High performance computing and numerical modeling

Volker Springel

Plan for my lectures

Lecture 1: Collisional and *collisionless* N-body dynamics

Lecture 2: Gravitational force calculation

Lecture 3: Basic gas dynamics

Lecture 4: Smoothed particle hydrodynamics

Lecture 5: Eulerian hydrodynamics

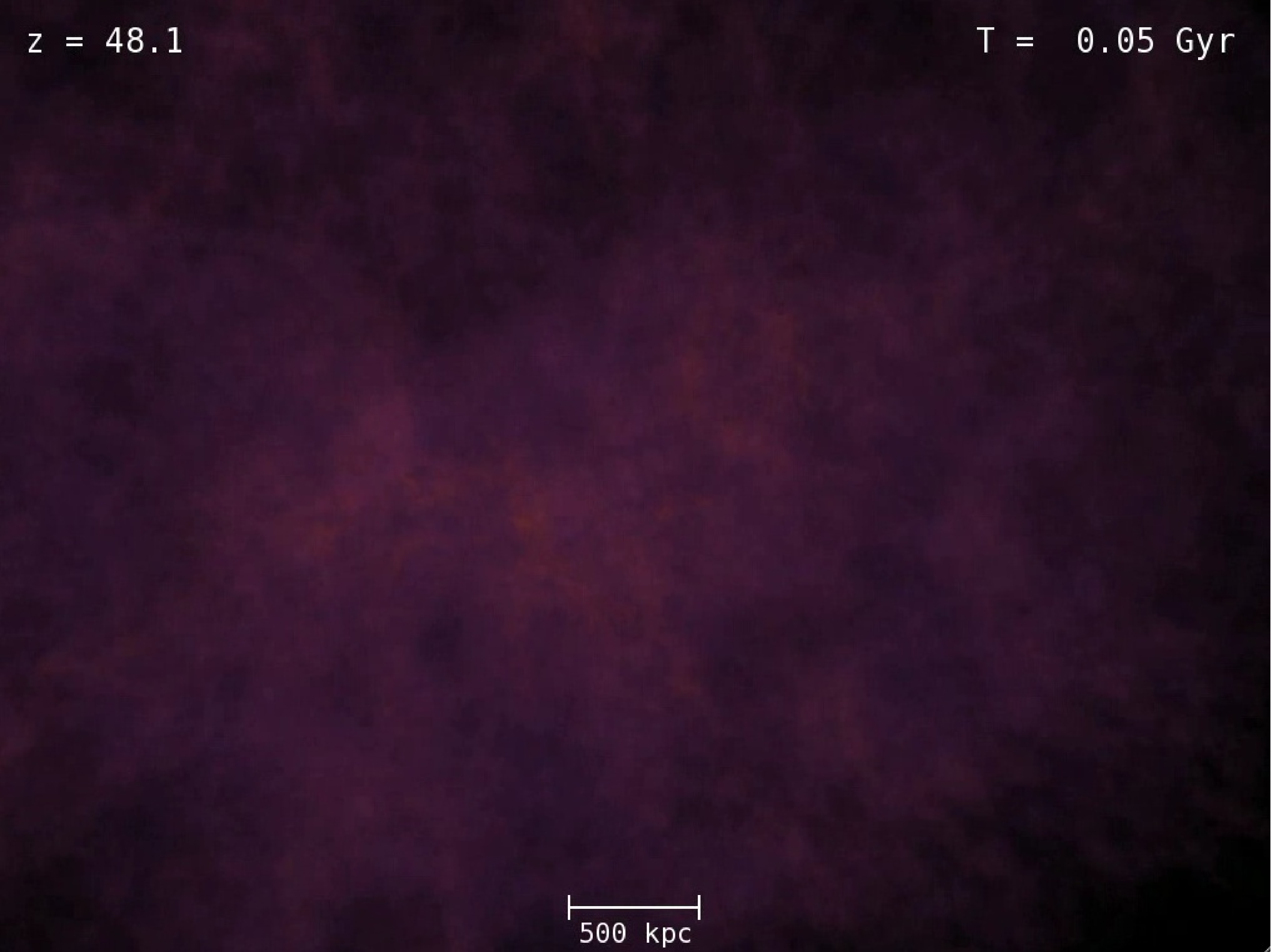
Lecture 6: Moving-mesh techniques

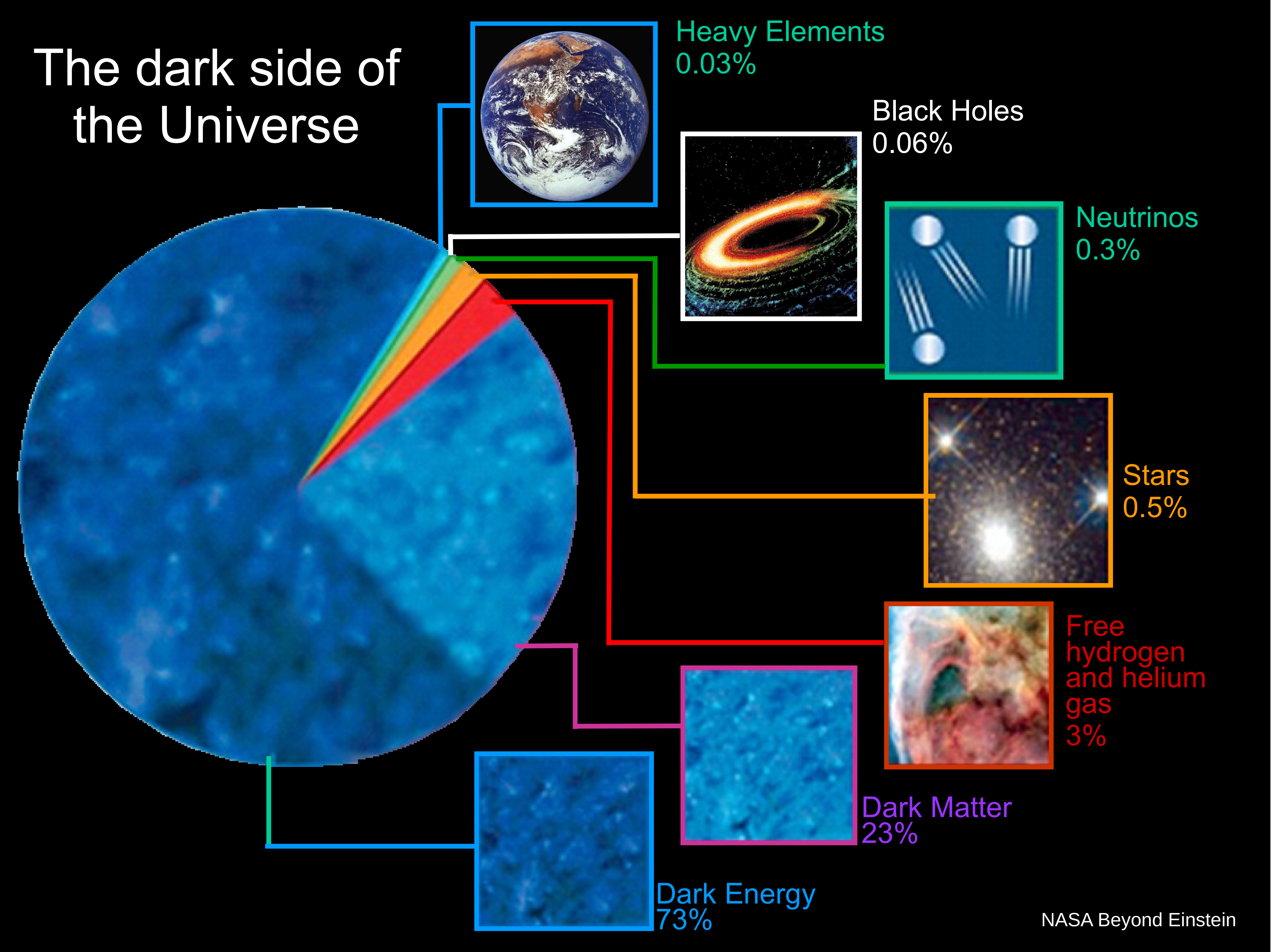
Lecture 7: Towards high dynamic range

Lecture 8: Parallelization techniques and current computing trends

Heidelberg Institute for Theoretical Studies
HITS
Universität Heidelberg

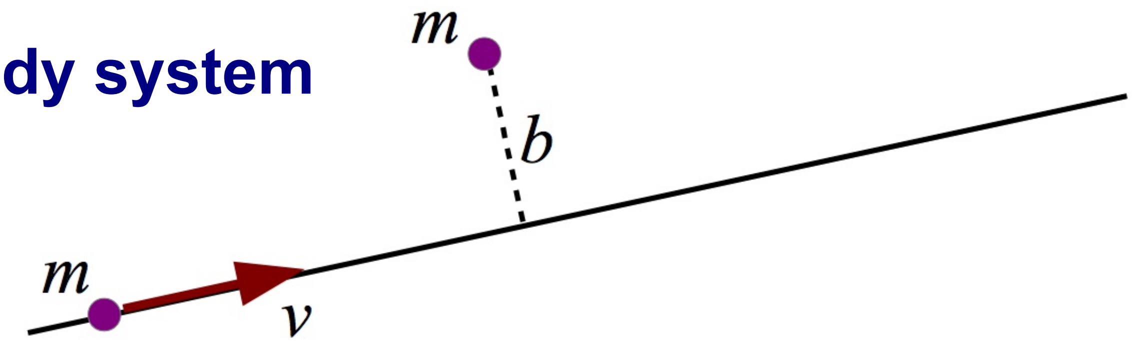
43rd Saas Fee Course
Villars-Sur-Ollon, March 2013


z = 48.1
T = 0.05 Gyr
500 kpc


The dark side of the Universe
Heavy Elements 0.03%
Black Holes 0.06%
Neutrinos 0.3%
Stars 0.5%
Free hydrogen and helium gas 3%
Dark Matter 23%
Dark Energy 73%
NASA Beyond Einstein

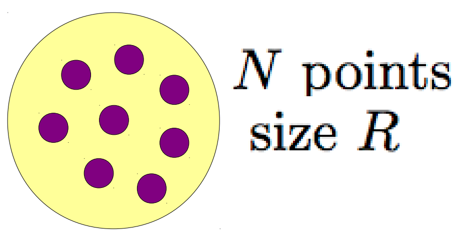
Basics of collisionless simulations

Relaxation time of an N-body system



Transverse momentum change:

$$\Delta p_\perp = m\Delta v_\perp = \int F_\perp \mathrm{d}t \;= \int \frac{Gm^2}{x^2+b^2}\frac{b}{\sqrt{x^2+b^2}}\frac{\mathrm{d}x}{v} = \frac{2Gm^2}{bv}$$



Particles encountered in one crossing in a ring

$$\mathrm{d}n = N\frac{2\pi b\,\mathrm{d}b}{\pi R^2}$$

Different encounters add incoherently:

$$(\Delta v)^2 = \int \left(\frac{2Gm}{bv}\right)^2 \mathrm{d}n \;= 8N\frac{Gm^2}{Rv}\int\frac{\mathrm{d}b}{b} = 8N\frac{Gm^2}{Rv}\;\ln\Lambda$$

Coloumb logarithm: $\Lambda = \ln\frac{b_{\mathrm{max}}}{b_{\mathrm{min}}}$

Typical specific energy of a particle: $$v^2 \simeq v_c^2 = \frac{GNm}{R}$$

Crossing time through the system: $$t_{\rm cross} = \frac{R}{v}$$

Relaxation time: $$t_{\rm relax} \equiv \frac{v^2}{(\Delta v)^2/t_{\rm cross}} = \frac{N}{8\ln\Lambda}\, t_{\rm cross}$$

But what about the Coloumb logarithm?

Maximal scattering: $\Delta v_\perp \simeq v.$

$$\frac{2Gm}{b_{\rm min} v} = v \qquad b_{\rm min} \simeq \frac{2R}{N}$$

Minimal scattering: $b_{\rm max} \simeq R.$

$$\longrightarrow \quad \Lambda \simeq \ln N/2.$$

Relaxation time of N-body system:

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

Small globular star cluster:

$$N \sim 10^5 \qquad t_{\rm cross} \sim \frac{3\,{\rm pc}}{6\,{\rm km/s}} \simeq \frac{1}{2}\,{\rm Myr}$$

This is a collisional system, and stellar encounters are important for the evolution.

Stars in a galaxy:

$$N \sim 10^{11} \qquad t_{\rm cross} \sim \frac{1}{100}\frac{1}{H_0}$$

Behaves as a collisionless system.

Dark matter particles in a galaxy (100 GeV WIMP):

$$N \sim 10^{77} \qquad t_{\rm cross} \sim \frac{1}{10 H_0}$$

The mother of all collisionless systems!

In an N-body model of a collisionless system, we must ensure that the simulated time is smaller than the relaxation time

$$t_{\rm sim} \ll t_{\rm relax}$$

We assume that the only appreciable interaction of dark matter particles is **gravity**

COLLISIONLESS DYNAMICS

Because there are **so many** dark matter particles, it's best to describe the system in terms of the **single particle distribution function**

$$f = f(\mathbf{x}, \mathbf{v}, t)$$

There are so many dark matter particles that they do not scatter locally on each other, they just respond to their collective gravitational field

Collisionless Boltzmann equation

Poisson-Vlasov System

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \mathbf{x}} \cdot \mathbf{v} + \frac{\partial f}{\partial \mathbf{v}} \cdot \left(-\frac{\partial \Phi}{\partial \mathbf{x}} \right) = 0$$

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

Phase-space is conserved along each characteristic (i.e. particle orbit).

The number of stars in galaxies is so large that the two-body relaxation time by far exceeds the Hubble time. Stars in galaxies are therefore also described by the above system.

This system of partial differential equations is very difficult (impossible) to solve directly in non-trivial cases.

The N-body method uses a finite set of particles to sample the underlying distribution function

"MONTE-CARLO" APPROACH TO COLLISIONLESS DYNAMICS

We discretize in terms of N particles, which approximately move along characteristics of the underlying system.

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

$$\Phi(\mathbf{x}) = -G \sum_{j=1}^{N} \frac{m_j}{\left[(\mathbf{x} - \mathbf{x}_j)^2 + \epsilon^2\right]^{1/2}}$$

The need for **gravitational softening**:

- Prevent large-angle particle scatterings and the formation of bound particle pairs.
- Helps to ensure that the two-body relaxation time is sufficiently large.
- Allows the system to be integrated with low-order integration schemes.

} Needed for faithful collisionless behavior

But how should we pick the gravitational softening length?

Let's first look at typical cosmological halos

$$M_{200} = 200 \times \rho_{\rm crit} \times \frac{4\pi}{3} R_{200}^3$$

$$v_{200}^2 \equiv \frac{GM_{200}}{R_{200}}$$

$$\rho_{\rm crit} = \frac{3H^2}{8\pi G}$$

Relations between halo virial quantities:

$$M_{200} = \frac{v_{200}^3}{10GH}$$

$$R_{200} = \frac{v_{200}}{10H}$$

Specific binding energy of a softened particle pair at vanishing distance

$$v_{\rm bind}^2 \simeq \frac{Gm}{\epsilon}$$

Specific energy of particles in the halo

$$v_{200}^2 \simeq (10GHM_{200})^{2/3}$$

For collisionless behavior, we must at least have:

$$v_{200}^2 > v_{\rm bind}^2$$

Let's introduce the mean particle distance: (for simplicity in a EdS universe)

$$\rho_{\rm crit} d^3 = m \qquad\qquad M_{200} = N \cdot m$$

Hence we get the condition: $$\epsilon \geq \left(\frac{3}{800\pi N^2}\right)^{1/3} d$$

For: $N = 5$ $$\epsilon \geq \frac{1}{30} d$$

But if we also recall the relaxation time of dark matter in halos:

$$t_{\rm relax} = \frac{N}{8\ln\Lambda} t_{\rm cross} \qquad\qquad t_{\rm cross} \simeq \frac{R_{200}}{v_{200}} = \frac{1}{10H}$$

We see that halos with well below 100 particles are typically always affected by relaxation over a Hubble time.

Compromise in practice: $$\epsilon \sim \left(\frac{1}{40} - \frac{1}{20}\right) d$$

Derivation of the collisionless cosmological equation of motion

Newtonian equation of motion

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = -\nabla_r \Phi + \frac{\Lambda c^2}{3}\mathbf{r}$$

$$\mathbf{u} = \dot{\mathbf{r}}$$

$$\frac{\mathrm{D}}{\mathrm{D}t} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla_r$$

$$\frac{\Lambda c^2}{3} \equiv \Omega_\Lambda H_0^2$$

Introduction of comoving coordinates

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

Hubble flow

peculiar velocity

$$\mathbf{u} = \dot{\mathbf{r}} = \dot{a}\mathbf{x} + a\dot{\mathbf{x}} = H(t)\mathbf{r} + \mathbf{v}$$

Carry out a variable transformation of the equations...

$$(\mathbf{r}, t) \rightarrow (\mathbf{x}, t)$$

$$\nabla_r \rightarrow \frac{1}{a}\nabla_x$$

$$\left(\frac{\partial}{\partial t}\right)_r \rightarrow \left(\frac{\partial}{\partial t}\right)_x + \left(\frac{\partial \mathbf{x}}{\partial t}\right)_r \nabla_x$$

Rewriting yields...

$$\left[\left(\frac{\partial}{\partial t}\right)_x + \frac{1}{a}\left(\mathbf{v}\cdot\nabla_x\right)\right]\left(\dot{a}\mathbf{x}+\mathbf{v}\right) = -\frac{1}{a}\nabla_x\Phi + \frac{\Lambda c^2}{3}a\mathbf{x}$$

And then...

$$\frac{\partial\mathbf{v}}{\partial t} + H(t)\mathbf{v} + \frac{1}{a}(\mathbf{v}\cdot\nabla_x)\mathbf{v} = -\frac{1}{a}\nabla_x\Phi - \ddot{a}\mathbf{x} + \frac{\Lambda c^2}{3}a\mathbf{x}$$

Recalling the Friedmann equation (in the matter dominated era)

$$\frac{\ddot{a}}{a} = -\frac{4\pi G}{3}\bar{\rho} + \frac{\Lambda c^2}{3}$$

yields the equation of motion in the form:

$$\frac{\mathrm{D}\mathbf{v}}{\mathrm{D}t} + H(t)\mathbf{v} = -\frac{1}{a}\nabla_x\Phi + \frac{4\pi G}{3}\bar{\rho}a\mathbf{x}$$

We define the peculiar gravitational potential as

$$\phi = \Phi - \frac{2\pi G}{3}\bar{\rho}a^2\mathbf{x}^2$$

This implies:

$$-\frac{1}{a}\nabla\phi = -\frac{1}{a}\nabla\Phi + \frac{4\pi G}{3}\bar{\rho}a\mathbf{x}$$

$$\nabla^2\phi = \nabla^2\Phi - 4\pi G\bar{\rho}a^2 = 4\pi G(\rho - \bar{\rho})a^2$$

So that we finally get the equations of motion as:

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

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

- Motion is created by density fluctuations around the background
- Infinite space is no problem any more

Two conflicting requirements complicate the study of **hierarchical** structure formation

DYNAMIC RANGE PROBLEM FACED BY COSMOLOGICAL SIMULATIONS

Want **small particle mass** to resolve internal structure of halos

Want **large volume** to obtain respresentative sample of universe

need large N

where N is the particle number

Problems due to a small box size:

- Fundamental mode goes non-linear soon after the first halos form. ⇨ Simulation cannot be meaningfully continued beyond this point.
- No rare objects (the first halo, **rich** galaxy clusters, etc.)

Problems due to a large particle mass:

- Physics cannot be resolved.
- Small galaxies are missed.

At any given time, halos exist on a large range of mass-scales !

Several questions come up when we try to use the N-body approach for collisionless simulations

- How do we compute the gravitational forces efficiently and accurately?
- How do we integrate the orbital equations in time?
- How do we generate appropriate initial conditions?
- How do we parallelize the simulation?

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

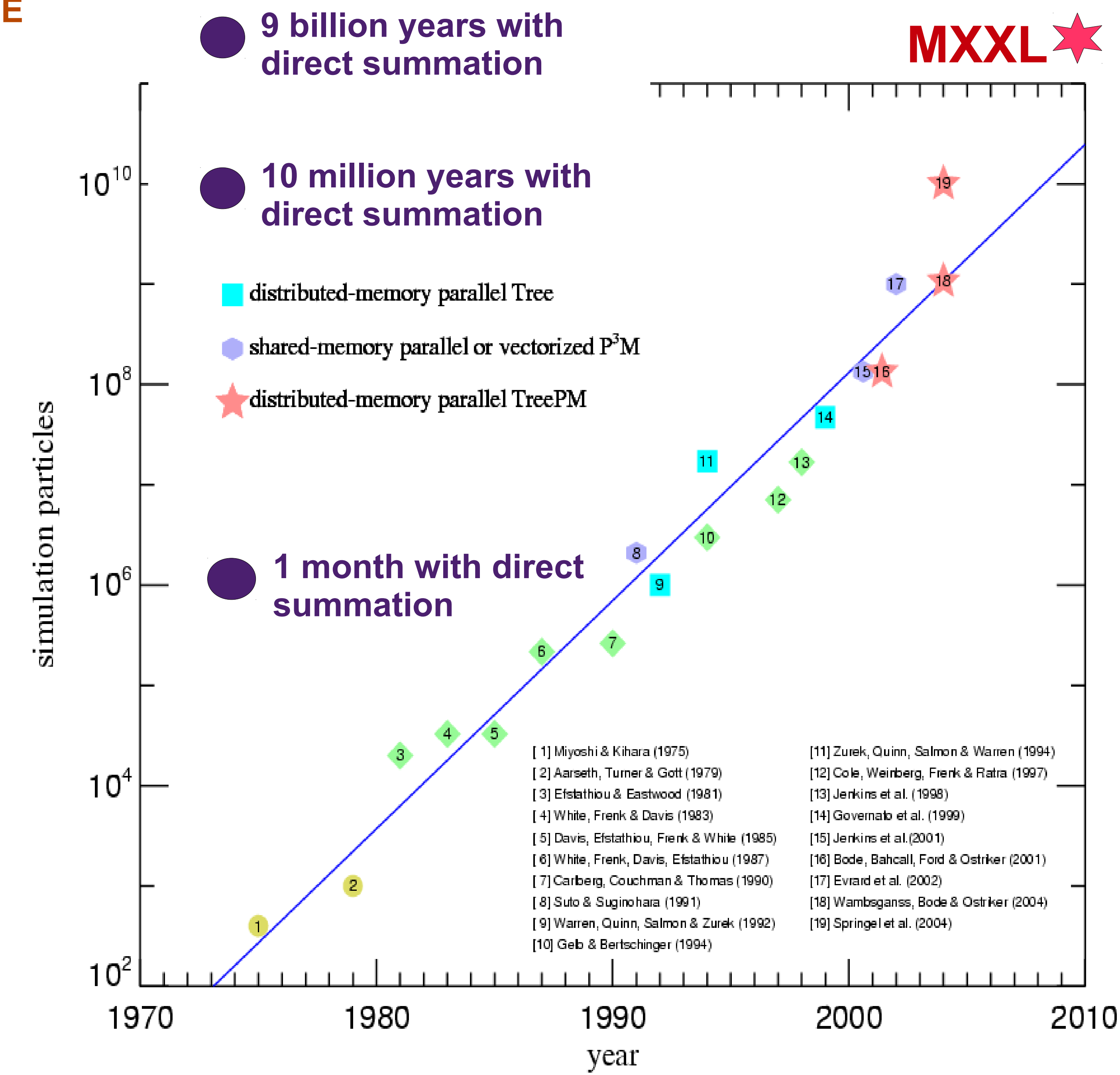
$$\Phi(\mathbf{x}) = -G \sum_{j=1}^{N} \frac{m_j}{\left[(\mathbf{x} - \mathbf{x}_j)^2 + \epsilon^2\right]^{1/2}}$$

Note: The naïve computation of the forces is an N^2 - task.

Cosmological N-body simulations have grown rapidly in size over the last three decades

"N" AS A FUNCTION OF TIME

- Computers double their speed every 18 months (Moore's law)
- N-body simulations have doubled their size every 16-17 months
- Recently, growth has accelerated further.



Time integration issues

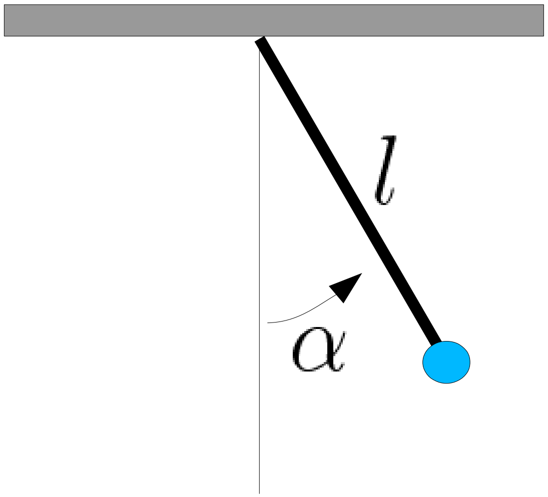
Time integration methods

Want to numerically integrate an **ordinary differential equation** (ODE)

$$\dot{\mathbf{y}} = f(\mathbf{y})$$

Note: $\mathbf{y}$ can be a vector

Example: Simple pendulum



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

$$y_0 \equiv \alpha \qquad y_1 \equiv \dot{\alpha}$$

$$\dot{\mathbf{y}} = f(y) = \begin{pmatrix} y_1 \\ -\frac{g}{l}\,\sin y_0 \end{pmatrix}$$

A numerical approximation to the ODE is a set of values $\{\mathbf{y}_0, \mathbf{y}_1, \mathbf{y}_2, \ldots\}$ 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 known, **explicit method**
- The error in a single step is $O(\Delta t^2)$, but for the N steps needed for a finite time interval, the total error scales as $O(\Delta t)$!
- 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}
- But still low order

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

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

4th order accurate.

$$\begin{aligned} k_1 &= f(y_n, t_n) \\ k_2 &= f(y_n + k_1 \Delta t/2, t_n + \Delta t/2) \\ k_3 &= f(y_n + k_2 \Delta t/2, t_n + \Delta t/2) \\ k_4 &= f(y_n + k_3 \Delta t/2, t_n + \Delta t) \\ y_{n+1} &= y_n + \left(\frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6}\right)\Delta t \end{aligned}$$

The Leapfrog

For a second order ODE: $\ddot{\mathbf{x}} = f(\mathbf{x})$

"Drift-Kick-Drift" version

$$
\begin{aligned}
x_{n+\frac{1}{2}} &= x_n + v_n \frac{\Delta t}{2} \\
v_{n+1} &= v_n + f(x_{n+\frac{1}{2}}) \Delta t \\
x_{n+1} &= x_{n+\frac{1}{2}} + v_{n+1} \frac{\Delta t}{2}
\end{aligned}
$$

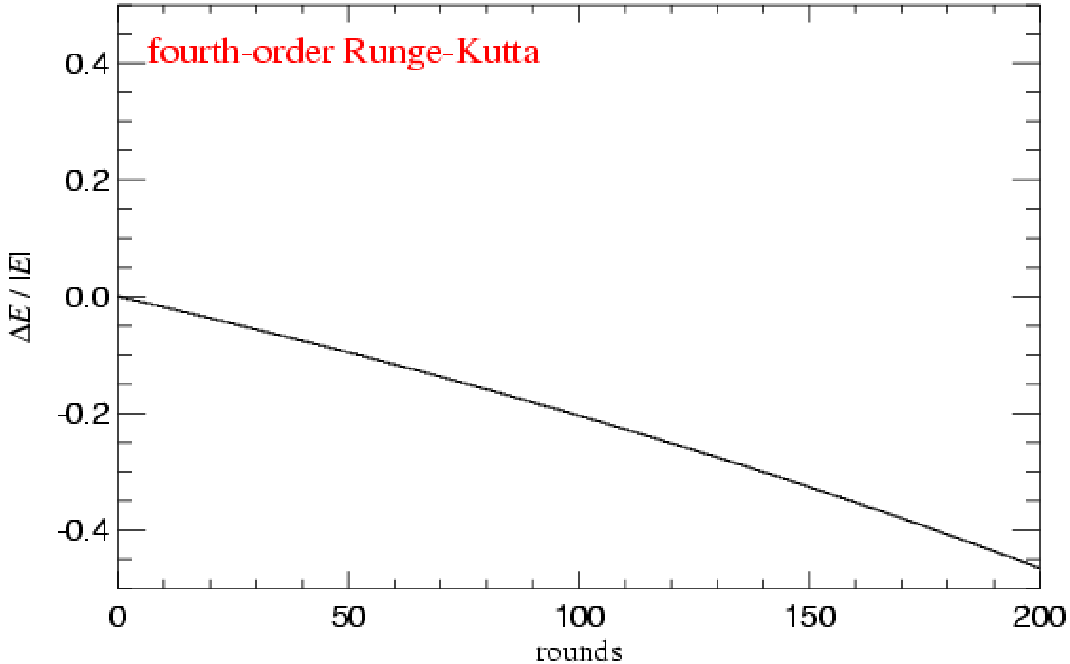
"Kick-Drift-Kick" version

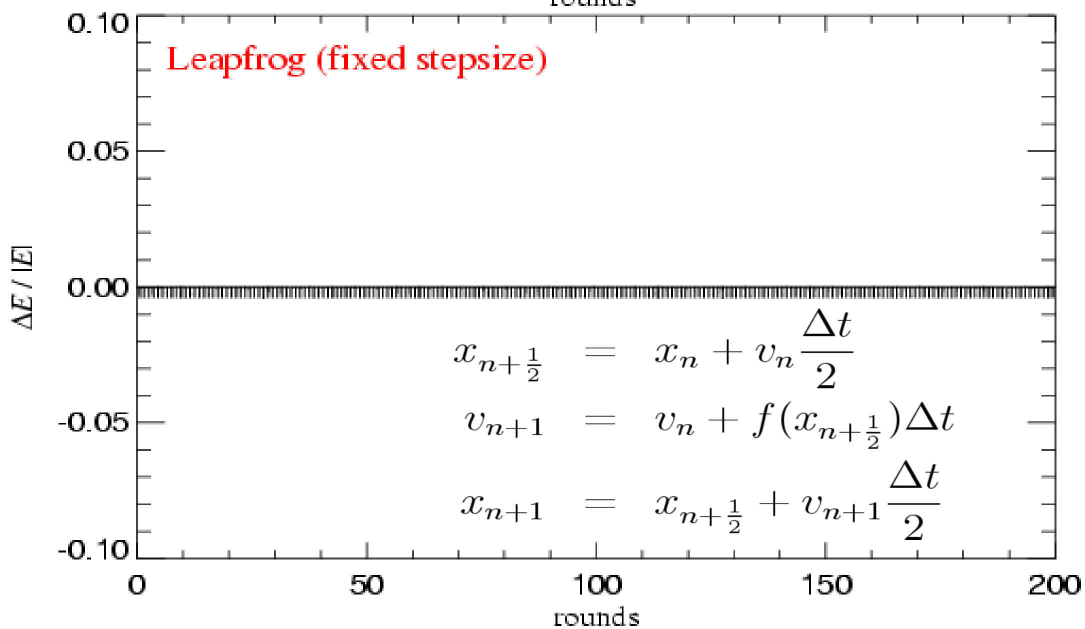
$$
\begin{aligned}
v_{n+\frac{1}{2}} &= v_n + f(x_n) \frac{\Delta t}{2} \\
x_{n+1} &= x_n + v_{n+\frac{1}{2}} \frac{\Delta t}{2} \\
v_{n+1} &= v_{n+\frac{1}{2}} + f(x_{n+1}) \frac{\Delta t}{2}
\end{aligned}
$$

- **2nd order accurate**
- **symplectic**
- can be rewritten into time-centered formulation

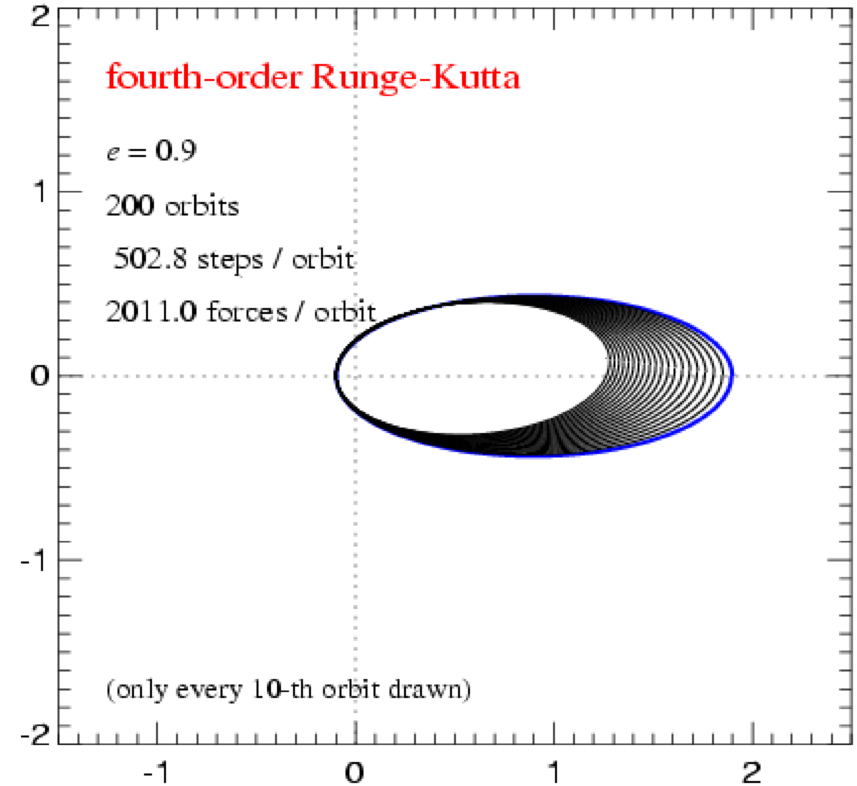
The leapfrog is behaving much better than one might expect...

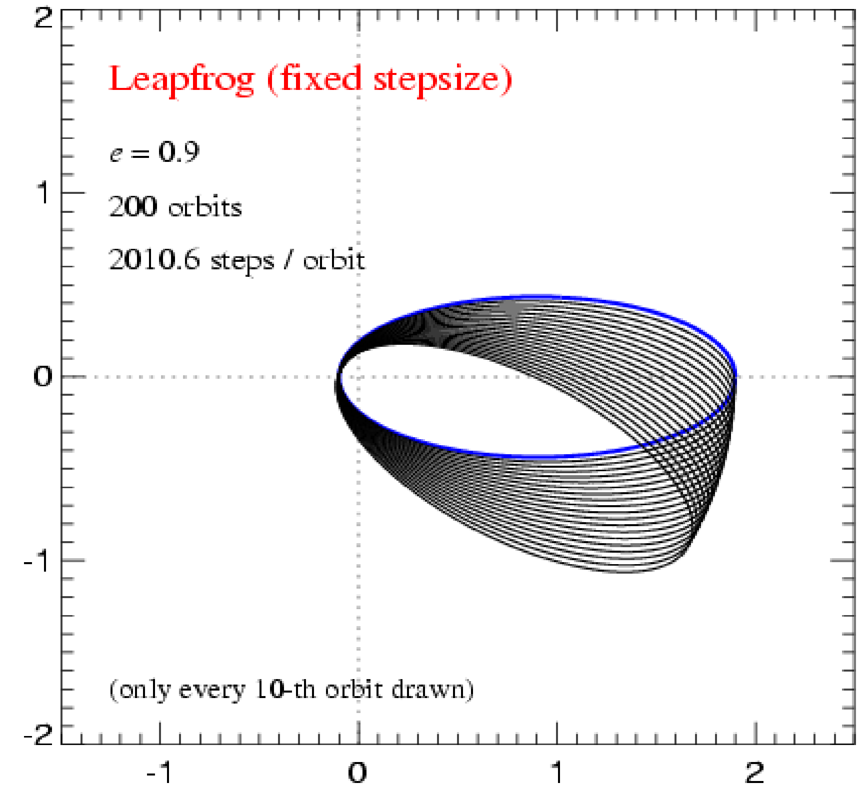
INTEGRATING THE KEPLER PROBLEM





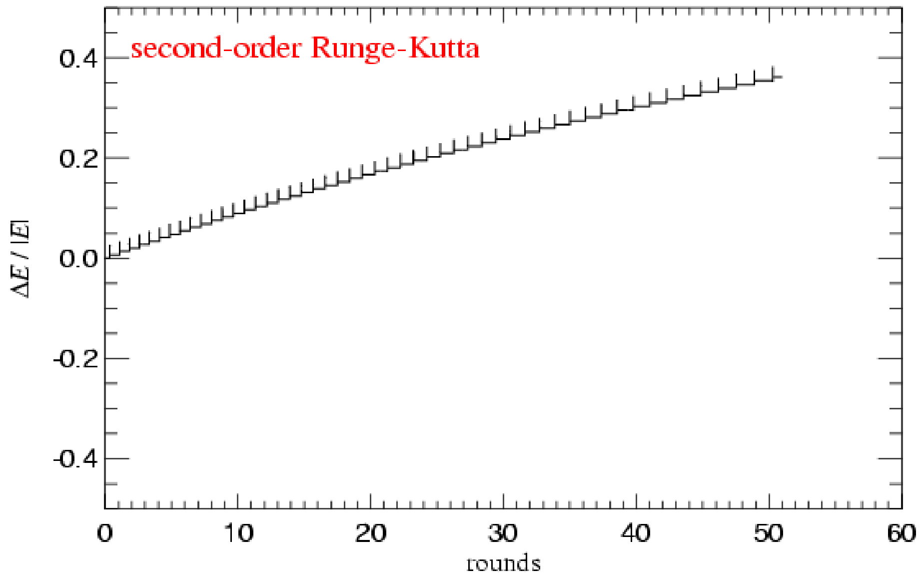
$$x_{n+\frac{1}{2}} = x_n + v_n \frac{\Delta t}{2}$$
$$v_{n+1} = v_n + f(x_{n+\frac{1}{2}}) \Delta t$$
$$x_{n+1} = x_{n+\frac{1}{2}} + v_{n+1} \frac{\Delta t}{2}$$

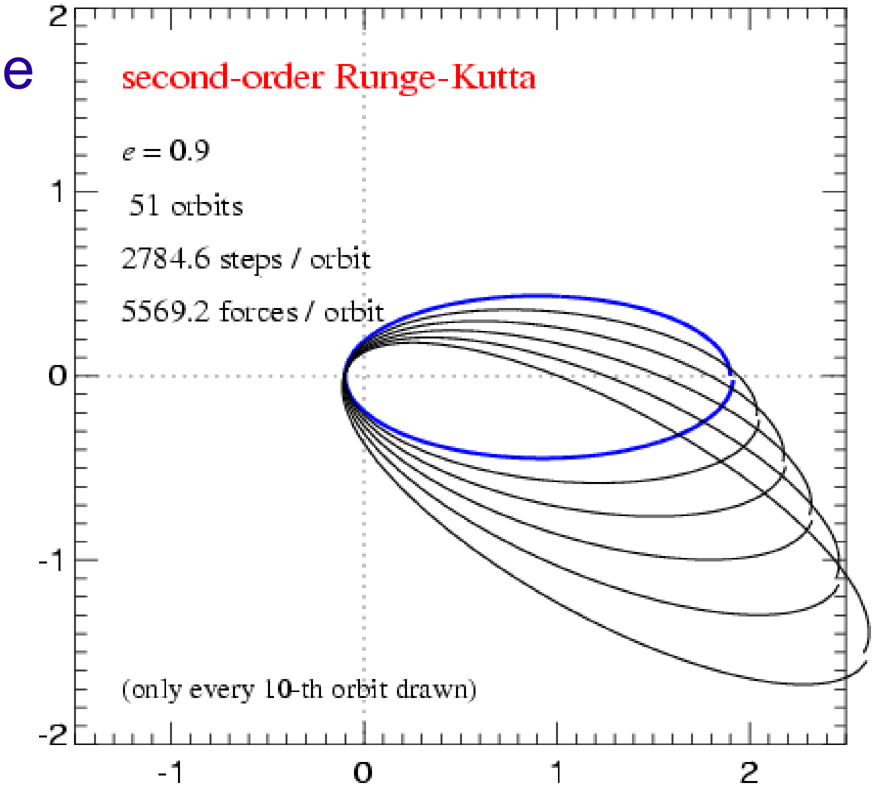


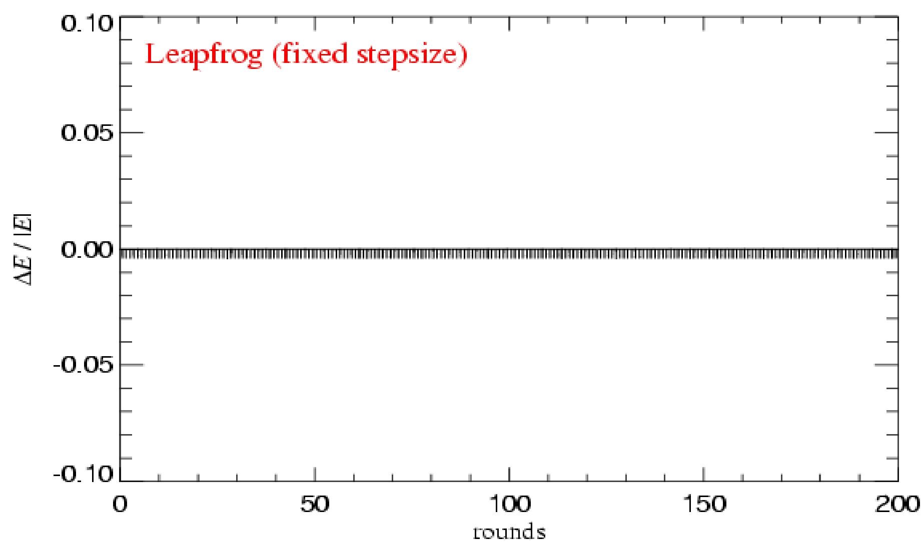


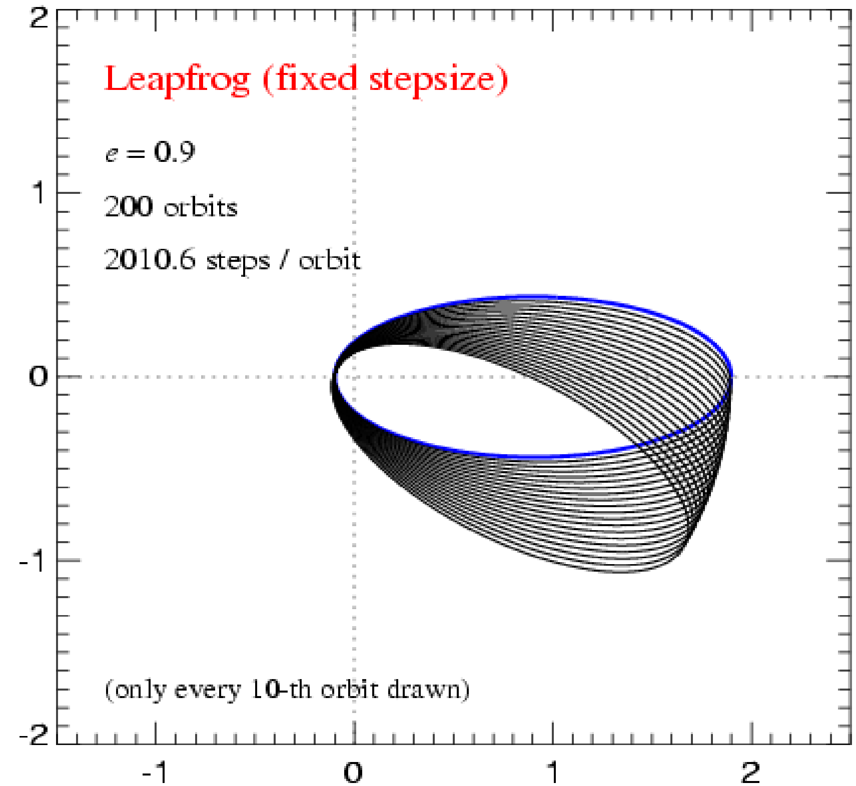
When compared with an integrator of the same order, the leapfrog is highly superior

INTEGRATING THE KEPLER PROBLEM



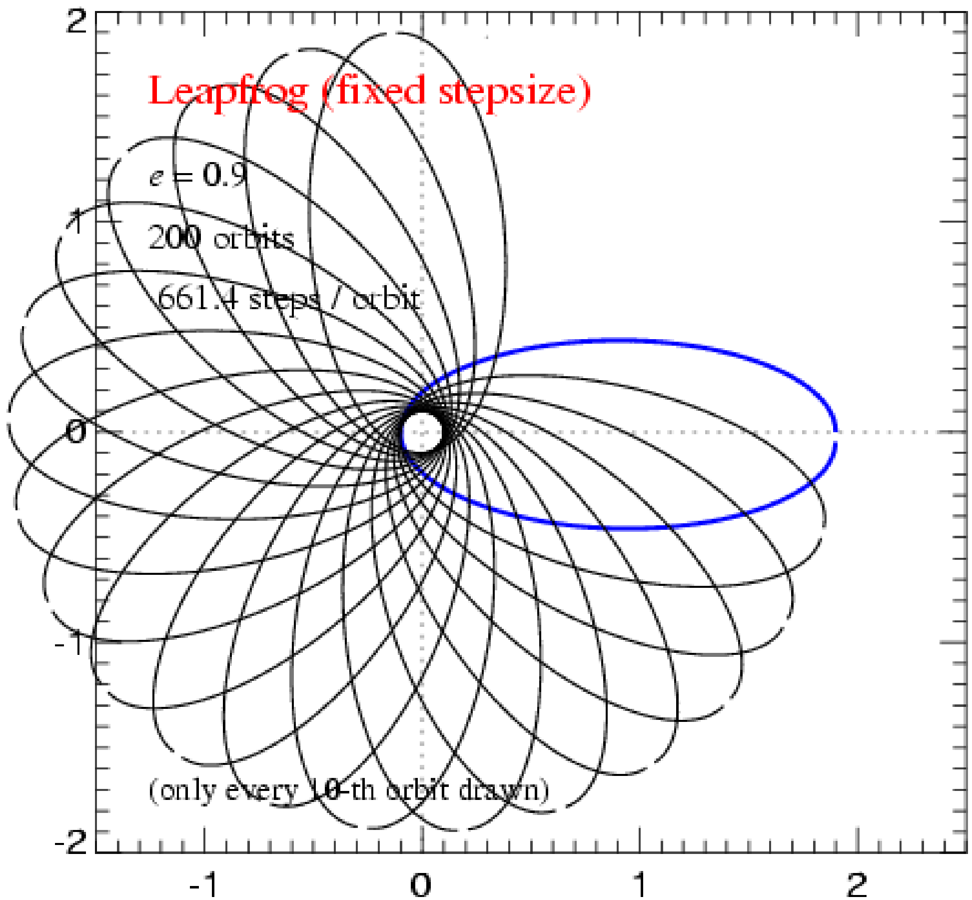


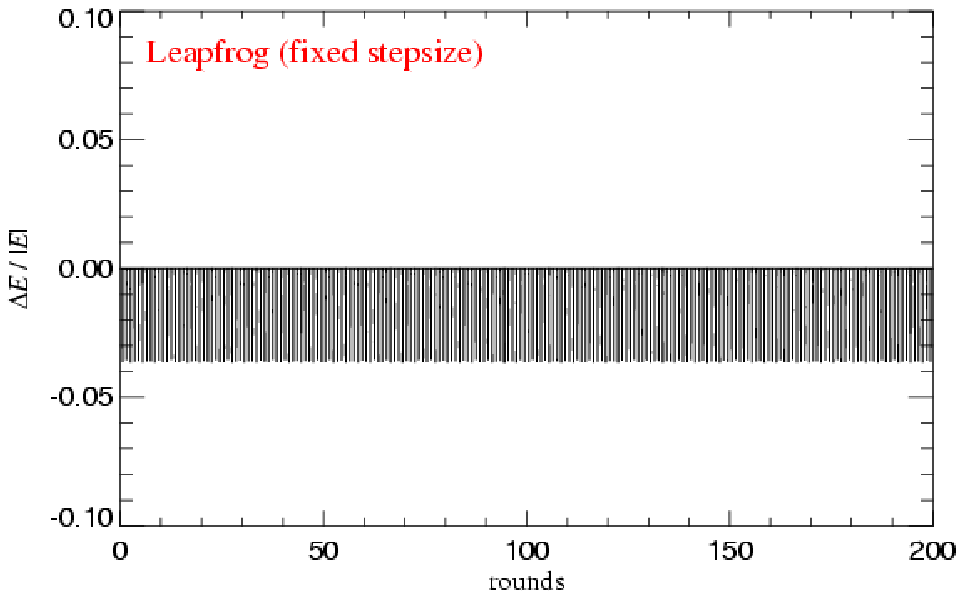




Even for rather large timesteps, the leapfrog maintains qualitatively correct behaviour without long-term secular trends

INTEGRATING THE KEPLER PROBLEM





What is the underlying mathematical reason for the very good long-term behaviour of the leapfrog ?

HAMILTONIAN SYSTEMS AND SYMPLECTIC INTEGRATION

$$H(\mathbf{p}_1, \ldots, \mathbf{p}_n, \mathbf{x}_1, \ldots, \mathbf{x}_n) = \sum_i \frac{\mathbf{p}_i^2}{2m_i} + \frac{1}{2}\sum_{ij} m_i m_j \phi(\mathbf{x}_i - \mathbf{x}_j)$$

The Hamiltonian structure of the system can be preserved in the integration if each step is formulated as a *canonical transformation*. Such integration schemes are called *symplectic*.

Poisson bracket

$$\{A, B\} \equiv \sum_i \left(\frac{\partial A}{\partial \mathbf{x}_i}\frac{\partial B}{\partial \mathbf{p}_i} - \frac{\partial A}{\partial \mathbf{p}_i}\frac{\partial B}{\partial \mathbf{x}_i} \right)$$

Hamilton's equations

$$\frac{\mathrm{d}\mathbf{x}_i}{\mathrm{d}t} = \{\mathbf{x}_i, H\}$$

$$\frac{\mathrm{d}\mathbf{p}_i}{\mathrm{d}t} = \{\mathbf{p}_i, H\}$$

Hamilton operator

$$\mathbf{H}f \equiv \{f, H\}$$

System state vector

$$|t\rangle \equiv |\mathbf{x}_1(t), \ldots, \mathbf{x}_n(t), \mathbf{p}_1(t), \ldots, \mathbf{p}_n(t), t\rangle$$

Time evolution operator

$$|t_1\rangle = \mathbf{U}(t_1, t_0)\ |t_0\rangle$$

$$\mathbf{U}(t + \Delta t, t) = \exp\left(\int_t^{t+\Delta t} \mathbf{H}\,\mathrm{d}t \right)$$

The time evolution of the system is a continuous canonical transformation generated by the Hamiltonian.

Symplectic integration schemes can be generated by applying the idea of operating splitting to the Hamiltonian

THE LEAPFROG AS A SYMPLECTIC INTEGRATOR

Separable Hamiltonian

$$H = H_{\text{kin}} + H_{\text{pot}}$$

Drift- and Kick-Operators

$$\mathbf{D}(\Delta t) \equiv \exp\left(\int_t^{t+\Delta t} \mathrm{d}t\, \mathbf{H}_{\text{kin}}\right) = \begin{cases} \mathbf{p}_i & \mapsto & \mathbf{p}_i \\ \mathbf{x}_i & \mapsto & \mathbf{x}_i + \frac{\mathbf{p}_i}{m_i}\Delta t \end{cases}$$

$$\mathbf{K}(\Delta t) = \exp\left(\int_t^{t+\Delta t} \mathrm{d}t\, \mathbf{H}_{\text{pot}}\right) = \begin{cases} \mathbf{x}_i & \mapsto & \mathbf{x}_i \\ \mathbf{p}_i & \mapsto & \mathbf{p}_i - \sum_j m_i m_j \frac{\partial \phi(\mathbf{x}_{ij})}{\partial \mathbf{x}_i}\Delta t \end{cases}$$

The drift and kick operators are symplectic transformations of phase-space !

The Leapfrog

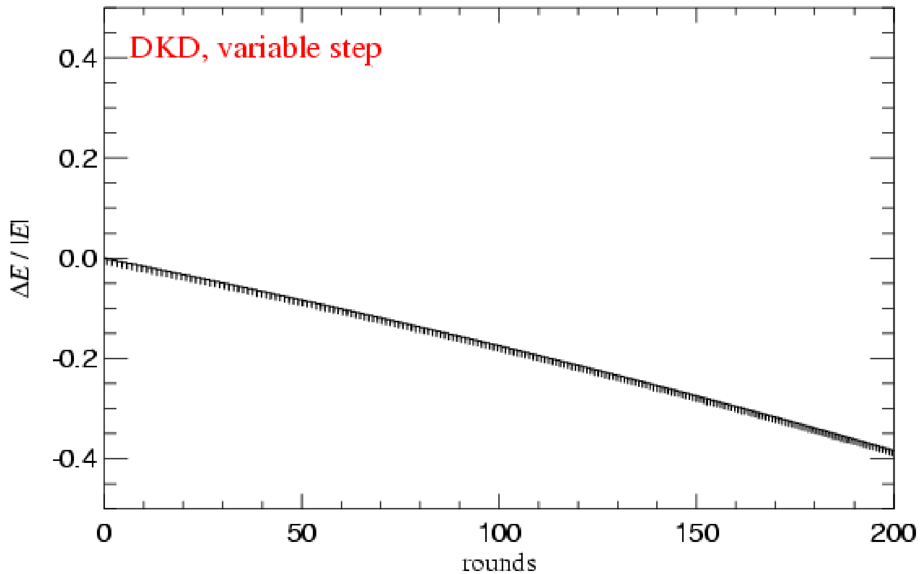
Drift-Kick-Drift: $$\tilde{\mathbf{U}}(\Delta t) = \mathbf{D}\left(\frac{\Delta t}{2}\right)\,\mathbf{K}(\Delta t)\,\mathbf{D}\left(\frac{\Delta t}{2}\right)$$

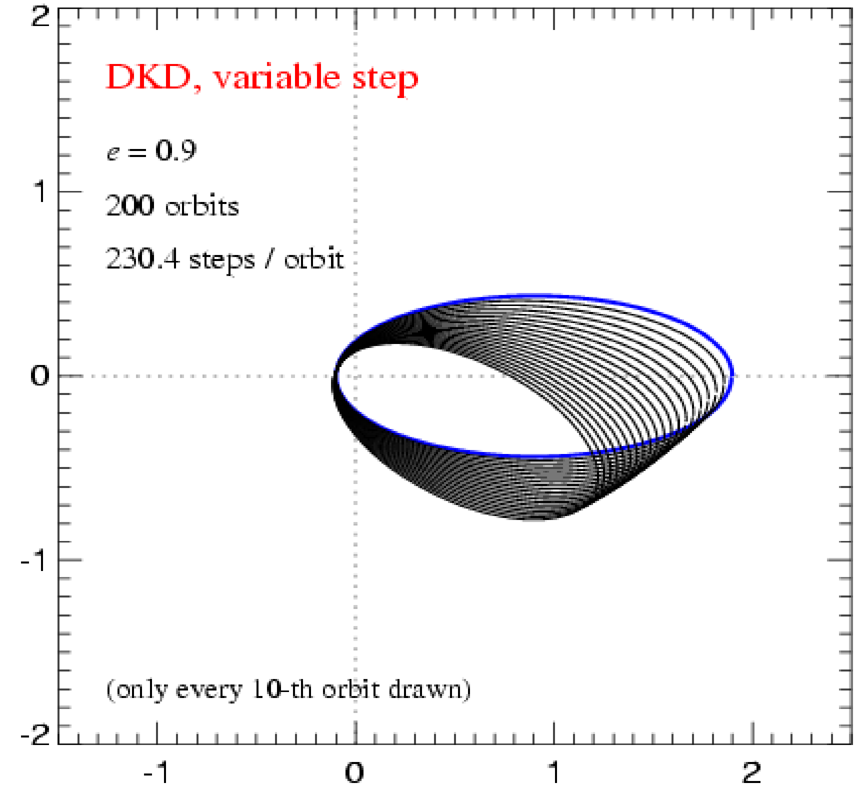
Kick-Drift-Kick: $$\tilde{\mathbf{U}}(\Delta t) = \mathbf{K}\left(\frac{\Delta t}{2}\right)\,\mathbf{D}(\Delta t)\,\mathbf{K}\left(\frac{\Delta t}{2}\right)$$

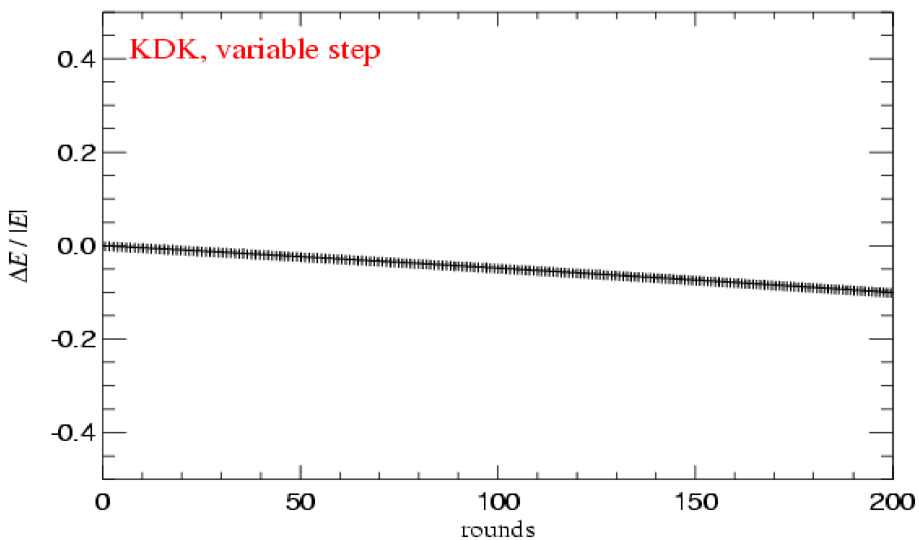
Hamiltonian of the numerical system: $$\tilde{H} = H + H_{\text{err}} \qquad H_{\text{err}} = \frac{\Delta t^2}{12}\left\{\left\{H_{\text{kin}}, H_{\text{pot}}\right\}, H_{\text{kin}} + \frac{1}{2}H_{\text{pot}}\right\} + \mathcal{O}(\Delta t^3)$$

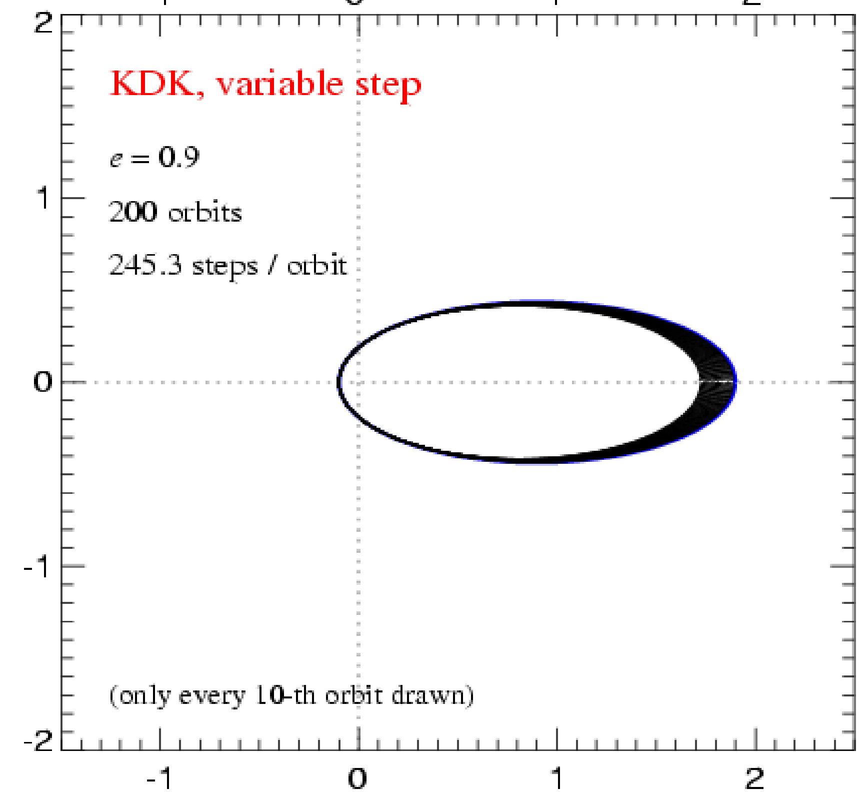
When an adaptive timestep is used, much of the symplectic advantage is lost

INTEGRATING THE KEPLER PROBLEM





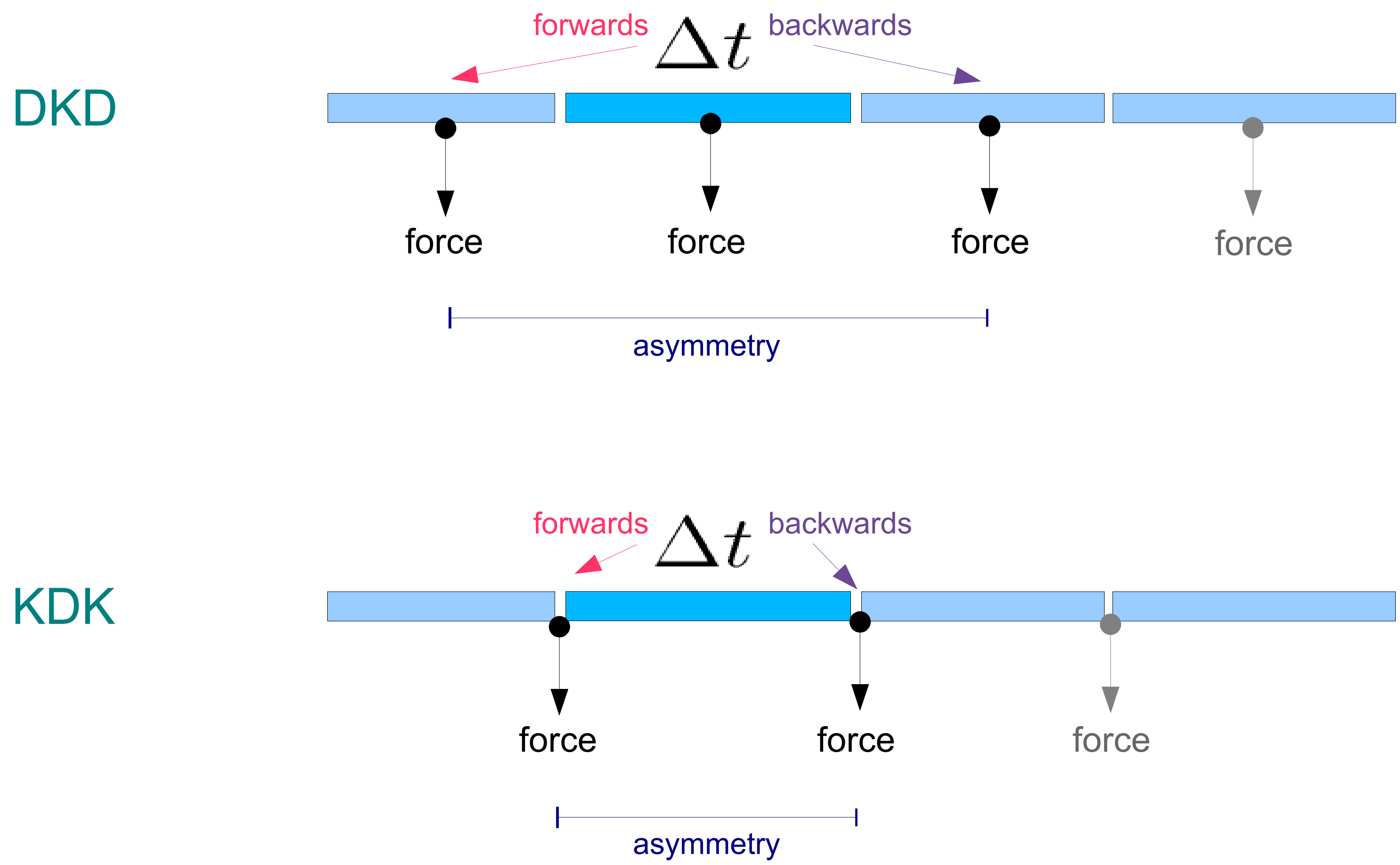




→ Going to KDK reduces the error by a factor 4, at the same cost !

For periodic motion with adaptive timesteps, the DKD leapfrog shows more time-asymmetry than the KDK variant

LEAPFROG WITH ADAPTIVE TIMESTEP



Collisionless dynamics in an expanding universe is described by a Hamiltonian system

THE HAMILTONIAN IN COMOVING COORDINATES

Conjugate momentum $\mathbf{p} = a^2 \dot{\mathbf{x}}$

$$H(\mathbf{p}_1, \ldots, \mathbf{p}_n, \mathbf{x}_1, \ldots, \mathbf{x}_n, t) = \sum_i \frac{\mathbf{p}_i^2}{2 m_i a(t)^2} + \frac{1}{2} \sum_{ij} \frac{m_i m_j \phi(\mathbf{x}_i - \mathbf{x}_j)}{a(t)}$$

Drift- and Kick operators

$$\mathbf{D}(t+\Delta t, t) = \exp\left(\int_t^{t+\Delta t} \mathrm{d}t\, \mathbf{H}_{\mathrm{kin}}\right) = \begin{cases} \mathbf{p}_i & \mapsto \quad \mathbf{p}_i \\ \mathbf{x}_i & \mapsto \quad \mathbf{x}_i + \frac{\mathbf{p}_i}{m_i} \boxed{\int_t^{t+\Delta t} \frac{\mathrm{d}t}{a^2}} \end{cases}$$

$$\mathbf{K}(t+\Delta t, t) = \exp\left(\int_t^{t+\Delta t} \mathrm{d}t\, \mathbf{H}_{\mathrm{pot}}\right) = \begin{cases} \mathbf{x}_i & \mapsto \quad \mathbf{x}_i \\ \mathbf{p}_i & \mapsto \quad \mathbf{p}_i - \sum_j m_i m_j \frac{\partial \phi(\mathbf{x}_{ij})}{\partial \mathbf{x}_i} \boxed{\int_t^{t+\Delta t} \frac{\mathrm{d}t}{a}} \end{cases}$$

Choice of timestep

For linear growth, fixed step in log(a) appears most appropriate... → timestep is then a constant fraction of the Hubble time

$$\Delta t = \frac{\Delta \log a}{H(a)}$$