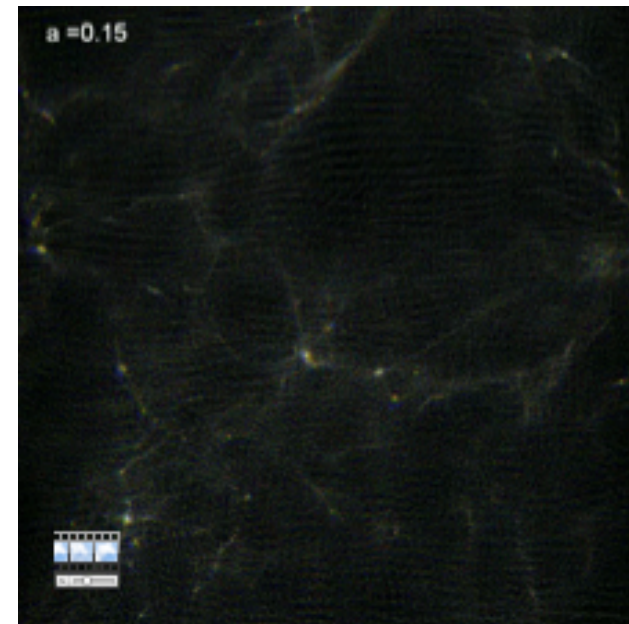
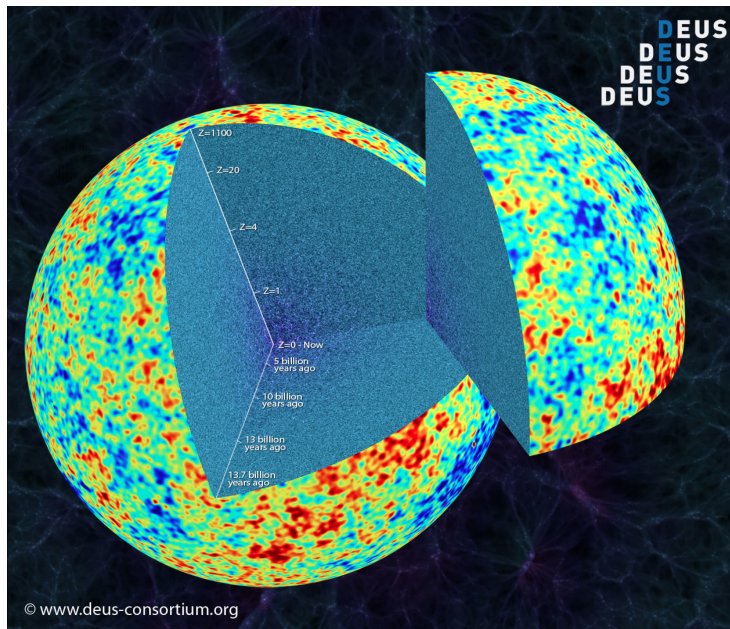


NUMERICAL SIMULATION OF THE DARK UNIVERSE



Jean-Michel ALIMI, Laboratory Universe and Theories

DEUS Consortium

www.deus-consortium.org

Numerical simulations of Dark Universe

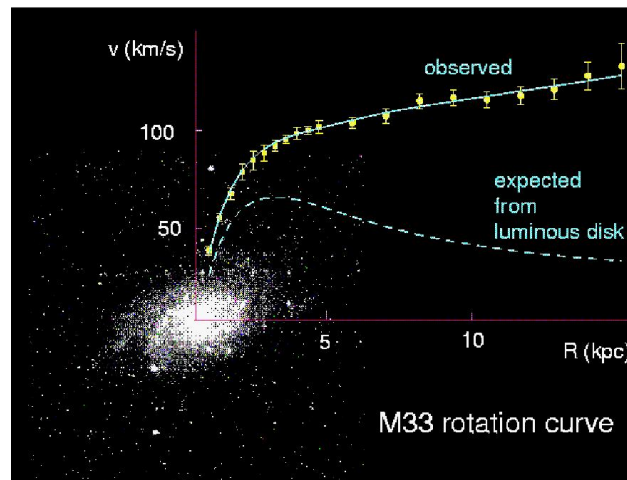
Why are we talking about a Dark Universe ?

« OBSERVATIONAL » EVIDENCES OF THE DARK UNIVERSE: DARK MATTER

For 80 years, Astronomy has accumulated evidence that the dominant form of matter in the Universe is dark and non-baryonic (DM: 85% + BM: 15%).

Dark matter came to the attention of astrophysicists due to discrepancies between the mass of large astronomical objects determined from their gravitational effects, and the mass calculated from the "luminous matter" they contain; such as stars, gas and dust.

Evidence for dark matter in spiral galaxies



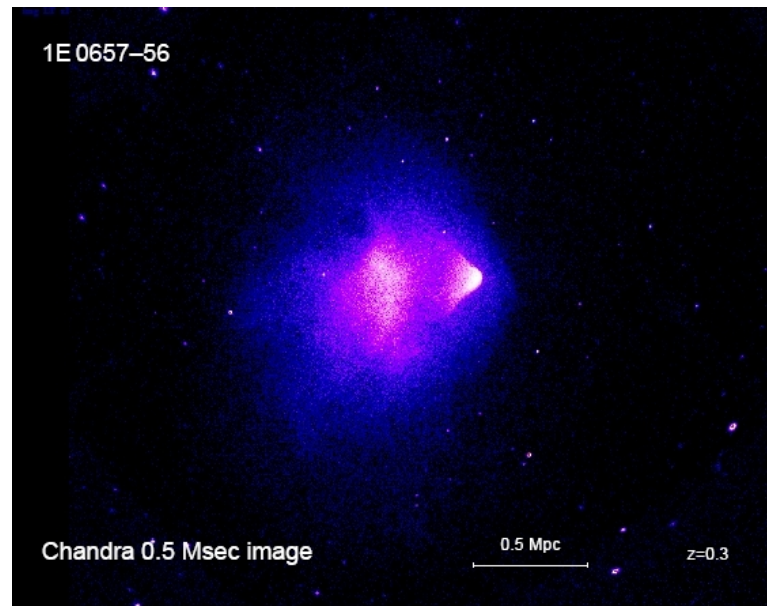
Most spiral galaxies show flat rotation curves out as far as we can trace them, even where no more stars are visible.

Therefore we conclude that the gravitational mass is more than 10 times more massive than the luminous mass.

« OBSERVATIONAL » EVIDENCES OF THE DARK UNIVERSE: DARK MATTER

For 80 years, Astronomy has accumulated evidence that the dominant form of matter in the Universe is dark and non-baryonic (DM: 85% + BM: 15%).

Evidence for dark matter in clusters of galaxies: Bullet Cluster



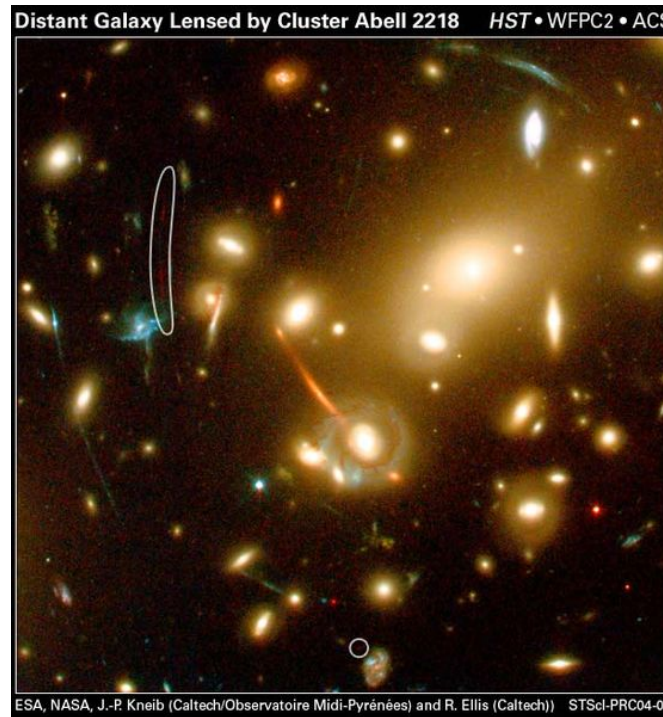
Comparison of images of the gas obtained by the Chandra X-ray telescope to « maps » of the gravitational field deduced from weak lensing observations.

The clear separation of dark matter and gas clouds is considered direct evidence that dark matter exists

« OBSERVATIONAL » EVIDENCES OF THE DARK UNIVERSE: DARK MATTER

For 80 years, Astronomy has accumulated evidence that the dominant form of matter in the Universe is dark and non-baryonic (DM: 85% + BM: 15%).

Evidence for dark matter in clusters of galaxies (lensing measures)

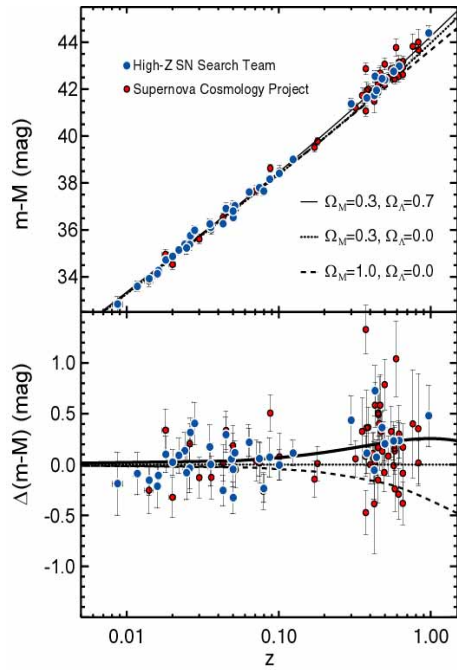


By measuring how the background galaxies are distorted by the foreground cluster, astronomers can measure the mass in the cluster. The mass in the cluster is more than five times larger than the inferred mass in visible stars, gas and dust.

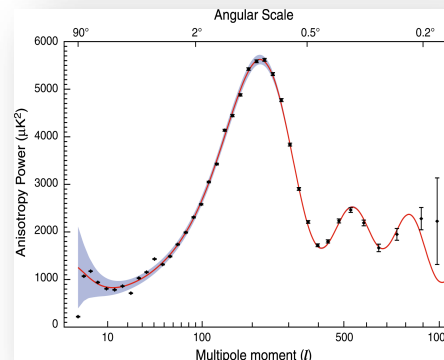
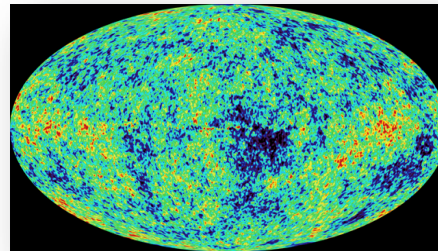
« OBSERVATIONAL » EVIDENCES OF THE DARK UNIVERSE: DARK ENERGY

Since a decade, we have solid observational evidence of cosmic acceleration, requiring yet another mysterious contribution to the total energy budget of the Universe, the dark energy.

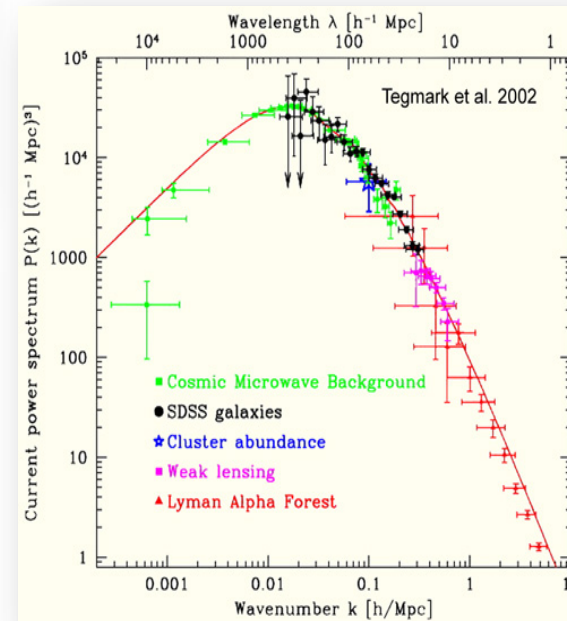
- SN Ia luminosity distance (SCP,HST,SNLS,ESSENCE)



- CMB anisotropy power spectra (WMAP)



- Matter P(k) (from 2dF and SDSS)

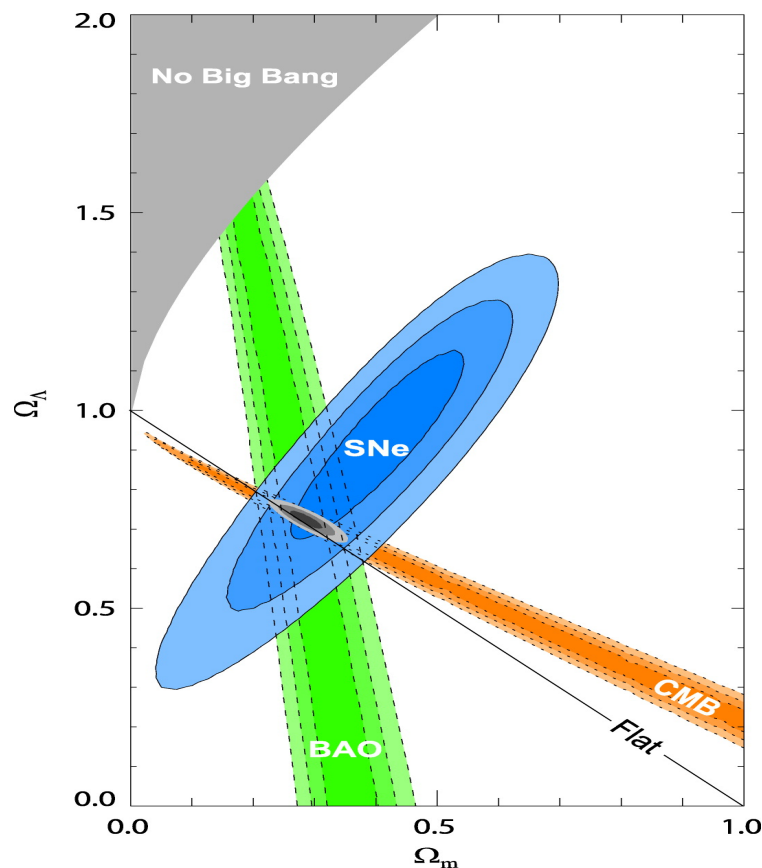


- BAO (detected in 2dF and SDSS), ISW-correlation (several galaxy surveys vs. WMAP)
Cluster Number Counts (Chandra detections) ...

« OBSERVATIONAL » EVIDENCES OF THE DARK UNIVERSE: DARK ENERGY

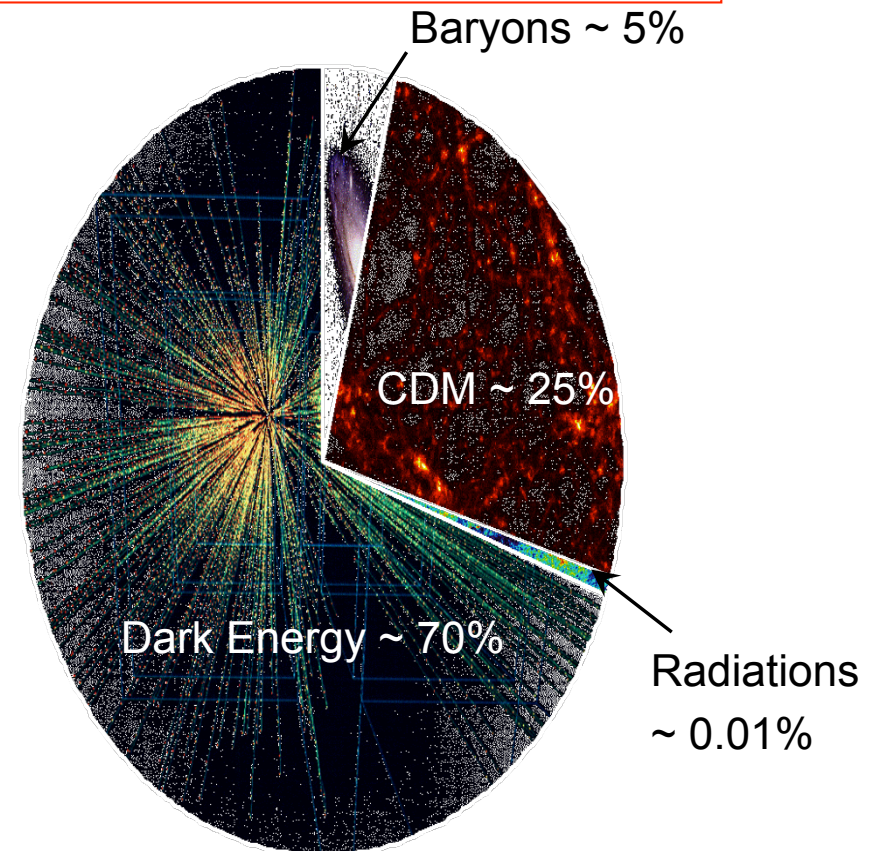
Since a decade, we have solid observational evidence of cosmic acceleration, requiring yet another mysterious contribution to the total energy budget of the Universe, the dark energy.

Cosmic complementarity



Kowalski et al. 2008

The Concordance Model Λ CDM



NUMERICAL SIMULATION OF THE DARK UNIVERSE

What is the nature of the Dark Matter ?

What is the nature of the Dark Energy ?

As the signatures of the nature of DM and DE depend on the detailed distribution of DM (may be of DE too) throughout the Universe, from cosmics all the way down to sub galactic scales, the question of the contents of the dark Universe and the origin of the cosmic structure are deeply related.

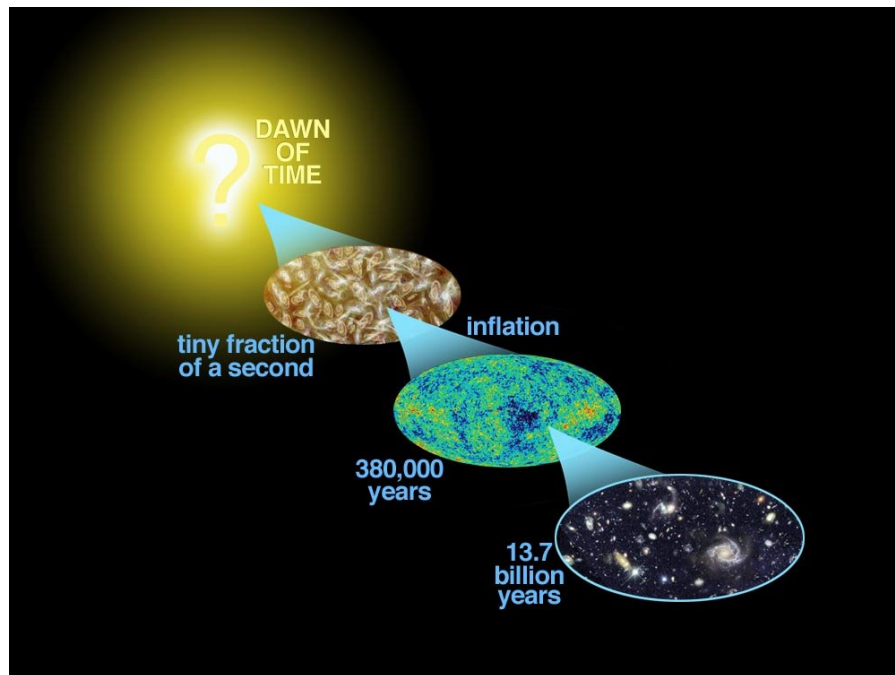
The origin of the cosmic structures in the Universe is as such a fundamental question in cosmology.

NUMERICAL SIMULATION OF THE DARK UNIVERSE

Usual paradigm of the cosmic structure formation model (evolution of the Universe) is:

Universe is spatially homogenous and isotropic, it is described by General Relativity
Its dynamics is given only by $a(t)$ through FLRW Equation

$$ds^2 = dt^2 - a(t)^2 \left[\frac{dr^2}{1 - kr^2} + r^2 d\theta^2 + r^2 \sin^2 \theta d\phi^2 \right] \quad H_*^2 = \left(\frac{\dot{a}}{a} \right)^2 = \frac{8\pi G}{3} \sum_i \rho_i, \quad \frac{\ddot{a}}{a} = -\frac{8\pi G}{6} \sum_i (\rho_i + 3p_i)$$



Primordial perturbations are seeded by quantum fluctuations and are stretched to cosmological scales by inflation

The shape and the amplitude of these perturbations are observed on the CMB.

Their growth by gravitational instability in an expanding universe leads to the cosmic structures we observe today. The gravitational interactions are modelled using quasi-Newtonian laws (taking into account the cosmic expansion)

Structure formation models attempts to reduce cosmology to an initial value problem.

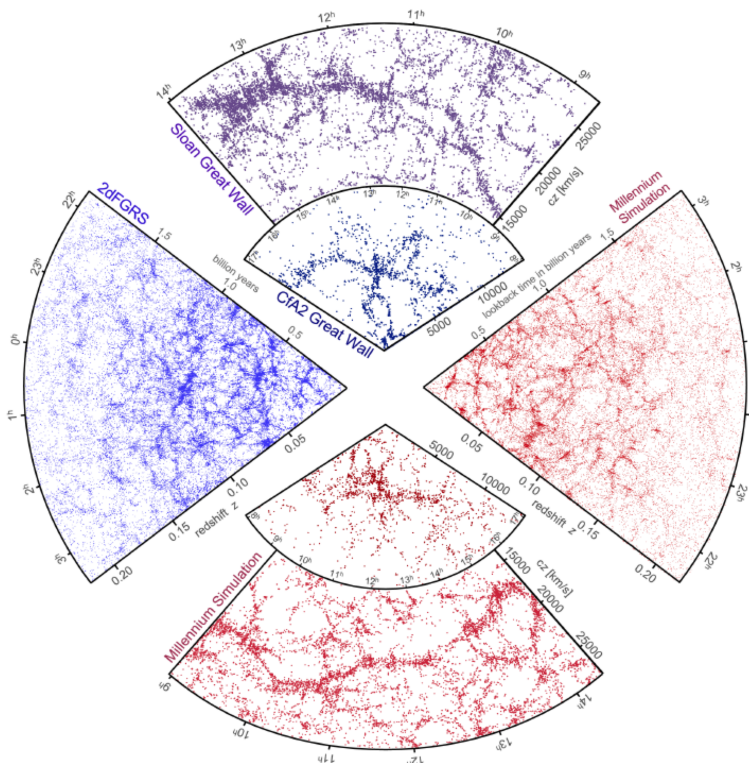
The purpose of cosmological simulations is to model the growth of structures in the Universe.

NUMERICAL SIMULATION OF THE DARK UNIVERSE

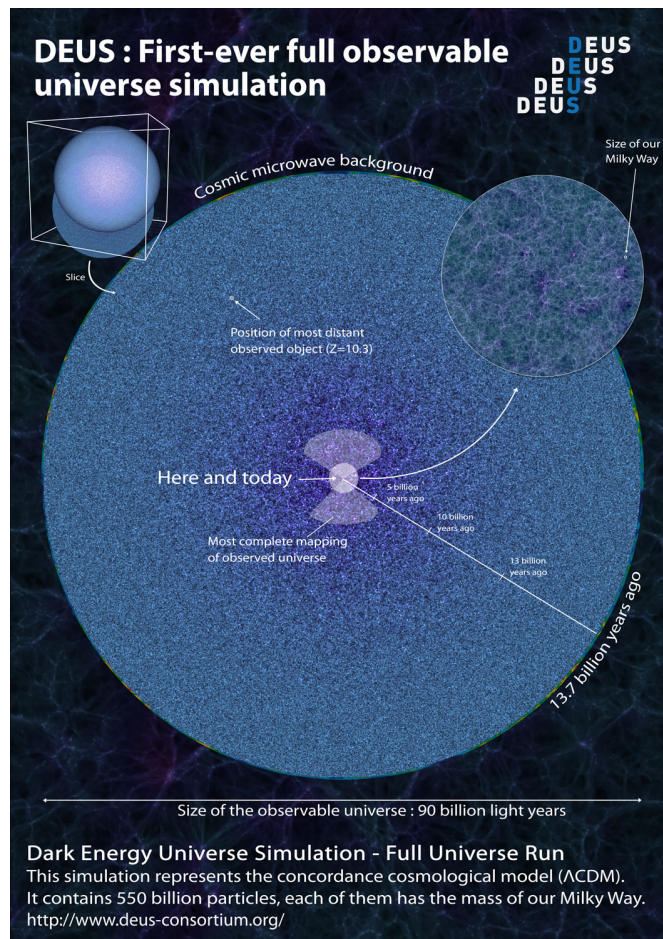
Numerical simulations of cosmic structure formation is also a powerful theoretical tool to interpret and to support present and future cosmological observations (redshift space).

Simulated and observed large-scale structure in the galaxy distribution

MOCK PIE DIAGRAMS COMPARED TO SDSS, 2DFGRS, AND CFA-2



Springel et al. (2006)



NUMERICAL SIMULATION OF THE DARK UNIVERSE

This lecture will organized around three main questions:

Why do we need to perform numerical simulation in cosmology ?

**How do we perform numerical simulation of
cosmic structure formation ?**

**What have we learned from numerical simulations
on cosmics structure formation ?**

**Many lectures on cosmic structure formation are available (see Bibliography)
(numerical methods, initial conditions...).**

**I shall discuss these aspects but mainly to show up the « logic » of the development
of numerous methods for cosmological numerical simulations,**

**To show up the links between these methods. I shall give also some remarks on
Optimization process, Supercomputer Architecture, Grand Challenge Project (DEUS)...
and some Results on large scale structure, halo profil,...**

Non Linear Gravity / Cosmology, Universality / Non Universality

Numerical simulations of Dark Universe OUTLINE

Numerical Simulation of the Dark Universe

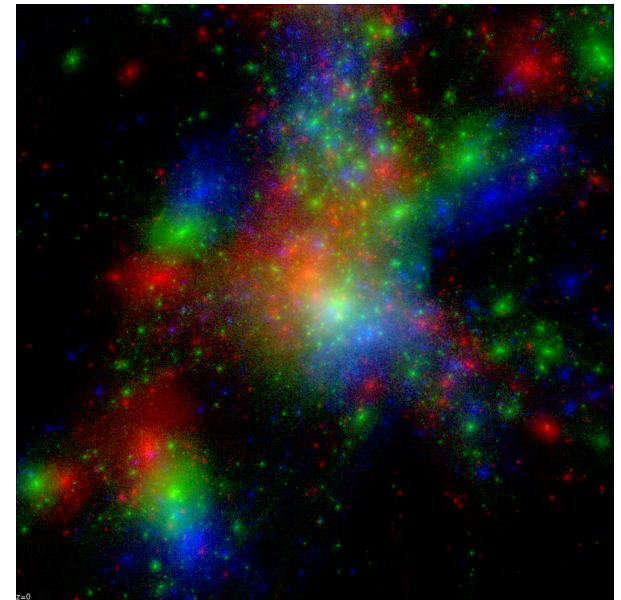
Introduction

I. Why do we need to perform numerical Simulation in cosmology ?

I. 1. Gravitational instability in an expanding universe.
N-body collisionless gravitational dynamics

I.2. Mean Field approximation.
Vlasov-Poisson system / N-body system

I.3. Why is approximate solutions of
the non linear gravitational dynamic
not sufficient ? cosmological observables.



Numerical Simulation of the Dark Universe

II. How can we perform numerical simulation of large scale structure formation

II. 2. Gravity Solver

Direct Methods, Tree Methods, PM Methods,
Hybrid Methods, AMR Methods,
...

II. 1. Numerous Methods: Time integration.

II. 3. Generation of Initial Condition

II. 6. Cosmological observables and analysis of numerical results

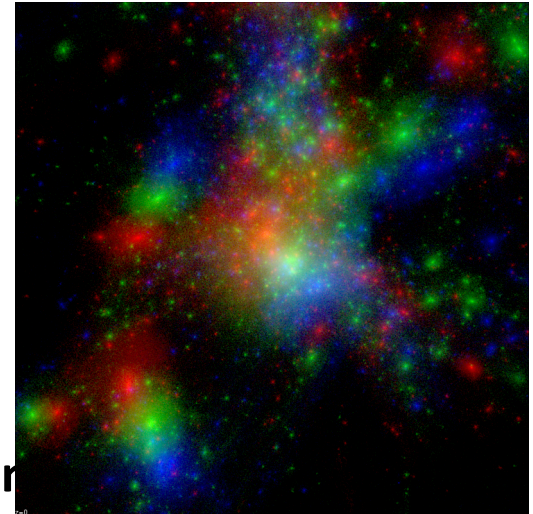
Correlation, Power Spectrum, Mass Function, Halo Profiles, Bulk Flow,
Redshift Space Distortions...

II. 5. Numerical and Physical Limitations

II. 7. To higher resolution: mass and spatial resolution

Parallel Implementations, Supercomputer architectures, Performance Results

II. 8. Cosmological consortia: Grand Challenge Simulation.



Numerical Simulation of the Dark Universe

III. What do we have learned from numerical simulations on large scale structure formation ?

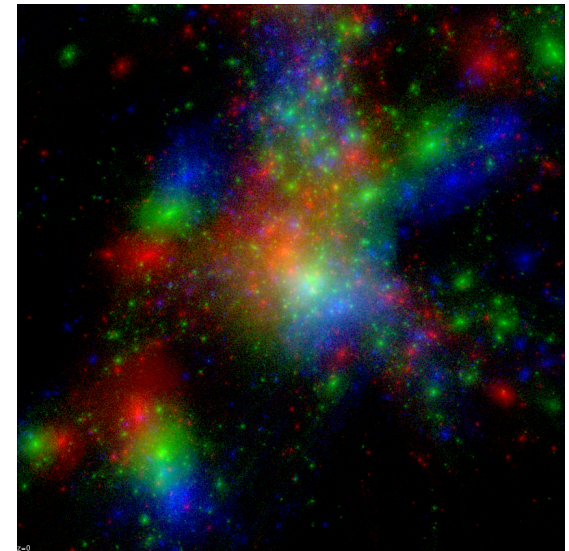
III. 1. DEUS: Results in Progress

III. 2. Large scale structure formation (Bias, Bulk Flow)

III. 3. Halo properties (Mass function, Profiles)

IV. Conclusion - Acknowledgments

V. Bibliography



What do we simulate?

Why do we need to perform numerical Simulation in cosmology ?

What do we want to simulate ? N-body collisionless gravitational dynamics

Let us compare some time scales.

A system of N particles interacting gravitationally with total mass M and a given size R reaches a dynamic equilibrium state on a timescale comparable to a few times the typical time t_{cr} , needed for a particle to cross the system

$$t_{cr} \approx \frac{1}{\sqrt{GM/R^3}} \left(\approx \frac{1}{\sqrt{G\rho}} \right)$$

t_{cr} is the response time needed to settle down to equilibrium.

If the system is initially out of equilibrium, this is reached through mixing in phase space due to fluctuations of the gravitational potential, a process called violent relaxation (Lynden-Bell 1967).

For dark matter halos, large scale cosmic structures

$$t_{cr} \approx t_U$$

Why do we need to perform numerical Simulation in cosmology ?

What do we simulate ? N-body collisionless gravitational dynamics

Let us compare time scales.

Once the system is in dynamic equilibrium a long term evolution is possible, driven by two-body relaxation, where energy is slowly exchanged between particles, and the system tends to evolve toward energy equipartition. The timescale t_{rel} for this process depends on the number of particles and on the geometry of the system (Spitzer 1987).

$$t_{rel} \approx \left[\frac{N}{10 \text{Log}(N)} \right] t_{cr}$$

N-body systems such as galaxies and dark matter halos have a relaxation time much longer than the life of the Universe and are thus considered collisionless systems.

Why do we need to perform numerical Simulation in cosmology ?

What is the N-body collisionless gravitational dynamics ?

A system of N particles ($N \gg 1$) interacting gravitationally defines a $6N+1$ dimensional phase space given by the N position and velocity vectors associated to each particle at each time t .

The solution of the N-body problem defines a trajectory in this phase space.

As the number of dark matter particles in cosmic structure is large enough, that is if the two body relaxation time is long compared to the time-frame one is interested in, they just respond to their collective gravitational field and a statistical description of the problem is possible.

This allows us to pass from a $6N+1$ to a $6+1$ dimension phase space.

Why do we need to perform numerical Simulation in cosmology ?

What is the N-body collisionless gravitational dynamics ?
Mean Field Approximation

We adopt a mean field description of the dynamical system in terms of a single particle distribution function $f(\mathbf{r}, \mathbf{v}, t)$, where $f(\mathbf{r}, \mathbf{v}, t)d\mathbf{r}d\mathbf{v}$ is proportional to the probability of finding a particle in a 6D element of volume $d\mathbf{r}d\mathbf{v}$ centered around position $\mathbf{r}$ and velocity $\mathbf{v}$ at time t .

Within this simplified framework the knowledge of the distribution function uniquely defines all the properties of the system.

The dynamic is described by the Vlasov equation.

$$\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \vec{v} \cdot \frac{\partial f}{\partial \vec{r}} - \frac{\partial \phi}{\partial \vec{r}} \cdot \frac{\partial f}{\partial \vec{v}} = 0 \quad \nabla^2 \phi(\vec{r}, t) = 4\pi G \rho(\vec{r}, t)$$

where $\rho(\vec{r}, t) = \int f(\vec{r}, \vec{v}, t) d\vec{v}$

Phase-space is conserved along each characteristic (i.e. particle trajectory).

Why do we need to perform numerical Simulation in cosmology ?

Mean Field approximation: Vlasov-Poisson system / N-body system

But this system of **partial** differential equations is very difficult (impossible) to solve directly in non-trivial cases. Given its high dimensionality (6+1), the Vlasov equation is usually solved by sampling the initial distribution function and then by evolving the resulting N-body system by means of numerical method that suppresses two body interactions at small scales (the interaction is softened)

Since the Vlasov equation states that f is constant along any trajectory $\{\mathbf{r}(t), \mathbf{v}(t)\}$, the trajectories obtained by time integration of N points $\{\mathbf{r}_i, \mathbf{v}_i\}$ sampled from the distribution function f at time $t = t_{\text{initial}}$ forms a representative sample of f at each time t .

Hence the problem reduces to solving Poisson's equation for a set of N particles and advancing them forward in time according to their equations of motion.

Why do we need to perform numerical Simulation in cosmology ?

Mean Field approximation: Vlasov-Poisson system / N-body system

In N-body approach, the initial phase space is splitted into small domains, each domain is represented by a (macro-) particle, and (macro-) particles are evolved selfconsistently using equations of (macro-) particle motion:

with potential given by the Poisson equation:

$$\frac{d\vec{r}}{dt} = \vec{v}$$
$$\frac{d\vec{v}}{dt} = -\vec{\nabla}\phi$$
$$\vec{\nabla}^2\phi = 4\pi G\rho_{tot}$$
$$\phi(\vec{r}) = -\sum_{j \neq i} G \frac{m_j}{|\vec{r} - \vec{r}_j|^2 + \varepsilon^2}$$

N-body approach can be seen as a Monte Carlo technique for Random sampling of the characteristics.

Why do we need to perform numerical Simulation in cosmology ?

Mean Field approximation: Vlasov-Poisson system / N-body system

We follow the growth of primordial fluctuations in an expanding Universe. It is convenient to re-write the equations in comoving variables $\mathbf{x} = a(t)^{-1} \mathbf{r}$ where the scale factor $a(t)$ satisfies Friedmann equation

Several questions come up now:

How do we compute the gravitational forces efficiently and accurately?
(Numerical techniques by using or not using a Mesh)

How do we integrate the orbital equations in time?
(Time integrator symplectic or not symplectic)

How do we generate appropriate initial conditions?
(Background / Perturbations)

Why do we need to perform numerical Simulation in cosmology ?

What do we simulate ? Which are the difficulties ?

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

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

If the particle mass is too large (or particle number N is too low), gravitational physics cannot be correctly resolved and smallest structures (dwarf galaxies) will be missed.



We want **smallest particle mass and the largest number of particles** to resolve internal structure of halos

If the computing volume is too small, fundamental mode goes non-linear soon after the first halos form and computation cannot be meaningfully continued beyond this point. Moreover, rare events, rare objects as most massive objects (rich clusters) or the first halo could be missed



We want **a large volume** to get a representative sample of the Universe.

Physics / Cosmology impose the largest N and the largest Volume

Numerical Approach / Analytical Approximation

Why do we need to perform numerical Simulation in cosmology ?

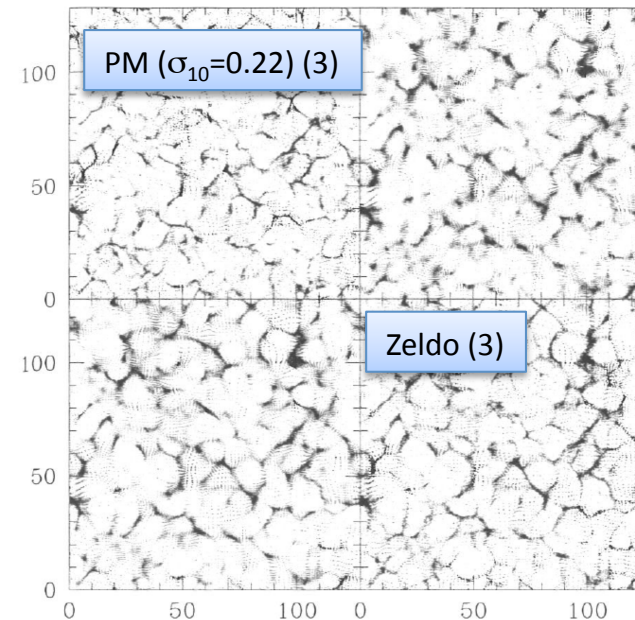
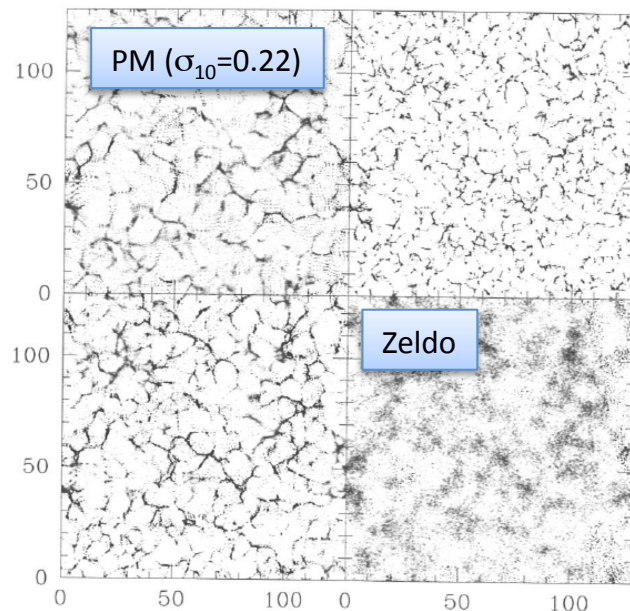
Cosmic structure formation can be described using approximations of non-linear gravitational dynamics ! Why do not use such approximations ?

Three kinds of approximations:

Approximation of the dynamics of the collapse (Zeldovich, perturbative theory...)

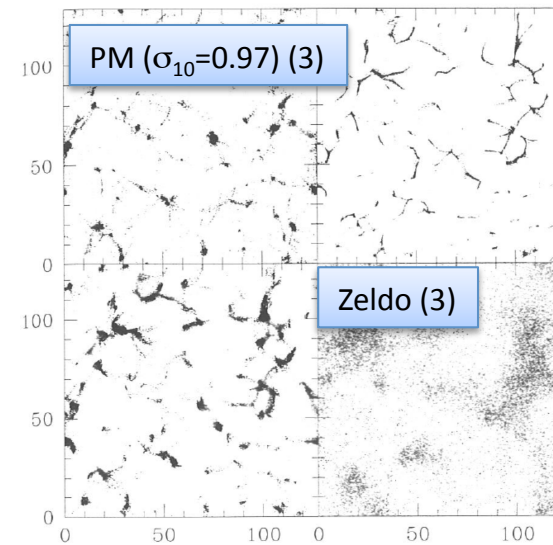
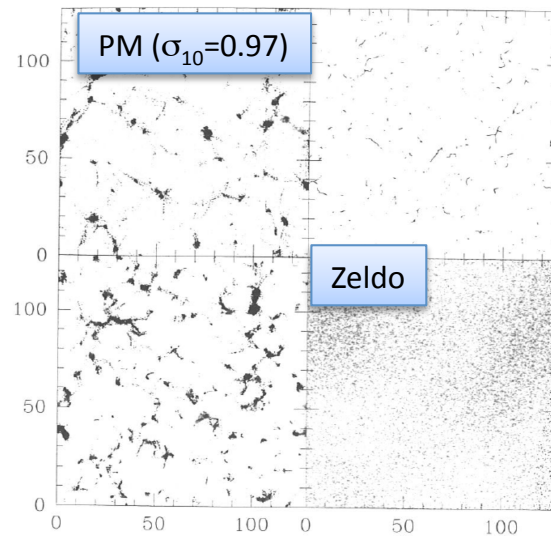
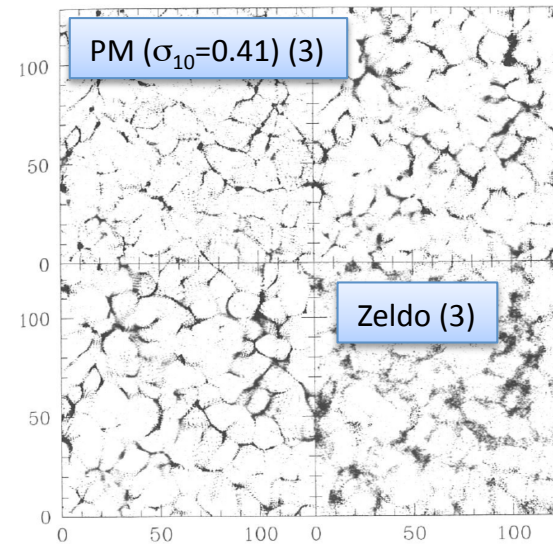
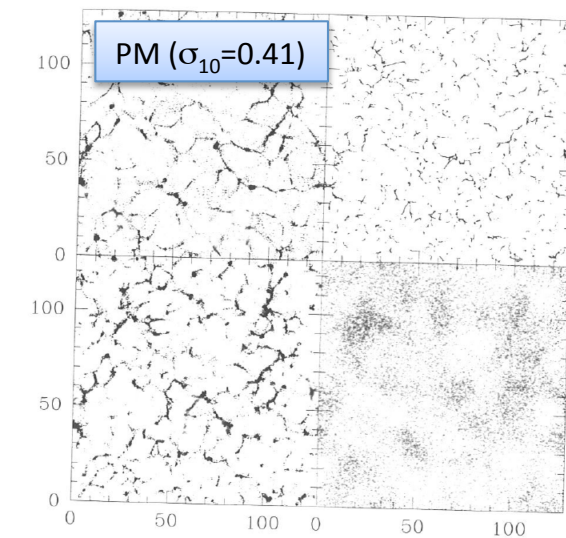
Approximation on the geometry of the collapse (spherical, ellipsoidal collapse...)

Approximation on the statistics (Press Schechter formalism, Excursion Set Theory...)



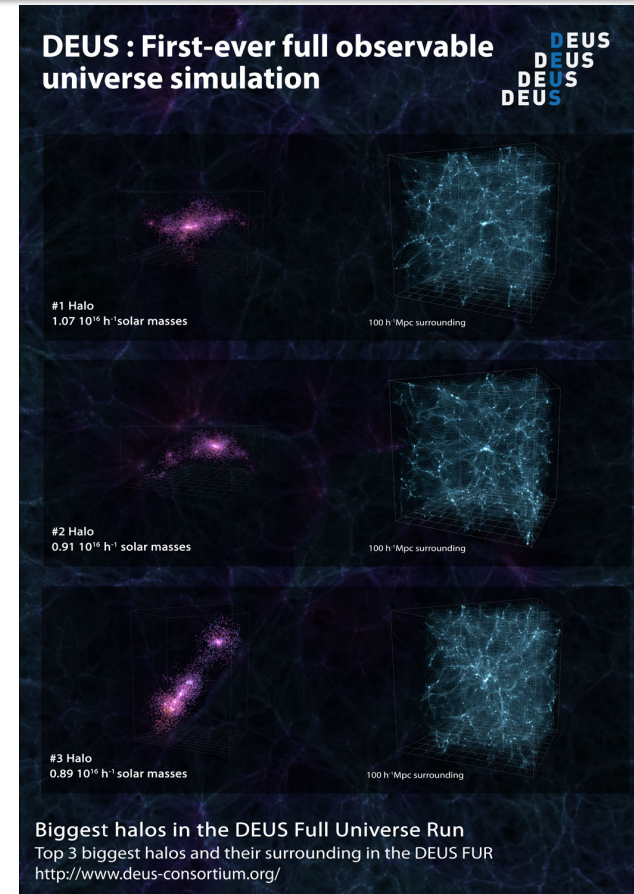
Why do we need to perform numerical Simulation in cosmology ?

Why do not use such approximations ? Comparison Approximation and « Exact » dynamics



Why do we need to perform numerical Simulation in cosmology ?

Why do not use such approximations ? Sphericity of Halos

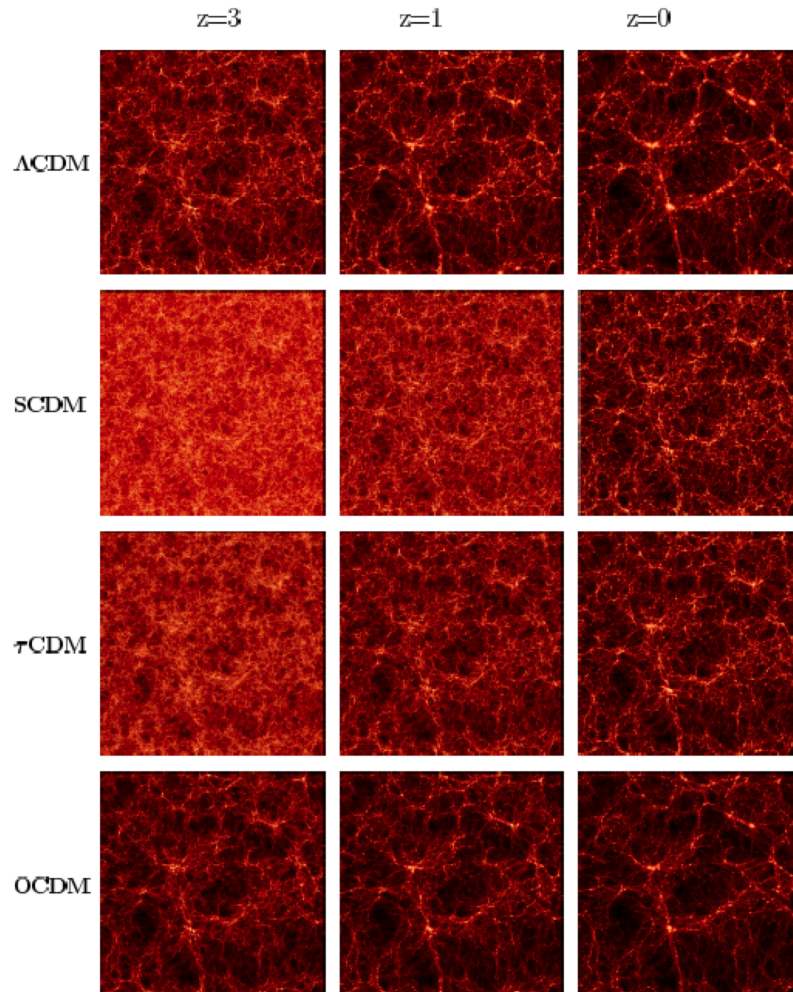


Non-sphericity for low mass and high mass halos

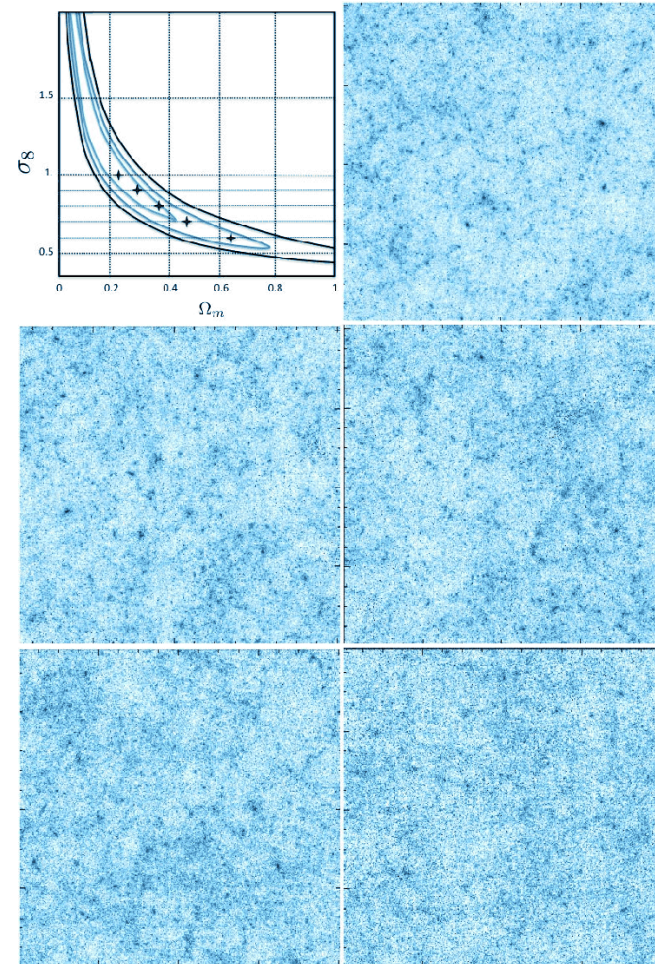
Each approximations is efficient to describe a specific aspect. The analytical approximations are probably the only way to deeply understand the origin of the mass function, the distribution of dark matter But none approximation is able to calculate and to describe correctly both all observables and the complexity of the cosmic structure formation process.

Why do we need to perform numerical Simulation in cosmology ?

Cosmic structure formation can be described using approximations of non-linear gravitational dynamics ! Why do not use such approximations ?



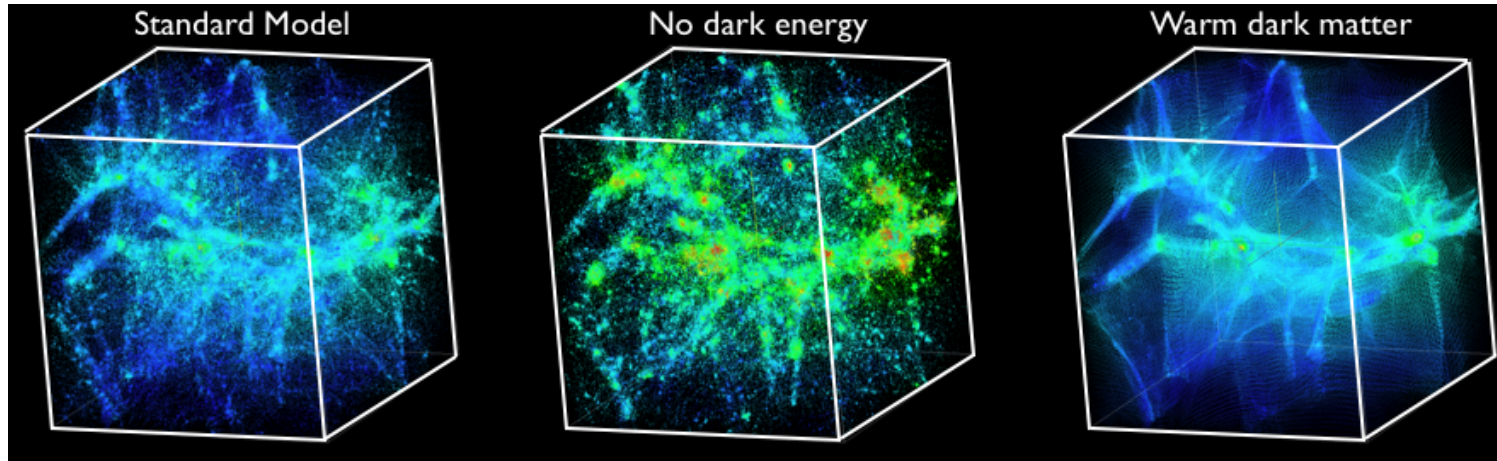
Virgo Consortium 1996



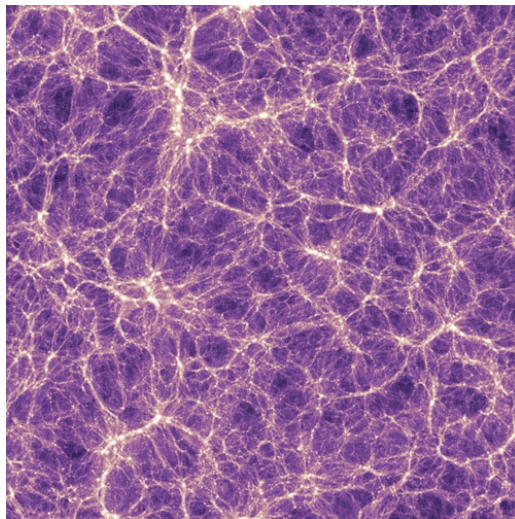
Horizon - Pires et al 2010

Why do we need to perform numerical Simulation in cosmology ?

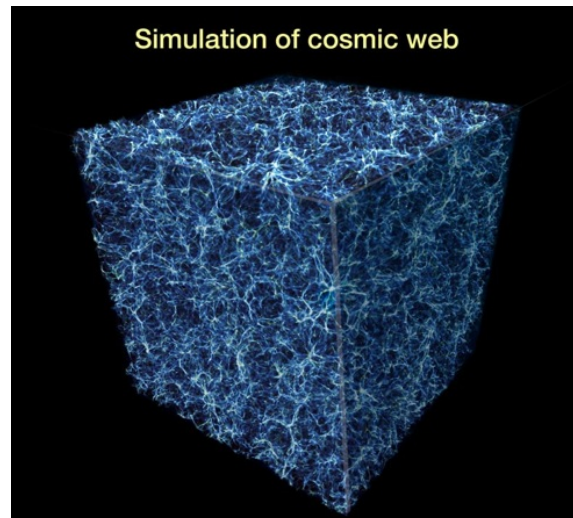
Cosmic structure formation can be described using approximations of non-linear gravitational dynamics ! Why do not use such approximations ?



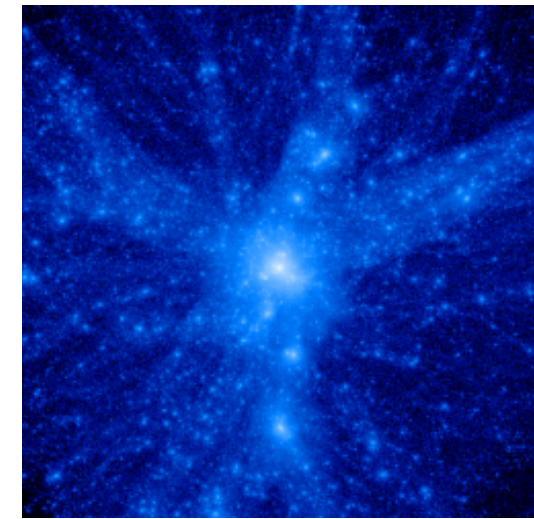
Heitmann,
Habib et al.
Argonne
National
Laboratory
2012.



Angulo et al, Millenium 2011



Loeb et al 2010

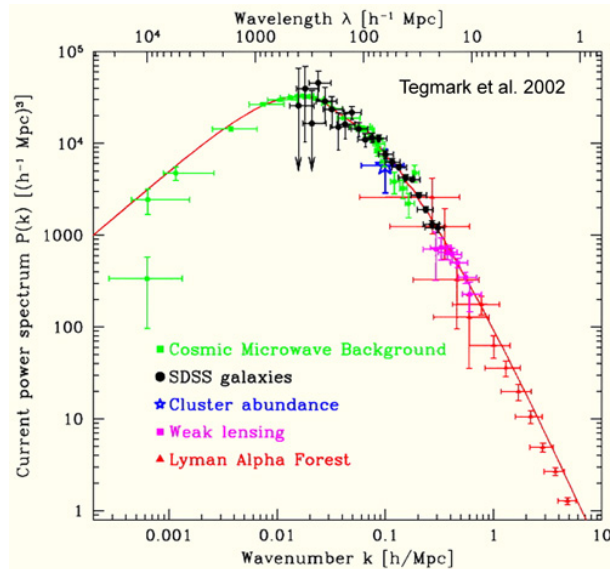


Borgani et al 2012, Trieste Num Group

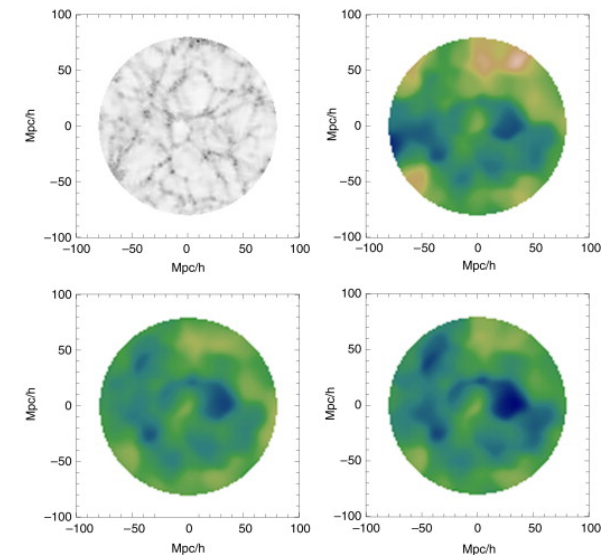
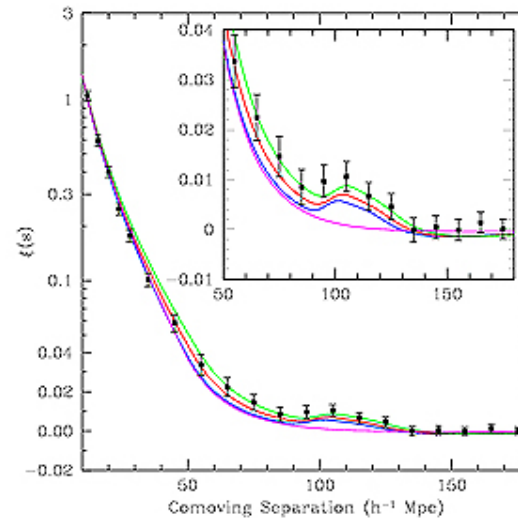
Why do we need to perform numerical Simulation in cosmology ?

What are these observables ?

Power spectrum



Correlation function ($\xi(r)$)
higher statistics

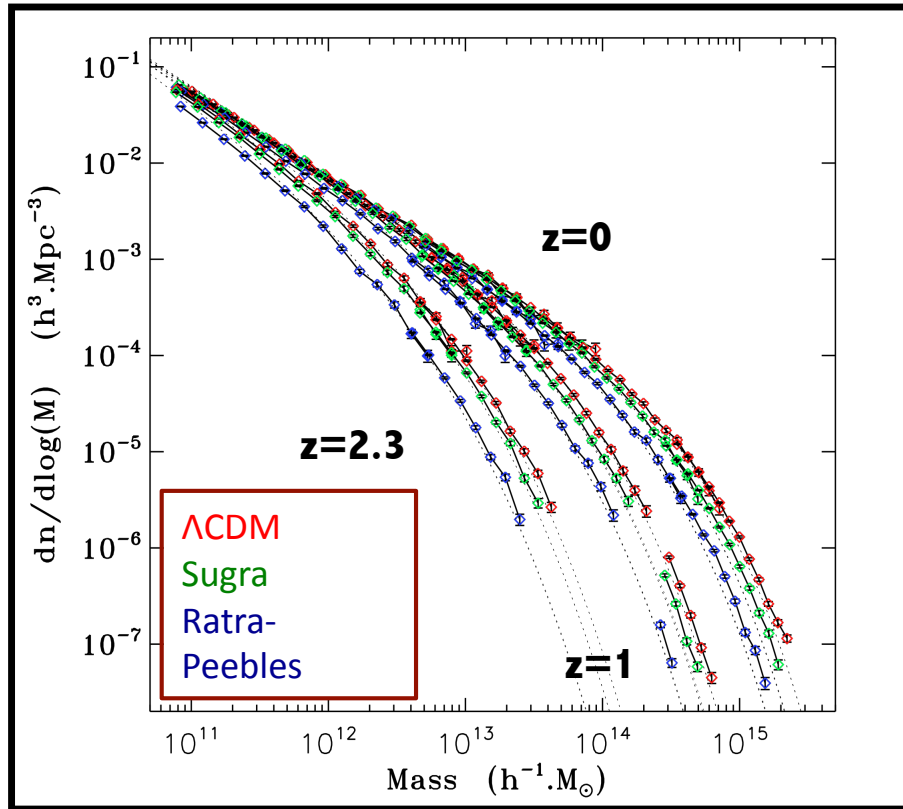


Velocity Field and Correlation in velocity space , bulk flow...

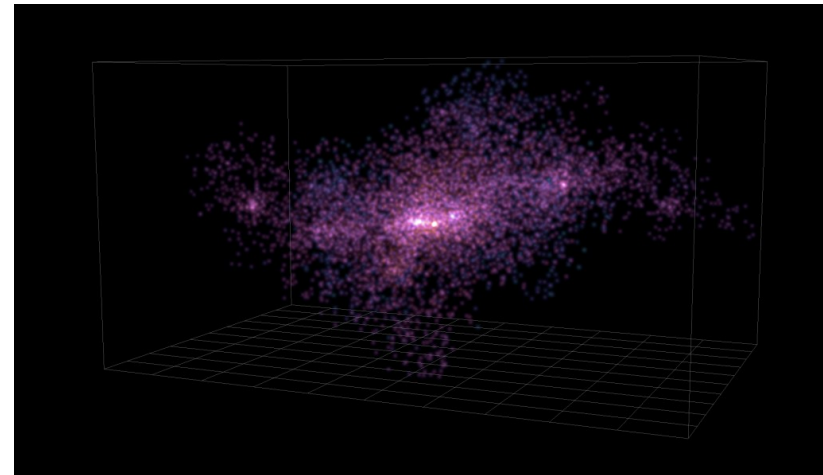
Why do we need to perform numerical Simulation in cosmology ?

What are these observables ?

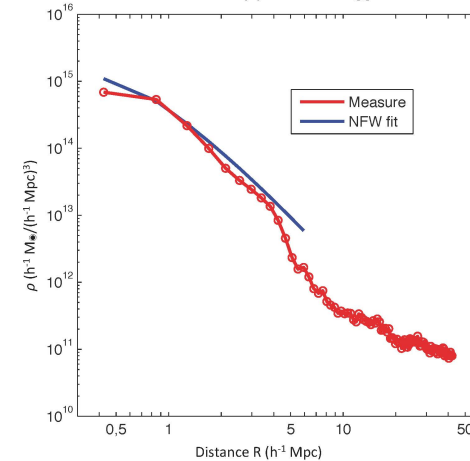
Mass function



Halo profile



DEUS Full Universe Run: Density profile for biggest halo vs NFW fit



Structural properties,
angular momentum,
concentration...

Sub-structures

Merger-Tree

Why do we need to perform numerical Simulation in cosmology ?

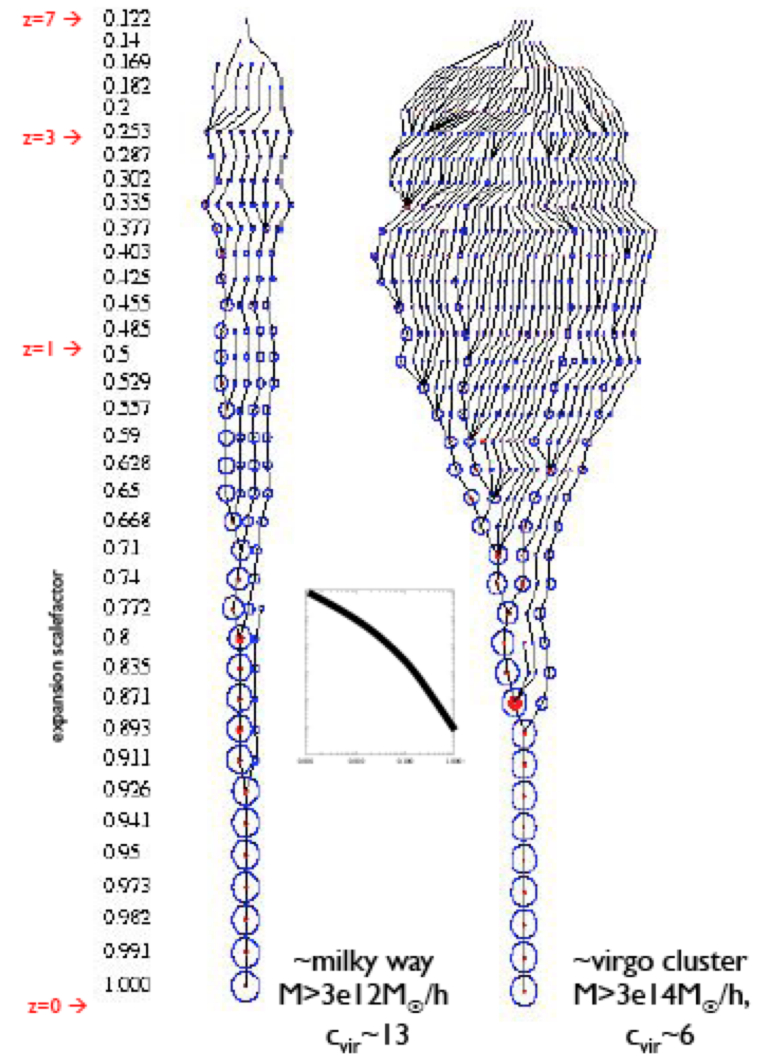
What are these observables ?

Sub-structures

Merger-Tree



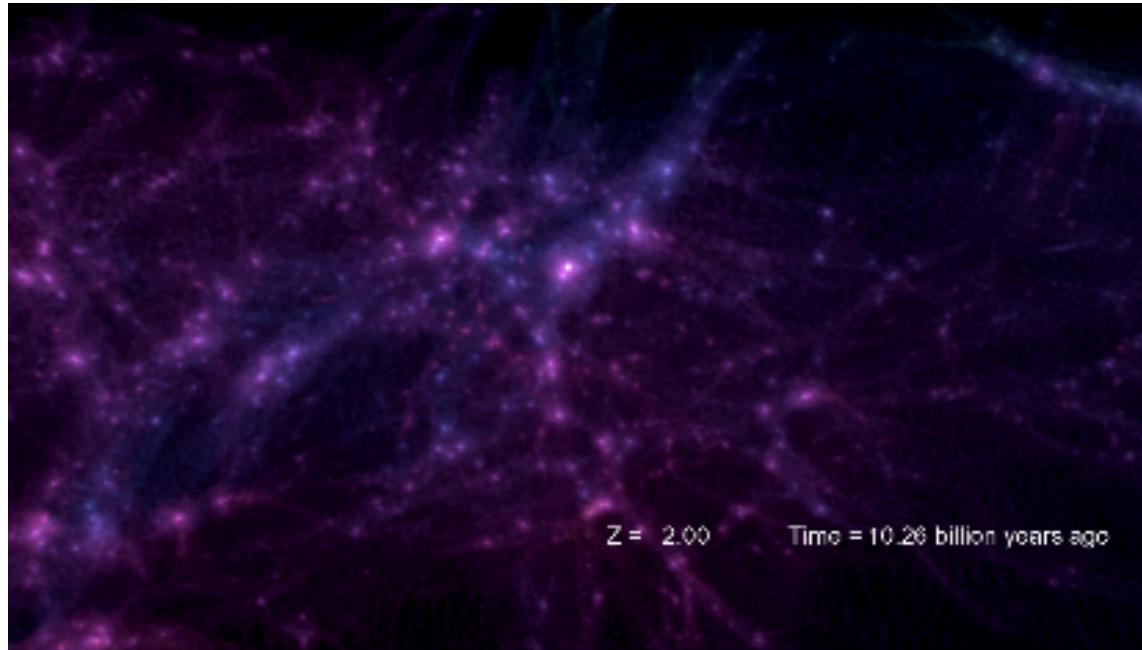
Kulhen et al 2008



Wechsler et al 2002

Why do we need to perform numerical Simulation in cosmology ?

Cosmic structure formation can be described using approximations of non-linear gravitational dynamics ! Why do not use such approximations ?



DEUS Consortium 2010

The process of structure formation is complex. The gravitational collapse in hierarchical models produces filaments, structures at the intersection of these filaments, clumps... Structures appear at all scales, structures merge... The power spectrum is not sufficient to describe the matter distribution. Higher order description and other statistics are often needed. We also want to know the number of objects formed, i.e. the halo mass function, the structure of these objects, the halo profile... Only a cross-analysis of numerous observables will better understand the formation of cosmic structures and allow to deduce the cosmological model.

Why do we need to perform numerical Simulation in cosmology ?

Why is an approximation of the non linear gravitational dynamics not sufficient?

Though numerical simulations are not an exact reproduction of the gravitational dynamics but because it does not exist any approximate solution which is able **both** to evaluate the evolution of the dark matter, its distribution on large range of scales, the structure of DM halos, the number of DM halos...

Numerical simulations are the only or at least an effective way to compute any cosmological observables.
And provided, in a numerical simulation we evaluate the accuracy with which we are able to calculate these observables, the numerical simulations is a powerful way to constrain and to discriminate between the cosmological models.

Numerical Simulation of the Dark Universe

II. How can we perform numerical simulation of large scale structure formation

II. 2. Gravity Solver

Direct Methods, Tree Methods, PM Methods,
Hybrid Methods, AMR Methods,
...

II. 1. Numerous Methods: Time integration.

II. 3. Generation of Initial Condition

II. 6. Cosmological observables and analysis of numerical simulation

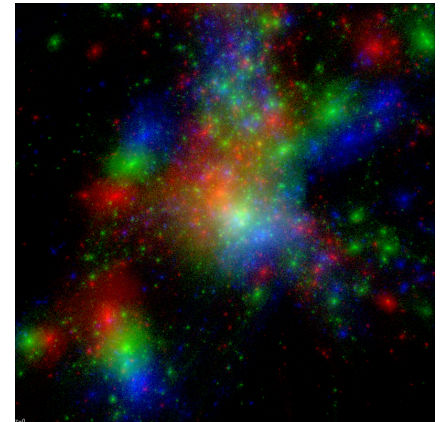
Correlation, Power Spectrum, Mass Function, Halo Profiles, Bulk Flow,
Redshift Space Distortions...

II. 5. Numerical and Physical Limitations

II. 7. To higher resolution: mass and spatial resolution

Parallel Implementations, Supercomputer architectures, Performance Results

II. 8. Cosmological consortia: Grand Challenge Simulation.



How can we perform numerical simulation of LSS formation

**Gravity Solver
Numerous Methods**

How can we perform numerical simulation of LSS formation

Gravity Solver: Direct Methods

Sum forces by direct particle-to-particle gravitational force:

$$\vec{F}_i = - \sum_{j \neq i} G \frac{m_i m_j (\vec{r}_i - \vec{r}_j)}{|\vec{r}_i - \vec{r}_j|^3} \quad \vec{F}_i = - \sum_{j \neq i} G \frac{m_i m_j (\vec{r}_i - \vec{r}_j)}{\left(|\vec{r}_i - \vec{r}_j|^3 + \varepsilon^2 \right)^{3/2}}$$

- 1) The problem is thus a set of non-linear second order ordinary differential equations relating the acceleration $d^2\mathbf{r}_i/dt^2 = \mathbf{F}_i/m_i$ with the position of all the (macro) particles in the system.
- 2) The gravitational force presents a singularity when the distance of two particles approaches 0, which can lead to arbitrarily large relative velocities.
In addition, given the non-linear nature of the equations, the singularities are movable, that is they depend on the specific choice of initial conditions (In contrast, all singularities in linear ordinary differential equations are independent of initial conditions).

How can we perform numerical simulation of LSS formation

Gravity Solver: Direct Methods and Softening of the force

The singularity may be avoided by introducing a smoothing length that is by modifying the gravitational interaction at small scales.

$$\vec{F}_i = - \sum_{j \neq i} G \frac{m_i m_j (\vec{r}_i - \vec{r}_j)}{\left(|\vec{r}_i - \vec{r}_j|^3 + \varepsilon^2 \right)^{3/2}}$$

Where $\varepsilon > 0$ is the softening, or smoothing length, that is a typical distance below which the gravitational interaction is « suppressed ».

This strategy effectively suppresses binary formation and strong gravitational interactions (Aarseth 1972...) ($\varepsilon \ll L$)

All N-body numerical methods in the following introduce in one way or another way such a smoothing length.

How can we perform numerical simulation of LSS formation

Gravity Solver: Direct Methods

Sum forces by direct particle-to-particle gravitational force:

$$\vec{F}_i = - \sum_{j \neq i} G \frac{m_i m_j (\vec{r}_i - \vec{r}_j)}{\left(|\vec{r}_i - \vec{r}_j|^3 + \varepsilon^2 \right)^{3/2}}$$

A state of the art, publicly available, serial direct N-body integrator is Aarseth's NBODY6 (2012) (time step for each particle, new version on GPU...)

Advantage:

Very Intuitive, First version very simple, Exact forces calculated on each particle

Disadvantage:

Takes N^2 summations to calculate force: Doable for $N \sim 10^6$, impossible for $N \sim 10^9$

Difficult to apply periodic boundary conditions

An amazing exemple rather oriented to study stellar dynamics: A computer which has been specifically developed and designed for computing the gravitational term.

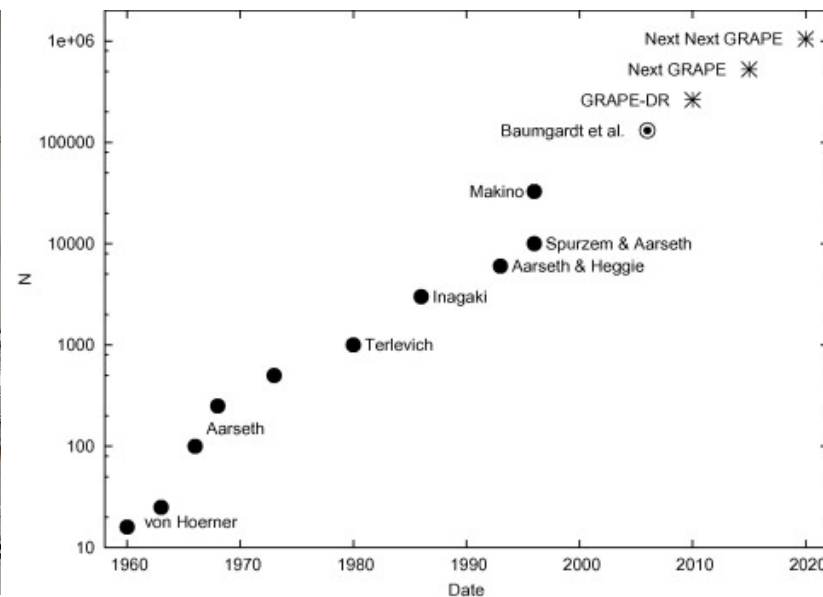
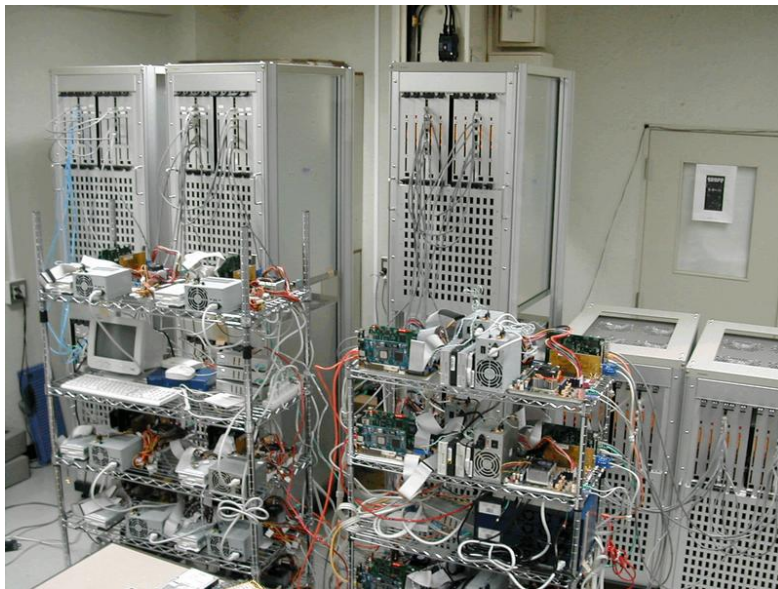
Gravity Pipe (abbreviated **GRAPE**) is a project which uses hardware acceleration to perform gravitational computations (GRAPE, GRAPE-2, GRAPE-4 , GRAPE-6...)

P. Hut, J. Makino

How can we perform numerical simulation of LSS formation

Gravity Solver: Direct Methods

An amazing exemple oriented to study stellar dynamics: A computer which has been specifically developped and designed to computer the gravitational term.
Gravity Pipe (abbreviated GRAPE) is a project which uses hardware acceleration to perform gravitational computations (GRAPE, GRAPE-2, GRAPE-4 , GRAPE-6...) P. Hut, J. Makino....



Number of particles used in N-body simulations up to and beyond core collapse, as a function of year of publication. The dot labeled Makino refers to calculations using the GRAPE-4. The circled dot denotes work in progress, using the GRAPE-6. The stars indicate predicted years of publication for runs using computers that are currently under development or planned to be built.

How can we perform numerical simulation of LSS formation

Gravity Solver: The N^2 - scaling of direct summation puts serious limitations on large N .

Two approximations on the Gravitational Potential:
Multipole Approximation / Harmonic Approximation

Tree Method

It consists to group distant particles together, and use their multipole expansion. The gravitational potential is approximated by **multipole expansion**

Fast Multipole Method

TREEPM Method
(Gadget)

Particle-Mesh Method

It consists to develop gravitational potential on harmonic functions (plane waves, spherical harmonics...)

P3M Method

AP3M Method

AMR Methods
Structured / No-Structured

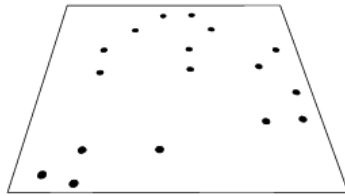
...Other Methods...

How can we perform numerical simulation of LSS formation

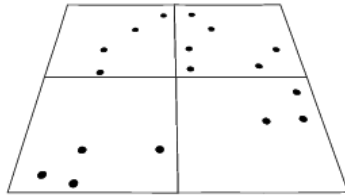
Gravity Solver: Tree Method

Oct-tree in two dimensions

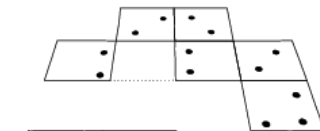
level 0



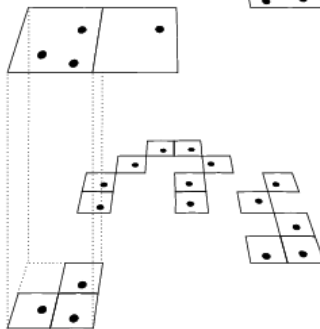
level 1



level 2



level 3

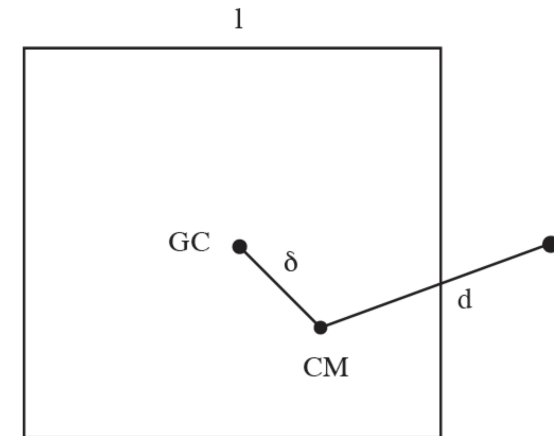


- Original reference: Barnes & Hut 1986, Nature, 324, 446-449
- The simulation volume is usually divided up into cubic cells via an octree (in a three dimensional space), so that only particles from nearby cells need to be treated individually (PP interaction), and particles in distant cells can be treated as a single large particle centered at its center of mass (or as low-order multipole expansion). This reduces strongly the number of particle-particle interactions that must be computed.
- Space divided recursively into a hierarchy of cells. The particles are organized in a tree-like structure based upon a cubical decomposition of the computational domain. Consequently, for each particle we « walk the tree » and add the forces from branchings that need no further unfolding into finer branches according some pre-selected « **opening criteria** »

How can we perform numerical simulation of LSS formation

Gravity Solver: Tree Method

- Original reference: Barnes & Hut 1986, Nature, 324, 446-449
- **The cell-opening criterion** is used to determine whether a cell is sufficiently distant for a force evaluation via multipoles. The simplest criterion is based on an opening angle parameter θ . We consider a cell where GC is the geometric center of the cell and CM the center of mass of the cell. If the size of the cell is l and the distance of the particle from the cell center of mass is d , the algorithm accepts the cell for a force evaluation if $l/d < \vartheta$. Smaller values of ϑ lead to more cell openings and more accurate forces.



How can we perform numerical simulation of LSS formation

Gravity Solver: Tree Method

Use hierarchical multipole expansion to account for distant particle groups

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

We expand

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

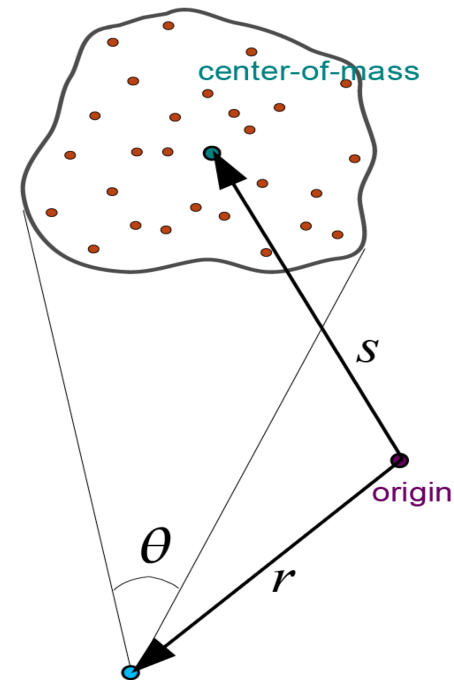
For $|\vec{x}_i - \vec{s}| \ll |\vec{r} - \vec{s}|$

We define $\vec{y} \equiv \vec{r} - \vec{s}$

and obtain

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

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



How can we perform numerical simulation of LSS formation

Gravity Solver: Tree Method

The multipole moments are computed for each node of the tree

Monopole moment:

$$M = \sum_i m_i$$

Quadrupole tensor:

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

Resulting potential/force approximation:

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

For a single force evaluation, not N single-particle forces need to be computed, but only of order $\log(N)$ multipoles: **Nlog(N) operations.**

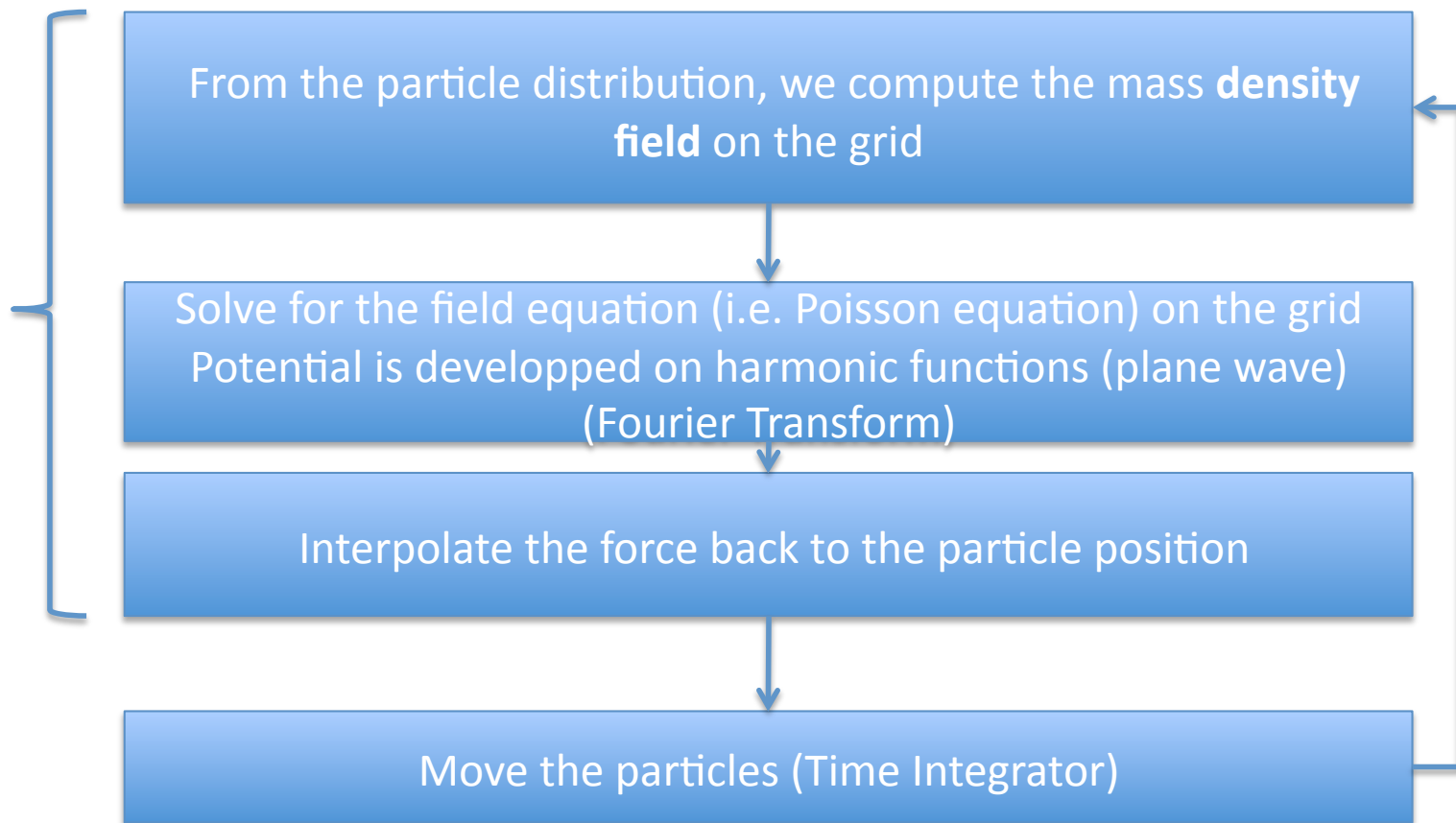
Bouchet & Hernquist 1988 and Hernquist et al; 1991 extended the tree code for the periodical boundary conditions adapted for cosmological simulations.

How can we perform numerical simulation of LSS formation

Gravity Solver: Particle-Mesh Methods

We distinguish a **continuous** space where the **particles** evolve and a **discrete** space (Grid) where is computed the **fields**: density, potential and forces.

4 Main Steps: at each timestep.



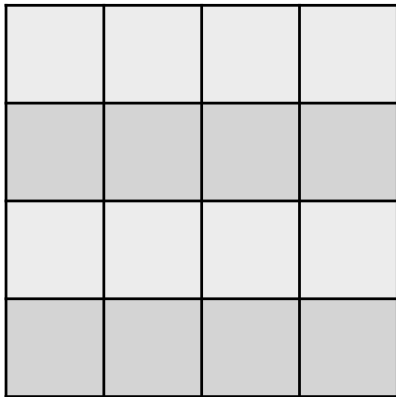
How can we perform numerical simulation of LSS formation

Gravity Solver: Particle-Mesh Methods: Density assignment

From the particle distribution, we compute the mass **density field** on the grid:

We assign to each particle 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

$\{x_p\}$ is the set of discret mesh centres



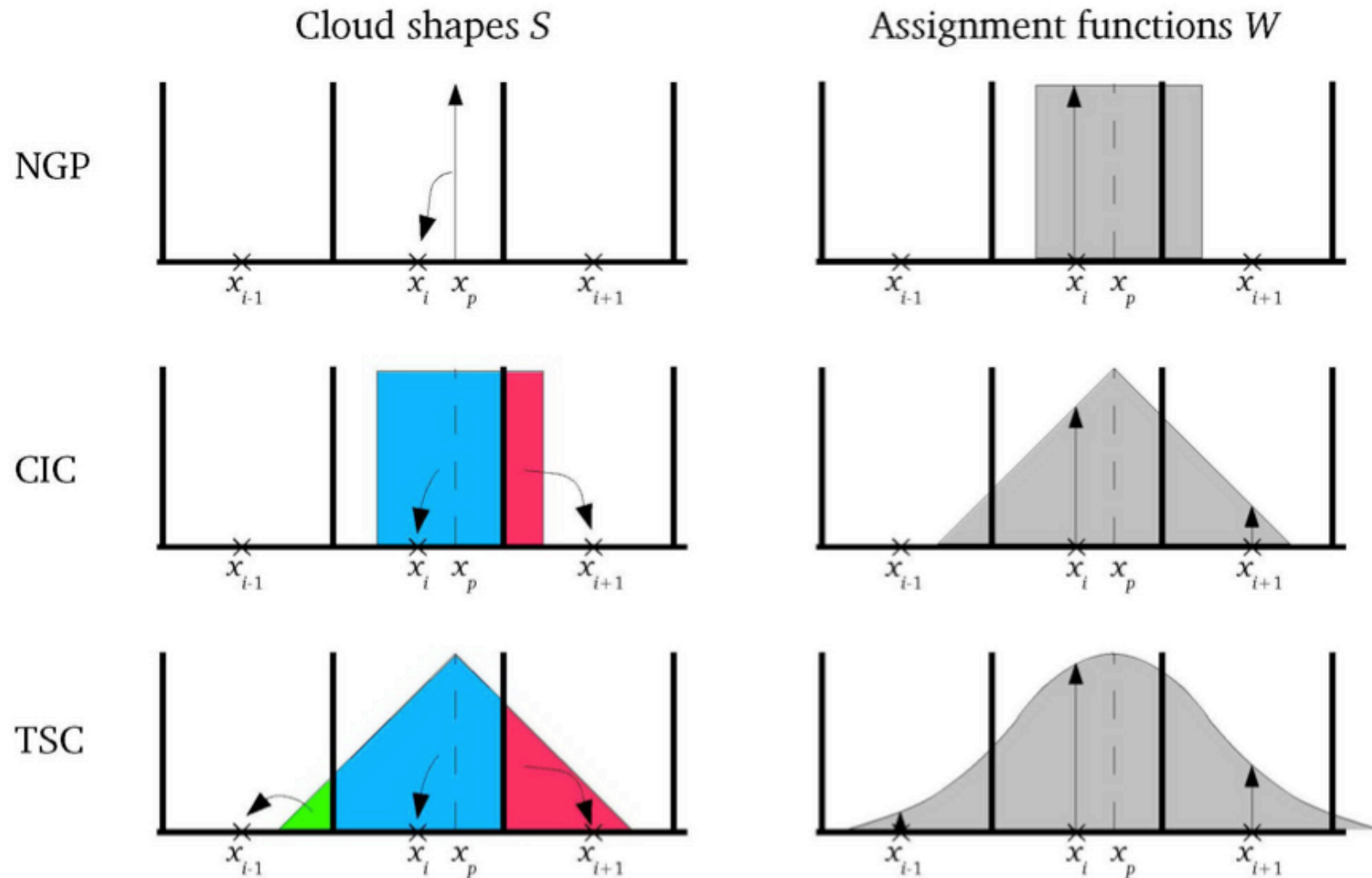
$$W^p(x_p - x_i) = \int_{x_i - \Delta x/2}^{x_i + \Delta x/2} S(x_p - x) dx$$

The total charge in the cell is

$$\rho_i = \frac{1}{\Delta x} \sum_{p=1}^{N_p} m_p W^p(x_p - x_i)$$

How can we perform numerical simulation of LSS formation

Usual particle shape functions and assignment schemes



How can we perform numerical simulation of LSS formation

Usual particle shape functions and assignment schemes

Name	Shape Function $S(x)$	# of cells involved	Properties of force
Nearest grid point (NGP)	$\frac{1}{\Delta x} \delta\left(\frac{x}{\Delta x}\right)$	$1^3=1$	Piecewise constant in cells
Clouds in cells (CIC)	$\frac{1}{\Delta x} \Pi\left(\frac{x}{\Delta x}\right)$	$2^3=8$	Piecewise linear continuous
Triangular shaped clouds (TSC)	$\frac{1}{\Delta x} \Theta\left(\frac{x}{\Delta x}\right)$	$3^3=27$	Continuous for derivative

The choice of interpolation scheme is a tradeoff between accuracy and computational expense: CIC / TSC

How can we perform numerical simulation of LSS formation

Potential is developed on harmonic functions (plane wave)
(Fourier Transform)

$$\frac{\partial^2 \phi}{\partial x^2} \propto \rho \quad -k^2 \tilde{\phi}(k) \propto \tilde{\rho}(k) \quad \text{Green Function : } G(k) = -\frac{1}{k^2}$$

$$-\frac{\partial \phi}{\partial x} = F \quad -ik \tilde{\phi}(k) = \tilde{F}(k) \quad \tilde{D}(k) = -ik$$

The inverse Laplacian operator ($-1/k^2$) is replaced by a finite difference approximation,
(other multiplicative factor in Fourier space, optionally including an anti-aliasing filter is possible),
(Hockney & Eastwood 1980)

For the CIC case, the finite difference approximation is identical to tri-linear interpolation.
The same assignment function needs to be used to ensure momentum conservation for
the interpolation force.

$$\rho_i \Delta_x^2 = \phi_{i+1} - 2\phi_i + \phi_{i-1} \quad \tilde{G}(k) = -(\Delta_x^2 / 4) / \sin^2\left(\frac{k\Delta_x}{2}\right)$$

$$F_i \Delta_x = -(\phi_{i+1} - \phi_{i-1}) \quad \tilde{D}(k) = -i \frac{\sin(k\Delta_x)}{\Delta_x}$$

(Instead of FFT, Poisson equation with Dirichlet boundary conditions on a Cartesian grid can be solved
by using multigrid method (Guillet and Teyssier 2011))

How can we perform numerical simulation of LSS formation

Gravity Solver: Particle-Mesh Methods

Advantages of the PM-scheme

This method has been extensively tested (Hockney and Eastwood 1980, Melott 1981, Bouchet et al 1984, Mellot 1997...). These authors presented a detailed theoretical analysis of this method. The evaluation of numerical effects due to the presence of the grid can be accurately performed (resolution $\sim 6\Delta x$, anisotropy (CIC) due to grid $\sim 2\Delta x$)

Method is very fast: $O(N_p) + O(N_g \log N_g)$ operations using FFT
Periodic boundary conditions are trivial
Simple to write and « parallelize »

A possible extension to increase the dynamic range ?

How can we perform numerical simulation of LSS formation

Gravity Solver: P3M: Particle-Particle/Particle-Mesh Methods

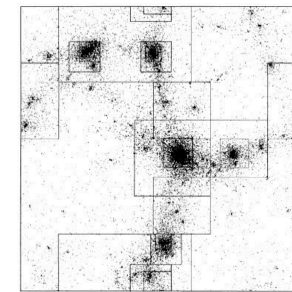
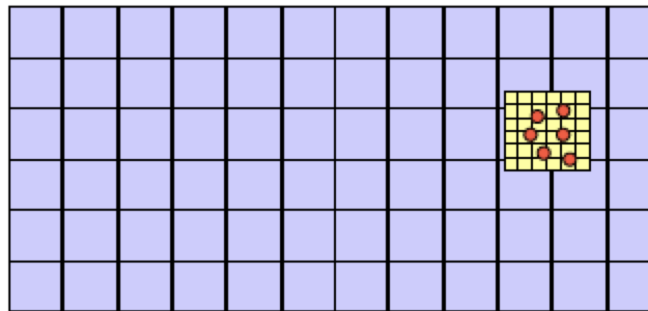
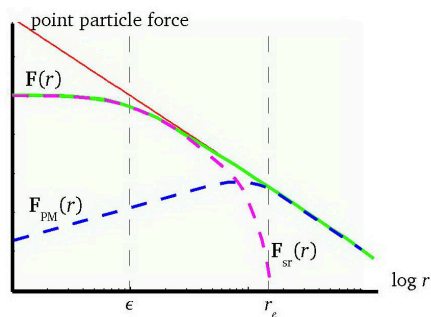
P3M: Particle – Particle / Particle Mesh (Efsthathiou et al. 1985)

- Combines particle-particle and particle-mesh methods
- At large distances, use particle-mesh to calculate gravitational potentials
- Up close, force computed by direct summation (N^2 summation)

Problem:

Melott 1997: PP Part, Two-body scattering in simulations violates the Poisson-Vlasov equations (collisionless hypothesis): $N \gg 1$, for highly clustered configuration, the PP force dominates the CPU time in the P3M scheme

AP3M scheme: (Adaptive P3M) Improves the P3M method by using additional subgrids at regions where clustering occurs (like APM, but with additional particle-particle summation) (**Couchman, H.M.P., “Mesh refined P3M: A fast adaptive N-body algorithm”, 1991**).



How can we perform numerical simulation of LSS formation

Gravity Solver: TreePM Methods

- Combine tree algorithm and particle-mesh algorithm:
- At large distances, use PM to calculate 'smooth' contribution to gravitational potential
- At small distances ($< 2dx$) use tree to calculate local neighbors' contributions
- Fast and efficient, high dynamic range.
- Example code: N-body part of Gadget-2 (Springel 2005, MNRAS, 364, 1105)
- Original method papers: Xu 1995 (ApJS, 98, 355), Bode & Ostriker 2003 (ApJS, 145, 1)

All the previous combined methods (P3M, AP3M, TreePM) are high-resolution N-body solvers based on the Particle In Cell method with a constant (small scale) force softening:

Adaptive force softening ?

How can we perform numerical simulation of LSS formation

Gravity Solver: AMR Methods

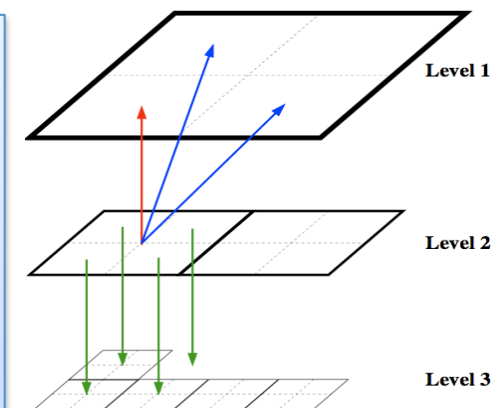
Adaptive Refinement: General remarks

PANDORA code: Villumsen, J.W., “A New Hierarchical PM Code for Very Large Scale Cosmological N-body Simulations”, ApJS, 71, 407, (1989)

ART code: Kravtsov, A.V., Klypin, A.A., Khokhlov, A.M., “ART: a new highresolution N-body code for cosmological simulations”, ApJS, 111, 73, (1997)

RAMSES code: R. Teyssier, Cosmological hydrodynamics with adaptive mesh refinement. a new high resolution code called RAMSES, A&A 385 (2002) 337–364.

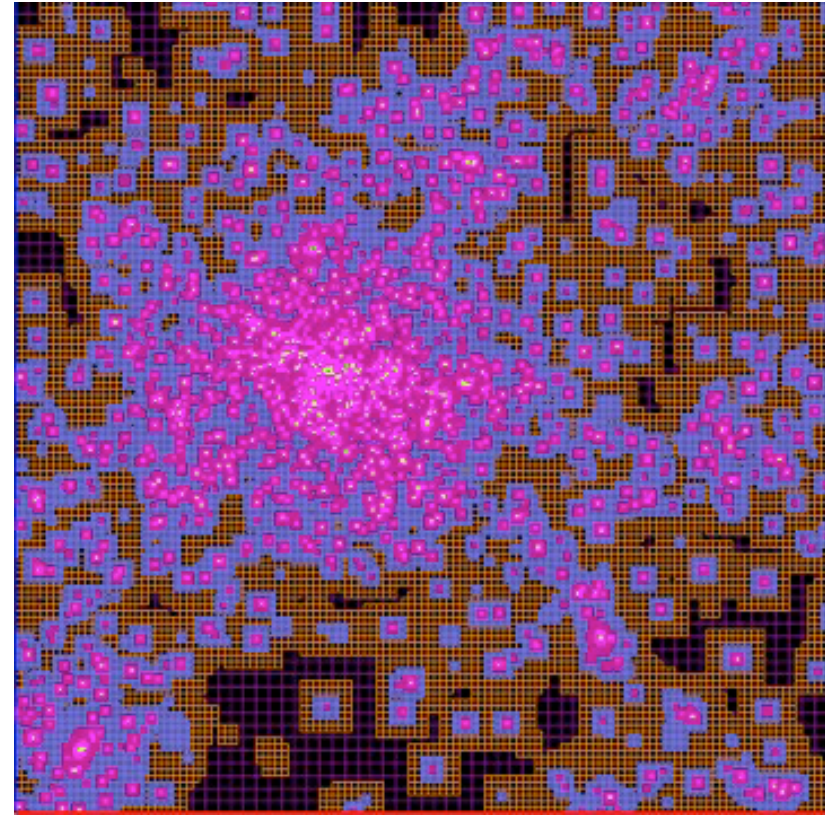
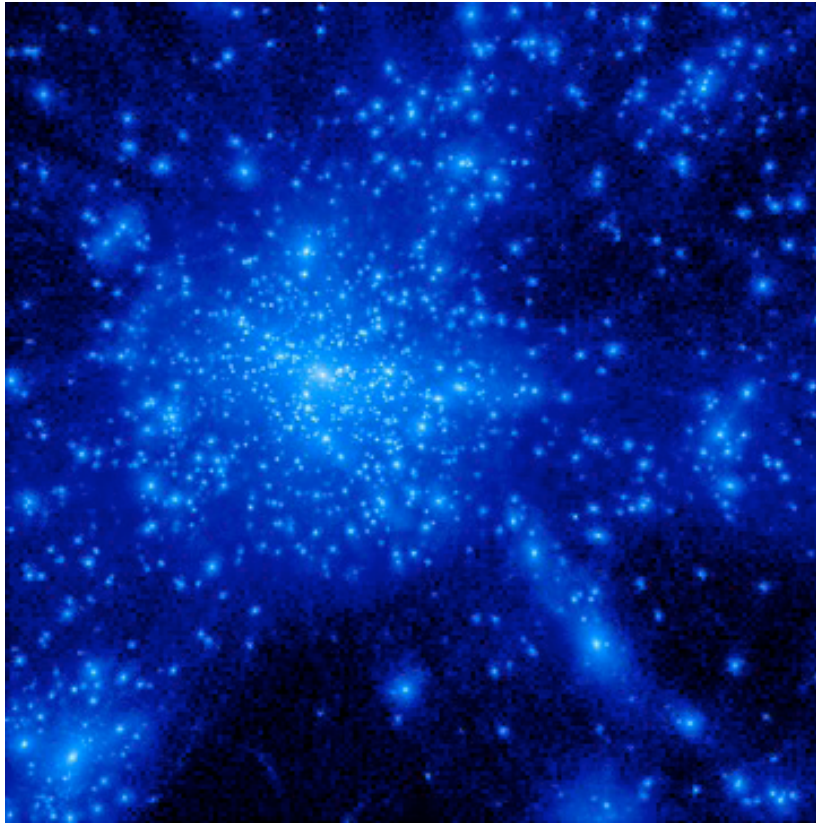
- Mesh is refined where the density exceeds a given threshold. Other quantity can be used as additional condition for refinement.
- Refinement field defines how refinement is done.
- Each cell can be split into 8 new cells, each having twice smaller size. This is ideal for tracing anisotropic structures such as filaments.
- Adjacent cells can differ not more than by one level
- Time-step decreases by factor two with each level



1 parent cell
6 neighboring parent cells
8 children octs

How can we perform numerical simulation of LSS formation

Gravity Solver: AMR Methods



Refinement in Ramses Code

How can we perform numerical simulation of LSS formation

Gravity Solver: AMR Methods

Two Main Points.

1. We have to solve Poisson equation on a domain with boundary conditions.
2. Time stepping has to be adaptive at each grid level

Firstly, the potential **on boundary condition** at level ℓ is deduced from level $\ell - 1$ through a linear reconstruction.

Secondly, using these specific boundary conditions, the potential can be computed using any efficient **relaxation method**. In RAMSES, the Gauss-Seidel (GS) method with **Red-Black Ordering** and **Successive Over Relaxation** (Press et al. 1992) is used. In two dimensions, for unit mesh spacing, the basic GS writes as

$$\phi_{i,j}^{n+1} = \frac{1}{4} \left(\phi_{i+1,j}^n + \phi_{i-1,j}^n + \phi_{i,j+1}^n + \phi_{i,j-1}^n \right) - \frac{1}{4} \rho_{i,j}$$

This iteration is applied first to update the potential for “black” cells defined by i odd and j odd or i even and j even, and then to update the potential for “red” cells defined by i odd and j even or i even and j odd.

How can we perform numerical simulation of LSS formation

Gravity Solver: AMR Methods N-body solver with Dirichlet Boundary conditions

Finally, the result is “over-corrected” using the so-called overrelaxation parameter ω

$$\phi_{i,j}^{n+1} = \omega \phi_{i,j}^n + (1 - \omega) \phi_{i,j}^{n+1} \quad \text{with} \quad 1 < \omega < 2$$

The speed of the algorithm relies on the correct choice for both ω and the initial guess $\phi_{i,j}^0$. For a regular ($N \times N$) cartesian mesh, the optimal over-relaxation parameter is known to be (Press et al. 1992)

$$\omega \approx \frac{2}{\left[1 + \left(\frac{\alpha\pi}{N}\right)\right]}$$

where $\alpha = 1$ for Dirichlet boundary conditions and $\alpha = 2$ for periodic boundary conditions.

« Let us consider a **128³** coarse grid, completely refined in a **256³** underlying fine grid. Solving first the Poisson equation on the coarse level using FFT, the solution is injected to the fine grid as a first guess. In this particular example, the optimal over-relaxation parameter is $\omega \approx 1.9$ (using [...] $\alpha = 2$) and **60** iterations are needed to damped the errors sufficiently ». (Ramses, Teyssier 2002)

« Note that for the ART code, the optimal value was found to be $\omega = 1.25$ (Kravtsov et al. 1997), using however a different approach to set up boundary conditions ».

How can we perform numerical simulation of LSS formation

Time Integration issues

How can we perform numerical simulation of LSS formation

Numerous Method: Time Integrator scheme
How to choose the Time Integrator scheme

Vlasov-Poisson is a Hamiltonian system. Vlasov equation can be written with a Poisson bracket as

$$\frac{\partial f}{\partial t} + \{f, H\} = 0 \quad \{f, H\} \equiv \sum_i \left(\frac{\partial f}{\partial \vec{x}_i} \frac{\partial H}{\partial \vec{p}_i} - \frac{\partial f}{\partial \vec{p}_i} \frac{\partial H}{\partial \vec{x}_i} \right)$$

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

The Hamiltonian structure of the system can be preserved (Energy Conservation) in the integration, if each step is formulated as a canonical transformation. Such integration schemes are called symplectic.

If the integration scheme introduces non-Hamiltonian perturbations, a completely different long-term behavior results.

How can we perform numerical simulation of LSS formation

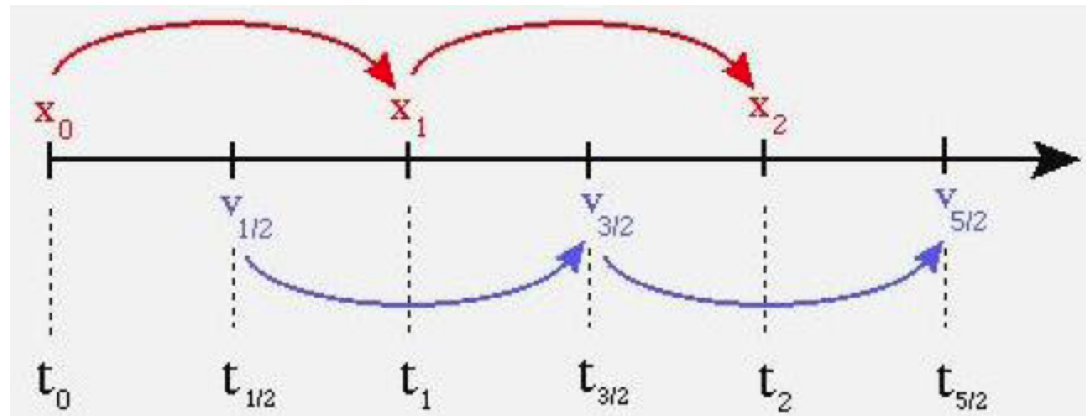
Numerous Method: Time Integrator scheme
How to choose the Time Integrator scheme

The time evolution of the system is a continuous canonical transformation generated by the Hamiltonian. **We need a symplectic integrator.**

The most commonly used time integration scheme for N-body simulations is the leapfrog method. **Leapfrog scheme is a symplectic integrator.**

$$v_{n+\frac{1}{2}} = v_{n-\frac{1}{2}} + a_n dt$$

$$x_{n+1} = x_n + v_{n+\frac{1}{2}} dt$$



Leapfrog integration consists to updating positions and velocities at interleaved time points

How can we perform numerical simulation of LSS formation

Numerous Method: Time Integrator scheme How to choose the Time Integrator scheme

With leap frog integrator, the specific properties of Hamiltonian systems will be preserve. A symplectic integrator conserves phase space volume and has no spurious dissipation. This is especially important in self-gravitating systems where a dissipation time scale that is linked to the dynamical time can lead to a runaway to spuriously large densities.

From empirical point of view, leap-frog scheme has other advantages over other methods.

- Leapfrog is a second order integrator requiring only one costly force evaluation per timestep and only one copy of the physical state of the system. This is particularly beneficial for N-body simulations where the cost of a force evaluation is very expensive and memory usage is often a critical concern.
- The force field in an N-body simulation is not very smooth, so higher order does not necessarily mean higher accuracy
- Leapfrog method is time-reversible. One can integrate forwrd n steps, and reverse the direction of integration and integrate backwards n steps to arrive at the same starting position.

How can we perform numerical simulation of LSS formation

Numerous Method: Time Integrator scheme

What happens if we use a non-symplectic time integrator ?

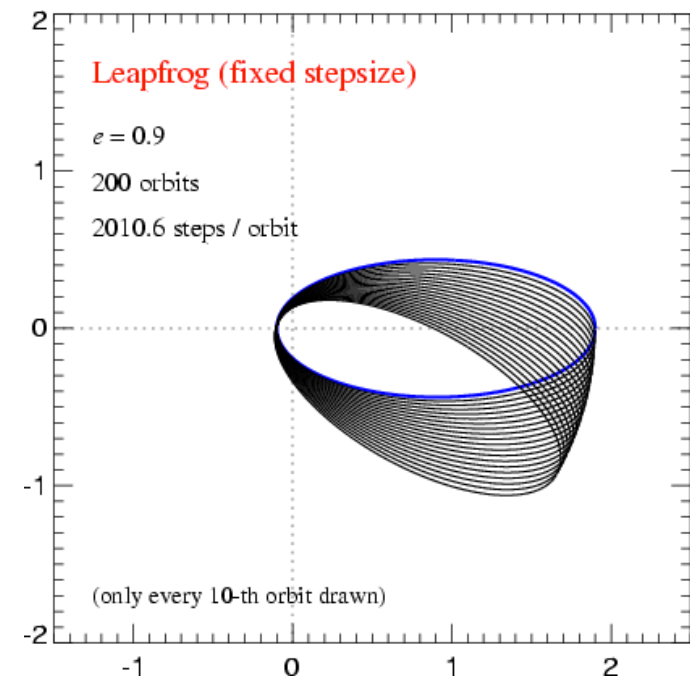
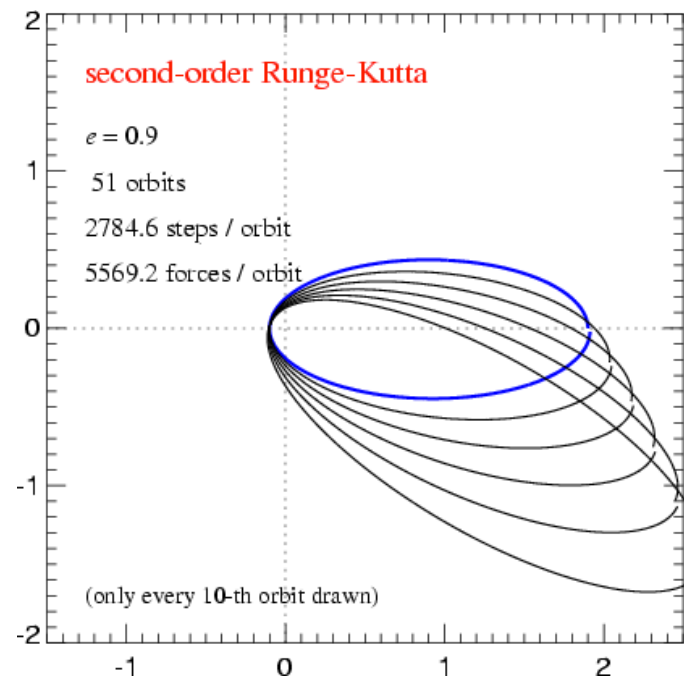
In a simple case. We compare the integration of the Kepler Problem (two bodies interact by a central force that varies in strength as the inverse square of the distance r between them) for different time integrators (symplectic and non-symplectic).

Implicit mid point rule

$$k_1 = f(y_n)$$

$$k_2 = f(y_n + k_1 dt)$$

$$y_{n+1} = y_n + \left(\frac{k_1 + k_2}{2} \right) dt$$



How can we perform numerical simulation of LSS formation

Numerous Method: Time Integrator scheme
What happens if we use a non-symplectic time integrator ?

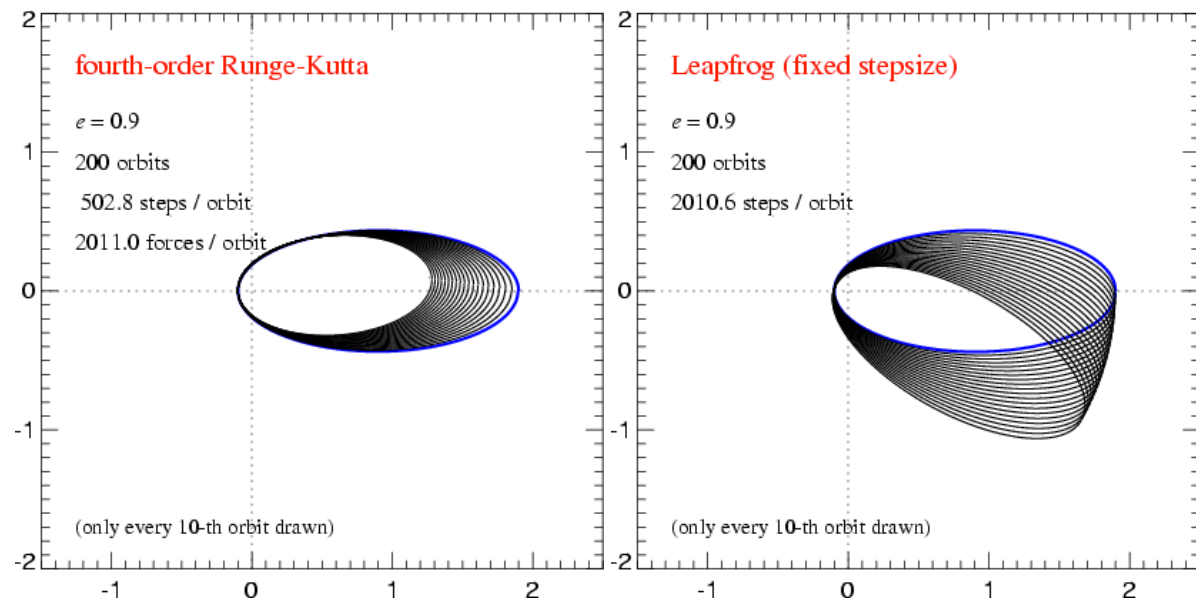
$$k_1 = f(y_n, t_n)$$

$$k_2 = f(y_n + k_1 dt/2, t_n + dt/2)$$

$$k_3 = f(y_n + k_2 dt/2, t_n + dt/2)$$

$$k_4 = f(y_n + k_3 dt/2, t_n + dt)$$

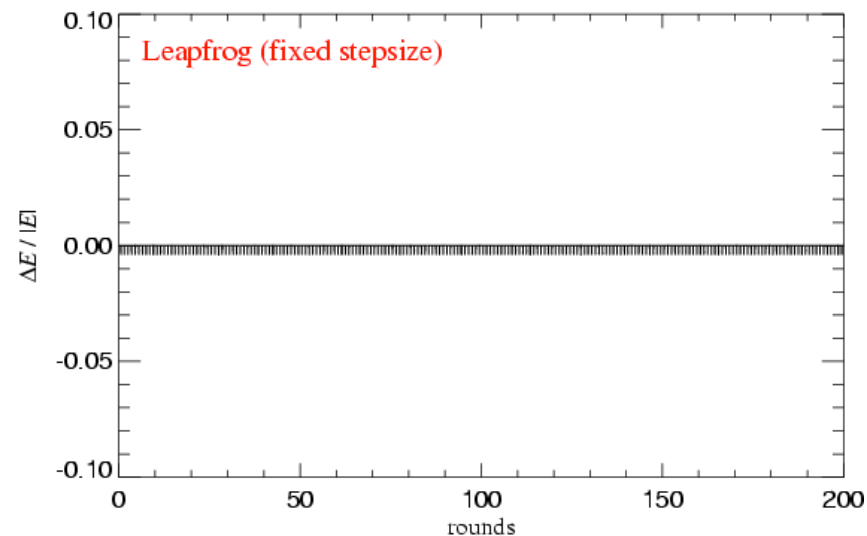
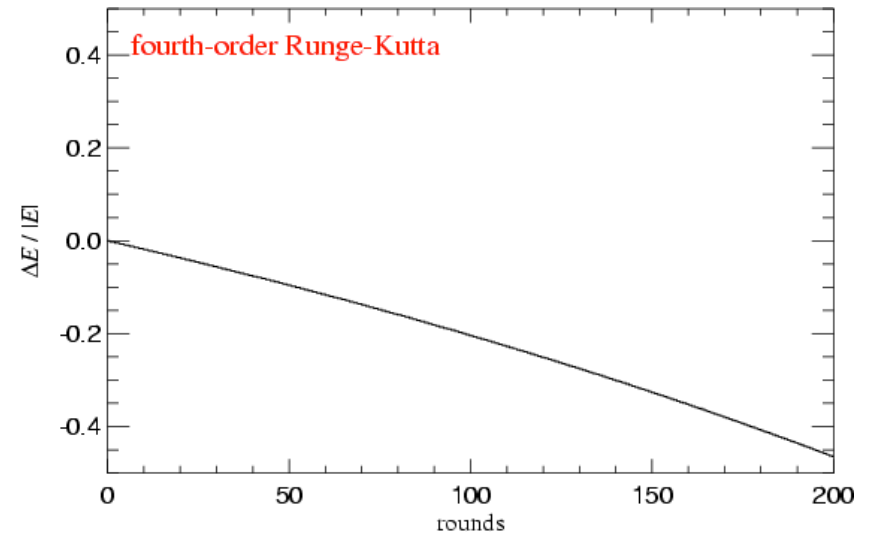
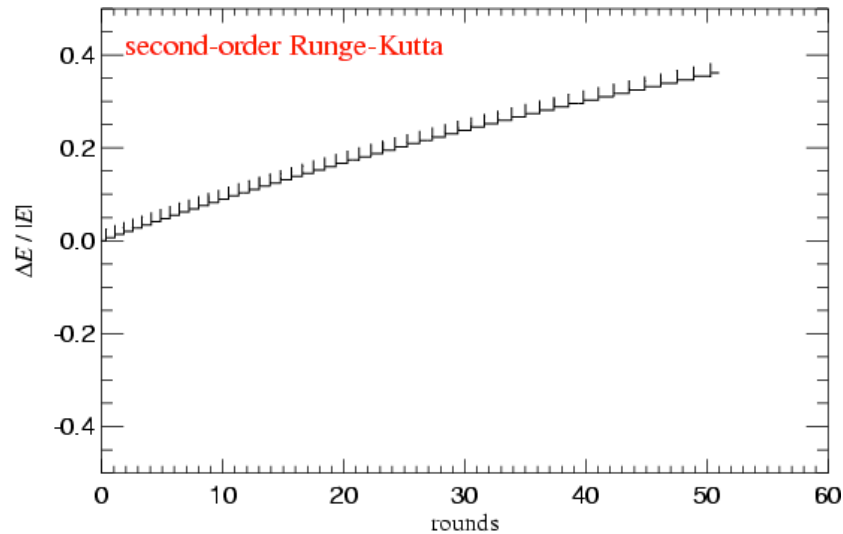
$$y_{n+1} = y_n + \left(\frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} \right) dt$$



How can we perform numerical simulation of LSS formation

Numerous Method: Time Integrator scheme

What happens if we use a non-symplectic time integrator ? Energy Conservation ?



How can we perform numerical simulation of LSS formation

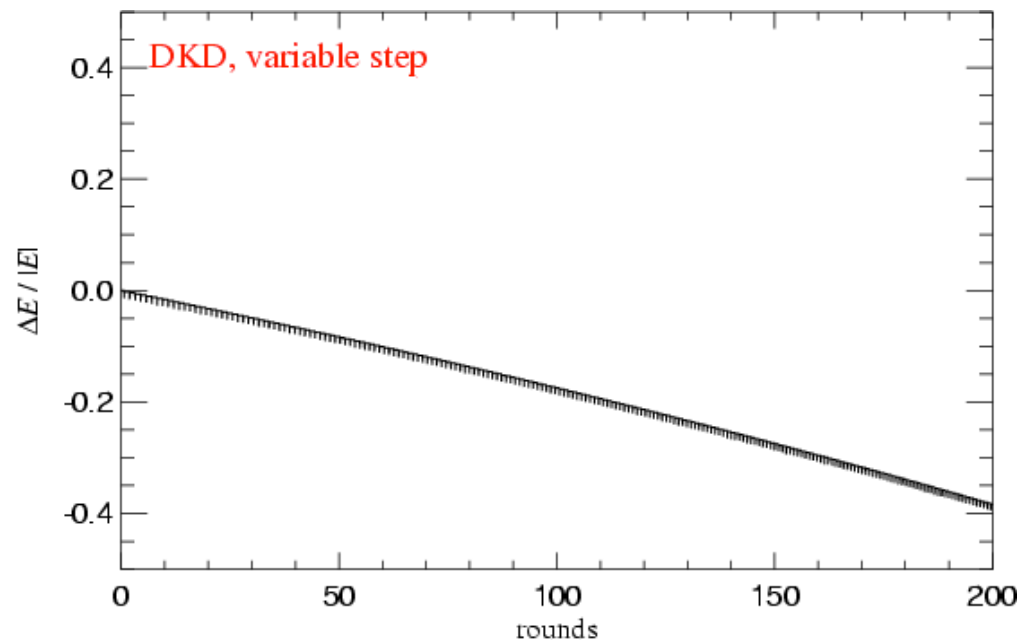
Numerous Method: Time Integrator scheme
What happens if we need adaptive timestep ?

“Drift-Kick-Drift” version

$$x_{n+\frac{1}{2}} = x_n + v_n \frac{dt}{2}$$

$$v_{n+1} = v_n + f(x_{n+\frac{1}{2}})dt$$

$$x_{n+1} = x_{n+\frac{1}{2}} + v_{n+1} \frac{dt}{2}$$



The time-step scheme is no more symplectic, the conservation of energy is lost

How can we perform numerical simulation of LSS formation

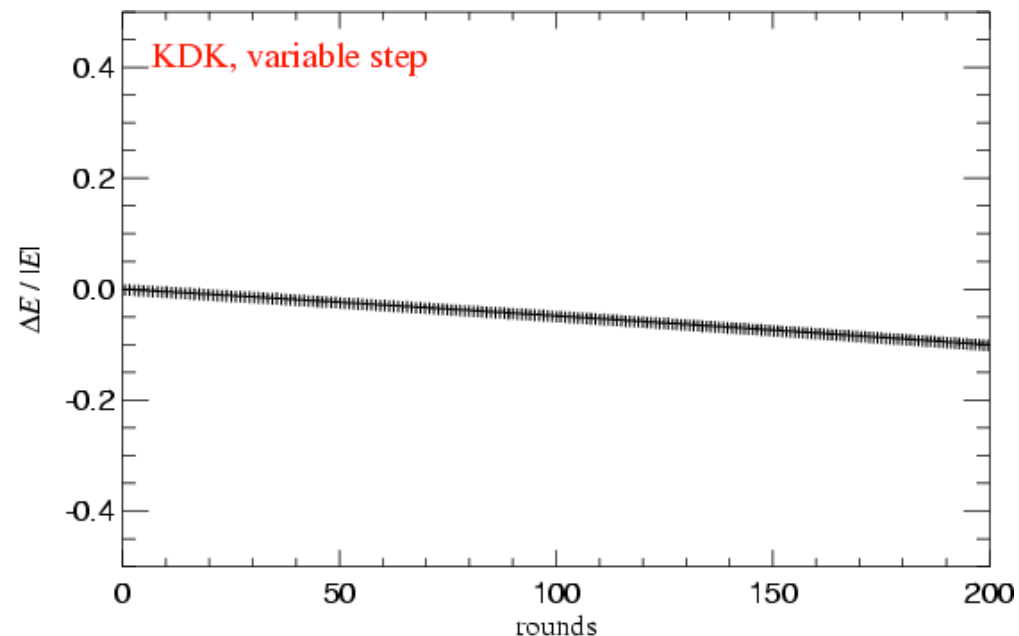
Numerous Method: Time Integrator scheme
What happens if we need adaptive timestep ?

“Kick-Drift-Kick” version

$$v_{n+\frac{1}{2}} = v_n + f(x_n) \frac{dt}{2}$$

$$x_{n+1} = x_n + v_{n+\frac{1}{2}} dt$$

$$v_{n+1} = v_{n+\frac{1}{2}} + f(x_{n+1}) \frac{dt}{2}$$



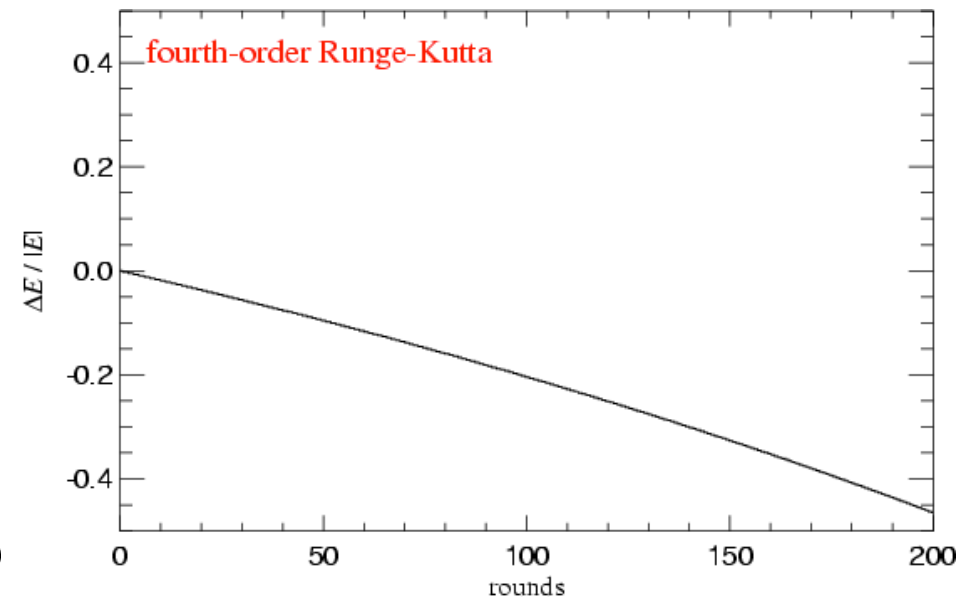
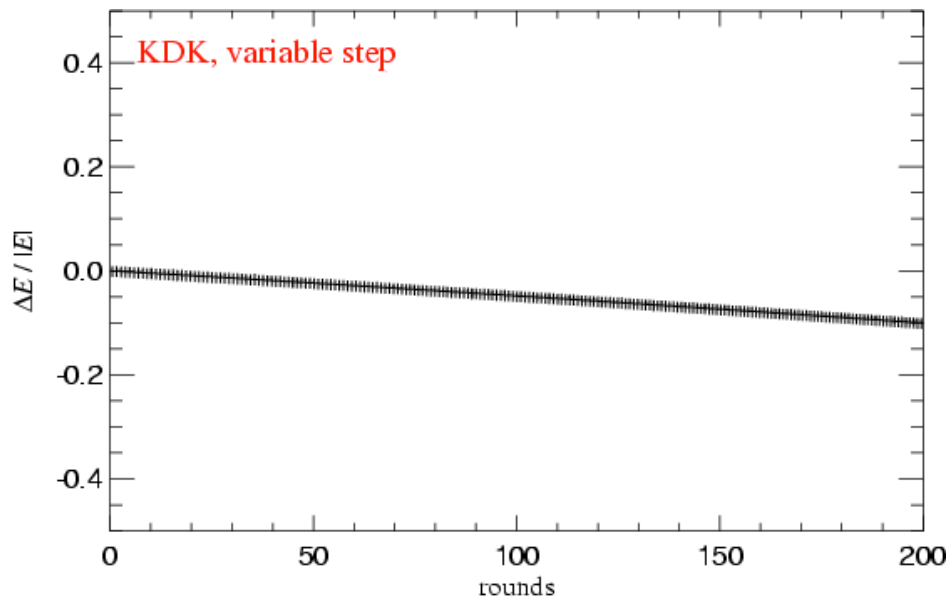
Going to KDK reduces the error by a factor 4, at the same cost !

See THE ASTRONOMICAL JOURNAL, 118:2532-2541, 1999 November, Preto & Tremaine

How can we perform numerical simulation of LSS formation

Numerous Method: Time Integrator scheme

KDK stays better than 4th order Runge-Kutta



How can we perform numerical simulation of LSS formation

Numerous Method: KDM is a quasi « leap frog » adaptive time step scheme

It reduces exactly to the second order leapfrog scheme for constant time steps

$$v_{n+\frac{1}{2}} = v_n - \nabla \phi_n \frac{dt_n}{2}$$

$$x_{n+1} = x_n + v_{n+\frac{1}{2}} dt_n$$

$$v_{n+1} = v_{n+\frac{1}{2}} - \nabla \phi_{n+1} \frac{dt_n}{2}$$

positions and velocities are updated first by a predictor step

That plays the role of a corrector step

It is implemented in AMR Codes (Ramses, ART)

How can we perform numerical simulation of LSS formation

Generation of Initial Conditions

How can we perform numerical simulation of LSS formation

Generation of Initial Conditions

We need to answer four questions.

What is the shape of the initial fluctuations ? This question is related to the physics of the primordial universe and the cosmic microwave background physics.

How is the amplitude of the initial fluctuations fixed in a cosmological simulation ? We could answer to this question by using linear theory and observations.

How does one generate the initial background of particles in a cosmological simulation ?

How does one generate the initial positions and velocities of particles in a cosmological simulation in agreement with the cosmological initial conditions fixed by Observations or Theory ?

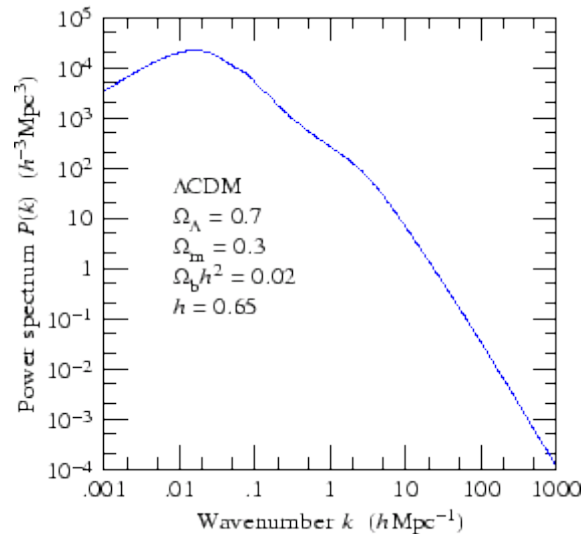
How can we perform numerical simulation of LSS formation

Generation of Initial Conditions

What is the shape of the initial fluctuations ?

The formation of cosmic structures is seen as a stochastic process. The most often this process is supposed Gaussian. As long as the fluctuations are linear, the power spectrum is only necessary to generate a possible realization of such a process (The extension to non-Gaussian case is possible).

The accurate computation of the power spectrum is obtained by taking into account the physics of the early universe and the linear growth of perturbations during the era dominated by the radiation (CAMB or CMBFAST). The cosmological parameters determines the shape of the power spectrum.



$$P(k, z) = A(z) k^n T^2(k, z)$$

- $A(z)$ amplitude is determined observationally
- k^n is the primordial power spectrum (early universe, inflation)
- $T(k, z)$ is the transfert function: contents of the Universe and physics of the CMB

How can we perform numerical simulation of LSS formation

Generation of Initial Conditions

What is the amplitude of the initial fluctuations ?

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

The filtered density field:

$$\sigma^2(R, z) = D_+^2(z) \int_0^\infty \frac{dk}{2\pi^2} k^2 P(k) \left[\frac{3j_1(kR)}{kR} \right]^2$$

Observational input:

$$\sigma_8 = 0.66 - 0.9 \quad R = 8h^{-1} \text{Mpc}$$

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

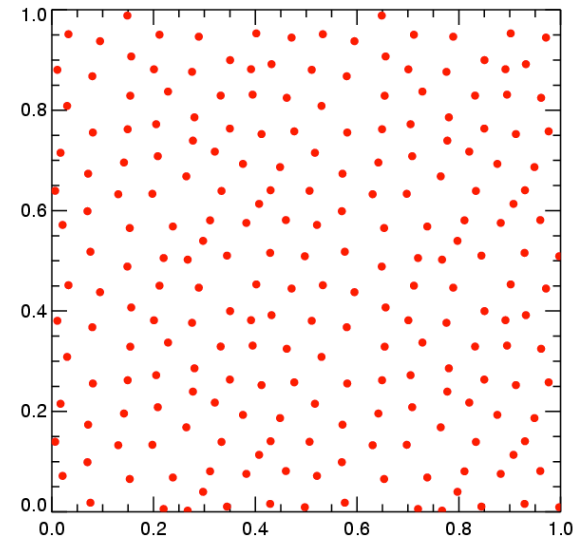
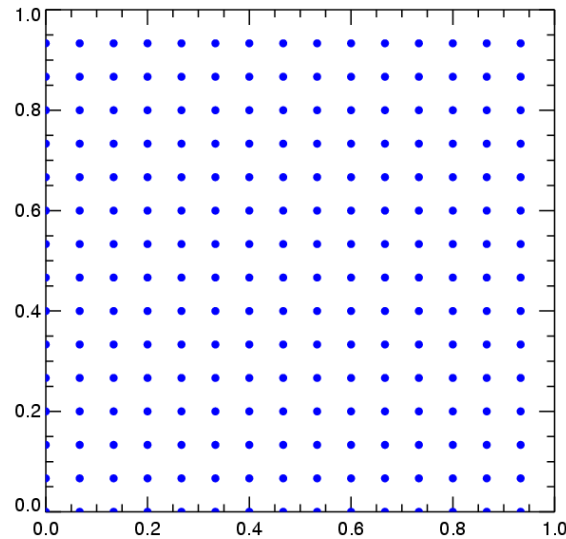
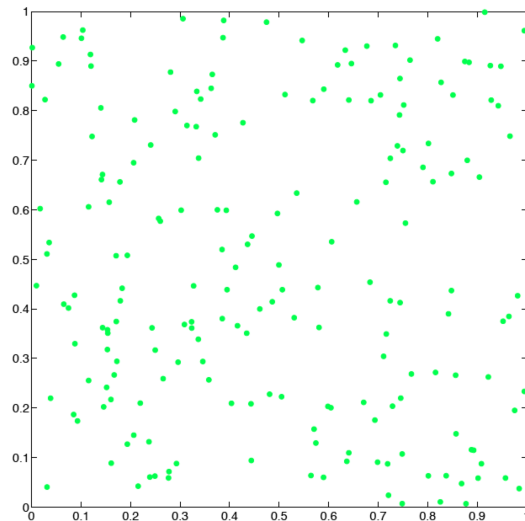
Fluctuation spectrum of initial conditions is fully specified.

How can we perform numerical simulation of LSS formation

Generation of Initial Conditions The Initial background

To create one « realization » of the perturbation spectrum, we need a model for an unperturbed density field (homogeneous)

POISSON / QUIET START / GLASS



Introduce some statistical noise: white noise, k-linear noise on cell scale

How can we perform numerical simulation of LSS formation

Generation of Initial Conditions Power spectrum: a perturbed background

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

Zeldovich approximation (Zeldovich 1970)

- A first-order (linear) Lagrangian collapse model. It can be expressed by one equation:

$$\vec{x}(\vec{q}, t) = \vec{q} + D_+(t) \vec{p}(\vec{q})$$

$$\vec{v}(\vec{q}, t) = \dot{\vec{x}}(\vec{q}, t) = \dot{D}_+(t) \vec{p}(\vec{q})$$

Where $\mathbf{q}$ is the initial position of a particle in N-body simulations and $\mathbf{x}(\mathbf{q}, t)$ is its position at time t . $D_+(t)$ is the linear growth function, $\mathbf{p}(\mathbf{q})$ is a *time-independent displacement vector*.

In the linear regime, the Zeldovich approximation reduces to

$$\delta(t) \approx D_+(t) \vec{\nabla} \cdot \vec{p}(\vec{q}) \Rightarrow \vec{\nabla} \cdot \vec{v} = -\dot{\delta}(t)$$

The Zeldovich approximation works well up to $\delta \sim 1$, where Eulerian linear perturbation theory breaks down.

How can we perform numerical simulation of LSS formation

Generation of Initial Conditions Power spectrum: a perturbed background

We generate the Fourier transform of the overdensity fields

$$\delta_{\vec{k}} = |\delta_{\vec{k}}| \exp(i\theta_{\vec{k}}) \quad \delta_{\vec{k}} = D_+(z) \sqrt{-2P(k, z=0) \ln x}$$
$$\theta_{\vec{k}} = 2\pi y$$

Where x and y are random numbers uniformly distributed in [0,1]

Inverse Fourier transform to get the real space density fluctuation

$$\delta_n = \delta(\vec{x}_n)$$

To get the velocity field and consequently the displacement field, and then positions and velocities for the particles, we use the linear approximation for the (no-rotational) velocity field

$$\vec{v}_{\vec{k}} = \frac{i\vec{k}}{k^2} \frac{\dot{D}_+}{D_+} \delta_{\vec{k}} \quad FFT^{-1} \text{ to get } \vec{v}_n = \vec{v}(\vec{x}_n)$$

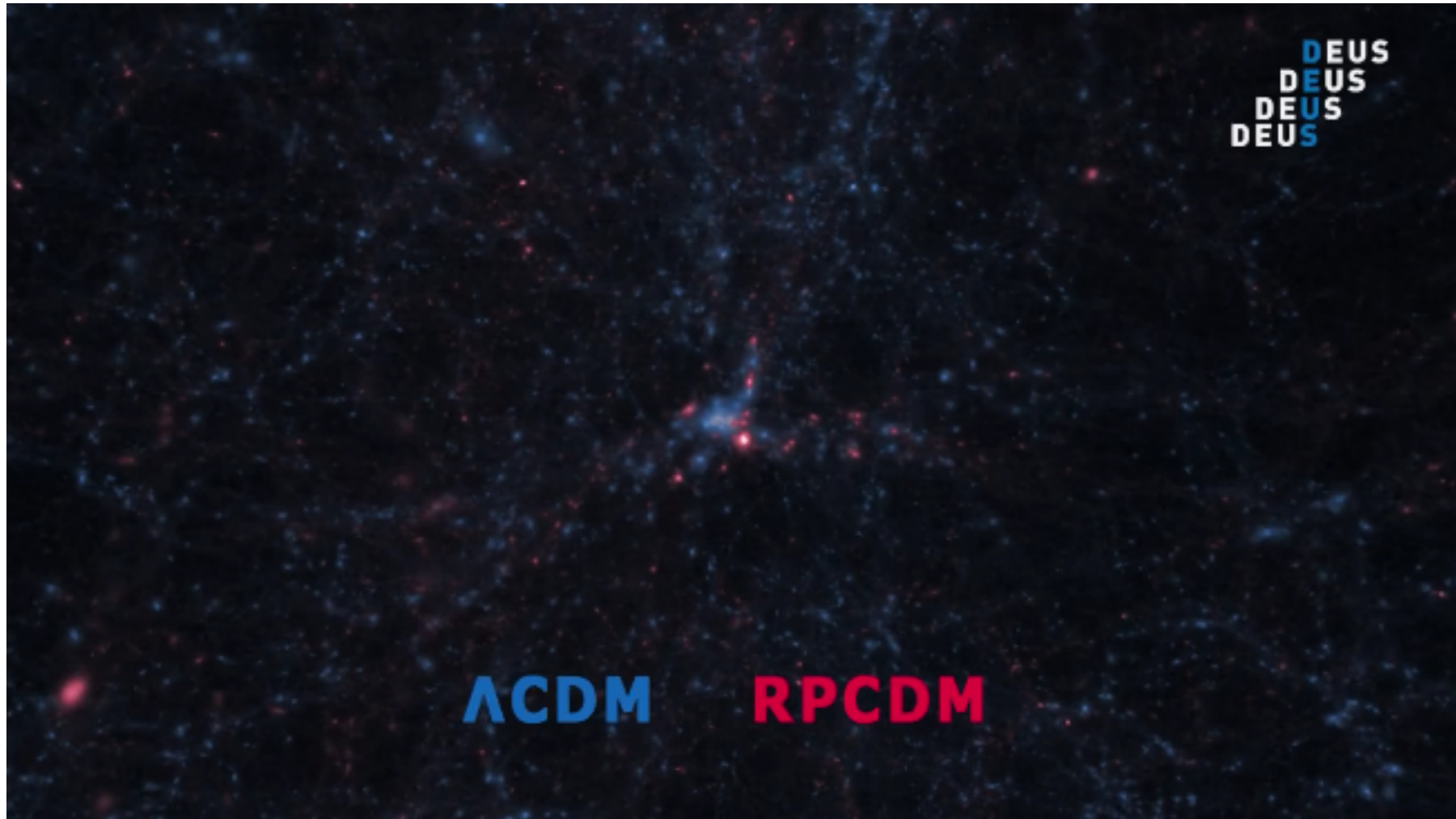
Note: the Zel'dovich approximation has incorrect second- and higher-order growth rates: it's worth considering higher-order approximation methods if you are doing something particularly sensitive to this (Crocce et al. 2006, MNRAS, 373, 369).

How can we perform numerical simulation of LSS formation

Examples for Numerical simulations of Dark Universe

How can we perform numerical simulation of LSS formation

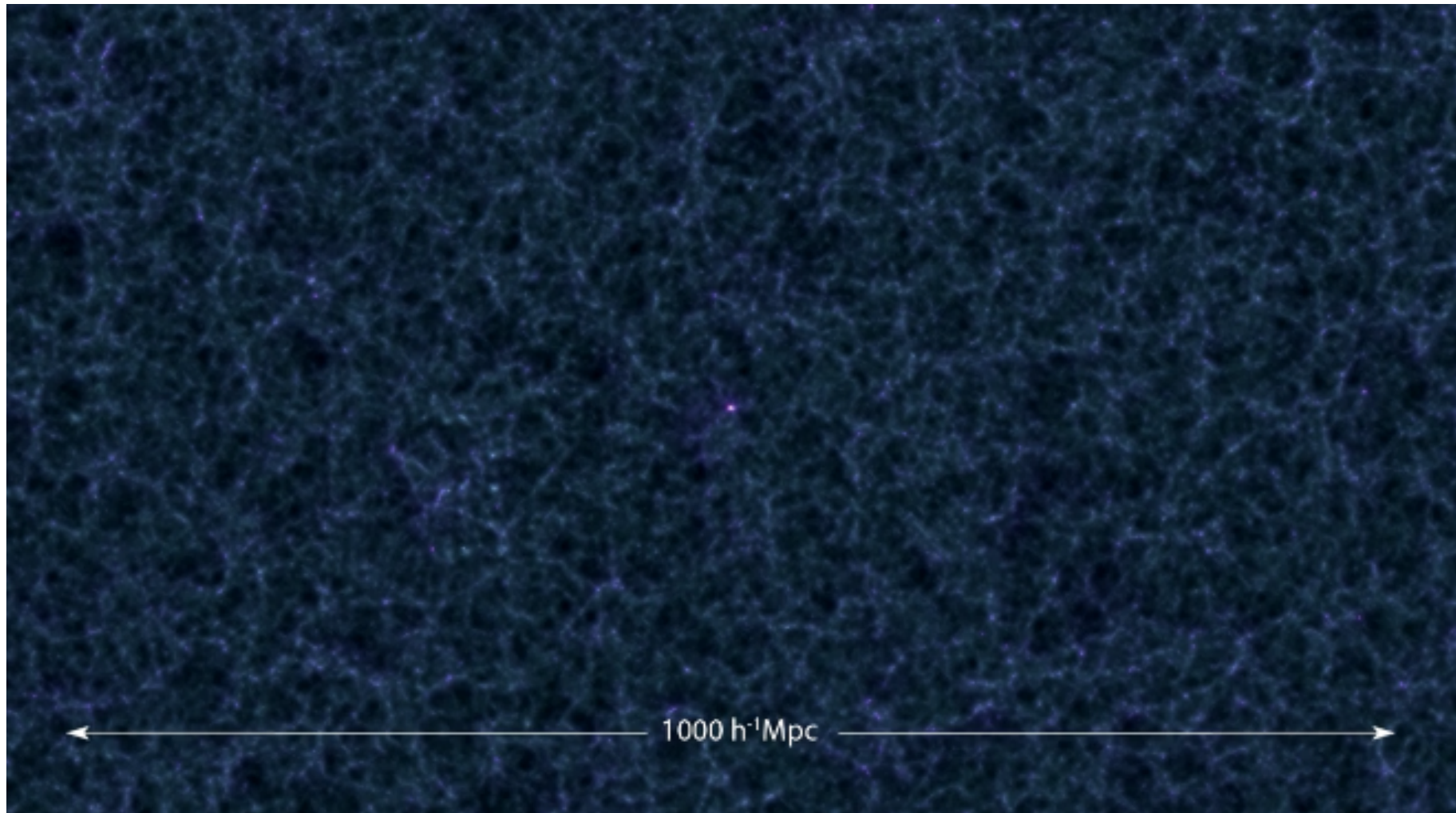
Numerical Simulation of the Dark Universe: A first illustration.



Dark Energy Universe Simulation: Λ CDM vs RPCDM

How can we perform numerical simulation of LSS formation

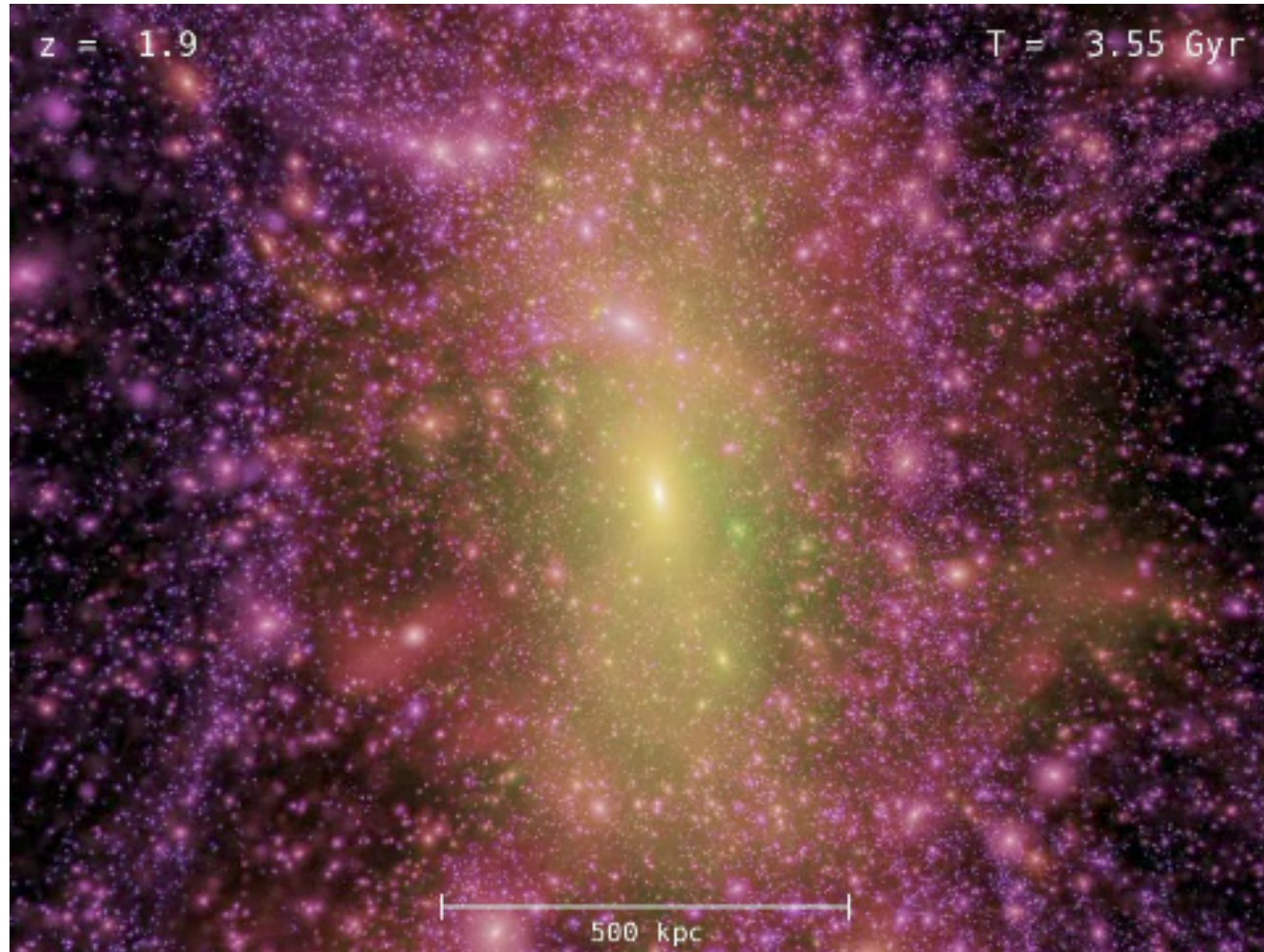
Numerical Simulation of the Dark Universe: A first illustration.



DEUS Full Universe Run: Λ CDM WMAP7 (Zoom on the biggest Halo in the Simulation)

How can we perform numerical simulation of LSS formation

Numerical Simulation of the Dark Universe: A first illustration.



Aquarius Project: Inside an Halo(<http://www.mpa-garching.mpg.de/aquarius/>)

**Numerical simulations of Dark Universe:
Other Aspects
Analysis Techniques – Numerical Limitations**

How can we perform numerical simulation of LSS formation

Cosmological Simulations: Analysis Techniques

- Cosmics structures formation models are stochastic: The initial conditions are random (with well-specified statistical properties), and their evolution is chaotic.
- No realistic model would claim to predict the exact structures we see in our Universe; at best, theorists can hope to construct models of the Universe that look like the « real world ». But how is this vague test quantified? Many statistics have been devised for this purpose.
- These imply also heavy numerical developments.

Ed. Bertschinger, Annu. Rev. Astron. Astrophys. 1998. 36:599–654

Today, the list is longer still....

Table 1 Statistical measures applied to galaxies and numerical simulations of structure formation

Category	Statistic	Name	Reference
Particle positions	$\xi(r)$	Two-point correlation function	Peebles 1980
	$P(k)$	Power spectrum	Bertschinger 1992
	$\xi(r_1, r_2, r_3)$	Three-point correlation function	Groth & Peebles 1977
	$B(k_1, k_2, k_3)$	Bispectrum	Peebles 1980
	ξ_N, ξ_N	N -point correlation functions and moments	Peebles 1980
	$P_0(V), P_N(V)$	Void probability function, cell counts	White 1979
	—	Percolation, minimal spanning tree statistics	Coles 1992
	—	Multifractal statistics	Martínez et al 1990
Density fields	$G(v)$	Genus of isodensity surfaces	Melott 1990
	—	Area of isodensity surfaces	Ryden 1988
	$v_i(v)$	Minkowski functionals	Mecke et al 1994
	$f(\delta)$	One-point density distribution	Kofman et al 1994
	$\langle \delta_c^N \rangle$	One-point cumulants (skewness, kurtosis, etc)	Peebles 1980
	—	Shape statistics	Davé et al 1997b
Velocity fields	$f(v)$	One-point velocity distribution (and moments)	Inagaki et al 1992
	$\mathcal{M}$	Mach number	Ostriker & Suto 1990
	$f(\theta)$	Velocity divergence distribution (and moments)	Bernardeau et al 1985
	$f(v_{12}), \sigma_{12}$	Pairwise radial velocity distribution and dispersion	Davis & Peebles 1983
Redshift space	$\xi(r_p, \pi), \xi(s)$	Redshift space correlation functions	Davis & Peebles 1983
	$P_s(k, \mu)$	Redshift space power spectrum	Cole et al 1995
Clusters or halos	$n(m)$	Mass distribution	Press & Schechter 1974
	$n(V_c)$	Circular velocity distribution	Gelb & Bertschinger 1994a
	$n(\sigma)$	Velocity dispersion distribution	Evrard 1989
	$n(T), n(L)$	Temperature and X-ray luminosity distributions	Cen & Ostriker 1994a

How can we perform numerical simulation of LSS formation

Numerical Limitations and Robustness of the Results ? Personal point of View.

In purely gravitational N-body simulations of structure formation, the numerical issues include dynamic range, force accuracy, and time integration accuracy.

Four distinct kinds of dynamic range are needed for a faithful simulation: time integration accuracy, mass resolution (number of particles), initial power spectrum sampling (range of wavenumbers present in the initial conditions), and spatial resolution (force-softening length compared with box size).

Each aspects can be tested separately, numerous tests exists which combine these effects for some simple cases, simple geometry...

But there is no complete theory of numerical effects in a cosmological context.

A good method for evaluating the accuracy of any numerical results, consist to check for a specific observable (correlation function, power spectrum...) the numerical convergence when one considers different mass resolution, spatial resolution...

For example, what does it happens when the spatial resolution is modified ? Does it exist a numerical convergence ? Can we say that for a given accuracy on a specific observable if the number of computing points needed has well been reached ? Ditto for mass resolution, time-step resolution, random phases selection... for any observable quantities.

How can we perform numerical simulation of LSS formation

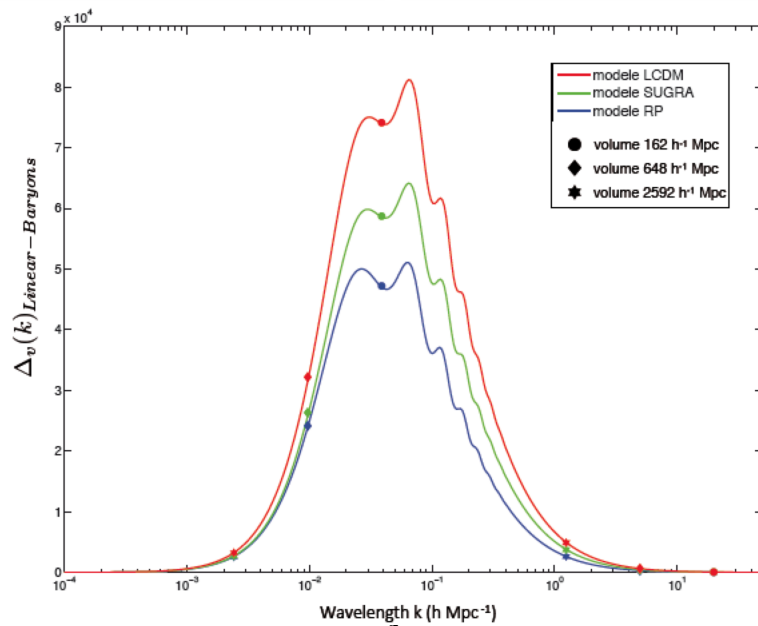
Numerical Limitations and Robustness of the Results ? Bulk Flow

According the observable quantity the numerical effects can be very different

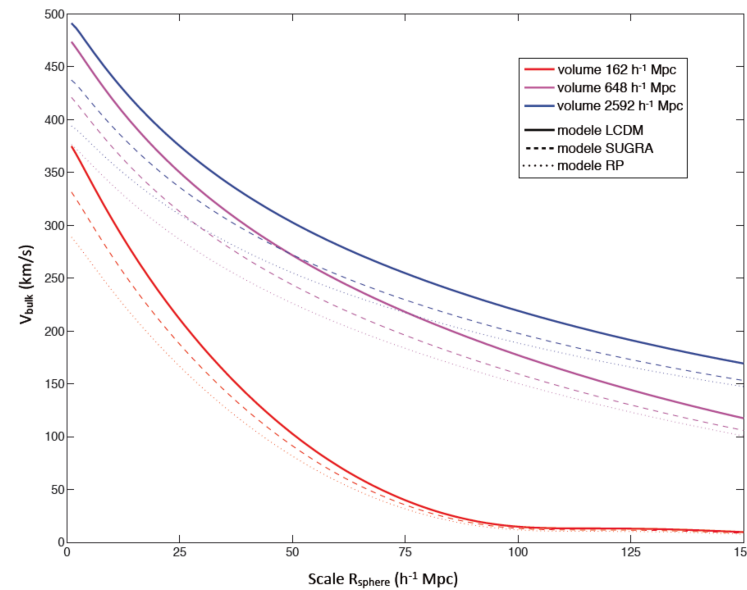
While estimating the density fluctuations on linear scales depend weakly on the box size, at the opposite, the numerical estimate of the bulk flow is strongly dependent on the box size

$$\vec{v}_{bulk}(R) = \frac{1}{N_{part, r < R}} \sum_i^{N_{part, r < R}} \vec{v}_i$$

$$|\vec{v}_{bulk}(R, z)| = \sqrt{\frac{1}{2\pi^2} \int_0^\infty k^3 P_v(k, z) W(kR)^2 d \ln k} = \sqrt{\frac{1}{2\pi^2} \int_0^\infty k^3 \frac{f(z)^2}{k^2} P_\delta(k, z=0) W(kR)^2 d \ln k}$$



$$\Delta_v^2(k) = \frac{1}{2\pi^2} k^3 P_v(k)$$

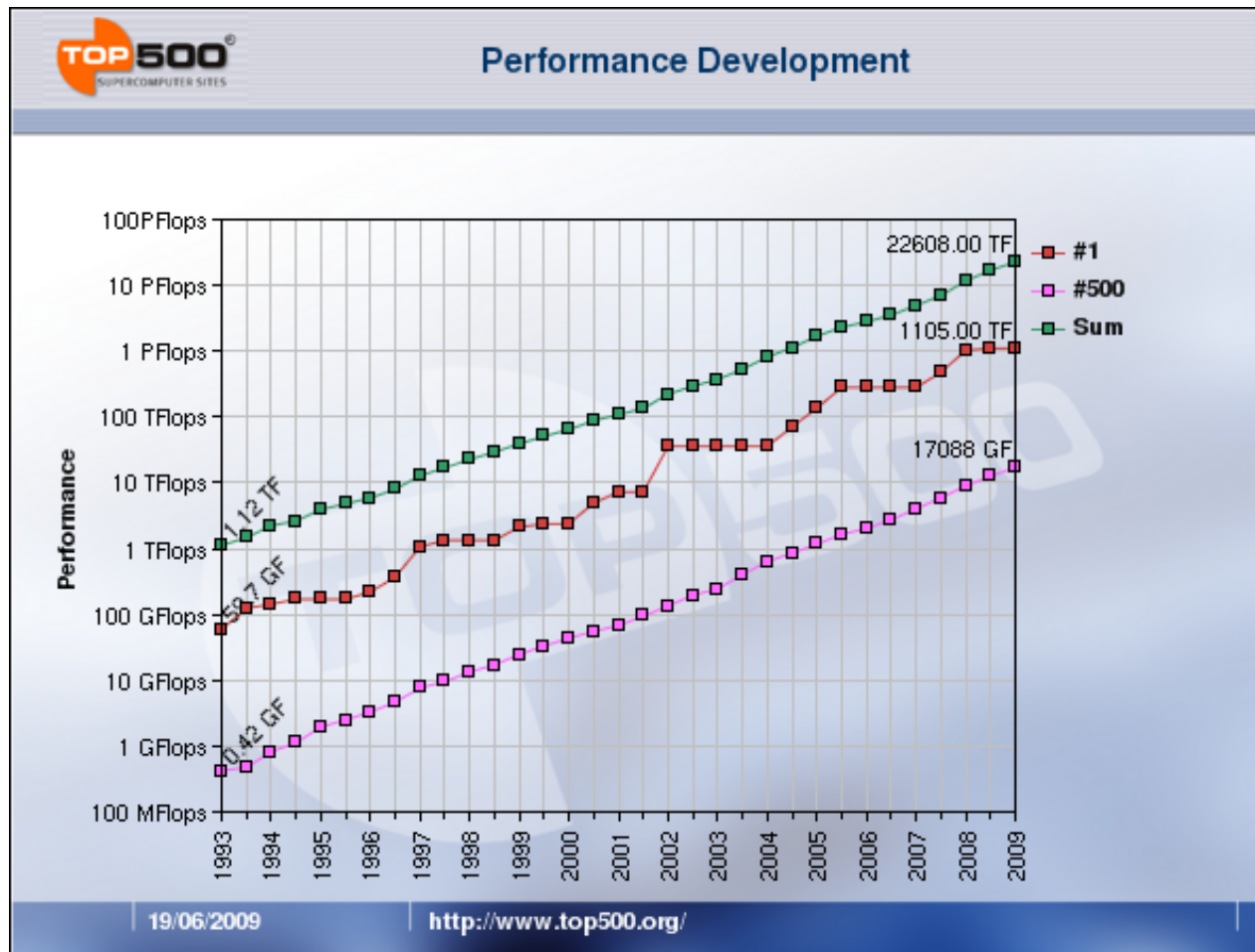


Numerical simulations and Supercomputers Parallelization – Architecture

How can we perform numerical simulation of LSS formation

To higher mass and spatial resolutions

The number of particles and the size of simulation volume are dictated by the available computational resources and methods of parallelization



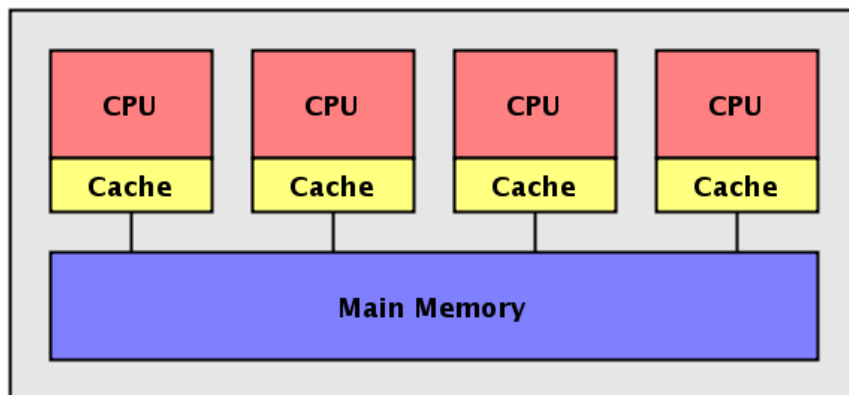
The most powerful computer are now parallel supercomputer. A parallel supercomputer is multiple-processor computer system with large memory capacity

How can we perform numerical simulation of LSS formation

Two Methods of parallelization according to the architecture of the supercomputer

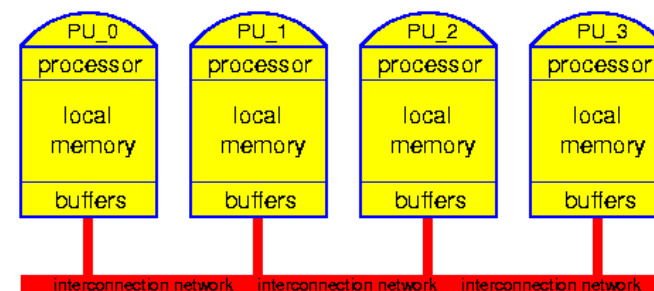
Parallel programming involves two major difficulties in addition to the task of solving the numerical problem in a serial code. First, there is the difficulty of how to divide the work and data evenly among the processors, and second, an efficient communication scheme between the processors needs to be devised.

OpenMP needs computer with shared memory. This memory refers to a large block of random access memory (RAM) that can be accessed by several different central processing units (CPUs) in a multiple-processor computer system.



MPI works on distributed memory (**in general much more memory available**) system. Distributed memory refers to a multiple-processor computer system in which each processor has its own private memory. Computational tasks can only operate on local data, and if remote data is required, the computational task must communicate with one or more remote processors.

DISTRIBUTED-MEMORY COMPUTER with 4 PUs



How can we perform numerical simulation of LSS formation

Message Passing Interface

MPI and OpenMP

Each MPI task can use many OpenMP threads. So, a task is not necessarily mapped on a core or a processor, but often it does.

After initialization each MPI task gets its unique id (rank). All MPI tasks are equal. For programming purposes it is convenient to name the rank=0 task as root and use it differently. Root (and some other tasks) can be allocated to different compute nodes with larger memory.

Exchange of data between tasks is done by library calls.

The Message Passing Interface (MPI) is an explicit communication scheme, i.e. it is entirely up to the user to control the communication.

Messages containing data can be sent between processors, both in synchronous (safer) and asynchronous modes.

There are collective communications and Point-to-Point (safer) Communications.

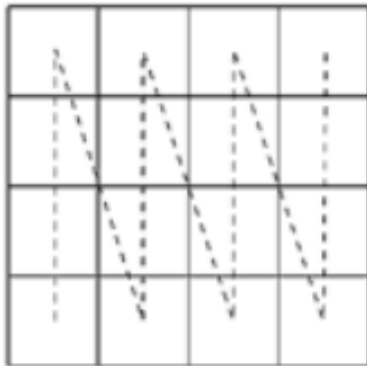
There are blocking (safer) and no-blocking instructions.

How can we perform numerical simulation of LSS formation

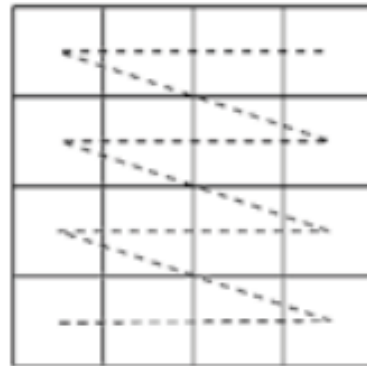
First Point: Domain decomposition for parallel computing

Numerous schemes of dynamic partitioning are possible

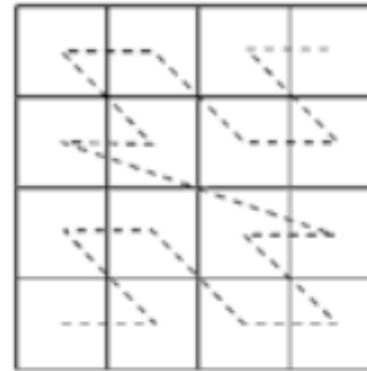
- Column, row or plane major (PM)
- Morton curves
- Peano-Hilbert curves
- User defined (angular, column+ PH...) (geometry of the dynamics)



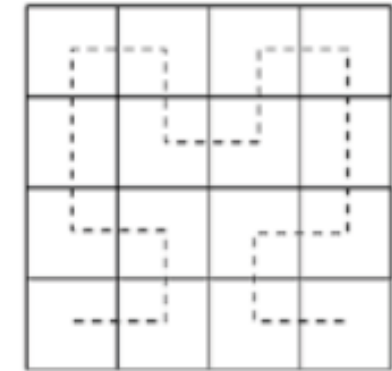
Column major



Row major



Morton

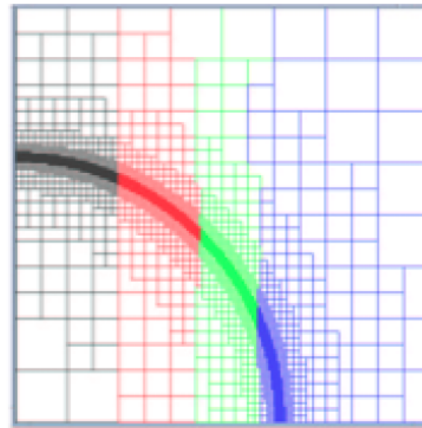


Hilbert

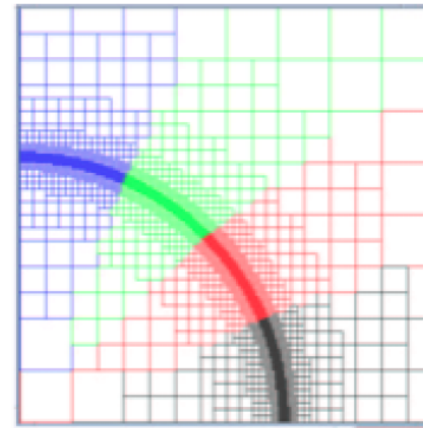
Load Balancing: Dynamic partitioning is performed every N steps by sorting each cell along chosen ordering and redistributing the mesh across processors.

How can we perform numerical simulation of LSS formation

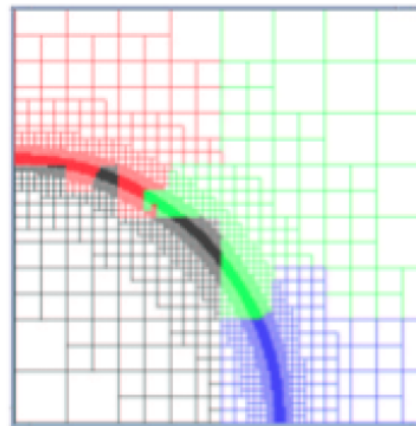
First Point: Domain decomposition for parallel computing



Column major



Angular



Hilbert

Is there an optimal load balancing strategy ?

How can we perform numerical simulation of LSS formation

An example: Domain decomposition for parallel computing in AMR Code

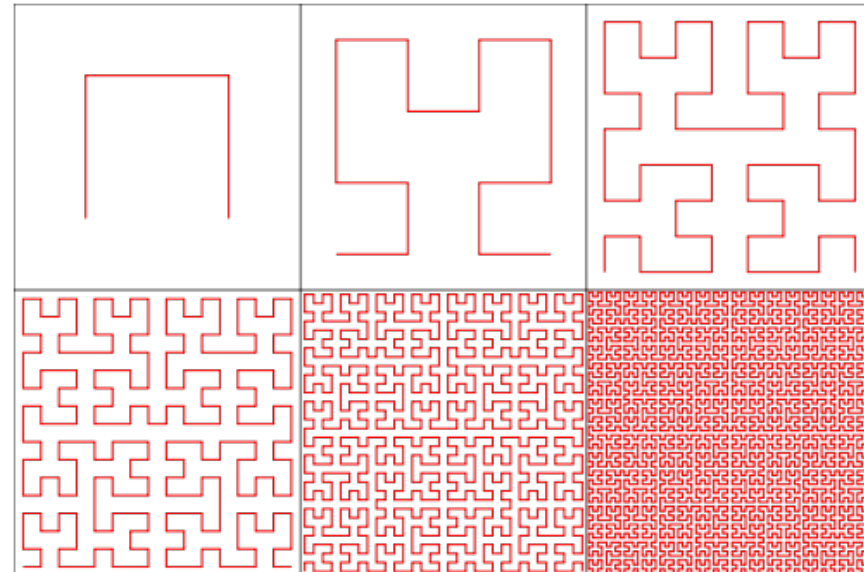
Parallel computing using the MPI library with a domain decomposition based on the Peano-Hilbert curve

Advantages:

- Peano-Hilbert curve is a space-filling curve.
- Two particles close in space are close on the Peano-Hilbert curve and therefore have close ident
- Algorithm inspired by gravity solvers (originally implemented on tree codes).
- tested, operational effective for large and complex problem size.

Disadvantage:

- Unintuitive and Unnatural for a exterior user. It needs to re-write the resulting data

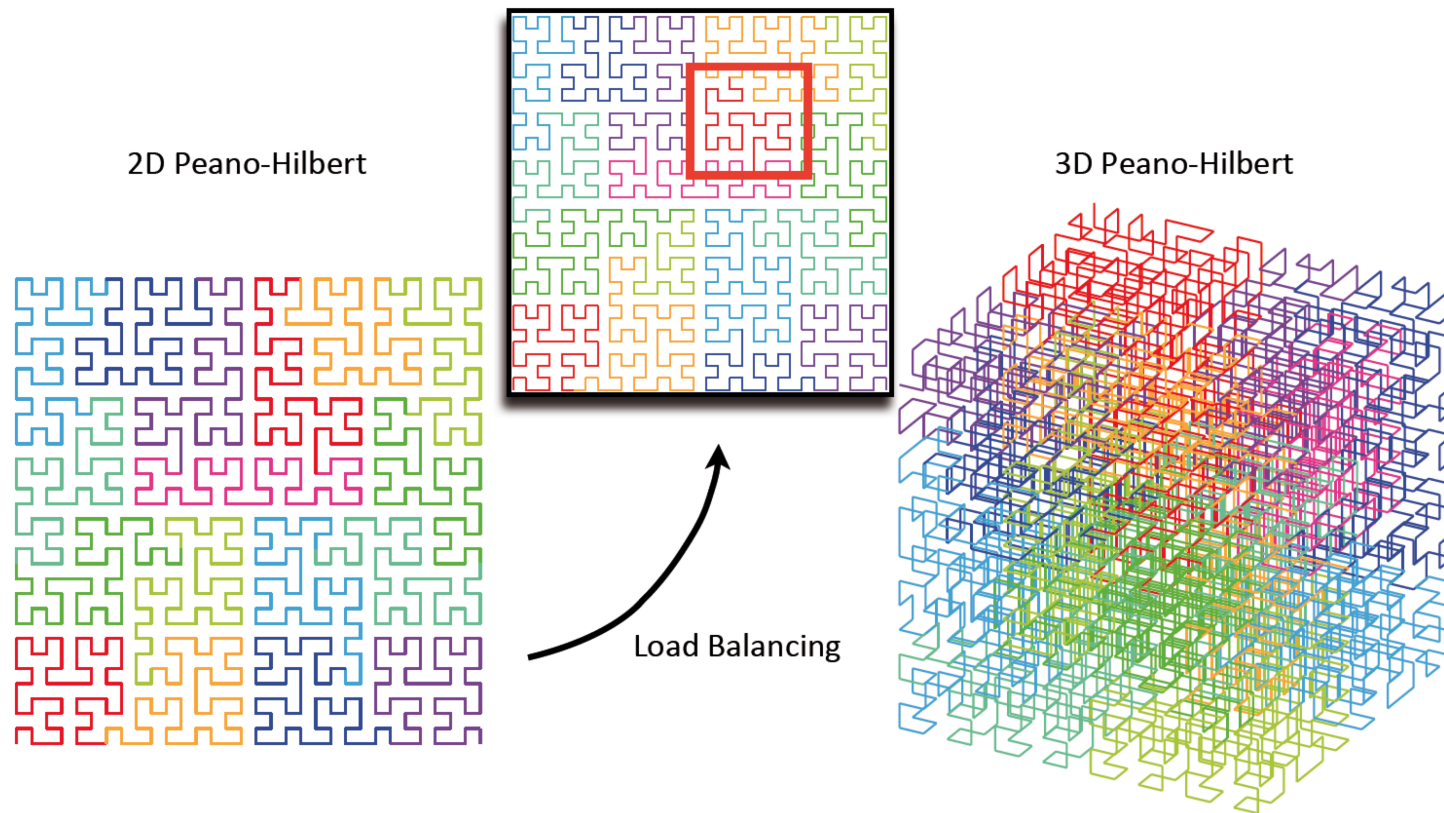


How can we perform numerical simulation of LSS formation

An example: Domain decomposition for parallel computing in AMR Code

Parallel computing using the MPI library with a domain decomposition based on the Peano-Hilbert curve

How does it proceed the load balancing ?



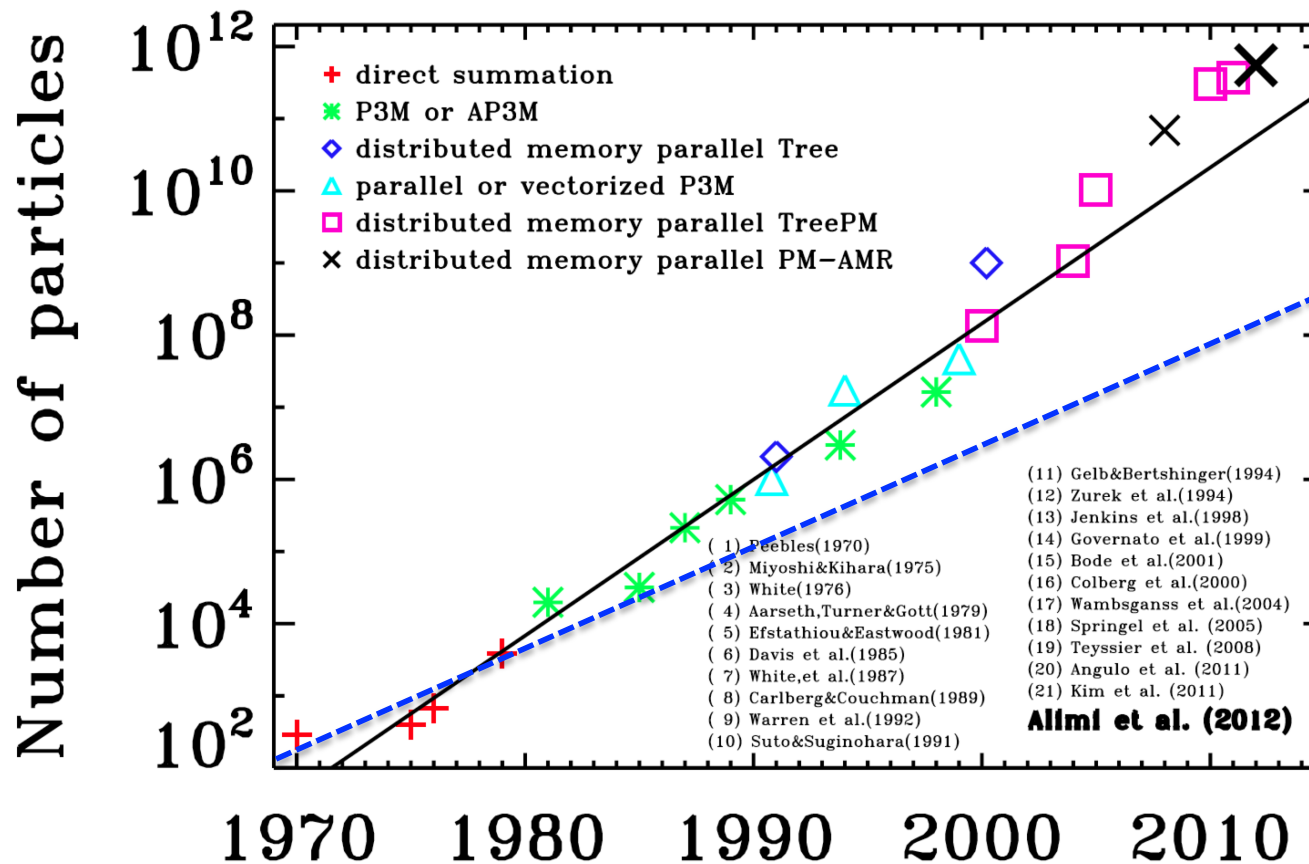
Numerical simulations of Dark Universe: Performances

How can we perform numerical simulation of LSS formation

Numerical Simulations of Dark Universe: Performances

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

Computers double their speed every 18 months (Moore's law) N-body simulations have doubled their size every 16 months. Recently, growth has accelerated further.



10⁶ 1month for PP,
10¹⁰ 10 millions Ye for PP

a "Moore"-like law with an increasing factor of 2 every 18 months underestimates the acceleration of state-of-the-art cosmological N-body simulations.

The mean evolution of the simulation size is taken from Springel et al. 2005. It is linear in logarithmic space, increasing by a factor of 10 every 4.55 years.

How can we perform numerical simulation of LSS formation

Numerical Simulations of Dark Universe: Performances

Larger volume



Larger statistics and rare events



Larger is the volume, smaller is the statistical error (simple variance) in the measured power spectrum

$$\sigma(k) \propto \sqrt{\frac{1}{N_k}} \propto \sqrt{\left(\frac{\Delta k}{k}\right)^2} \propto \frac{1}{kL_{\text{Box}}}$$

N_k is the number of independant Fourier modes used for estimating the Power spectrum.

How can we perform numerical simulation of LSS formation

Cosmological consortia: Grand Challenge Simulation.

« Virgo » (Millenium 1, 2, XXL, UK, Germany...),
« Horizon Run » (Canada, Korea, USA),
« MICE » (Spain ICE, UK, Germany)
« Bolchoi » (Nuevo Mexico USA, Santa Cruz USA, Potsdam Germany)
« Cosmic Emulators » (Coyote Simulation, Los Alamos, UC Berkeley, ICC Barcelona Spain)
....
Brasil ? South America

« **DEUS** » (**Dark Energy Universe Simulation**) (www.deus-consortium.org)

The goal of the DEUS project (Dark Energy Universe Simulation) is to investigate the imprints of dark energy on cosmic structure formation through high-performance numerical simulations:

Λ CDM , DE dynamical models.

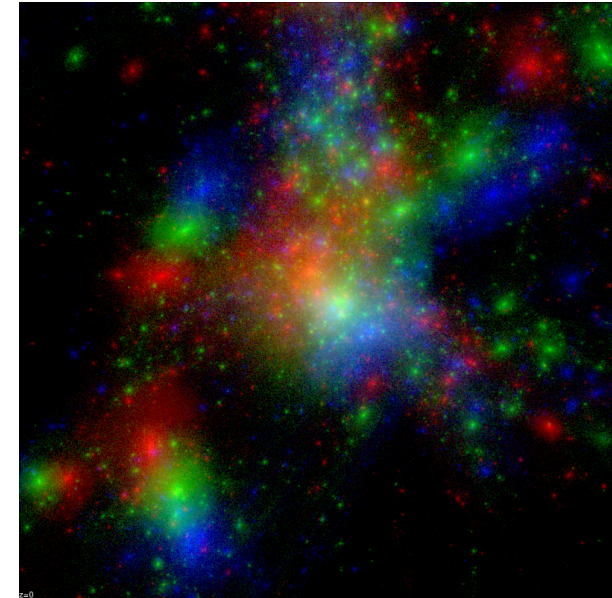
Realistic Models and Toys Models

DEUS Series, DEUS Full Universe Run

...DEUS Multi-Fluids...

Dark Energy Universe Simulation

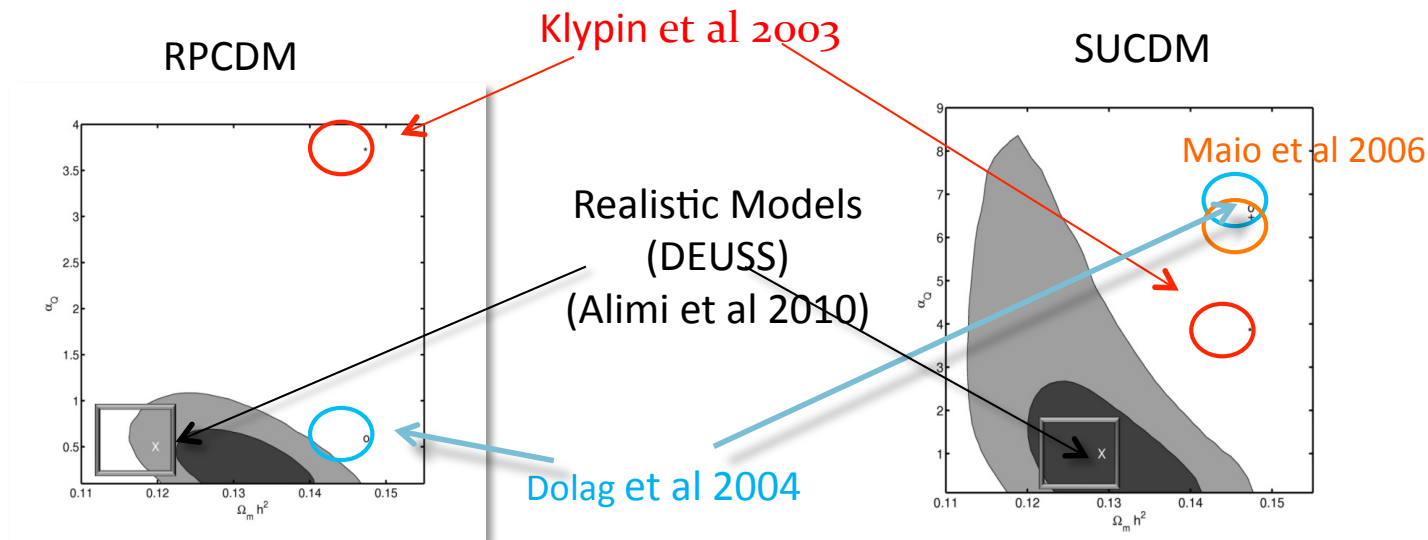
- The Cosmic expansion is accelerated
- What is the nature of the Dark Energy that drives this acceleration ? Probably, the most challenging problem in Cosmology, in Physics.
- How can we distinguish between DE Models ?
- What can we learn on DE from LSS Formation ?
/
- How LSS formation process is affected by the presence of Dark Energy



Developping the largest cosmological DM simulations to date with realistic DE component, involving billions of particules, highest spatial resolution for the largest set of simulated Universe, our challenge is to reproduce with unprecedented details the cosmic structure formation process and answer to these fundamental questions both from theoretical point of view and by providing useful results for the present and future cosmological surveys as SDSS, Planck, DES, Euclid, ... **DEUS Series**

**DEUS Full Universe Runs: The first-ever full observable Universe Simulations:
 Λ CDM , DE dynamical models. **DEUS FUR****

Likelihood analysis of the combined SNIa UNION dataset and WMAP data.
Flat Universe, CAMB modified to take into account δQ clustering.



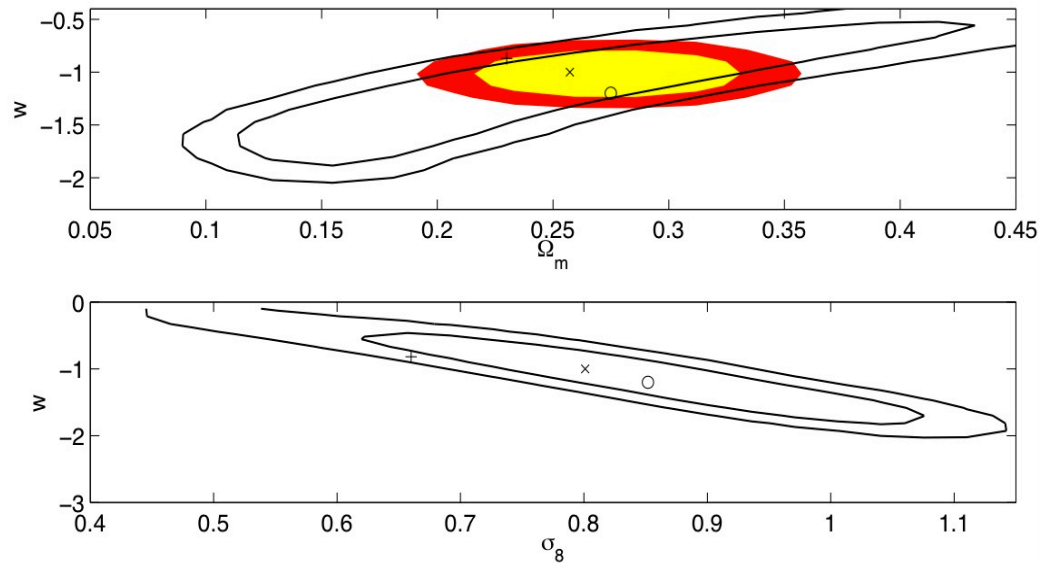
- Constraints on Ω_m et $\Omega_{(\Lambda,Q)}$ from Union SNe Ia data set (Kowalski et al 2008)
- Constraints on $\Omega_b, \Omega_{CDM}, \sigma_8$ from WMAP5 (Komatsu et al 2008).

Conclusion Low slope, $\Omega_m h^2$ slightly lower than in Λ CDM

- Λ CDM vs QCDM's: frozen vs dynamical DE
- RPCDM vs SUCDM: varying $w(z)$ (/w constant)

DEUS: Realistic Models for DEUS FUR

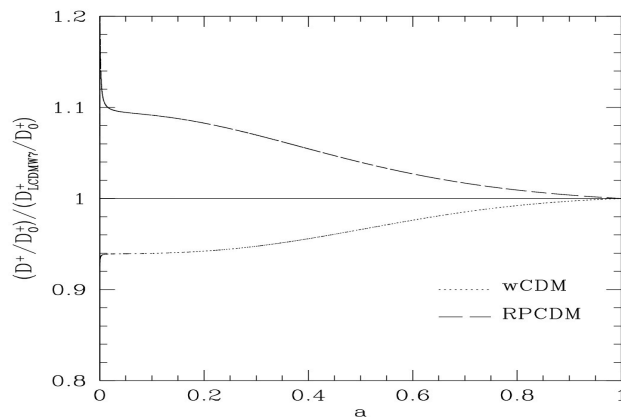
From Observational Data to Cosmological Parameters



1 and 2 σ likelihood contours in the w - Ω_m (top panel) and w - σ_8 (bottom panel) planes respectively.

The solid lines corresponds to marginalized limits from WMAP7-yr data, while the red-yellow contours in the top panel are from the UNION dataset.

The symbols corresponds to Λ CDM (+), Λ CDM-W7 (x) and w CDM (o).



With this choice of cosmological parameters the two non-standard dark energy models exhibit a linear growth of the density perturbations that is specular relative to that of the concordance model.

DEUS: Realistic Models

Cosmological parameters table.

Parameters	Λ CDM	RPCDM	SUCDM	W'CDM
H_0 (km/s/Mpc)	72	72	72	72
Ω_{cdm}	0.26	0.23	0.25	0.275
$\Omega_b h^2$	0.02273	0.02273	0.2273	0.2258
σ_8^{lin}	0.8	0.66	0.73	0.852
α	0	0.5	1	/
$\lambda(\text{eV})$	2.4×10^{-3}	4.9	2.1×10^3	/
A_s	2.1×10^{-9}	2.0×10^{-9}	2.1×10^{-9}	/
n_s	0.951 (0.963)	0.951 (0.963)	0.951	0.963
w_0	-1	-0.87	-0.94	-1.2
w_1	0	0.08	0.19	0

Flat Universe $\Omega_{\Lambda,Q}=1-\Omega_m$

Dark Energy Universe Simulation

LARGE SET OF UNIVERSE VOLUMES (+ 25 SIMULATIONS),
 HIGH SPATIAL RESOLUTION AND MASS: $2.5 \text{ h}^{-1} \text{ kpc}$ to $21 \text{ h}^{-1} \text{ Gpc}$, $2.5 \cdot 10^8 \text{ h}^{-1} M_{\odot}$ to $10^{16} \text{ h}^{-1} M_{\odot}$
 INITIAL REDSHIFT DEEP IN LINEAR REGIME

Box Size	<u>Force Resolution</u>	<u>Mass Resolution</u>	<u>Number of Particles</u>	Initial Redshift	<u>Cosmological Models</u>	Calculateur (Nb of Proc)
$162 \text{ h}^{-1} \text{ Mpc}$	$2.5 \text{ h}^{-1} \text{ kpc}$	$\sim 2 \cdot 10^9 \text{ h}^{-1} M_{\odot}$	512^3	~ 90	$\Lambda 1_1$, SU1_1, RP1_1	Titane (64)
$162 \text{ h}^{-1} \text{ Mpc}$	$2.5 \text{ h}^{-1} \text{ kpc}$	$\sim 2.5 \cdot 10^8 \text{ h}^{-1} M_{\odot}$	1024^3	~ 130	$\Lambda 1_2$, SU1_2, RP1_2	Blue Gene/P (4096)
$648 \text{ h}^{-1} \text{ Mpc}$	$20 \text{ h}^{-1} \text{ kpc}$	$\sim 1.5 \cdot 10^{11} \text{ h}^{-1} M_{\odot}$	512^3	~ 55	$\Lambda 4_1$, SU4_1, RP4_1	-
$648 \text{ h}^{-1} \text{ Mpc}$	$10 \text{ h}^{-1} \text{ kpc}$	$\sim 1.75 \cdot 10^{10} \text{ h}^{-1} M_{\odot}$	1024^3	~ 90	$\Lambda 4_2$, SU4_2, RP4_2	Blue Gene/P (4096)
$648 \text{ h}^{-1} \text{ Mpc}$	$5 \text{ h}^{-1} \text{ kpc}$	$\sim 2 \cdot 10^9 \text{ h}^{-1} M_{\odot}$	2048^3	~ 90	$\Lambda 4_4$, RP4_4	Blue Gene/P (32768)

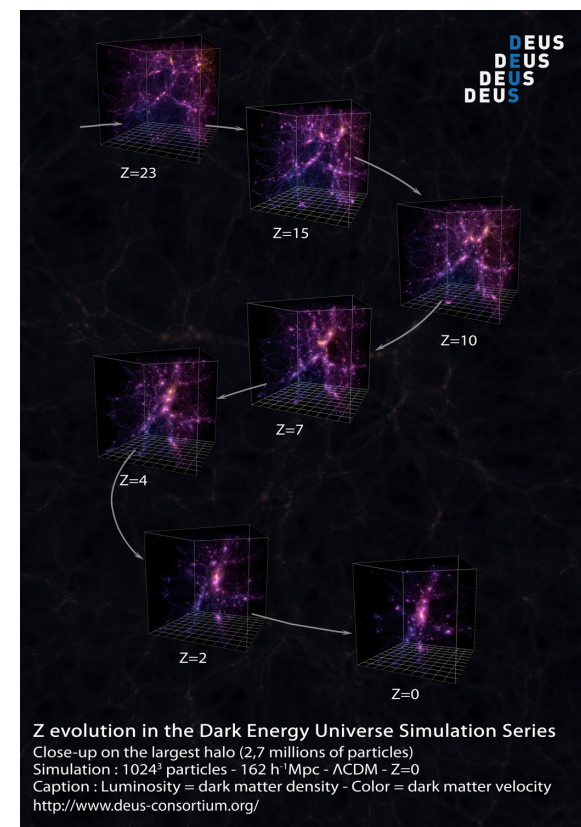
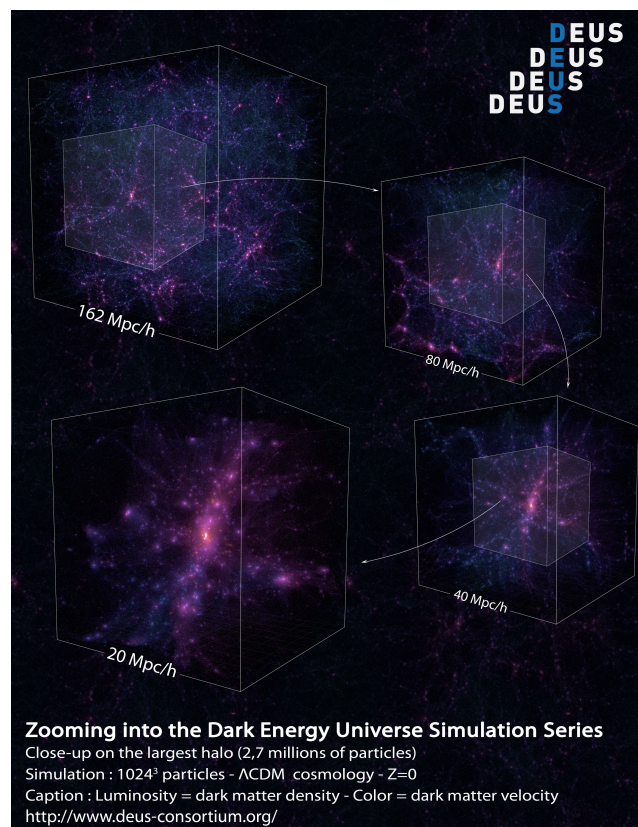
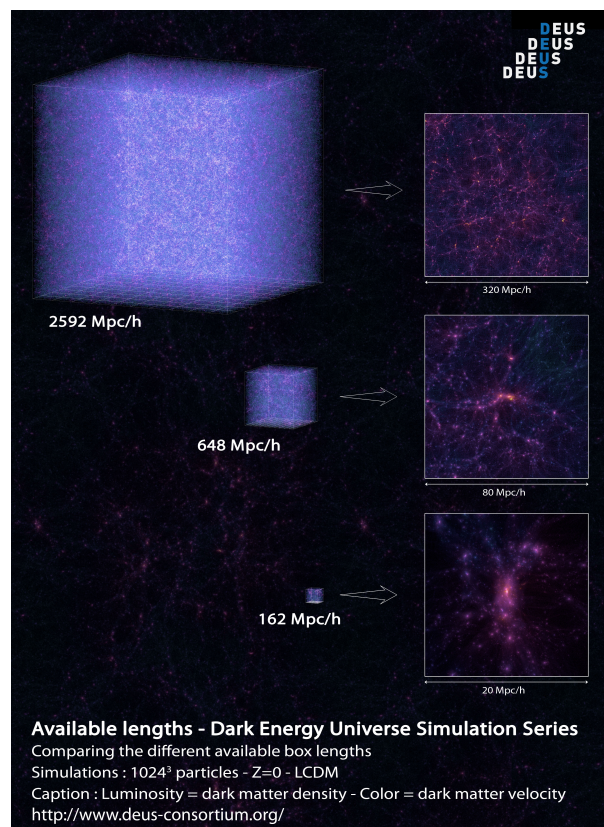
Dark Energy Universe Simulation

LARGE SET OF UNIVERSE VOLUMES (+ 25 SIMULATIONS),
 HIGH SPATIAL RESOLUTION AND MASS: $2.5 \text{ h}^{-1} \text{ kpc}$ to $21 \text{ h}^{-1} \text{ Gpc}$, $2.5 \cdot 10^8 \text{ h}^{-1} M_{\odot}$ to $10^{16} \text{ h}^{-1} M_{\odot}$
 INITIAL REDSHIFT DEEP IN LINEAR REGIME

Box Size	Force Resolution	Mass Resolution	Number of Particles	Initial Redshift	Cosmological Models	Calculateur (Nb of Proc)
$1296 \text{ h}^{-1} \text{ Mpc}$	$40 \text{ h}^{-1} \text{ kpc}$	$\sim 1. \cdot 10^{12} \text{ h}^{-1} M_{\odot}$	512^3	~ 40	$\Lambda 8_1$, SU8_1, RP8_1	-
$2592 \text{ h}^{-1} \text{ Mpc}$	$40 \text{ h}^{-1} \text{ kpc}$	$\sim 1. \cdot 10^{12} \text{ h}^{-1} M_{\odot}$	1024^3	~ 55	$\Lambda 16_2$, SU16_2, RP16_2	Blue Gene/P (4096)
$2592 \text{ h}^{-1} \text{ Mpc}$	$20 \text{ h}^{-1} \text{ kpc}$	$\sim 1.5 \cdot 10^{11} \text{ h}^{-1} M_{\odot}$	2048^3	~ 55	$\Lambda 16_4$, RP16_4	Blue Gene/P (24576)
$5184 \text{ h}^{-1} \text{ Mpc}$	$40 \text{ h}^{-1} \text{ kpc}$	$\sim 1. \cdot 10^{12} \text{ h}^{-1} M_{\odot}$	2048^3	~ 40	$\Lambda 32_4$, RP32_4	Blue Gene/P (24576)
$10368 \text{ h}^{-1} \text{ Mpc}$	$40 \text{ h}^{-1} \text{ kpc}$	$\sim 1. \cdot 10^{12} \text{ h}^{-1} M_{\odot}$	4096^3	~ 100	$\Lambda 64_8$	Curie Thin Nodes (9728)
$21000 \text{ h}^{-1} \text{ Mpc}$ <i>Full Universe RUN</i>	$40 \text{ h}^{-1} \text{ kpc}$	$\sim 1. \cdot 10^{12} \text{ h}^{-1} M_{\odot}$	8192^3	~ 100	$\Lambda 128_16$ RP128_16 W'128_16	Curie Thin Nodes (80 000)

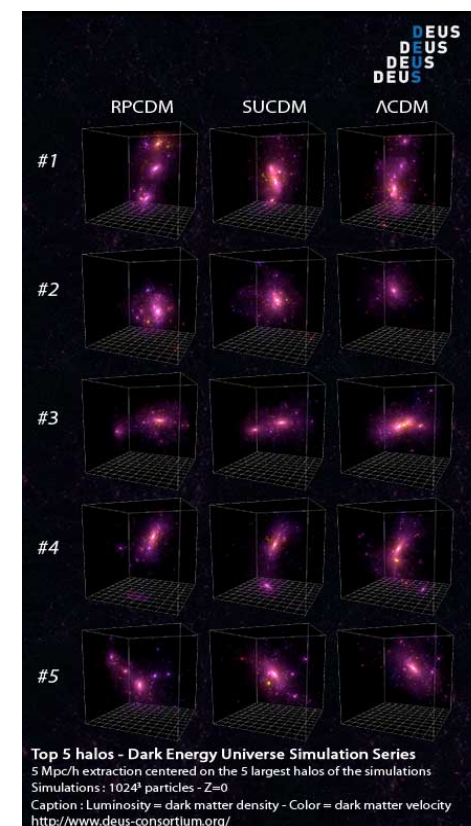
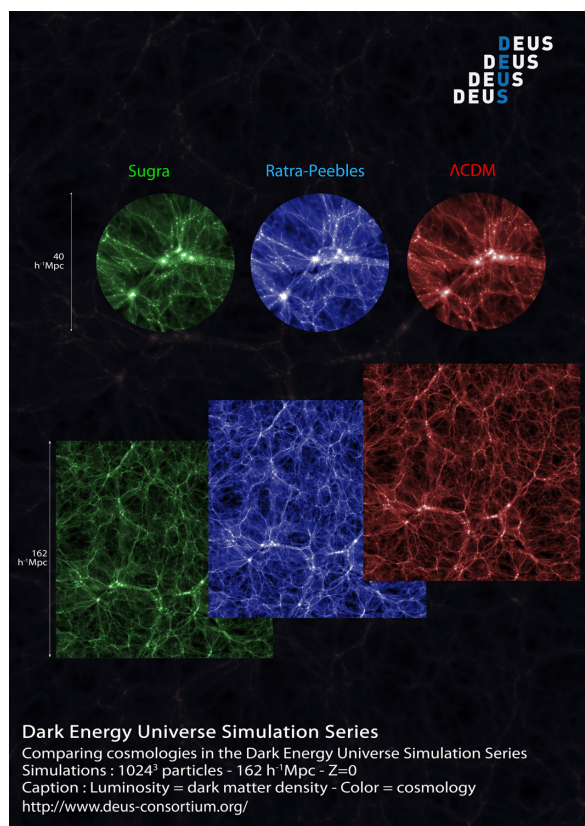
Dark Energy Universe Simulations : A large set of simulations

Large set of Universe Volumes (+ 25 simulations),
Very High spatial resolution: $2.5 \text{ h}^{-1} \text{ kpc}$ to $21 \text{ h}^{-1} \text{ Gpc}$,
Very High mass resolution: $2.5 \cdot 10^{10} \text{ h}^{-1} M_{\odot}$ to more than $10^{16} \text{ h}^{-1} M_{\odot}$ Halos
Initial redshift deep in linear regime



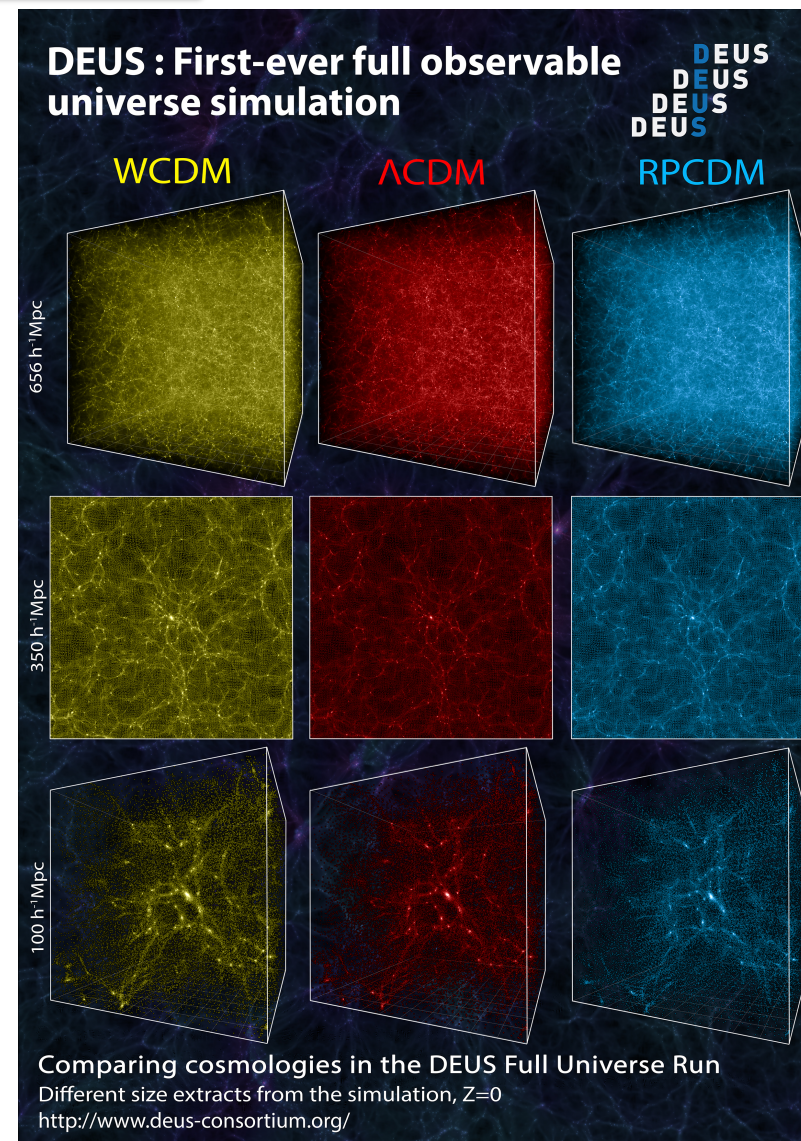
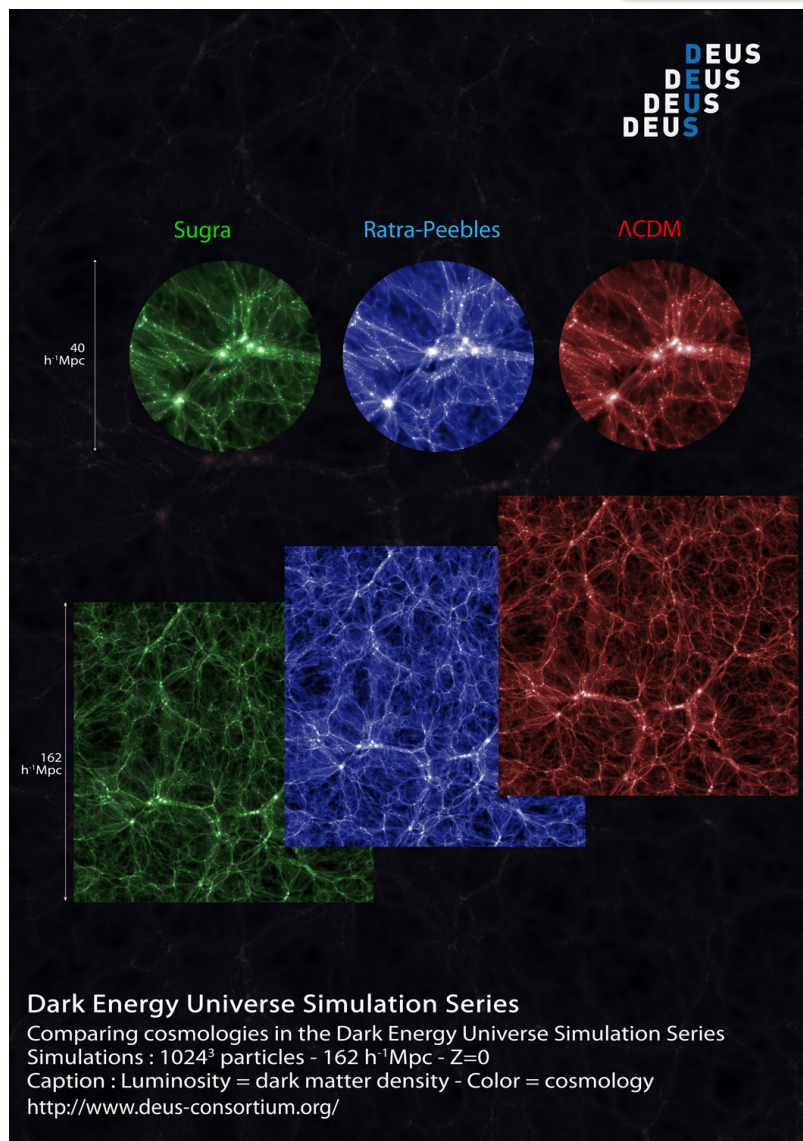
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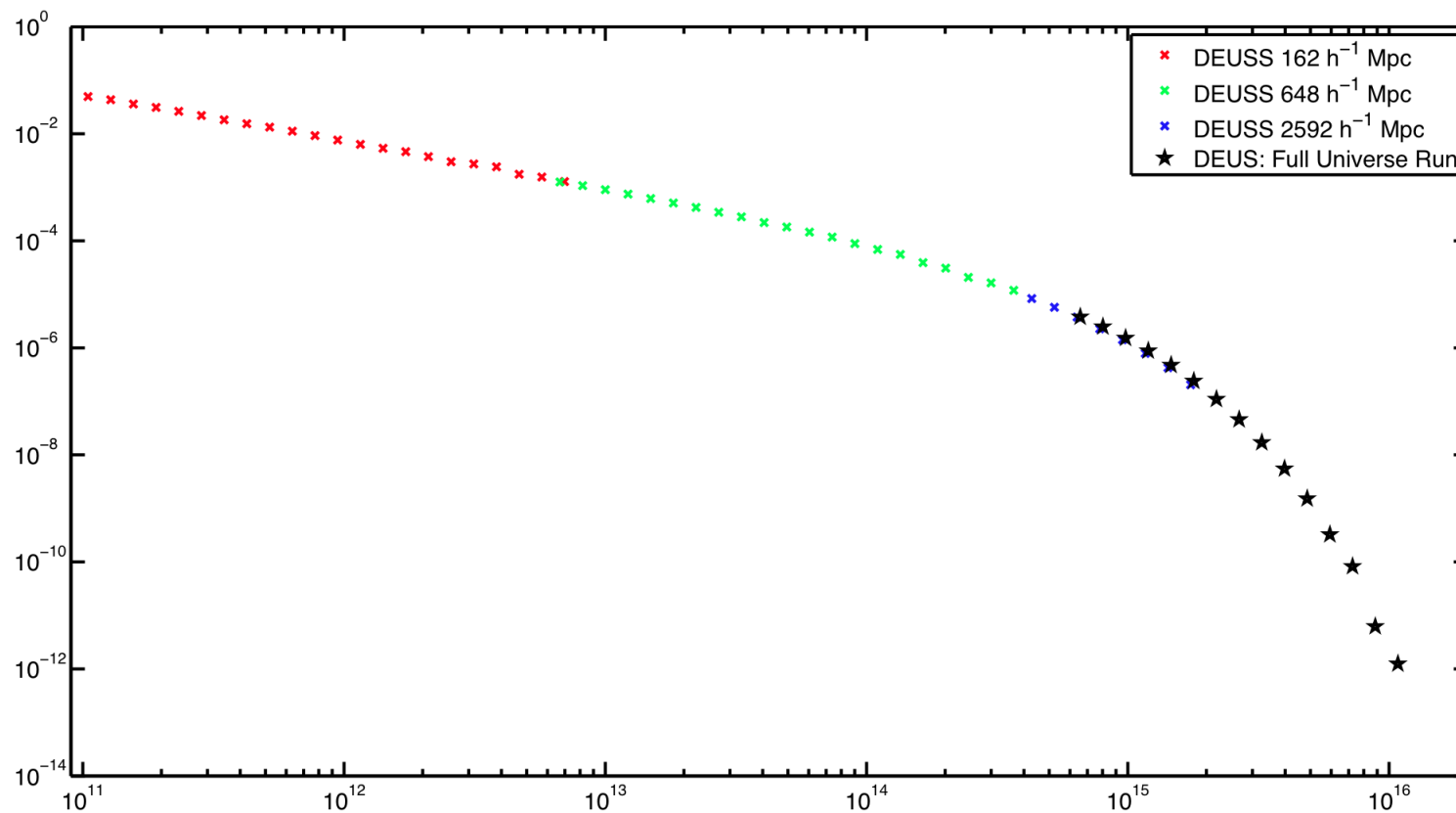
Dark Energy Universe Simulation : A large set of simulations

DEUSS / DEUS FUR



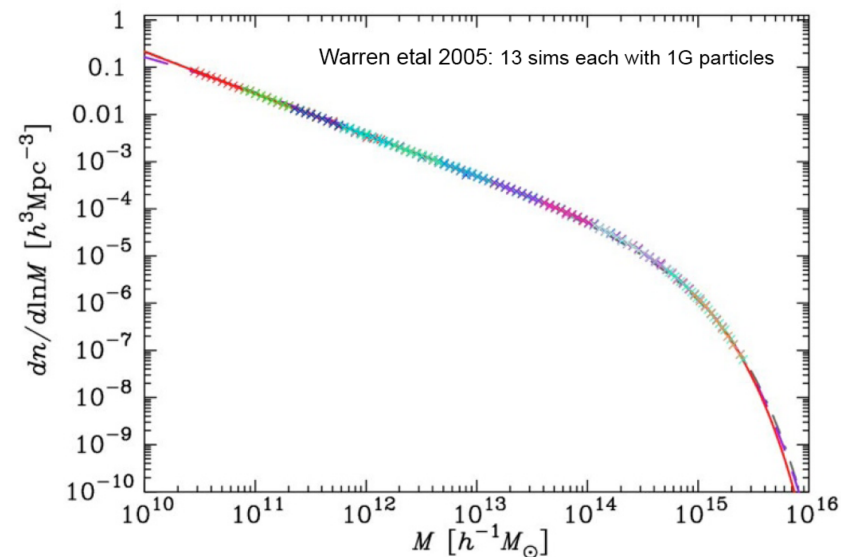
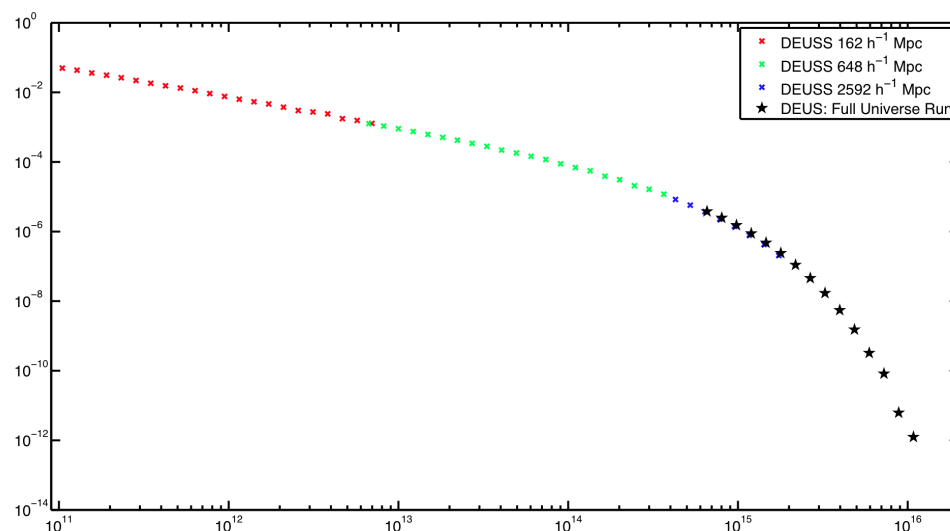
Dark Energy Universe Simulation : A large set of simulations

**Halo Mass Function:
Universality/No Universality, Extreme large Massive Halos...**



Dark Energy Universe Simulation : A large set of simulations

Halo Mass Function: Universality/No Universality, Extreme large Massive Halos...



Dark Energy Universe Simulation : a huge job to optimize

Optimisation Phase: The big first problem is the scalability of the computation.

We need weak-scaling configuration : the same simulation with a smaller number of node

TABLE I

CHARACTERISTICS OF THE TEST RUN SIMULATIONS IN WEAK-SCALING CONFIGURATION.

Particles	MPI Task Number	MPI Task Memory	Nodes Number
1024^3	74	8Go	10
2048^3	594	8Go	75
4096^3	4752	8Go	594
8192^3	38016	8Go	4752

To improve scalability, different communication schemes have been implemented in addition to the default method already present in the original version of Gravity Solver « RAMSES » and based on asynchronous MPI operations (Isend/Irecv). Synchronous communications (Send/Recv, Bcast) have been implemented for certain levels of refinements (particularly the coarser ones). Such optimisations have proven to be highly dependent on the MPI library as well as the IB topology. This has required the implementation of specific tuning of the system with BULL HPC experts during the preparatory phase

Dark Energy Universe Simulation : a huge job to optimize

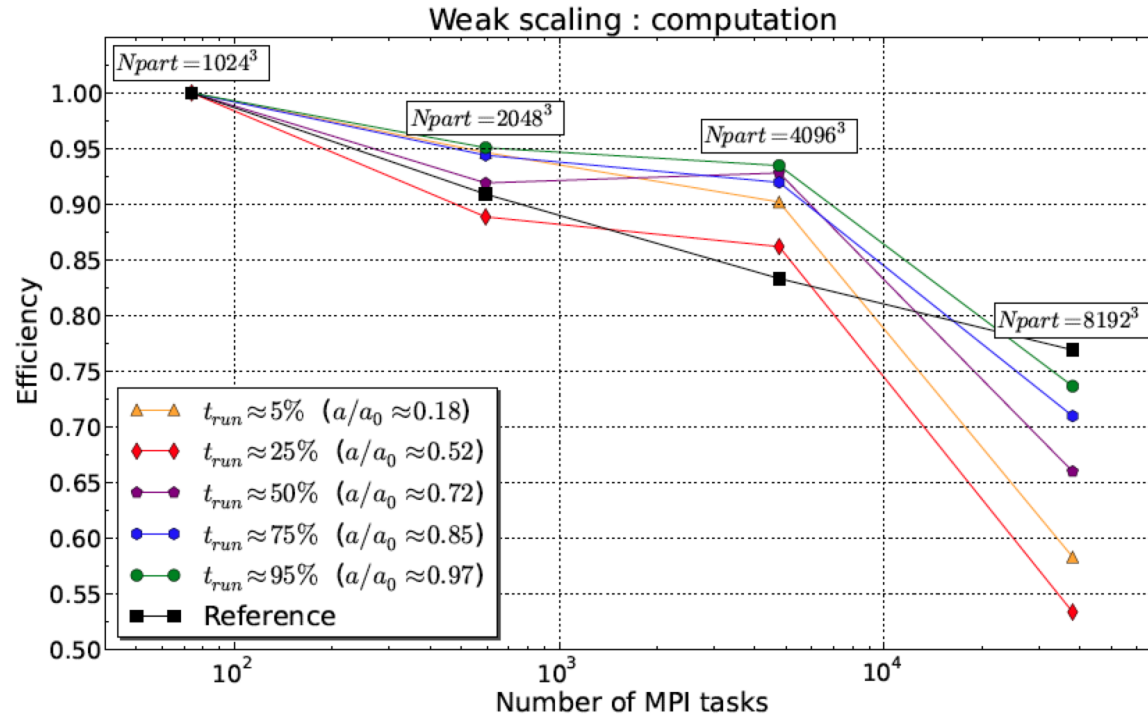


Fig. 7. Efficiency of N-body/Poisson solver as a function of the number of MPI tasks in a weak-scaling configuration. The reference corresponds to 74 MPI tasks. The efficiency is shown at the beginning of the run (yellow), at 1/4th (red), half (purple), 3/4th (blue) and at the end of the run (green). The efficiency is first of the order of 60%, it falls to about 55% during a short time when the first refinements are triggered and finally it increases to 75%. Multigrid acceleration allows us to reach higher efficiencies comparatively to the efficiency of an ideal PM-FFT code in black.

Dark Energy Universe Simulation : a huge job to optimize

Optimisation Phase: The memory usage.

Memory usage has been one of the major challenge of the simulation.

The computation has to satisfy the absolute condition of using less than 64 GB per node, i.e. less than 8 GB per MPI process. Any “swap” generated by a local memory excess leads to a prohibitive execution time. Thus, to evaluate the memory use in the weak-scaling configurations, a set of preparatory tests has been designed. The goals of these tests have been to determine the best parametrization of the triggering levels of the adaptive mesh refinement from a physical point of view (essentially the final choice of the threshold sets the refinement to 14 particles per cell) for different scenarios of memory usage.

The execution of these tests has represented a milestone toward the realization of the project.

These have allowed us to to maximize the accuracy of the calculation of the dynamical evolution of the particles given the available amount of memory on each node of CURIE Thin.

Dark Energy Universe Simulation : a huge job to optimize

Optimisation Phase: The memory usage.

During the initialization phase, nine processes communicate with all 38016 processes using the original communication scheme of the « RAMSES » code which was based on point-to-point communications.

Because of these 9 tasks use up to 16 GB of memory when the MPI libraries are configured for the optimal execution speed (via OpenMPI options), thus altering the normal run of the simulation till its complete crash.

The use of OpenMPI parameters with low memory footprint has solved the problem, however this resulted in lockups of the code.

An "intermediate" parametrization has been finally chosen, including a relaxation of the option scheme of the generic point-to-point communication originally used in favor of BCAST(broadcast) instructions which have reduced the maximum memory used per processes by about 35%, thus limiting the memory usage of the 9 processes considered to 8 GB.

Dark Energy Universe Simulation : a huge job to optimize

Optimisation Phase: The memory usage.

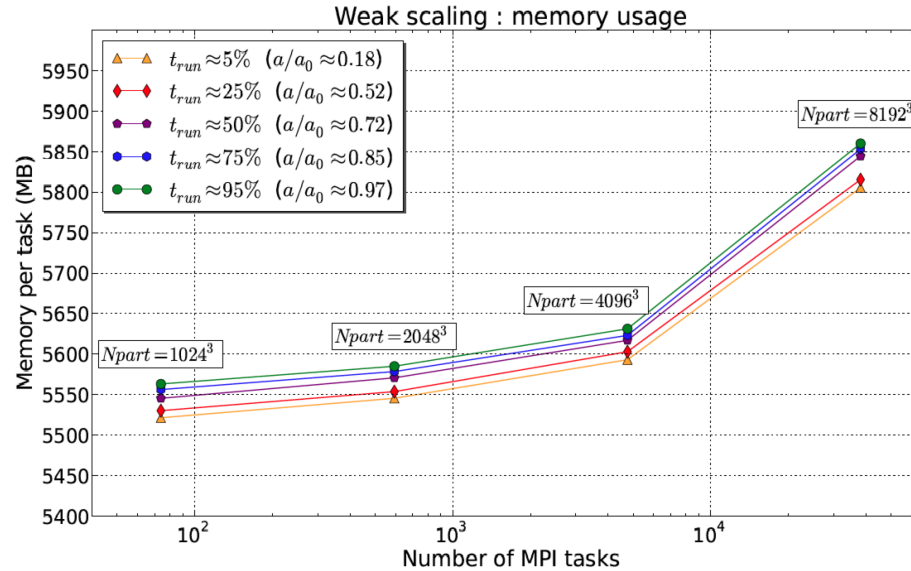
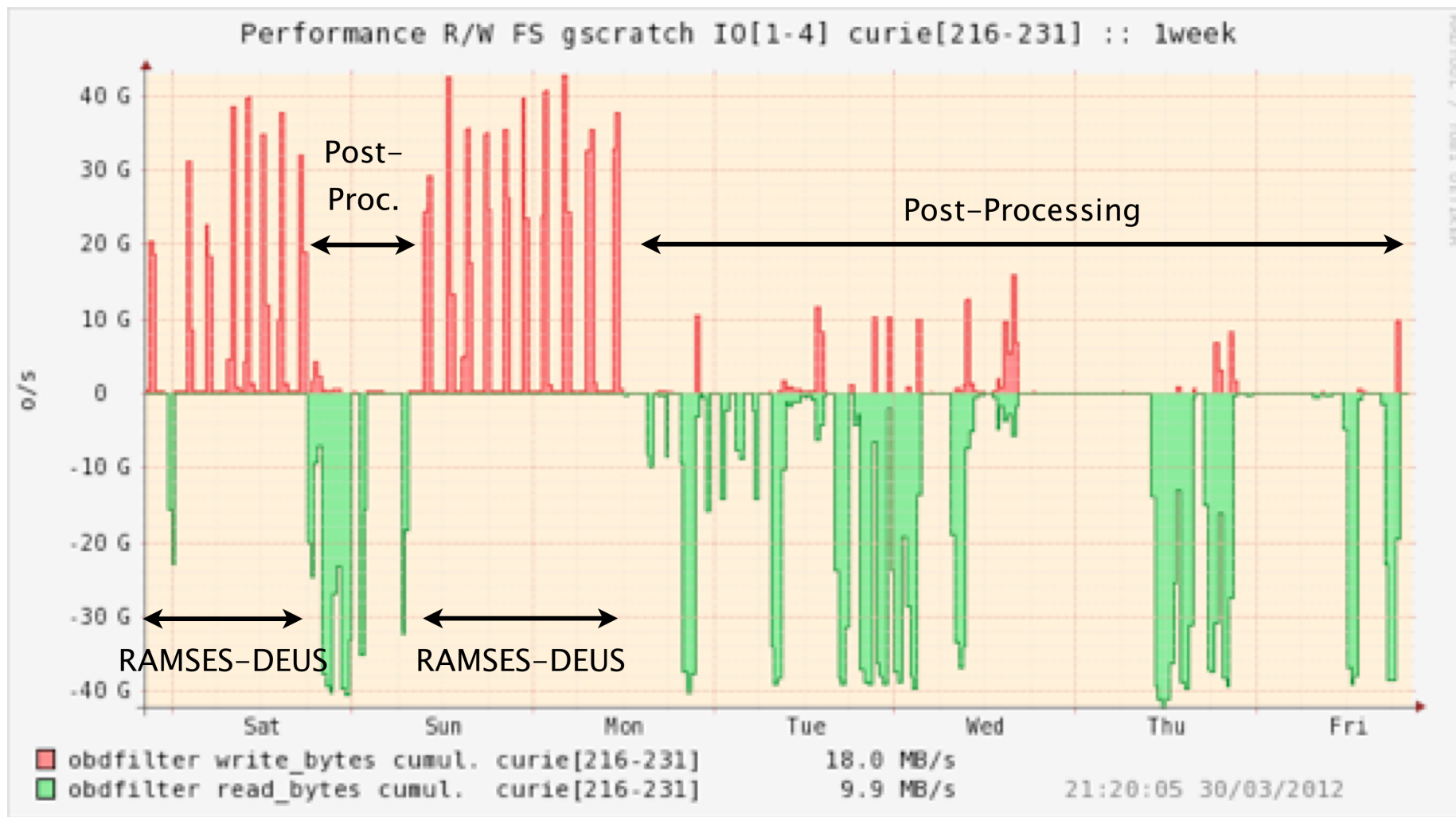


Fig. 8. Mean memory usage as a function of number of MPI tasks in a weak-scaling configuration: beginning of the run (orange), at 1/4th (red), half (purple), 3/4th (blue) and at the end of the run (green). The control of memory usage (including the one from MPI buffers) achieved at the 5% level was a key point for the success of the run.

All these optimizations have led to an average use of memory per process illustrated in Figure 8. The majority of arrays are allocated during the initialization phase of the code, the average memory used increases very little during the run and remains below 6 GB per process. We can see that there is a good scalability in memory since increasing the number of MPI tasks from 74 to 38016 increase the memory usage by 5% only

Dark Energy Universe Simulation : a huge job to optimize

Optimisation Phase: I/O Performances.



Dark Energy Universe Simulation : a huge job to optimize

Optimisation Phase: I/O Performances.

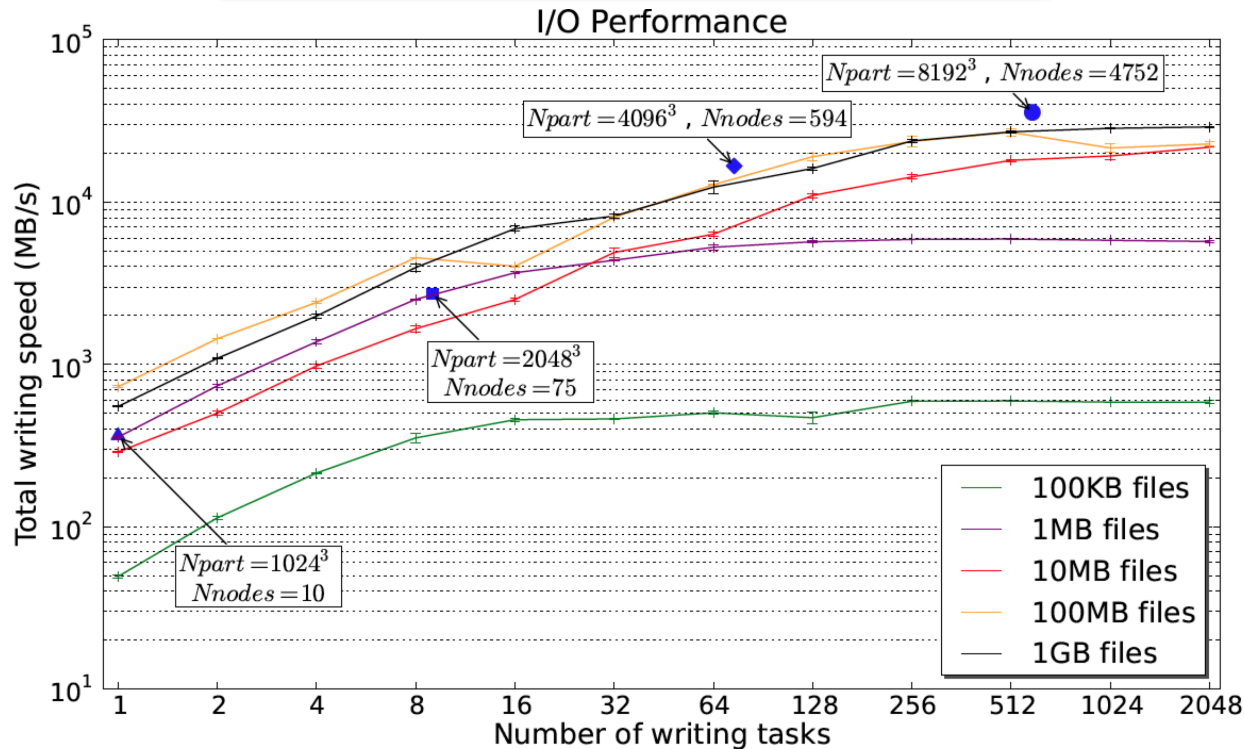


Fig. 9. Writing speed as a function of number of MPI tasks: green is for 100 KB files, purple 1 MB, red 10 MB, yellow 100 MB, black 1 GB like in our run. This is measured using a benchmark on less than 128 nodes. Blue points correspond to the average writing speed during the whole Full Universe Run (4752 nodes/38016 MPI tasks), and the weak scaling simulations. The token system was tuned to saturate the bandwidth allocated for our simulations.

Dark Energy Universe Simulation : a huge job to optimize

Optimisation Phase: Post Processing Workflow

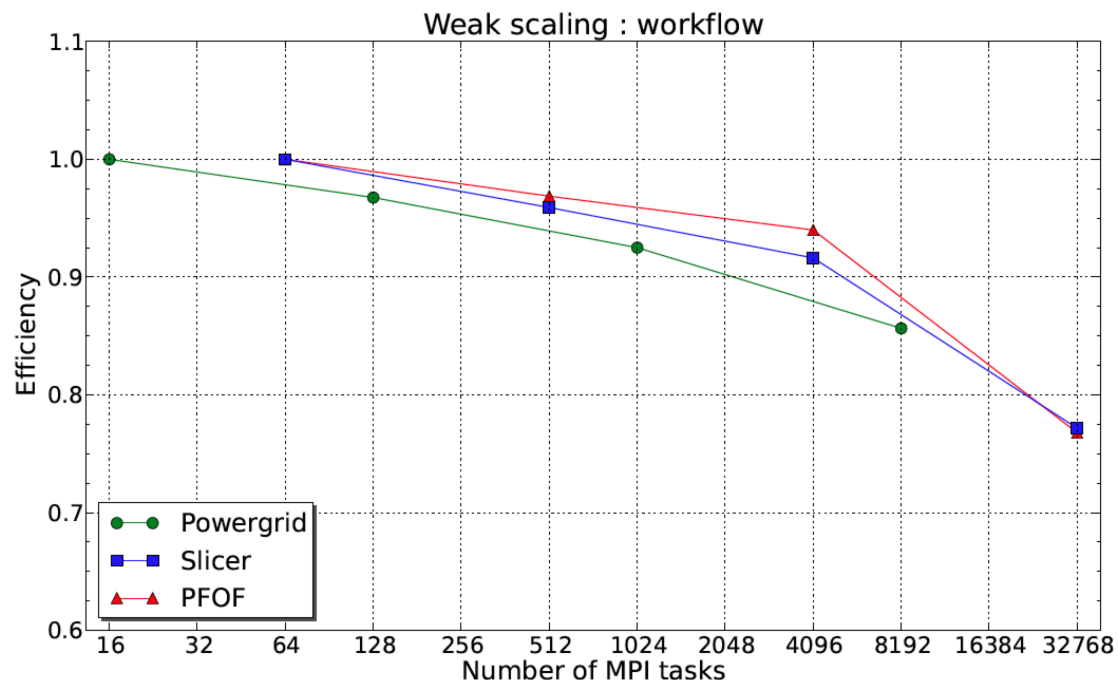
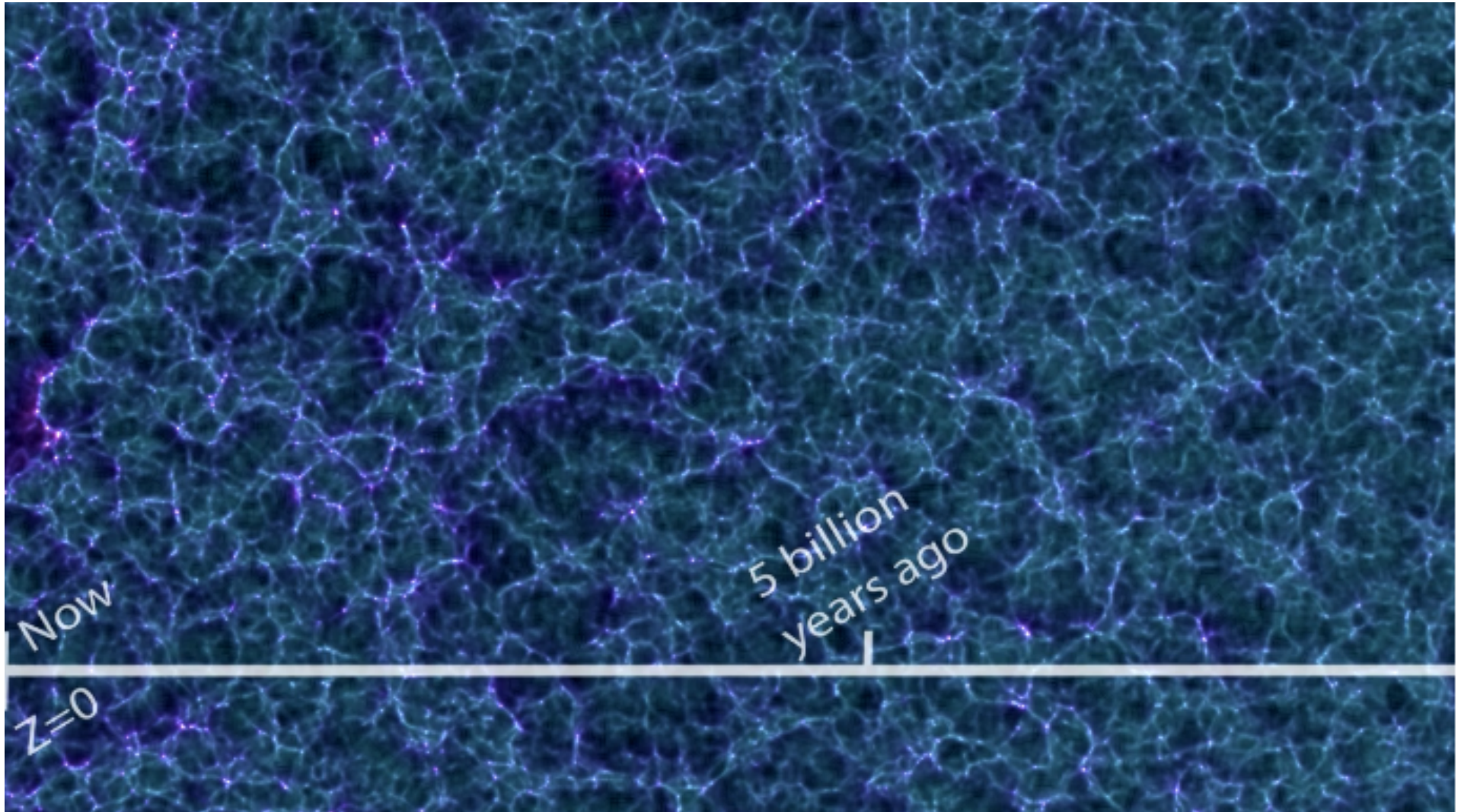


Fig. 10. Efficiency of programs developed to process data generated during the DEUS FUR simulation as a function of the number of MPI tasks. The efficiency obtained is satisfactory: The computation of the power spectrum for validating the results of RAMSES-DEUS corresponds to green curve. The redistribution of these data along the Peano-Hilbert curve in cubic splitting is the blue curve. The efficiency of the detection of massive halos by the percolation algorithm "Friends of Friends" [24] is represented in red.

Dark Energy Universe Simulation



Redshift Space from the Big to the present Λ CDM DEUS FUR

Numerical Simulation of the Dark Universe

III. What do we have learned from numerical simulations on large scale structure formation ?

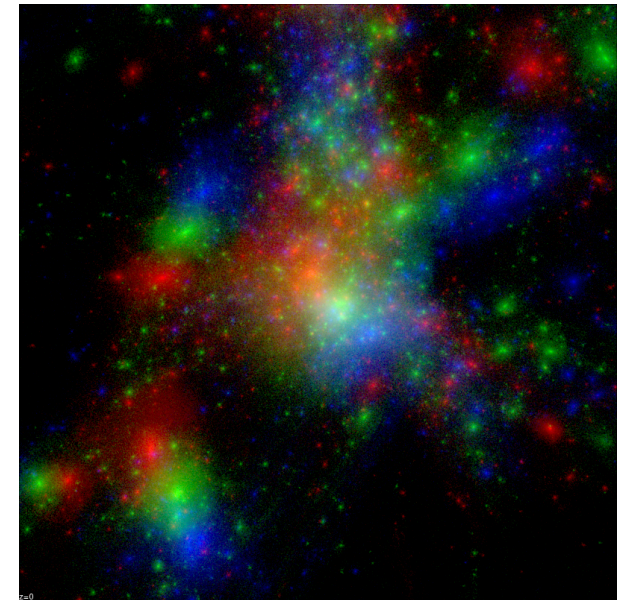
III. 1. DEUS: Some Results in Progress

III. 2. Large scale structure formation (Bias, Bulk Flow)

III. 3. Halo properties (Mass Function, Profil)

IV. Conclusion - Acknowledgments

V. Bibliography



What do we have learned from numerical simulations on LSS formation ?

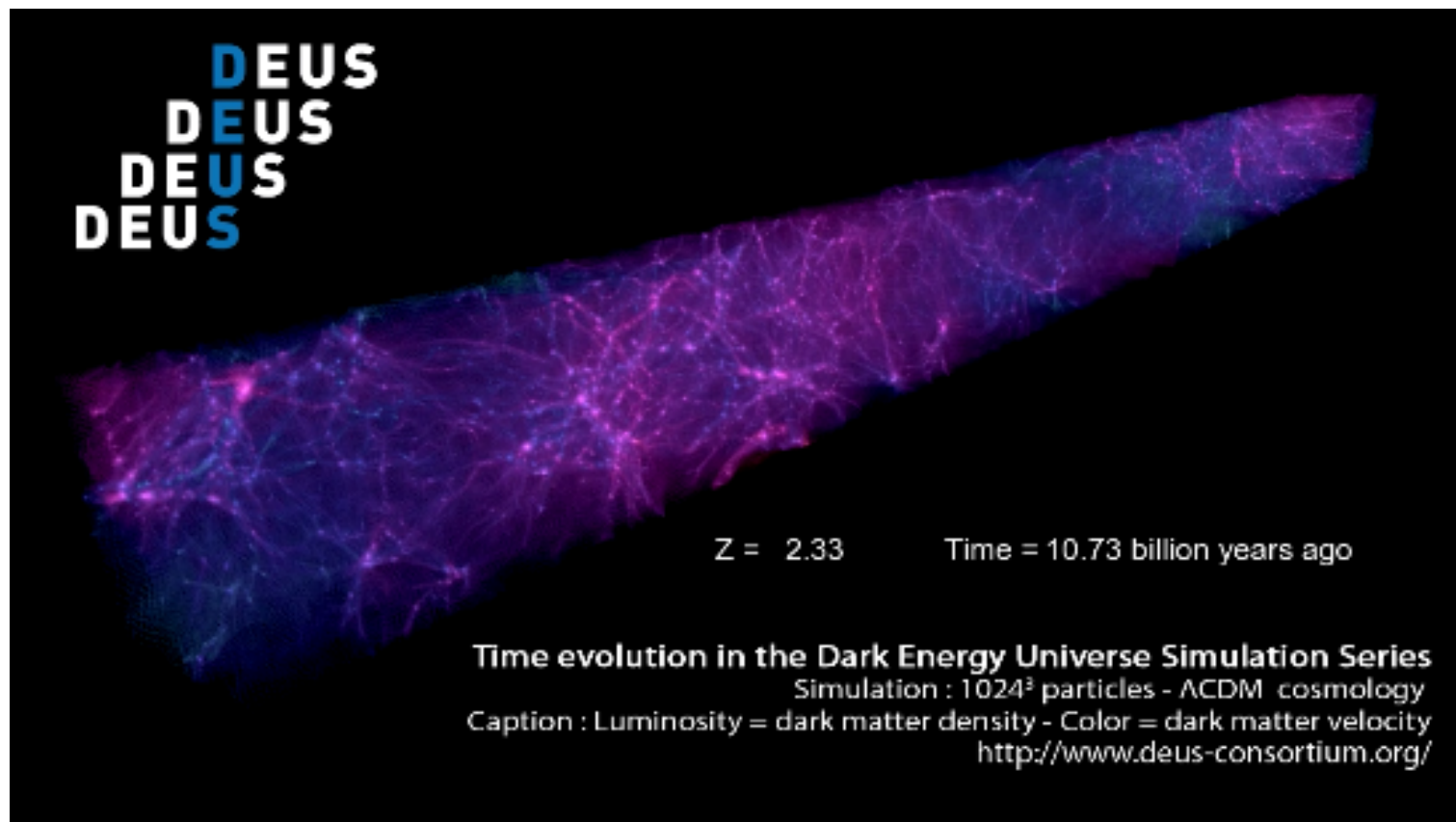
General Properties of LSS Formation

What have we learned from numerical simulations on LSS formation ?

Cosmological Models: General Properties

Large Scale Structure Evolution

The growth by gravitational instability in an expanding universe of the primordial matter fluctuations leads to the cosmic structures we observe today.

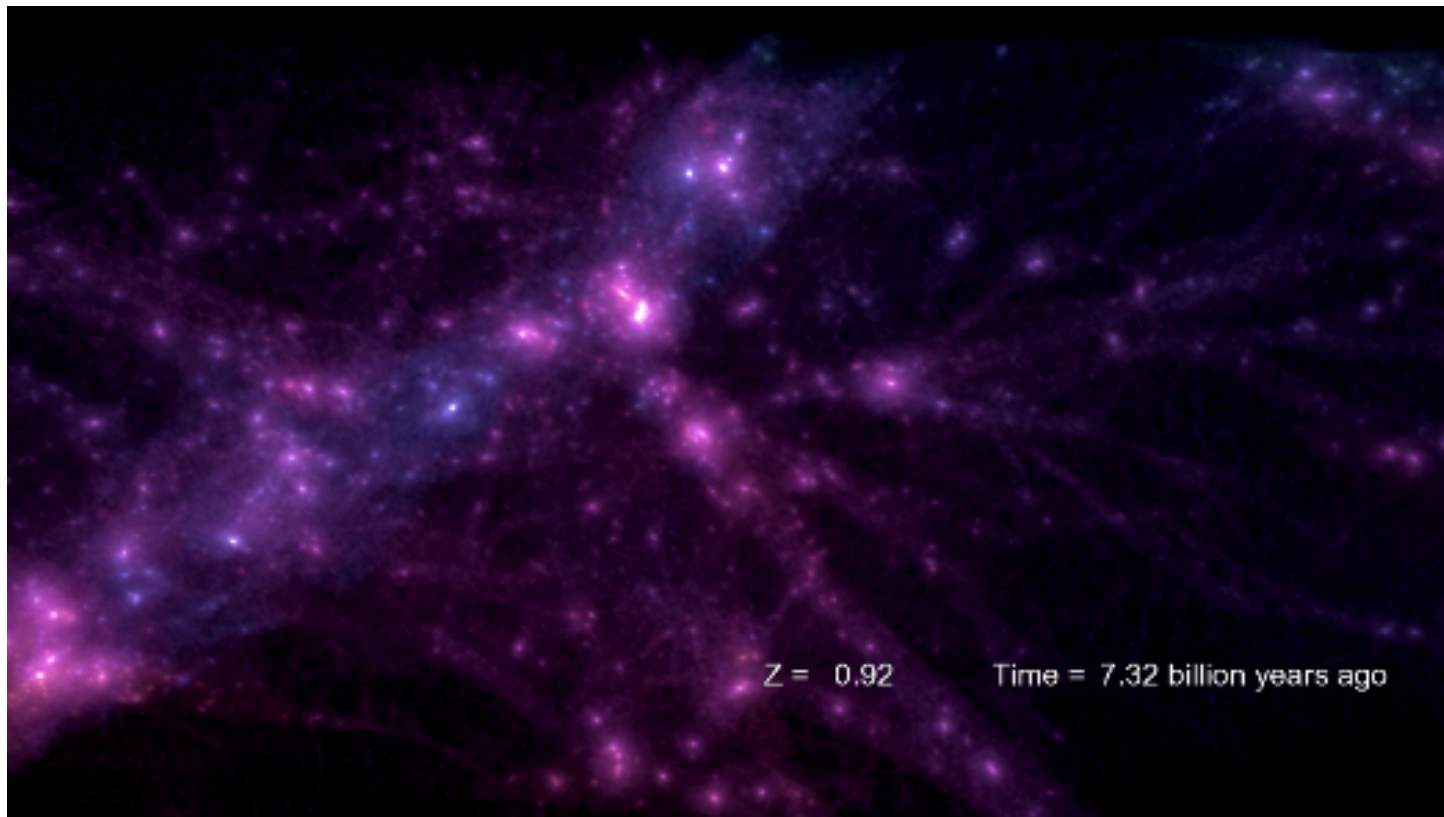


What have we learned from numerical simulations on LSS formation ?

Cosmological Models: General Properties

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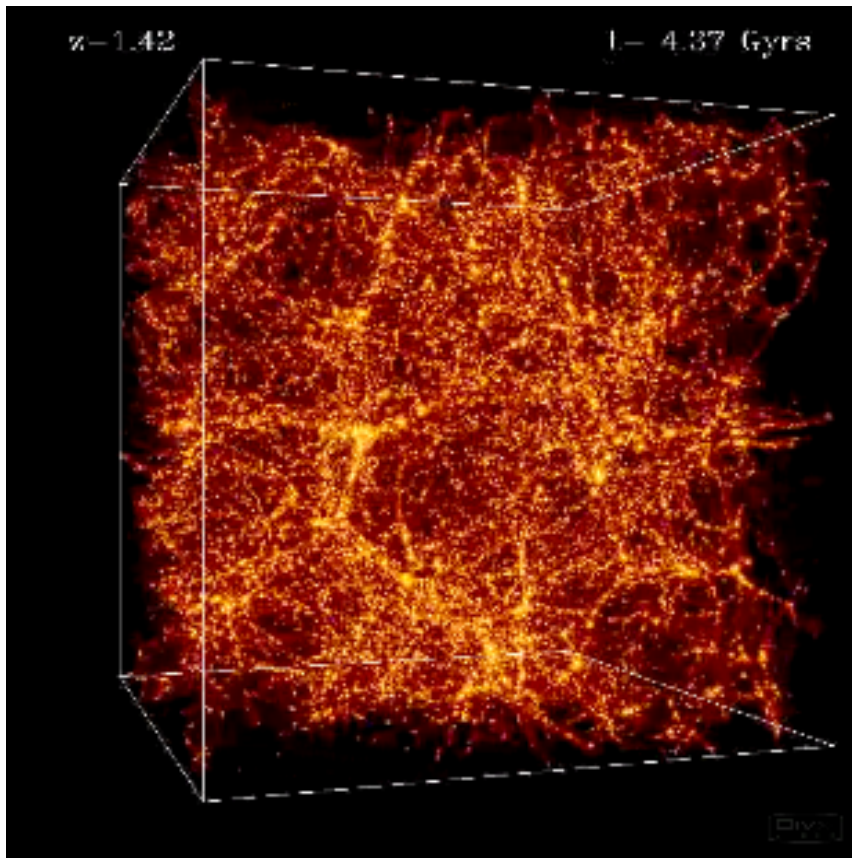


What have we learned from numerical simulations on LSS formation ?

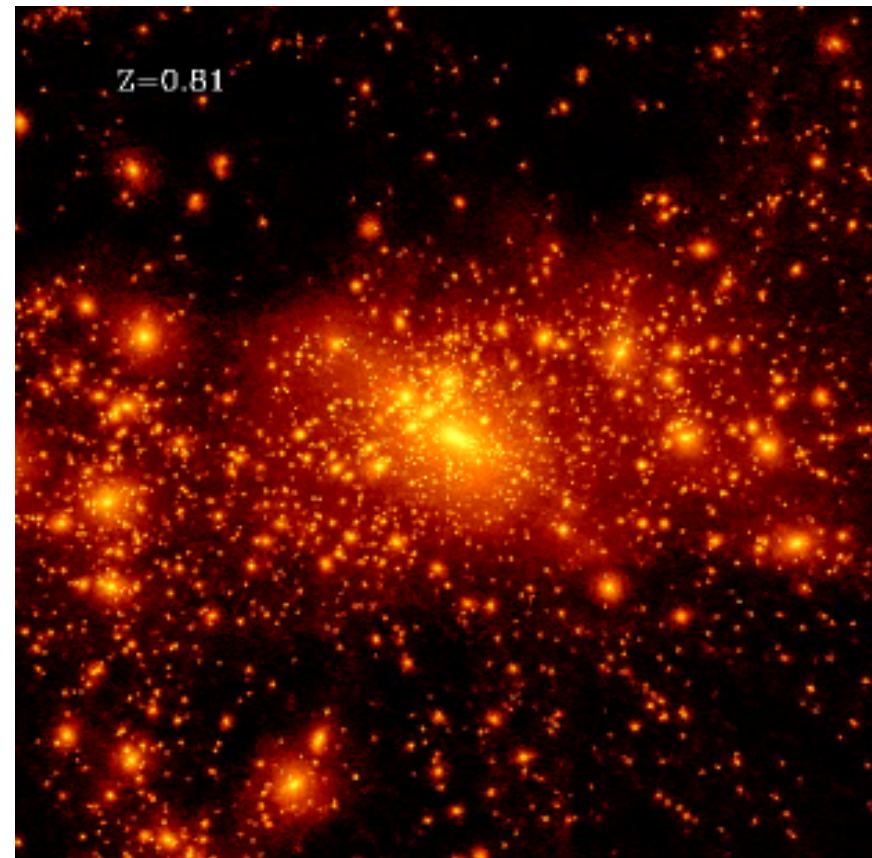
Cosmological Models: General Properties

Large Scale Structure Morphology

Filaments in hierarchical models, large voids, complexity of DM Halos formation....



LSS 60 Mpc, Kravtsov, Klypin et al.; ART Code.



Formation of a MWsize halo, Klypin, Kravtsov et al, ART Code.

What do we have learned from numerical simulations on LSS formation ?

**Numerical Simulation to support for
Observational projects**

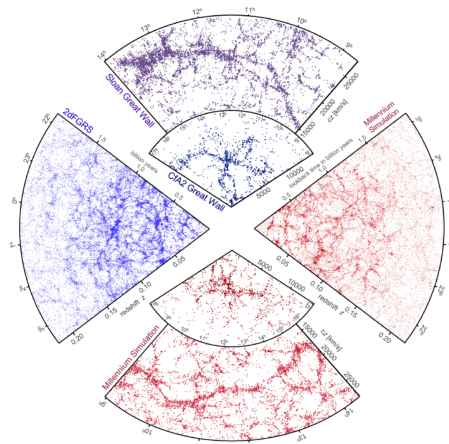
What have we learned from numerical simulations on LSS formation ?

Numerical Simulation and Observational Projects

Numerical simulations of cosmic structure formation
Is a powerful theoretical tool to support present and future cosmological observations (redshift space).

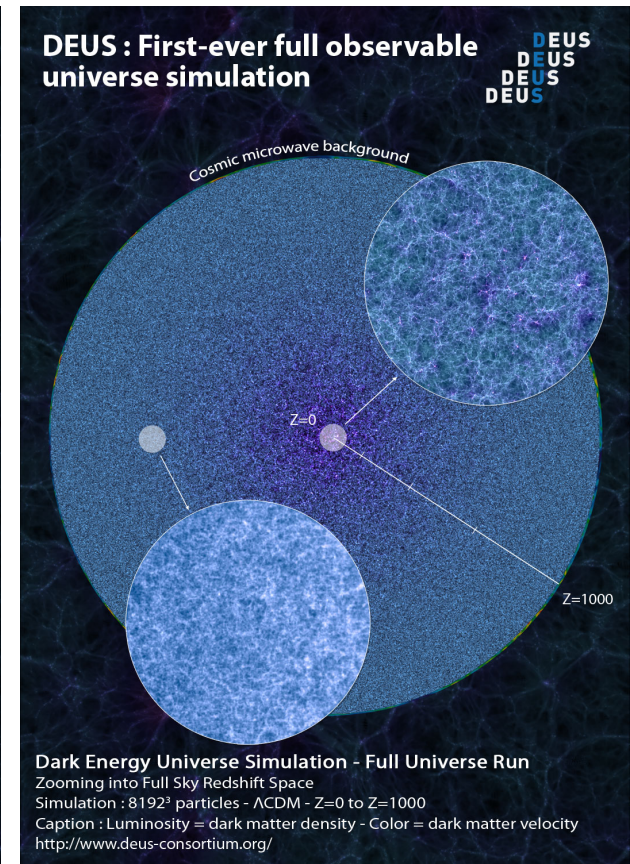
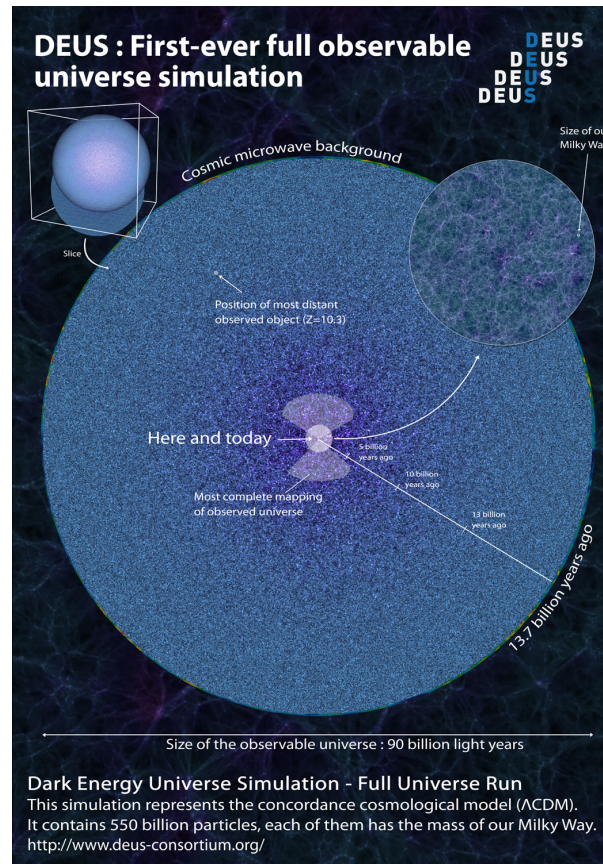
Simulated and
observed large-
scale structure
in the galaxy
distribution

MOCK PIE
DIAGRAMS
COMPARED TO
SDSS, 2DFGRS,
AND CFA-2

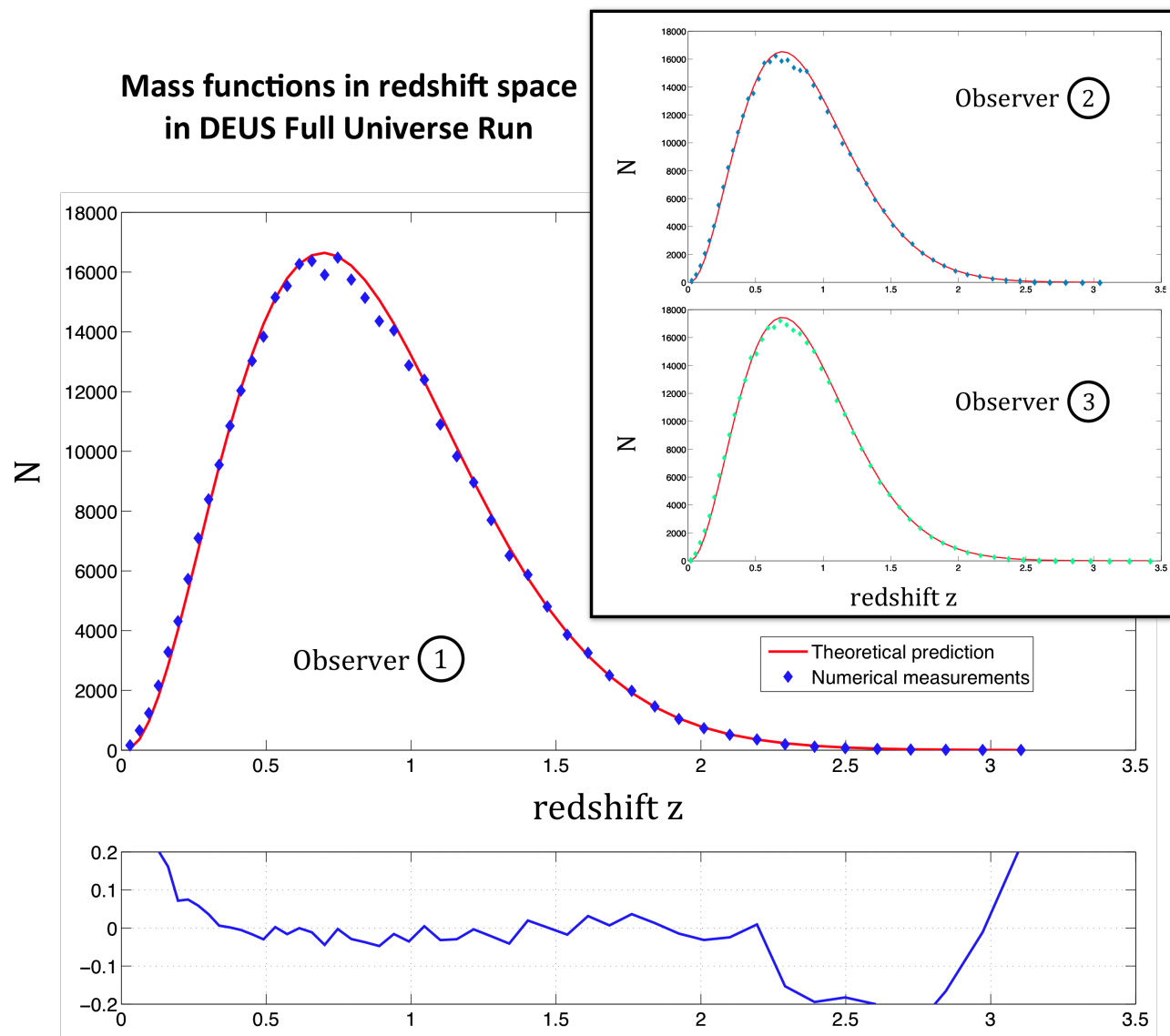


Springel et al. (2006)

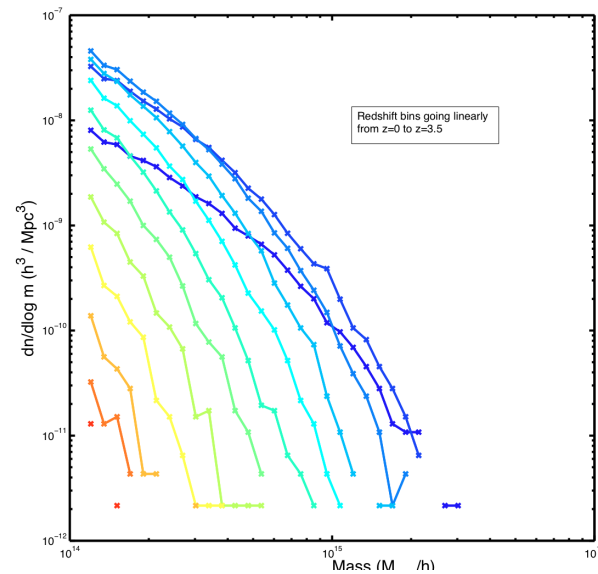
Total full sky lightcone
($z \approx 1100$).
All galaxy cluster in the
observable Universe.
 $10^{14} h^{-1} M_{\odot}$ (galaxy cluster)
when does such a halo
form ? ($z \approx 4$)!



DEUS Full Universe Run: Halos Mass Function in Redshift Space

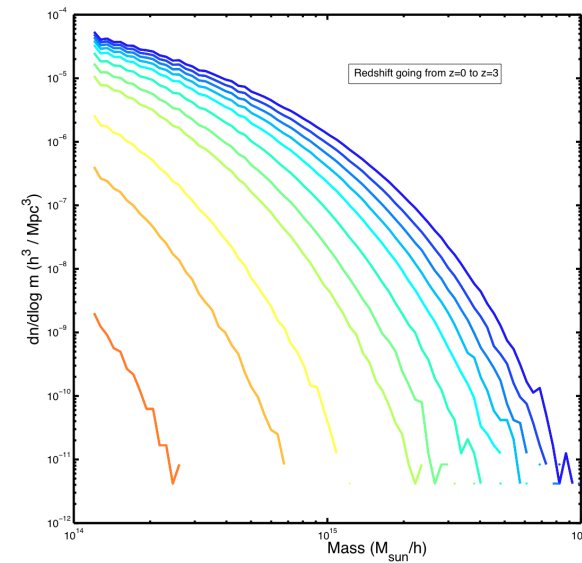


DEUS Full Universe Run: Halos Mass Function in Redshift Space

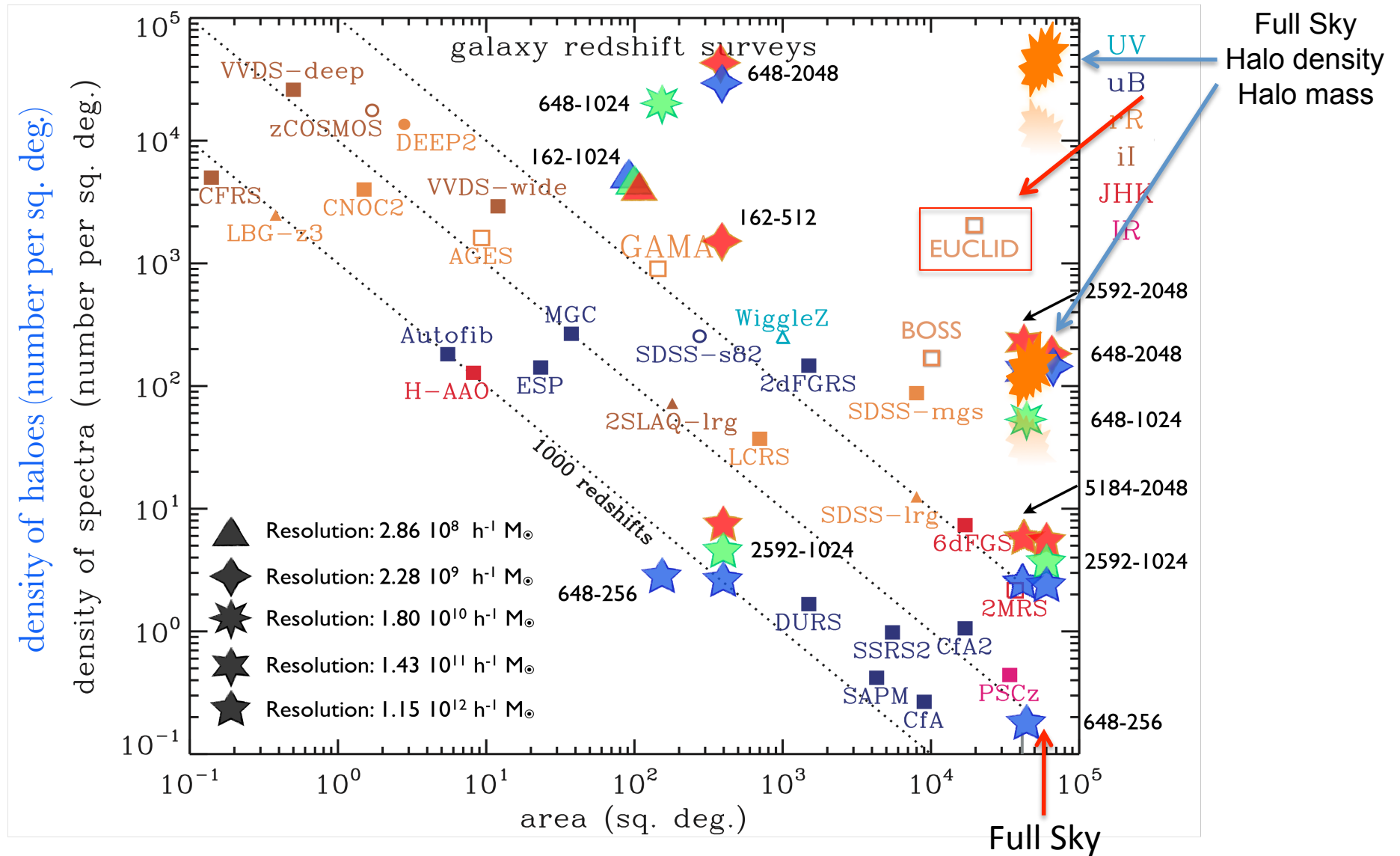


Redshift Space

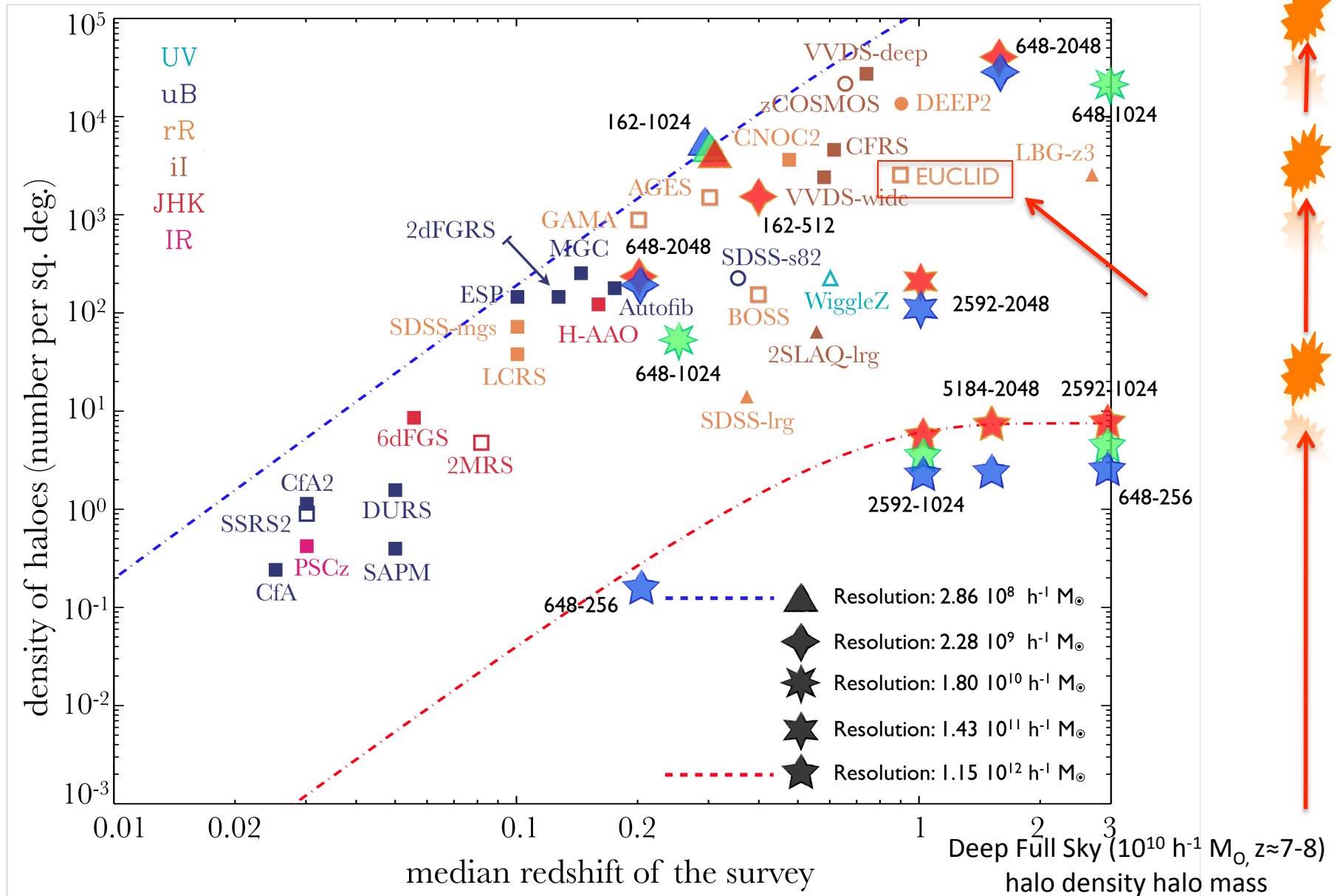
Comoving Space



Observational motivations for DEUS FUR : Redshift Space



Observational motivations for DEUS FUR : Redshift Space

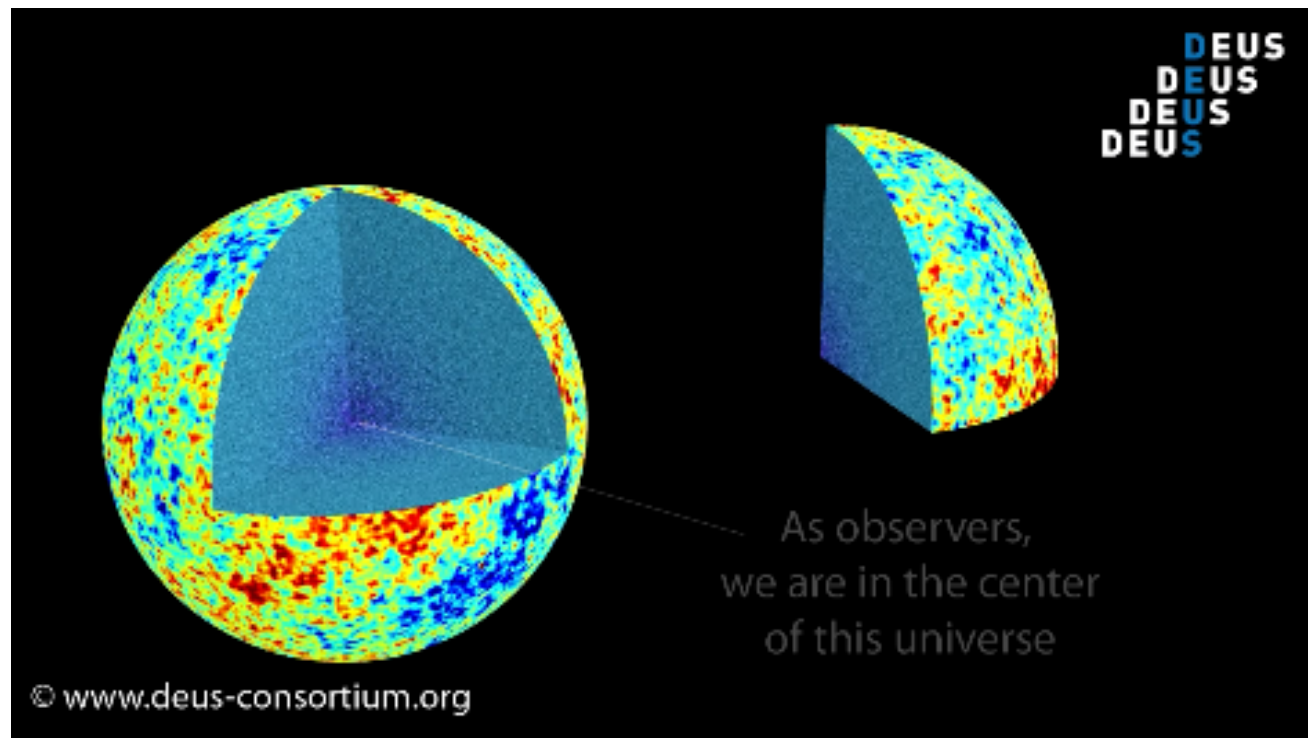


What have we learned from numerical simulations on LSS formation ?

Numerical Simulation and Observational Projects

**Numerical simulations of cosmic structure formation
Is a powerful theoretical tool to support present and future cosmological
observations (redshift space).**

Numerical simulations are useful for upstream calibration, definition,
preparation of instruments and beyond observational projects.



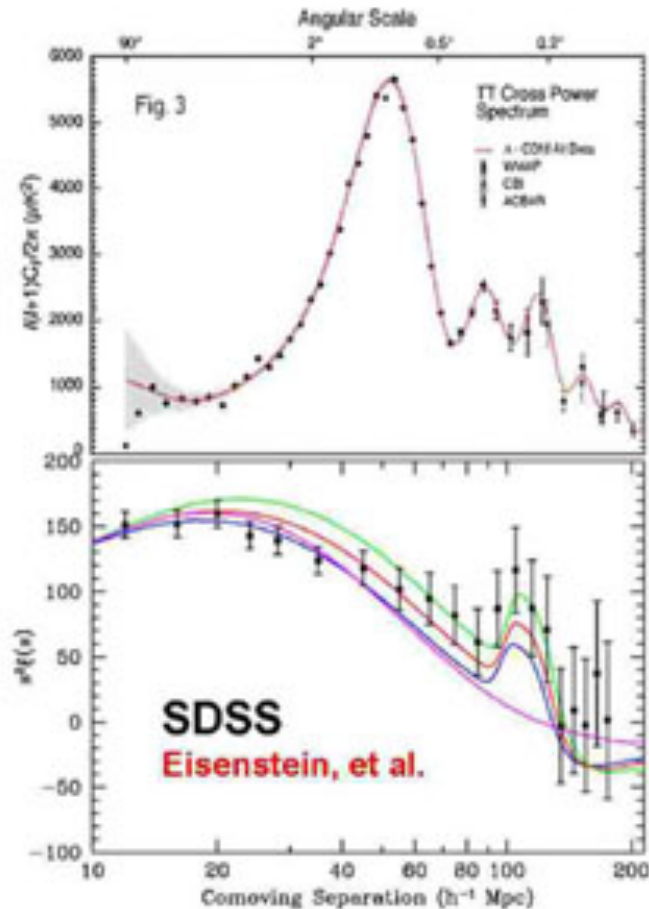
What do we have learned from numerical simulations on LSS formation ?

**Baryonic Acoustic Oscillation:
A probe of the Dark Energy**

What do we have learned from numerical simulations on LSS formation ?

•Baryonic Acoustic Oscillations

Large Scale Structure: Matter distribution, BAO...



Before decoupling between matter and radiation ($z = 1100$) the primordial density fluctuations gave rise to pressure waves (i.e. acoustic oscillations) in the photon-baryon fluid. At decoupling, these oscillations were frozen, leaving their imprint in the CMB, and in the distribution of baryons and dark matter (Peebles & Yu, Sunyaev & Zeldovitch (1970)). This imprint in the fluctuation of the cosmic microwave background, corresponding to the main peak in the CMB power spectrum, and ~ 150 Mpc in the large-scale distribution of galaxies at redshift $z \approx 0.3$ (SDSS-I collaboration (Eisenstein et al 2005)). The phases and amplitudes of BAO in the galaxy power spectrum can be used as cosmological probes to constrain different cosmological models and especially the equation of state parameter w of dark energy.

SDSS-I (47 000, 10%, $z \approx 0.3$), SDSS-II (1 million), BOSS (1.5 million, 25 %, $z \approx 0.8$, $V_{\text{BOSS}} = 5 \times V_{\text{SDSS-II}}$).

larger and larger volume / **non-linear structure growth**, redshift space effects, and biasing

What do we have learned from numerical simulations on LSS formation ?

« PERTURBATION THEORY RELOADED. II. NONLINEAR BIAS, BARYON ACOUSTIC OSCILLATIONS, AND MILLENNIUM SIMULATION IN REAL SPACE », D. Jeong and E. Komatsu

ApJ, 691:569–595, 2009 January 20

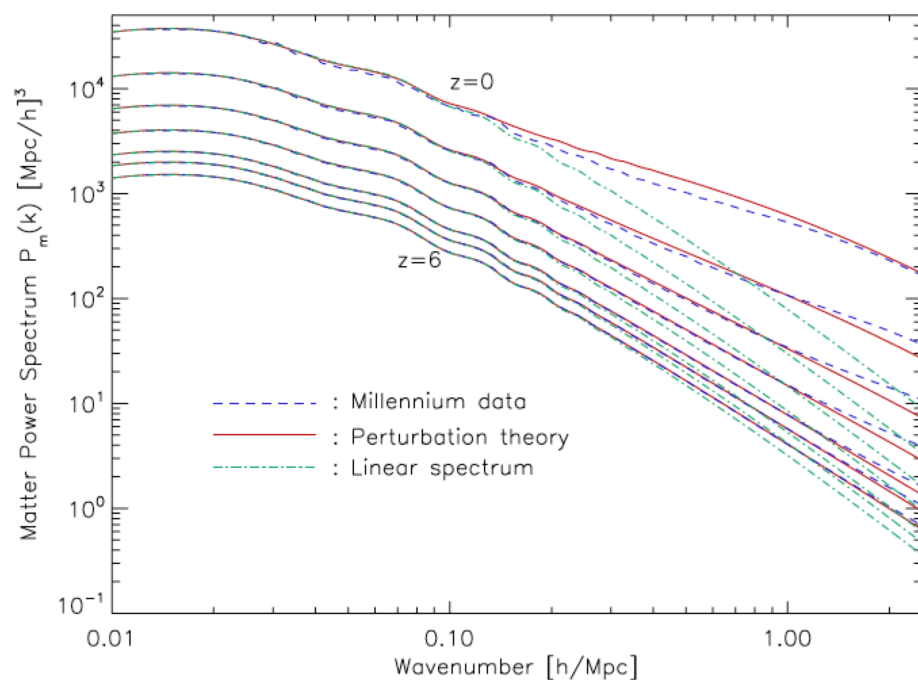


Figure 1. Matter power spectrum at $z = 0, 1, 2, 3, 4, 5$, and 6 (from top to bottom) derived from the Millennium Simulation (dashed lines), the third-order PT (solid lines), and the linear PT (dot-dashed lines).

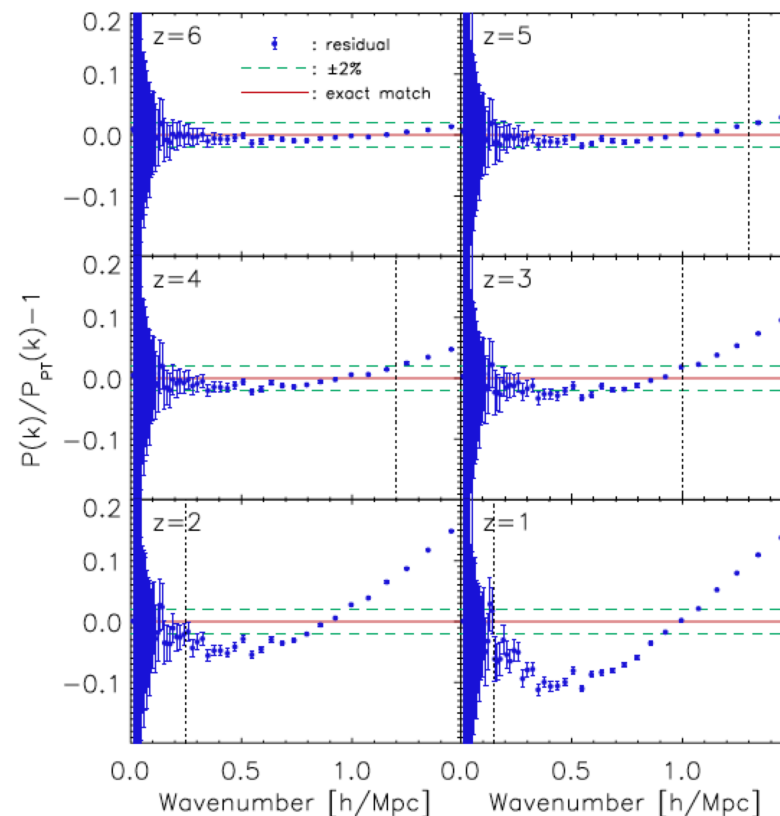
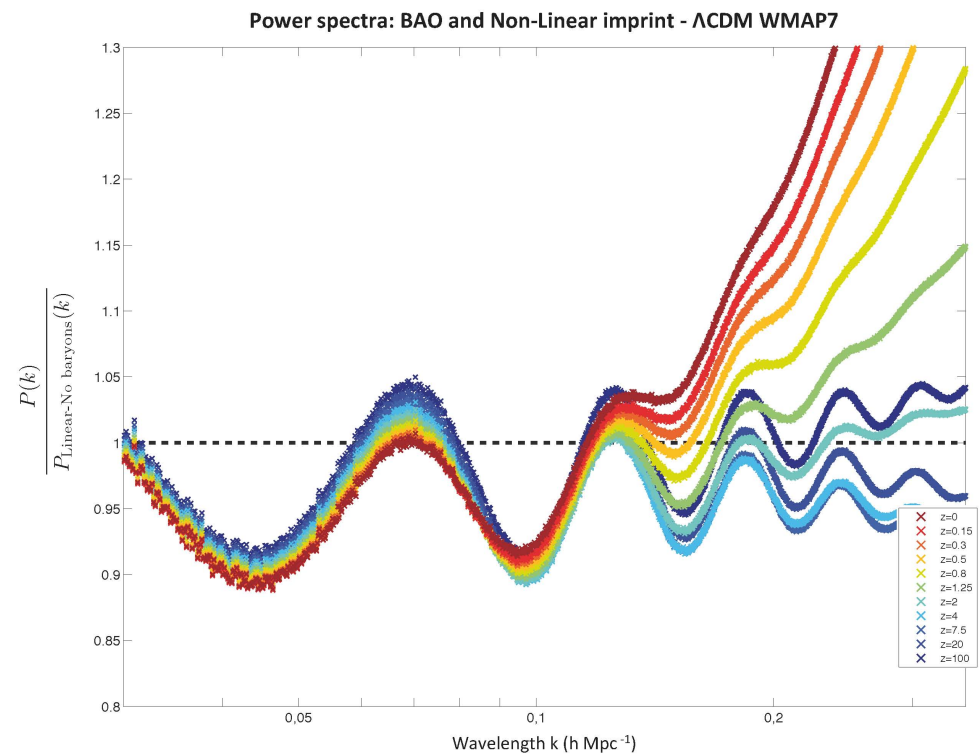
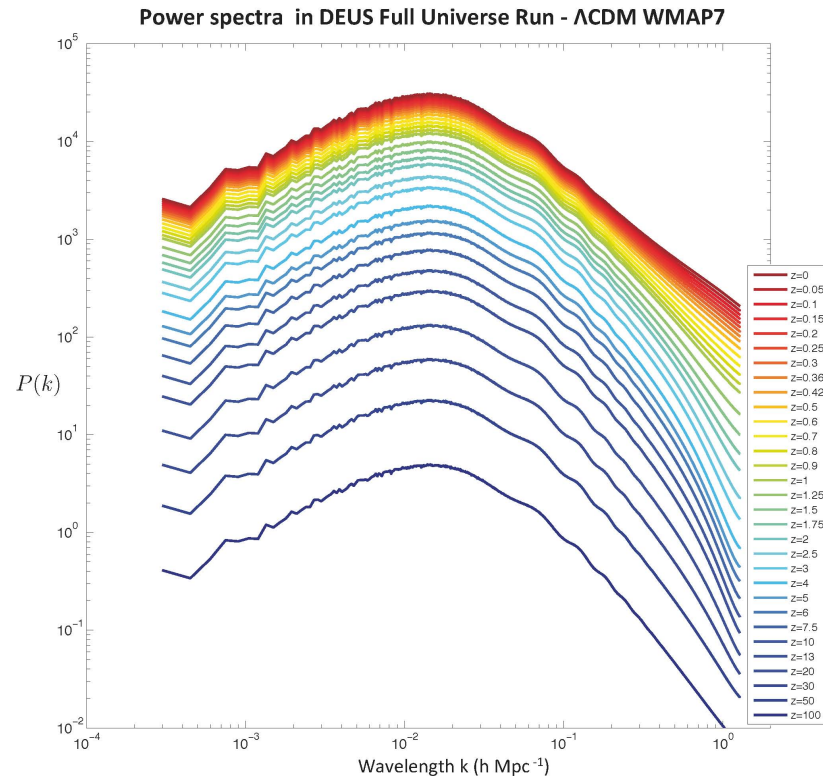


Figure 3. Fractional difference between the matter power spectra from the third-order PT and that from the Millennium Simulation, $P_m^{\text{sim}}(k)/P_m^{\text{PT}} - 1$ (dots with error bars). The solid lines show the perfect match, while the dashed lines show $\pm 2\%$ accuracy. We also show $k_{\text{max}}(z)$, below which we trust the prediction from the third-order PT, as a vertical dotted line.

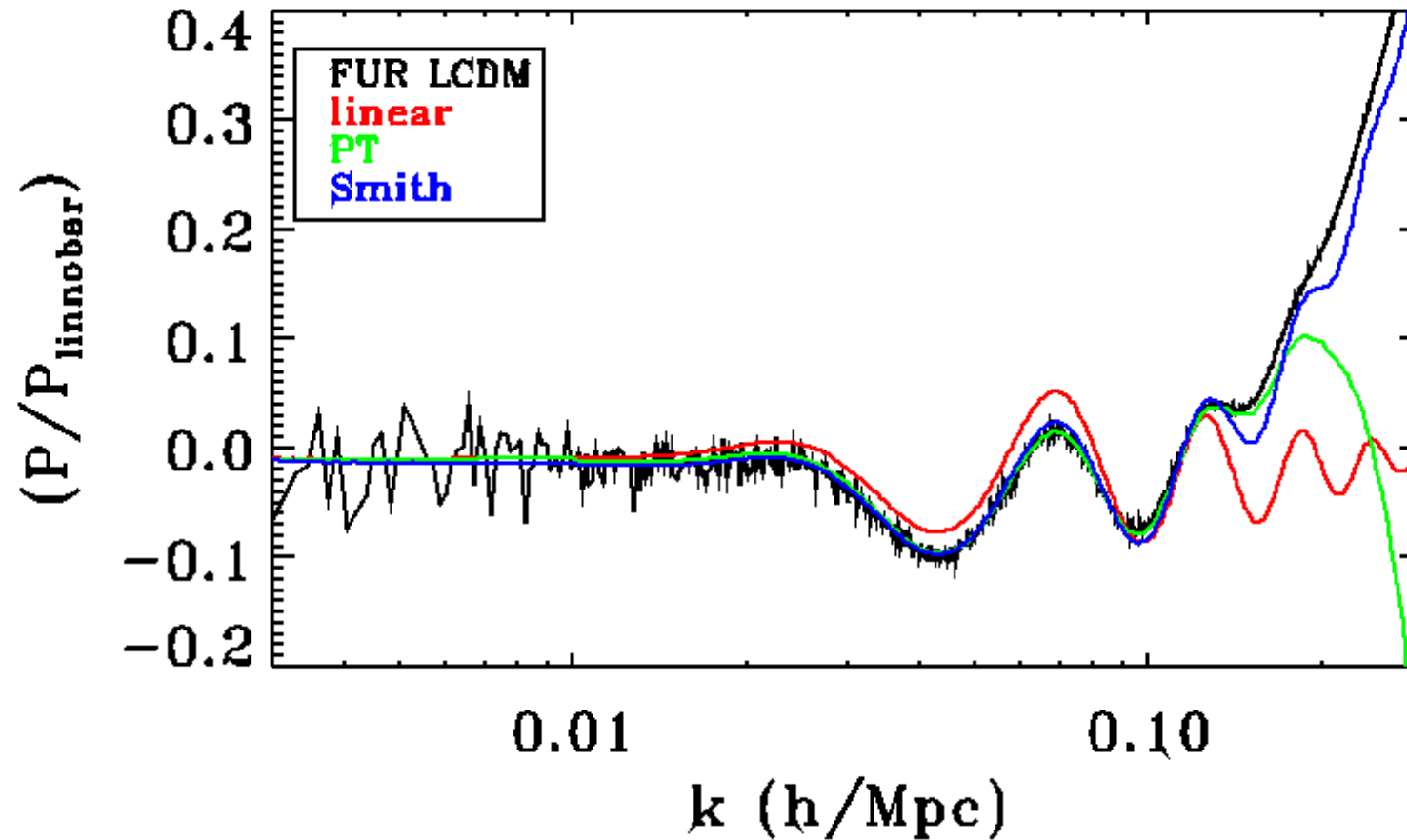
What do we have learned from numerical simulations on LSS formation ?

Power Spectrum In DEUS: BAO - non linear dynamics effects



What have we learned from numerical simulations on LSS formation ?

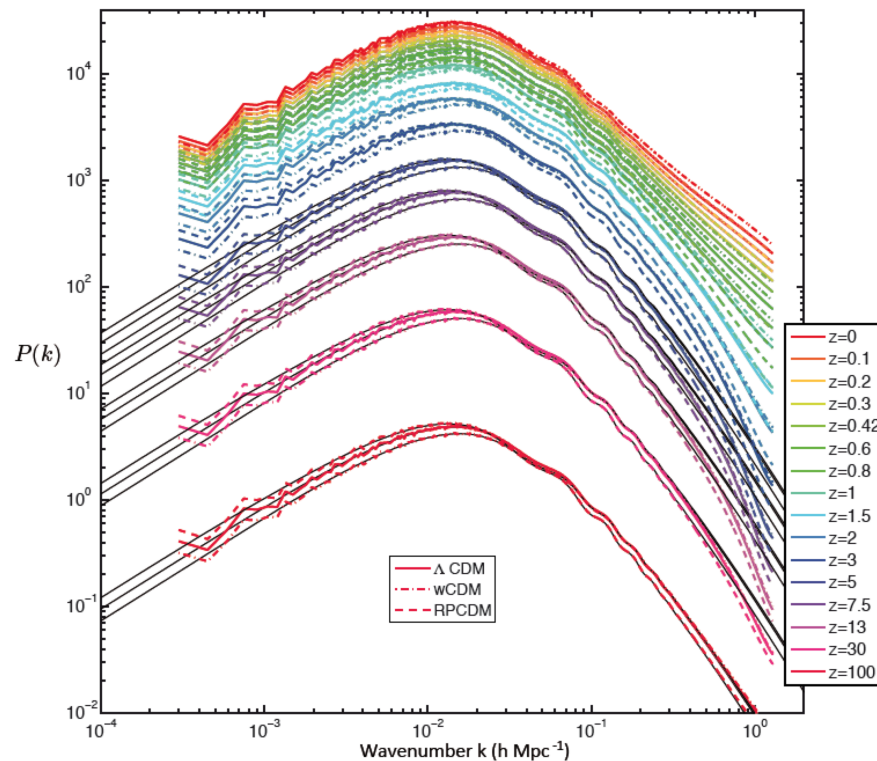
Power Spectrum In DEUS: BAO - non linear dynamics effects



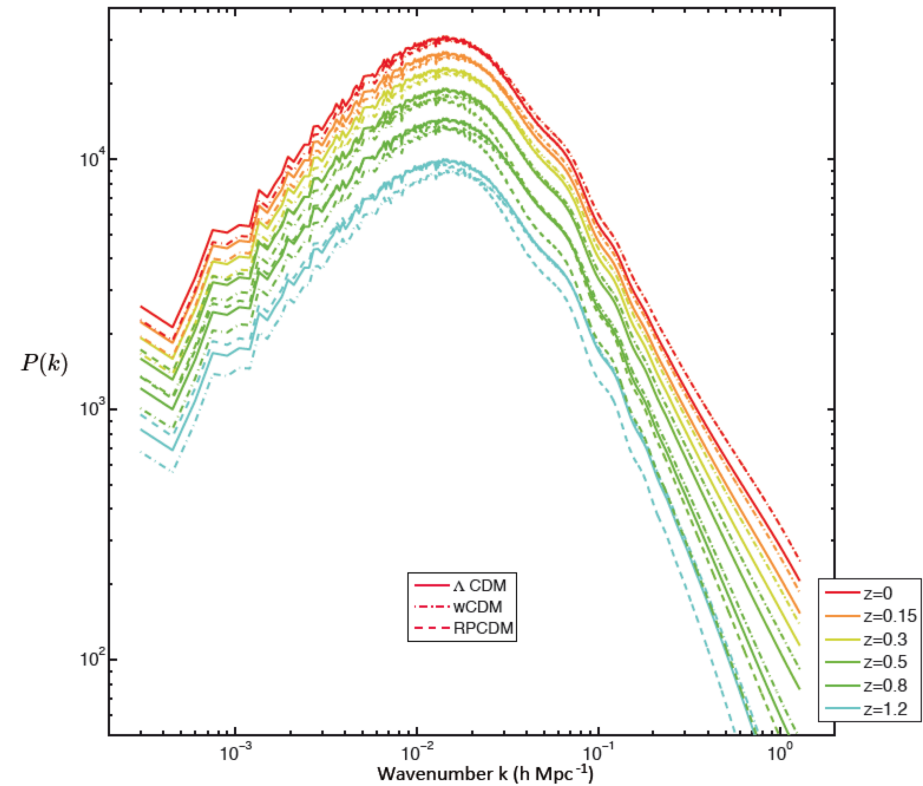
What have we learned from numerical simulations on LSS formation ?

Power spectrum Comparison in Λ CDM- w CDM-RPCDM

Power spectra in DEUS Full Universe Runs:
 Λ CDM - w CDM - RPCDM WMAP7



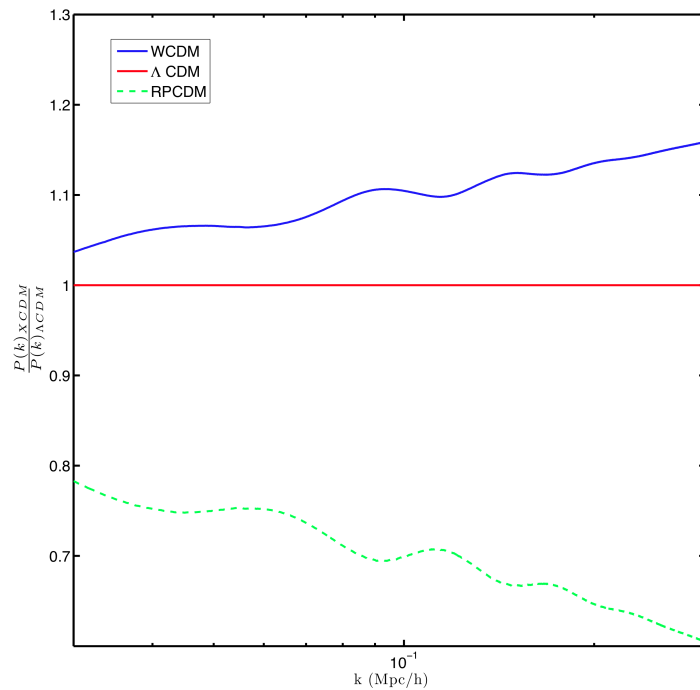
Zoom on power spectra in DEUS Full Universe Runs:
 Λ CDM - w CDM - RPCDM WMAP7



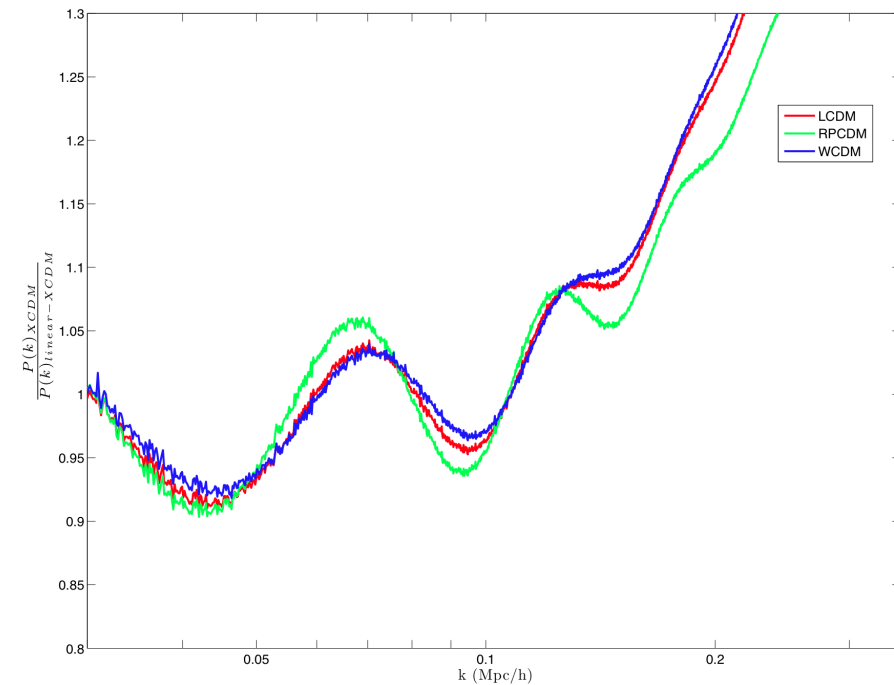
What have we learned from numerical simulations on LSS formation ?

Large Scale Structure: Matter distribution, BAO...

BAO: Dark Energy Probe



$$\frac{P_{XCDM}(k)}{P_{\Lambda CDM}(k)}$$

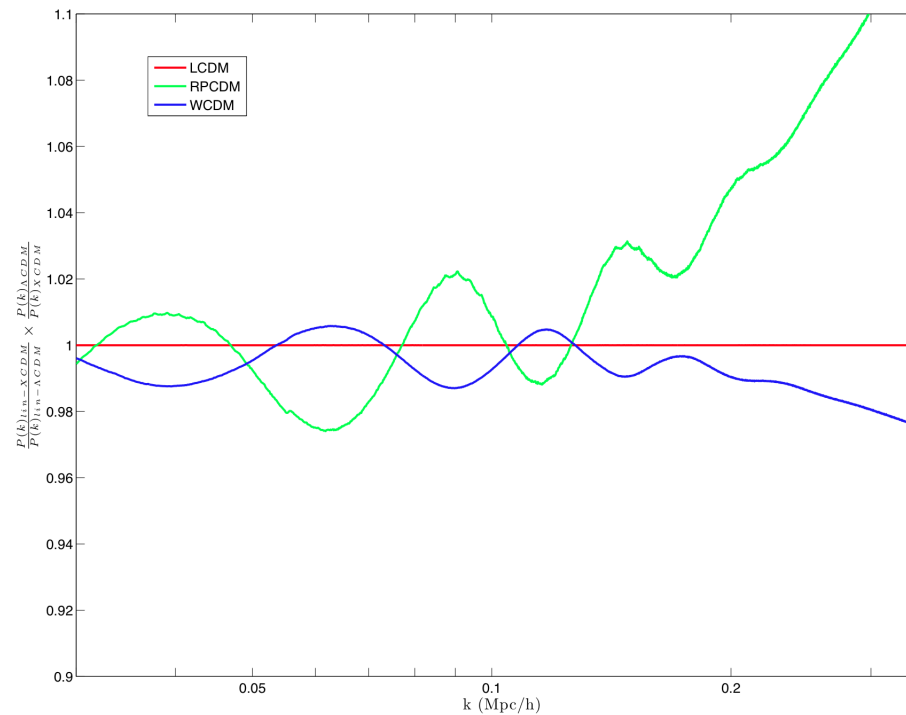


$$\frac{P_{XCDM}(k)}{P_{XCDM-linear_no_baryon}(k)}$$

What have we learned from numerical simulations on LSS formation ?

Large Scale Structure: Matter distribution, BAO...

BAO: Dark Energy Probe



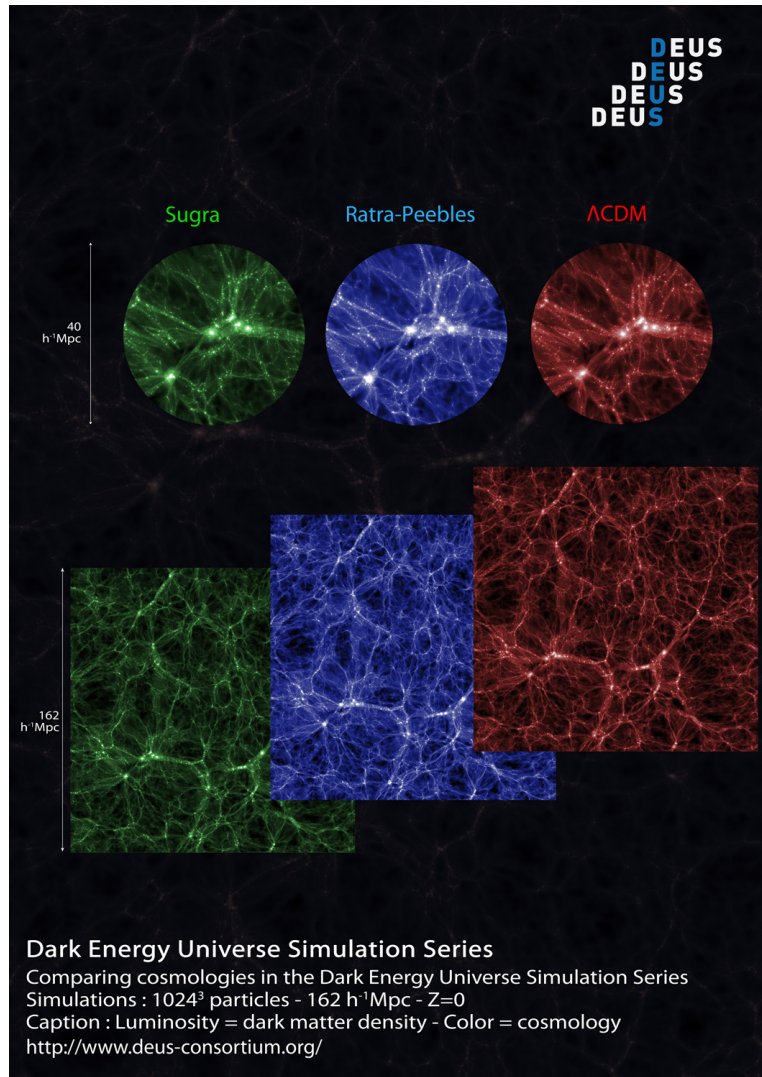
$$\frac{P_{\Lambda\text{CDM}}(k)}{P_{\text{XCDM}}(k)} \frac{P_{\text{XCDM-linear_no_baryon}}(k)}{P_{\Lambda\text{CDM-linear_no_baryon}}(k)}$$

What do we have learned from numerical simulations on LSS formation ?

Halo Spatial Distribution: Bias and Dark Energy

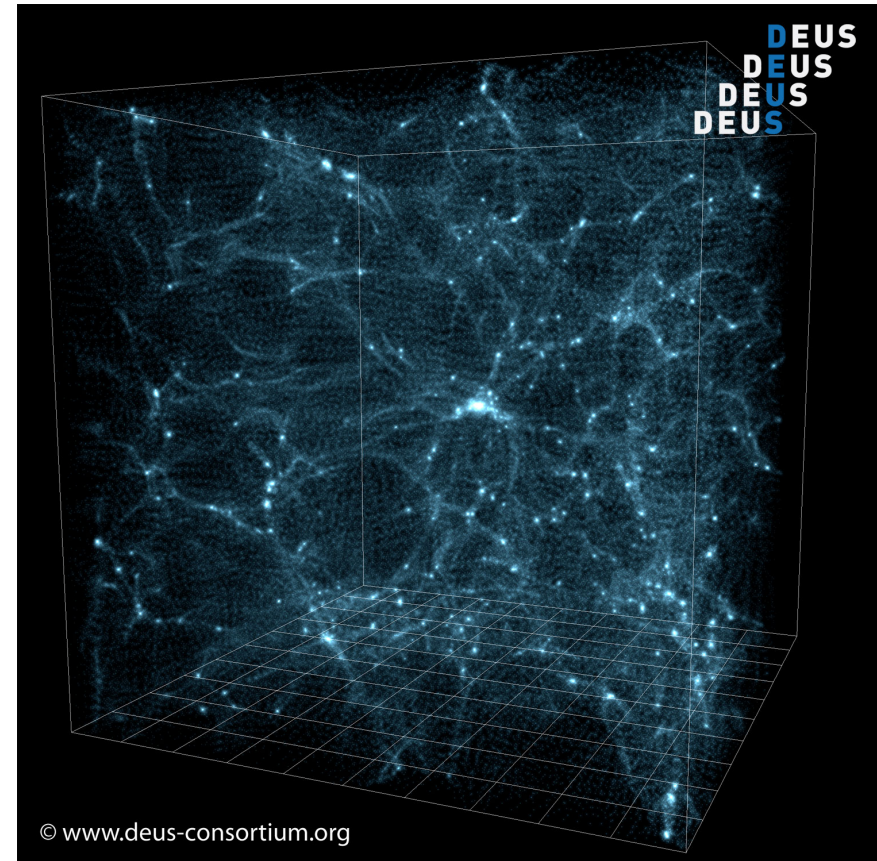
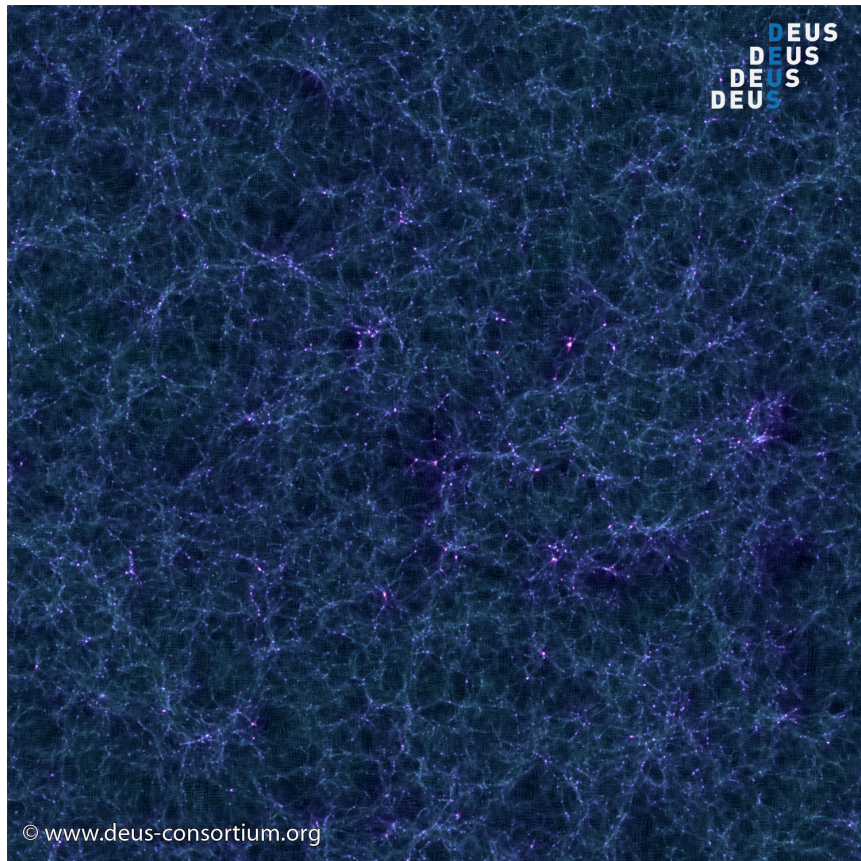
What have we learned from numerical simulations on LSS formation ?

Large Scale Structure: Matter distribution, Halos Distribution, Bias Halos / Matter...



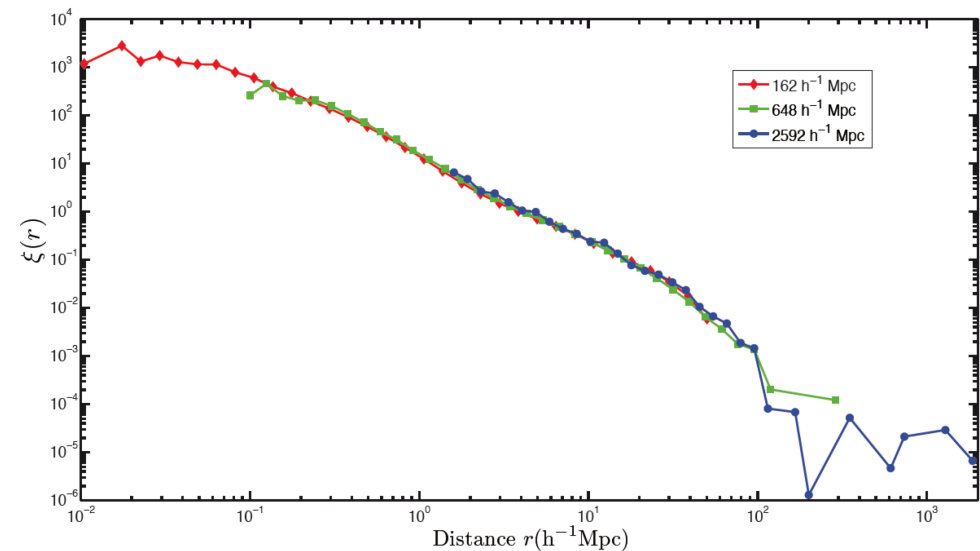
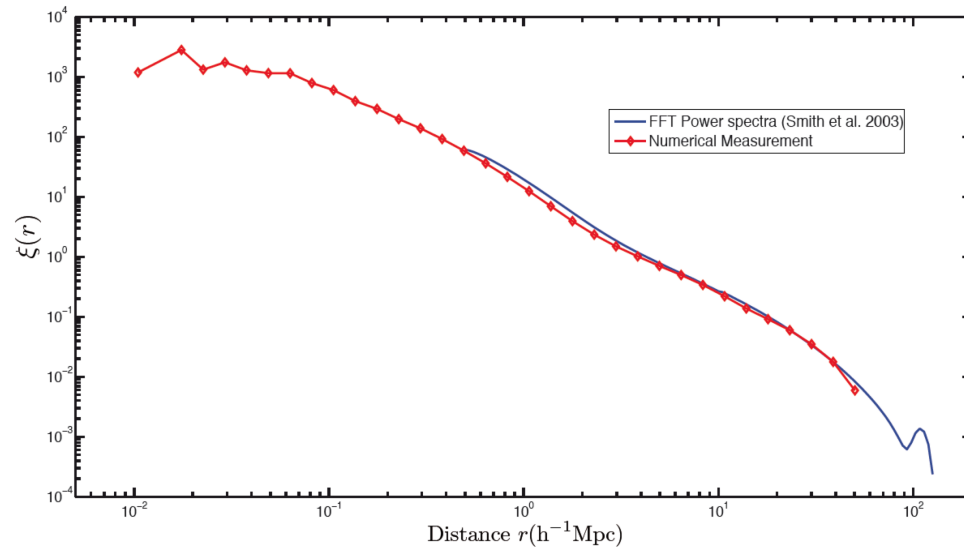
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Large Scale Structure: Matter distribution, Halos Distribution, Bias Halos / Matter...

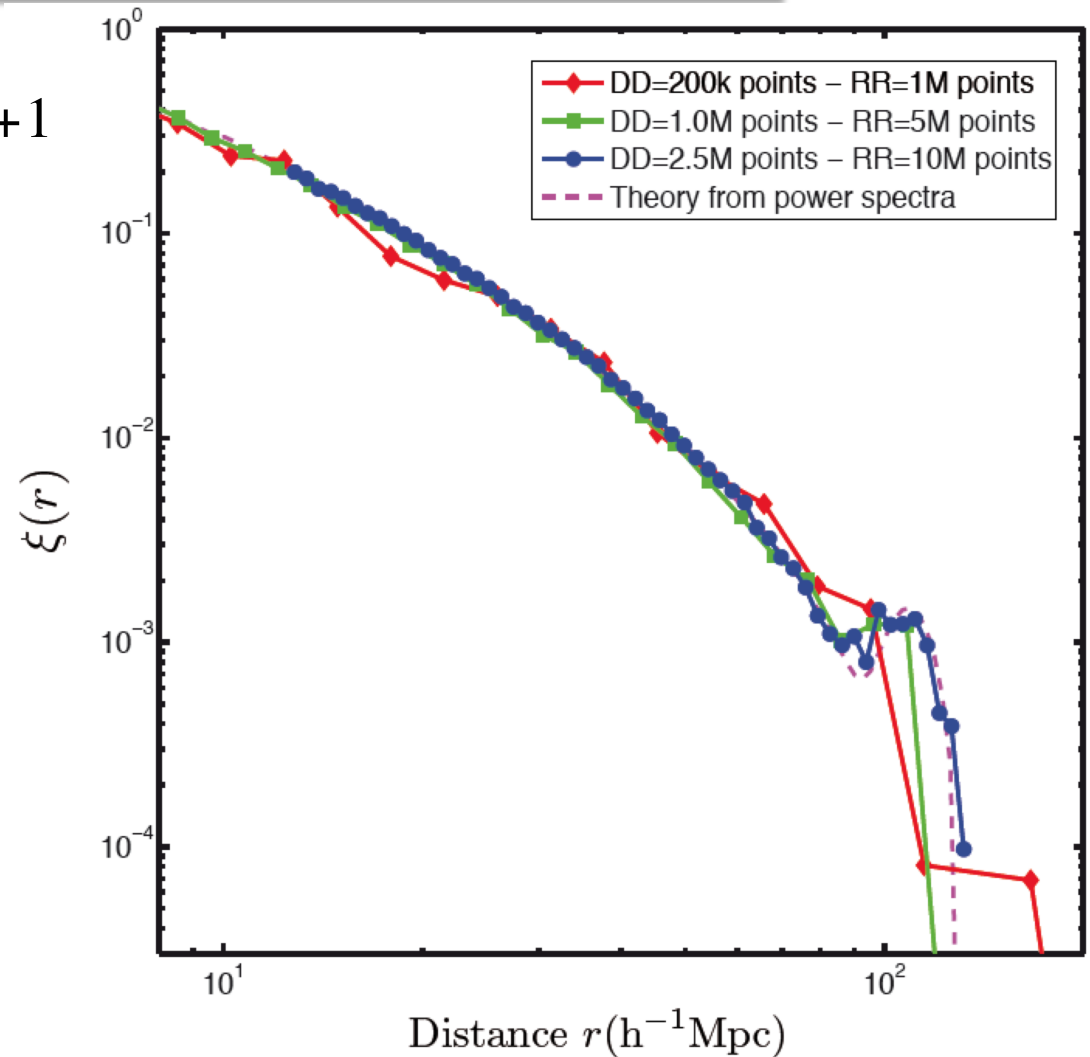


What have we learned from numerical simulations on LSS formation ?

Large Scale Structure:
Matter distribution, Halos Distribution, Bias Halos / Matter...

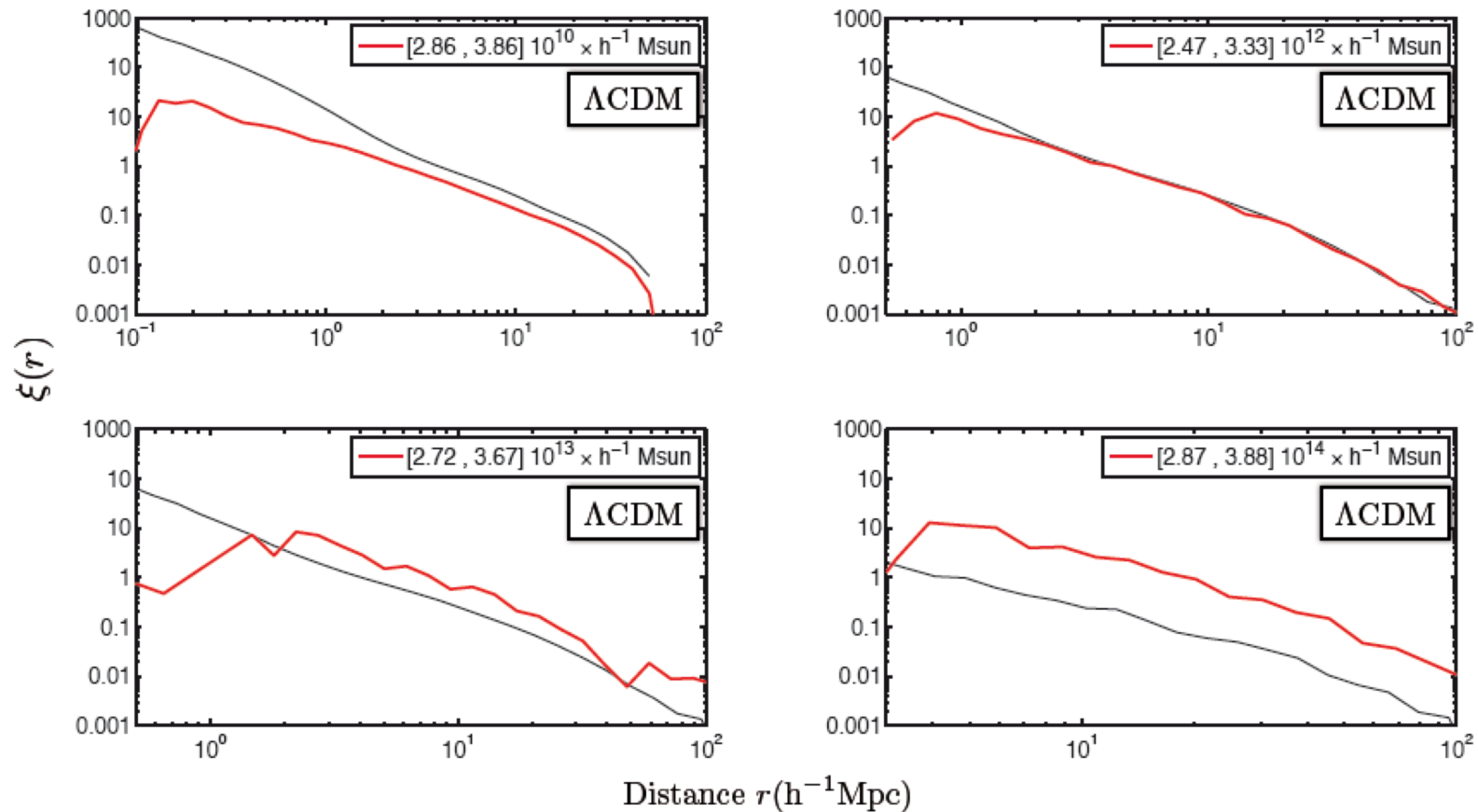
$$\xi(r) = \frac{n_R(n_R - 1)}{n_D(n_D - 1)} \frac{DD}{RR} - 2 \frac{n_R - 1}{n_D} \frac{DR}{RR} + 1$$

Landy and Szalay 1993
(see Peebles 1980, Blanchard and Alimi 1988...)



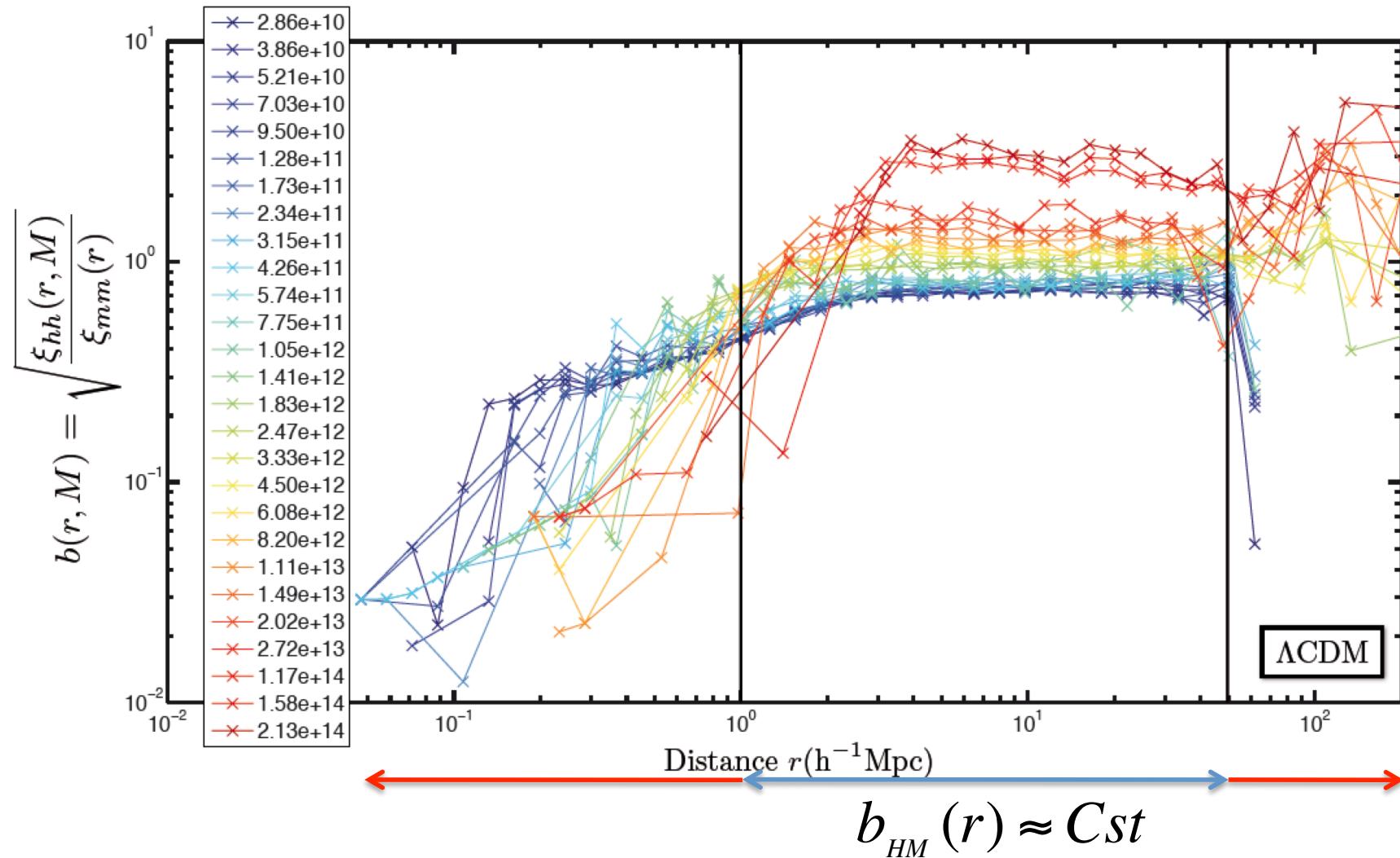
What have we learned from numerical simulations on LSS formation ?

Halos Distribution, Bias Halos / Matter...



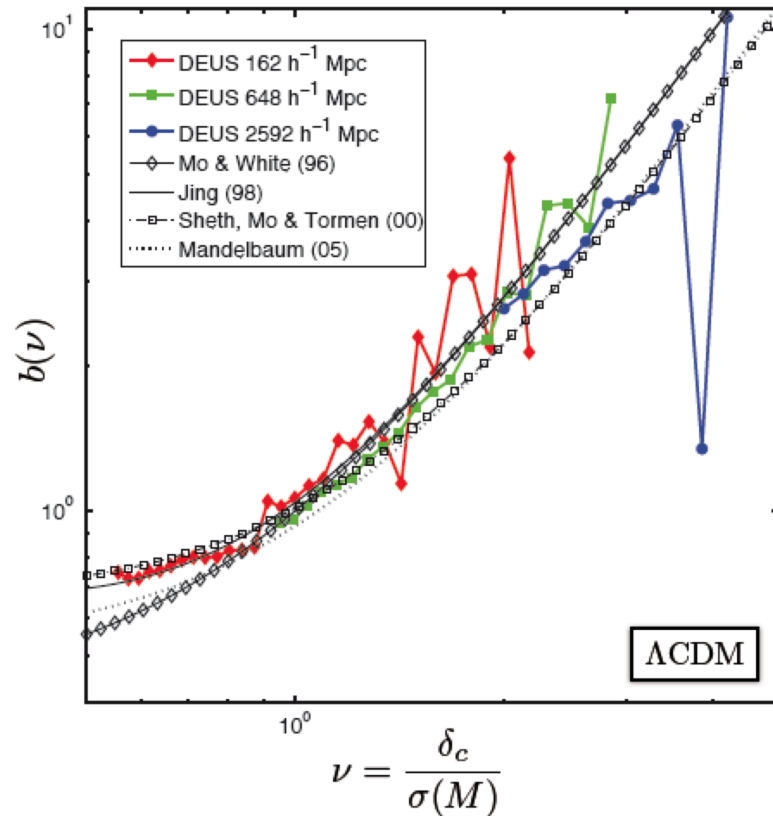
What have we learned from numerical simulations on LSS formation ?

Halos Distribution, Bias Halos / Matter... scale dependence



What have we learned from numerical simulations on LSS formation ?

Halos Distribution, Bias Halos / Matter... Comparison to some models



$$b_{\text{Mo \& White}} = 1 + \frac{v^2 - 1}{\delta_c}$$

$$b_{\text{Sheth}} = 1 + \frac{dv^2 - 1}{\delta_c} + 2 \frac{p/\delta_c}{(1 + (dv^2)^p)} \text{ with } d = 0.707, p = 0.3$$

$$b_{\text{Jing}} = \left(\frac{0.5}{v^4} + 1 \right)^{0.06 - 0.02n} \times \left(1 + \frac{v^2 - 1}{\delta_c} \right) \text{ with } n = -2$$

$$b_{\text{Mandelbaum}} = 1 + \frac{av^2 - 1}{\delta_c} + 2 \frac{p}{\delta_c (1 + (av^2)^p)} \text{ with } a = 0.73, p = 0.15$$

What have we learned from numerical simulations on LSS formation ?

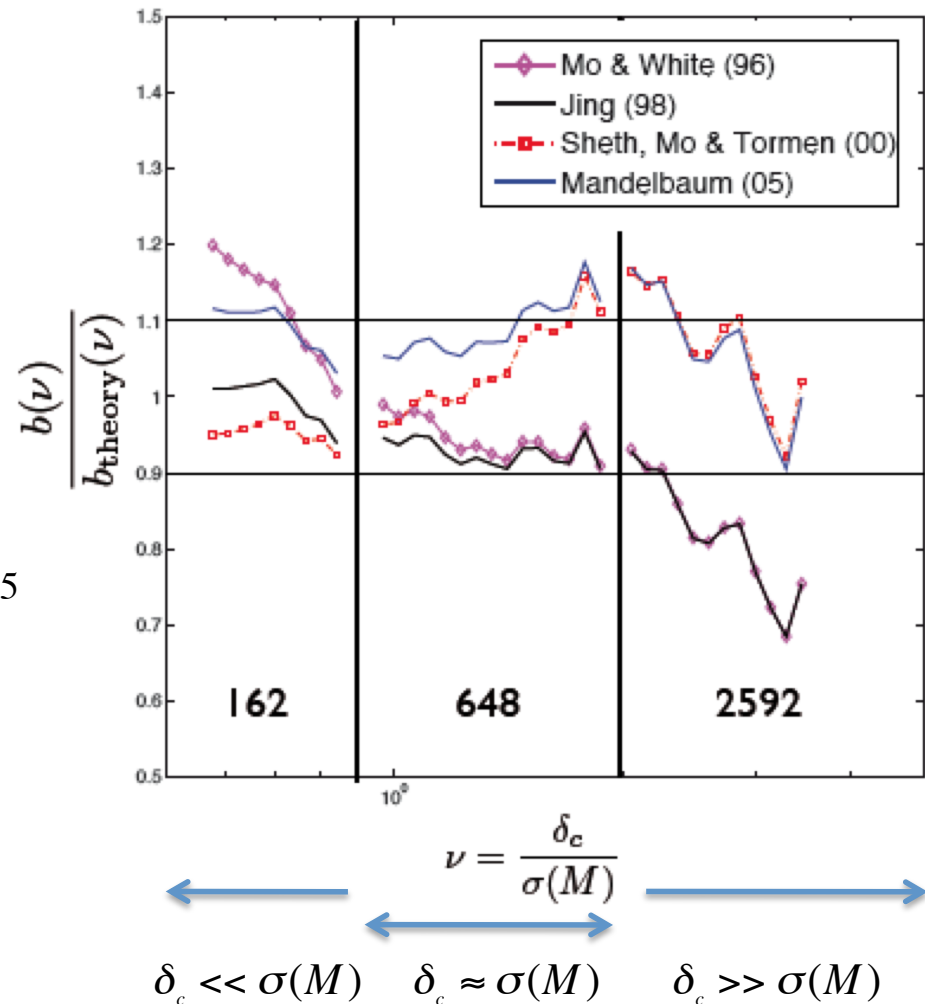
Halos Distribution, Bias Halos / Matter... Comparison to some models

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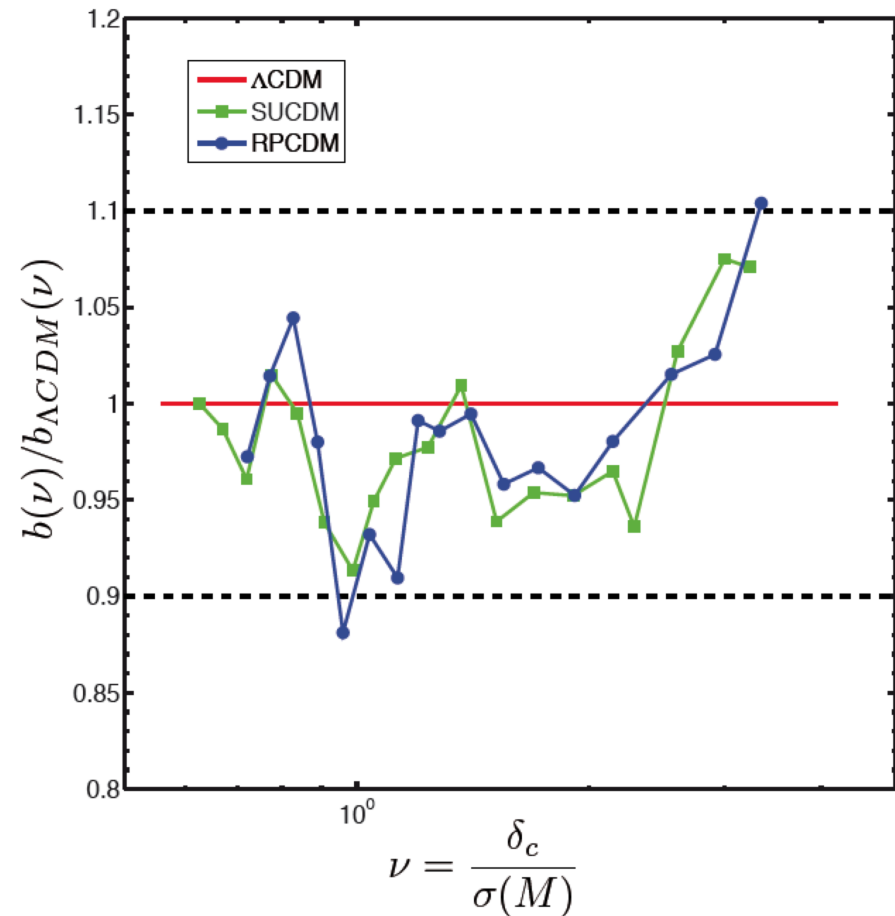
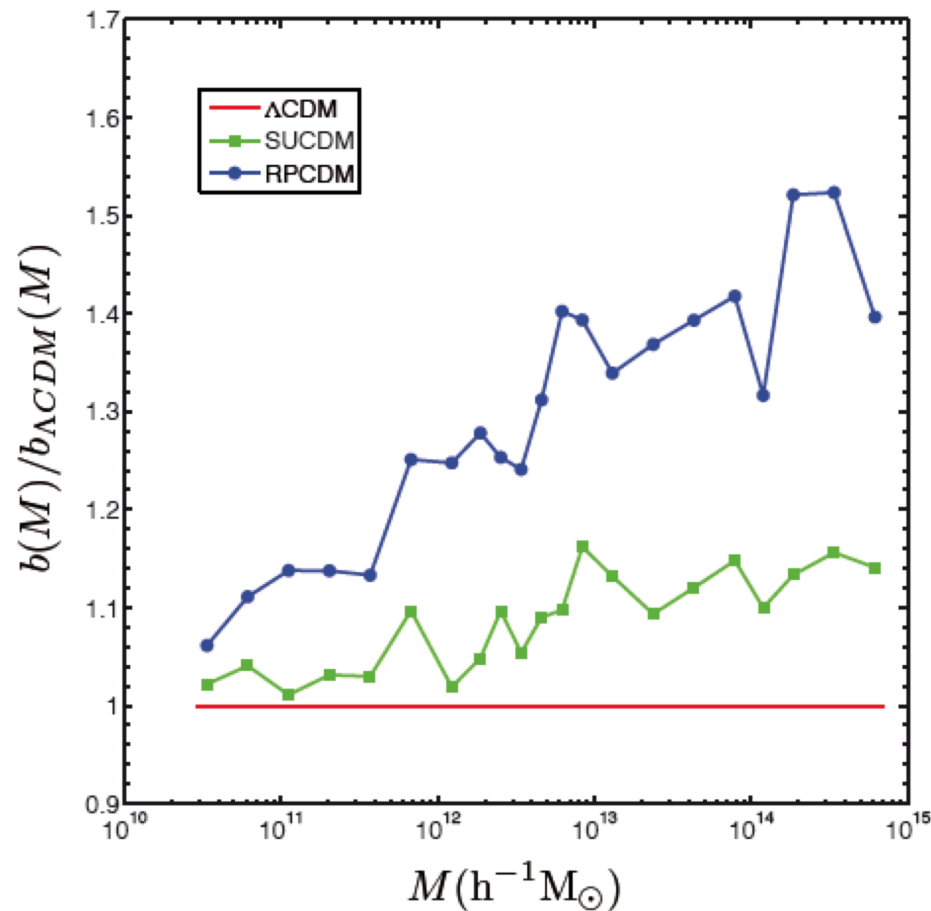
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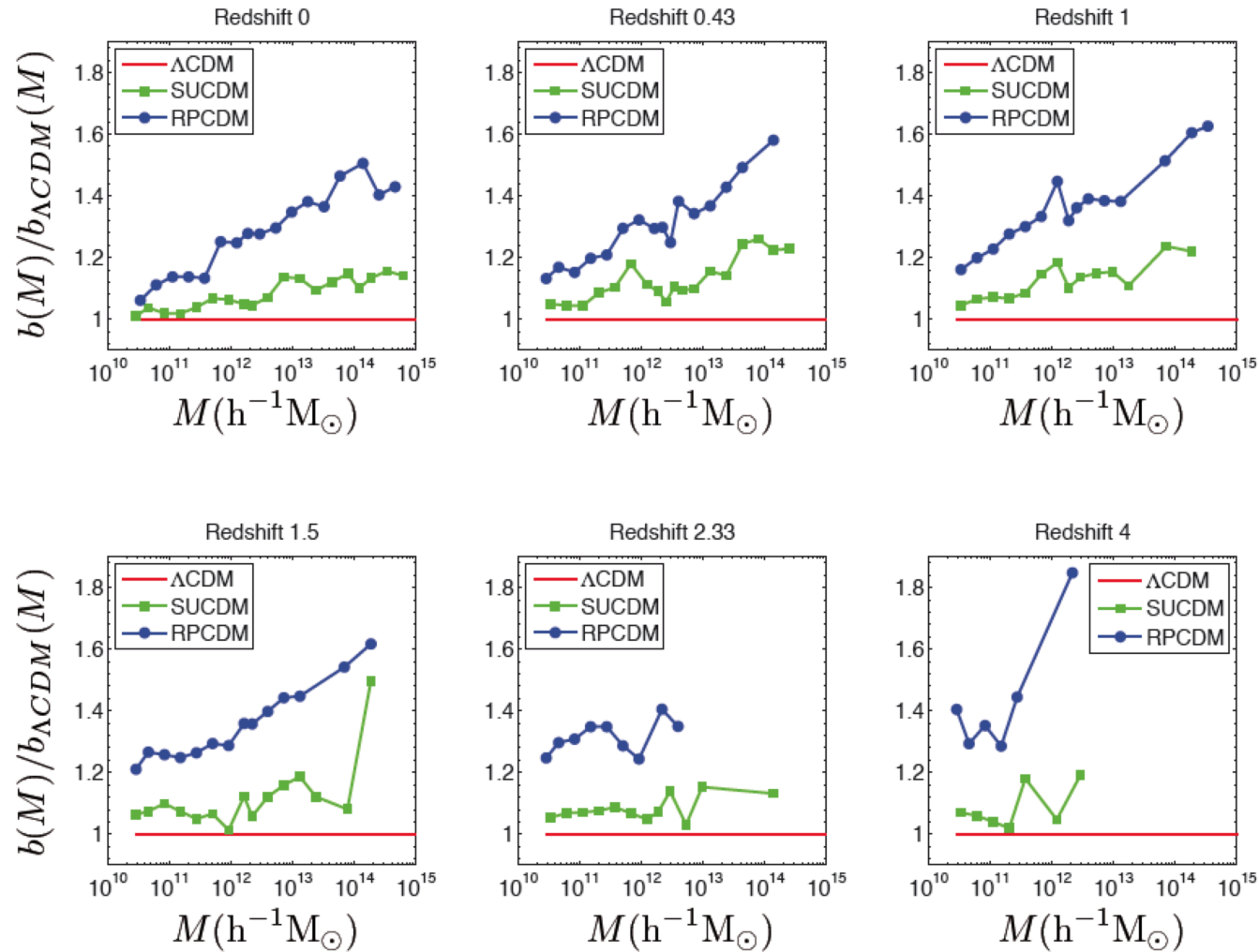
What have we learned from numerical simulations on LSS formation ?

Bias Halos / Matter... Mass dependence and Cosmology



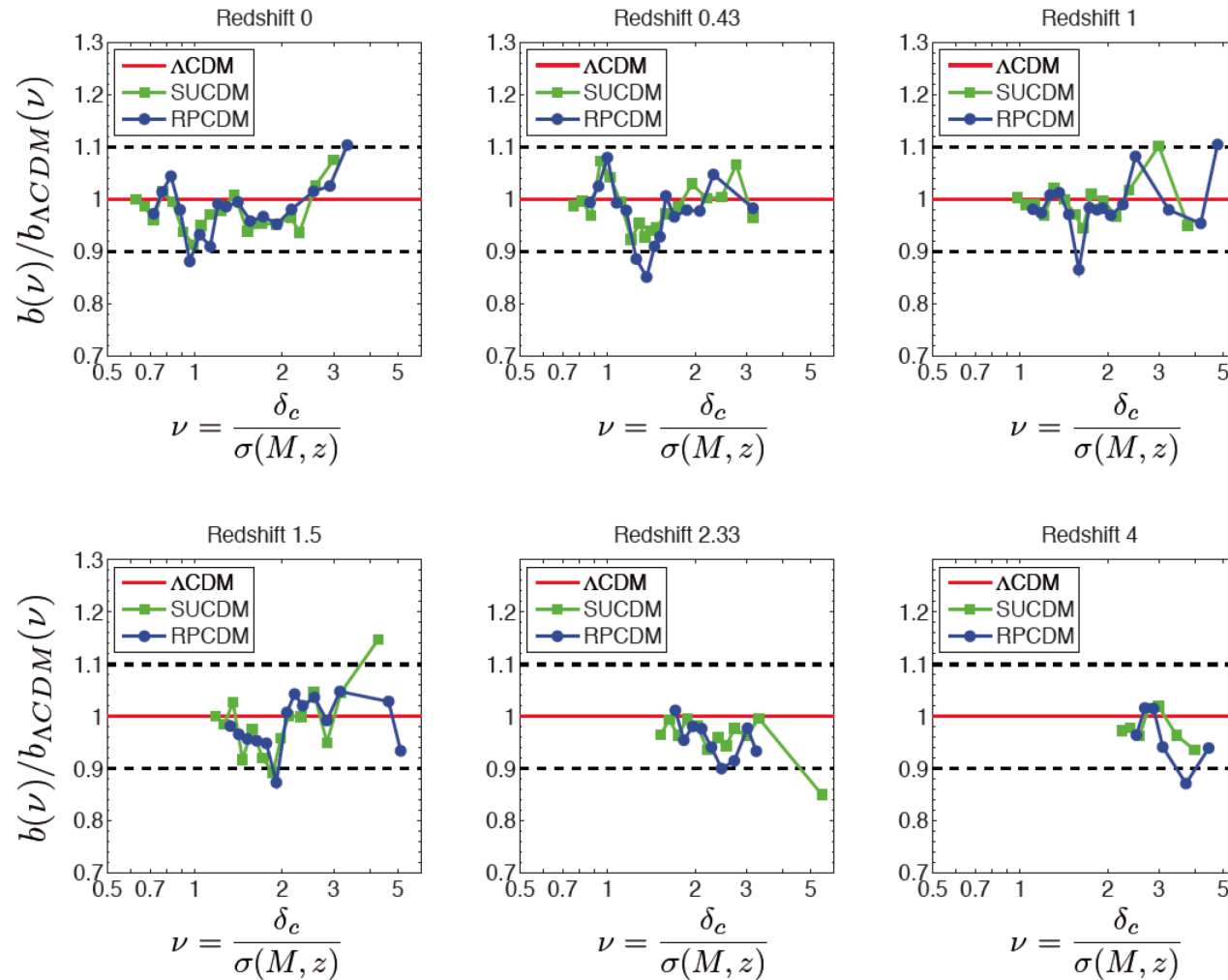
What have we learned from numerical simulations on LSS formation ?

Bias Halos / Matter... Redshift dependence and Cosmology



What have we learned from numerical simulations on LSS formation ?

Bias Halos / Matter... Redshift dependence and Cosmology



What do we have learned from numerical simulations on LSS formation ?

Origin of cosmological bulk flow

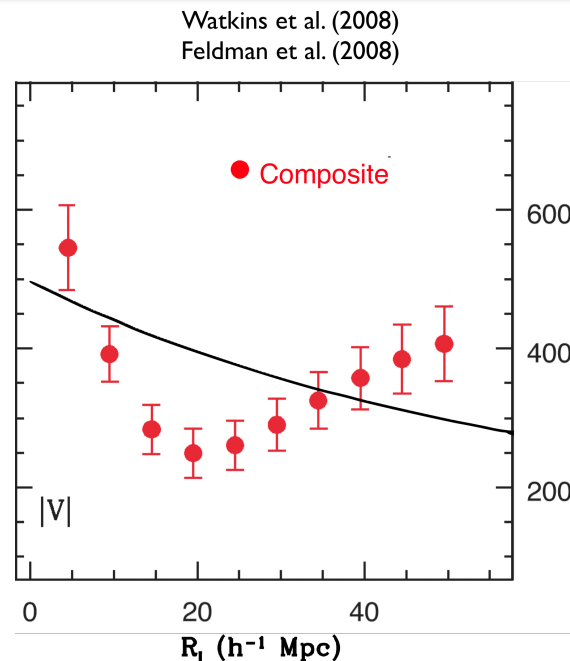
What have we learned from numerical simulations on LSS formation ?

Large Scale Structure: Bulk Flow

Abnormal Observational signal on **Bulk Flow** in velocity surveys

(Watkins et al 2008, Feldman et al 2008, Lavaux et al 2009 (2MRS survey (redshift survey)...))

High deviation from linear predictions.



$$v_{bulk}(R) = \left\| \frac{1}{N_{h,r < R}} \sum_i^{N_{h,r < R}} \vec{v}_i \right\|$$

Mean of the (peculiar) velocity fields present in a sphere of radius R centered on the Milky Way

$$v_{bulk} = \sqrt{\langle \bar{v}^2 \rangle} = \sqrt{\frac{1}{2\pi^2} \int_0^\infty dk k^2 P_v(k) \hat{W}(kR)^2}$$

Is this signal a cosmological one or is it an unlikely event?

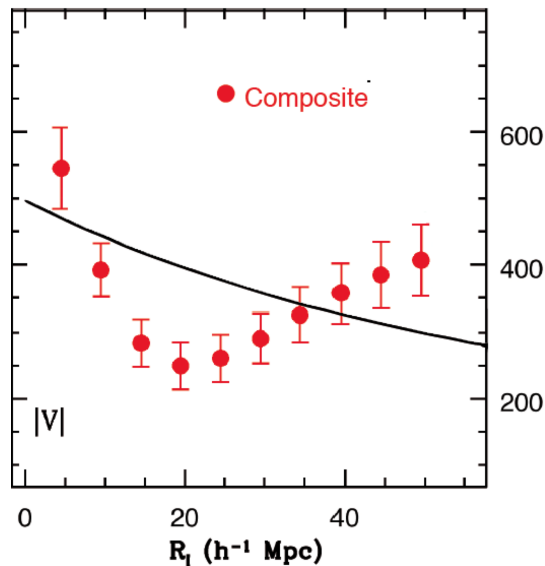
Is (Λ)Cold **D**ark **M**atter Scenario ruled out?

What have we learned from numerical simulations on LSS formation ?

Large Scale Structure: « Anomalous » Bulk Flow

For gaussian initial conditions, is such a V_{bulk} possible ?
Is it not a rare event ?

As a first approximation, we can characterize the Watkins curve by two data points: depletion at $16 h^{-1} \text{ Mpc}$ and bump at $53 h^{-1} \text{ Mpc}$. We then compute the Probability to get such a event from initial condition statistics.



$$P(v_{R_1}, v_{R_2}) \propto \frac{2}{\pi} \frac{v_{R_1}^2 v_{R_2}^2}{|\det M|^{3/2}} \times \exp \left(-\frac{1}{2} \vec{V}^\dagger M^{-1} \vec{V} \right)$$

$$\gamma_{i,j} = \frac{1}{2\pi^2} \int_0^\infty k^3 P_v(k) \hat{W}(kR_i) \hat{W}(kR_j) d\ln k.$$

Strong correlation between scales R_{16} and R_{53} , M is the correlation matrix containing non-diagonal terms, (tail of a 2D maxwellian).

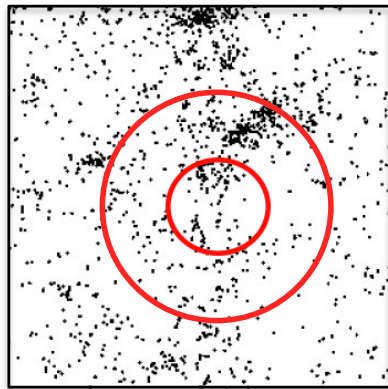
$$P \approx 1.58 \%$$

Watkins V_{bulk} could be a rare event realization in ΛCDM !

What have we learned from numerical simulations on LSS formation ?

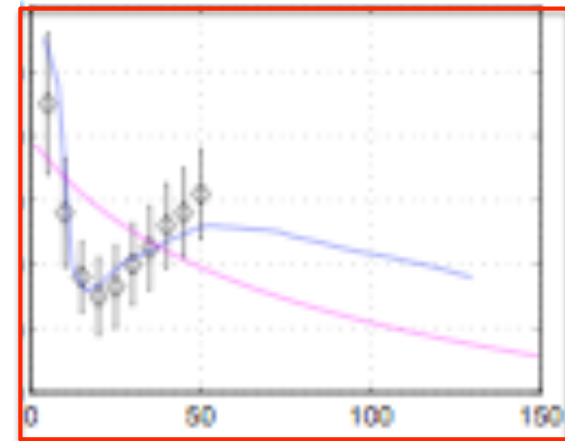
Large Scale Structure: « Anomalous » Bulk Flow

DEUS: Λ CDM-WMAP5 , $648 h^{-1}$ Mpc.



From 20.000 random centers
(environments)

$$\vec{V}_{bulk}(R) \quad \sigma_R$$



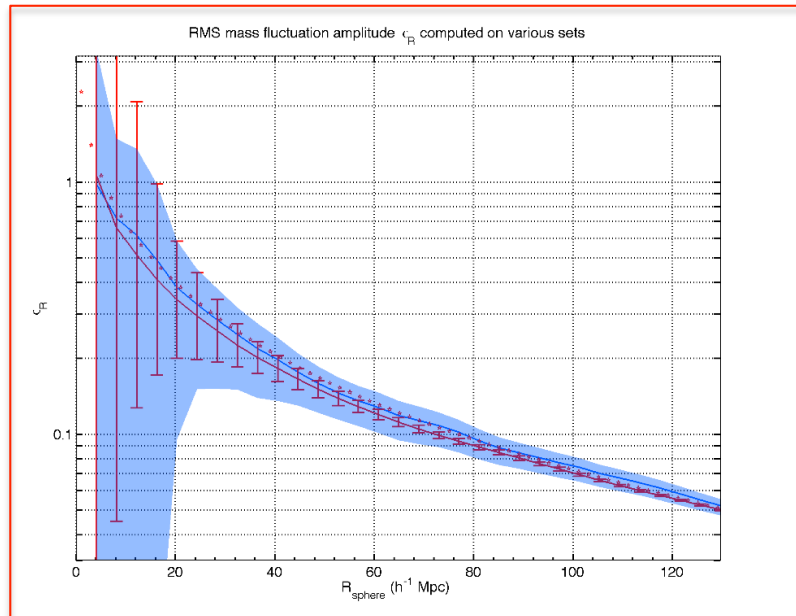
Using Watkins observational data points: We isolate an observational-like sample at 95% (χ^2 analysis done on all observational 10 data points) : 255 out of 20.000.

Rare events ($P \approx 1.56\%$)
in (very good) agreement with the previous estimation.

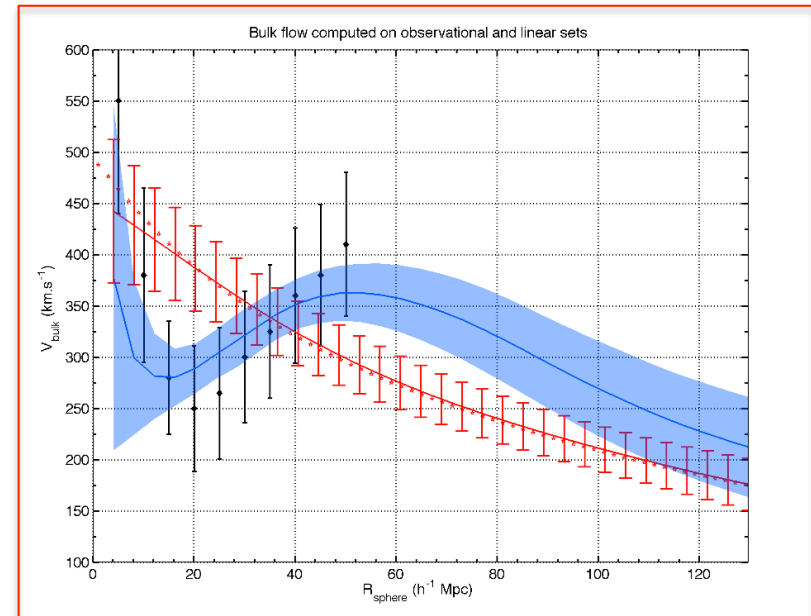
What have we learned from numerical simulations on LSS formation ?

Large Scale Structure: « Anomalous » Bulk Flow

Watkins Bulk Flows Numerical Catalog (255)



$\sigma(R)$ in good agreement
with linear predictions



$$\|\vec{V}_{\text{Bulk}}(R)\|$$

seems to diverge from the linear prediction.

But $\vec{V}_{\text{Bulk}}(R)$ is directional

To solve this Contradiction.
What is the Dynamical Origin of Bulk Flow ?

What have we learned from numerical simulations on LSS formation ?

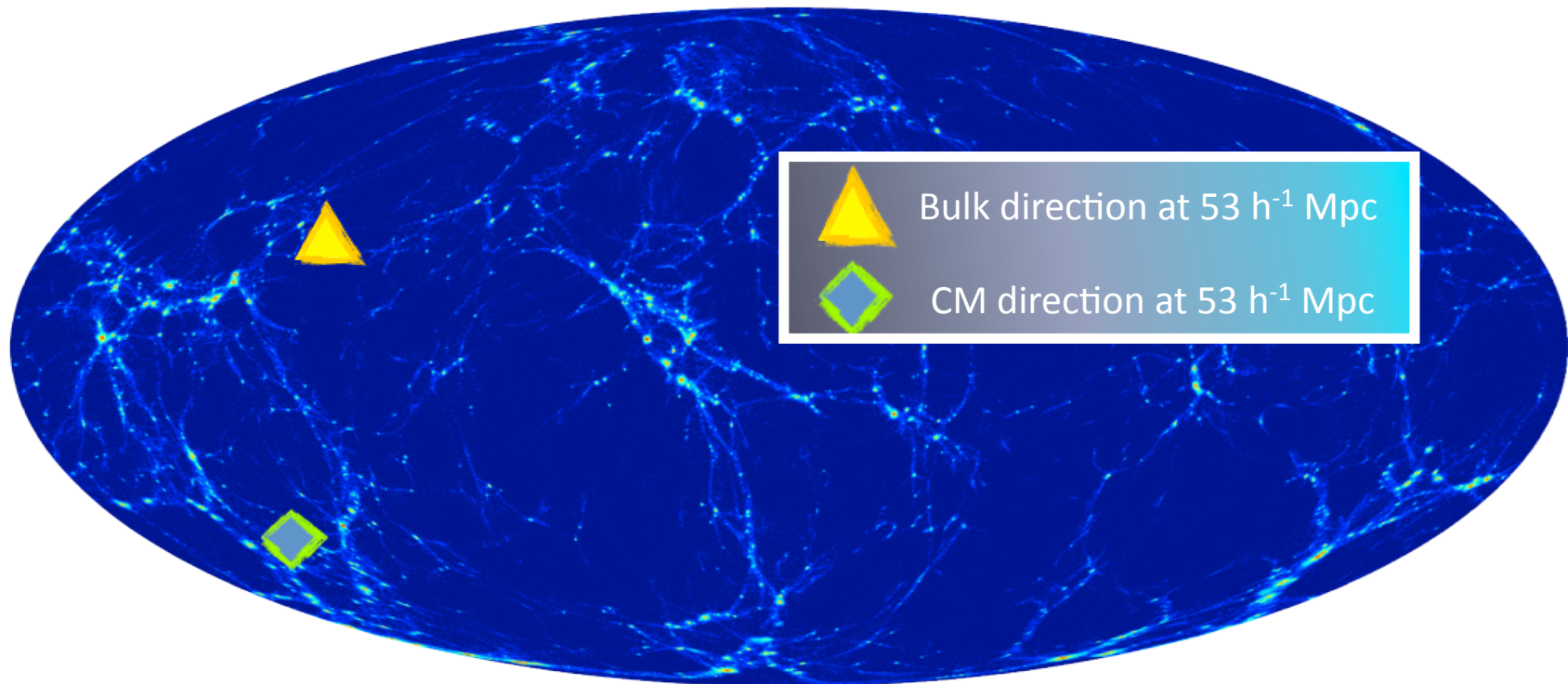
Large Scale Structure: « Anomalous » Bulk Flow

We suppose such a Watkins event, What is the Dynamical Origin of Bulk Flow ?

Directionality suggests an asymmetry in matter distribution.

We then qualitatively study the direction of the bulk flow versus the direction of the center of mass;

For a Watkins Numerical event, Mollweide projection ($53 h^{-1} \text{ Mpc}$)



Clearly distinct direction

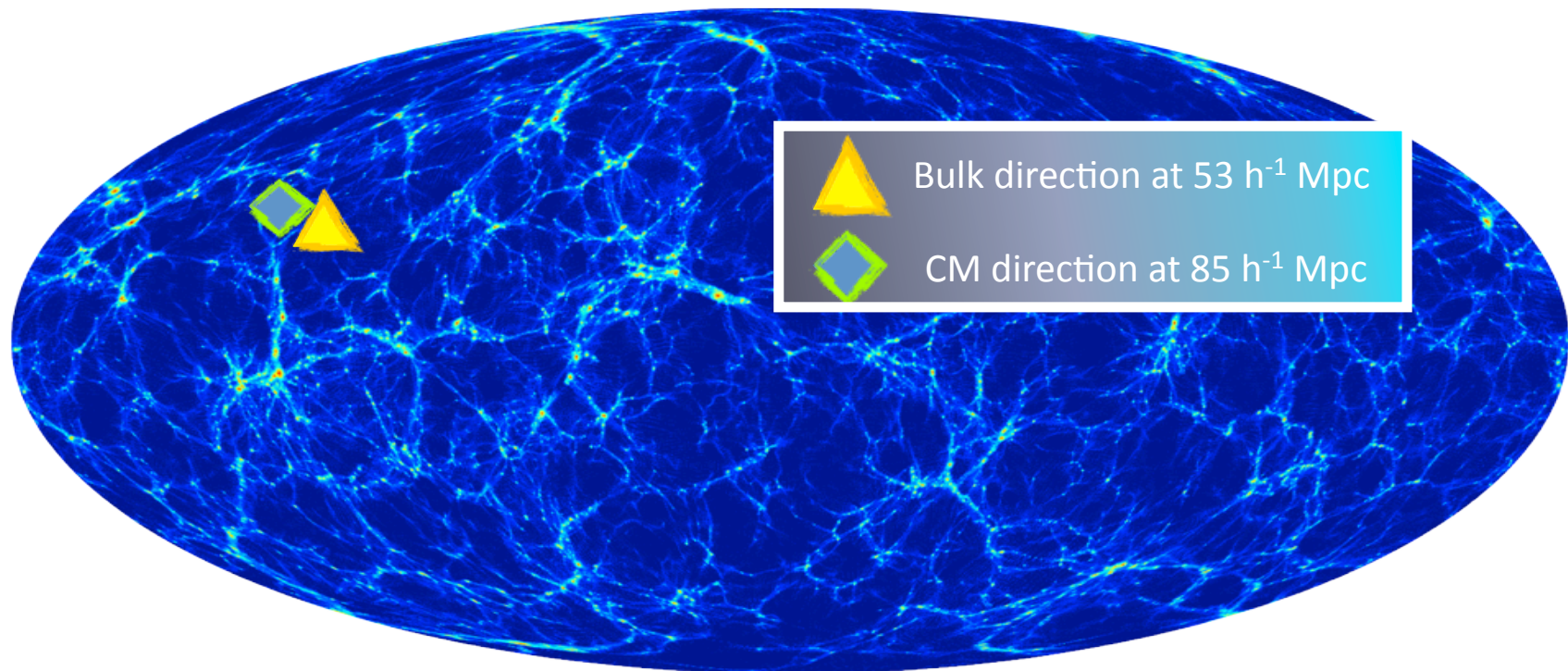
What have we learned from numerical simulations on LSS formation ?

Large Scale Structure: « Anomalous » Bulk Flow

We suppose such a Watkins event, What is the Dynamical Origin of Bulk Flow ?

Directionality suggests an asymmetry in matter distribution.

We then qualitatively study the direction of the bulk flow versus the direction of the center of mass;
For a Watkins Numerical event, Mollweide projection at larger scale ($85 h^{-1} \text{ Mpc}$)



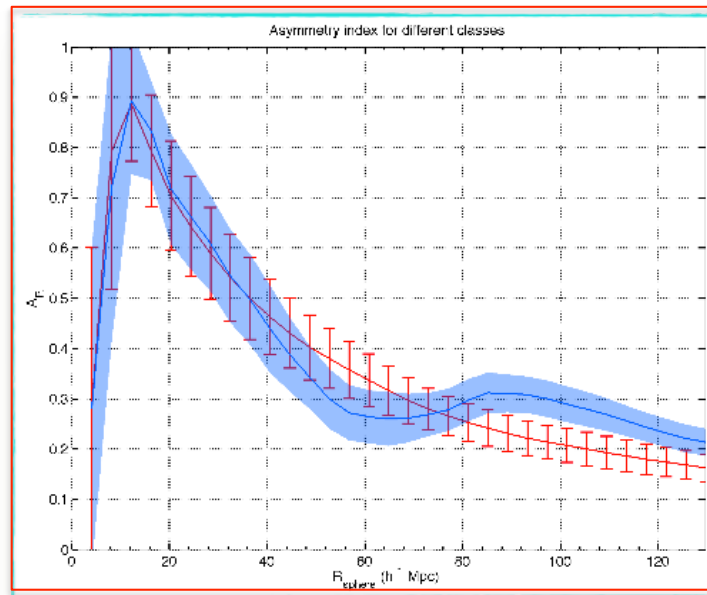
Clearly similar direction

What have we learned from numerical simulations on LSS formation ?

Large Scale Structure: « Anomalous » Bulk Flow

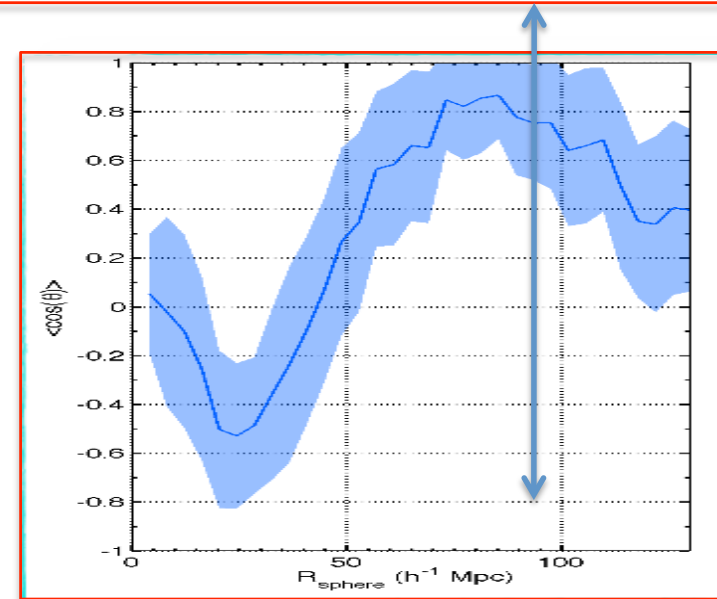
What is the Dynamical Origin of Bulk Flow ?

We compare the mean $\|\vec{C}(R)\|$ for the complete Watkins bulk flow numerical catalog and for the Linear bulk flow numerical catalog:



~ 85 h⁻¹ Mpc (bump)
~ 55 h⁻¹ Mpc (depletion)

Which scales shows an alignment between the direction of asymmetry in a shell and the direction of the Bulk Flow at 53 h⁻¹ Mpc ?



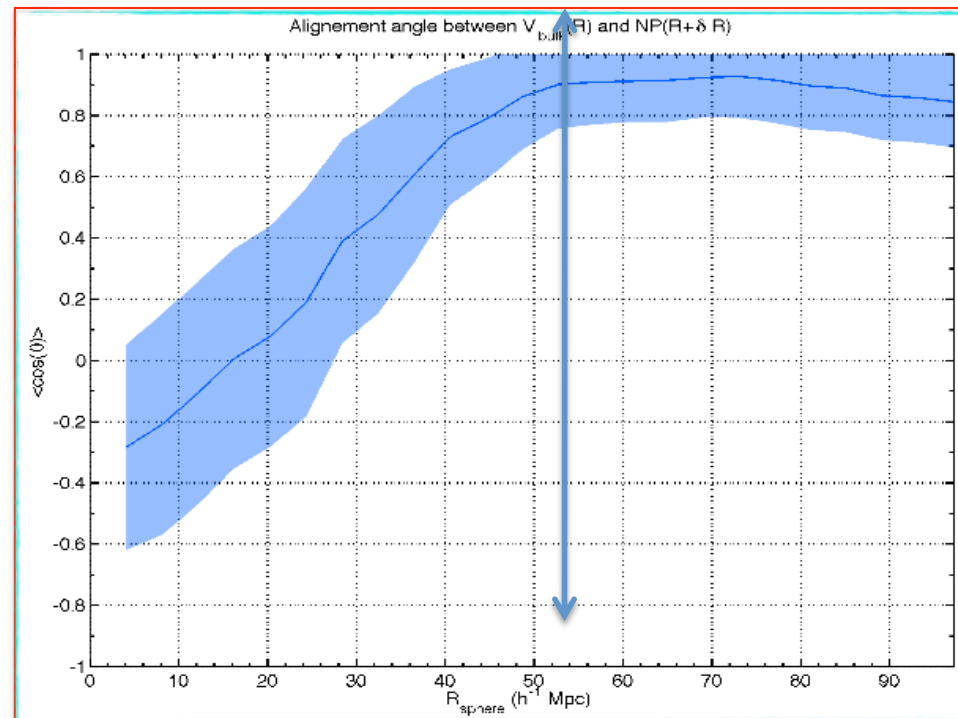
$\vec{V}_{Bulk}(53h^{-1}Mpc) \cdot (\vec{C}(R + dR) - \vec{C}(R))$
Alignment scale at ~ 85 h⁻¹ Mpc
(85 = 53 + 32)

What have we learned from numerical simulations on LSS formation ?

Large Scale Structure: « Anomalous » Bulk Flow

What is the Dynamical Origin of Bulk Flow ?

For all events from the complete Watkins bulk flow numerical catalog, we compute the scalar product of the bulk flow at radius R with the direction of the asymmetry in spheres of radius $R+32$



$$\vec{V}_{Bulk}(R) \cdot \vec{C}(R + 32h^{-1} Mpc)$$

Alignment scale from $53 h^{-1} Mpc$.

What have we learned from numerical simulations on LSS formation ?

Large Scale Structure: « Anomalous » Bulk Flow

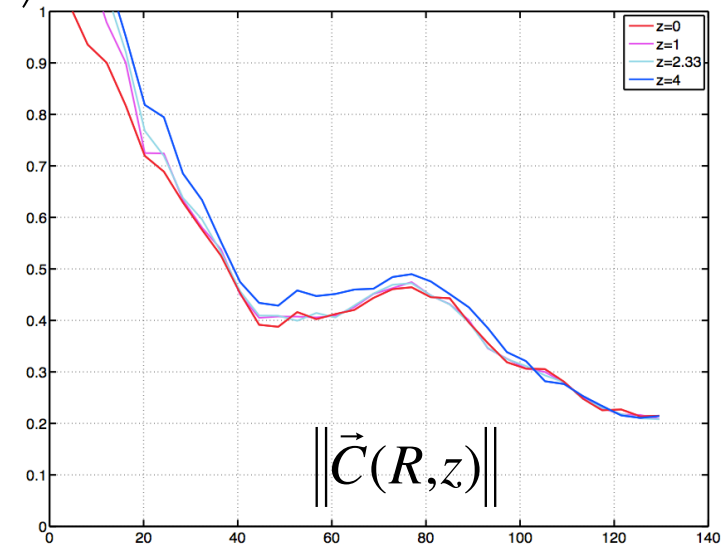
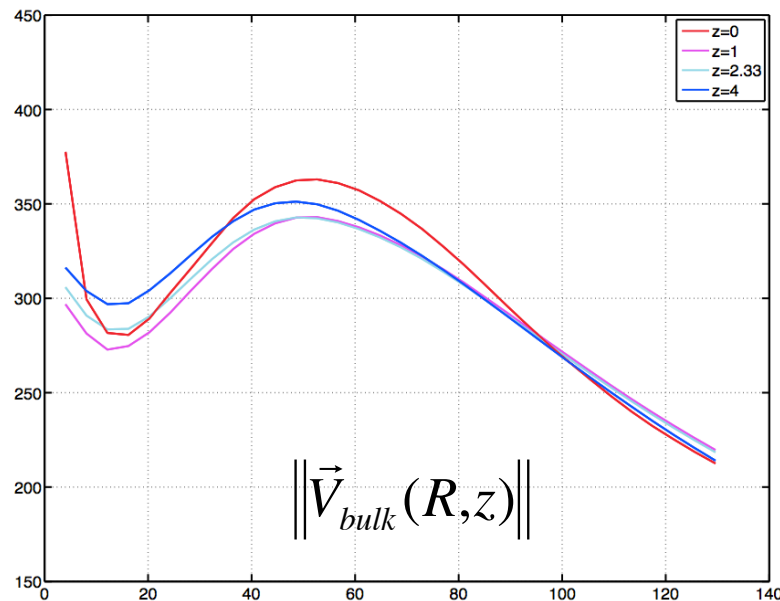
**We confirm that V_{bulk} is a linear quantity even for such a rare event.
Its evolution satisfies the linear evolution, idem for the asymmetry factor**

$$\|\vec{V}_{\text{Bulk}}(R,z)\| = \sqrt{(H(z) f(z))^2 \int P_\delta(k,z) W^2(kR) dk}$$

$$\|\vec{V}_{\text{Bulk}}(R,0)\| = \sqrt{(H(0) f(0))^2 \int P_\delta(k,0) W^2(kR) dk}$$

$$P_\delta(k,z) = \left(\frac{D_+(z)}{D_+(0)} \right)^2 P_\delta(k,0)$$

$$\|\vec{V}_{\text{bulk}}(R,z)\| = \left(\frac{H(z) f(z) D_+(z)}{H(0) f(0) D_+(0)} \right) \|\vec{V}_{\text{bulk}}(R,0)\|$$

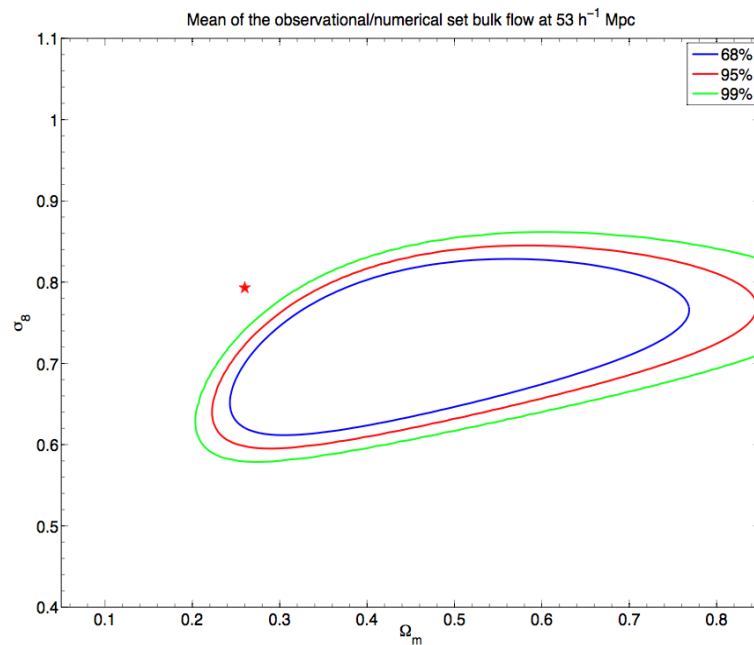


What have we learned from numerical simulations on LSS formation ?

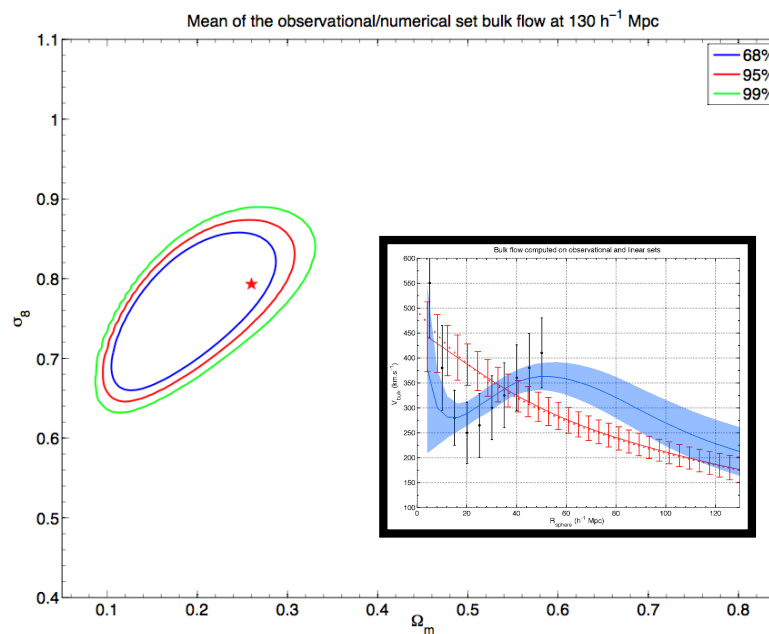
Large Scale Structure: « Anomalous » Bulk Flow

Where is the cosmology ?

Likelihood analysis on the Vbulk data for the Watkins Bulk Flow catalog ($R \leq 53 \text{ h}^{-1} \text{ Mpc}$ and $R \leq 130 \text{ h}^{-1} \text{ Mpc}$)



Wrong cosmological parameters ($R \leq 53 \text{ h}^{-1} \text{ Mpc}$).



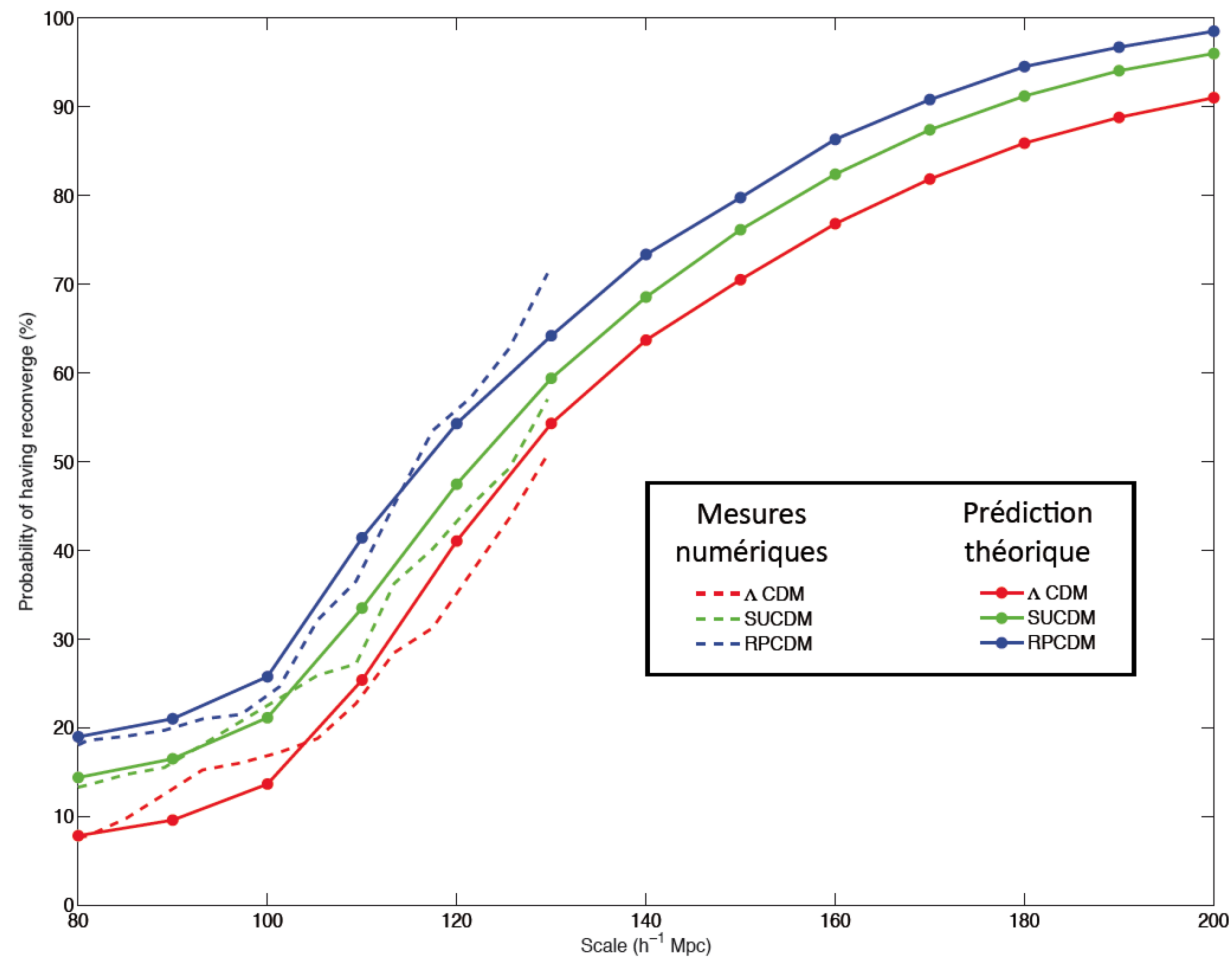
Correct cosmological parameters ($R = 130 \text{ h}^{-1} \text{ Mpc}$).

Convergence on large scale: A probe for Cosmology

DEUS : Anomalous cosmic flow, a challenge for Λ CDM

Convergence on large scale: A probe for Cosmology

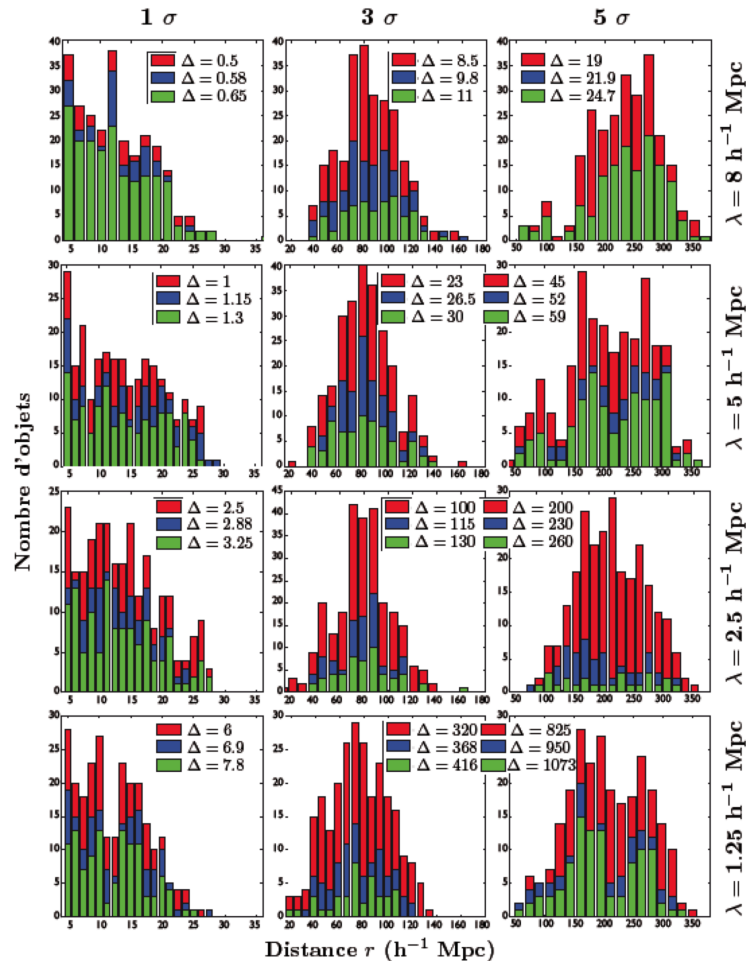
3-Point Probability !!!



What have we learned from numerical simulations on LSS formation ?

Large Scale Structure: « Anomalous » Bulk Flow

What is the origin of the assymetry, responsible of the anomalous bulk Flow ?



Distance to the high peaks in density.

Gaussian distribution:

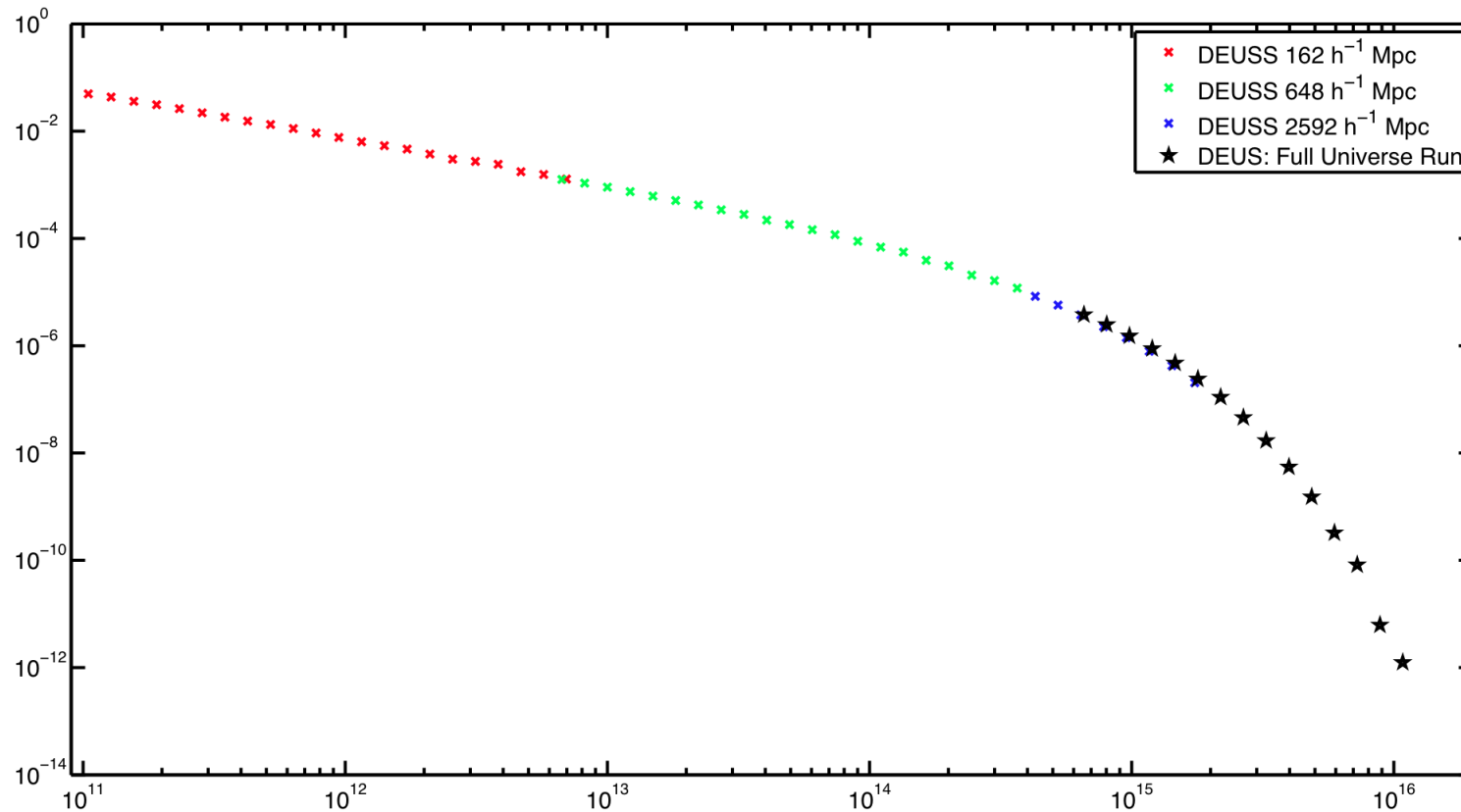
Smoothing Length	3σ
$8 h^{-1} \text{ Mpc}$	$\mu=82 h^{-1} \text{ Mpc}$ ($\sigma=24 h^{-1} \text{ Mpc}$)
$5 h^{-1} \text{ Mpc}$	$\mu=79 h^{-1} \text{ Mpc}$ ($\sigma=22 h^{-1} \text{ Mpc}$)
$2.5 h^{-1} \text{ Mpc}$	$\mu=79 h^{-1} \text{ Mpc}$ ($\sigma=22 h^{-1} \text{ Mpc}$)
$1.25 h^{-1} \text{ Mpc}$	$\mu=76 h^{-1} \text{ Mpc}$ ($\sigma=26 h^{-1} \text{ Mpc}$)

What do we have learned from numerical simulations on LSS formation ?

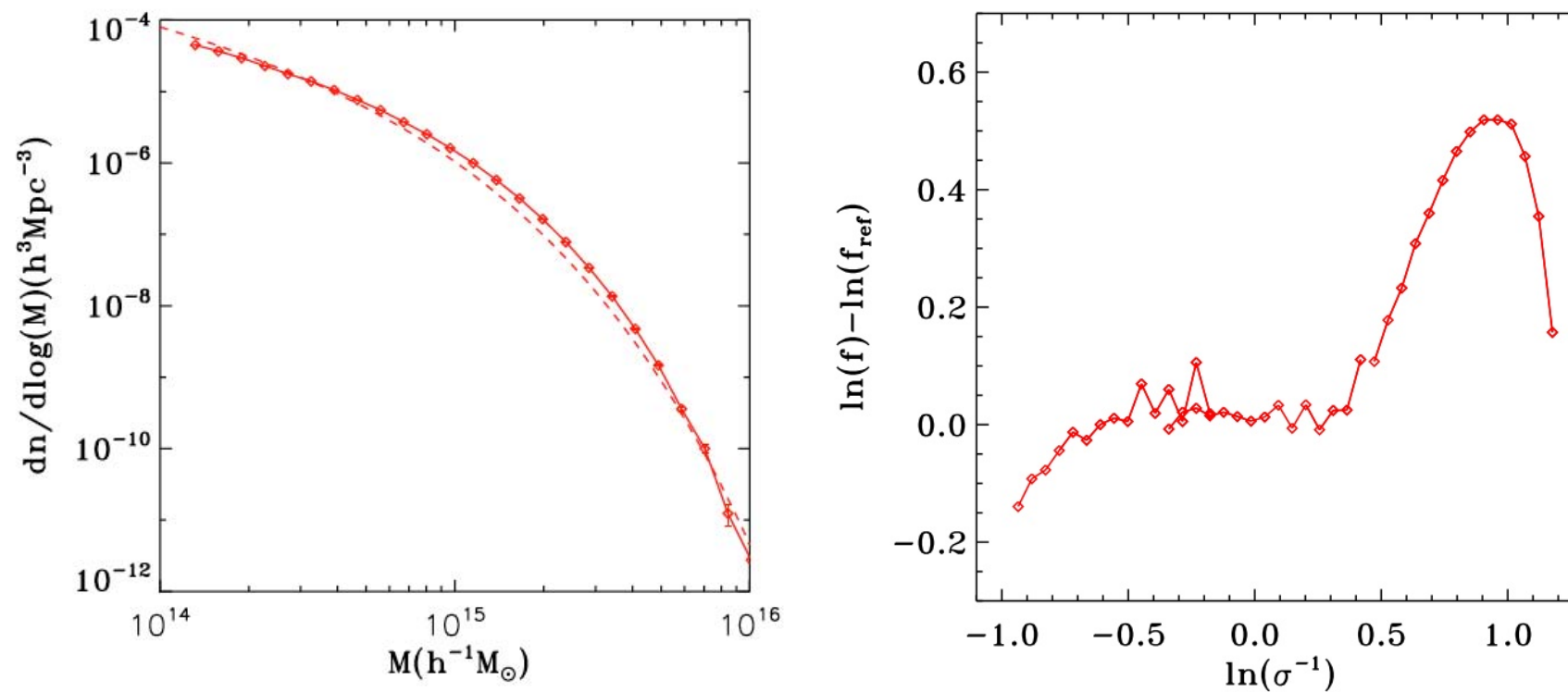
Halos Mass Function

What have we learned from numerical simulations on LSS formation ?

Halo Mass Function: Universality/No Universality, Extreme large Massive Halos...



DEUS Full Universe Runs: Halos Mass Function



Mass function: strong deviation to Jenkins fit

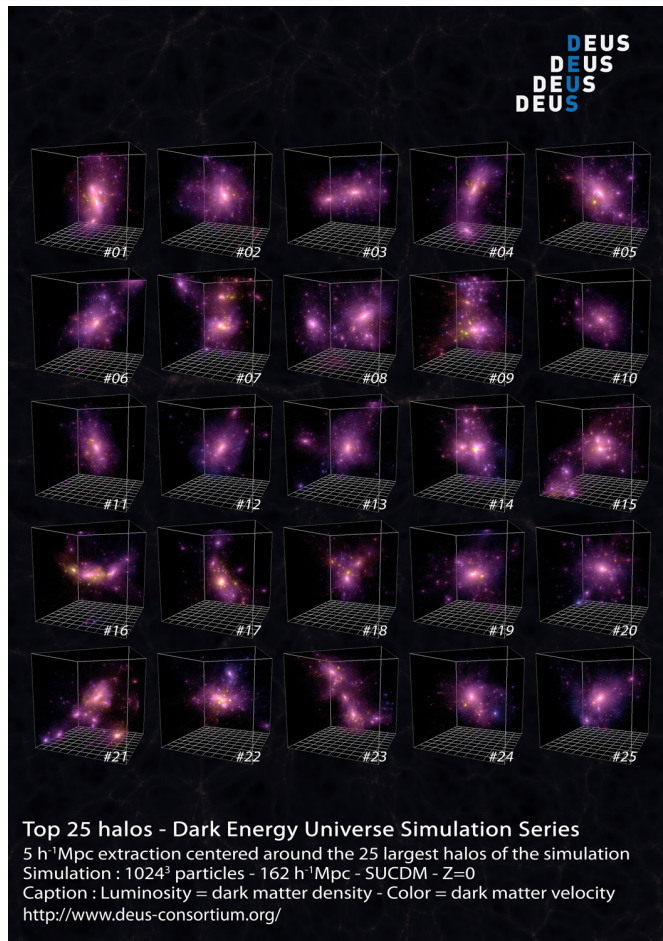
What do we have learned from numerical simulations on LSS formation ?

Dark Matter Halos Profil

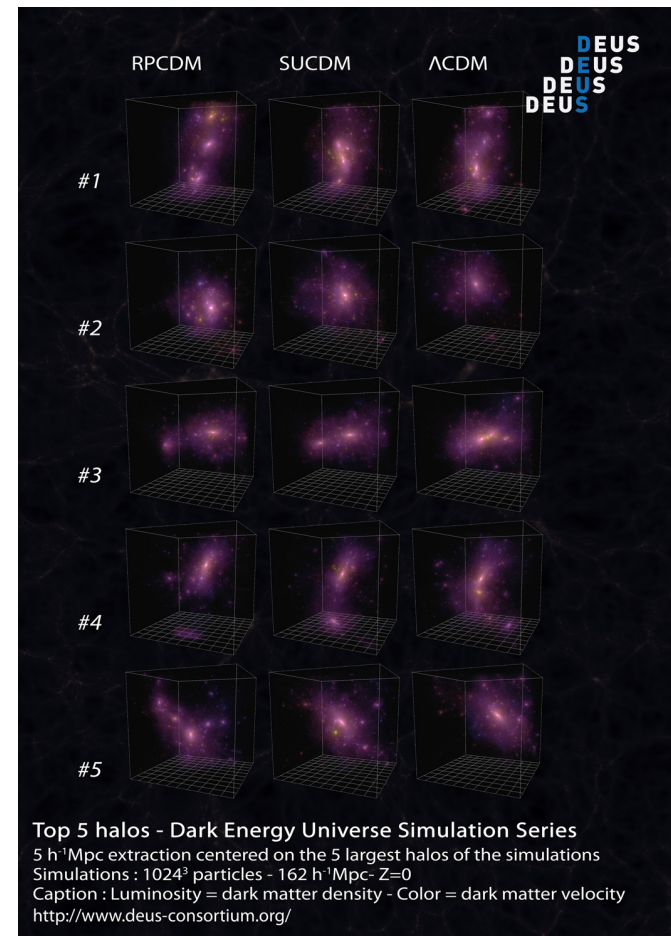
What have we learned from numerical simulations on LSS formation ?

Dark Matter Halos properties

In a specific cosmological model
a large diversity of halos



Different halos for
different cosmological models



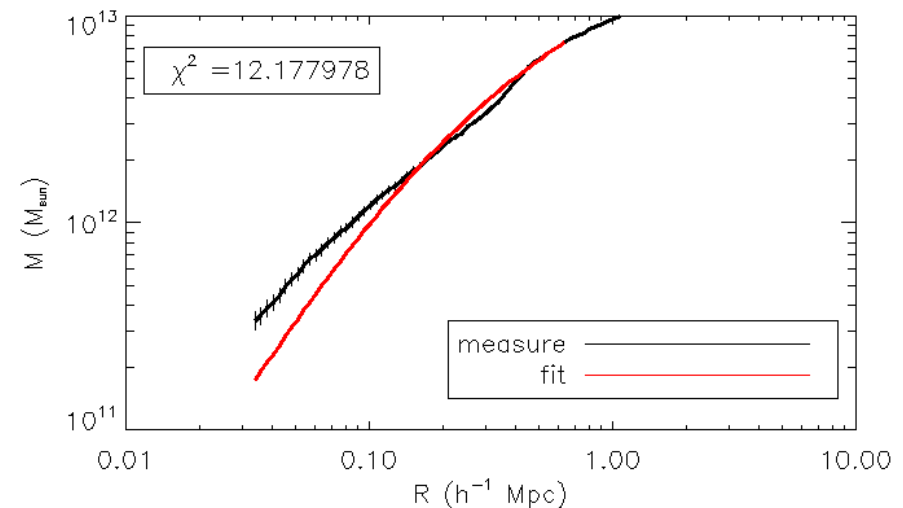
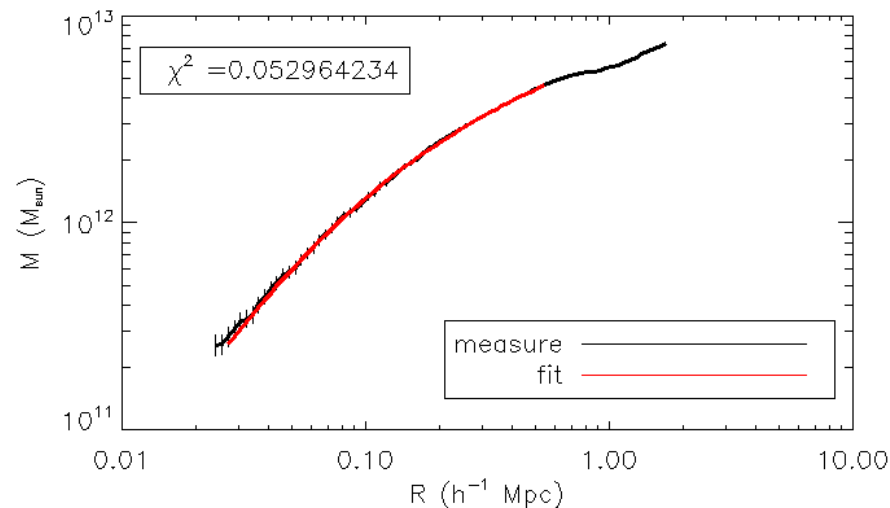
What have we learned from numerical simulations on LSS formation ?

Dark Matter Halos properties

NFW profile widely used, but effectively all halos are not well described by NFW.



$$\rho(r) = \frac{\rho_0}{\frac{r}{r_s} \left(1 + \frac{r}{r_s} \right)^2}$$

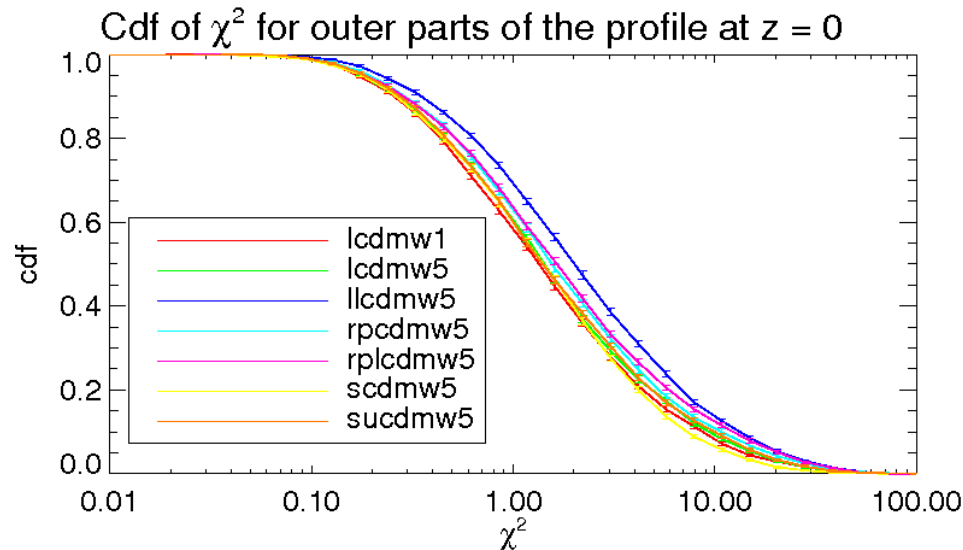


We fit NFW profile for each halo and characterize the goodness of the best NFW fit by the parameter χ^2 .

What have we learned from numerical simulations on LSS formation ?

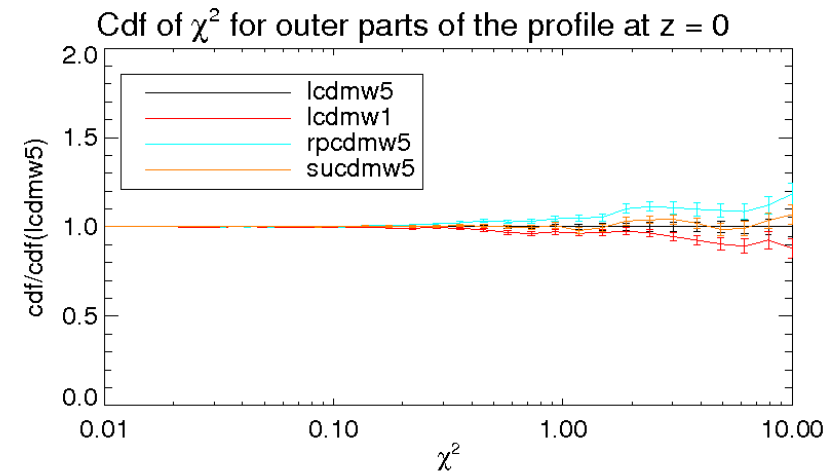
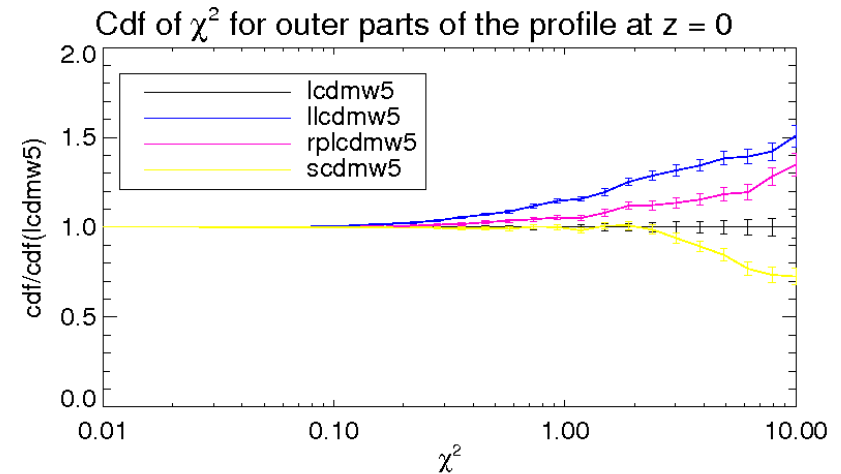
Dark Matter Halos properties

Number of ill fitted halos is dependant on the cosmology



Provides physical information on the collapse process

χ^2 contains cosmological information

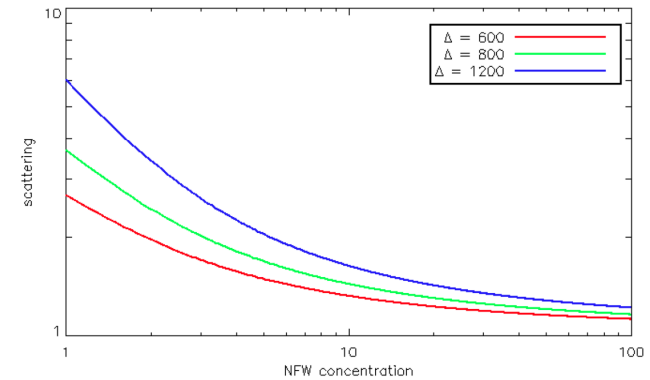
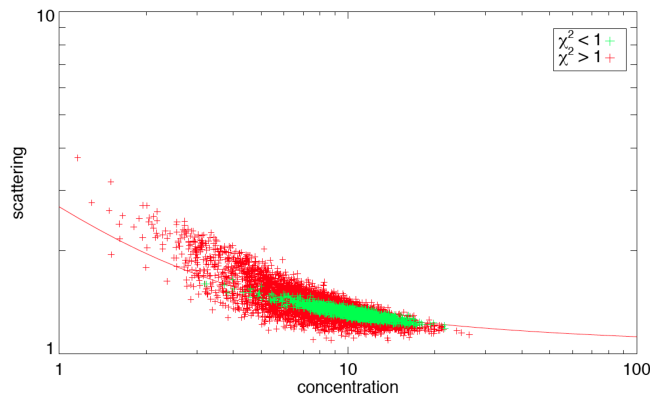


What have we learned from numerical simulations on LSS formation ?

Dark Matter Halos properties

Instead of Concentration / We define a new parameter,
which does not depend on the profil : the Sparsity

$$s_{\Delta} = \frac{M_{200}}{M_{\Delta}} \left(c_{NFW} = \frac{R_{Vir}}{R_s} \right)$$



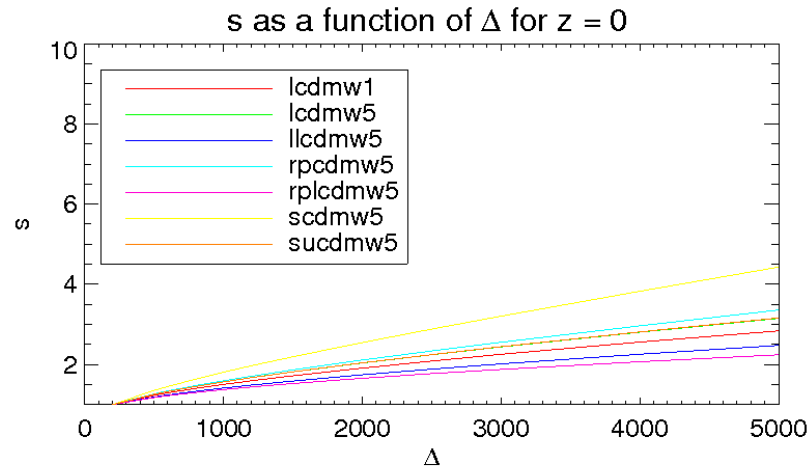
The relation between the sparsity S and the NFW concentration C can be computed theoretically. It is well verified on the simulation.

S is anti-correlated with the NFW concentration c .

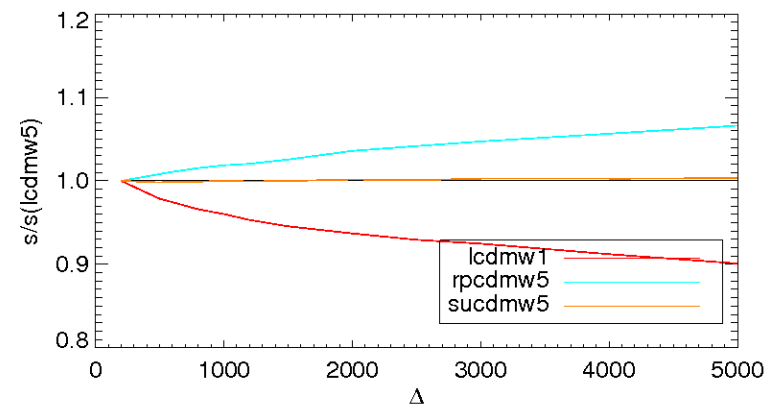
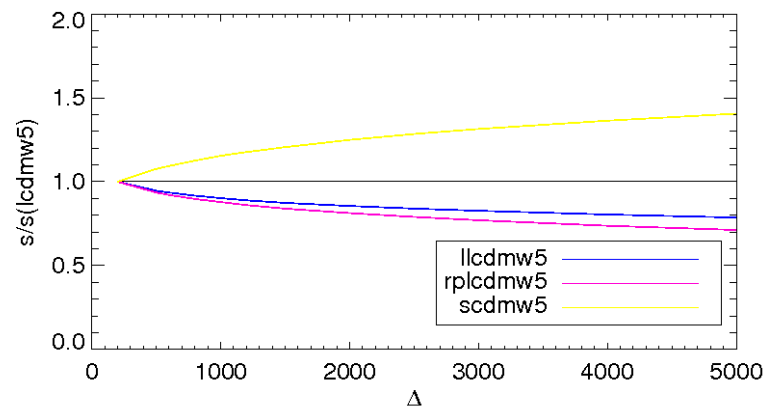
What have we learned from numerical simulations on LSS formation ?

Dark Matter Halos properties

The sparsity parameter depends on cosmology



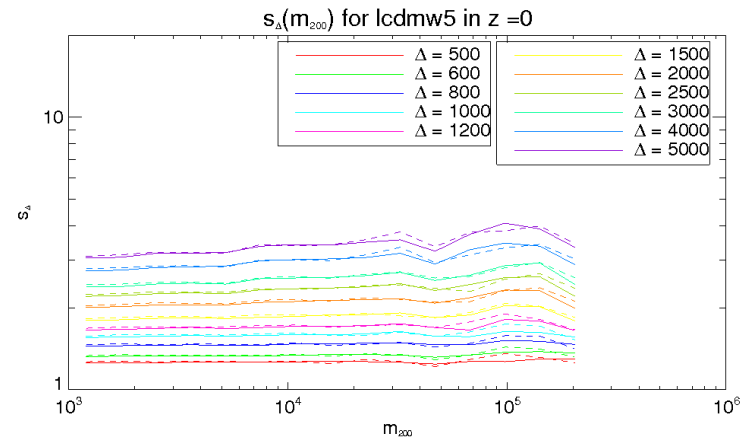
and



What have we learned from numerical simulations on LSS formation ?

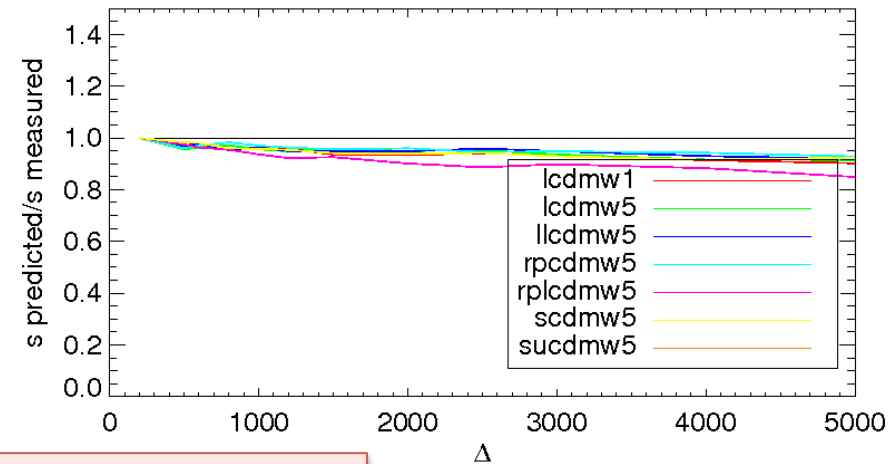
Dark Matter Halos properties

As sparsity parameter is (almost) independant of the mass.
(If the profile is $\propto r^{-3}$ at large radius, it is natural).



The sparsity parameter can be predicted using the mass function: .

$$\int \frac{1}{M_{\Delta}} \frac{dn}{d \ln M_{\Delta}} d \ln M_{\Delta} = s \int \frac{1}{M_{vir}} \frac{dn}{d \ln M_{vir}} d \ln M_{vir}$$



A new probe for the cosmology

What have we learned from numerical simulations of Dark Universe ?

CMB-Galaxy Correlation and
Sachs-Wolfe effect using Ray tracing in Numerical Simulation.

Nature of Dark Matter and
sub-halos abundances: Millenium II Simulation

.... All aspects of the Cosmology....

Conclusion

« Vouloir conclure c'est la bêtise »

Gustave Flaubert.

The numerical simulation activity is rapidly evolving, as computational resources continue to grow, enabling larger, more complicated, and more realistic simulations to be performed.

As Dark matter dynamics can be studied with high precision in cosmological N-body simulations. The simulation allows high-precision measurements of the dark matter clustering, like halo mass function, power spectrum, bulk flow, halo profil... abundance of dark matter substructure...etc.

The simulation Is a powerful theoretical tool to probe the nature of Dark Matter and Dark Energy.

The simulation is a powerful theoretical tool to support present and future cosmological observations (redshift space).

The next decade promises to be filled with exciting challenges and the potential for great discoveries. It is safe to say that the field of Numerical Simulations of the Dark Universe will not run out of things to do.

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Niklas Zennström and Janus Friis (SKYPE)....

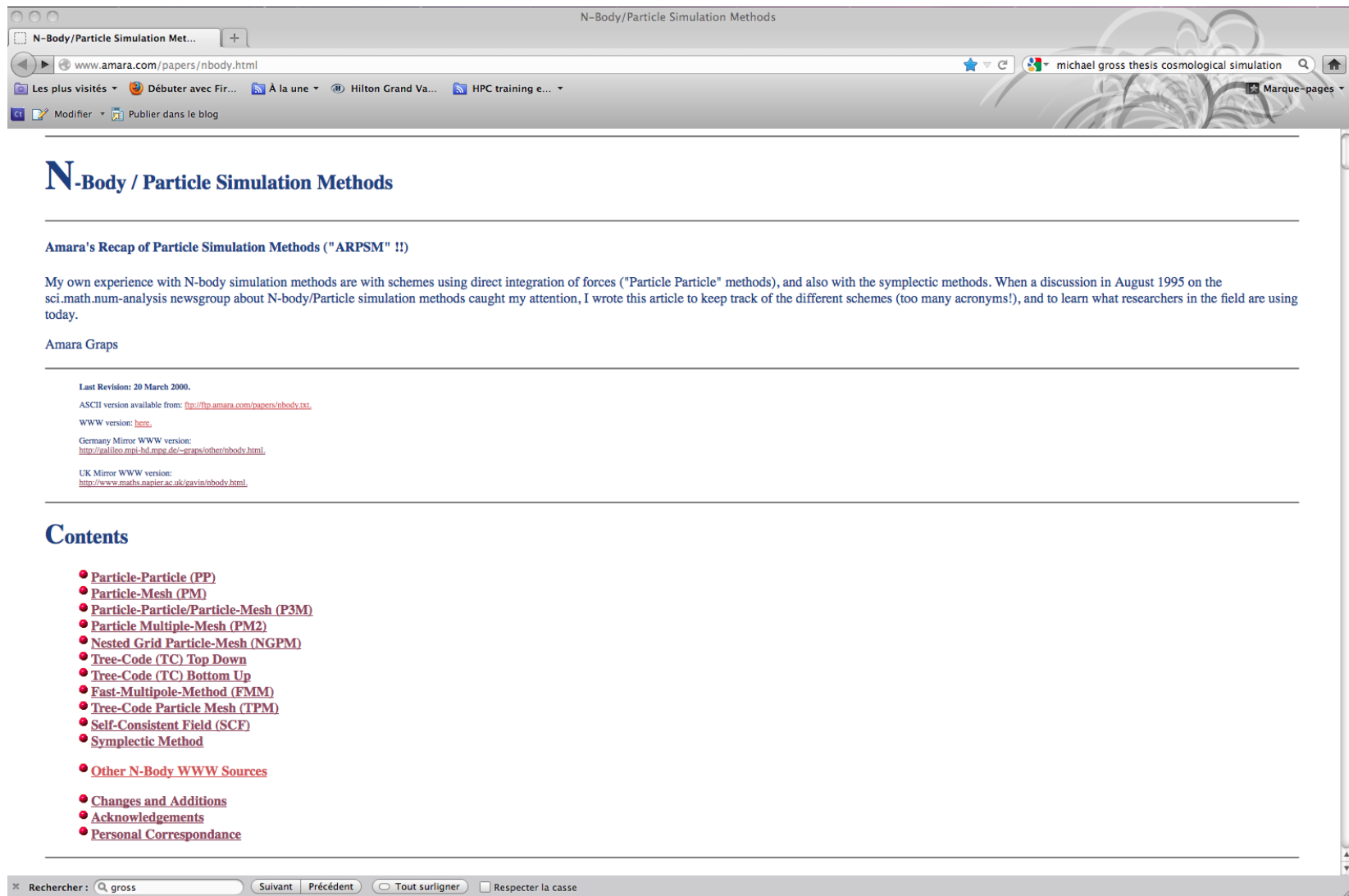
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Bibliography

A survey of all known N-body methods: <http://www.amara.com/papers/nbody.html>



The screenshot shows a web browser window displaying the "N-Body/Particle Simulation Methods" page. The browser's address bar shows the URL "http://www.amara.com/papers/nbody.html". The page title is "N-Body / Particle Simulation Methods". The content includes a section titled "Amara's Recap of Particle Simulation Methods ('ARPSM' !!)" with a paragraph about the author's experience with N-body simulation methods. Below this, there is a section for "Amara Graps" with links to the last revision (20 March 2000), an ASCII version, and WWW versions in Germany and the UK. A "Contents" section lists various simulation methods: Particle-Particle (PP), Particle-Mesh (PM), Particle-Particle/Particle-Mesh (P3M), Particle Multiple-Mesh (PM2), Nested Grid Particle-Mesh (NGPM), Tree-Code (TC) Top Down, Tree-Code (TC) Bottom Up, Fast-Multipole-Method (FMM), Tree-Code Particle Mesh (TPM), Self-Consistent Field (SCF), and Symplectic Method. There are also links for "Other N-Body WWW Sources", "Changes and Additions", "Acknowledgements", and "Personal Correspondance". The browser's search bar at the bottom shows "gross" and navigation buttons like "Suivant", "Précédent", "Tout surligner", and "Respecter la casse".

N-Body/Particle Simulation Methods

Amara's Recap of Particle Simulation Methods ("ARPSM" !!)

My own experience with N-body simulation methods are with schemes using direct integration of forces ("Particle Particle" methods), and also with the symplectic methods. When a discussion in August 1995 on the sci.math.num-analysis newsgroup about N-body/Particle simulation methods caught my attention, I wrote this article to keep track of the different schemes (too many acronyms!), and to learn what researchers in the field are using today.

Amara Graps

Last Revision: 20 March 2000.
ASCII version available from: <http://ftp.amara.com/papers/nbody.txt>.
WWW version: [here](#).
Germany Mirror WWW version:
<http://galileo.mpi-hd.mpg.de/~graps/other/nbody.html>.
UK Mirror WWW version:
<http://www.maths.napier.ac.uk/gavin/nbody.html>.

Contents

- [Particle-Particle \(PP\)](#)
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- [Particle Multiple-Mesh \(PM2\)](#)
- [Nested Grid Particle-Mesh \(NGPM\)](#)
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Rechercher : gross Suivant Précédent Tout surligner Respecter la casse

Bibliography

Codes you can download and use

Enzo: <http://enzo.googlecode.com>

Gadget: <http://www.mpa-garching.mpg.de/gadget/>

FLASH: <http://flash.uchicago.edu/>

RAMSES: http://irfu.cea.fr/Projets/Site_ramses/RAMSES.html

TPM: <http://www.astro.princeton.edu/~bode/TPM/index.html>

Hydra: http://coho.mcmaster.ca/hydra/hydra_consort.html

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