CODES IC's Cosmological Nbody Simulations ISYA 2018, Colombia, Socorro Octavio Valenzuela

Reasons to use N-body Simulations

Exploring the role on non-linear dynamical evolution, hard to do in analytical way for more than 2 bodies Studying non-equillibrium, transient processes in a selfconsistent way.

The Galactic Bulge and Sagittarius (Dynamical Feedback in action)

- The Sagittarius
- satellite
- being disrupted by a
- with the
- Milky Way

Ibata 1994
 I Stripping and Stirring

Spiral Arms and disk rings secularly or tidally triggered? Purcell,



What about M31? Dynamical state of its satellites? MV

Biasing interpretation of observations? From disk? Migrations. Bulge. From satellites?



Halo Archeology







Galaxy - Galaxy interactions (HST)

High redshift Galaxies





Galaxy at z=1



Gonzalez-Samaniego, Valenzuela, Colir

width = 111 kpc

















Cosmic Large Scale Structure growth is a complex multi scale process Transient process are quite slow so they bias our interpretation

Avoid these reasons:

- Easier than analytic solution
- The only robust solution
- The most realistic approach

Nbody simulations are just another approach to dynamical problems

- Very useful, but you have to test, and test the robustness of results
- Compare if possible against analytic solutions
- Convergence studies of solutions is your guide most of the time, because frequently there is not an analytical solution

You have a powerful toy, be careful



Kinetic description in terms of Vlasov-Poisson





General Structure of N-body codes

- Density/Force Call conditions probler
- Time Integration



Initial Conditions: The Art



Galaxies, halos, etc



Poisson Self-gravity



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

Full self-consistency

Ideally we would like ... for Isolated dynamical systems

Method I: Phase Space • Fully Self-consistent

 But...PSF available only for idealized symmetric systems



Random sampling?

Quiet Start (Sellwood), cosmological neutrinos??

Inhibits scatter

Prendergast & Tomer (1970)

- This method works for axisymmetric (flattened) potentials and an adopted form for f(E,Lz)
- Iterate
 - 1. guess an initial $\rho(r,z)$
 - 2. solve for Φ (e.g. using Poisson solver)
 - 3. compute a new $\rho(r,z) = \int f d^3 v$
 - complete steps 2 & 3 until changes in ρ are small (8 – 10 iterations)

Because

Halo disk

interactio

Adaptable and yields a good equilibrium

But the final stage is not always what we wanted Sometimes not converging

Starts assuming a spherical disk from the point of view of the halo

Excelent for controlled experiments

Implementation Widrow Dubinsky for MW/M31



Cosmological.

GENERATING INITIAL CONDITIONS

SUPERIMPOSING DENSITY PERTURBATIONS



$$\delta(\vec{x}) = \sum \hat{\delta}(\vec{k}) e^{-i\vec{k}\cdot\vec{x}} \qquad P(k) = \left\langle \left| \hat{\delta}(\vec{k}) \right|^2 \right\rangle_{|\vec{k}|=k}$$

Inflation theory

$$P_i(k) = Ak^n$$
 with $n = 1$ (Harrision - Zeldovich spectrum)

1

• transferring P(k) across recombination

$$P(k) = T^2(k)P_i(k)$$



 $\delta(\vec{x}) = \sum \hat{\delta}(\vec{k}) e^{-i\vec{k}\cdot\vec{x}}$

 $P(k) = \left\langle \left| \hat{\delta}(\vec{k}) \right|^2 \right\rangle$



CDIM, WDIM,SIDIM, SIFDIM, massive Neutirinos $P(k) = T^2(k)P_i(k)$ Mod Gravity, contrasted with CIMB

FFT

SUPERIMPOSING DENSITY PERTURBATIONS

$$\delta(\vec{x}) = \sum \hat{\delta}(\vec{k}) e^{-i\vec{k}\cdot\vec{x}} \qquad P(k) = \left\langle \left| \hat{\delta}(\vec{k}) \right|^2 \right\rangle_{|\vec{k}|=k}$$

RMS deviation at scale 2Pi/k

 remember linear perturbation theory*: Is a continuous media, collisionless plasma, Boltzmann moments 		
density contrast:	$\frac{\partial \delta}{\partial t} + \frac{1}{a} \nabla \cdot \vec{u} = 0$	mass conservation
peculiar velocity field:	$\frac{\partial \vec{u}}{\partial t} + \frac{\dot{a}}{a}\vec{u} = -\frac{1}{a}\nabla\Phi$	momentum conservation
	$\Delta \Phi = 4\pi G a^2 \overline{\rho} \delta$	Poisson's equation

$$\delta(\vec{x}) = \sum \hat{\delta}(\vec{k}) e^{-i\vec{k}\cdot\vec{x}} \qquad P(k) = \left\langle \left| \hat{\delta}(\vec{k}) \right|^2 \right\rangle_{|\vec{k}|=k}$$

• remember linear perturbation theory*:

$$\frac{\partial^2 \delta}{\partial t^2} + 2 \frac{\dot{a}}{a} \frac{\partial \delta}{\partial t} - 4\pi G \overline{\rho} \delta = 0 \quad \text{evolution of matter density}$$

$$\delta(x,t) = D(t)\delta_0(x)$$

$$\boxed{P(k) = D^2(t)P_0(k)}$$

SUPERIMPOSING DENSITY PERTURBATIONS

Zel'dovich approximation:

$$\vec{x}(t) = \vec{q} + D(t)\vec{S}(\vec{q})$$

Ansatz based upon the idea to

displace particles from their initial positions on a regular mesh

Zel'dovich approximation:



general solution:

$$D(t) = \frac{5}{2}\Omega_0 \frac{\dot{a}}{a} \int_{t_0}^{t} \frac{1}{\dot{a}^2} dt'$$

SUPERIMPOSING DENSITY PERTURBATIONS

Zel'dovich approximation:

$$\vec{x}(t) = \vec{q} + D(t)\vec{S}(\vec{q})$$

• in practice...

$\vec{q} = \text{regular grid, i.e. } q_{klm}$

$$D = \frac{5}{2}\Omega_0 \frac{\dot{a}}{a} \int_{t_0}^t \frac{1}{\dot{a}^2} dt'$$

$$\vec{S}(\vec{q}) = -\nabla \Psi(\vec{q})$$

D(t): determines the initial redshift of the simulation

S(q): determines the direction of displacement

$$\Psi(\vec{q}) = FFT^{-1}(\hat{\Psi}(\vec{k}))$$
$$\hat{\Psi} = \hat{\delta}_0 (k) \frac{1}{k^2}$$
$$\hat{\delta}_0 (k) = \sqrt{P_0(k)}R_{\vec{k}} e^{i\varphi_{\vec{k}}}$$
$$R_{\vec{k}} e^{i\varphi_{\vec{k}}} = R_1 + iR_2$$
$$R_1, R_2 = \text{Gauss}(0, 1)$$

Zel'dovich approximation:

positions

$$\vec{x}(t) = \vec{q} + D(t)\vec{S}(\vec{q})$$

velocities

$$\dot{\vec{x}}(t) = \dot{D}(t)\vec{S}(\vec{q})$$

SUPERIMPOSING DENSITY PERTURBATIONS

2nd order Lagrangian perturbation theory

$$\vec{x}(t) = \vec{q} + D(a)S(\vec{q}) - D^{(2)}S^{(2)}(\vec{q})$$

Higher accuracy IC's, why??

CODES: Which one is the best code? • Adaptive: Tree codes,

Adaptive: Tree codes, Adaptive Mesh Refinement (AMR)

- Particle-Particle
- Fixed Shape, GRIDS, Orthogonal Base


- Los resultados de la simulación son confiables para ~2

 (Athanassoula et al. 2000).
- Las unidades usadas son tales que: $G = M_T = a_s = 1$

PP Codes

 \square

- Challenge: Time of calculation Scales as N^2 (harder go further than 1e6 particles)
- Can be used for collision less systems (galaxies, LSS) but they are not that efficient
- Very Useful for high density systems (clusters, galaxy nucleus, binaries decay)

Criteria

- Accuracy: Geometry, capture of relevant processes, good handling of numerical effects, quality of integration
- Efficiency: Speed, with the right accuracy

Grids



- By far the most efficient methods to solve for the gravitational field use grids
 - Cartesian, cylindrical polar, or spherical
 - polar grids have additional advantages

Shape may imply disadvantages when systems evolves quickly in shape

• Cylindrical, spherical CODES: Which Operiod Strike Spherical, something else? best?

- Caution, good geometric choice for the beginning
- What happens if it evolves?

Accuracy decreases

Fixed Shape, GRIDS, Orthogonal Base

Modern codes currently used many techniques

- PP-Regularization (analytical 2 body solution for close encounters: binary formation and destruction)
- PM (PM + Perturbative solution)
- Tree's
- Hybrid's
- AP3M(AMR-fixed + pp)
- Tree-GRAPE (Tree-pp)
- Tree-GPU ()
- AMR
- Hybrid´s

PM CODES

• numerically integrate Poisson's equation

$$\Delta \Phi(\vec{g}_{k,l,m}) = 4\pi G \rho(\vec{g}_{k,l,m})$$

$$\vec{F}(\vec{g}_{k,l,m}) = -m\nabla\Phi(\vec{g}_{k,l,m})$$



sounds like a waste of time and computer resources, but **exceptionally fast** in practice

COMPUTATIONAL COSMOLOGY

SomePM caveats

- FFT is very efficient
- Regular grid wastes computation time, if the dynamical range is large (from galaxies to the universe, from stars-to galaxies)
- Nested PM grids?
- Aliasing effects
- Careful that the Grid-Box-N of particles do not trigger artificial structure (your project)

Force + integrator accuracy



The Particle-Particle Particle-Mesh (P³M) Scheme:



 This extends the PM method with a direct summation of short-range forces on the scale of the mesh cells.

GOOD: Increases substantially the spatial dynamic range

 BAD: Highly-clustered states (when the short range force calculations dominate) are very costly to evolve

 Mesh-refinements may be placed on clustered regions (as in the AP³M and Hydra codes developed by Hugh Couchman et al) but this suffers from high complexity (which makes it very difficult to parallelize) and ambiguities on the optimal choice of refinement placement.

look Marios's and Peder's talks **Tree Algorithms**

Tree algorithms

Oct-tree in two dimensions







•The idea here is to use the fact that the contribution to the potential of far-away masses is given by the first few terms of a multipole expansion.

$$\Phi(\mathbf{r}) = -G\sum_{i}rac{m_{i}}{|\mathbf{r}-\mathbf{x}_{i}|}$$

We expand:

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

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



dipole contribution vanishes outside each node

•And get:

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

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GADGET - 2

A code for cosmological simulations of structure formation

General

- Description
- Features
- Authors and History
- Acknowledgments
- News

Software

- Download
- Requirements
- License
- Mailing List
- Change-Log
- Examples

Documentation

- Code Paper
- Users Guide
- Code Reference

Publications

Aplicaciones Lugares Escritorio

Scientific Papers

look Juan Carlos Classes and projects

Features

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- lightarrowners in the second s
- Optional TreePM method, where the tree is used for short-range gravitational forces only while long-range forces are computed with a FFT-based particle-mesh (PM) scheme. A second PM layer can be placed on a high-resolution region in 'zoom'-simulations.
- Periodic boundary conditions, either by means of the Ewald summation technique or based on the FFT algorithm used in the TreePM scheme. Simulations that only follow gas dynamics without self-gravity can be run in periodic boxes with arbitrary aspect ratios, and also in 2D, if desired.
- Smoothed particle hydrodynamics with fully adaptive smoothing lengths and a novel entropy conserving formulation of SPH.
 - Signal-velocity parameterisation of the artificial viscosity, as suggested by Monaghan.
- Individual timesteps for all particles. In the TreePM scheme, long-range and short-range forces are integrated with different timesteps.
 - Work-load balanced domain decomposition and dynamic tree updates.
- Efficient cell-opening criteria for the gravitational tree-walk.
- Support for parallel I/O and a number of different output formate, including the UDE5 format

GADGET is a versatile TreeSPH N-body code for cosmological applications PRINCIPLE CHARACTERISTICS OF GADGET

- Gravity solver based on a TREE or TreePM algorithm
- Hydrodynamics is followed by means of SPH
- Timesteps can be individual and adaptive
- Code is parallelized with MPI for distributed memory architectures
- Code is written in C and is highly portable
- A basic version of the code is publicly available

GADGET has evolved over the years and is in a process of continuous change

MAJOR EVENTS IN GADGET'S DEVELOPMENT







N-body Solver (KD-Tree Method, PKDGRAV) and Smoothed Particle Hydrodynamics
Physics: Gravity, Hydrodynamics, Atomic Chemistry (Radiative Heating, Cooling)
Subgrid Physics: Star Formation, Supernova Feedback, Planetesimal Collisions

> Wadsley, Stadel & Quinn 2003, Stadel Pr Governato et al 2005, Nature

Likely the future in paralelization efficiency. CHARM++, P-Cello code

5. ChANga (Charm N-body GrAvity solver)

http://librarian.phys.washington.edu/astro/index.php/Research:ChaNGa http://www-hpcc.astro.washington.edu/tools/changa.html

 Barnes-Hut tree code (where leaves can be > 1 particle and there is multipole expansion for far away particles)

- Softening not as Plummer but cubic spline
- In gravity only mode seems to work well for > 128k cores

 Multi-stepping for timesteps allowed (which does not mean it is smart to use it)

 Excellent work-load balance (= integrations and particles are well distributed between the used CPUs) thanks to CHARM++ runtime system http://charm.cs.uiuc.edu/software

The quest for higher resolution...

as perturbations collapse, their size shrinks by orders of magnitude as matter collapses to overdensities in excess of 1e6...

an additional shrinking can be due to expansion if integrating on a grid fixed in comoving coordinates

fixed uniform grid methods are therefore not suitable to study halo structure in the highly nonlinear regime or galaxy formation

The AMR Approach

 Efficient, reliable finite element methods for uniform grids have been developed for solving the Poisson and gasdynamics equations.

 The <u>Adaptive Mesh Refinement</u> (AMR) methods increase the dynamic range of grid-based numerical algorithms beyond the limits imposed by existing hardware.

- The methods have numerous applications in different fields of physics, engineering, etc.
- Now gaining popularity in astrophysics and cosmology



Structured vs unstructured AMR



Structured: hierarchy of rectangular grids or irregularly shaped meshes of cubic cells

ectangular Unstructured: highly flexible eshes of refinement meshes, efficient for cases of complicated region geometry and Arepo uses son beyindgries; more sophisticated data Like this one structures and algorithms

Refining cell by cell



Taken to its limit, one can think of tree of individual cells or small groups of cells (quads – 4 cells in 2D, octs – 8 cells in 3D)

In this case, the refinement can be controlled on the level of individual cells, which allows meshes with complicated geometries to match complicated features in the systems (shocks, filaments etc.)

This approach is used in ART, FLASH, AMIGA, RAMSES

Cosmological and Galatic AMR codes

□ AP³M (N-body)

H. Couchman 1991 publicly available: http://coho.mcmaster.ca/hydra/ap3m/ap3m.html

ENZO (N-body + gasdynamics) G. Bryan & M. Norman 1996 publicly available: cosmos.ucsd.edu/enzo/

Adaptive <u>Refinement Tree</u> (N-body + gasdynamics) Kravtsov, Klypin & Khokhlov 1997; Kravtsov 1999; Kravtsov, Klypin & Hoffman 2002

Cosmological an AMR codes

Includes SN,AGN, MHD, MG MPI paralellization

RAMSES (N-body + gas dynamics) R. Tesyer (<u>http://irfu.cea.fr/Projets/Site_ramses/</u> <u>RAMSES.html</u>)

This morning simulation...



http://popia.ft.uam.es/AMIGA/

MLAPM/AMIGA



A publicly available AMR N-body code that uses PM and multigrid approaches to solve the Poisson equation and integrate particle trajectories

Detailed description of the publicly available
In Alexander Knebe website

this morning alter the break

AP3M: HYDRA

Particle-Particle PM schemes (P³M)

Idea: Supplement the PM force with a direct summation short-range force at the scale of the mesh cells. The particles in cells are linked together by a chaining list.

Offers much higher dynamic range, but becomes slow when clustering sets in.

In AP³M, mesh-refinements are placed on clustered regions



Can avoid clustering slow-down, but has higher complexity and ambiguities in mesh placement

Codes that use AP³M: HYDRA

DRA (C

(Couchman)

AP³M code (Adaptive P³M)



y give ew chance to this d of code *subgrids introduced adaptively in an AP³M simulation around collapsing halos* P³M algorithm achieves higher resolution by complementing low-res PM force, with higher resolution small-separation force calculated via direct PP Calculation (hence the name: PPPM or P³M)

as matter collapses into halos
 PP part of the calculation carries
 larger and larger burden.
 Simulation slows down or stalls.

Idea behind AP³M: reduce PP load by using PM force calculation on subgrids introduced in high particle density regions

Critical for any adaptive Nbody method: avoid jumps from one accuracy level to another

.UqA1911.



Gravity force in the AP³M code is stitched together from different grids and PP calculation at the smallest separations

The same gravity solver (albeit w/o PP part) is used in another AMR code – Enzo

refinement criteria AMR

opening angle for Tree

FIG. 1.—The pairwise force as a function of radius calculated on a 32^3 periodic mesh with two levels of refinement. The heavy continuous line is the calculated force, and the dots indicate the modulus of the error in the force. The curves at the top of the plot indicate the components of the force (×100) calculated from the base mesh (level 0), the refinements, and the corresponding direct sums.

Couchman 1991

Precursor: Zeus Descendent: P-Cello (ask me)

Enzo



The first AMR N-body + Eulerian gasdynamics code in cosmology

Initially developed by Greg Bryan & Michael Norman in 1996-1998 at UIUC and NCSA. Currently is developed and maintained by M. Norman's group at UC San Diego.

publicly available (code and documentation: cosmos.ucsd.edu/enzo



Figure 1. A 2D adaptive mesh refinement example showing a three-level, four-grid hierarchy.



Adaptive Refinement Tree (ART) code



 The ART code refines (and derefines) mesh cells individually.

 We use a fully-threaded oct tree data structure (hence, the ART name) to support the refinement mesh hierarchy. The cost is only 2.5 storage words per cell. [Khokhlov 1998]

 This allows for flexible adaptive refinement structure that can be easily modified. The meshes can effectively match the complex geometry of filaments, sheets, and clumps in a cosmological simulation.





Frames 49

HD_00002_x,0 HD

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E pur si muove: Galiliean-invariant cosmological hydrodynamical simulations on a moving mesh

AREPO

Authors: Volker Springel (MPA)

Comments: accepted in MNRAS, 67 pages, 50 figures.

Hydrodynamic cosmological simulations at present usually employ either the Lagrangian smoothed particle hydrodynamics (SPH) technique, or Eulerian hydrodynamics on a Cartesian mesh with (optional) adaptive mesh refinement (AMR). Both of these methods have disadvantages that negatively impact their accuracy in certain situations, for example the suppression of fluid instabilities in the case of SPH, and the lack of Galilean-invariance and the presence or overmixing in the case of AMR. We here propose a novel acheme which largely eliminates these weaknesses. It is based on a moving unstructured mesh defined by the Voronoi tessellation of a set of discrete points. The mesh is use solve the hyperbolic conservation laws of ideal hydrodynamics with a finite volume appreach, based on a second-order unsplit Goduno vscheme with the velocity of the local flow, one obtains a Lagrangian formulation of contin hydrodynamics that does not suffer from the mesh distortion limitations inherent in other mesh-based Lagrangian schemes. In this mode, our new method is fully Galilean-invariant, unlike ordinary Eulerian methods in the reatment of shocks is also retained, will be spatial resolution automatically and continuously, and hence inherits the principal advant of SPH for simulations of cosmological simulations where highly supersonic bulk flows are common. In addition, the new scheme can adjust its spatial resolution automatically and continuously, and hence inherits the principal advant of SPH for simulations of cosmological simulations where highly accuracy of Eulerian methods in the teatment of shocks is also retained, while the treatment of contac discontinuities improves. We liscus how this approach is partically for the gas that allows the new method to be seamlessly combined with a high-resolution dust time-step approach for finit here at the principal edvant of shocks is also retained, while the treatment of contact discontinuously, and hence inherits the principal advant of SPH for simulations of cosmological simulati







Solvers

Gravity solver:

FFT solver on the uniform (I=0) grid covering the entire volume relaxation solver for I>0 [Gauss-Seidel + SOR + Chebyshev accel] potential on child refinement cells is inherited from the parent cells potential from the previous step is used as initial guess for the next step

Eulerian gasdynamics solver:

2nd order Godunov solver with piecewise linear reconstruction [van Leer 1979; Collela & Glaz 1985; Khokhlov 1998]

Particles: are treated using standard particle -mesh methods cloud in cell density assignment and force interpolation 2nd order leapfrog time integration, interpolation and loss of 2nd order accuracy at the refinement mesh interfaces...

□ Time integration on each refinement level *l* is done with time step $dt_l = dt_0/2^l$, where dt_0 is the global time step on l=0, set so that the *CFL condition* is satisfied for cells on all levels

Relaxation ART gravity solver Relaxation

when you have a nonlinear equation poisson or can not use spectral method

$$\nabla^2 \phi = \rho \quad \longrightarrow \quad \frac{\partial \phi}{\partial \tau} = \nabla^2 \phi - \rho.$$

relaxation equation

relaxation iteration:

$$\phi_i^{n+1} = \phi_i^n + \frac{\Delta\tau}{\Delta^2} \left(\sum_{j=1}^6 \phi_{Nb(j)}^n - 6\phi_i^n \right) - \rho_i \Delta\tau$$

although in general relaxation is not a fast method, we have no choice with irregular meshes of ART...

However, convergence of relaxation iteration is much much faster if we use potential solution from the previous step as initial guess to initialize the relaxation

red-black Gauss-Seidel relaxation scheme with successive overrelaxation (SOR) further speeds up the convergence (Hockney & Eastwood 1988; also, Numerical Recipes)

$$\phi_*^{n+1} = \omega \phi^{n+1} + (1-\omega)\phi^n,$$

Problema de optimización: Técnica de relajación.



HACC in a Nutshell

Long-range/short range force splitting:

S. Habib et al. 2016, New Astronomy

- Long-range: Particle-Mesh solver, C/C++/MPI, unchanged for different architectures, FFT performance dictates scaling (custom pencil decomposed FFT)
- Short-range: Depending on node architecture switch between tree and particle-particle algorithm; tree needs "thinking" (building, walking) but computationally less demanding (BG/Q, X86, KNL), PP easier but computationally more expensive (GPU)
- Overload concept to allow for easy swap of short-range solver and minimization of communication (reassignment of passive/active in regular intervals)
- Adaptive time stepping, analysis on the fly, mixed precision, custom I/O, ...


Aurrent State-of-the-Art Gravity-Only Simulations



Nonlinear Structure Formation Simulations with HACC

HACC: Extreme-scale, particle-based framework for computational cosmology

- Very high levels of performance across multiple architectures (BG/Q, GPU, KNL,...)
- Focus on absolute, not relative, performance; first production science code to break 10 PFlops sustained

Portability

- Uses multiple algorithms and implementations across architectures, yet 95% of code base remains unchanged
 - Programming model: C++/MP| + X (X=OpenMP/CUDA/OpenCL/assembly)

Science Targets

- Large-scale structure probes of cosmology
- Exploration of effects of massive neutrinos, dynamical dark energy equation of state, ...
- Focus on large surveys



Weak Scaling up to 96 Racks; Strong Scaling, 1024³ Particles



3

Simulation Challenges Now and in the Future

- Computational Challenges: Next-generation computing opportunities and difficulties
 Exascale hardware/architecture challenge
- Modeling Challenge: Gravity + gasdynamics, subgrid models, galaxy/ group/cluster modeling
 Scalable gravity + cosmological gasdynamics
- Statistical Challenges: Cosmology as a statistical inverse problem, emulators, machine learning
 Robust emulation



Move. Integration Time Step



MOUDI/Particits ligitly lies



Motion/ Particles Trejectories

- X = F(x)/m = a(x) (Initial Condition problem)
- . ■ X=V
- V = a(x)

How to proceed?

- A classic problem in Ordinary Diferential Equations
- Several Methods

Time integration methods

Want to numerically integrate an ordinary differential equation (ODE) $\dot{\mathbf{y}}=f(\mathbf{y})$

Note: y can be a vector

Example: Simple pendulum

$$\ddot{\alpha} = -\frac{g}{l}\,\sin\alpha$$



$$y_{0} \equiv \alpha \quad y_{1} \equiv \dot{\alpha}$$
$$\dot{\mathbf{y}} = f(y) = \begin{pmatrix} y_{1} \\ -\frac{g}{l} \sin y_{0} \end{pmatrix}$$

A numerical approximation to the ODE is a set of values $\{y_0, y_1, y_2, \ldots\}$ at times $\{t_0, t_1, t_2, \ldots\}$

There are many different ways for obtaining this.

Explicit Euler method

$y_{n+1} = y_n + f(y_n)\Delta t$

- Simplest of all
- Right hand-side depends only on things already non, explicit method
- The error in a single step is O(Δt²), but for the N steps needed for a finite time interval, the total error scales as O(Δt) !
- Never use this method, it's only first order accurate.

Implicit Euler method

$$y_{n+1} = y_n + f(y_{n+1})\Delta t$$

- Excellent stability properties
- Suitable for very stiff ODE
- Requires implicit solver for y_{n+1}



Figure 16.1.1. Euler's method. In this simplest (and least accurate) method for integrating an OD he derivative at the starting point of each interval is extrapolated to find the next function value. The nethod has first-order accuracy.

Implicit mid-point rule

$$y_{n+1} = y_n + f\left(\frac{y_n + y_{n+1}}{2}\right)\Delta t$$

- 2nd order accurate
- Time-symmetric, in fact symplectic
- But still implicit...

Runge-Kutta methods

whole class of integration methods

2nd order accurate

$$k_1 = f(y_n)$$

$$k_2 = f(y_n + k_1 \Delta t)$$

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

4th order accurate.

$$k_{1} = f(y_{n}, t_{n})$$

$$k_{2} = f(y_{n} + k_{1}\Delta t/2, t_{n} + \Delta t/2)$$

$$k_{3} = f(y_{n} + k_{2}\Delta t/2, t_{n} + \Delta t/2)$$

$$k_{4} = f(y_{n} + k_{3}\Delta t/2, t_{n} + \Delta t)$$

$$y_{n+1} = y_{n} + \left(\frac{k_{1}}{6} + \frac{k_{2}}{3} + \frac{k_{3}}{3} + \frac{k_{4}}{6}\right)\Delta t$$



1.3. Fourth-order Runge-Kutta method. In each step the derivative is evaluated initial point, twice at trial midpoints, and once at a trial endpoint. From these de ion value (shown as a filled dot) is calculated. (See text for details.)

Which one shall we use?

- Euler? Tiny steps? Accuracy? Better avoid the explicit form. What about implicit one? Seems a good one?
- Runge-Kutta (order? 4th, higher?)
- Mid point
- Burlish-Stoher (prediction, correction at the end of interval, see N. Recipes)
- Commonly used and very good integrators

Are we done?

We try to represent this: Evolution with a constant Hamiltonian (Volume in Phase Space, defined by Conserved Integrals of Motion or by Symmetries)



Most of the N-body codes use an scheme called Leap-Frog

Why is that?

- Cheap in terms of computation
- Symplectic

The Leapfrog Integrator

For second-order problems like (4) in which f depends only on x, the second-order *Leapfrog* integration scheme is widely used. Its simplicity makes it an attractive alternative. However, it requires us to make a modification to the way we have been thinking about how -- and when -- our data are defined.

Up to now, we have assumed (quite reasonably) that all data are *synchronous* -- that is, all the components of the vector x_i are defined at the same time t_i . However, in second-order systems at

$$v_{i+1/2} = v(i + \frac{1}{2}\delta t), \quad i = 0, 1, 2, \dots$$
 (23)

With this definition, we can write down a statement of the Leapfrog scheme that advances x_i to x_{i+1} and $v_{i+1/2}$ to $v_{i+3/2}$:

$$\begin{aligned} x_{i+1} &= x_i + v_{i+1/2} \,\delta t \,, \\ v_{i+3/2} &= v_{i+1/2} + f(x_{i+1}) \,\delta t \,, \end{aligned} \tag{24}$$

It is depicted graphically below. Notice the *symmetry* between the ways x and v are advanced in time. You can easily verify by expanding out the Taylor series

$$v(t + \frac{1}{2}\delta t) = v(t) + \frac{1}{2}\delta t f(t) + O(\delta t^2)$$
(25)

that this scheme does indeed give second-order accuracy in x. In fact, it is formally equivalent to the Mid-point or second-order predictor-corrector methods.



Of course, initial conditions are rarely specified at the staggered times required by the leapfrog scheme! Typically, we must use a so-called ``self-starting" scheme (like Euler, Mid-point or Runge-Kutta-4) to take the first half step and establish the value of $v_{1/2}$. The program leapfrog.e



In situations where we are interested in long-term small changes in the properties of a nearly periodic orbit, and where even small systematic errors would mask the true solution, time-reversible integrators such as the Leapfrog scheme are essential.

Time-Reversibility

You might well ask, ``Since we have to start off with one of the other schemes anyway, and since the Mid-point method is already very simple to program, why should I ever bother with the Leapfrog scheme?" The answer is that, unlike any of the other methods we have described, the Leapfrog integrator is *time reversible* -- and that property gives it some very important advantages.

To see the time reversibility explicitly, reconsider equation (24) and imagine that we wished to ``reverse our tracks'' and step backward from $(t_{i+1}, x_{i+1}, v_{i+3/2})$ to $(t_i, x_i, v_{i+1/2})$. Applying the

algorithm, we do the following:

$$\begin{aligned}
v_{i+1/2} &= v_{i+3/2} + f(x_{i+1}) (-\delta t), \\
x_i &= x_{i+1} + v_{i+1/2} (-\delta t),
\end{aligned}$$
(26)

But these are precisely the steps (in reverse) that we took to advance the system in the first place! In other words, if we use the Leapfrog scheme to integrate forward in time, then reverse the velocities (and the sign of the timestep) and use the same integrator to return to time t = 0, we will arrive *precisely* our starting point -- not approximately, as would be the case with the other integrators, but exactly, at least up to rounding error. Verify this for yourself by modifying <code>leapfrog.c</code> to reverse itself and integrate backwards after integrating forward for some interval -- 10 time units, say.

The Leapfrog scheme is time reversible because of the symmetric way in which it is defined. None of the earlier schemes have this property, because they all evaluate derivatives in an asymmetrical way. For example, in the Euler method, it is clear that the forward and backward steps would not cancel out precisely -- they use different derivatives, evaluated at different times. In the Mid-point method, which uses an estimate of the derivative at the center of the range, that estimate is still based on an extrapolation from the *left-hand* side of the interval. On time reversal, the corresponding estimate would be based on the derivative at the right-hand edge, and would *not* vield precisely the same result. The difference is small, but it is enough to prevent the scheme from

Symplectic integrators are designed for the numerical solution of Hamilton's equations, which read

$$\dot{p} = -\frac{\partial H}{\partial q}$$
 and $\dot{q} = \frac{\partial H}{\partial p}$,

where q denotes the position coordinates, p the momentum coordinates, and H is the Hamiltonian (see Hamiltonian mechanics for more background).

The time evolution of Hamilton's equations is a symplectomorphism, meaning that it conserves the symplectic two-form $dp \wedge dq$. A numerical scheme is a symplectic integrator if it also conserves this two-form.

Symplectic integrators possess as a conserved quantity a Hamiltonian which is slightly perturbed from the original one. By virtue of these advantages, the SI scheme has been widely applied to the calculations of long-term evolution of chaotic Hamiltonian systems ranging from the Kepler problem to the classical and semi-classical simulations in molecular dynamics.

Most of the usual numerical methods, like the primitive Euler scheme and the classical Runge-Kutta scheme, are not symplectic integrators.

Splitting methods for separable Hamiltonians

A widely used class of symplectic integrators is formed by the splitting methods.

Assume that the Hamiltonian is separable, meaning that it can be written in the form

$$H(p,q) = T(p) + V(q).$$
 (1)

This happens frequently in Hamiltonian mechanics, with T being the kinetic energy and V the potential energy.

Then the equations of motion of a Hamiltonian system can be expressed as

$$\dot{z} = \{z, H(z)\}\tag{2}$$

where $\{\cdot, \cdot\}$ is a Poisson bracket, and z = (q,p). By using the notation $D_H = \{\cdot, H\}$, this can be re-expressed as

$$\dot{z} = D_H z$$
.

The formal solution of this set of equations is given as

$$z(\tau) = \exp(\tau D_H) z(0). \tag{3}$$

When the Hamiltonian has the form of eq. (1), the solution (3) is equivalent to

$$z(\tau) = \exp[\tau (D_T + D_V)]z(0). \tag{4}$$

The SI scheme approximates the time-evolution operator $\exp[\tau(D_T + D_V)]$ in the formal solution (4) by a product of operators as

$$\exp[\tau (D_T + D_V)] = \prod_{i=1}^k \exp(c_i \tau D_T) \exp(d_i \tau D_V) + O(\tau^{n+1}), \tag{5}$$

where c_i and d_i are real numbers, and k is an integer, which is called the order of the integrator. Note that each of the operators $\exp(c_i \tau D_T)$ and $\exp(d_i \tau D_V)$ provides a symplectic map, so their product appearing in the right hand side of (5) also constitutes a symplectic map. In concrete terms, $\exp(c_i \tau D_T)$ gives the mapping

$$\begin{pmatrix} q \\ p \end{pmatrix} \mapsto \begin{pmatrix} q' \\ p' \end{pmatrix} = \begin{pmatrix} q + \tau c_i \frac{\partial T}{\partial p}(p) \\ p \end{pmatrix} \qquad \qquad \begin{pmatrix} q \\ p \end{pmatrix} \mapsto \begin{pmatrix} q \\ p - \tau d_i \frac{\partial V}{\partial q}(q) \end{pmatrix}.$$

The symplectic Euler method is the first-order integrator with k = 1 and coefficients

$$c_1 = d_1 = 1.$$

The Verlet method is the second-order integrator with k = 2 and coefficients

$$c_1 = c_2 = \frac{1}{2}, \qquad d_1 = 1, \qquad d_2 = 0.$$

A third order sympectic integrator (with k = 3) was discovered by Ronald Ruth in 1983. ^[1] One of the ma

$$c_1 = \frac{2}{3}, \qquad c_2 = -\frac{2}{3}, \qquad c_3 = 1, \\ d_1 = \frac{7}{24}, \qquad d_2 = \frac{3}{4}, \qquad d_3 = -\frac{1}{24}$$

A fourth order integrator (with k = 4) was also discovered by Ruth in 1983 and distributed privately to the This fourth order integrator was published in 1990 by Forest and Ruth and also independently discovere

$$c_1 = c_4 = \frac{1}{2(2 - 2^{1/3})}, \quad c_2 = c_3 = \frac{1 - 2^{1/3}}{2(2 - 2^{1/3})},$$
$$d_1 = d_3 = \frac{1}{2 - 2^{1/3}}, \quad d_2 = -\frac{2^{1/3}}{2 - 2^{1/3}}, \quad d_4 = 0.$$

To determine these coefficients, the Baker-Campbell-Hausdorff formula can be used. Yoshida, in particu

Pendulum example

We can motivate the study of geometric integrators by considering the motion of a pendulum.

Assume that we have a pendulum whose bob has mass m = 1 and whose rod is massless of length $\ell = 1$. Take the acceleration due to gravity to be g = 1. Denote by q(t) the angular displacement of the rod from the vertical, and by p(t) the pendulum's momentum. The Hamiltonian of the system, the sum of its kinetic and potential energies, is

$$H(q, p) = T(p) + U(q) = \frac{1}{2}p^2 - \cos q$$

which gives Hamilton's equations

$$(\dot{q},\dot{p})=(p,-\sin q).$$

It is natural to take the configuration space Q of all q to be the unit circle \mathbb{S}^1 , so that (q,p) lies on the cylinder $\mathbb{S}^1 \times \mathbb{R}$. However, we will take $(q, p) \in \mathbb{R}^2$, simply because (q,p)-space is then easier to plot. Define $z(t) = (q(t),p(t))^T$ and $f(z) = (p, -\sin q)^T$. Let us experiment by using some simple numerical methods to integrate this system. As usual, we select a constant step-size h and write $z_k := z(kh)$ for $k \ge 0$. We use the following methods.

$$\begin{aligned} z_{k+1} &= z_k + hf(z_k) \text{ (explicit Euler),} \\ z_{k+1} &= z_k + hf(z_{k+1}) \text{ (implicit Euler),} \\ z_{k+1} &= z_k + hf(q_k, p_{k+1}) \text{ (symplectic Euler),} \\ z_{k+1} &= z_k + hf((z_{k+1} + z_k) / 2) \text{ (implicit midpoint rule).} \end{aligned}$$

(Note that the symplectic Euler method treats q by the explicit and p by the implicit Euler method.)



Simple pendulum: trajectories

Approximate solutions



Figure 4. A Kepler problem of high eccentricity evolved with different simple time integration schemes, using an equal time-step in all cases. Even



pin, Valenzuela, Colin, Quinn 08

A combination of a pseudo simplectic scheme and a time step prescription seems to have a slow departure from the Hamiltionian solution



Hut, Makino, McMillan 1995

- Implicit: An iterative solution at each step (expensive, in the 90's, now?)
 Why shall we care?
- Worth trying

Why shall we care? Allows larger time steps without compromising accuracy?

Anyone?

ANY ONE?

Lessons

 Do not feel overwhelm: Code development and use is now a transdisciplinary group project.

- You are capable to learn the skills for your interest
- Advice: choose carefully the tool for the problem
- Test. Test and test afterwards
- You pretend to have a numerical dynamical experiment including some properties of the observed galaxy/universe not the actual universe inside the computer
- You are trying to test hypothesis not creating the universe ()but looks like
- Sometimes impossible to catch a numerical problem after the simulation has been run

- More eficiente Integrators
- More flexible and accurate Solvers
- More efficient parallelization
- New strategy Boltzmann solver??