NUMERICAL SIMULATIONS OF GALAXY FORMATION AND THE INTERGALACTIC MEDIUM

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1. Cosmological simulation methods
2. Numerical studies of galaxy formation
3. QSO absorption lines and the IGM
4. Cosmology with the Lyα forest

LECTURE 1

COSMOLOGICAL SIMULATION METHODS

1. Motivation

2. N-body simulations
   General approach
   Initial conditions
   N-body methods
   Numerical considerations
   Testing
   Some results

3. Hydrodynamic simulations
   Why hydrodynamics?
   Methods: grids, SPH
   Numerical considerations
   Cooling, photoionization
   Star formation and feedback
   Testing

Cosmological Questions

- Is the gravitational instability hypothesis basically correct?
- If so, what were the properties of the primordial fluctuations, and what was their physical origin?
- What is the dark matter?
- What are the values of Ω and Λ?

- How did galaxies form?
- What processes determine galaxy morphology, luminosity, size, and color?
- What is the relation between the large scale distribution of mass and the distributions of observable objects: galaxies, QSO absorbers, X-ray clusters, etc.?

The Inflation + Cold Dark Matter Model

- Structure formed by gravitational instability.

- Primeval fluctuations were Gaussian and scale-invariant ($n = 1$).
  Non-scale-invariant spectrum from inflation.
  Non-Gaussian fluctuations from inflation.
  Non-scale-invariant or non-Gaussian fluctuations from something else (e.g., topological defects).

- Dark matter consists predominantly of "cold" collisionless particles.
  Some dark matter is hot.
  Baryons are a substantial component.
  There is no non-baryonic dark matter.

- $\Omega_0 = 1$ and $\Lambda_0 = 0$.
  $\Omega_0 < 1$ *and the universe is open.*
  $\Omega_0 < 1$ *and* $\Lambda_0/3H_0^2 = 1 - \Omega_0$.

Numerical Simulations

We turn to numerical computations when analytic techniques break down or become too inaccurate.

Numerical simulations are themselves approximate because of

- numerical errors
- activity below resolution scale
- simplifications of physics

Some sources of numerical errors:

    roundoff errors
    finite step errors
    discreteness effects
    bugs
    limited dynamic range

Numerical errors and physical simplifications can both have serious effects. But numerical techniques can be powerful if one understands their limitations.

Uses of Cosmological Simulations

Provide physical understanding.
Make observable predictions for testing models.
Aid interpretation of observations.

More specifically:

- Understand qualitative predictions of theoretical models.
  See how variations of input assumptions affect final results.
  Compare to analytic or semi-analytic models.
- Test validity of analytic approximations and techniques.
- Make detailed, quantitative predictions for confrontation with observations.
  Requires that computations accurately represent model predictions.
  Requires judging uncertainties in observations.
- Synthesize results of disparate observations.
  Simulation provides full information about geometry, history, physical conditions.
- Model observations in detail, to reveal possible selection effects and biases, estimate statistical uncertainties.
- Test sensitivity and power of analysis methods.

The N-body Method

In principle, an N-body simulation is an attempt to solve the collisionless Boltzmann equation,

$$\frac{df(\mathbf{x},\mathbf{v},t)}{dt} = \frac{\partial f}{\partial t} + \mathbf{v}\cdot\vec{\nabla}f - \vec{\nabla}\Phi\frac{\partial f}{\partial \mathbf{v}} = 0,$$

in concert with the Poisson equation

$$\nabla^2\Phi = 4\pi G\int d^3v\ m\ f(\mathbf{x},\mathbf{v},t).$$

Direct, 6-dimensional integration of f is usually impractical.

In the N-body approach, one follows the orbits of representative mass elements, a.k.a. particles.

Schematically:

- Start with initial positions and velocities.
- Compute gravitational potential from particle distribution.
- Compute accelerations from potential gradients.
- Update velocities and positions.
- Repeat.

Gravitational forces must be "softened" in order to suppress 2-body scattering.

Initial Conditions

To initialize a simulation with $N_p = N^3$ particles:

(1) Generate linear density field on an N^3 grid.
Starting in $\mathbf{k}$-space, draw real and imaginary parts of $\delta_\mathbf{k}$ from independent Gaussian distributions with variance $P(k)/2$. FFT to get $\delta(\mathbf{x})$.
Simulation can only represent initial $P(k)$ over range $k = 1$ to $k = k_{\rm Nyq} = N/2$.

(2) Create "uniform" particle distribution: Poisson, grid, or glass.

(3) Perturb particles and assign velocities using the Zel'dovich approximation (Lagrangian linear perturbation theory):

$$\Delta\mathbf{x}(\mathbf{q},t) \;\equiv\; \mathbf{x}(\mathbf{q},t) - \mathbf{q} \;=\; \mathbf{g}_0(\mathbf{q})\frac{D(t)}{D(t_0)}\left(\frac{3}{2}\Omega_0 H_0^2 a_0\right)^{-1}$$

$$\mathbf{v} \;=\; a(\dot{\Delta\mathbf{x}}) \;=\; \frac{\dot{D}}{D}(a\Delta\mathbf{x}) \;\approx\; \Omega^{0.6} H(a\Delta\mathbf{x})$$

$D(t) =$ growing mode growth rate of linear perturbations

$\mathbf{q} =$ comoving position in an unperturbed universe

$\mathbf{g}_0 =$ gravitational acceleration at $t = t_0$

Can instead use 2nd-order perturbation theory solution to suppress transients, start at later redshift (Scoccimarro, astro-ph/9711187).

Equations of Motion

Newtonian approximation to GR valid for $R \ll ct$ and $v \ll c$. Acceleration determined by peculiar gravitational potential.

In comoving coordinates and Newtonian approximation, equations of motion are:

$$\begin{aligned}
&\dot{\mathbf{x}} = \mathbf{u} \\
&\dot{\mathbf{u}} + 2\frac{\dot{a}}{a}\mathbf{u} = -\frac{\nabla\phi}{a} \\
&\nabla^2\phi = 4\pi G a^2 \overline{\rho}\delta(\mathbf{x}).
\end{aligned}$$

$a(t)$ is determined by integrating the Friedmann equation.

The Poisson equation can be expressed in terms of Fourier components:

$$\begin{aligned}
&\nabla^2 \int d^3k\; e^{2\pi i\mathbf{k}\cdot\mathbf{x}}\; \phi_{\mathbf{k}} = (4\pi G a^2 \overline{\rho}) \int d^3k\; e^{2\pi i\mathbf{k}\cdot\mathbf{x}}\; \delta_{\mathbf{k}} \\
\Longrightarrow\quad &-4\pi^2 k^2 \int d^3k\; e^{2\pi i\mathbf{k}\cdot\mathbf{x}}\; \phi_{\mathbf{k}} = (4\pi G a^2 \overline{\rho}) \int d^3k\; e^{2\pi i\mathbf{k}\cdot\mathbf{x}}\; \delta_{\mathbf{k}} \\
\Longrightarrow\quad &\phi_{\mathbf{k}} = -(4\pi G a^2 \overline{\rho})\frac{\delta_{\mathbf{k}}}{4\pi^2 k^2}.
\end{aligned}$$

N-body codes compute $\phi(\mathbf{x})$ by direct summation over particles or particle groups, by FFT using the result above, or by a combination.

Example: The Particle-Mesh (PM) Algorithm

At each step:

(1) Compute $\delta(\mathbf{x})$ from particle distribution by cloud-in-cell (CIC) or TSC interpolation onto a rectangular grid.

(2) Compute $\phi(\mathbf{x})$ on the grid by FFT:

$$\phi_{\mathbf{k}} = -(4\pi G a^2 \overline{\rho})\mathcal{G}(\mathbf{k})\frac{\delta_{\mathbf{k}}}{4\pi^2 k^2}.$$

Automatically imposes periodic boundary condition.

(3) Compute gravitational accelerations by finite-differencing potential. Forces automatically softened on grid scale.

(4) Update particle velocities and positions, using 2nd-order "leapfrog" integration scheme.

Leading alternatives

- $\mathrm{P}^3\mathrm{M}$: As above, but add small scale forces computed by direct summation, imposing softening.
- Tree: Compute accelerations by direct summation (with softening), grouping distant particles into nodes. Use Ewald summation to get fully periodic boundary condition.
- Relaxation: Solve for $\phi(\mathbf{x})$ by finite-differencing on grid, using relaxation scheme.

Numerical Desiderata

Based on "N-body Constitution" of Katz, Quinn, Stadel, & Lake.

- Gravitational softening large enough to suppress 2-body relaxation. Many particles per softening volume in objects of interest.
- Timesteps small enough to eliminate 2-body scattering due to integration errors.
  Roughly, $\Delta t < 0.1(G\rho)^{-1/2}$, $N_{\rm steps} = \frac{t_0}{\Delta t} \sim 4500(10 \text{ kpc}/\epsilon_{\rm grav})$
- Time integration scheme that is at least 2nd-order, and preferably time-reversible and/or symplectic. (See Quinn et al., astro-ph 9710043.)
- Simulation volume large enough that (a) no one object dominates evolution, (b) fundamental mode remains in linear regime.
- Starting redshift high enough to ensure accuracy of Zel'dovich approximation.

Resolution

An N-body simulation has several different resolution limits.

Force resolution: Set by gravitational softening. Determines smallest physical scale on which results are reliable.

Mass resolution: Set by particle mass. Determines
minimum scale that can be represented in initial conditions
accuracy of gravitational evolution
detail with which final conditions can be studied
minimum mass of object that can be reliably modeled

Time resolution: Set by timestep. *Should* always be matched to force resolution. High force resolution requires high time resolution, which can be aided by individual particle timesteps.

PM is fastest method for $\epsilon_{\rm grav} \sim L_{\rm box}/N_p^{1/3}$.
Other methods can achieve $\epsilon_{\rm grav} < L_{\rm box}/N_p^{1/3}$, hence higher force resolution for given N_p. The value of this is a subject of debate.

Tests of N-body Simulations

Tests against analytic solutions:
- linear theory
- higher-order perturbation theory
- collapse of 1-d plane wave
- spherical collapse
- spherical hole

Self-similar evolution from scale-free initial conditions.

Convergence tests with individual code, comparing runs with varying timesteps, force resolution, particle number, box size, etc.

Comparison between results of different codes.

Some Important Results

- Nonlinear evolution of Gaussian initial conditions produces walls, filaments, tunnels, voids.
  Like ZA prediction, even in hierarchical models.
- Dead models: HDM, $n = 0$ initial $P(k)$, CCDM.
- Distinguishing biased, $\Omega = 1$ model from unbiased, low-Ω model is hard.
- Strongly non-Gaussian models generally fare worse than Gaussian models.
- No one definitive clustering statistic, but combination of several is powerful.
- Matching power-law $\xi(r)$ requires well-placed features in initial $P(k)$ or scale-dependent bias on small scales.
- Press-Schechter formalism and its extensions work surprisingly well.
- Stable clustering *ansatz* not valid for $\xi(r) < 100$.
- Universal density profile from hierarchical clustering. (?)
- Collisionless collapse erases substructure. (?)
- Mergers probably play important role in evolution of galaxy population from $z = 3$ to $z = 0$.

Key shortcoming of N-body simulations: they show where the mass is, but not where the galaxies are.

Hydrodynamic Cosmological Simulations

Motivation:

- See whether models produce realistic galaxies and galaxy groups.
- Predict "bias" between galaxies and mass *a priori*.
- Predict X-ray and SZ properties of cluster IGM.
- Predict absorption properties of galaxies, diffuse IGM.
- Understand physics of galaxy formation, cluster formation, IGM evolution.

Essential differences between gas and collisionless matter:

- Gas doesn't interpenetrate. It shocks, converting kinetic energy to thermal energy.
- Gas equations of motion include pressure gradients.
- Gas can dissipate energy by cooling.
- Gas can be converted into (collisionless) stars.

Radiative transfer rarely included at present.

Gas Equations

$$\frac{\partial \rho}{\partial t} = -\vec{\nabla} \cdot (\rho \mathbf{v}) \quad \text{mass conservation}$$

$$\frac{\partial \mathbf{v}}{\partial t} = -\vec{\nabla}\Phi - \frac{\vec{\nabla} P}{\rho} + \mathbf{a}_{\mathrm{visc}} \quad \text{momentum conservation}$$

$$\frac{\partial \epsilon}{\partial t} = -\frac{P}{\rho}\vec{\nabla} \cdot \mathbf{v} + \frac{Q_{\mathrm{visc}}}{\rho} + \frac{Q - \Lambda(\rho, T)}{\rho} \quad \text{energy conservation}$$

$$P = (\gamma - 1)\rho\epsilon \quad \text{equation of state}$$

Computational Methods

- Eulerian grid:
  Solve gas equations by finite difference on fixed grid.
  Use artificial viscosity or shock-capturing scheme.
  Can include embedded high-resolution mesh or adaptive regridding.

- Lagrangian grid:
  Similar, but mesh distorts to put more cells in high density regions.

- Smoothed particle hydrodynamics (SPH):
  Represent fluid elements by particles, which move with flow, retain memory of thermal energy.
  Compute densities and pressure gradients by weighted (smoothed) sums over neighbors.
  Use artificial viscosity to prevent interpenetration, produce shocks.
  Smoothing length scales with density $\Longrightarrow$ high spatial resolution in high density regions.

$$\rho = \sum m_i W(r_i/h)$$
$$\vec{\nabla} P = \sum P_i \vec{\nabla} W(r_i/h).$$

Numerical Considerations

Timestep must satisfy Courant condition, $\Delta t_i \lesssim 0.3 h_i / c_i$, where h and c are smoothing length, sound speed.

If there is a minimum Δt, then h should be increased to satisfy Courant condition. Time resolution and spatial resolution explicitly linked.

Cooling times can be very short. Usually solve thermal energy equation implicitly or semi-implicitly.

Ionization and recombination times can be very short. May solve abundance equations by equilibrium.

Star Formation and Feedback

Representative algorithm:

- Density threshold criterion (perhaps supplemented).
- Eligible gas forms stars at rate

$$\frac{d\rho_\star}{dt} = -\frac{d\rho_g}{dt} = \rho_g \frac{c_\star}{t_g}$$

  where t_g is maximum of $(t_{\rm dyn}, t_{\rm cool})$ and $c_\star$ is dimensionless efficiency parameter.
- Gas converted to collisionless "star" particles.
- Feedback energy distributed to surrounding gas as thermal and/or kinetic energy.

Star formation rate is essentially governed by rate at which gas cools on galactic scale.

Alternatives: bursts, triggering events, slow extended star formation

True effect of feedback is a major uncertainty.

Tests of Hydrodynamic Simulations

Tests against analytic solutions:

shock tube
collapse of 1-d plane wave
spherical collapse
spherical hole

Self-similar evolution from scale-free initial conditions, with or without cooling.

Convergence tests with individual code, comparing runs with varying timesteps, force resolution, particle number, box size, etc.

Comparison between results of different codes.