Cosmological Simulations

Marco Baldi - Bologna University

XIV Tonale Winter School on Cosmology - 5-10/XII/2021

an introduction to Cosmological Simulations

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an introduction to

Cosmological Simulations

(and how to use them to test the Dark Universe)

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Two main types of characters in the numerical cosmology business

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"Hardcore" code developers

- Very good at programming.
- Know every single detail of the code structure and workflow
- Could develop the whole code from scratch
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- Focus on the interpretation and analysis of the outputs
- Develop very sophisticated analysis tools

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Outline

Cosmological Simulations: What, Why, and How?

- What are Cosmological Simulations?
- Motivations and applications of creating synthetic universes
- The 3 main steps of cosmological simulations
- The (cosmological) N-body problem: gravitational dynamics of a collisionless system in an expanding space
- Before starting: initial conditions for cosmological simulations
- Solving gravity for a system of N particles: the PM method
- Solving gravity for a system of N particles: the Tree method
- Solving gravity for a system of N particles: the Multigrid method
- Time integration

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Cosmological Simulations: What else?

- Beyond LCDM cosmologies: motivations and classification
- Modifying N-body algorithms to include additional physics
- Dark Energy implementations
- Modified Gravity implementations: the example of *f(R)*
- Dark Matter models: massive neutrinos et al.

References

Cosmological Simulations: What, Why, and How?

- V. Springel, High-Performance Computing and numerical modelling, (2014) arXiv:1412.5187
- Kuhlen et al., Numerical Simulations of the Dark Universe: state of the art and next decade (2012) Phys.Dark.Univ.

Cosmological Simulations: What else?

- M. Baldi, Dark Energy Simulations (2012), Phys.Dark.Univ.
- C. Llinares (2020), Simulations Techniques for Modified Gravity (2018), Int.J.Mod.Phys.D

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[countable, uncountable] a situation in which a particular set of conditions is created artificially in order to study or experience something that could exist in reality

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... otherwise you fall into one of Borges Paradoxes (J. L. Borges, "On the exactitude of Science", 1946, inspired by Lewis Carroll's Sylvie and Bruno, 1895)

"... in that Empire, the Cartographer's art achieved such a degree of perfection that the Map of a single Province occupied an entire City, and the Map of the Empire, an entire Province. In time, these vast Maps were no longer sufficient. The Guild of Cartographers created a Map of the Empire, which perfectly coincided with the Empire itself. But Succeeding Generations, with diminished interest in the Study of Cartography, believed that this immense Map was of no use, and not Impiously, they abandoned it to the Inclemency of the Sun and of numerous Winters. In the Deserts of the West ruined Fragments of the Map survive, inhabited by Animals and Beggars; in all the Country there is no other Relic of the Geographical Disciplines."

(from Viajes de Varones Prudentes, Suárez Miranda, book IV, chap. XIV, Lérida, 1658. Quoted by Jorge Luis Borges, Historia universal de la infamia "Etcetera," Buenos Aires, 1935).

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"What a useful thing a pocket-map is!" I remarked.

"That's another thing we've learned from your Nation," said Mein Herr, "mapmaking. But we've carried it much further than you. What do you consider the largest map that would be really useful?"

"About six inches to the mile."

"Only six inches!" exclaimed Mein Herr. "We very soon got to six yards to the mile. Then we tried a hundred yards to the mile. And then came the grandest idea of all ! We actually made a map of the country, on the scale of a mile to the mile!"

"Have you used it much?" I enquired.

"It has never been spread out, yet," said Mein Herr: "the farmers objected: they said it would cover the whole country, and shut out the sunlight ! So we now use the country itself, as its own map, and I assure you it does nearly as well."

from Lewis Carroll, Sylvie and Bruno Concluded, Chapter XI, London, 1895

Why doing Cosmological Simulations?

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1. To model the evolution of structures in the Universe into the non-linear regime not directly accessible with analytical tools

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- 6. More motivations at the end...

How

do Cosmological Simulations work?

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Setting up the stage

Cosmological Simulation -> an artificial replica of the cosmos aimed at studying its real properties and evolution.

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Not an easy task as the Universe is:

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- Very OLD —> replica should be evolved for a long time, i.e. approximations and numerical errors may propagate and accumulate (need for a way to control the accuracy of the simulation)

However, we can rely on some simplifying (yet reasonable) statements...
- **Cosmological Principle**: the universe is homogeneous and isotropic over sufficiently large scales (at any time of its evolution)

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Bad news!

The homogeneity scale is quite large, a few hundred comoving Mpc

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Bad news!

Gravity is a long-range non-screenable force... we will have to solve a global problem (where every part of the system interacts with any other part)

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 $\Delta T/T \approx \delta \rho_b / \rho_b \approx 10^{-5}$

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 $(\delta \rho / \rho)_{\rm obs} \approx 1$

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Well...

at least we know what we require from our simulation techniques

Primordial density field $z_{\rm CMB} \approx 10^3, a_{\rm CMB} \approx 10^{-3}$



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evolve the density field of the Universe under the effect of gravity from the point where we can predict it analytically to today

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How? Discretisation Approaches

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Density field



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1) Discretise **space** —> Eulerian methods

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Density on a grid (mapping)



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i.e. coarse-graining the field on a given set of space-filling volume elements

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Density field

Particle distribution (sampling)



i.e. sampling the density through a set of discrete point-like tracers called "particles", which carry a given mass and which have nothing to do (in general) with physical or fundamental particles

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How? Formalising the Problem

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where the gravitational potential is given by Poisson's equation:

$$\nabla_r^2 \Phi = 4\pi G\rho$$

$$\mathbf{r} = a\mathbf{x}$$

For cosmological systems, one needs to take into account the expansion of space, so that it is convenient to work in comoving coordinates:

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$$\mathbf{r} = a\mathbf{\hat{x}}$$
 comoving coordinate
physical velocity
 $\mathbf{u} = \dot{\mathbf{r}} = \dot{a}\mathbf{x} + a\dot{\mathbf{x}} = H(t)\mathbf{r} + \mathbf{v}$
peculiar velocity

This allows to rewrite the equation of motion and the Poisson equation

as

$$\dot{\mathbf{v}} = -H(t)\mathbf{v} - \frac{1}{a}\nabla_x\phi$$

$$\nabla_x^2 \phi = 4\pi G \bar{\rho} a^2 \delta$$

Where ϕ is the peculiar potential and $\delta \equiv \delta \rho / \bar{\rho}$ is the density contrast

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$$\dot{\mathbf{p}}_i = -\nabla_x \phi(\mathbf{x}_i)$$

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where we now have to write the peculiar potential for a set of N pointlike massive particles:

$$\phi(\mathbf{x}_i) = -\frac{1}{a} \sum_{j \neq i} \frac{Gm_j}{|\mathbf{x}_i - \mathbf{x}_j|}$$

How? The 3 main steps

The steps of an N-body simulation

1. Initial Conditions:

The gravitational N-body problem amounts to integrate a system of first order differential equations:

$$\dot{\mathbf{x}}_i = \mathbf{p}_i / a^2$$

 $\dot{\mathbf{p}}_i = -\nabla_x \phi(\mathbf{x}_i)$

We therefore need initial conditions for $\, {\bf x} \,$ and $\, {\bf \dot x} \,$ for all the particles in the system

The steps of an N-body simulation

2. Gravitational Solver

It will be the core of our calculation, and requires to compute the source term for the acceleration equation for any given configuration of the particles' distribution.

In other words, it is the method to obtain the source term on the RHS of the differential equations:

$$\dot{\mathbf{p}}_i = -\nabla_x \phi(\mathbf{x}_i)$$

which requires computing the peculiar gravitational potential

$$\phi(\mathbf{x}_i) = -\frac{1}{a} \sum_{j \neq i} \frac{Gm_j}{|\mathbf{x}_i - \mathbf{x}_j|}$$

at every particle's position

The steps of an N-body simulation

3. Time integration

Once the source term (i.e. the acceleration on all particles) has been computed, and the initial configuration of the system is known (particles' positions and velocities at a given time) the dynamics must be integrated by **moving the system forward in time**, thereby updating positions and velocities of all particles:

> $\mathbf{x}(t) \to \mathbf{x}(t + \Delta t)$ $\mathbf{p}(t) \to \mathbf{p}(t + \Delta t)$

How? Setting up initial conditions

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Euler equation

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1

Poisson equation

$$\nabla_x^2 \phi = 4\pi G \bar{\rho} a^2 \delta$$

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These three equations can be combined into one second-order differential equation for the evolution of the density contrast:

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Which is solved by the growth function $D(a) : \delta(a) = D(a)\delta_0$

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All these derivations are valid only in the linear regime, i.e. when $\delta \ll 1$ For $\delta \sim 1$ this treatment breaks down ($\delta > 1$ would imply negative densities), but as long as $\delta \ll 1$ it provides a way to obtain δ from observations (of P(k)). How?

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We want to translate the temperature fluctuations observed in the CMB (well in the linear regime, $\delta \ll 1$) into initial conditions for particles' positions and velocities. First, convert the angular power spectrum of temperature fluctuations in a 3D density power spectrum



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Take Poisson's Equation and substitute the density growth solution

$$\delta(a) = D(a)\delta_0$$
$$\nabla^2 \phi = 4\pi G a^2 \bar{\rho} \delta = 4\pi G a^2 \frac{\bar{\rho}_0}{a^3} D(a)\delta_0$$

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This implies

$$\nabla^2 \phi = \frac{D(a)}{a} \nabla^2 \phi_0 \Rightarrow \phi(a) = \frac{D(a)}{a} \phi_0$$

So that in matter domination ($D(a) \sim a$) one has $\phi(a) \sim {
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and integrate it:

$$a\mathbf{v} = -\int \nabla \phi dt = -\nabla \phi_0 \int \frac{D(a)}{a} dt$$

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and substitute its solution D(a):

$$\ddot{D} + 2H\dot{D} = 4\pi G \frac{\bar{\rho_0}}{a^3} D \quad \rightarrow \quad \frac{1}{a^2} \frac{\partial(a^2 D)}{\partial t} = 4\pi G \frac{\bar{\rho_0}}{a^3} D$$

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To get:

$$\dot{\mathbf{x}} = \frac{\mathbf{v}}{a} = -\frac{\nabla\phi_0}{a^2} \int \frac{D(a)}{a} dt = -\frac{\nabla\phi_0}{a^2} \frac{a^2 \dot{D}}{4\pi G\bar{\rho}_0} = -\frac{D\dot{\nabla}\phi_0}{4\pi G\bar{\rho}_0}$$

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Now integrate the latter to get the Zel'dovich approximation:

$$\dot{\mathbf{x}} = -\frac{D\nabla\phi_0}{4\pi G\bar{\rho_0}} \Rightarrow \mathbf{x}(a) - \mathbf{x}_0 = -\frac{\nabla\phi_0}{4\pi G\bar{\rho}_0}D(a) \sim -\frac{a\nabla\phi(a)}{4\pi G\bar{\rho}_0}$$

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so that we can define the displacement field as

$$\psi \equiv \mathbf{x} - \mathbf{x}_0 = -\frac{a\nabla\phi(a)}{4\pi G\bar{\rho}_0}$$

that allows to evolve particles' positions in the linear regime

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Take the Fourier transform of the displacement field:

$$\psi = -\frac{a\nabla\phi(a)}{4\pi G\bar{\rho}_0} \rightarrow \psi_k = \frac{a(i\mathbf{k})\phi_k}{4\pi G\bar{\rho}_0}$$

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and of Poisson's Equation:

$$\nabla^2 \phi = 4\pi G a^2 \frac{\bar{\rho}_0}{a^3} D(a) \delta_0 \quad \to \quad -k^2 \phi_k = \frac{4\pi G \bar{\rho}_0}{a} \delta_k$$

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then substitute:

$$\psi_k = \frac{a(i\mathbf{k})}{4\pi G\bar{\rho}_0} \frac{4\pi G\bar{\rho}_0}{ak^2} \delta_k = i\mathbf{k}\frac{\delta_k}{k^2}$$

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Now use the power spectrum (from CMB observations) to obtain a statistical realisation of the density field δ_k :

$$P(k) = \langle |\delta_k|^2 \rangle \Rightarrow \delta_k = \sqrt{P(k)} A_k e^{i\varphi_k}$$

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where $A_k e^{i\phi_k} = B_1 + iB_2$ and B_1, B_2 are drawn from a Gaussian distribution. Finally, one gets:

$$\mathbf{x} - \mathbf{x}_0 = \psi \to (\mathbf{x} - \mathbf{x}_0)_k = i\mathbf{k}\frac{\delta_k}{k^2}$$
$$\dot{\mathbf{x}} = \frac{\dot{D}}{D}\psi \to \mathbf{v}_k = a\frac{\dot{D}}{D}\psi_k$$

Fourier transforming back to position space we obtain the desired initial conditions for the simulation.

Unperturbed positions (homogeneous grid)







How? Solving gravity

Now that we have an initial particle distribution with well-defined values of \mathbf{x} and \mathbf{v} we need to solve the dynamics:

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 or $\dot{\mathbf{p}}_i = -\nabla_x\phi(\mathbf{x}_i)$

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for which we need to know the gravitational potential:

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Compute force on particle *i* given by all other particles $j \neq i$ in the simulation domain

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Requires order of *N*² operations, which **quickly becomes prohibitive for large** *N*

We know that the relaxation time of a system of N objects interacting through gravity is given by

$$t_{\rm relax} = \frac{N}{8\ln N} t_{\rm cross}$$

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The system will behave as collision less when evolving over a time span $\,t\ll t_{
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$$N \sim 10^{67}$$
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So dark matter in a galaxy is evolving collisionlessly throughout the whole cosmic history. This is true also for (standard cold) dark matter in any larger cosmic volume



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So we know that (standard cold) dark matter in the Universe is expected to behave as a collision less system. However, we will sample it with mass elements representing a (huge) ensemble of fundamental particles (so N is much lower than in reality):

$$m_{\chi} \approx 100 \,\mathrm{Gev}/c^2 \qquad \Rightarrow$$

 $m_{\mathrm{sim}} \approx 10^8 - 10^{10} \,\mathrm{M_{\odot}}/h$

One simulation particle represents ~ 10⁶⁰ dark matter particles!

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Still, as long as we can ensure $t_{relax} \gg t_{sim}$ the system can still remain collisionless, and the orbits of the simulation particles will faithfully represent the motion of the fundamental particles

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- ϵ too small implies:
- possible collisional effects in the system
- integration of low-impact parameter orbits very expensive
Solving gravity: a note on collisionless systems

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- ϵ typically 2-4% of the mean inter-particle separation

Step 2: Solving gravity

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for which we need to know the peculiar potential ϕ that follows:

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How? Solving gravity: Particle-Mesh

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A possible way to solve for the gravitational potential is the so-called particle-mesh (PM) method, which exploits the properties of the Poisson's equation in Fourier space.

Instead of computing ϕ by direct summation on all particles, the solution to the gravitational Poisson's Equation

$$\nabla_x^2 \Phi = 4\pi G a^2 \rho(\mathbf{x})$$

can be obtained through a convolution of the density field $\rho(\mathbf{x})$ with a Green's Function

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

Example: for vacuum boundary conditions (i.e. the density goes to zero at infinity) one has:

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

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The PM method exploits the convolution theorem:

in Fourier space the convolution becomes a simple multiplication (between the Fourier transform of the Green's Function g_k and the Fourier transform of the density field ρ_k) so that the gravitational potential in Fourier space Φ_k can be simply computed as:

$$\Phi_k = g_k \cdot \rho_k$$

Therefore, the PM method requires three mathematical operations to solve for the gravitational potential:

- 1. Compute the Fourier transform of the density field ρ_k
- 2. Multiply the density field in Fourier space with the Green's function to obtain the potential $\Phi_k = g_k \cdot \rho_k$
- 3. Compute the inverse Fourier transform of the potential to position space to get $\Phi_k \to \Phi(\mathbf{x})$

However, in a system of N discrete particles, one does not have a density field, which has to be computed starting from the particles.

Therefore, the PM algorithm is made of four different steps, only one of which is the actual potential computation:

- A. **Density assignment** (from particle's position to a density field)
- B. Potential computation (comprising the 3 mathematical operations discussed above)
- C. Computation of the force (acceleration) field from the potential
- D. Assign the forces to individual particles

Step A: Density assignment

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We can give particles a "shape" *S(x)* with a corresponding volume of uniform density, and assign to each mesh cell the fraction of the particle's mass that falls inside the cell.

If we call $\mathbf{x_m}$ the position of the cell centres and \mathbf{x}_i the position of particle *i* the overlap of a cell (i.e. the fraction of the particle's volume falling in the cell) is given by:

Step A: Density assignment

$$W(\mathbf{x}_{\mathrm{m}} - \mathbf{x}_{i}) = \int_{\mathbf{x}_{\mathrm{m}} - \frac{h}{2}}^{\mathbf{x}_{\mathrm{m}} + \frac{h}{2}} S(\mathbf{x}' - \mathbf{x}_{i}) d\mathbf{x}'$$



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where we have defined:

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

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and the density on the grid is:

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

Step A: Density assignment



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Shape function: a Dirac delta A single particle contributes all its mass to the cell it belongs to Density in the cell $\rho = 4 m / h^3$



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Shape function: a cubic volume of side *h* A single particle contributes some mass to 8 different grid cells

This is called Cloud-In-Cell, or CIC

Step A: Density assignment

Some popular Shape Functions for the density assignment



For the force assignment (step D), the same assignment function used for step A needs to be used **to ensure momentum conservation**.

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Step B: Potential Computation

Once the density field in real space has been obtained, in order to compute the gravitational potential **we first need to get its Fourier transform**. If we assume a **periodic** density field in a cubic box of size L, this can be expressed as a Fourier series:

/ \

$$\rho(\mathbf{x}) = \sum_{\mathbf{k}} \rho_k e^{i\mathbf{k}\cdot\mathbf{x}} \quad \text{where} \quad \mathbf{k} \in \frac{2\pi}{L} \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix}$$

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One can do the same thing for the potential

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$$\Phi(\mathbf{x}) = \sum_{\mathbf{h}} \Phi_k e^{i\mathbf{k}\cdot\mathbf{x}}$$

 $\mathbf{k} \in \frac{2\pi}{L} \left(\begin{array}{c} n_1 \\ n_2 \\ n_1 \end{array} \right)$

and after substitution, the Poisson equation reads:

$$\nabla^2 \Phi = 4\pi G \rho(\mathbf{x}) \Rightarrow \nabla^2 \left(\sum_{\mathbf{k}} \Phi_k e^{i\mathbf{k} \cdot \mathbf{x}} \right) = 4\pi G \left(\sum_{\mathbf{k}} \rho_k e^{i\mathbf{k} \cdot \mathbf{x}} \right)$$

Step B: Potential Computation

The derivative on the LHS can be easily performed:

$$\sum_{\mathbf{k}} \left(-k^2 \Phi_k \right) e^{i\mathbf{k} \cdot \mathbf{x}} = 4\pi G \sum_{\mathbf{k}} \rho_k e^{i\mathbf{k} \cdot \mathbf{x}}$$

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As the equality must hold for each Fourier mode k, this gives the solution for the gravitational potential in Fourier space:

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From which we see that the Green's function for the Poisson's equation with periodic boundary conditions is given by:

$$g_k = -\frac{4\pi G}{k^2}$$

Step B: Potential Computation

We can now Fourier transform back the gravitational potential to real space, and have a potential field defined in each of the grid cells.

$$\mathcal{F}^{-1}(\Phi_k) = \Phi(\mathbf{x}_{\mathrm{m}})$$

We can now compute the forces at the cells' centers...

Step C: Force Computation

Once the gravitational potential in real space is known, one has to compute the force field in each of the grid cells. This is done by approximating the force field by finite differencing:

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Possible finite differencing schemes:

2nd order:

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

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4th order:

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

Step D: Force assignment

Once the force field on the grid cells in real space is known, in order to evolve the particles system one needs to compute the forces (or the accelerations) on the particles' positions.
Solving gravity: PM force computation

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Once the force field on the grid cells in real space is known, in order to evolve the particles system one needs to compute the forces (or the accelerations) on the particles' positions.

This is done by interpolation:

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

where the same interpolation kernel W that was used for the density assignment in Step A MUST be used to ensure for momentum conservation

Solving gravity: the Particle-Mesh method Advantages and disadvantages of the PM method

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The main **disadvantage** of the PM algorithm is the fact that the **spatial resolution is limited to the mesh size** (h in our examples).

This is a very serious problem for astrophysical and (most importantly) for cosmological simulations, where the dynamic range of the problem is large: systems of interest may be unresolved as they cluster below the mesh scale

LookBack	Time: 13.89	134 Gyr		ioMpc

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How? Solving gravity: Tree methods

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A different method to solve the N-body problem is the so-called **Tree algorithm**: the simulation domain is recursively divided into subdomains (tree nodes) forming the different levels of a hierarchical tree structure.

The main goal of such procedure is to group distant particles together in the potential calculations and approximate their gravitational potential with a multipole expansion. This reduces the complexity of the algorithm to O(N log[N]).

Basic structure of a hierarchical tree:



ROOT node (the entire simulation domain)

Basic structure of a hierarchical tree:



CHILD nodes - level 1 (1/8th of the simulation domain)

Basic structure of a hierarchical tree:



And so on until child nodes have at most 1 particle

CHILD nodes - level 2 (1/64th of the simulation domain)









Why is the tree advantageous?

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Consider a group of particles at positions x_i with their center of mass at position s.



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So, we want to compute:

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

we can expand the factor:

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

for

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



Why is the tree advantageous?

One gets (with some tedious calculations):

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

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Why is the tree advantageous?



Why is the tree advantageous?

The group of particles can correspond to a particular Tree node



of mass

S

r

origin

Why is the tree advantageous?

The group of particles can correspond to a particular Tree node

So the following multipole moments can be computed and stored for all tree nodes:

• Monopole:

$$M = \sum_{i} m_{i}$$

• Quadrupole tensor:

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

and the resulting potential is:

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

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Often (as e.g. in Gadget2-3) only the Monopole is used, so that one can replace the N_{node} interactions with a single interaction for its center of mass:

$$-G\sum_{i=1}^{N_{\text{node}}} \frac{m_i}{|\mathbf{r} - \mathbf{x}_i|} \to -G\frac{M}{|\mathbf{y}|}$$



The accuracy of the approximation can be adjusted by defining what "distant" means.



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This is done by setting a threshold for the angle θ under which a given tree node (i.e. a group of particles) is "seen" from the target particle on which the potential is to be computed. Such threshold (dividing sufficiently distant nodes from closer ones) is called **OPENING ANGLE**



Advantages and disadvantages of the Tree method

The main **advantages** of the tree method are the following:

- There is no intrinsic restriction to the dynamic range that can be achieved: spatial resolution automatically increases in regions where particles cluster
- It is possible to adjust the accuracy of the force calculation by tweaking the tree opening angle
- The speed of the algorithm does not strongly depend on the level of clustering

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The main **disadvantage** of the tree method is that for highly homogeneous matter distributions (as e.g. the cosmic density field at high redshifts) **the almost vanishing force on each particle is the result of the cancellation of many larger contributions**. This makes it numerically expensive to obtain high accuracy in the force calculation.

How?

Solving gravity: the Tree-PM method (if you can't beat them, join'em!)
In order to overcome the latter disadvantage of the Tree method, and to exploit the high speed of the PM method, many N-body codes implement a combination of the Tree and PM algorithms, called the Tree-PM method. The idea is the following:

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1: Start from Poisson's equation in Fourier space

$$\phi_k = \frac{4\pi G}{k^2} \rho_k$$

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the PM method in Fourier space

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where the short-range potential features the complementary error function

$$\phi^{\rm short}(r) = -\frac{Gm}{r} \operatorname{erfc}\left(\frac{r}{2r_s}\right)$$

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The Tree-PM force splitting



The Tree-PM force splitting



How? Solving gravity: Multi-grid methods

A different procedure to solve the Poisson equation is given by approximating the Laplace operator ∇^2 on a grid. Consider a 1D version of Poisson's equation:

$$\nabla^2 \phi = \frac{\partial^2 \phi}{\partial x^2} = 4\pi G \delta(x)$$

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If the potential ϕ and the density δ are discretised at N equallyspaced points with spacing h the Laplace operator can be approximated as:

$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i \simeq \frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{h^2}$$

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so that Poisson's equation becomes:

$$\frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{h^2} = 4\pi G\delta_i$$

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$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i \simeq \frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{h^2}$$

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Generalising to 2D one gets:

$$\left(\nabla^2 \phi\right)_{i,j} \simeq \frac{\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1} - 4\phi_{i,j}}{h^2} = 4\pi G \delta_{i,j}$$

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5-points stencil

Update of a black cell depends only on values of red cells: Red-Black sweep: first update half of the cells (all the black ones) and then the other half (all the red ones) using the updated values of the black cells

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7-points stencil

Update of a black cell depends only on values of red cells: Red-Black sweep: first update half of the cells (all the black ones) and then the other half (all the red ones) using the updated values of the black cells

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Therefore, the solution of Poisson equation corresponds to finding the zeros of the function

$$[f(\phi)]_{i,j,k} \equiv \left(\nabla^2 \phi\right)_{i,j,k} - 4\pi G \delta_{i,j,k}$$

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Solving this by matrix inversion is computationally prohibitive for large grids as complexity grows like $\mathcal{O}(N^3)$ but can be solved iteratively using Newton-Raphson's method.

A short recap of Newton-Raphson's method.

For a 1D function f(x) the zeros of the function (i.e. the values \tilde{x} for which $f(\tilde{x}) = 0$) can be found iteratively starting from a guess $\tilde{x}^{(0)}$ with the rule :

$$\tilde{x}^{(n+1)} = \tilde{x}^{(n)} - \frac{f(\tilde{x}^{(n)})}{f'(\tilde{x}^{(n)})}$$

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Therefore, for our function $[f(\phi)]_{i,j,k}$ we will have:

$$\phi_{i,j,k}^{(n+1)} = \phi_{i,j,k}^{(n)} - \frac{f_{i,j,k}}{\frac{\partial f_{i,j,k}}{\partial (\phi_{i,j,k})}}$$

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which can be iterated until

$$|\phi_{i,j,k}^{(n+1)} - \phi_{i,j,k}^{(n)}| < \epsilon$$

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Convergence can be fastened by using multi-grid acceleration:

- 1) map the target grid guess on a coarser grid (restriction)
- 2) get a (faster) solution for the large-scale structure on a coarser grid
- 3) repeat steps 1-2 until reaching a minimum grid resolution
- 4) map to a finer grid (prolongation) and use as a guess for new iteration on the finer grid
- 5) repeat step 4) until reaching again the target grid resolution

As only neighbouring points in the grid communicate with each other at every iteration (7-points stencil) information propagates only by one cell per iteration: convergence is slow.



How? Solving gravity: comparing solvers

Particle-Mesh

Solve

$$\nabla_x^2 \Phi = 4\pi G a^2 \rho(\mathbf{x})$$

by summing individual potential contributions over all volume elements

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

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Direct summation (Tree)

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

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Multi-grid (Newton-Raphson)

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$$\nabla_x^2 \Phi = 4\pi G a^2 \rho(\mathbf{x})$$

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$$\left(\frac{\partial^2 \phi}{\partial x^2}\right)_i \simeq \frac{\phi_{i+1} + \phi_{i-1} - 2\phi_i}{h^2}$$
Gravity solvers compared

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Does not rely on the superposition principle

Works also for non-linear Poisson-like equations

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How? Time integration

Step 3: Time integration

Once the force (hence the acceleration) on each particle is known, the system has to be moved **forward in time (positions and velocities)**



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

Step 3: Time integration

Once the force (hence the acceleration) on each particle is known, the system has to be moved **forward in time (positions and velocities)**



Time-reversible and explicitly energy conserving

What else? Extending to non-standard models

Standard Cosmology after Planck



The Universe after Planck: 6 parameters to fit all data

- $\Omega_{\rm b} = 0.049$ $\Omega_{\rm CDM} = 0.265$ $\Omega_{\Lambda} = 0.6844$ $\sigma_8 = 0.831$
- $n_s = 0.9645$ $\tau = 0.079$

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Standard ACDM cosmology is based on a series of assumptions:

- Cosmological Principle (homogeneity & isotropy);
- Gaussian and Adiabatic initial conditions;
- Dark Matter is Cold and Collisionless;
- Neutrinos are massless;
- Dark Energy is a Cosmological Constant;
- GR is the complete theory of gravity;

The Dark Energy problem

Starting point: observational evidence of an accelerated expansion





Can we explain this somehow?

The Dark Energy problem

Starting point: observational evidence of an accelerated expansion





"Until it is solved, the problem of the dark energy will be a roadblock on our path to a comprehensive physical theory"

S. Weinberg

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Simpson et al. 2016

SDSS-II

0.6

VVDS

VIPERS

This work

0.8

0.6

0.5

0.4

0.3

0.2

6dFGS

(z)

fσ₈ (

Testing the assumptions of the Standard Model



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DARK ENERGY MODELS BEYOND THE COSMOLOGICAL CONSTANT

This will be just a purely phenomenological classification, based on the expected effects on structure formation and how these will affect N-body simulation methods.

For a more formal classification, see e.g. *Pourtsidou et al. (2013) Skordis et al. (2015)*

	time evolution	spatial fluctuations	interactions
Λ	×	×	×

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Interacting DE (Coupled and Extended Quintessence, Modified Gravity)	a dynamical (scalar) degree of freedom	fluctuations sourced by the interaction	non-minimally coupled to matter

An interaction between a matter field and a scalar field can be described by a source term in the respective continuity equations:

$$\nabla_{\mu}T_{\nu}^{\mu(\phi)} = -QT^{(\mathrm{DM})}\nabla_{\nu}\phi \qquad \nabla_{\mu}T_{\nu}^{\mu(\mathrm{DM})} = +QT^{(\mathrm{DM})}\nabla_{\nu}\phi$$

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$$\dot{\rho}_{\rm DM} + 3H\rho_{\rm DM} = +Q\rho_{\rm DM}\dot{\phi} \qquad \ddot{\phi} + 3H\dot{\phi} + \frac{dV}{d\phi} = -Q\rho_{\rm DM}$$

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By perturbing these equations at linear order one obtains a dynamical equation for the field perturbations:

$$\left(\frac{\partial^2}{\partial t^2} - \nabla^2\right)\delta\phi = \frac{dV}{d\phi}(\delta\phi) + Q\delta_{\rm DM}$$

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that in the so-called quasi-static limit ($\partial^2 \delta \phi / \partial t^2 \ll \nabla^2 \delta \phi$) gives:

$$\nabla^2 \delta \phi = -\frac{dV}{d\phi} (\delta \phi) - Q \delta_{\rm DM}$$

and assuming a flat potential ($dV/d\phi \ll \delta_{\rm DM}$):

$$\nabla^2 \delta \phi \approx -Q \delta_{\rm DM} \Rightarrow \delta \phi \approx -Q \Phi$$

By combining this relation with the linear perturbations equations of the matter field (Amendola 2004), one obtains a modified version of the gravitational instability equation:

$$Q = 0 \quad \ddot{\delta} + 2H\dot{\delta} - \frac{3}{2}\Omega\delta = 0$$

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Scalar fifth-forces are tightly constrained from solar system tests of gravity, need to allow for a non-universal coupling so that CDM is coupled and baryons are uncoupled ($Q_c \neq 0, Q_b = 0$):

$$\ddot{\delta}_{c} + \left(2H - 2Q\dot{\phi}\right)\dot{\delta}_{c} - \frac{3}{2}H^{2}\left[\left(1 + 2Q^{2}\right)\Omega_{c}\delta_{c} + \Omega_{b}\delta_{b}\right] = 0$$
$$\ddot{\delta}_{b} + 2H\dot{\delta}_{b} - \frac{3}{2}H^{2}\left[\Omega_{c}\delta_{c} + \Omega_{b}\delta_{b}\right] = 0$$

This implies an effective violation of the Weak Equivalence Principle:

$$\vec{a}_{\rm CDM} = -\vec{\nabla}\Phi(1+2Q^2) + 2Q\dot{\phi}\vec{v}_{\rm CDM} \qquad \vec{a}_{\rm b} = -\vec{\nabla}\Phi$$

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The term $2Q\dot{\phi}\vec{v}_{\rm CDM}$ is called "friction term" and arises from momentum conservation:

$$\frac{d\vec{p}}{dt} = \frac{d(m(\phi)\vec{v})}{dt} = m(\phi)\vec{a} + \frac{dm}{d\phi}\dot{\phi}\vec{v}$$

Standard Coupled Quintessence: interacting DM and non-interacting baryons:



In interacting DE the coupling determines two different gravitational forces for dark matter and baryons:

Particle-Mesh (for interacting DE)



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I) Assign mass to grid nodes for one species only, obtain density on the grid

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non-linear Regime



Marco Baldi - Cosmological Simulations - marco.baldi5@unibo.it

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An alternative approach to the Dark Energy problem is to modify General Relativity in the low curvature regime by changing the gravitational Action. One of the most popular models of this modified gravity approach is f(R):

$$S = \frac{1}{16\pi G} \int d^4x \sqrt{-g} f(R) + S_m(g_{\mu\nu}, \Psi_m)$$

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By varying this Action with respect to the metric tensor, with a similar procedure as for the standard GR Action, one gets the f(R) field eqs:

$$f_R R_{\mu\nu} - \frac{1}{2} f(R) g_{\mu\nu} - \nabla_\mu \nabla_\nu f_R + g_{\mu\nu} \Box f_R = 8\pi G T_{\mu\nu}$$

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By varying this Action with respect to the metric tensor, with a similar procedure as for the standard GR Action, one gets the f(R) field eqs:

where we have defined $f_R \equiv df/dR$

In GR one has $f(R) = R - 2\Lambda$ so that $f_R = 1$ and $\Box f_R = 0$

On the contrary, if f_R is a function of R one has $\Box f_R \neq 0$ so that f_R corresponds to a new propagating scalar degree of freedom.

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A particularly relevant model of f(R) gravity is given by the choice (Hu & Sawicki 2007):

$$f(R) = R - m^2 \frac{c_1 (R/m^2)^n}{c_2 (R/m^2)^n + 1} \qquad m^2 \equiv \frac{8\pi G\rho_0}{3}$$

because this allows to reproduce exactly the background evolution of a ACDM cosmology by setting:

$$\frac{c_1}{c_2} = 6 \frac{\Omega_{\Lambda}}{\Omega_{\rm M}}$$

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In this setup the f(R) model will differ from the standard Λ CDM cosmology only at the level of linear and non-linear perturbations

Trace of the modified Einstein equations:

$$3\Box f_R + f_R R - 2f(R) = -8\pi G(\rho - 3p)$$

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By perturbing this equation at linear order (posing $f_R = \overline{f}_R + \delta f_R$):

$$\left(\frac{\partial^2}{\partial t^2} - \nabla^2\right)\delta f_R = -M^2(f_R)\delta f_R + \frac{8\pi G}{3\bar{f}_R}\delta\rho_{\rm M}$$

That in the quasi-static approximation becomes:

$$\nabla^2 \delta f_R = M^2(f_R) \delta f_R - \frac{8\pi G}{3\bar{f}_R} \delta \rho_{\rm M}$$

that is the same equation we saw for interacting dark energy. However, differently from the case of interacting Dark Energy, in f(R) one CANNOT assume $M^2(f_R)\delta f_R \ll \delta \rho_{\rm M}$ NOT TRUE

$$\nabla^2 \delta f_R = M^2(f_R) \delta f_R - \frac{8\pi G}{3\bar{f}_R} \delta \rho_{\rm M}$$

if one can not neglect the $M^2(f_R)\delta f_R$ term, the equation is no longer linear and superposition principle does not hold.

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This can be rewritten as:

$$\nabla^2 f_R = \frac{1}{3c^2} \left(\delta R - 8\pi G \delta \rho\right) \qquad \delta R = \bar{R}(a) \left(\sqrt{\frac{\bar{f}_R(a)}{f_R}} - 1\right) \quad (\star)$$

with the solution of the field configuration affecting structure formation through

$$\nabla^2 \Phi = \frac{16\pi G}{3} \delta \rho - \frac{1}{6} \delta R$$

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Not possible to solve (\star) using PM or Tree methods. Need to resort on the iterative Newton-Raphson approach (Newton-Gauss-Seidel relaxation method)

$$\nabla^2 f_R = \frac{1}{3c^2} (\delta R - 8\pi G \delta \rho)$$

If superposition principle does not hold, it is not possible to solve the equation using PM or Tree methods. Need to resort on the iterative Newton-Raphson approach (Newton-Gauss-Seidel relaxation method)

This has been implemented in several simulation codes after the first simulations performed by *Oyaizu et al. 2008*:

Ecosmog (Li et al. 2012) MG-Gadget (Puchwein et al. 2013) Isis (Llinares et al. 2014) MG-Arepo (Arnold et al. 2019)



The MG-Gadget code (Puchwein, MB, Springel 2013) is one of the available codes for cosmological N-body simulations in Modified Gravity cosmologies

- The field equation $\nabla^2 f_R = \frac{1}{3c^2} (\delta R - 8\pi G \delta \rho)~~{\rm is~discretized~in}$ position space

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• Once f_R is known, $\delta R(f_R)$ is also known, and the Poisson equation can be solved by adding up the standard and the MG contributions

Why doing Cosmological Simulations (for extended cosmological models)?



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* MUST be there: $\Sigma_i m_{\nu} \gtrsim 0.06 \text{eV}$ $\Omega_{\nu} = \frac{\Sigma_i m_{\nu_i}}{93.14 h^2 \text{eV}}$

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 $k [h \text{ Mpc}^{-1}]$
The effect of Massive Neutrinos

 $m_v = 0.17; 0.3; 0.53 \text{ eV}$



[see also Bird, Viel & Haehnelt 2012]

Nonlinear suppression of the matter $P(k) \sim 15\%$ larger than linear predictions at k~1-2 h/Mpc (critical range of scales for WL surveys)

MB et al. 2014



MB et al. 2014



MB et al. 2014



MB et al. 2014



The deviations expected for a non-zero neutrino mass and for an f(R) theory of gravity are suppressed below observational resolution if both phenomena coexist \rightarrow **RISK OF MISINTERPRETING THE DATA**!!!

Peel, MB et al., A&A 2018 (arXiv:1805:05146)



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Peel et al. 2018

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Summary and conclusions

- Cosmological simulations are a necessary tool to predict the properties and the evolution of cosmological observables
- Newtonian simulations can very well describe the evolution of the universe over a wide range of scales (large-scale relativistic effects can be included in post-processing for scales close to the horizon)
- **Different methods** have been developed to solve for the selfgravitational evolution of a system of N particles representing (i.e. sampling) the cosmic density field: **PM, Tree, TreePM, Multigrid**
- These methods may need to be combined and /or modified to include additional physics beyond the standard LCDM model for which they have been developed, such as non-trivial Dark Energy and Modified Gravity models
- Extended simulations may be the only way to predict characteristic features of such models allowing to distinguish them from standard LCDM

DUSTGRAIN fR5, m_v=0.1 eV CDM

100 Mpc/h



z = 0.00

Thank you!

DUSTGRAIN fR5, m_v=0.1 eV Neutrinos

