Relativistic Simulations for Cosmology

Julian Adamek (University of Zurich)

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Lecture I — The spacetime of N-body simulations

Newtonian description of an N-body system

Newton's second law:

$$\mathbf{F} \equiv \mathbf{p}' = m\mathbf{a} \tag{1}$$

In "Newtonian" cosmology, $\mathbf{p}$ is the *comoving* momentum, $'$ denotes the derivative w.r.t. *conformal* time (denoted as τ in this lecture), and the acceleration vector is given by the gradient of the *peculiar* gravitational potential ϕ as

$$\mathbf{a} = -a\nabla\phi\,, \tag{2}$$

where a is the *scale factor* and ∇ is the gradient operator in *comoving* coordinates.

NB: In many treatments the *peculiar velocity* $\mathbf{v}$ is used as the phase-space coordinate, assuming the classical relation

$$\mathbf{v} = \frac{\mathbf{p}}{ma}\,, \tag{3}$$

leading to the acceleration equation

$$\mathbf{v}' + \mathcal{H}\mathbf{v} = -\nabla\phi\,, \tag{4}$$

where $\mathcal{H} \equiv (\ln a)'$ is the conformal Hubble rate. In a relativistic context, the momentum will often turn out to be the more useful quantity.

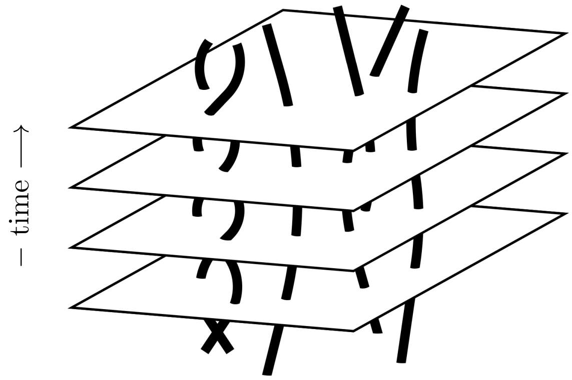
The Newtonian gravitational potential solves the Poisson equation

$$\Delta\phi = 4\pi G a^2 \delta\rho\,. \tag{5}$$

There are different approaches to solve the N-body dynamics numerically.

- Using the Green's function method to write a formal solution for eq. (5) one can avoid to solve for the potential ϕ explicitly and instead obtains a sum over two-body forces for eq. (1).
- One can discretise (sample) the potential field ϕ and the density field ρ and approximate eq. (5) by a finite-difference equation; here ρ is obtained through some *particle-to-mesh projection*. The finite-difference equation is then inverted numerically and the gradient is evaluated at the particle positions by *force interpolation*.

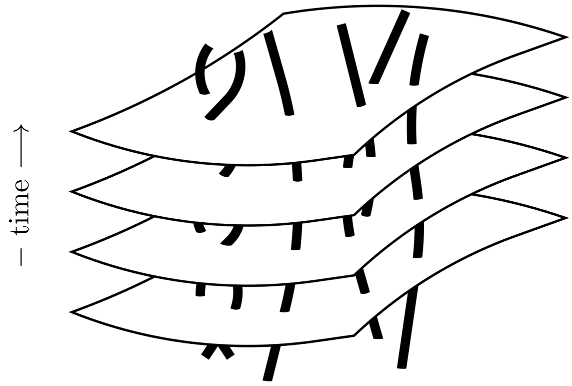
A simulation integrates the equations forward in time from some initial Cauchy data. Each integration "step" represents the solution at a fixed point in time.



Example: Kick-drift-kick scheme Given the particle positions, compute the forces (e.g. via the potential); update the peculiar velocities ("kick"). Move the particles according to their new velocities ("drift"). Repeat.

3+1 formulation of general relativity

The general relativistic view follows naturally: Each integration "step" represents the solution on a three-dimensional equal-time hypersurface of the four-dimensional spacetime.



Questions:

- What is a "good" foliation?
- Under which conditions is the Newtonian treatment a good approximation?
- How should one go about interpreting the solution, e.g. with regards to observations?

The ADM metric:

$$g_{\mu\nu} dx^\mu dx^\nu = -\alpha^2 d\tau^2 + \gamma_{ij} \left(dx^i + \beta^i d\tau\right) \left(dx^j + \beta^j d\tau\right) \tag{6}$$

The ADM (Arnowitt, Deser & Misner) metric provides a generic 3+1 decomposition of the metric, where α is called the *lapse function*, β^i is called the *shift vector*, and γ_{ij} is the induced (spatial) metric on the equal-time hypersurfaces.

The lapse α, the shift β^i and the spatial metric γ_{ij} are new fields that exist on the equal-time hypersurfaces. They play a similar role to the gravitational potential in Newton's second law, which is replaced by the *geodesic equation*:

$$\mathbf{p}' = -\sqrt{m^2 + \gamma^{ij} p_i p_j} \nabla \alpha + p_i \nabla \beta^i - \frac{\alpha p_i p_j \nabla \gamma^{ij}}{2\sqrt{m^2 + \gamma^{kl} p_k p_l}} \tag{7}$$

Here, ∇ is the spatial gradient that uses partial derivatives (not covariant ones).

Note that in eq. (7) we have already dropped the assumption that $p^2 \ll m^2$. In the Newtonian limit where the latter is true we might instead write

$$\mathbf{p}' \simeq -m\nabla\alpha\,. \tag{8}$$

In full generality the relation between comoving momentum and peculiar velocity becomes

$$v^i = \frac{\alpha\gamma^{ij}p_j}{\sqrt{m^2 + \gamma^{kl}p_k p_l}} - \beta^i\,. \tag{9}$$

Example: Kick-drift-kick scheme Given a solution for α, β^i, γ_{ij} (we will discuss those at length later) the "kick" step would use eq. (7) and the "drift" step would use eq. (9) for the position update.

The solution for the metric has to obey the *Hamiltonian constraint* (the time-time component of Einstein's equation) on the hypersurface,

$${}^3\mathcal{R} - K_{ij}K^{ij} + K^2 = 16\pi G\rho\,, \tag{10}$$

where the *extrinsic curvature tensor* K_{ij} is given by

$$K_{ij} = \frac{1}{2\alpha}\left(D_i\beta_j + D_j\beta_i - \gamma'_{ij}\right)\,, \tag{11}$$

(D_i is the covariant derivative on the hypersurface).

NB: In eq. (10) the energy density ρ is given by the projection of the stress-energy onto the unit normal vector of the hypersurface, $\rho \equiv n_\mu n_\nu T^{\mu\nu}$. This is in general *not* the same as the density in the fluid rest frame (if such a concept even exists).

We are still free to choose the *foliation* (i.e. the time coordinate) as well as the coordinate functions on the equal-time hypersurfaces. In particular, eq. (10) is true for any foliation!

Case $\alpha = a(\tau)$, $\beta^i = 0$ (comoving synchronous gauge): here $\mathbf{p} \equiv 0$ is a trivial solution to eq. (7) but the complicated particle dynamics are incorporated into the coordinate chart. Hence γ_{ij} becomes non-perturbative as soon as the particle configuration does, and becomes ill-defined when particle orbits cross! The relation of the solution to observations is obscured by the complex structure of γ_{ij}; for instance, the path of photons is often *very far* from a straight line under this chart.

Empirically it is evident that charts should exist where photons *do* travel almost along straight lines (this is how we interpret almost all our observations). Such a chart should have α, β^i, γ_{ij} such that the gradients in eq. (7) are small (take the limit $m \to 0$ to find the geodesic equation for photons). This situation is called *weak-field* gravity.

Linearised weak-field gravity

The linear regime of weak-field gravity has been studied extensively. We may write

$$\begin{aligned}
\alpha &= a\left(1 + A\right)\,, &(12)\\
\gamma_{ij}\beta^j &= -a^2\left(\nabla_i B + B_i\right)\,, &(13)\\
\gamma_{ij} &= a^2\left[\delta_{ij}\left(1 + 2H_L\right) - 2\left(\nabla_i\nabla_j - \frac{1}{3}\delta_{ij}\Delta\right)H_T + \nabla_i E_j + \nabla_j E_i + 2C_{ij}\right]\,, &(14)
\end{aligned}$$

with B_i and E_i transverse ($\delta^{ij}\nabla_i B_j = \delta^{ij}\nabla_i E_j = 0$) and C_{ij} transverse and traceless.

NB: Due to our freedom to choose the time coordinate (one "scalar") and the coordinate functions on the hypersurface (one three-vector which can be decomposed into its longitudinal and transverse parts) we are free to set two of the scalars A, B, H_L, H_T and one of the transverse vectors B_i, E_i to arbitrary functions.

Question: Neglecting vector and tensor perturbations (which are absent in Newtonian gravity) how do we recover the Newtonian limit?

The Hamiltonian constraint, linearised in the metric variables, reads

$$-\Delta H_L + 3\mathcal{H}H_L' - 3\mathcal{H}^2 A + \mathcal{H}\Delta B - \frac{1}{3}\Delta^2 H_T = 4\pi G a^2 \delta\rho\,. \tag{15}$$

Here we define $\delta\rho = \rho - \bar{\rho}$, where $\bar{\rho}$ is the function that enters the Friedmann equation to which a is the solution. For an N-body ensemble the computation of ρ requires knowledge about the metric, since for a classical point-particle we have

$$\rho_{\text{particle}}(\mathbf{x}) = \delta^{(3)}(\mathbf{x} - \mathbf{x}_{\text{particle}})\frac{\sqrt{m^2 + \gamma^{ij}p_i p_j}}{\sqrt{\gamma}}\,. \tag{16}$$

In the limit where $p^2 \ll m^2$ the physical density from the N-body ensemble therefore is

$$\rho = \bar{\rho}\frac{n}{\bar{n}}\left(1 - 3H_L\right)\,, \tag{17}$$

where n is the "bare" number density in coordinate space.

Let us now examine the geodesic equation in the limit $p^2 \ll m^2$,

$$\mathbf{v}' + \mathcal{H}\mathbf{v} = -\nabla\left(A - \mathcal{H}B - B'\right)\,, \tag{18}$$

which requires that the gravitational potential in a simulation should satisfy

$$\phi_{\text{sim}} \simeq A - \mathcal{H}B - B' \tag{19}$$

to a good approximation.

If anisotropic stress can be neglected, the trace-free part of the space-space component of Einstein's equations also imply that

$$H_L + A + \frac{1}{3}\Delta H_T + 2\mathcal{H}\left(H_T' - B\right) + \left(H_T' - B\right)' = 0\,, \tag{20}$$

which can be rearranged to

$$A - \mathcal{H}B - B' + 2\mathcal{H}H_T' + H_T'' = -H_L - \frac{1}{3}\Delta H_T + \mathcal{H}B\,. \tag{21}$$

Inserting into the Hamiltonian constraint we get

$$\Delta\left(A - \mathcal{H}B - B'\right) + \Delta\left(2\mathcal{H}H_T' + H_T''\right) + 3\mathcal{H}H_L' - 3\mathcal{H}^2 A = 4\pi G a^2\bar{\rho}\left[\frac{n}{\bar{n}}\left(1 - 3H_L\right) - 1\right]\,. \tag{22}$$

A Newtonian code solves

$$\Delta\phi_{\text{sim}} = 4\pi G a^2\bar{\rho}\left[\frac{n}{\bar{n}} - 1\right]\,. \tag{23}$$

Case $B = 0$, $H_T = 0$ (Newtonian gauge): we have $A = -H_L = \phi_{\text{sim}}$ from eqs. (19) and (20), but eq. (23) is only a good approximation to eq. (22) if "$\Delta\phi_{\text{sim}} \gg 3\mathcal{H}\phi'_{\text{sim}} + 3\mathcal{H}^2\phi_{\text{sim}}$" and "$(n/\bar{n}) - 1 \gg 3(n/\bar{n})\phi_{\text{sim}}$". Both conditions are generally met on scales much smaller than the homogeneity scale but fail to be met at ultra-large scales.

Case $H_L = 0$, $3\mathcal{H}^2 A = \Delta\left(2\mathcal{H}H'_T + H''_T\right)$ (N-body gauge[1]): works well on large scales but gauge condition is unusual. It turns out that after the radiation-matter transition $A \to 0$ and $H_T \to$ constant $\neq 0$. On small scales B becomes relatively large and therefore the weak-field assumption is not satisfied well.

Generally speaking there exists a whole family of gauges (so-called *Newtonian motion gauges*) that engenders Newtonian equations of motion at large scales. They typically have $H_T \neq 0$. Some of them fulfill the weak-field condition at all (cosmological) scales.

The cosmologist's choice: Poisson gauge

The ADM variables in Poisson gauge are written as

$$\begin{aligned} \alpha &= a e^{\psi} \,, & (24) \\ \gamma_{ij}\beta^j &= -a^2 B_i \,, & (25) \\ \gamma_{ij} &= a^2 e^{-2\phi}\left(\delta_{ij} + h_{ij}\right) \,, & (26) \end{aligned}$$

where B_i (the gravitomagnetic potential responsible for "frame dragging") is transverse and h_{ij} (the tensor perturbation, e.g. from gravitational waves) is transverse and traceless. Since those two are always very small I will linearise in them (i.e. I only keep them if they are multiplied with a background term), but shall keep ϕ and ψ nonperturbatively. It follows that

$$\gamma = a^6 e^{-6\phi} \,, \tag{27}$$

and the Hamiltonian constraint reads

$$e^{2\phi}\Delta\phi - \frac{1}{2}e^{2\phi}\left(\nabla\phi\right)^2 + \frac{3}{2}\left(\mathcal{H} - \phi'\right)^2 e^{-2\psi} = 4\pi G a^2 \rho \,, \tag{28}$$

and for an N-body ensemble the density is computed relativistically as

$$\rho = \bar{\rho}_{\text{rest}} \frac{n}{\bar{n}} \left\langle \frac{\sqrt{m^2 a^2 + p^2 e^{2\phi}}}{ma} \right\rangle e^{3\phi} \,, \tag{29}$$

where $\bar{\rho}_{\text{rest}}$ is the rest-mass density in the background model.

Let us say we want to truncate eq. (28) at order ϕ (typically we have $\phi \sim 10^{-5}$). If nonrelativistic matter is the dominant source of the gravitational fields we can estimate $\Delta\phi/\mathcal{H}^2 \sim \delta\rho/\bar{\rho} \sim O(1)$, $\phi' \sim \mathcal{H}\phi$, $v^2 \sim \phi$ (e.g. virial limit) and $\nabla\phi/\mathcal{H} \sim \mathbf{v}$. Truncating consistently we find

$$\left(1 + 2\phi\right)\Delta\phi - \frac{1}{2}\left(\nabla\phi\right)^2 - 2\mathcal{H}\phi' - 3\mathcal{H}^2\psi = 4\pi G a^2 \left[\bar{\rho}_{\text{rest}}\frac{n}{\bar{n}}\left(1 + \frac{1}{2}\left\langle v^2\right\rangle + 3\phi\right) - \bar{\rho}\right] . \tag{30}$$

If only sourced by nonrelativistic matter, the difference between ϕ and ψ is very small as it is sourced by the anisotropic stress roughly as $\Delta(\phi - \psi)/\mathcal{H}^2 \sim v^2$. It is therefore fair to treat it on the same

[1] I deviate slightly from the original definition introduced in Fidler et al., JCAP 09 (2016) 031. For further reading, see also Fidler et al., JCAP 12 (2017) 022, Adamek, Phys. Rev. D 97 (2018) and Adamek & Fidler, JCAP 09 (2019) 026.

footing as B_i or h_{ij}, i.e. only keep $(\phi - \psi)$-terms that are multiplied by background terms. From the space-space component of Einstein's equation one then finds

$$\Delta^2 (\phi - \psi) = \left(3\nabla^i\nabla^j - \delta^{ij}\Delta\right) (\nabla_i\phi\nabla_j\phi + 4\pi G T_{ij}) \,. \tag{31}$$

For an N-body ensemble the relativistic shear stress is computed as

$$T_{ij} = \bar{\rho}_{\text{rest}} \frac{n}{\bar{n}} \left\langle \frac{p_i p_j}{m\sqrt{m^2 + a^{-2}e^{2\phi}p^2}} \right\rangle e^{3\phi} \,. \tag{32}$$

In the nonrelativistic limit this is well approximated by $T_{ij} = a^2 \rho \langle v_i v_j \rangle$.

The gravitomagnetic potential can be computed from the momentum constraint as

$$\Delta^2 B_i = 16\pi G a^2 \left(\nabla_i \nabla^j - \delta_i^j \Delta\right) T_j^0 \,, \tag{33}$$

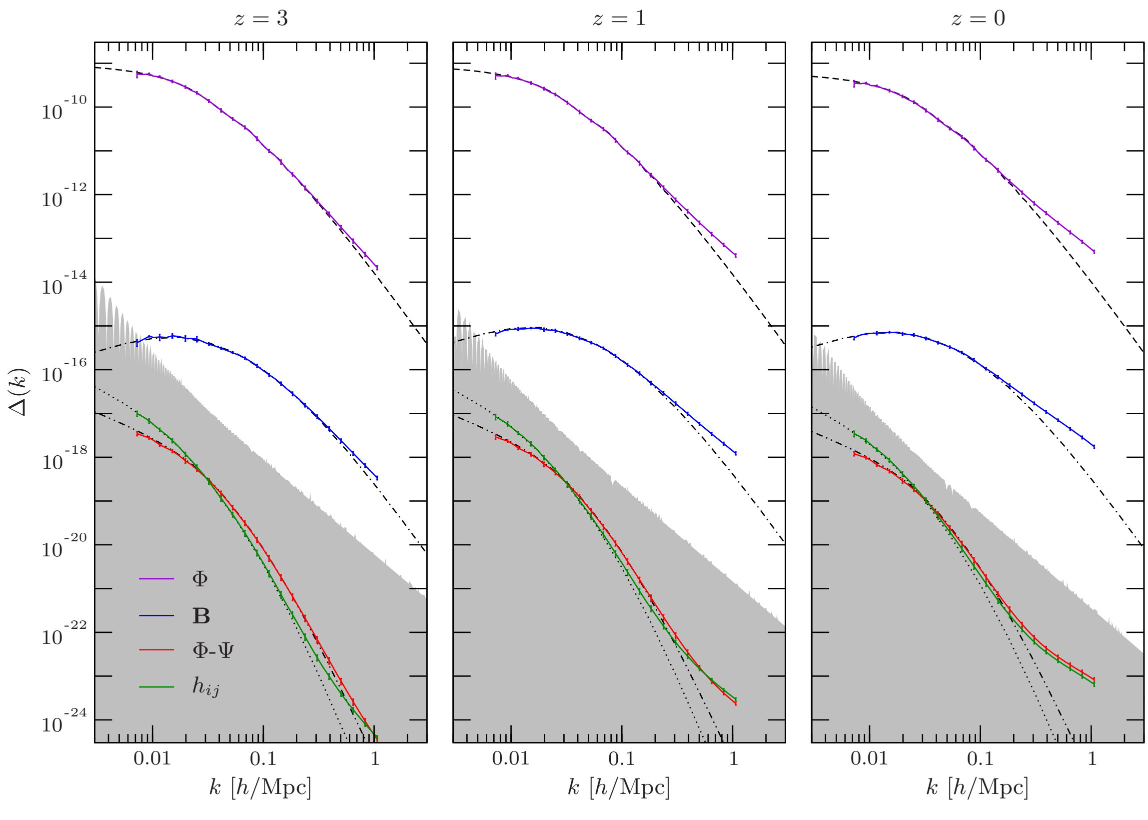
where the N-body ensemble produces a relativistic momentum density

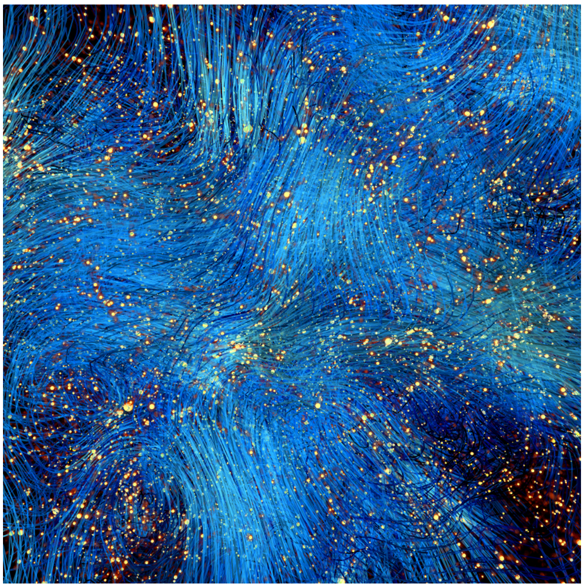
$$T_i^0 = \bar{\rho}_{\text{rest}} \frac{n}{\bar{n}} \left\langle \frac{p_i}{ma} \right\rangle e^{3\phi - \psi} \,. \tag{34}$$

Finally, the tensor perturbation is sourced as

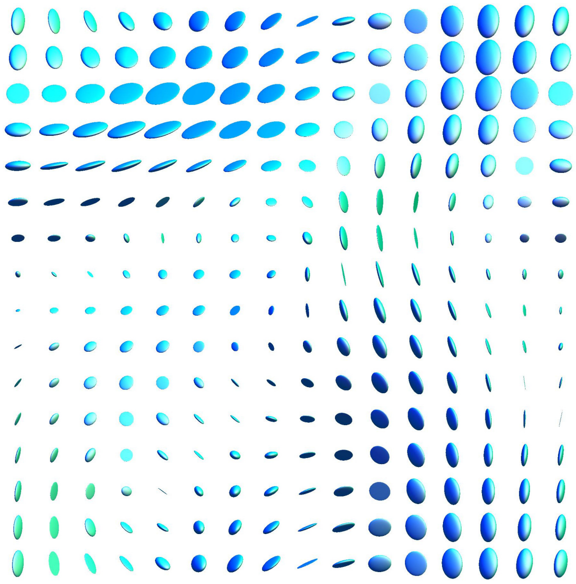
$$\Delta^2 \left(h''_{ij} + 2\mathcal{H} h'_{ij} - \Delta h_{ij}\right) = \\ \left[4\left(\nabla_i\nabla^k - \delta_i^k\Delta\right)\left(\nabla_j\nabla^l - \delta_j^l\Delta\right) - 2\left(\nabla_i\nabla_j - \delta_{ij}\Delta\right)\left(\nabla^k\nabla^l - \delta^{kl}\Delta\right)\right] (\nabla_k\phi\nabla_l\phi + 4\pi G T_{kl}) \,. \tag{35}$$

NB: The tensor perturbation contains the propagating degrees of freedom of GR. The fact that the scalar-vector-tensor decomposition of the metric in Poisson gauge allows us to isolate this contribution makes large GR cosmological simulations tractable.





Left: Visualisation of the gravitomagnetic potential in an N-body simulation [Adamek et al., Nature Phys. 12 (2016) 346-349].



Right: Visualisation of the tensor perturbation in an N-body simulation [Adamek et al., Class. Quant. Grav. 31 (2014) 23, 234006].

Summary (Lecture I):

- N-body dynamics in Poisson gauge differ from Newtonian dynamics at large scales (even in ΛCDM cosmology). However,
- Poisson gauge ensures weak-field conditions for the metric, making interpretation easier (though subtleties still need to be addressed — see Lecture II),
- additional (relativistic) sources for the gravitational fields can be added easily and consistently,
- hyperbolic nature of GR does not immediately jeopardise numerical performance (tensor modes can be approximated or neglected altogether).
- Other useful gauges exist (e.g. Newtonian motion gauges) but in all cases there are subtleties in the interpretation of the solution found by the N-body simulation. This will be the topic of the next lecture.

Further reading

- For more details on the 3+1 formulation of general relativity, see Chapters 1 and 2 of Baumgarte & Shapiro, *NUMERICAL RELATIVITY – Solving Einstein's Equations on the Computer.*
- Some details on relativistic N-body dynamics formulated in Poisson gauge can be found in sections 2 and 3 of Adamek et al., JCAP 11 (2017) 004. A full code description can be found in Adamek et al., JCAP 07 (2016) 053 which is however slightly outdated compared to the most recent implementation (note in particular a change in convention for the scalar metric variables).
- The relativistic interpretation of Newtonian simulations has been discussed extensively in the literature, see e.g. Chisari & Zaldarriaga, Phys. Rev. D 83 (2011) 123505 for an example. The issue is essentially solved through the introduction of Newtonian motion gauges, see e.g. Fidler et al., JCAP 12 (2017) 022.