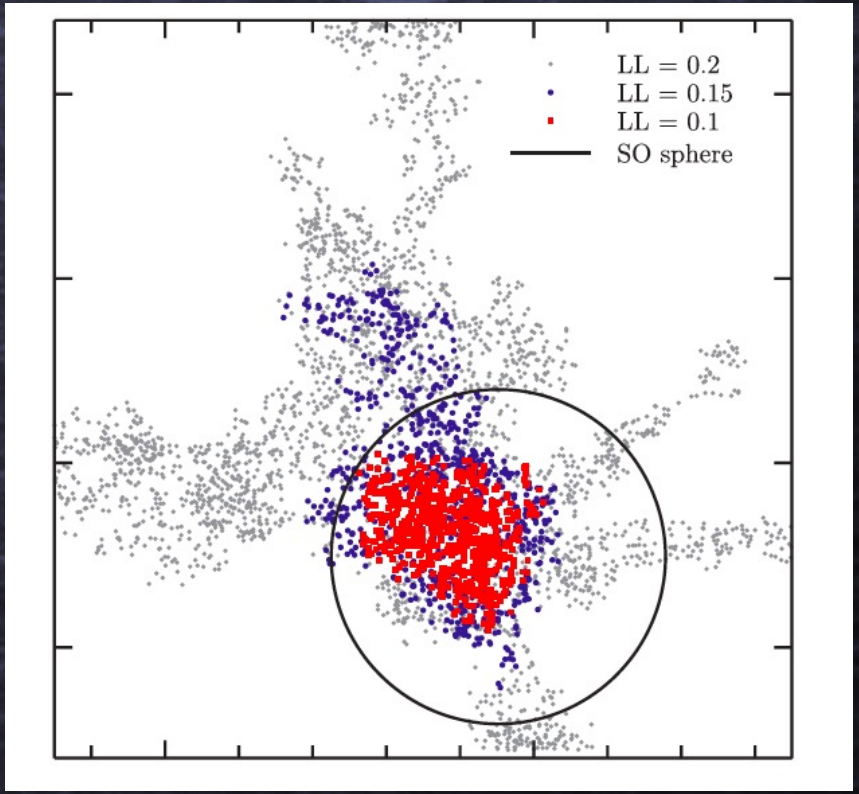

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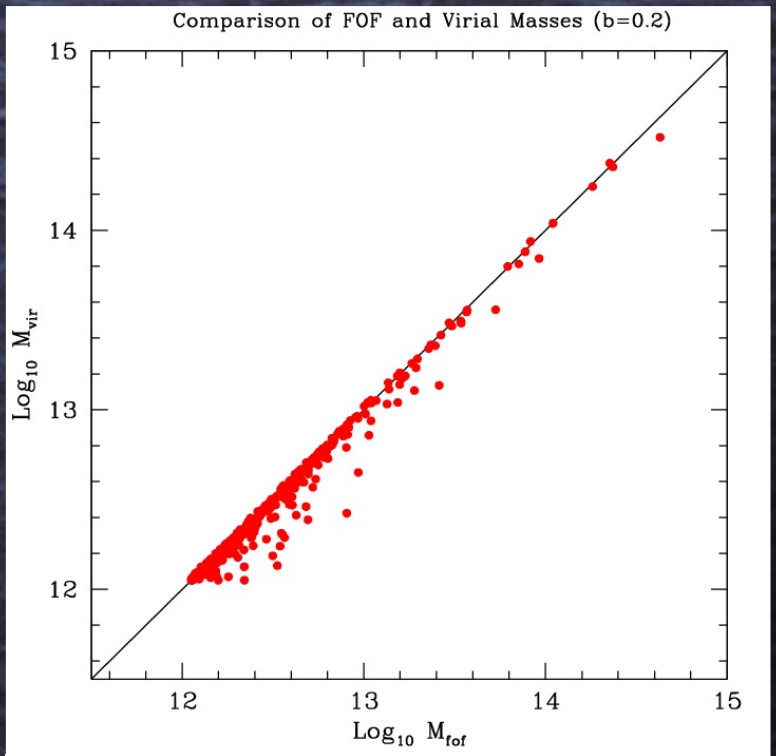
    - Problems with linking bridges….
    - How to choose the linking length?
    - Good agreement between FoF mass and Virial mass for

b ~0.17-0.2

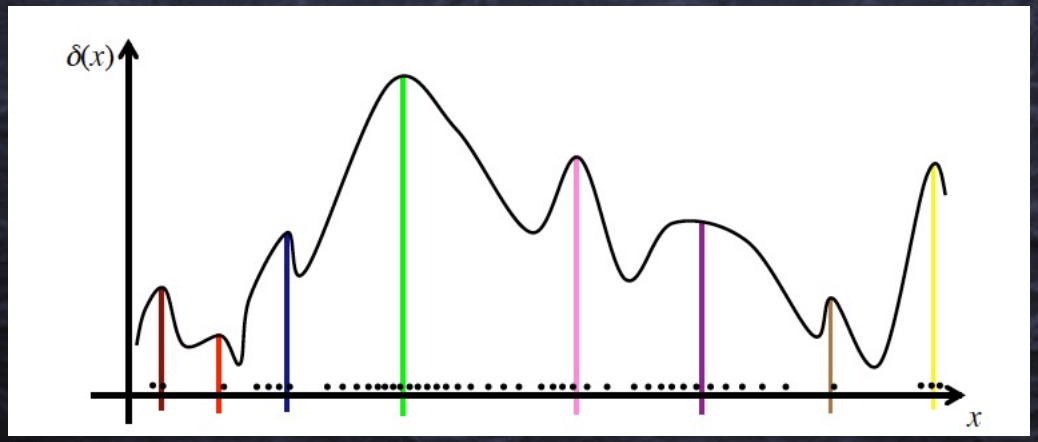


$$M_{vir} = \frac{4\pi}{3} \Delta \rho_{crit} r_{vir}^3$$

Δ Is the virial overdensity estimated by the Spherical collapse model. $\Delta \approx 97$ for ΛCDM.

Halo finders

- *Density Peak collector*
  - Estimate the smooth density field on a mesh from particles.
  - Identify local peaks as centers for halos.

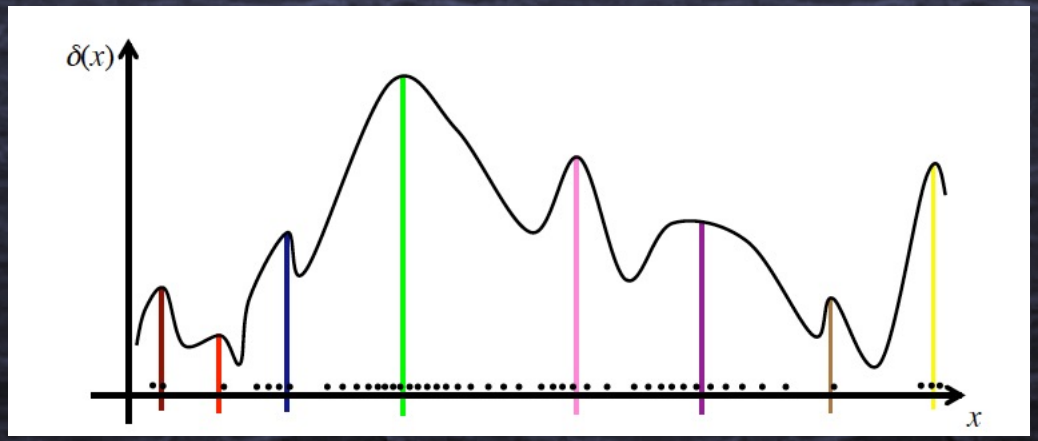


Collect particles in spherical shells around the peaks until M_{vir} is reached.

Can identify halos and sub-halos.

Halo finders

- *Density Peak collector & velocity information*
  - *Can use particle velocities to interactively remove gravitationally unbound particles*



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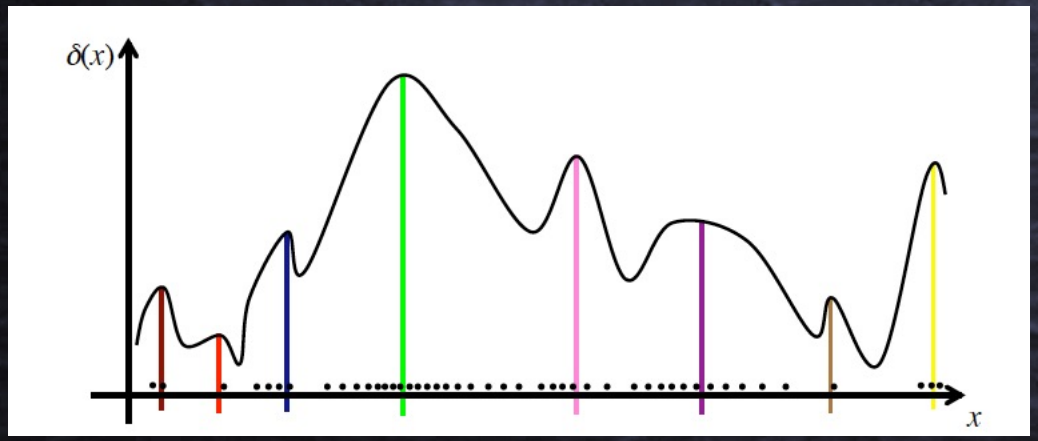
Examples of Density Peak Halo finders



- **SO** (Press & Schechter 1974)
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- **MHF** (Gill, Knebe & Gibson 2004)
- **PSB** (Kim & Park 2005)
- **VOBOZ** (Neyrinck et al. 2005)
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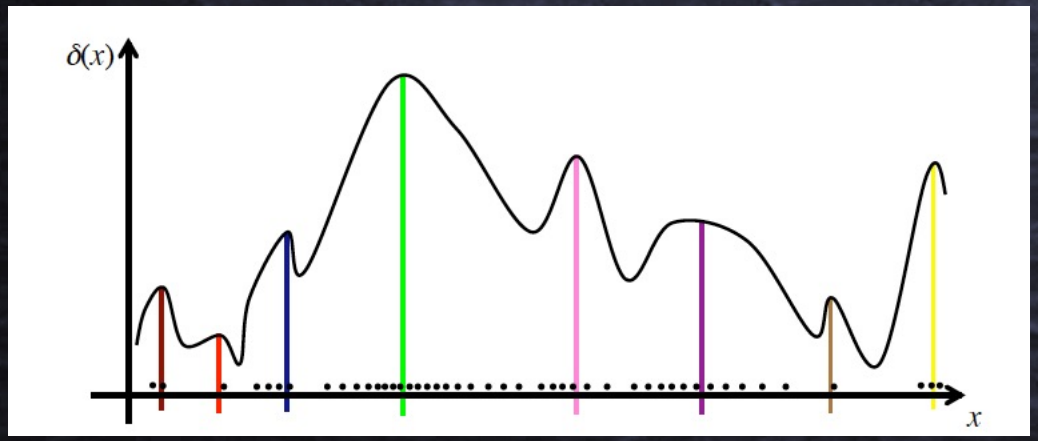

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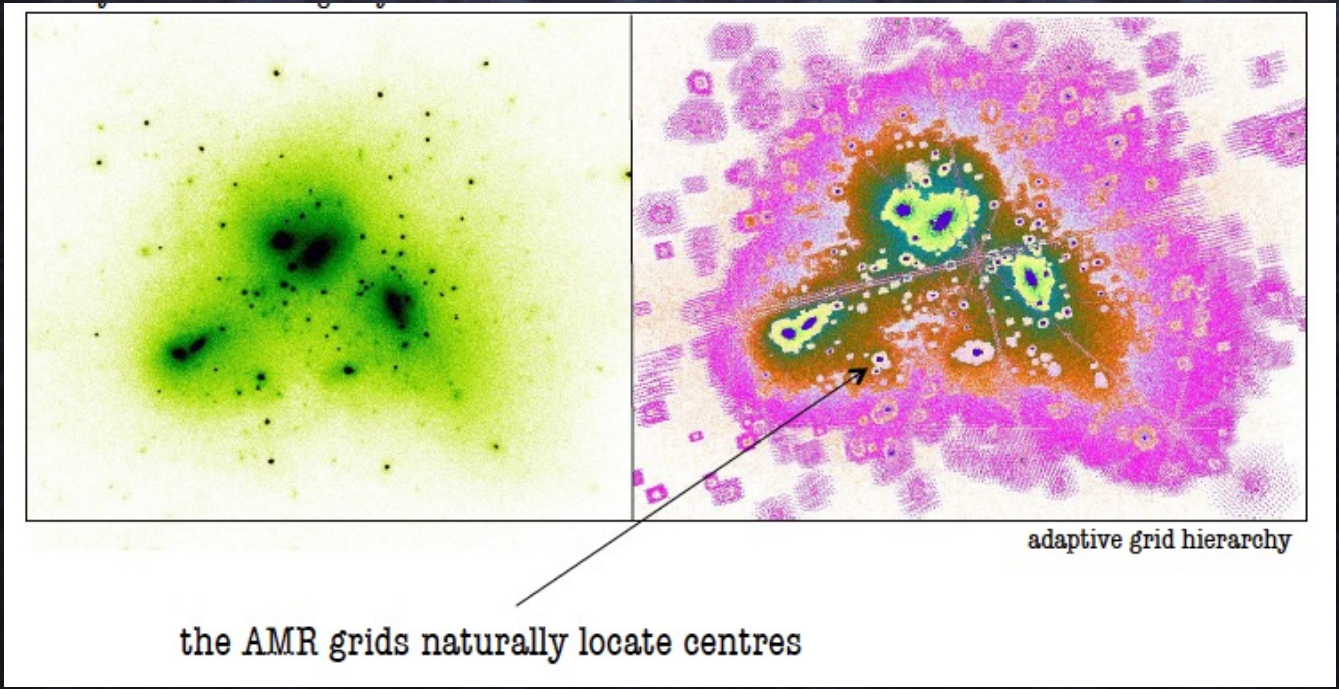
Halo finders

AMIGA HALO FINDER (AHF)

http://popia.ft.uam.es/AHF

Density field is constructed in a hierarchy of staggered meshes (AMR). Halos are found for density peaks in each refinement level.



Halo finders

AMIGA HALO FINDER (AHF)

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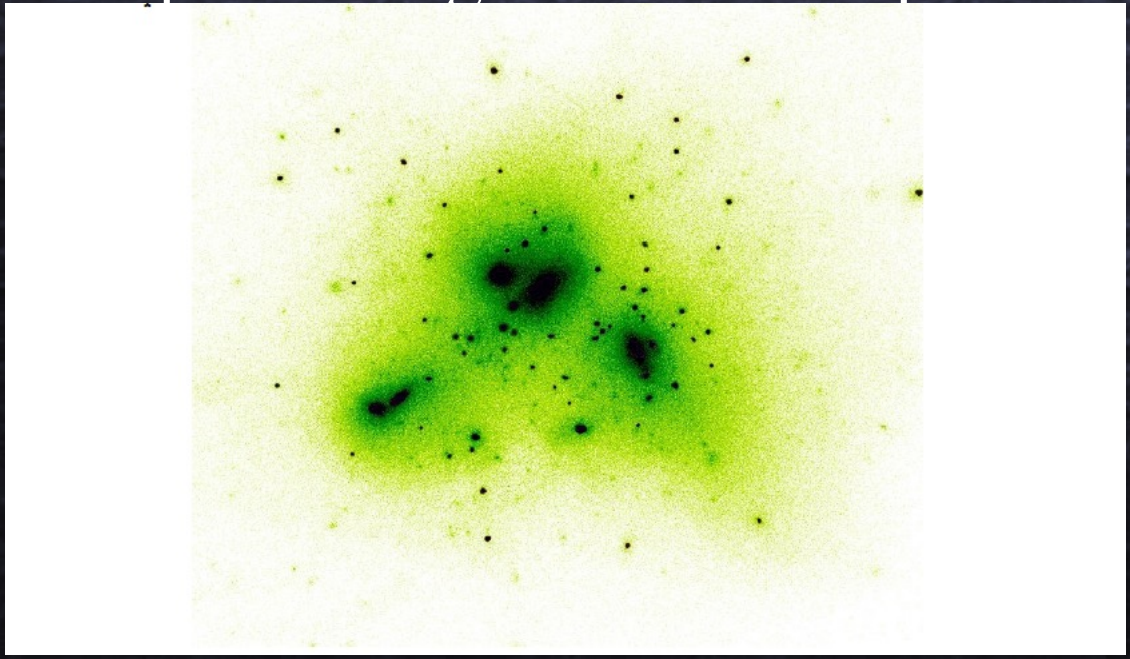
Identifies main halos and all substructures, at all levels. Then for each one do unbinding procedure and computes integral and radial profiles of quantites



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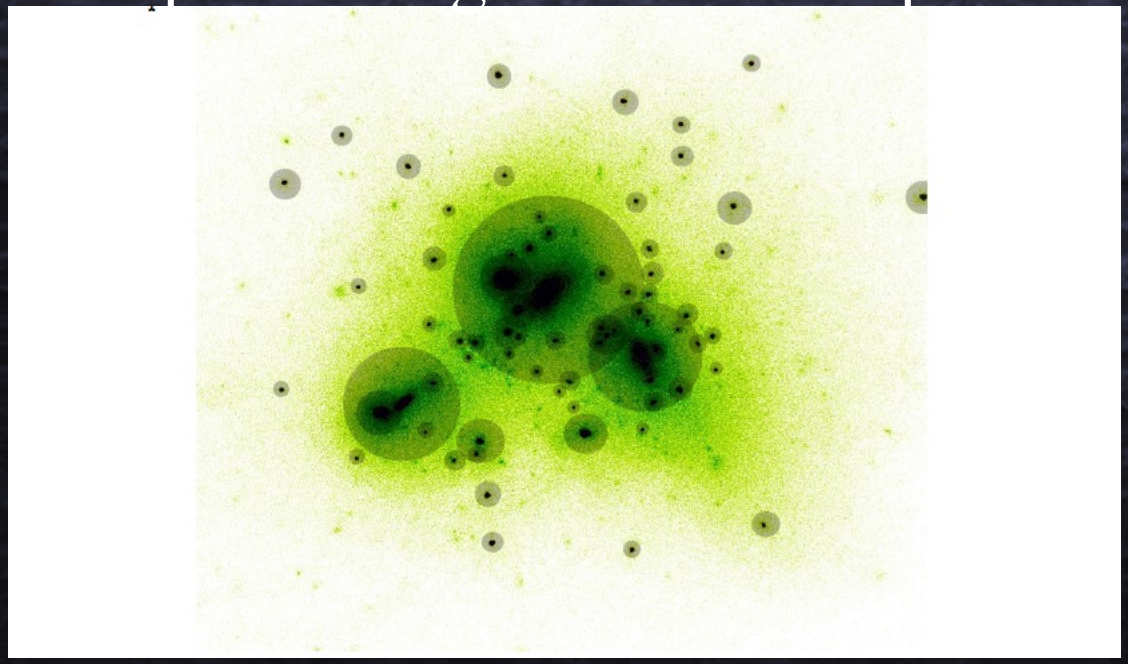


Halo finders

6D Phase Space halo finders

6DFOF (Diemand+06)

Search particles closer than a given distance in phase space

$$\frac{(\vec{x}_i - \vec{x}_j)^2}{(b_x \Delta x)^2} + \frac{(\vec{v}_i - \vec{v}_j)^2}{(b_v \Delta v)^2} < 1 \qquad \Delta x = \frac{B}{\sqrt[3]{N}} \qquad \Delta v \approx \sigma_v$$

ROCKSTAR: (Behroozi+13 ApJ)

https://bitbucket.org/gfcstanford/rockstar/

One of the most popular codes for analysing large volume simulations with $N > 10^{12}$ particles

Adaptive hierarchical FoF in 6D phase space.

Halo finders

ROCKSTAR:
(Behroozi+13 ApJ)
https://bitbucket.org/gfcstanford/rockstar/

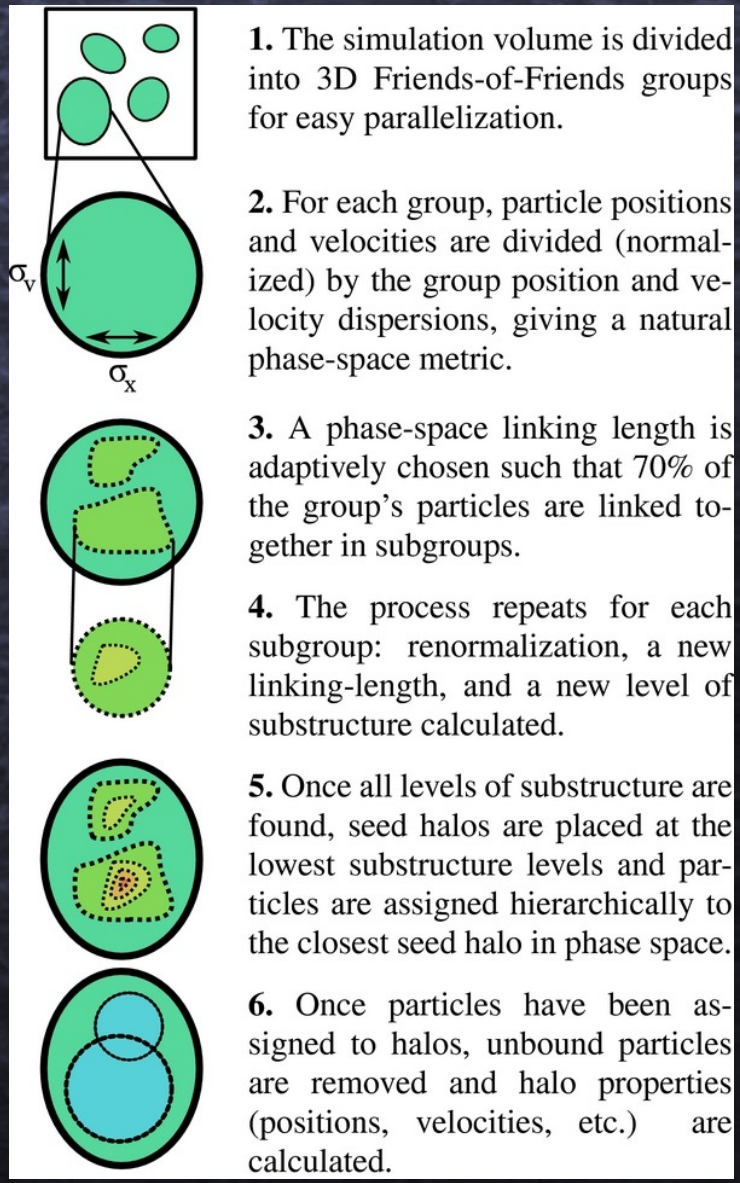
Obtains all hierarchy of halos and sub halos.

Uses information from previous timesteps to identify progenitors.

Can be used later for producing merger trees using

CONSISTENT TREES software

https://bitbucket.org/pbehroozi/consistent-trees/src/main/



1. The simulation volume is divided into 3D Friends-of-Friends groups for easy parallelization.

2. For each group, particle positions and velocities are divided (normalized) by the group position and velocity dispersions, giving a natural phase-space metric.

3. A phase-space linking length is adaptively chosen such that 70% of the group's particles are linked together in subgroups.

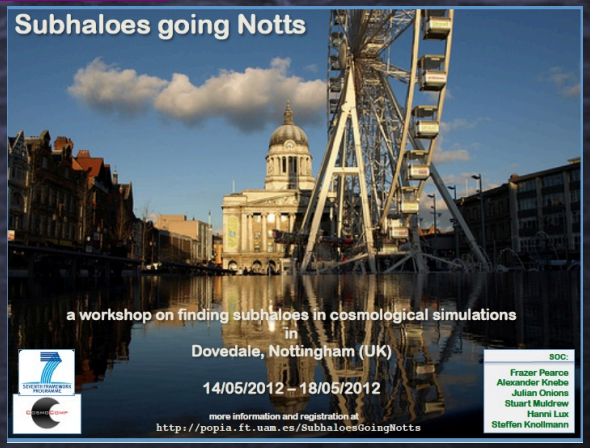
4. The process repeats for each subgroup: renormalization, a new linking-length, and a new level of substructure calculated.

5. Once all levels of substructure are found, seed halos are placed at the lowest substructure levels and particles are assigned hierarchically to the closest seed halo in phase space.

6. Once particles have been assigned to halos, unbound particles are removed and halo properties (positions, velocities, etc.) are calculated.

Halo finders

Comparison projects for halo finders:



Monthly Notices of the ROYAL ASTRONOMICAL SOCIETY

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Haloes gone MAD★: The Halo-Finder Comparison Project

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Subhaloes gone Notts: subhaloes as tracers of the dark matter halo shape

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N-body Simulations: things to look at

- Mass and force resolutions:
  - Dark halos identified with less than ~100 particles are usually not very trustable.
  - Check the gravitational smoothing choice: ε (typically ~ 1/20-1/40 $L/N^{1/3}$ see also Mansfield+21)
  - Distances less than ~3 x ε or 2-3 cell sizes in AMR are also subject to numerical errors dues to unresolved gravitational forces.
  - Center of halos are subject to two body relaxation. Apply convergence criteria ($t_{relax} \simeq {}^{N}/_{8 \ln N}\ t_{cross} > 1/2\ t_{Universe}$) (Power+ 03) for profiles.
  - Distances larger than ½ box size are affected by periodic conditions. Important for clustering measures.
  - Cosmic Variance effects due to Box size L (Power & Knebe 2006)
- Time steps:
  - Too large timesteps can introduce large errors in the particle trajectories. (see e.g. Quinn+97)
    - For fixed timesteps, a rule of thumb is $N_{step} > 6000(10kpc/\varepsilon)$ to integrate a Hubble time. (Lake+95)
- Starting redshift
  - Best if started as earlier as possible. Depends on Box size and LPT used (Knebe+ 09)

Questions?

SUMMARY

- Collisionless N-body simulations are still an indispensable tool in Cosmology.
- There has been an enormous technical development in the N-Body codes in the last 15 years.
  - From 10 billion particles in 2005 (Millenium) to today's 2 trillion particles FLAGSHIP
- We have been able to discover the main features of the late stages of non linear gravitational evolution of a collisionless dark matter fluid and test predictions about the distribution and internal structure of dark matter halos. But it lacks a fundamental ingredient: Baryonic matter which is responsible for most of the observations from galaxies.
- The N-body results can be complemented with some sort of modelling of the galaxy properties the dark halos are hosting (e.g. HOD, SHAM, SAM, or more recently, Machine Learning techniques)
- But for a self consistent picture of the cosmological galaxy formation, and to account for the effects of collisional matter, gas and star formation modelling has to be included in a simulation.
- Therefore, gas-dynamical simulations are the ultimate tool for properly understanding the combined gravitational evolution of the multiphase fluid that led to the formation of the structures we see today from our place in the Universe.

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- *Cosmological N-Body simulation: Techniques, Scope and Status, Bagla (arxiv/0411043)*
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- *Simulations techniques for cosmological simulations. K. Dolag et al arxiv/0801.1023*

Important papers to read.

- **Mansfield & Avestruz, 2021,** *How biased are halo properties in cosmological simulations?, MNRAS, 500, 3309.*
- Ludlow ***et al 2009,*** **Numerical convergence of simulations of galaxy formation: the abundance and internal structure of cold dark matter haloes MNRAS, 488, 3663**
- M. Zemp et al: *An optimum time-stepping scheme for N-body simulations*, MNRAS . 376 (2007) 273–286
- ***T. Quinn****, et al* . Time stepping N-body simulations, (1997), arXiv/9710043.
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