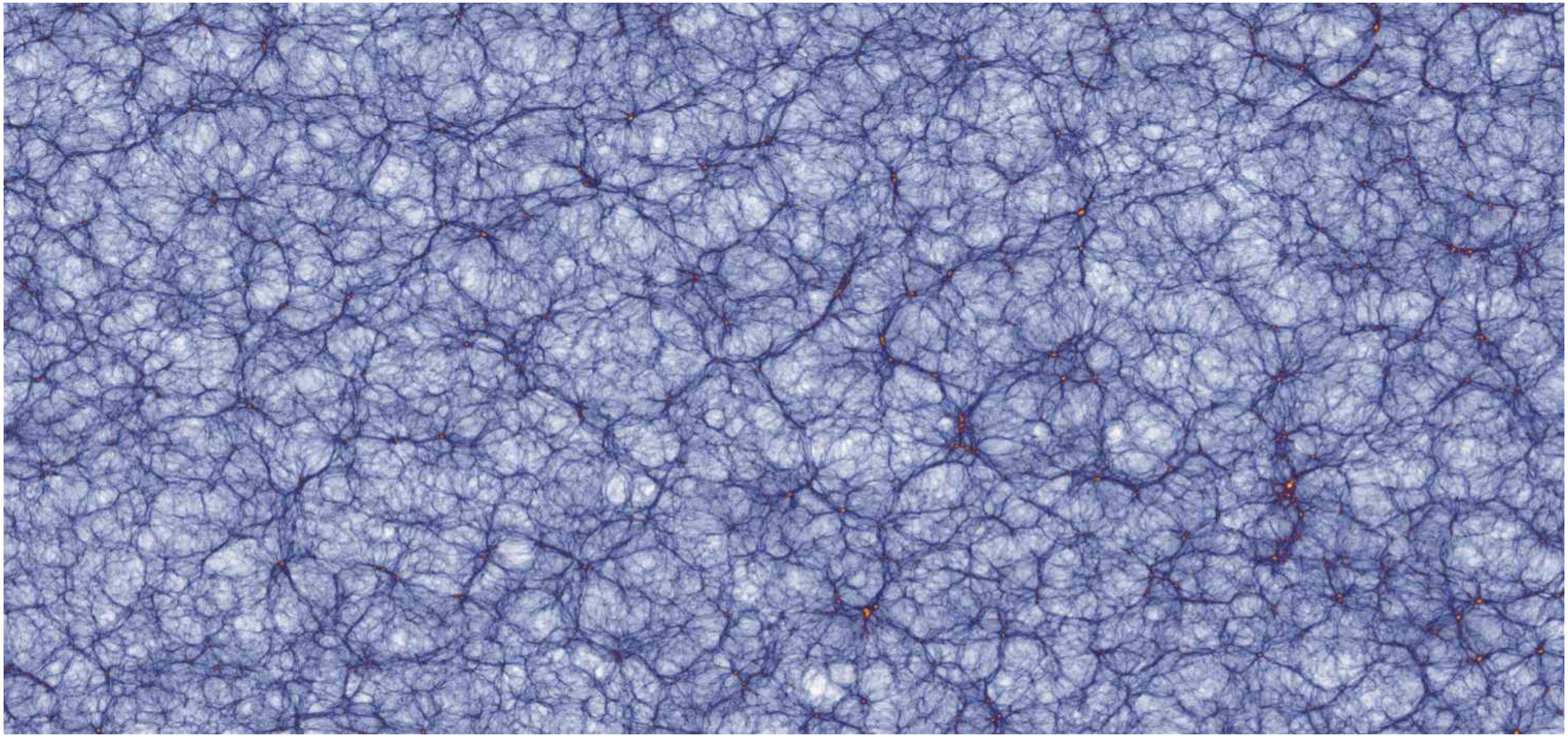
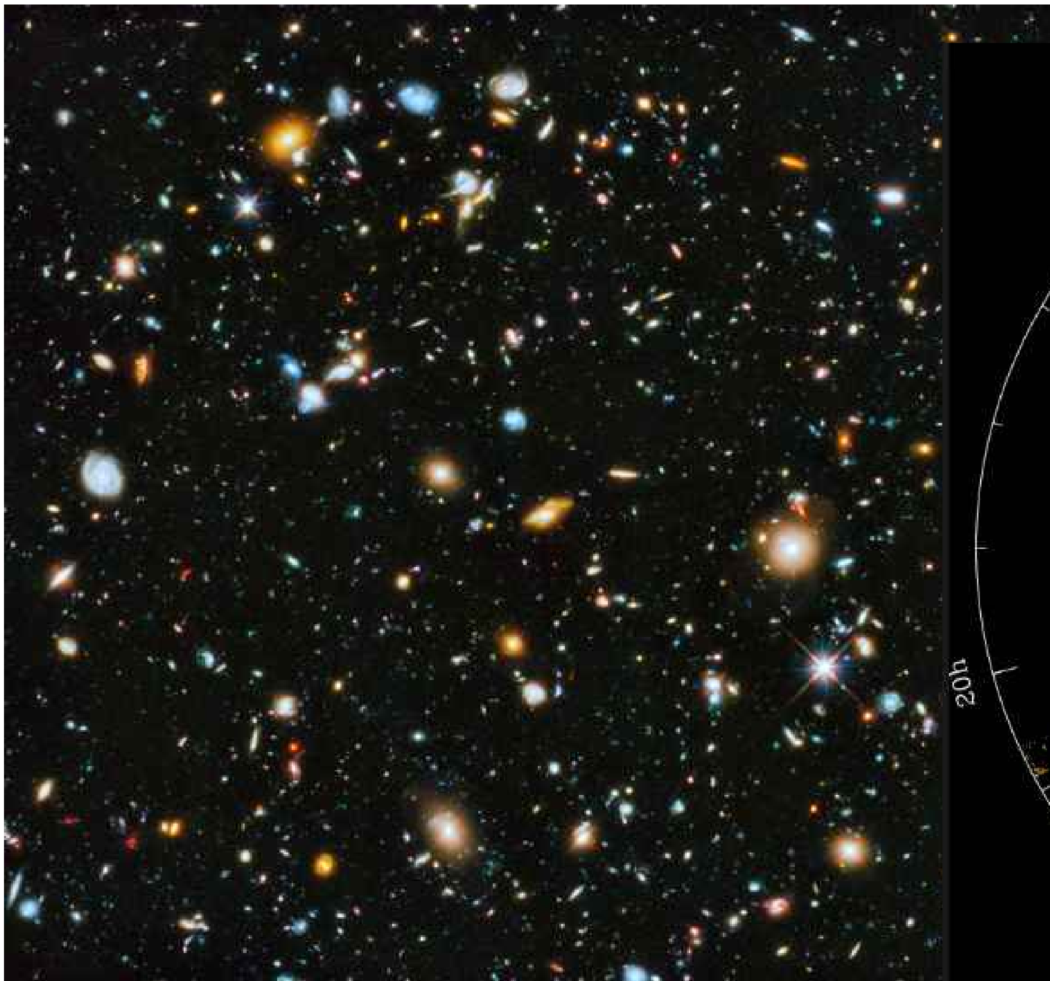
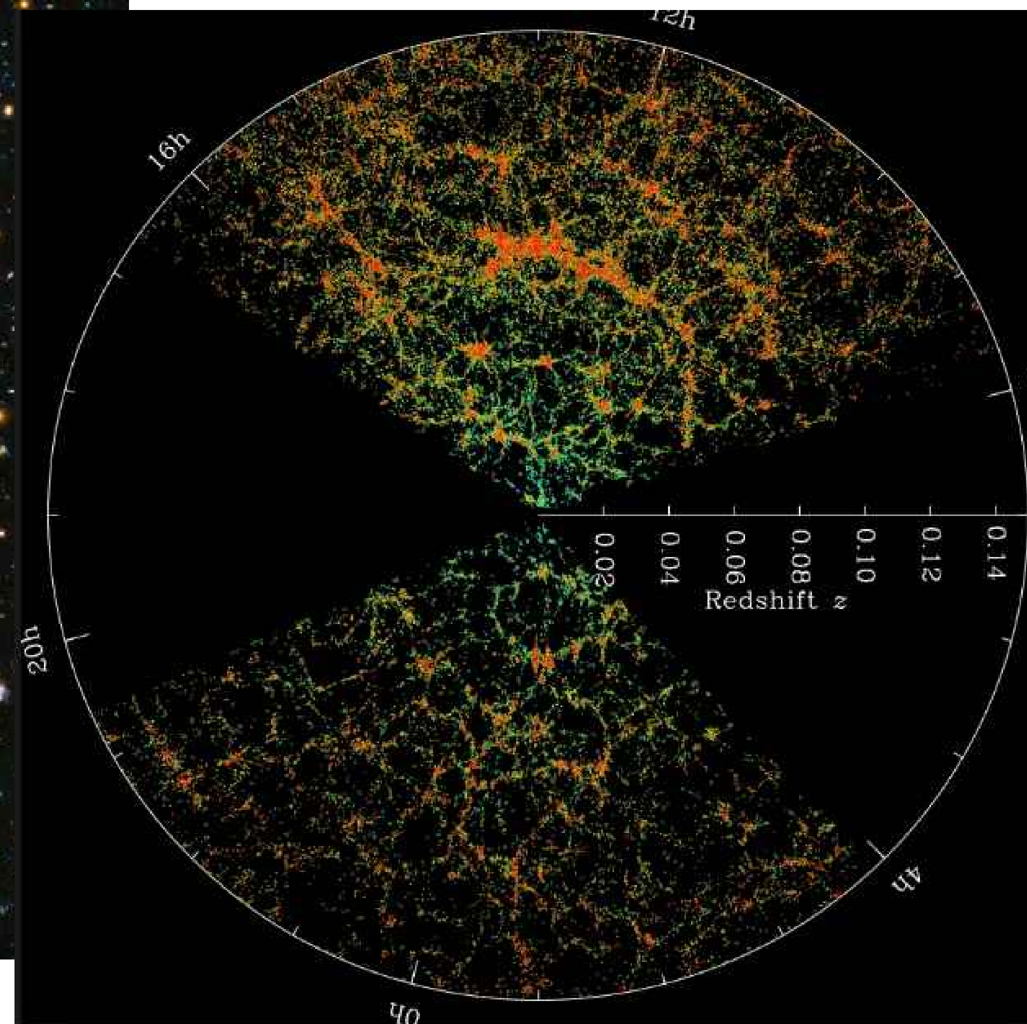
Simulating the formation of structure in the Universe

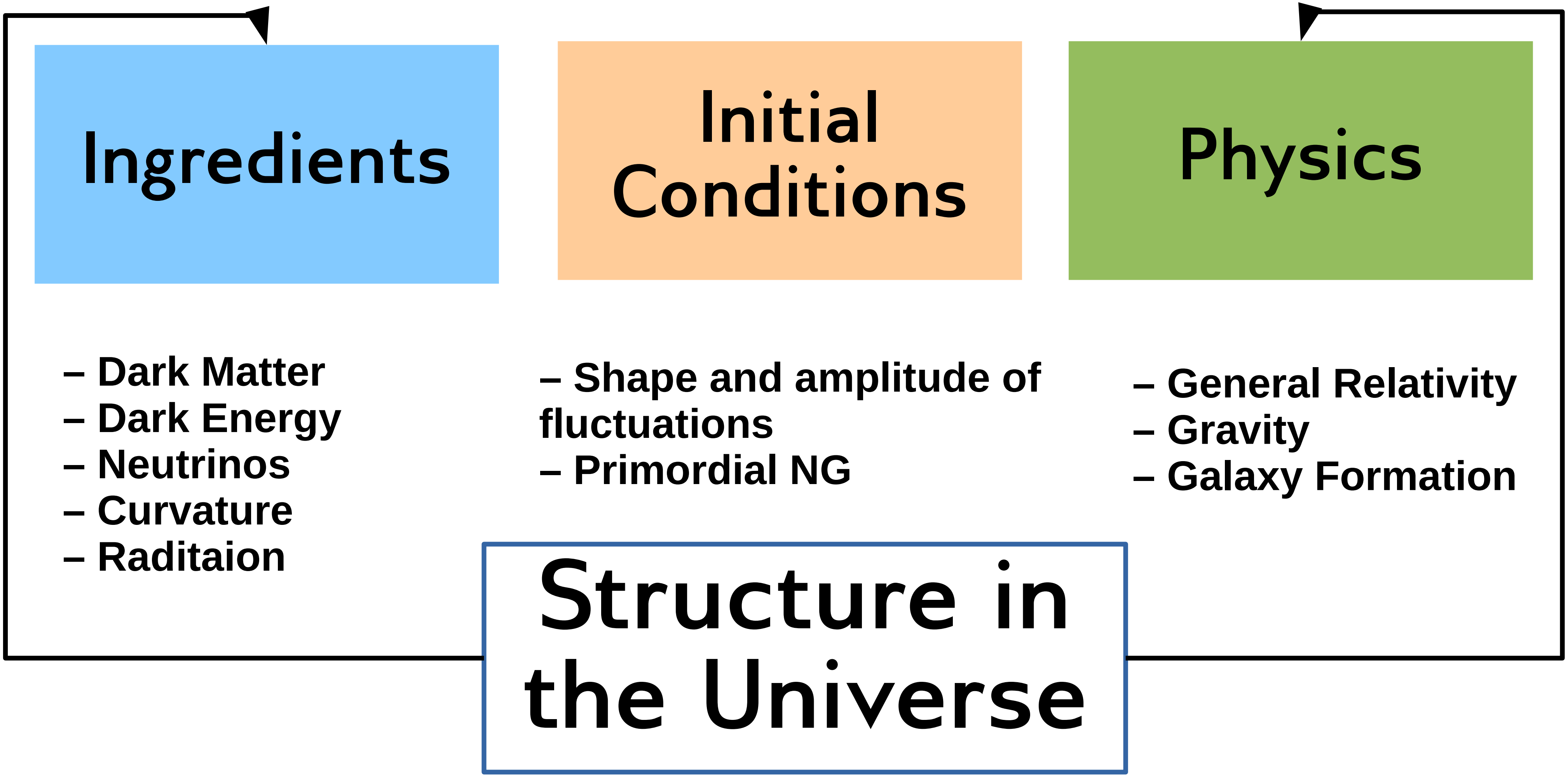


Raul E. Angulo

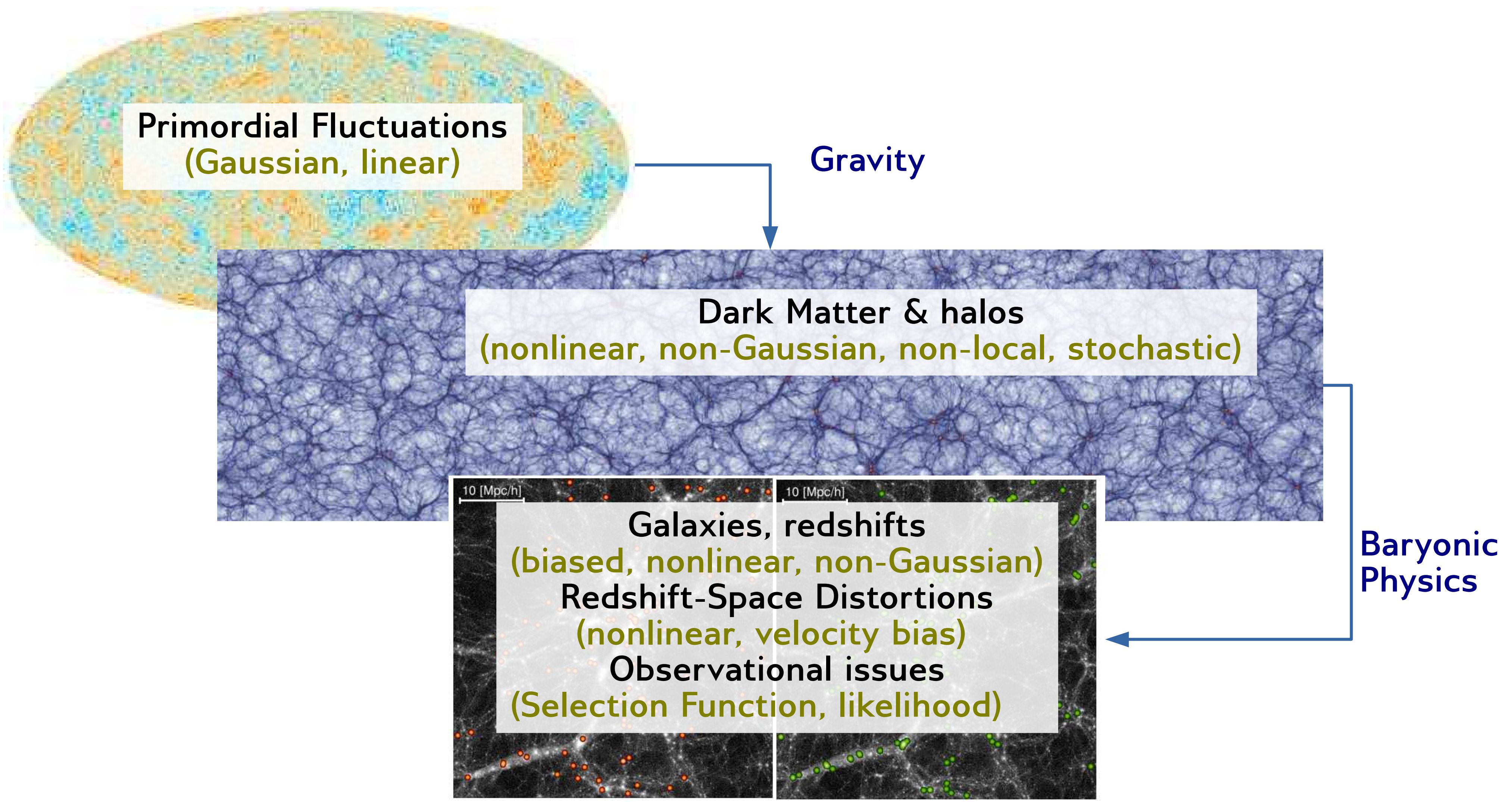
How can we explain the very diverse universe we observe and use it to infer fundamental physics






Ingredients
Initial Conditions
Physics
– Dark Matter
– Dark Energy
– Neutrinos
– Curvature
– Raditaion
– Shape and amplitude of fluctuations
– Primordial NG
– General Relativity
– Gravity
– Galaxy Formation
Structure in the Universe

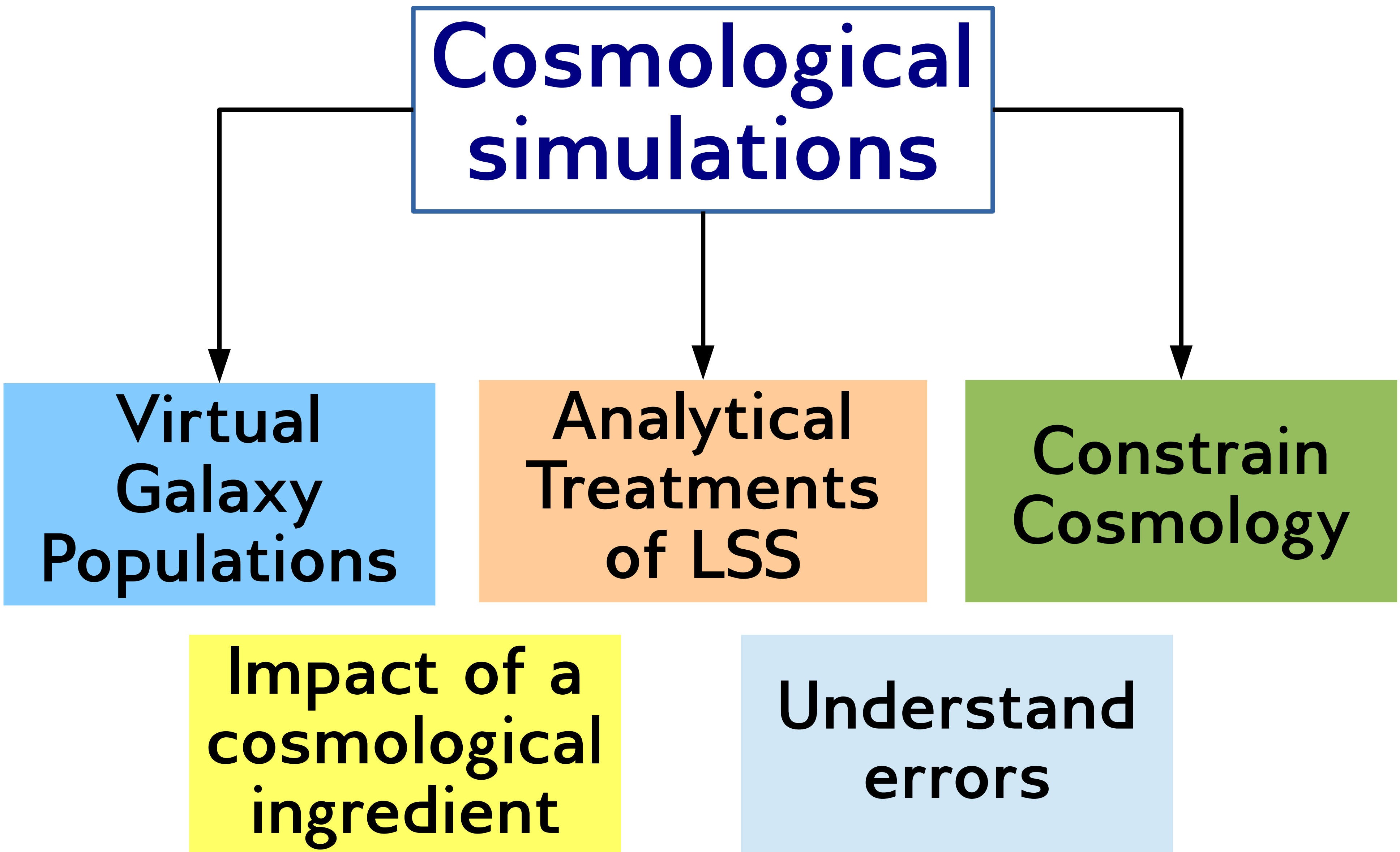
Explaining the structure in the Universe is a solvable (but very hard) problem.



Numerical simulations are the most accurate way to understand 13.7 billion years of nonlinear evolution in the Universe

Simulations have been essential in the establishment of the ”cosmology standard model”

Numerical simulations are an essential tool for precision cosmology



→ Background

→ Methods

→ Current State of the Art

→ The next decade

→ Open questions & challenges

Assumptions made in the simplest case

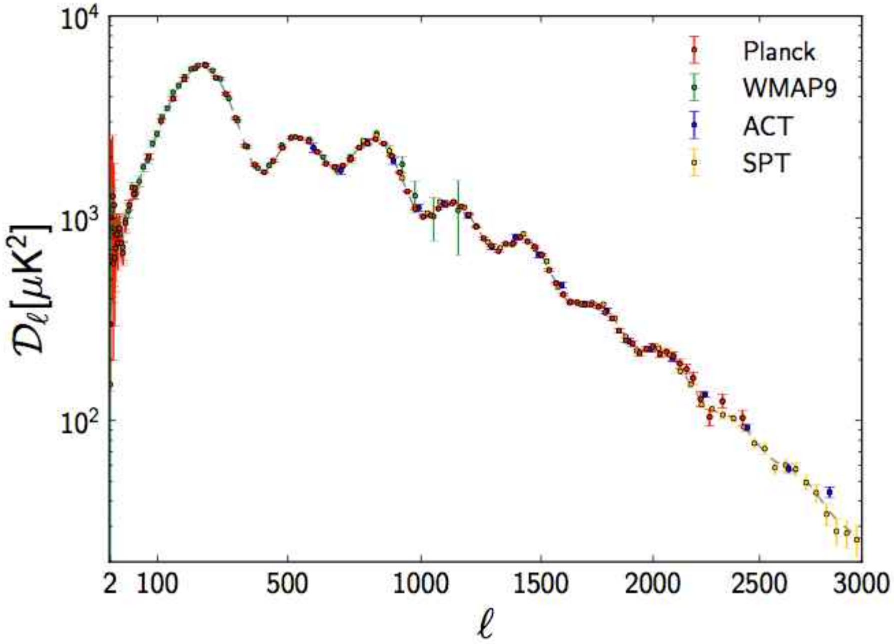
Usually referred to as dark-matter (gravity) only simulations

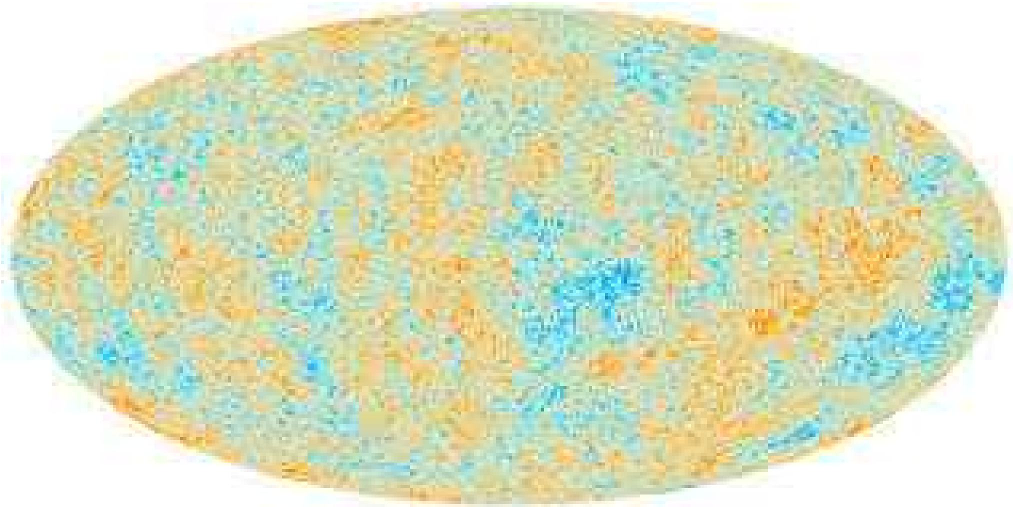
GR at the background level

Dark Matter as the main gravitating ingredient

Newtonian Gravity as the only force to consider

Evidence for dark matter





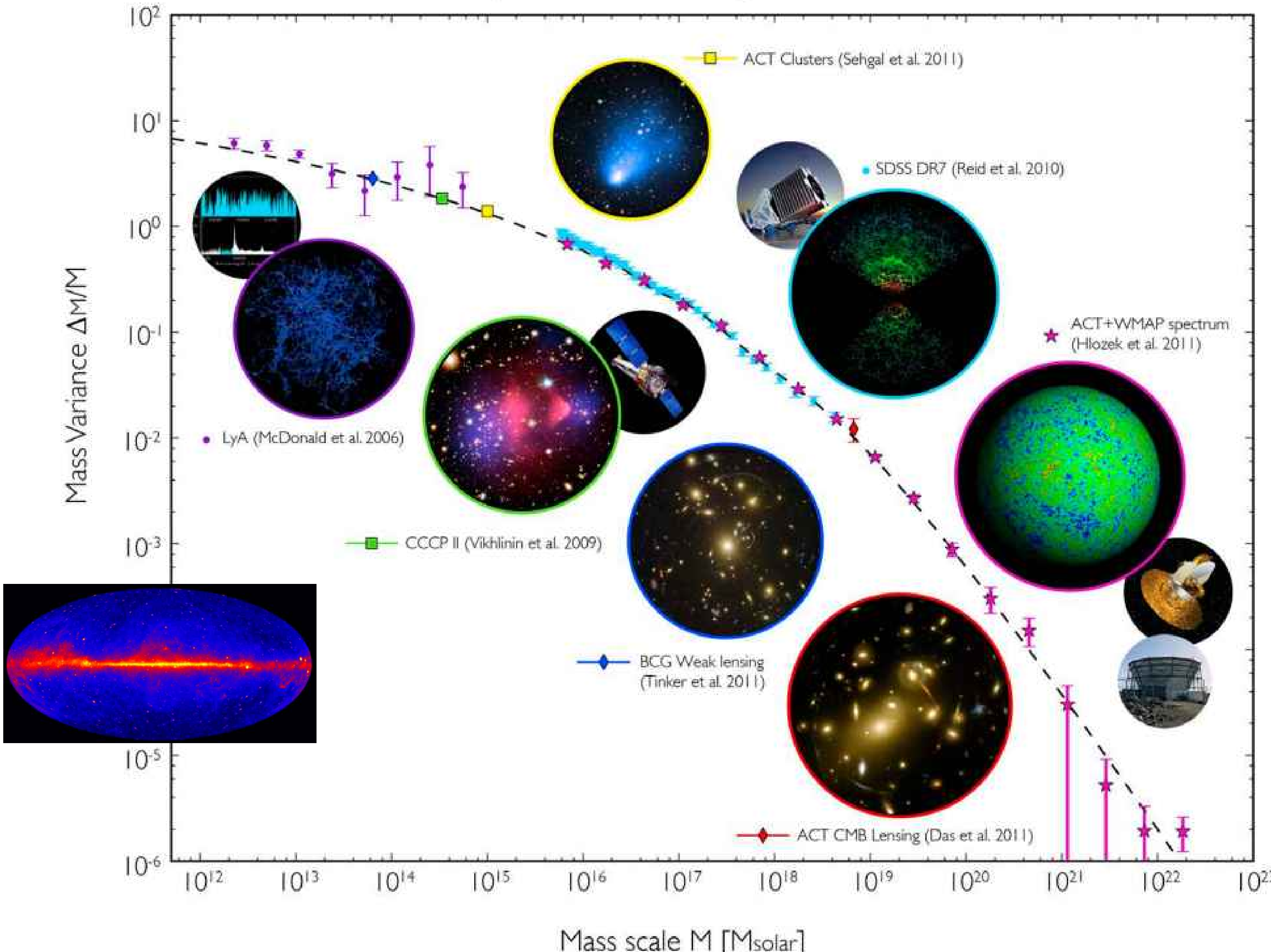
Planck data alone "detects" dark matter at a 25σ level!

Further evidence from, e.g.

- Rotation Curves of galaxies
- Galaxy clusters
- Gravitational Lensing
- Galaxy clustering

Hint on properties: Dark matter interacts only gravitationally and dœs not couple directly to radiation

Evidence supporting the simplest case



Primack 2015

In the simplest case, cosmological simulations are reduced to simulating the evolution of a

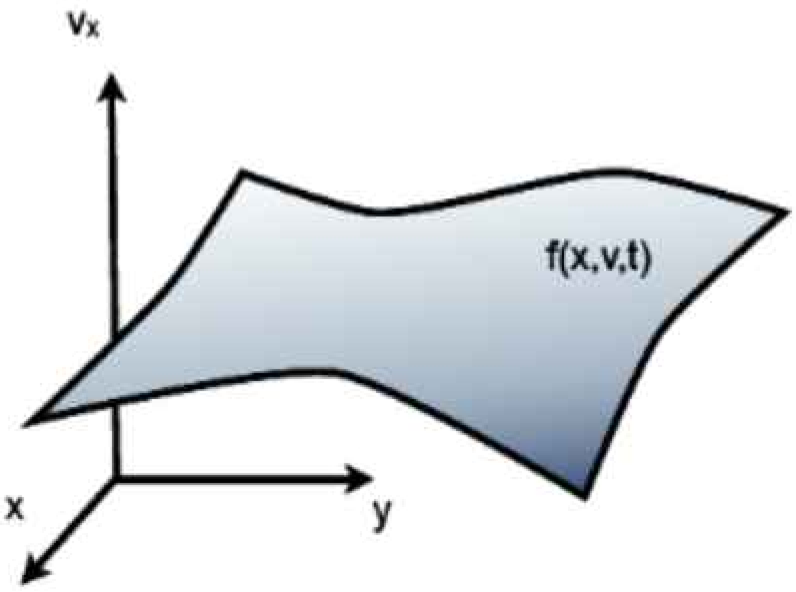
initially smooth,
cold,
classical,
collisionless

fluid under the effect of self-gravity in an expanding Universe.

Simply solve the respective Hamiltonian equations of motion for $N \to \infty$ particles

Simulating structure formation in the Universe

Most of the mass in the Universe is in the form of an unknown elementary particle: the Cold Dark Matter

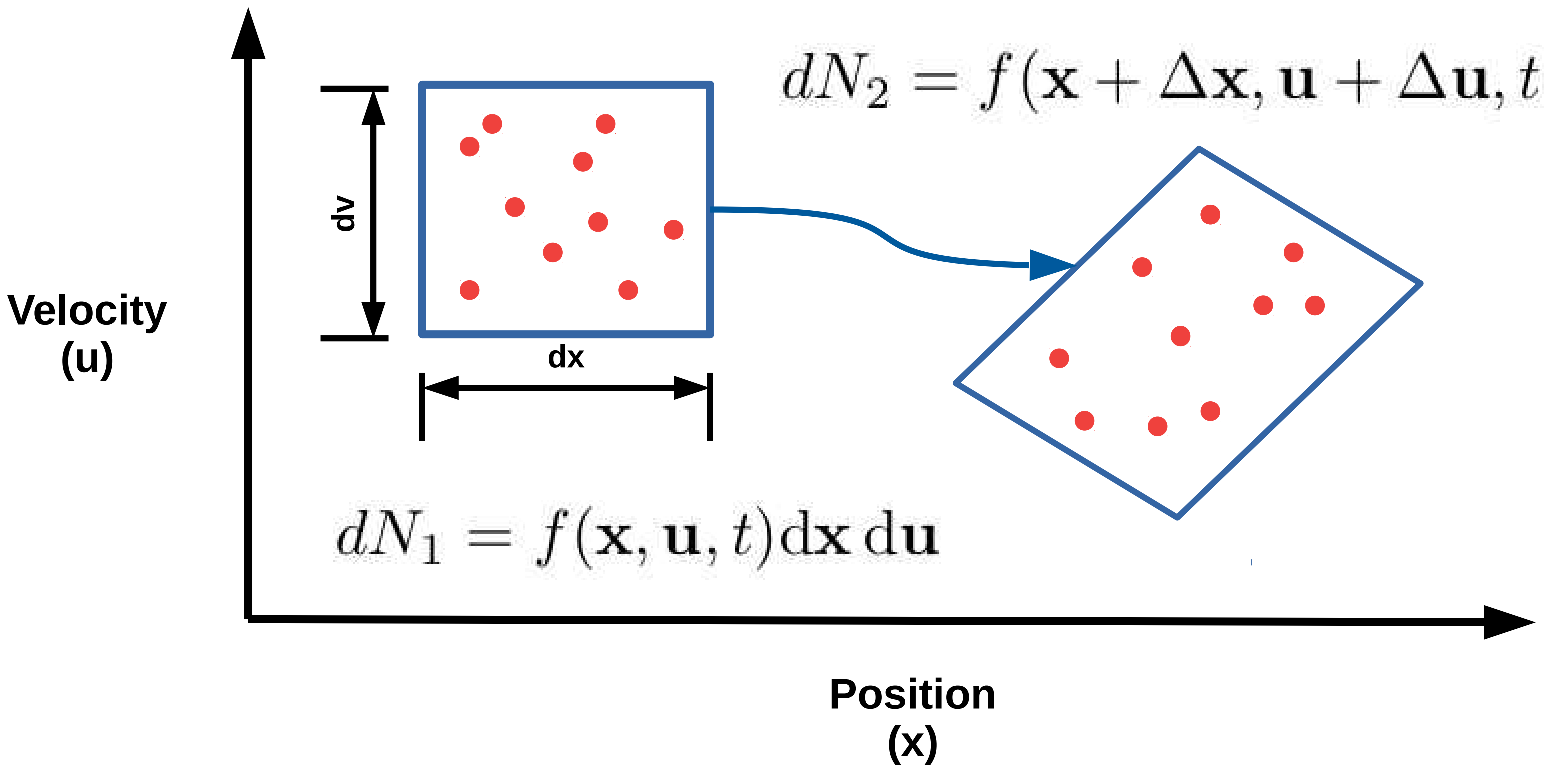


dark matter properties

- Cold
- Collisionless
- Gravity-only
- Smooth

...but simulating trillions of micro-physical CDM particles is impossible

CDM forms a "sheet": A continuous 3D surface embedded in a 6D space



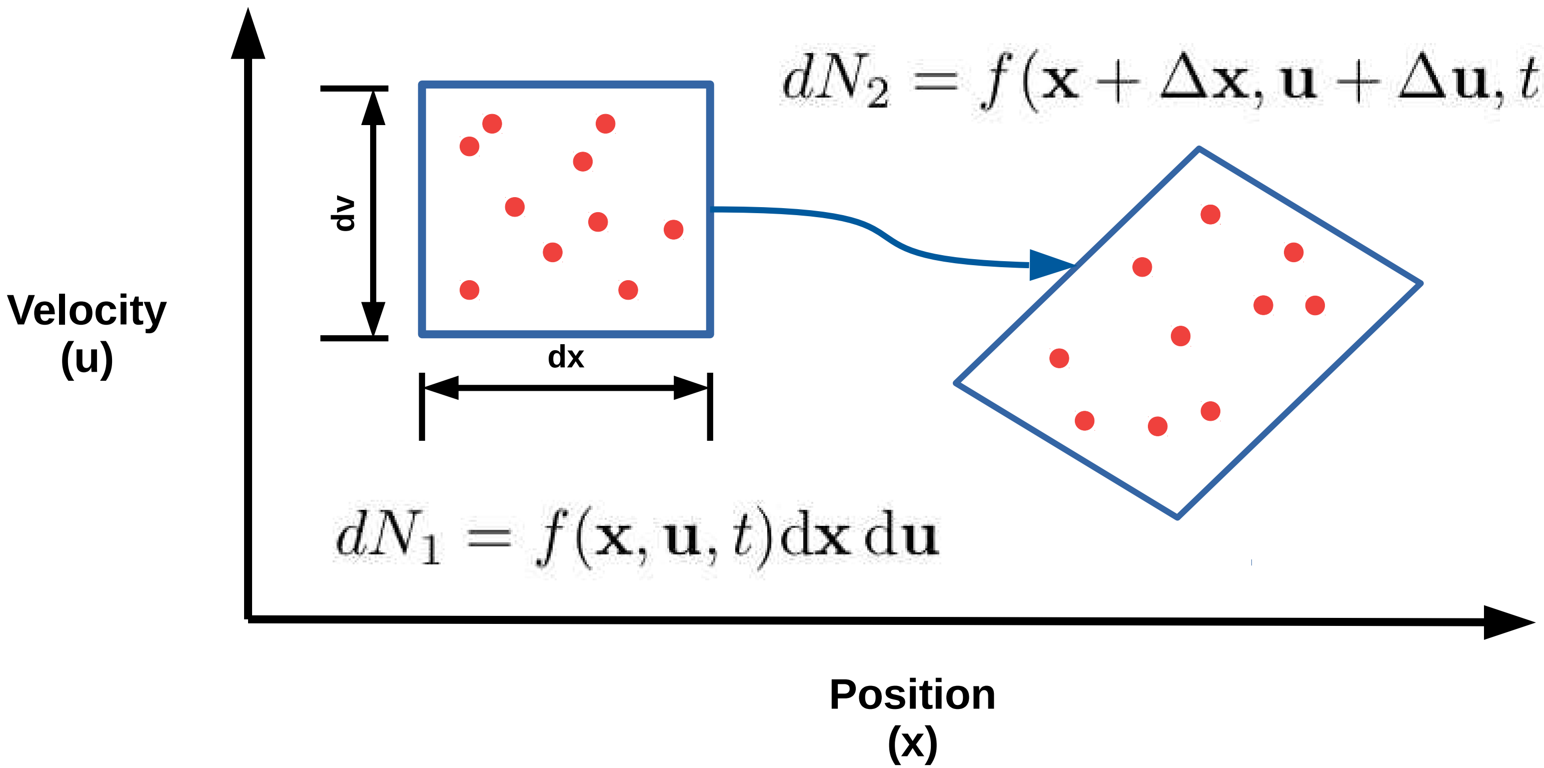
$$dN_2 = f(\mathbf{x} + \Delta\mathbf{x}, \mathbf{u} + \Delta\mathbf{u}, t + \Delta t)\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{u}$$

$$dN_1 = f(\mathbf{x}, \mathbf{u}, t)\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{u}$$

$$dN_1 - dN_2 = \Delta_{coll}$$

Taylor expanding dN2 at first order:

$$dN_2 = f(\mathbf{x}, \mathbf{v}, t)\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{u} \; + \frac{\partial f}{\partial t} + \dot{\mathbf{x}} \cdot \nabla_x f + \dot{\mathbf{u}} \cdot \nabla_u f$$



$$dN_2 = f(\mathbf{x} + \Delta\mathbf{x}, \mathbf{u} + \Delta\mathbf{u}, t + \Delta t)\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{u}$$

$$dN_1 = f(\mathbf{x}, \mathbf{u}, t)\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{u}$$

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{x}} f + \mathbf{F}(\mathbf{x}) \cdot \nabla_{\mathbf{u}} f = \frac{\partial \Delta_{coll}}{\partial t}$$

and using Newton's law:

$$\dot{\mathbf{x}} = \mathbf{u}$$

$$\dot{\mathbf{v}} = \mathbf{F}(\mathbf{x})/m$$

The Vlassov-Poisson Equation

$$0 = \frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{x}} f + \mathbf{F}(\mathbf{x}) \cdot \nabla_{\mathbf{u}} f$$

$$\nabla^2 \Phi = \frac{4\pi G}{a} \int f \mathrm{d}^3 v.$$

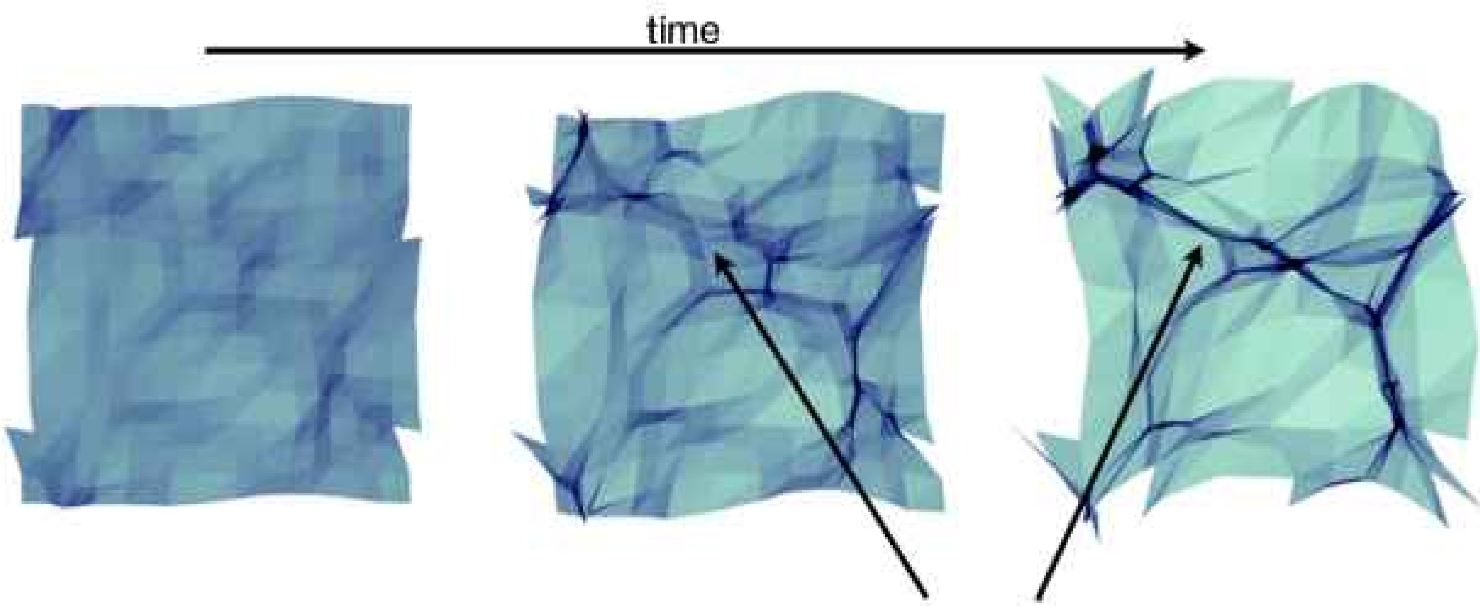
CDM Sheet Properties

→ phase-space is conserved along characteristics

→ It can never tear

→ It can never intersect

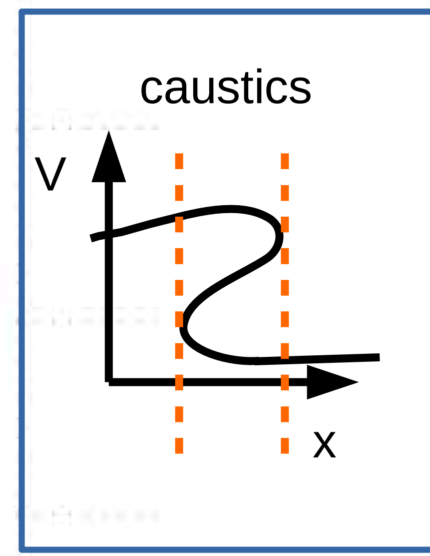
Credit: Oliver Hahn



shell crossing

multi-stream regions appear

density, velocity = sum over many cells



- → Background
- → **Methods**
- → Current State of the Art
- → The next decade
- → Open questions & challenges

→ **Methods**

- → The N-body method
- → Initial Conditions
- → Force Calculation
- → Time-stepping
- → The computational challenges

Solving Vlassov-Poisson via Moments

Taking velocity moments of the VP

$$\int \mathrm{d}^3\mathbf{u}\,\mathcal{U}_k \left[\frac{\partial f}{\partial t} + \mathbf{u}\cdot\nabla_{\mathbf{x}} f + \mathbf{F}(\mathbf{x})\cdot\nabla_{\mathbf{u}} f\right] = 0$$

$$\begin{aligned}
\mathcal{U}_k = 0 \quad &: \quad \frac{\partial n}{\partial t} + \frac{1}{m}\nabla(\mathbf{v}) = 0 \\
\mathcal{U}_k = \mathbf{u} \quad &: \quad \frac{\partial \mathbf{v}}{\partial t} + \frac{1}{m}\nabla\sigma = \rho\mathbf{F}(\mathbf{x}) \\
\mathcal{U}_k = \mathbf{u}^2 \quad &: \quad \frac{\partial \sigma}{\partial t} + \frac{1}{m}\nabla\pi \\
\ldots &
\end{aligned}$$

Linearising the continuity and momentum equations

Taking moments of the VP

$$\rho = \bar{\rho}(1+\delta)$$
$$\mathbf{u} = \bar{\mathbf{u}} + \mathbf{v}$$

$$\begin{aligned} \dot{\delta} + \frac{1}{a}\nabla \cdot \mathbf{v} &= 0 \\ \dot{\mathbf{v}} + H\mathbf{v} &= -\frac{1}{a}\nabla\phi \\ \nabla^2\phi &= \frac{3}{2a}H_0^2\Omega_m\delta \end{aligned}$$

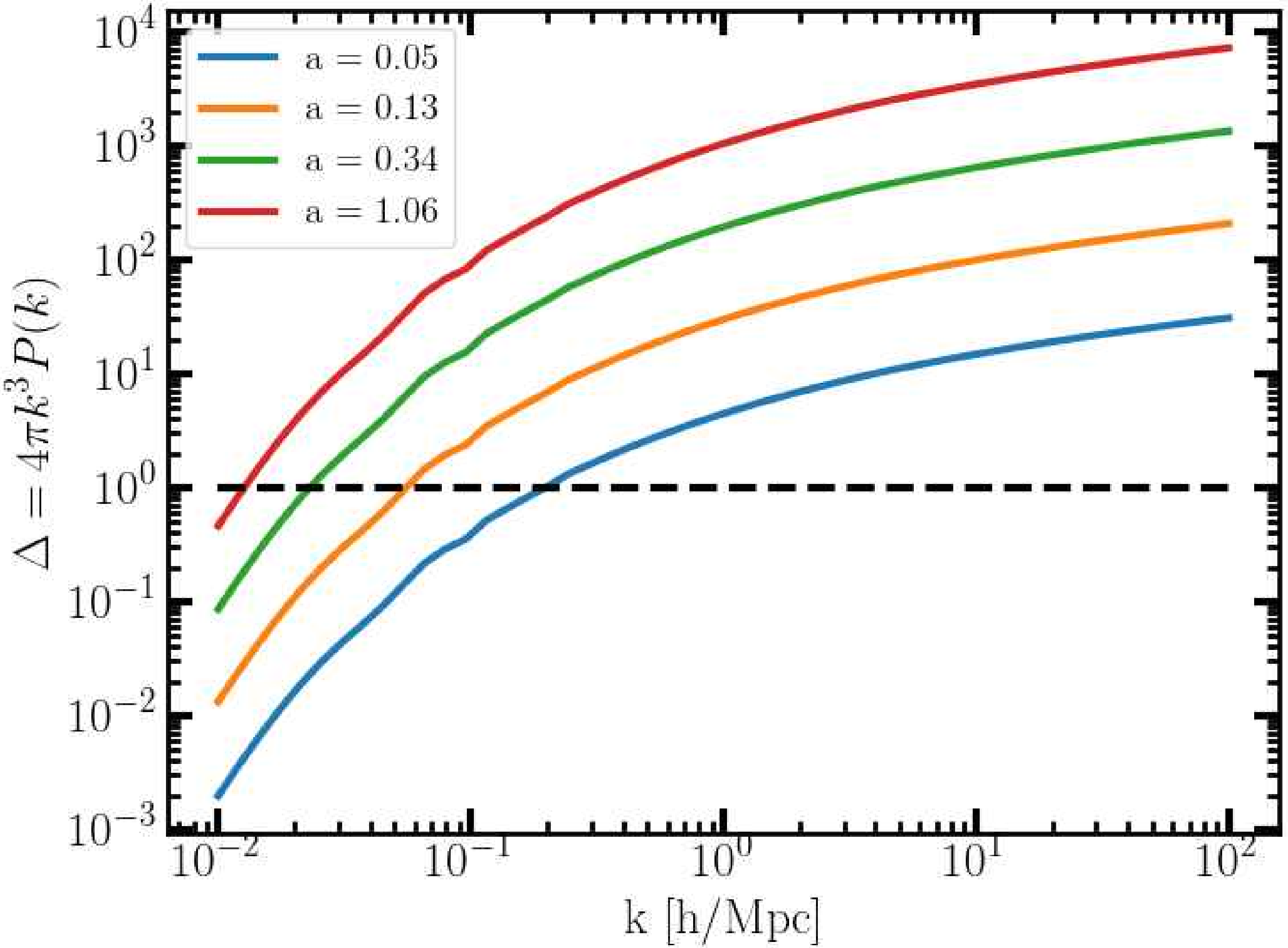
$$\ddot{\delta} + 2H\dot{\delta} - \frac{3}{2a}H_0^2\Omega_m\delta = 0$$

$$\delta(\mathbf{v}) = D(t)\delta(t_0, \mathbf{v})$$

$$D(t) \propto \frac{H(t)}{H_0}\int_0^t \mathrm{d}a[\Omega_m/a + \Omega_\lambda]^{-3/2}$$

Linearising the continuity and momentum equations

Taking moments of the VP



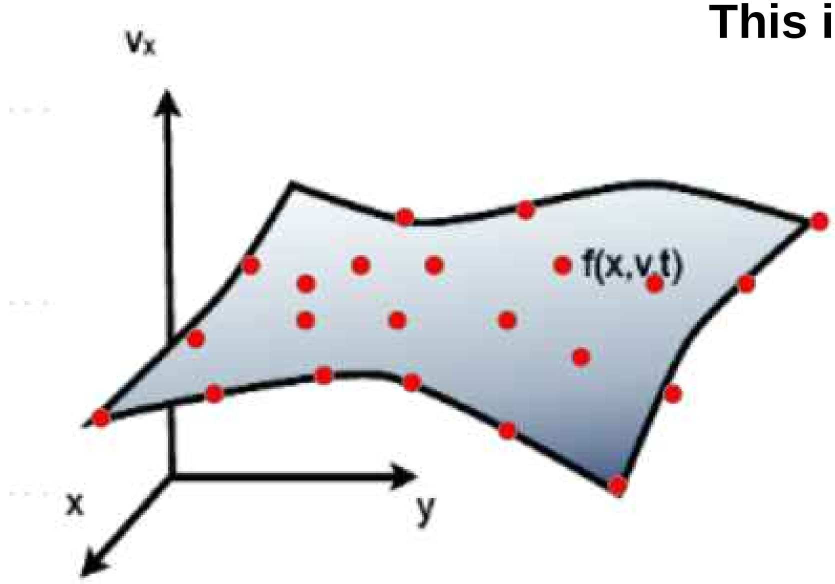
Solving Vlassov-Poisson via a Montecarlo sampling and coarse-graining

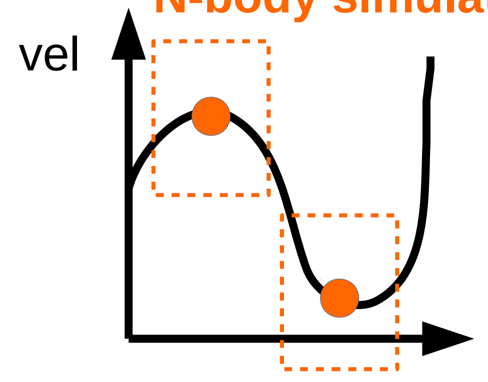
The "method of characteristics" is used to solve the Vlassov-Poisson partial differential equation.

$$H(p,x) = \frac{p^2}{2m} + \Phi(x)$$

The solution yields the equation of motions of the Hamiltonian of classical mechanics

This is the correct solution as N goes to infinity





The N-body equation

An apparently simple equation, is in fact quite hard to solve and very quickly becomes nonlinear

$$\ddot{\mathbf{x}} = -G \sum_{i}^{N} \frac{m_i \left(\mathbf{x} - \mathbf{x}_i\right)}{\left|\mathbf{x} - \mathbf{x}_i\right|^3}$$

Exact solutions exists only for N=2!
(This lead to discussions about the destiny of the Solar System)

Time-stepping

How do we numerically solve the 2nd order differential equation?

$$\ddot{\mathbf{x}} = -G\sum_{i}^{N}\frac{m_i\left(\mathbf{x}-\mathbf{x}_i\right)}{|\mathbf{x}-\mathbf{x}_i|^3}$$

Defining, W = [x, v]:

$$\frac{d\mathbf{W}}{dt} = \mathcal{F}(\mathbf{W})$$

And in a finite-differences form:

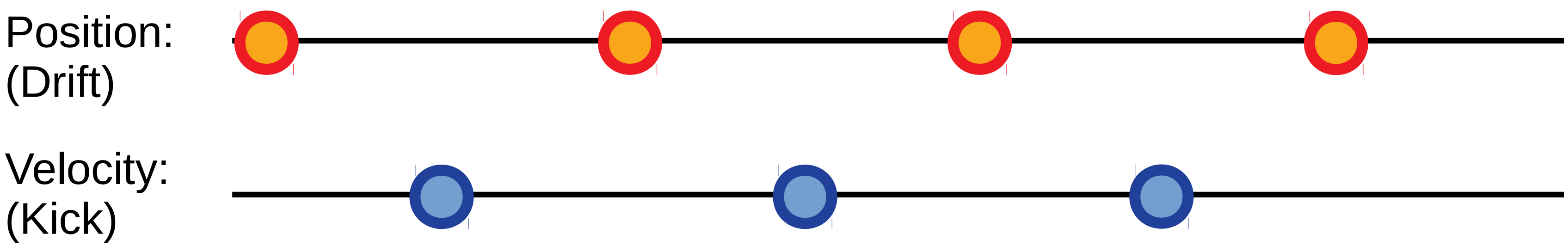
$$\mathbf{W}^{(l+1)} = \mathbf{W}^{(l)} + \sum_{i}^{n}\frac{(\Delta t)^i}{i!}\frac{\partial^i\mathcal{F}[\mathbf{W}^{(l)}]}{\partial^i t}$$

The zero-th order is called “forward Euler”. Runge-Kutta Methods aim at using higher order temrs

Time-stepping

A leapfrog scheme is simplectic, preserves the simplicity of first-order time-integrators

$$\mathbf{x}^{l+1} = \mathbf{x}^{l} + \Delta t\, \mathbf{v}^{l+1/2} + \mathcal{O}(\Delta t^3)$$
$$\mathbf{v}^{l+1/2} = \mathbf{v}^{l-1/2} + \Delta t\, \mathbf{a}^{l} + \mathcal{O}(\Delta t^3)$$

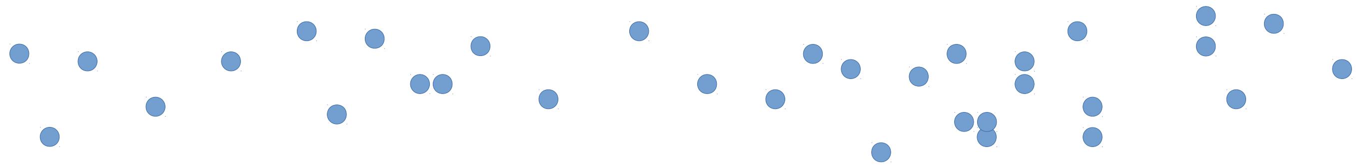


For large N, individually adaptive time-steps are mandatory (at the loss of time-reversibility):

$$\Delta t_i \simeq \eta \sqrt{1/a_i}$$

Force calculation

The problem is to estimate the gravitational interaction of A set of N discrete particles

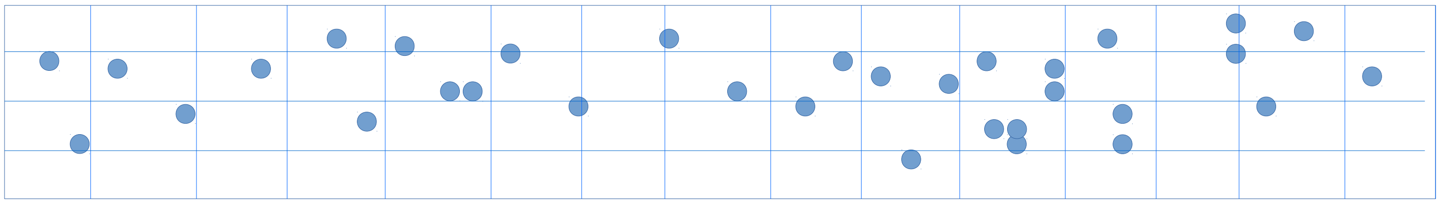


$$\ddot{\mathbf{x}} = -G \sum_{i}^{N} \frac{m_i \left(\mathbf{x} - \mathbf{x}_i\right)}{\left|\mathbf{x} - \mathbf{x}_i\right|^3}$$

For each particle, we need the add up the contribution of N-1 particles. Thus, this is a NxN problem!

Force calculation

The problem is to estimate the gravitational interaction of
A set of N discrete particles



Interpolation Methods

1) Nearest Grid Point (0th order)

2) Clouds-in-Cells (1st order)

3) Triangular shaped cloud (2nd order)

$$\nabla^2\phi = \frac{4\pi G}{a}(\rho - \bar{\rho})$$

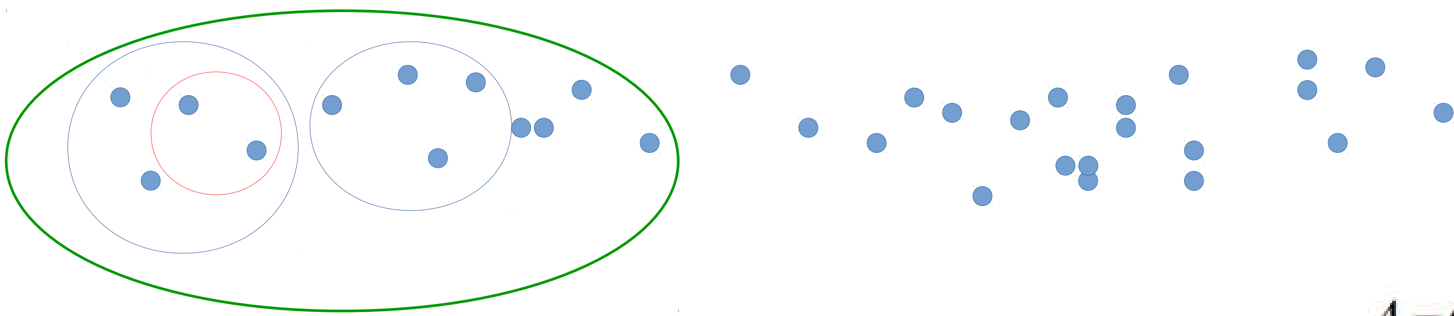
$$\nabla^2\phi \propto \delta \quad \Leftrightarrow \quad \tilde{\phi} \propto -\tilde{\delta}/k^2$$

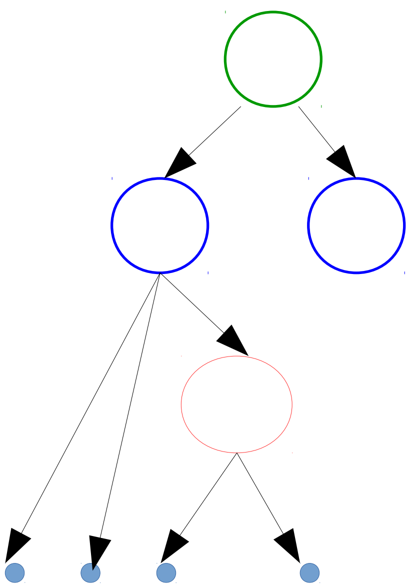
$$\mathbf{a} = -\boldsymbol{\nabla}\phi \quad \Leftrightarrow \quad \tilde{\mathbf{a}} \propto -\frac{i\mathbf{k}}{k^2}\tilde{\delta}$$

Fast, easy to parallelise, portable FFT libraries, scales as N;
but poor load balance, limited & uniform spatial resolution, global timesteps

Force calculation

The problem is to estimate the gravitational interaction of
A set of N discrete particles





$$\phi(\mathbf{x}_i) = -\sum_{j=1\ldots N} \frac{4\pi G}{a|\mathbf{x}_i - \mathbf{x}_j|}$$

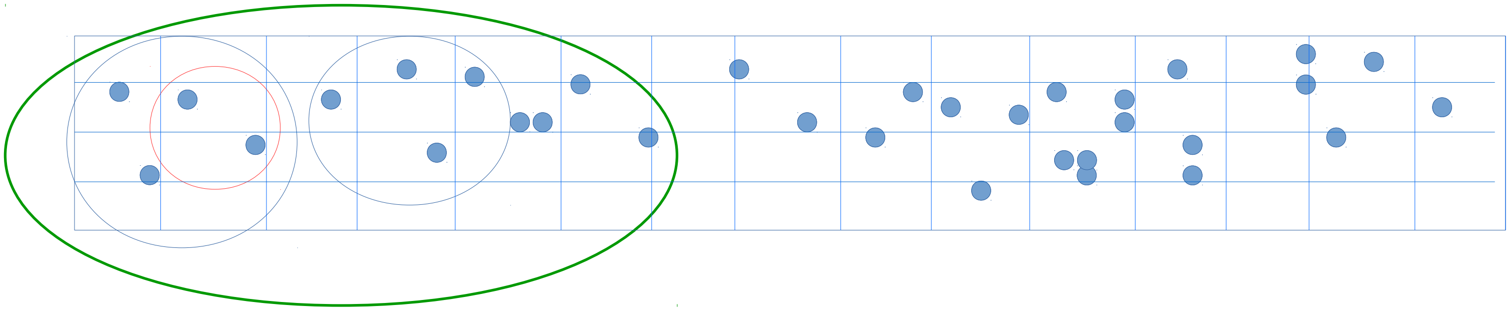
$$\frac{1}{|x - x_j|} = \frac{1}{|(x - \lambda) - (x_j - \lambda)|}$$

$$\frac{1}{|\mathbf{y} + \boldsymbol{\lambda} - \mathbf{x_j}|} \simeq \underbrace{\frac{1}{|y|}}_{\text{monopole}} - \mathbf{y} \cdot \underbrace{\frac{\boldsymbol{\lambda} - \mathbf{x}_j}{|\mathbf{y}|^3}}_{\text{dipole}} + \ldots$$

The decision to open a node is given by a desired accuracy.
The efficiency depends on the clustering but ~ N log(N), allows
Individual timesteps, good load/cpu balances.

Force calculation

The problem is to estimate the gravitational interaction of
A set of N discrete particles



Alternatives

1) Adaptive Mesh refinement

2) Ewald summation for trees

3) Direct Summation

4) Fast Multipole methods

$$\phi_{\boldsymbol{k}} = \phi_{\boldsymbol{k}}^{\rm long} + \phi_{\boldsymbol{k}}^{\rm short}$$

$$\phi^{\rm short}(\boldsymbol{x}) = -G \sum_i \frac{m_i}{r_i} {\rm erfc}\left(\frac{r_i}{2r_s}\right)$$

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

Force calculation

A regularization of force calculations is needed to avoid Unrealistic close-encounters and large-angle scatterings

$$\ddot{\mathbf{x}} = -G\sum_i^N \frac{m_i\left(\mathbf{x}-\mathbf{x}_i\right)}{|\mathbf{x}-\mathbf{x}_i|^3} \quad \longrightarrow \quad \ddot{\mathbf{x}} = -G\sum_i^N \frac{m_i(\mathbf{x}-\mathbf{x}_i)}{(|\mathbf{x}-\mathbf{x}_i|^2+\epsilon^2)^{3/2}}$$

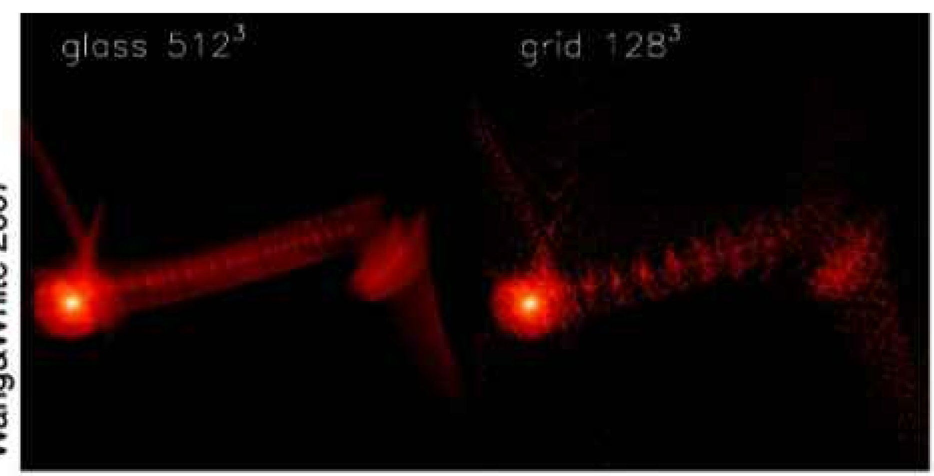
Forces are limited to:

$$\max[|\ddot{\mathbf{x}}|] = \frac{2Gm_i}{3^{3/2}\epsilon^2}$$

$$\epsilon \sim (V/N)^{1/3}$$

Collisionless Relaxation

Phase Mixing
Chaotic Mixing
Violent Relaxation
Landau Damping



Wang&White 2007

Initial Conditions

The problem is to create a realisation of particles compatible
With the statistical properties observed in the CMB

Eulerian (x) to Lagrangian (q) mapping)

$$\frac{\partial \mathbf{x}}{\partial dt} + \mathbf{v} \cdot \nabla \mathbf{x} \rightarrow \frac{\partial \mathbf{x}}{\partial dt}$$

The continuity equation becomes:

$$\frac{\partial \mathbf{v}}{\partial t} = \frac{-1}{a} \nabla \phi$$

$$\mathbf{v} = -\frac{\nabla \phi}{a} \int \mathrm{d}t \frac{D}{a}$$

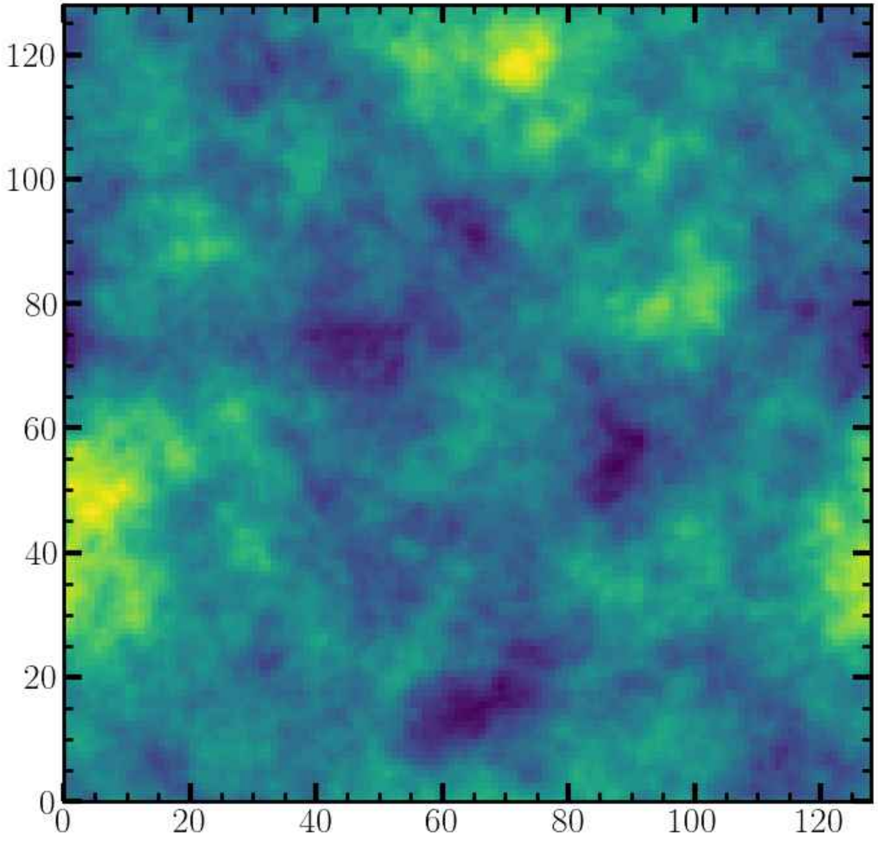
The Zel'dovich Approximation

$$\mathbf{v} = -\frac{2a\dot{D}}{3H_0^2 \Omega_m} \nabla \phi$$

$$\mathbf{x} = \mathbf{q} - \frac{2aD}{3H_0^2 \Omega_m} \nabla \phi$$

Initial Conditions

The problem is to create a realisation of a potential field
Compatible with the statistical properties of the CMB



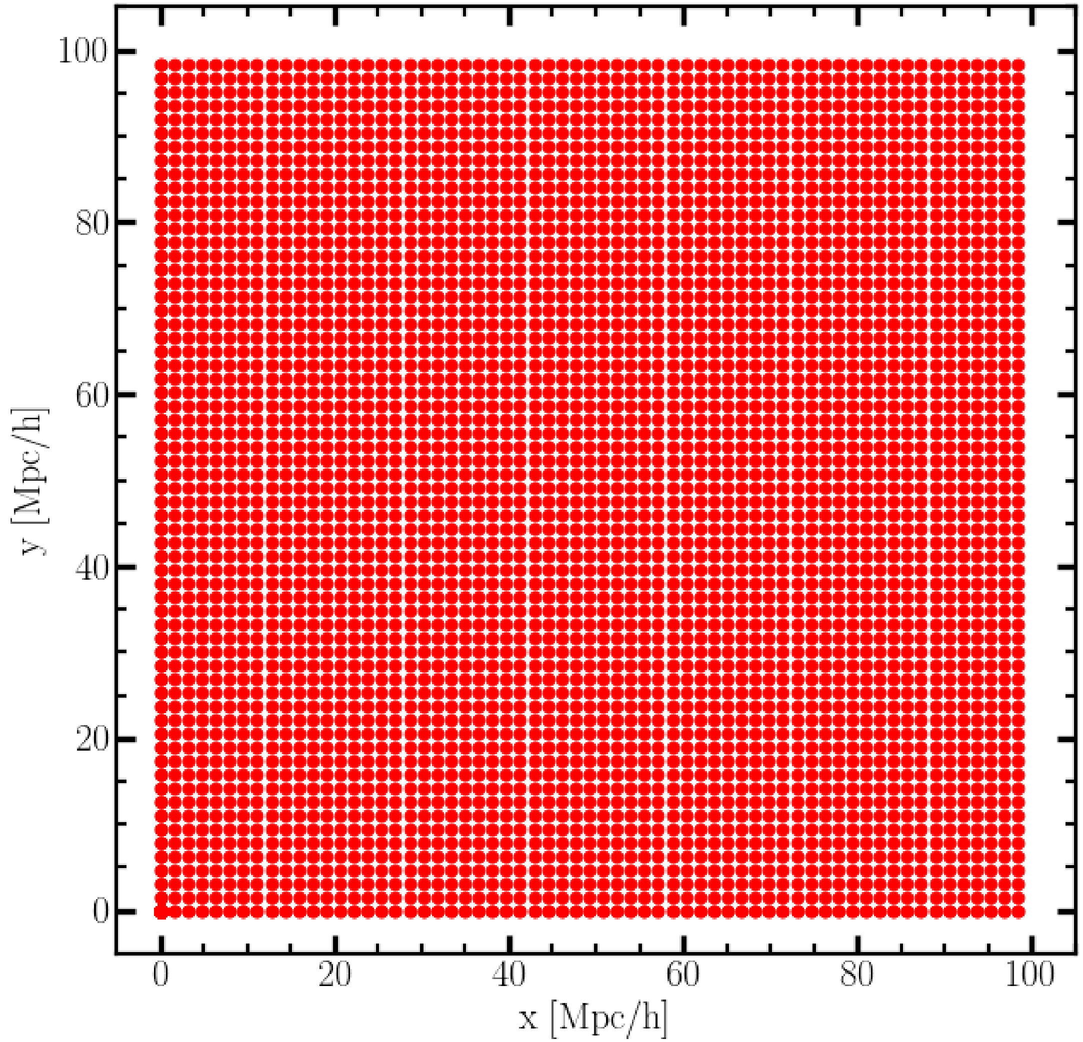
$$\delta_R = \mathcal{G}(0, \sqrt{P(\mathbf{k})})$$
$$\delta_I = \mathcal{G}(0, \sqrt{P(\mathbf{k})})$$

$$A(\mathbf{k}) = \delta_I^2 + \delta_R^2 = \frac{x}{\sigma} \exp[-x^2/2\sigma^2]$$
$$\theta(\mathbf{k}) = \mathcal{U}[0, 2\pi]$$

$$\tilde{\phi} \propto -\tilde{\delta}/k^2$$

Initial Conditions

An initially homogeneous (grid or glass usually) are initialised with the position and velocity consistent with those of a potential field



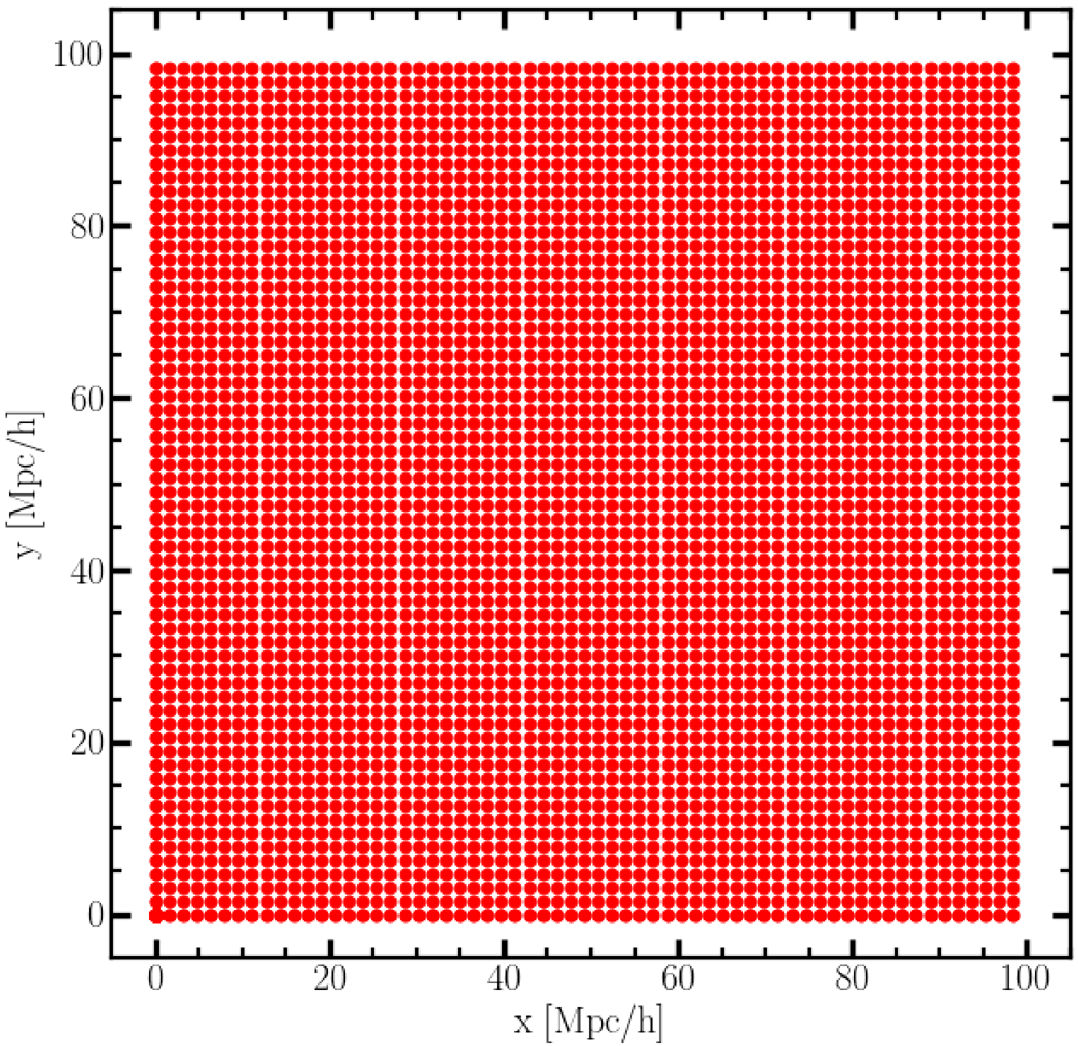
The Zeldovich Approximation

$$\mathbf{v} = -\frac{2a\dot{D}}{3H_0^2\Omega_m}\nabla\phi$$

$$\mathbf{x} = \mathbf{q} - \frac{2aD}{3H_0^2\Omega_m}\nabla\phi$$

Initial Conditions

The Zoldivich Approximation predicts triaxial collapse and The appearance of halos, filaments, walls, and voids



$$\int_V \mathrm{d}\mathbf{q} = \int_V \mathrm{d}\mathbf{x}\,(1+\delta(\mathbf{x}))$$

$$1+\delta(\mathbf{q}) = \left|\frac{\partial \mathbf{x}}{\partial \mathbf{q}}\right|^{-1}$$

$$= \frac{1}{(1+D\lambda_1)(1+D\lambda_2)(1+D\lambda_3)}$$

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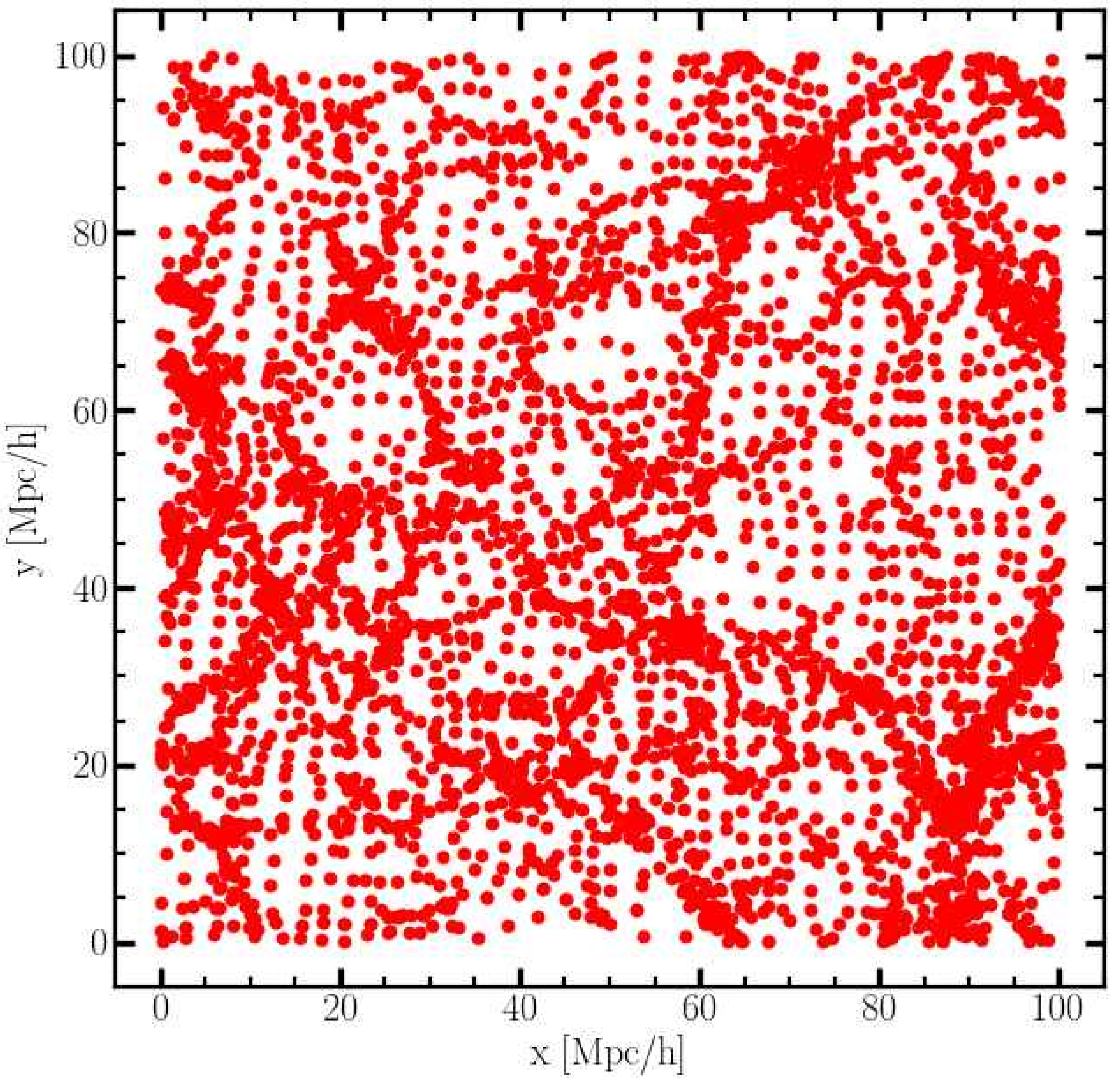

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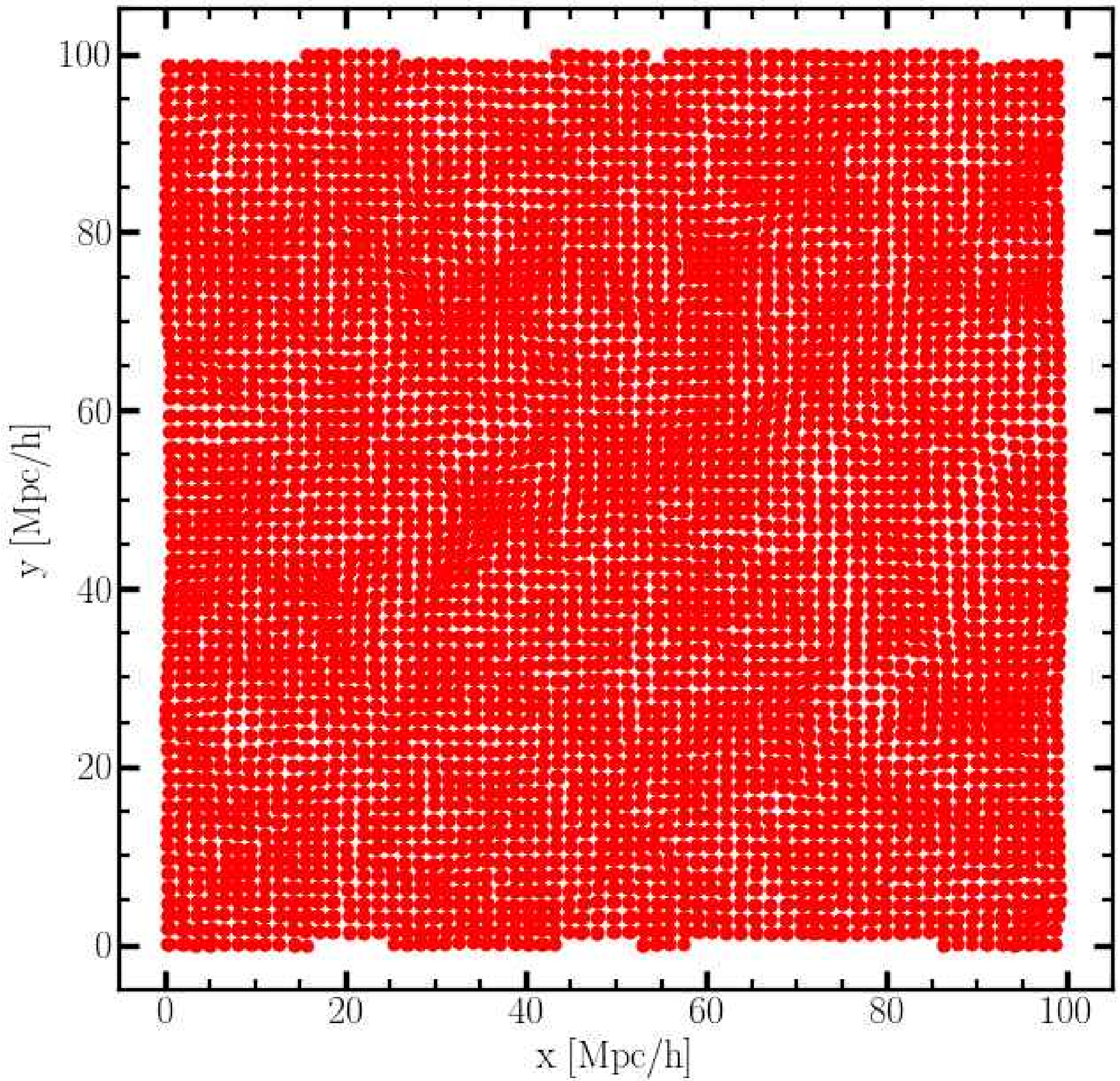
Our own N-body code!



An N-body code

→ Compute ICs

Loop over N timesteps

→ Kick velocities dt/2

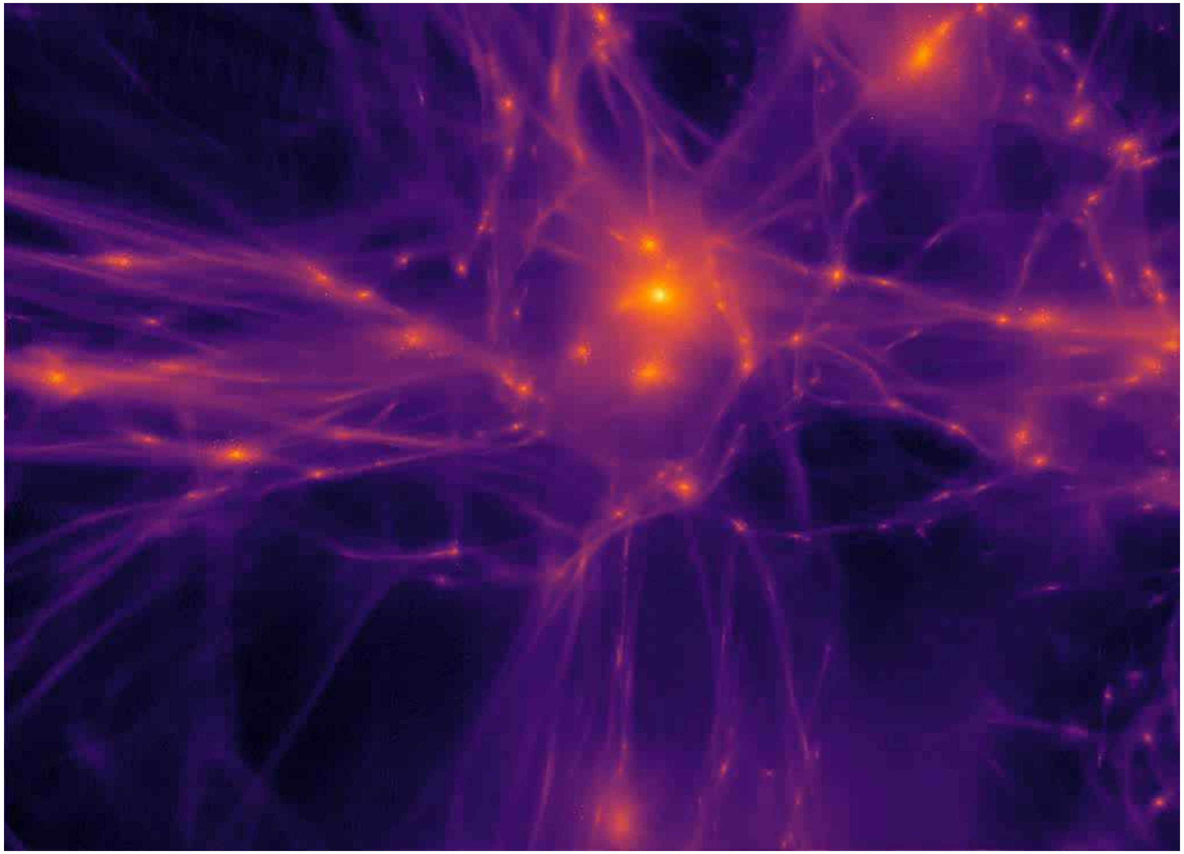
→ Drift particles dt

→ Compute forces

→ Kick velocities dt/2

Leap frog symplectic integrator

Our own N-body code!



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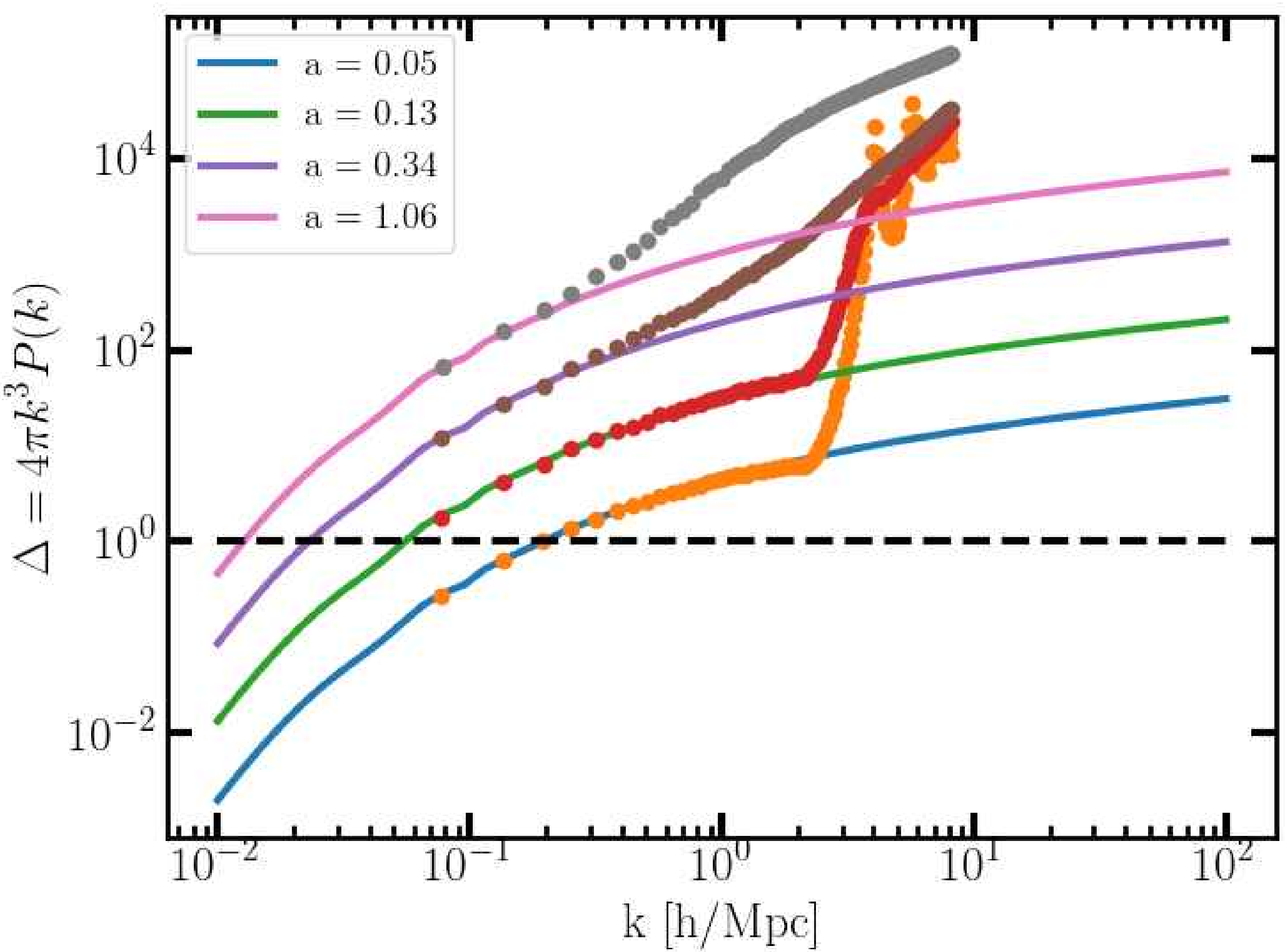
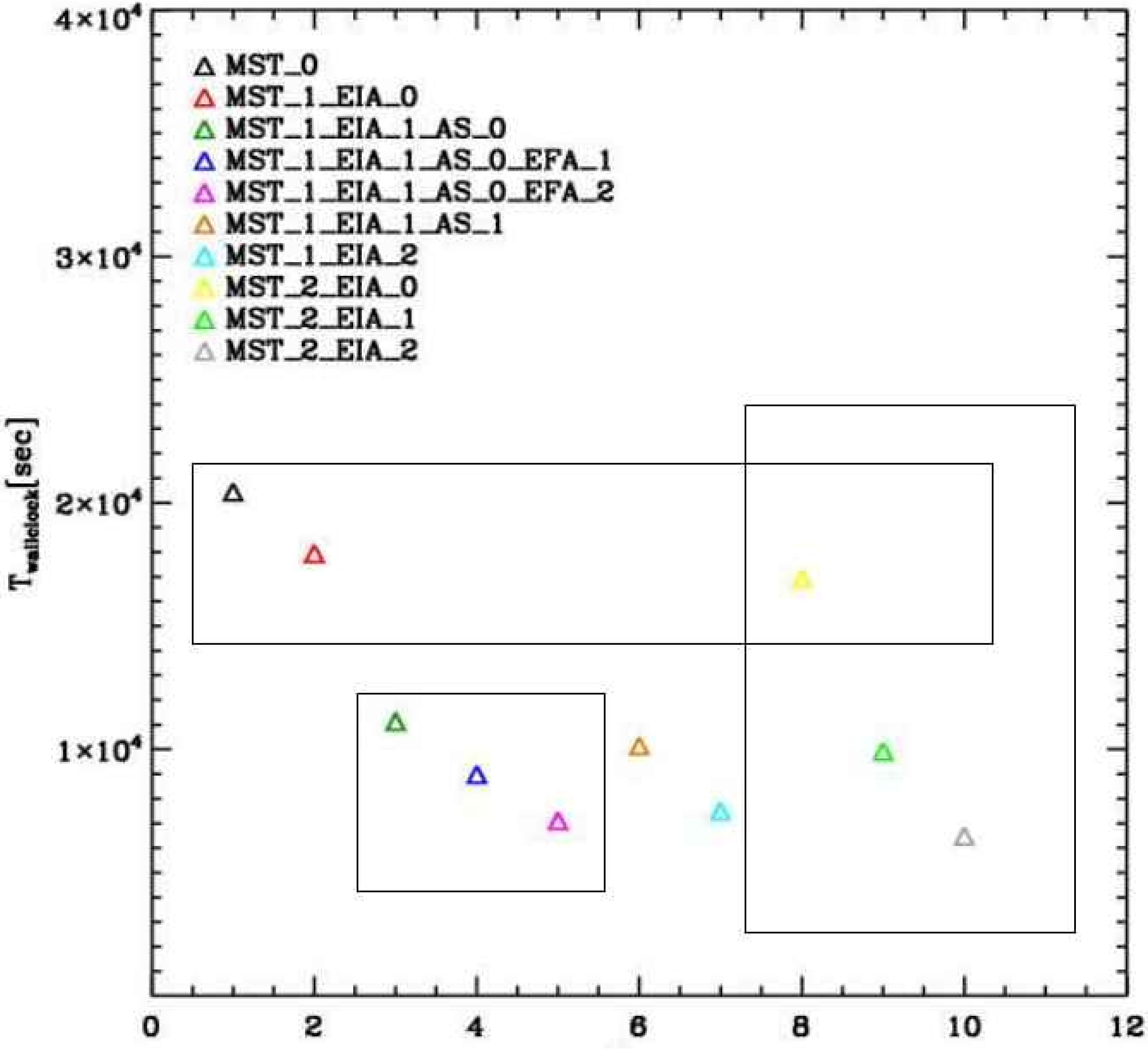


Number of particles is not precision

Force and time integration parameters can change execution times by factors of a few



MST: Maximum allowed timestep

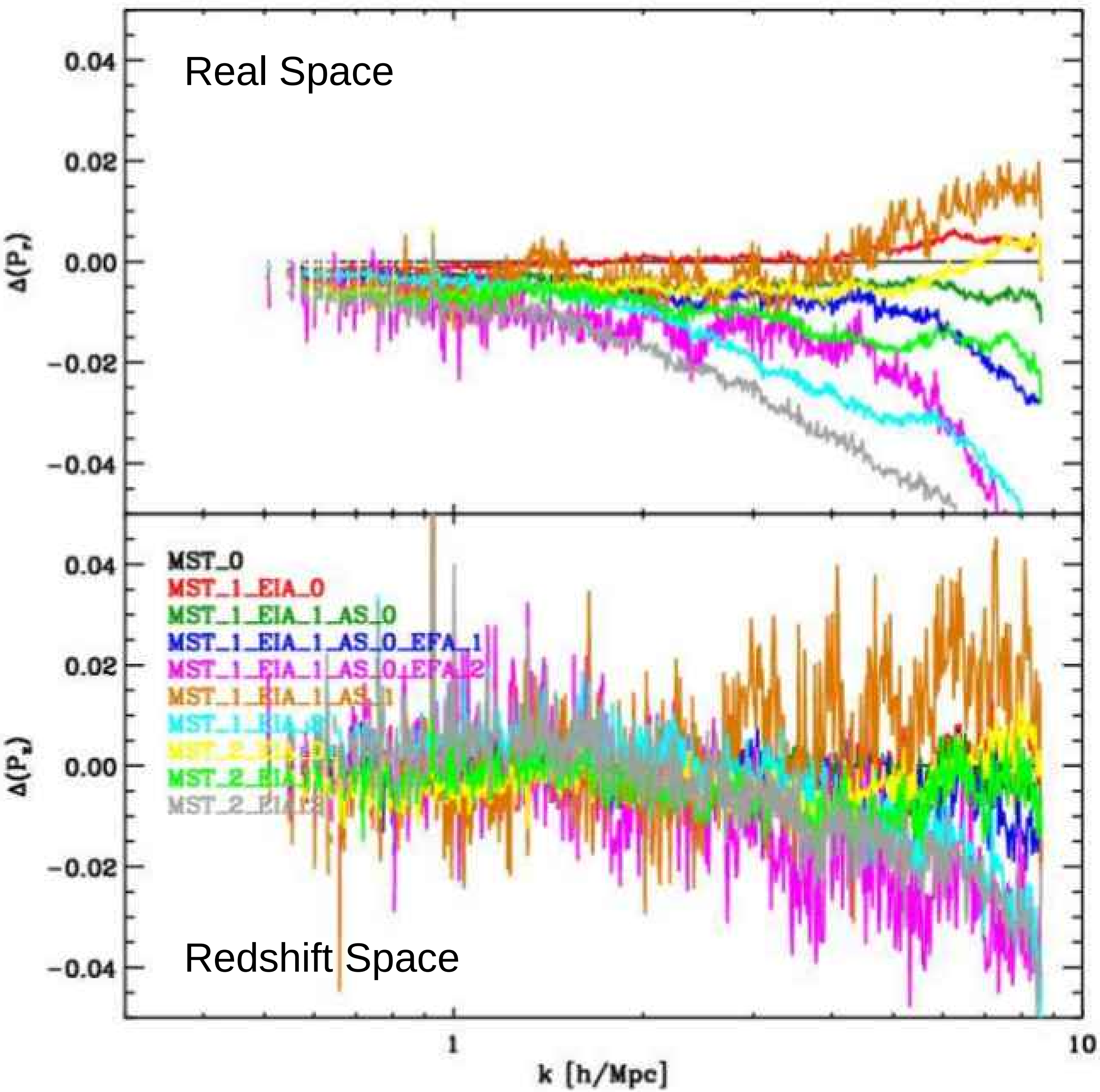
EIA: Error in time Integration

AS: Smoothing applied to mesh force

EFA: Error in Force Calculation

Number of particles is not precision

Errors on the power spectra induced by numerical errors



MST: Maximum allowed timestep

EIA: Error in time Integration

AS: Smoothing applied to mesh force

EFA: Error in Force Calculation

Not including:
1) Starting redshift
2) Transients from the ICs
3) Softening Length

The computational challenge

Modern cosmological simulations pose hard problems in terms of execution time, RAM consumption, and data handling

CPU and load Imbalances

Quadrillion force calculations with large anisotropies
and very different dynamical timescales

RAM

Above hundreds of Tb of RAM necessary to hold basic information
Additional requirements memory imbalances and data analyses

I/O & Disk Space

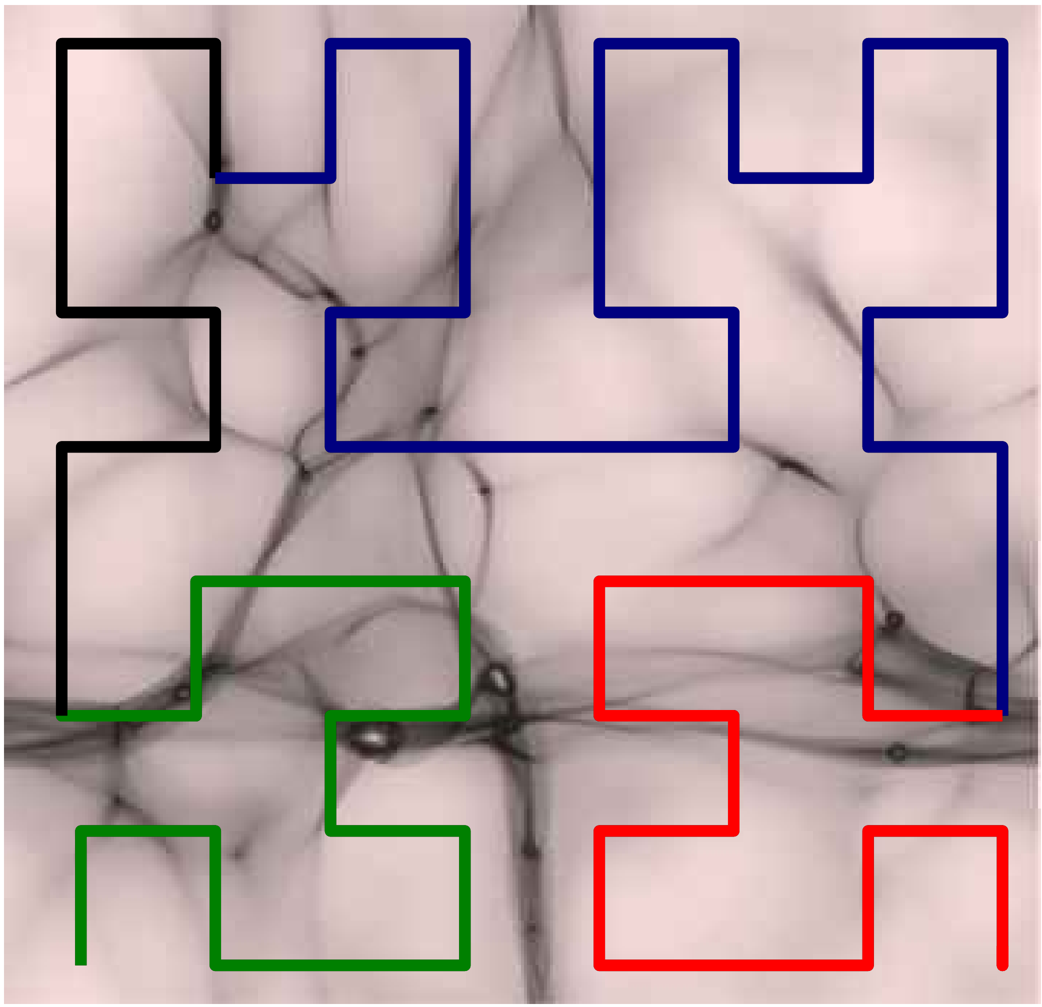
Data products can be en excess of dozens of Petabytes.

We require a combination of extremely efficient and scalable algorithms, and a large Supercomputer!

MXXL

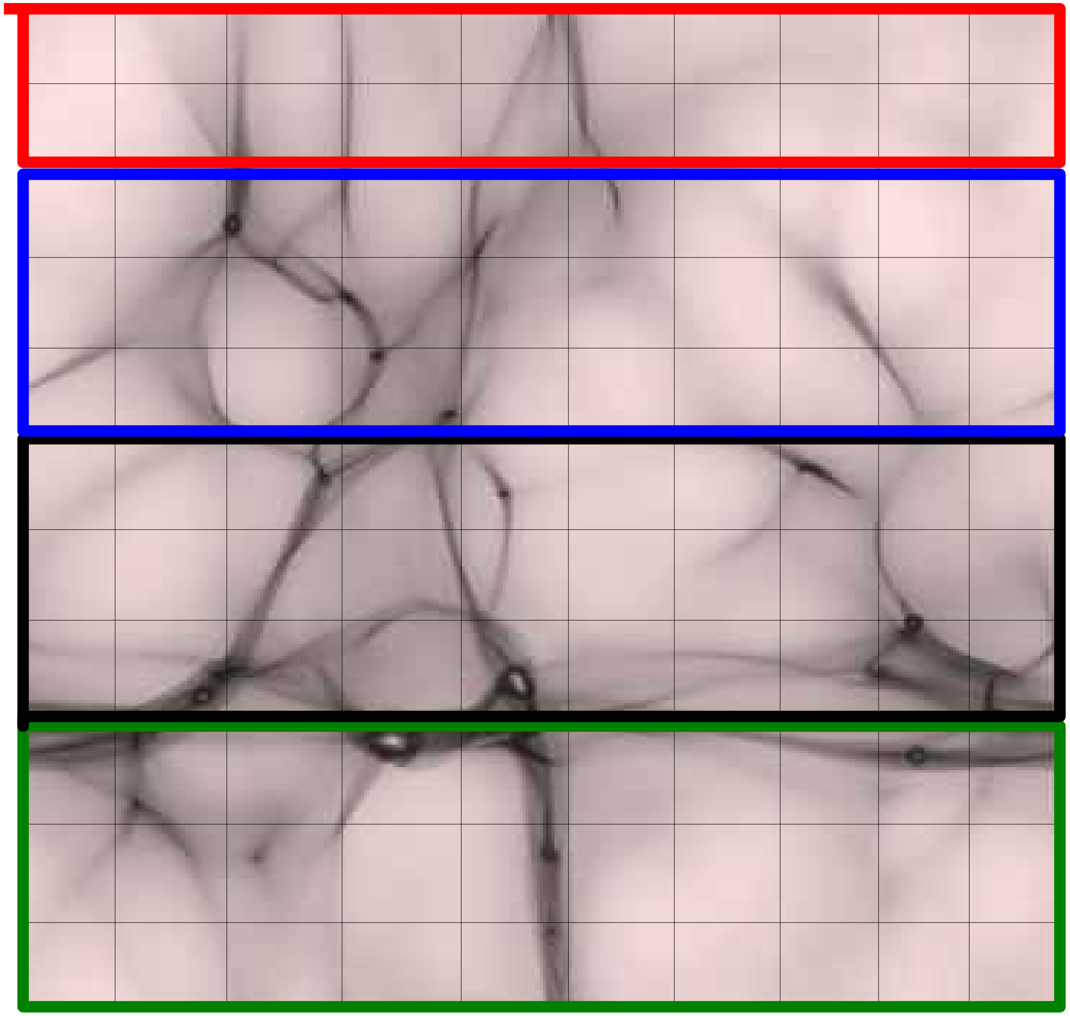
- L = 3000 Mpc/h
- N = 6720^3 particles
- € = 10 kpc/h
- M = 6.18×10^9 Msun/h

Computational domain decomposition



MPI Task #1
MPI Task #2
MPI Task #3
MPI Task #4

Force Calculation



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