





Initial Conditions for Cosmological Simulations: The next generation

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European Research Council Established by the European Commission

COSMO-SIMS

Overview:

The precision challenge: high order, convergence, discreteness

Michaux et al. (2020, TBS)

with Michaël Michaux, Cornelius Rampf, Raul Angulo

Massive Neutrinos

with Christian Partmann, Christian Fidler, Cornelius Rampf

More accurate ICs for Eulerian Codes: **Field level PT based on Semiclassical Dynamics**

with Cora Uhlemann, Cornelius Rampf, Mateja Gosenca

COSMICWEB:

Cosmological ICs in the Cloud

with Michael Buehlmann (also Adrian Jenkins for EAGLE/PANPHASIA integration)

Atelier DE, Mai 18 2020

Partmann et al. (2020)

Uhlemann+2019, OH+2020, in prep.

Buehlmann & Hahn (2020, in prep.)

Simulation workflow



background movie: Ralf Kaehler, Tom Abel & OH

The precision challenge: high order, convergence, discreteness

with Michaël Michaux, Cornelius Rampf, Raul Angulo

Michaux et al. (2020, TBS)

Equations of motion

Collisionless dynamics (for dark matter), weak field Newtonian limit, assume can subtract out mean field (no backreaction)

$$\frac{\partial f_m}{\partial t} + \frac{p_i}{ma^2} \frac{\partial f_m}{\partial x^i} - m \frac{\partial \phi}{\partial x^i} \frac{\partial f_m}{\partial p_i} = 0$$
$$\nabla^2 \phi = 4\pi G a^2 (\rho - \overline{\rho})$$
$$\rho = ma^{-3} \int d^3 p f_m(x, p)$$

describes collisionless fluid with self-gravity



continuum limit with only long-range interactions

no relativistic species

no horizon-scale (GR) effects

NASA/CXC/M. Weiss

Cold limit – cosmic distribution function

NO hot components (apart from neutrinos)

Lagrangian submanifold (Hamilton-Jacobi GF) describes full phase space



Cold limit – Boltzmann hierarchy

Get fluid variables by marginalising over momenta

$$\begin{split} n(\mathbf{x},t) &:= \int \mathrm{d}^3 p \ f(\mathbf{x},\mathbf{p},t) & \text{0th moment} \\ \pi_i(\mathbf{x},t) &:= \int \mathrm{d}^3 p \ p_i \ f(\mathbf{x},\mathbf{p},t) & \text{1st moment} \\ \Pi_{ij}(\mathbf{x},t) &:= \int \mathrm{d}^3 p \ p_i p_j \ f(\mathbf{x},\mathbf{p},t) & \text{2nd moment} \\ \end{split}$$

in cold monokinetic case, 2nd and all higher moments can be expressed in terms of 0th and 1st, **until shell-crossing happens**, $\Pi_{ij} = \pi_i \pi_j$ then hierarchy is in general infinite...

in monokinetic regime

These are just the standard fluid equations with a time-dependent Poisson equation.

Shell-crossing

gives rise to cosmic structure, and marks the end of current PT



Lagrangian Perturbation Theory

(for single fluid with cold initial data)

Lagrangian map

$$\boldsymbol{x}(\boldsymbol{q},t) = \boldsymbol{q} + \boldsymbol{\Psi}(\boldsymbol{q},t)$$

Density can be written as overdensity

$$\rho(\boldsymbol{x},t) = \overline{\rho}(t) \left[1 + \delta(\boldsymbol{x},t)\right]$$

Overdensity given by Jacobian

$$\delta(\boldsymbol{x},t) = \frac{1}{J(\boldsymbol{q},t)} - 1$$



Canonical equations of motion can be combined to second order to give in conformal time

$$\mathbf{x}'' + \mathcal{H}\mathbf{x}' = -\nabla\phi$$
 $\nabla_x^2 \phi = \frac{3}{2}\mathcal{H}\Omega_m\delta$ $\mathcal{H} = a'/a$

Final equation underlying all of LPT is

$$J \left(\delta_{ij} + \Psi_{i,j}\right)^{-1} \left(\Psi_{i,j}'' + \mathcal{H}\Psi_{i,j}'\right) = \frac{3}{2}\mathcal{H}^2\Omega_m(J-1) \qquad J = \det\left[\delta_{ij} + \Psi_{i,j}\right]$$

We want to solve this as a perturbative series (D is small parameter)

$$\Psi(\mathbf{q},\tau) = \sum_{n=1}^{\infty} D(\tau)^n \, \Psi^{(n)}(\mathbf{q})$$

Buchert (1994), Catelan (1995), Bouchet+(1995)

nLPT: UV sensitivity of ICs and N-body simulations



LPT to third order

expand in displacement field $x = q + \psi$

$$\psi_{3\text{LPT}}(\boldsymbol{q},t) = \psi^{(1)}(\boldsymbol{q}) D_{+} + \psi^{(2)}(\boldsymbol{q}) D_{+}^{2} + \psi^{(3)}(\boldsymbol{q}) D_{+}^{3}$$

Buchert (1994), Catelan (1995), Bouchet+(1995)

Displacement potentials

$$\boldsymbol{\psi}^{(i)} = \boldsymbol{\nabla}_{\boldsymbol{q}} \phi^{(i)} + \boldsymbol{\nabla}_{\boldsymbol{q}} \times \boldsymbol{A}^{(i)}$$

Terms get increasingly bluer

...thereby become increasingly more UV sensitive

UV truncation at Nyquist mode (= finite resolution) becomes visible

Results at z=0 in nonlinear insensitive to this due to gravity

Michaux+2020

Discrete evolution vs. fluid evolution

Lagrangian description, evolution of fluid element

 $\mathbb{Q} \subset \mathbb{R}^3 \to \mathbb{R}^6 : \mathbf{q} \mapsto (\mathbf{x}_{\mathbf{q}}(t), \mathbf{v}_{\mathbf{q}}(t))$



The N-body approximation:

cover distribution function with N 'coarse-graining' particles



Convergence of LPT and N-body...

I've talked a lot about discreteness and Vlasov in the past. Here is a new take:

(simple cubic)

Particle motion on small scales not isotropic. Can be calculated for Bravais lattices:



Agreement of nLPT and N-body in weakly non-linear regime, *but* only after correcting for discreteness



Michaux+2020

... discreteness effects large at early times. can push late with 3LPT...

but also Garrison+2016

Discreteness — impact on low-z power spectrum

effect on PS at z=0 wiped out by non-linearity (scale-mixing), not at higher z



Michaux+2020

discreteness effects strongest at high z

very slow convergence with particle number ($\propto k_{
m Nv}^3$)

Possible Solution: Interpolating in phase space

Abel, Hahn & Kaehler 2012 Schandarin et al. 2012



Defines density etc. everywhere in space...

But too costly for 'precision cosmology' workhorse simulations, instead: start late...

The convergence radius of LPT

How long can we trust LPT for a given simulation?

"Up to some point before shell-crossing!" - but can we be more precise?



Theoretical estimate:

$$R > D_{+}^{\text{theory}} = \frac{\mathrm{T}}{\|\nabla_i \nabla_j \varphi_{\text{ini}}\|} \qquad \mathrm{T} \simeq 10^{-1.5} - 10^{-1}$$

Rampf+2015 estimate, cf. also Saga+2018



Work in progress: How does this translate into accuracy of z=0 statistics?

In principle this means: we can start late, and we probably should start late...

Impact of nLPT vs. discreteness on low-z spectra



best results with high order LPT and low starting redshift (counter to common lore!)

Conclusions 1:

- N-body simulations limited by discreteness effects
- Can achieve per cent level accuracy up to particle Nyquist
- Requires late starts, high order LPT
- Unfortunately, we only know how to do this for single fluid... incl. baryons, neutrinos in nLPT framework still ongoing work

Efficient Simulations with Massive Neutrinos

with Christian Partmann, Christian Fidler, Cornelius Rampf

Partmann+2020

Cosmic Neutrinos

- Weak constraints for the neutrino mass sum from particle physics: $\Sigma m_{\nu} < 1.1 \,\mathrm{eV}$ [Katrin 2019]
- Cosmic neutrinos are omnipresent in the Universe: $n_{\nu} = \mathcal{O}(100 \,\mathrm{cm}^{-3})$
 - Neutrinos change the Hubble expansion rate due to **non-relativistic transition**: $\Omega_{\nu} \propto a^{-4} \rightarrow \Omega_{\nu} \propto a^{-3}$
 - Free streaming on small scales due to high thermal velocities
- Best constraints come from cosmology! $\Sigma m_{\nu} < 0.12 \,\mathrm{eV}$ [Planck 2018]

 \rightarrow Future cosmological observations (Euclid, LSST) will determine the absolute neutrino mass scale



Approaches to simulate neutrinos

Linear-response + Particles

Bird+2018



Problem: GR effects not included

Maybe we don't need to simulate neutrinos Partmann+2020:

- The **Weak field limit** of general relativity includes leading order GR effects but also non-linear clustering on small scales [Fidler 2017]
- Use **gauge freedom** of GR to absorb neutrino corrections $\gamma(x, t)$ in the definition of the coordinate system:



 $\xrightarrow{x^{\mathrm{Nm}} = x + L(x,t)} \quad \partial_t^2$

$$^{2}x^{\mathrm{Nm}} = -\nabla\Phi^{\mathrm{N}}(x^{\mathrm{Nm}}) + H\partial_{t}x^{\mathrm{Nm}}$$

- In the Newtonian motion gauge (Nm), particles move on Newtonian trajectories
- Nm space-time is fixed by a Nm gauge condition (2nd order PDE for L)

But see also COSIRA (Tram+2019): opposite approach: add corrections to potential over course of N-body simulation

(slide courtesy C. Partmann)

Oliver Hahn (Lagrange/UCA/OCA)

Add neutrinos in post-processing gauge-trafo

Density map in Nm gauge for $m_{\nu} = 0.1 \, \mathrm{eV}$

This already includes neutrinos partially through the Hubble friction (background effect) Coordinate transformation from Nm gauge to N-boisson gauge (implicitly used in N-body codes [Fidler 2018])

L Includes effects of neutrinos and GR on the perturbation level



Partmann+, 2020

(slide courtesy C. Partmann)

Competitive to full phase-space sampling



only caveat: currently more involved post-processing for lightcones (needs some more work)

Partmann+, 2020

(slide courtesy C. Partmann)

More accurate ICs for Eulerian Codes: Field level PT based on Semiclassical Dynamics

with Cora Uhlemann, Cornelius Rampf, Mateja Gosenca

Uhlemann+2019, OH+2020, in prep.

Precision CDM+baryon two-fluid simulations

N-body two-fluid sims have dominant discreteness errors



Perturbative Dynamics in a Field Framework I



After shell crossing, dynamics becomes complicated, but before, can absorb most dynamics into time coordinate and spatial expansion Lagrangian map

$$\mathbf{q} \mapsto \mathbf{x}(\mathbf{q}; a) = \mathbf{q} + \boldsymbol{\xi}(\mathbf{q}; a)$$

Lagrangian perturbation theory

$$\xi_i(\boldsymbol{q};a) = \sum_{n=1}^{\infty} \xi_i^{(n)}(\boldsymbol{q})$$

$$\boldsymbol{\xi}^{(1)} = -a \, \boldsymbol{\nabla}_{\mathbf{q}} \varphi_g^{(ini)}$$
$$\boldsymbol{\xi}^{(2)} = -a^2 \, \frac{\boldsymbol{\nabla}_{\mathbf{q}}}{\Delta_{\mathbf{q}}} \mu_2^{(ini)}$$

but how do we translate this for Eulerian codes (RAMSES,ENZO,Nyx) that want density and velocity?

. . .

at first order, Zeldovich, just straight lines...

Perturbative Dynamics in a Field Framework II

 $\bullet^{(x,t=a)}$ Zel'dovich approximation: particle moves on straight line

Transition amplitude for fluid element to go from q to x in time a

Rewrite these simple trajectories as a classical action

$$S_0(\boldsymbol{x}, \boldsymbol{q}; a) = \frac{1}{2}(\boldsymbol{x} - \boldsymbol{q}) \cdot \frac{\boldsymbol{x} - \boldsymbol{q}}{a}$$

Apply Feynman trick to get propagator

$$K_0(\boldsymbol{x}, \boldsymbol{q}; a) = N \exp\left\{rac{\mathrm{i}}{\hbar}S_0(\boldsymbol{x}, \boldsymbol{q}; a)
ight\}$$

then evolve field $\psi_0(\boldsymbol{x}; a) = \int \mathrm{d}^3 q \, K_0(\boldsymbol{x}, \boldsymbol{q}; a) \, \psi_0^{(\mathrm{ini})}(\boldsymbol{q})$

Recover moment hierarchy of evolved field by taking gradients

$$\rho = \psi \psi^* \qquad \mathbf{j} = \frac{i\hbar}{2} \left(\psi \nabla \psi^* - \psi^* \nabla \psi \right) \qquad \dots$$

Uhlemann, Rampf, Gosenca & OH (2019) see also Short&Coles (2006)

(q,t=0)

Why should this work? (for fluid dynamicists)

Madelung representation (polar decomposition)

$$\psi = \sqrt{\rho} \exp\left(-\frac{i}{\hbar}\phi_v\right)$$

Transforms Schroedinger-Poisson equation into

$$\partial_a \rho - \nabla \cdot \left[\rho \nabla \phi_v \right] = 0$$
$$\partial_a \phi_v - \frac{1}{2} (\nabla \phi_v)^2 = \frac{\hbar^2}{2} \frac{\nabla^2 \rho}{\rho}$$

continuity eq.

Bernoulli eq. + quantum corr.

RHS has important singularities! (see later)

Compare this to cosmic fluid equations for irrotational ICs

See Uhlemann, Rampf, Gosenca & OH (2019) for formal proofs of classical limits.

Perturbative Dynamics in a Field Framework III

Obtain a field version of Zeldovich trajectories:



Interference = multi-streaming

Uhlemann, Rampf, Gosenca & OH (2019)

Perturbative Dynamics in a Field Framework III

This can be expanded to n-th order LPT, propagator solves SE

$$\begin{split} \mathrm{i}\hbar\partial_a K &= \hat{H}K \qquad \hat{H} \equiv -\frac{\hbar^2}{2}\boldsymbol{\nabla}_x^2 + V_{\mathrm{eff}}(\boldsymbol{x};a) \\ V_{\mathrm{eff}}^{(1)} &= 0 \\ V_{\mathrm{eff}}^{(2)} &= \frac{3}{7}\nabla^{-2}\left[\left(\nabla^2\varphi_{\mathrm{g}}^{(\mathrm{ini})}\right)^2 - \left(\nabla_i\nabla_j\varphi_{\mathrm{g}}^{(\mathrm{ini})}\right)^2\right] \end{split}$$

end-point approx. to path integral gives "DKD" propagator, equiv. to 2.5LPT in h->0 limit

Order by order this turns out to be more accurate than nLPT



Due to underlying Hamiltonian, symplectic structure is preserved, unlike in LPT, where only 1LPT is exactly symplectic

Uhlemann, Rampf, Gosenca & OH (2018)

Random Initial Conditions



ICs=Gaussian Random Field with cosmo spectrum 256³ resolution (images show slice)

Advantages

continuous density and momentum fields "perfectly consistent with N-body particles" exact mass conservation



paper in prep.

To flow potentially, or not to flow potentially

Poincaré, or Kelvin-Helmholtz invariant is a constant of motion

$$\Gamma \equiv \oint_{C(a)} \boldsymbol{v} \cdot d\boldsymbol{x} = \int_{S^{(\text{ini})}} (\boldsymbol{\nabla}^{\text{L}} \times \boldsymbol{v}^{(\text{ini})}) \cdot d\boldsymbol{S}^{(\text{ini})} = 0, \text{ if no initial vorticity}$$

this is only true in 1LPT non-perturbatively...

In propagator framework, this translates to

$$\frac{1}{2\pi\hbar}\oint_{C(a)} \nabla \phi_{\mathbf{v}} \cdot d\mathbf{x} = n_{+} - n_{-} = 0 , \quad n_{\pm} \in \mathbb{N} \quad \text{implying vorticity is a} \\ \text{conserved topological charge}$$



'roton' pair production
in multi-stream region

Uhlemann, Rampf, Gosenca & OH (2018)

COSMICWEB: Cosmological ICs in the Cloud

with Michael Buehlmann

Buehlmann et al. (2020, in prep.)

Cosmological Zoom Simulations

Focus computational resources on object of interest

- "what happens inside a galaxy far far away will not influence our galaxy"
- use coarser resolution for distant regions
- high resolution, complex and computationally expensive physics for individual object

see Buehlmann & Hahn 2020, in prep. for details (also eff. of zooms)





slide courtesy M. Buehlmann

MUSIC 1 — zoomin' since 2011

very widely used in community for zoom simulations supports all major codes (Gadget, RAMSES, Arepo, ENZO, ART, GIZMO, Nyx,...)

https://bitbucket.com/ohahn/music



Motivation for the cosmICweb platform

Where to go from MUSIC1 towards MUSIC2 ecosystem



1: create ICs from cosmo parameters and random seed

2: running simulation, storing snapshots

3: structure finding and linking across time: merger trees

4: for each halo, findLagrangian patch (origin)5: for chosen halo, refine that patch in ICs

6: run zoom simulation with additional physics, etc.

cosmlCweb: A database and web interface for 1. Finding the right objects to resimulate 2. Obtaining initial conditions for these objects 3. Referencing objects in articles / papers

slide courtesy M. Buehlmann

Overview of cosmICweb – modular architecture



Buehlmann+, in prep

Overview of cosmlCweb – Data

Currently:

slide courtesy M. Buehlmann

locally hosted simulations:

- set of DM-only simulations ranging from 60 to 1000 Mpc³
- AGORA and RHAPSODY from existing zoom-projects
- data hosted at OCA

EAGLE simulations: Evolution and Assembly of GaLaxies and their Environments

- baryonic physics & DM-only simulations from the EAGLE project
- data hosted by VIRGO consortium (externally)

		size [h ⁻¹ Mpc]	cosmo.	DM resolution $[h^{-1}M_{\odot}]$	[b]	snapshots [z _{max} – z _{min}]	structure finder	N_{\min}^e
local	150MPC 150MPC_lowres 300MPC_lowres AGORA RHAPSODY RHAPSODY_NewCosmo	150 150 300 300 60 1000 1000	[P1] [P1] [P1] [W1] [W2] [P1]	$\begin{array}{c} 2.70 \times 10^8 \\ 2.16 \times 10^9 \\ 2.14 \times 10^9 \\ 1.71 \times 10^{10} \\ 1.21 \times 10^8 \\ 6.46 \times 10^{10} \\ 7.99 \times 10^{10} \end{array}$		$\begin{array}{c} 101 \ [12-0] \\ 101 \ [12-0] \\ 101 \ [12-0] \\ 101 \ [12-0] \\ 101 \ [12-0] \\ 101 \ [12-0] \\ 101 \ [12-0] \\ 101 \ [12-0] \\ 101 \ [12-0] \end{array}$	ROCKSTAR ROCKSTAR ROCKSTAR ROCKSTAR ROCKSTAR ROCKSTAR	100 500 100 500 1000 1000 1000
EAGLE	Ref-L0025N0376 L0025N0376 Ref-L0100N1504 L0100N1504	16.94 16.94 67.77 67.77	[P2] [P2] [P2] [P2]	6.57×10^{6} 7.63×10^{6} 6.57×10^{6} 7.63×10^{6}	√ √	29 [20.3 – 0] 29 [20.3 – 0] 29 [20.3 – 0] 29 [20.3 – 0]	FoF & SUBFIND FoF & SUBFIND FoF & SUBFIND FoF & SUBFIND	1000 1000 1000 1000

Why EAGLE? : PANPHASIA field decomposition!

Get in touch if you'd like to add yours!

[b]: run with baryonic physics

"Big data": Distribution of proto-halo shapes

0.30

0.25

0.20

 $M \in (3,6) \times 10^{10} h^{-1} M_{\odot}$

 $M \in (1,2) \times 10^{11} h^{-1} M_{\odot}$

 $M \in (1,2) \times 10^{12} h^{-1} M_{\odot}$

 $M \in (1,2) \times 10^{13} h^{-1} M_{\odot}$

slide courtesy M. Buehlmann



 $\lambda_1 \ge \lambda_2 \ge \lambda_3 > 0$ semi-axes of proto-halo

split by mass: more massive halos are more spherical

split by environment: at the same mass, more isolated halos are more spherical



 $M \in (1,2) \times 10^{14} h^{-1} M_{\odot}$ 0.15prolateness p0.10 0.05prolate 0.00 oblate -0.05-0.100.00 0.050.10 0.150.20 0.250.30 0.35ellipticity e0.30 $M \in (1,2) \times 10^{11} h^{-1} M_{\odot}$ $M \in (1,2) \times 10^{13} h^{-1} M_{\odot}$ 0.25 $M(10r_{\rm vir}) / M(r_{\rm vir})$ low $M(10r_{\rm vir}) / M(r_{\rm vir})$ low $M(10r_{\rm vir}) / M(r_{\rm vir})$ high $M(10r_{\rm vir}) / M(r_{\rm vir})$ high 0.20 0.15prolateness p0.10 0.05prolate 0.00oblate -0.05-0.100.000.050.100.150.200.250.300.35ellipticity econtours contain 10%, 50% and 90% of data cf. BBKS 1986

MUSIC 2 — towards a whole ecosystem for ICs

The roadmap...

Do get in touch if you want to be early adopter!

MUSIC2 monofonIC beta release: early 2020

single resolution (=only full cosmological volume) version

- direct integration of CLASS
- up to 3LPT
- PLT corrections
- new propagator approach for Eulerian baryons
- still modular architecture: multi code, easily extensible
- MPI+threads (no more limits)
- call directly from within your sim code (in prep.)

MUSIC2 cosmICweb beta release: early 2020

- cosmological ICs in the cloud
- reproducibility of zooms
- towards "one" numerical universe
- integrates with MUSIC1 update

MUSIC2 polyfonIC late 2020-early 2021 multi resolution (=zoom) version

- will replace MUSIC1
- MPI+threads



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