Time integration issues

Time integration methods

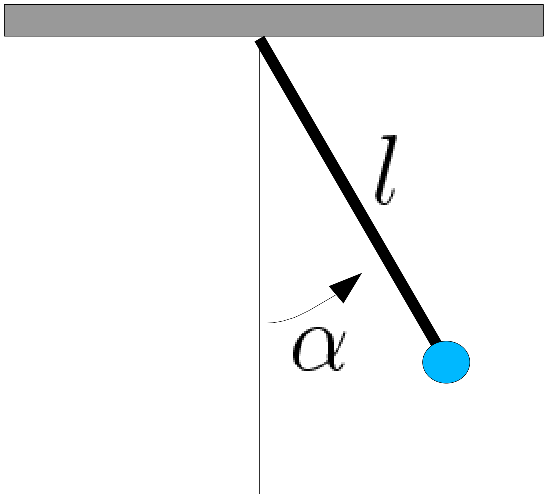
Want to numerically integrate an **ordinary differential equation** (ODE)

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

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 non, **explicit method**
- The error in a single step is O(Δt^2), 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}

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

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

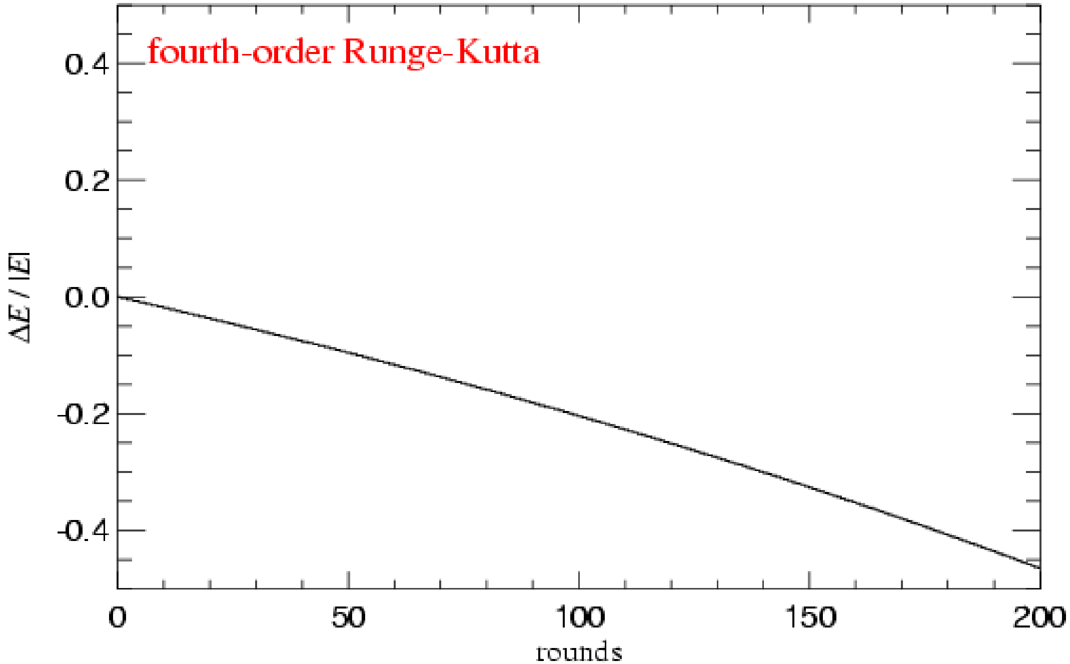
"Kick-Drift-Kick" version

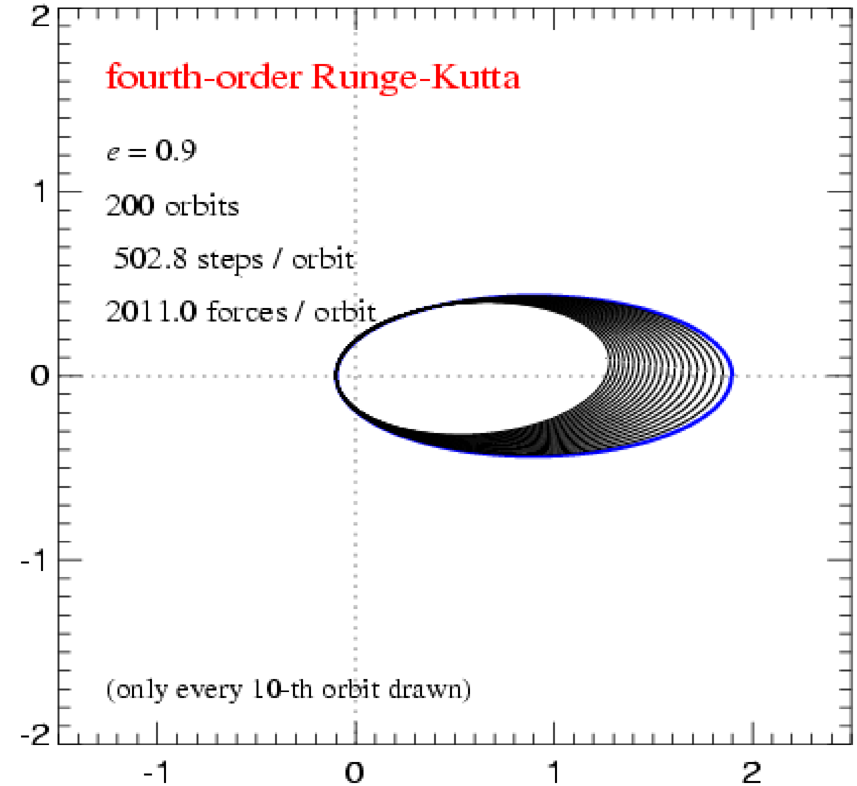
$$
\begin{aligned}
v_{n+\frac{1}{2}} &= v_n + f(x_n)\frac{\Delta t}{2} \\
x_{n+1} &= x_n + v_{n+\frac{1}{2}} \frac{\Delta t}{2} \\
v_{n+1} &= v_{n+\frac{1}{2}} + f(x_{n+1})\frac{\Delta t}{2}
\end{aligned}
$$

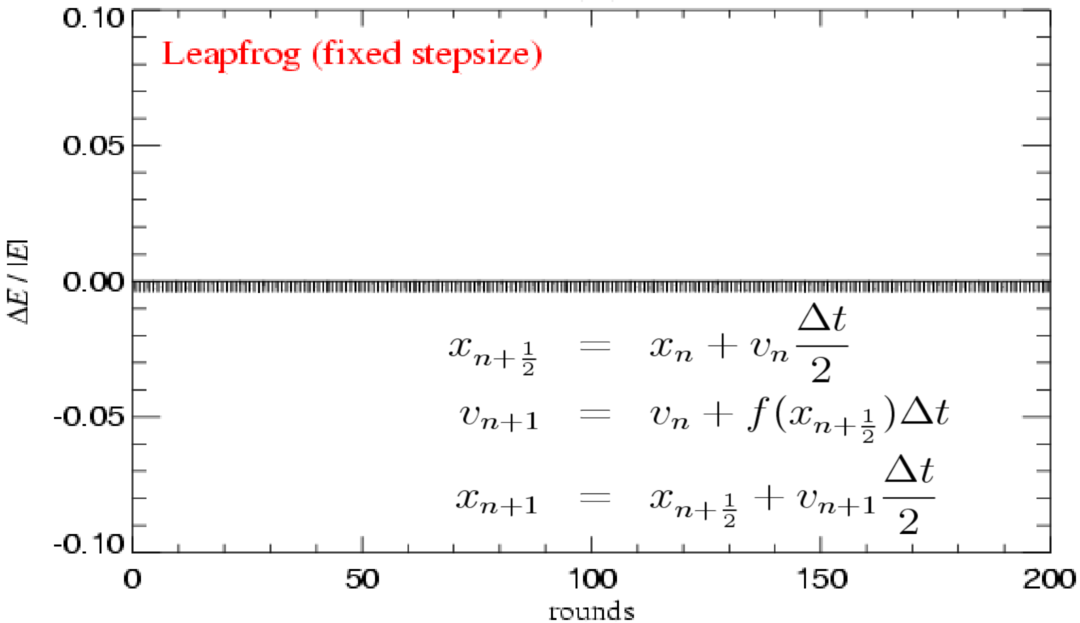
- **2nd order accurate**
- **symplectic**
- can be rewritten into time-centred formulation

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

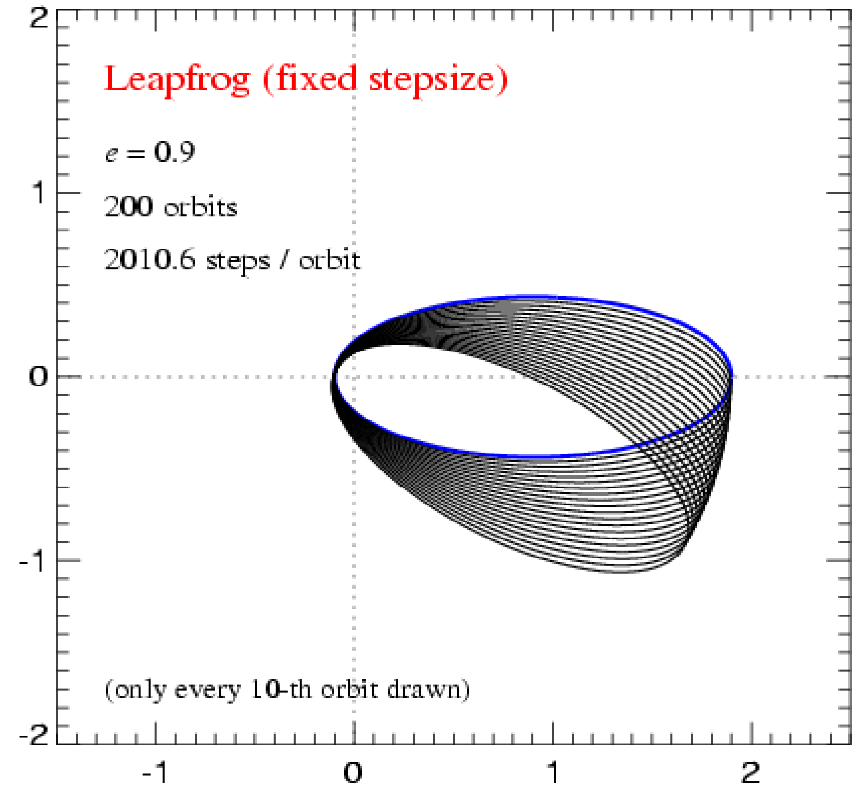
INTEGRATING THE KEPLER PROBLEM





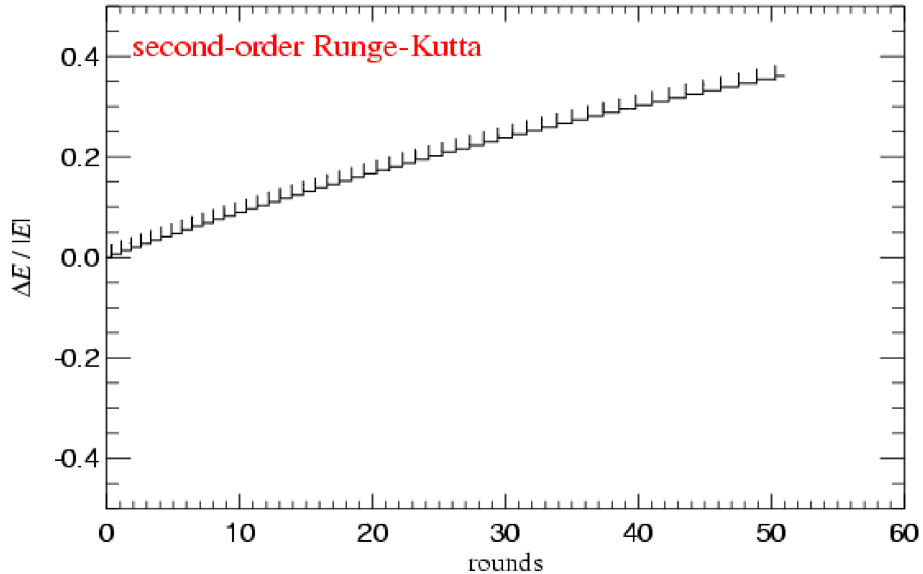


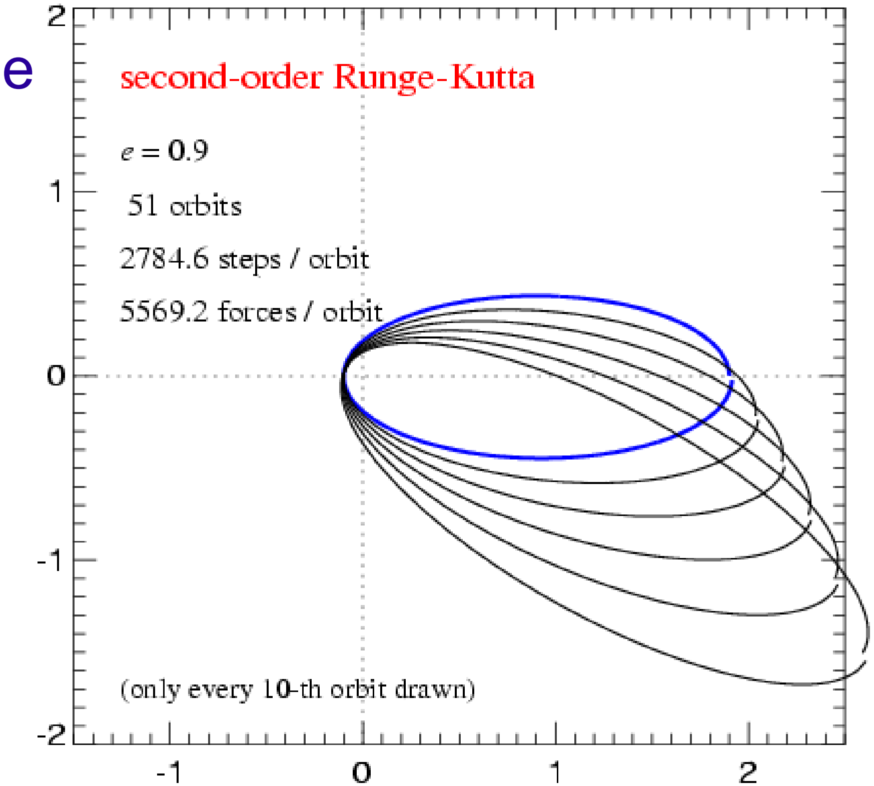
$$x_{n+\frac{1}{2}} = x_n + v_n \frac{\Delta t}{2}$$
$$v_{n+1} = v_n + f(x_{n+\frac{1}{2}})\Delta t$$
$$x_{n+1} = x_{n+\frac{1}{2}} + v_{n+1} \frac{\Delta t}{2}$$

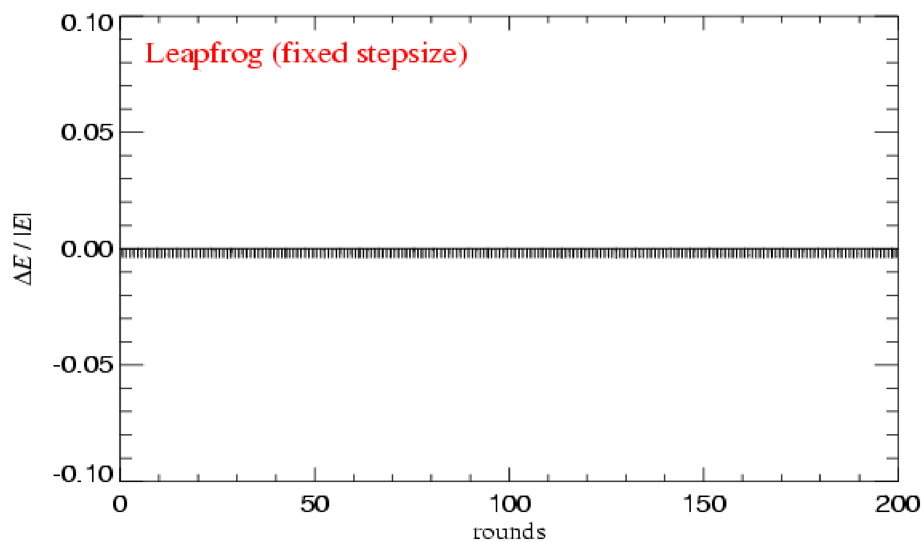


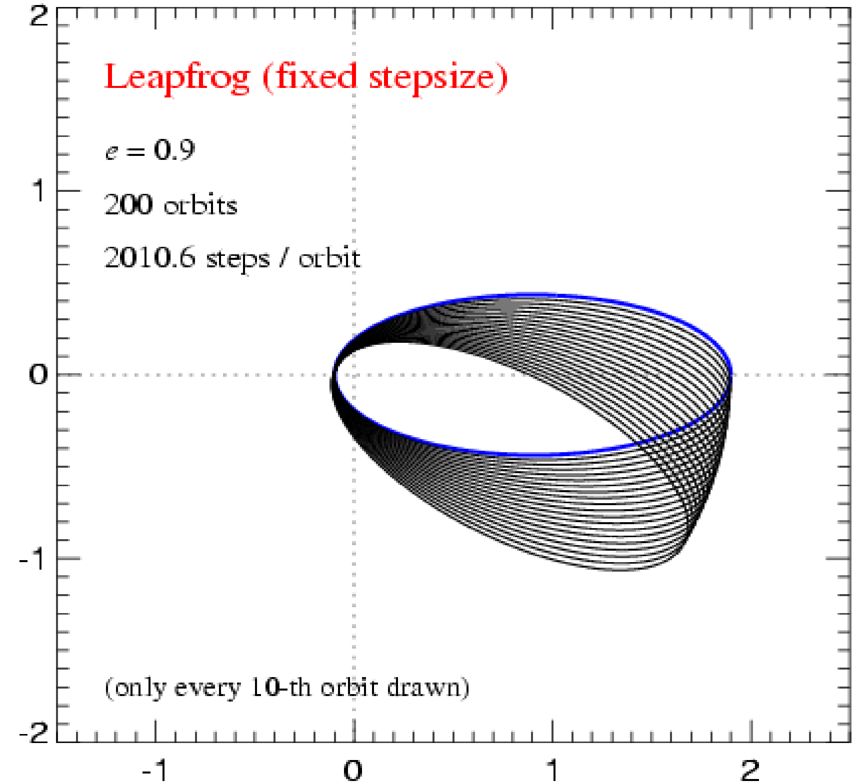
When compared with an integrator of the same order, the leapfrog is highly superior

INTEGRATING THE KEPLER PROBLEM



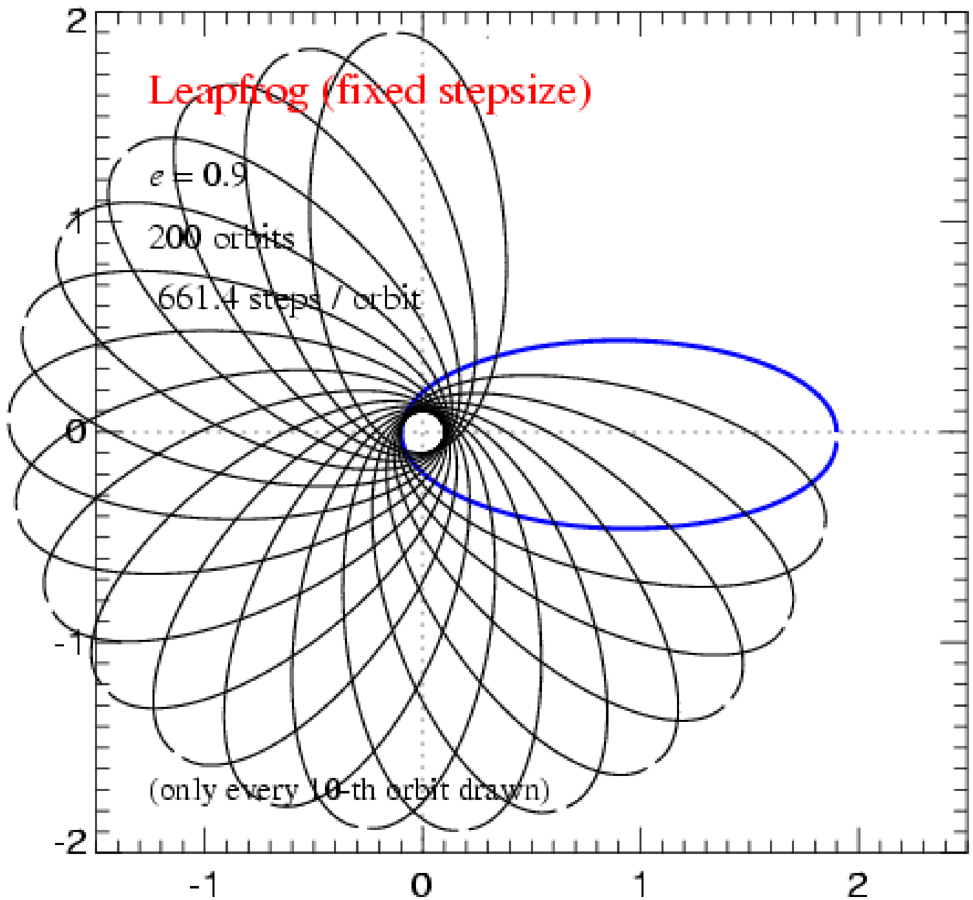


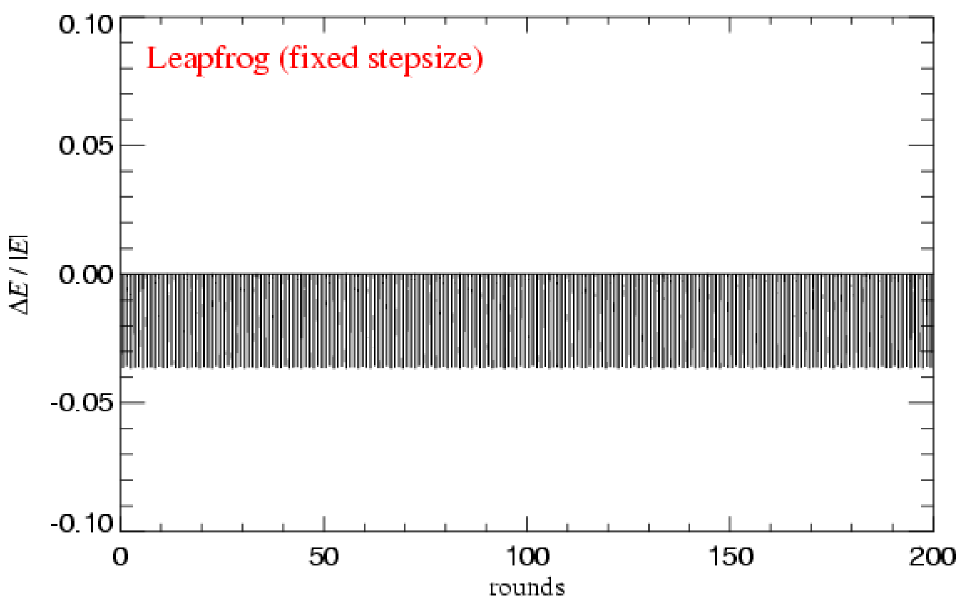




Even for rather large timesteps, the leapfrog maintains qualitatively correct behaviour without long-term secular trends

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

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

If the integration scheme introduces non-Hamiltonian perturbations, a completely different long-term behaviour results.

The Hamiltonian structure of the system can be preserved in the integration if each step is formulated as a *canoncial 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

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

Drift- and Kick-Operators

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

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

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:

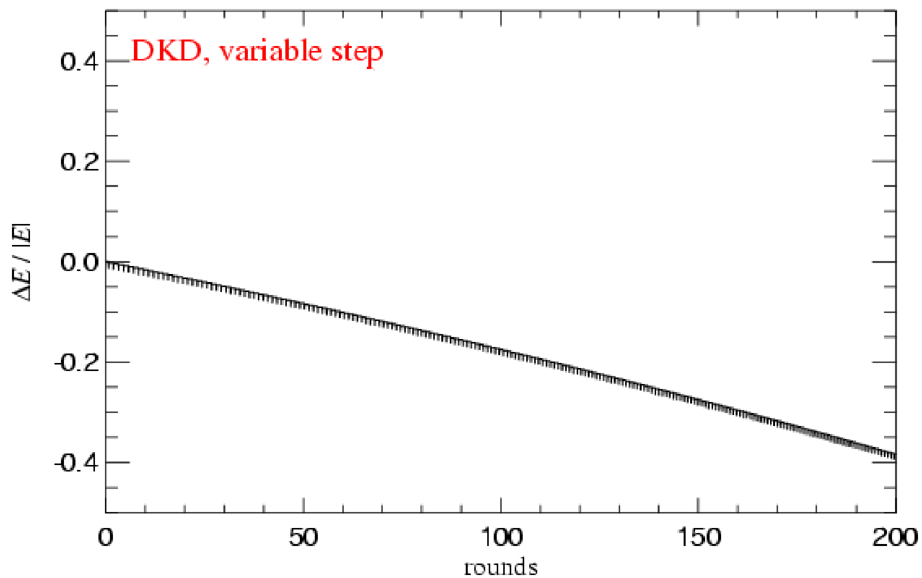
$$\tilde{\mathbf{U}}(\Delta t) = \mathbf{K}\left(\frac{\Delta t}{2}\right)\,\mathbf{D}(\Delta t)\,\mathbf{K}\left(\frac{\Delta t}{2}\right)$$

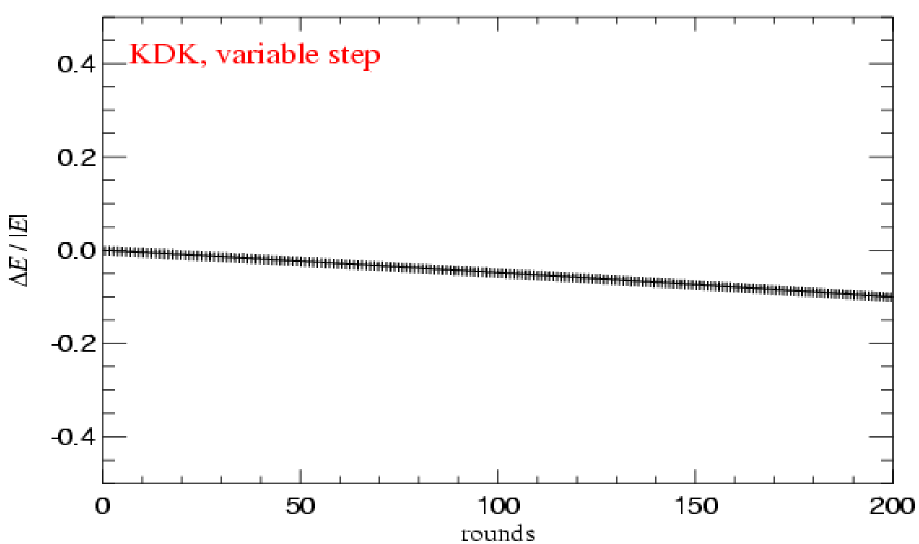
Hamiltonian of the numerical system:

$$\tilde{H} = H + H_{\rm err} \qquad H_{\rm err} = \frac{\Delta t^2}{12}\left\{\left\{H_{\rm kin}, H_{\rm pot}\right\}, H_{\rm kin} + \frac{1}{2}H_{\rm pot}\right\} + \mathcal{O}(\Delta t^3)$$

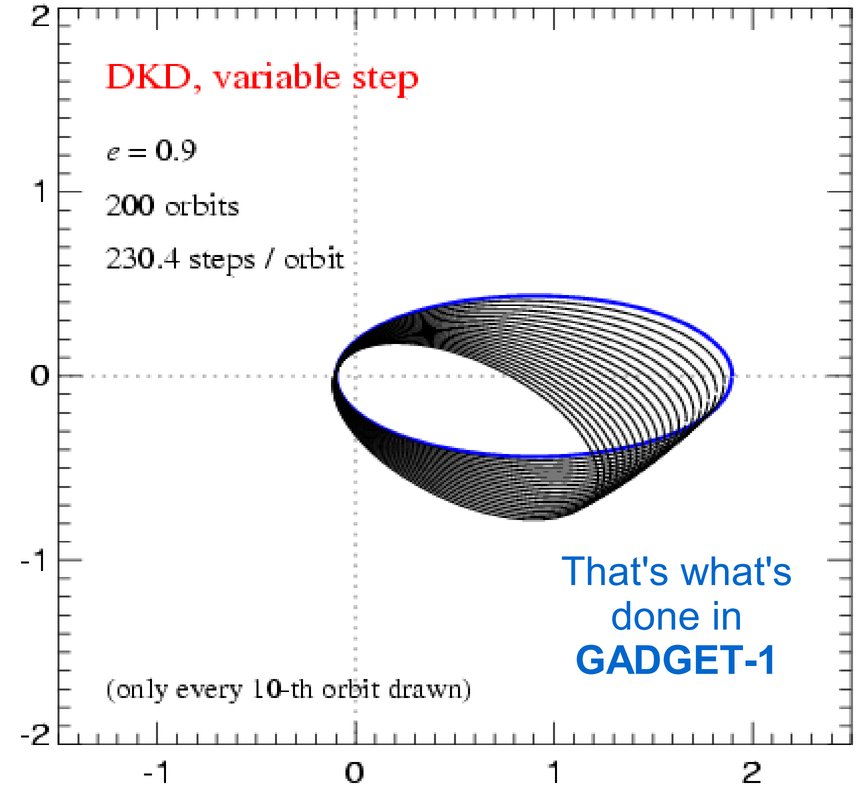
When an adaptive timestep is used, much of the symplectic advantage is lost

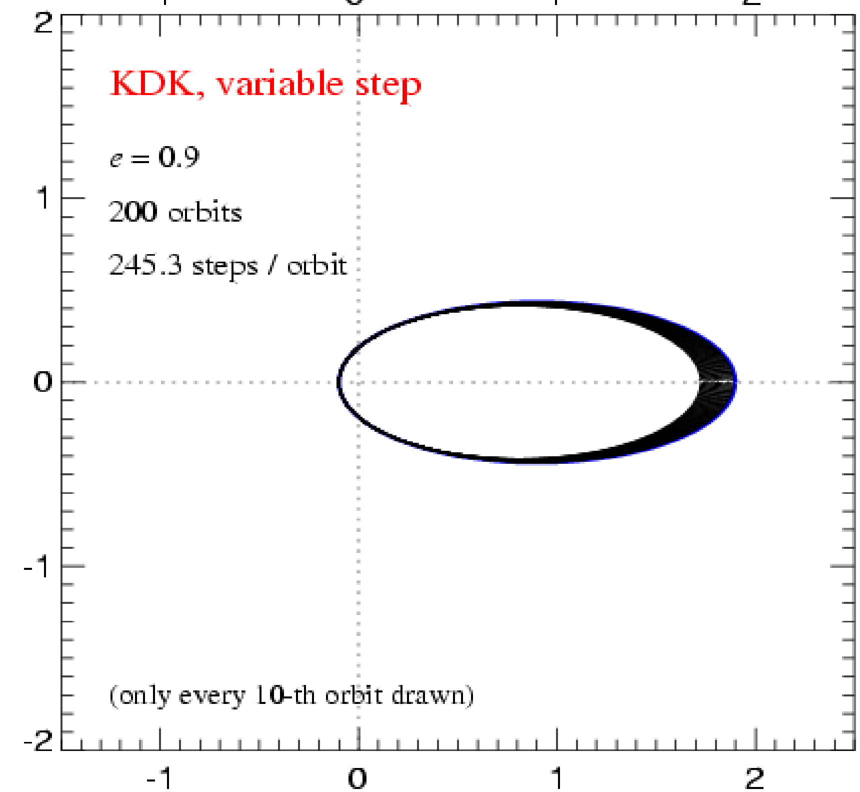
INTEGRATING THE KEPLER PROBLEM





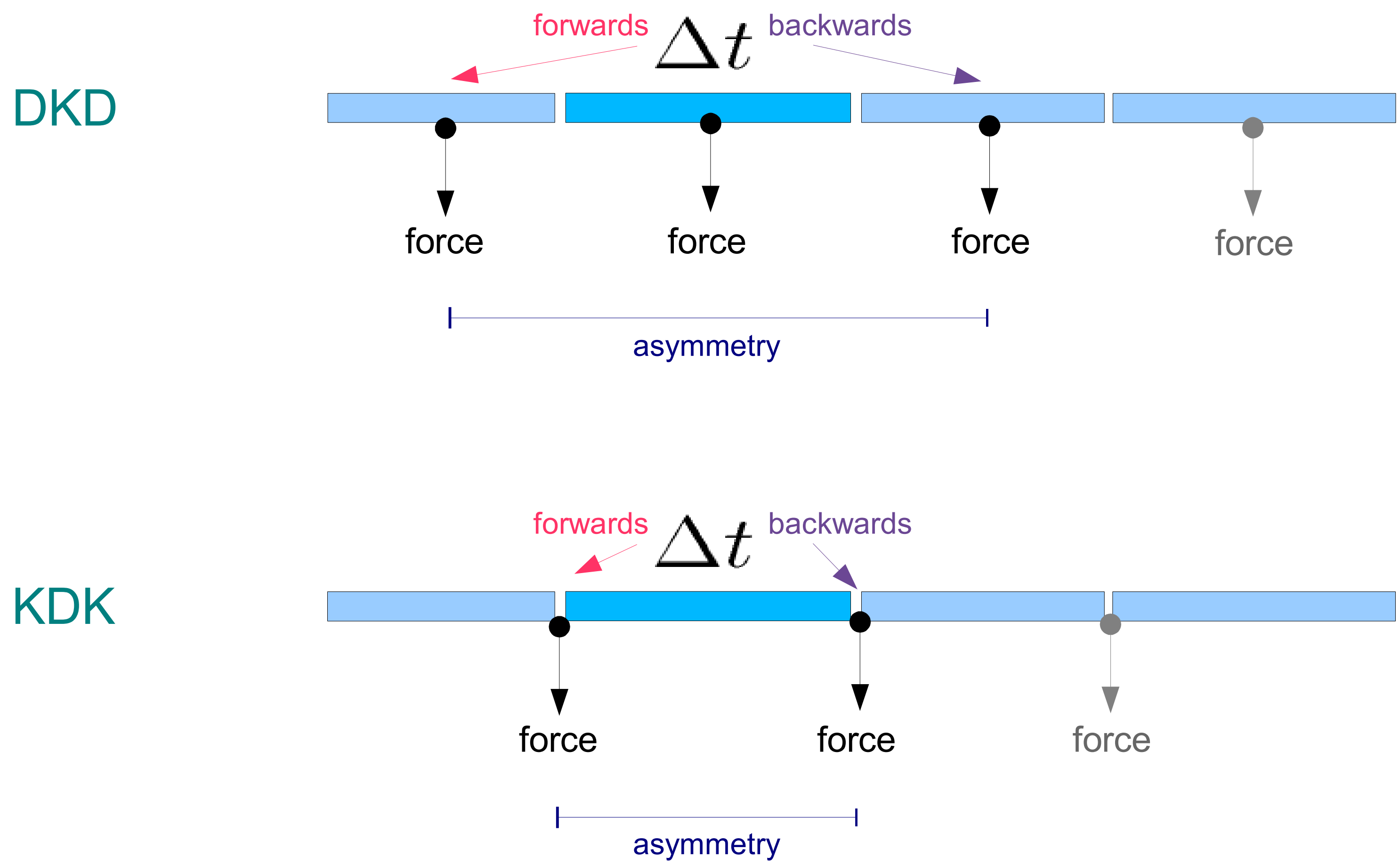
→ Going to KDK reduces the error by a factor 4, at the same cost !





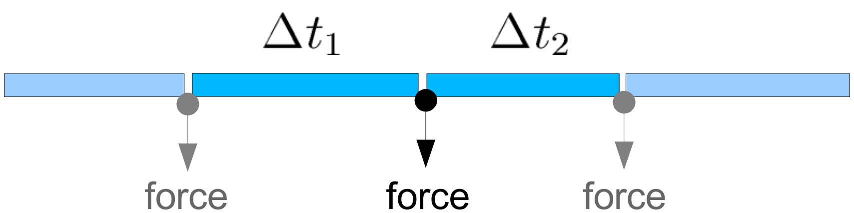
For periodic motion with adaptive timesteps, the DKD leapfrog shows more time-asymmetry than the KDK variant

LEAPFROG WITH ADAPTIVE TIMESTEP

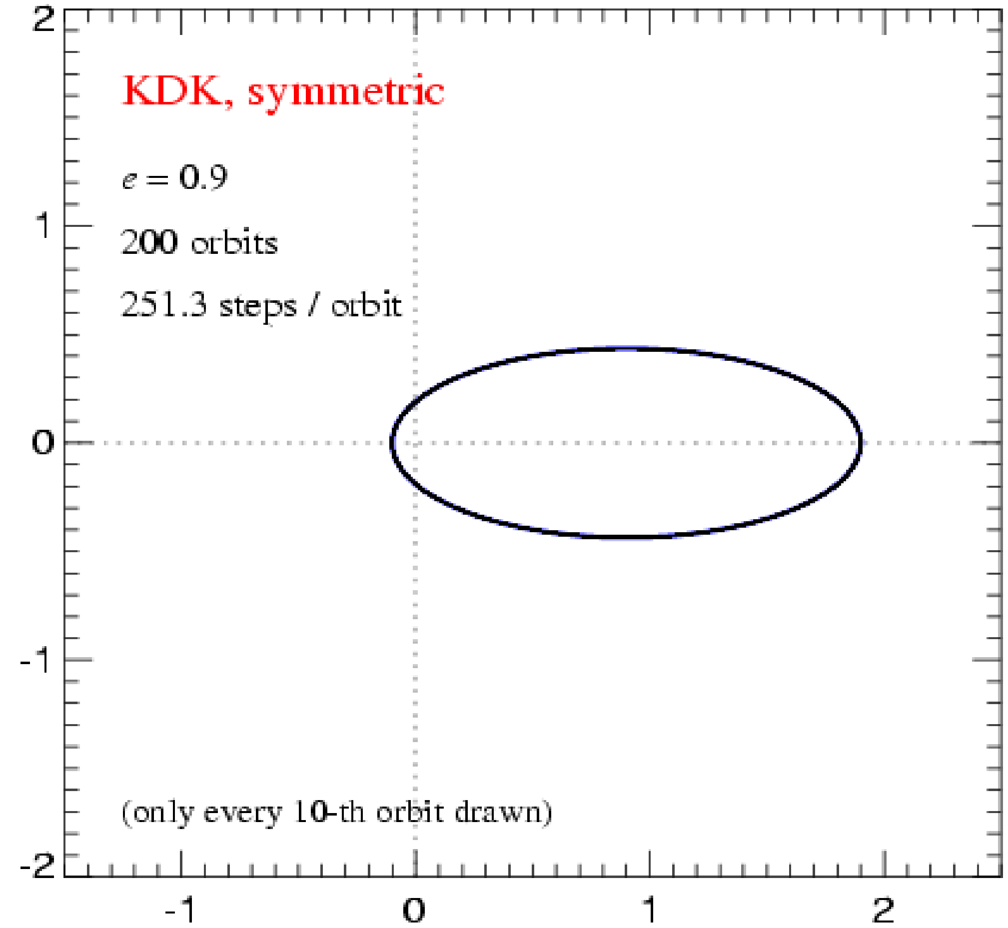


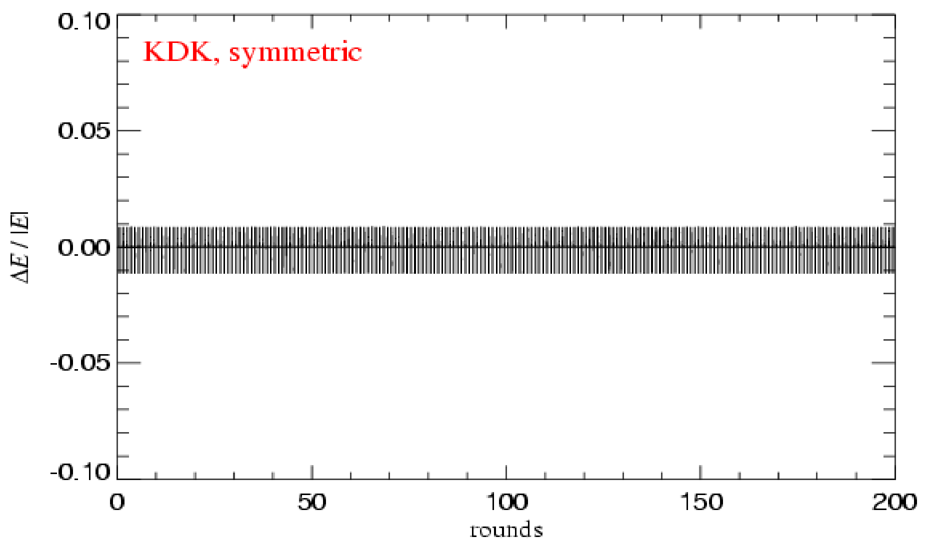
The key for obtaining better long-term behaviour is to make the choice of timestep time-reversible

INTEGRATING THE KEPLER PROBLEM



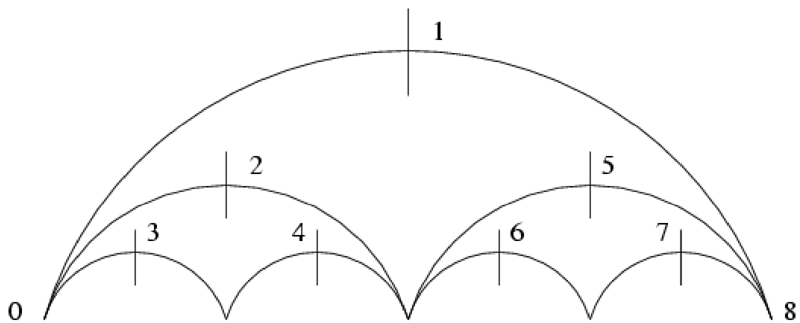
$$\frac{\Delta t_1 + \Delta t_2}{2} = f(\mathbf{a}, \mathbf{v})$$



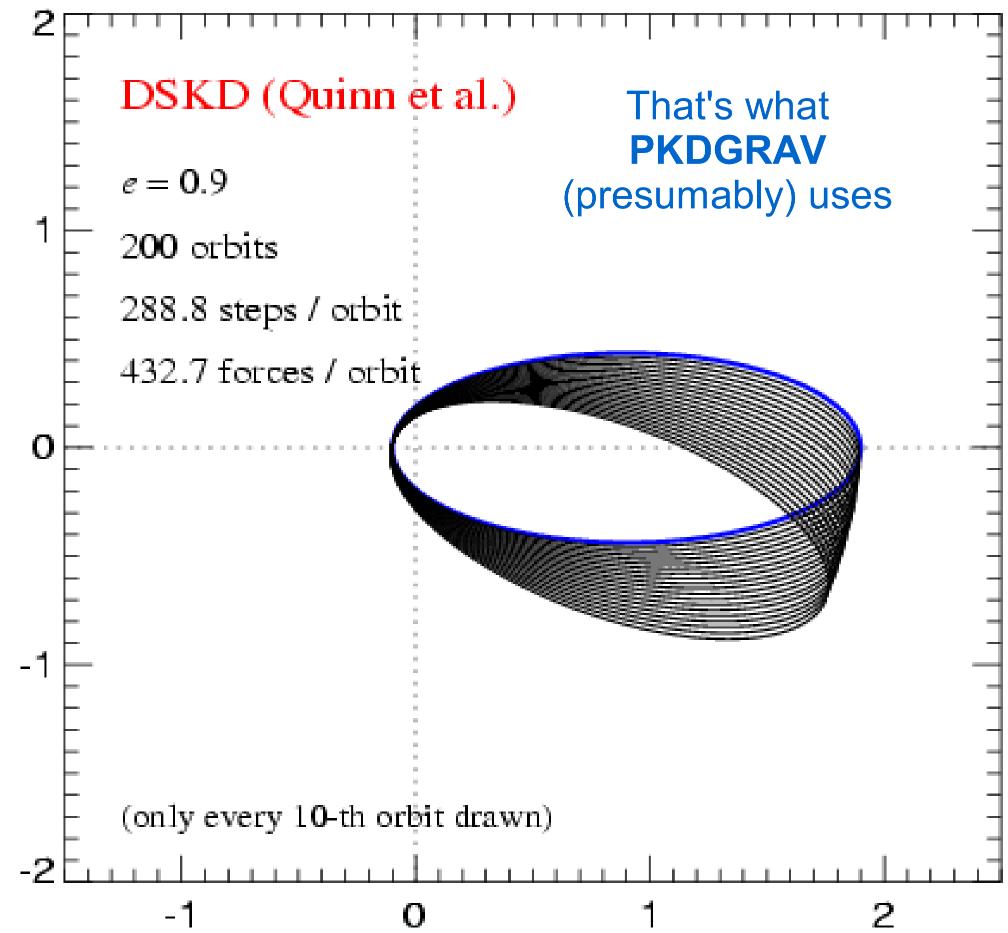


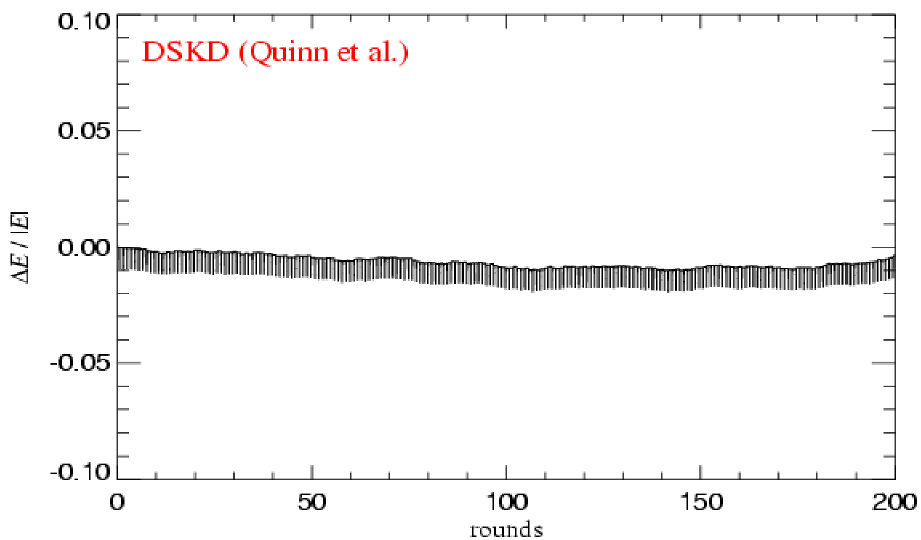
Symmetric behaviour can be obtained by using an implicit timestep criterion that depends on the end of the timestep

INTEGRATING THE KEPLER PROBLEM



Quinn et al. (1997)



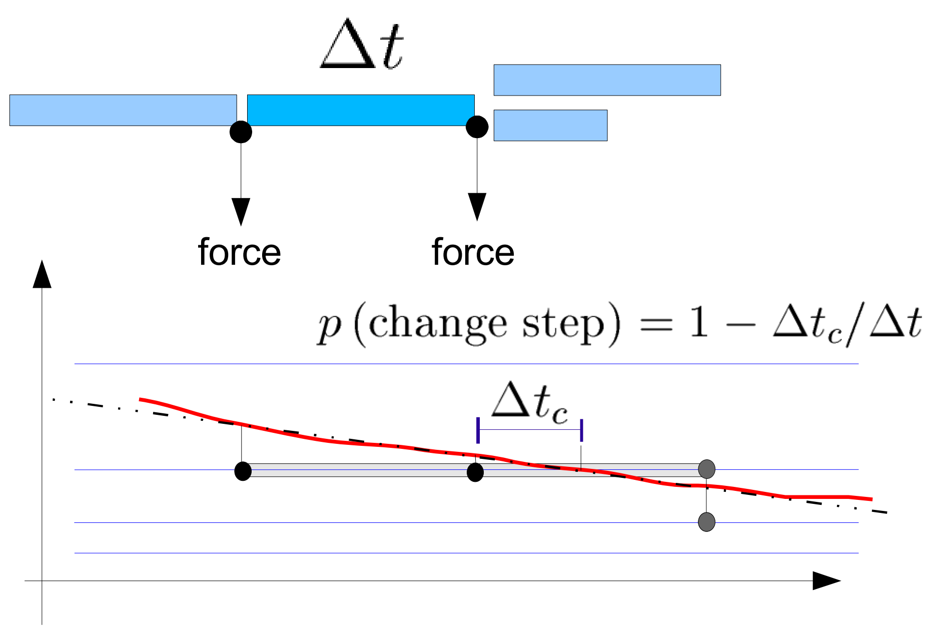


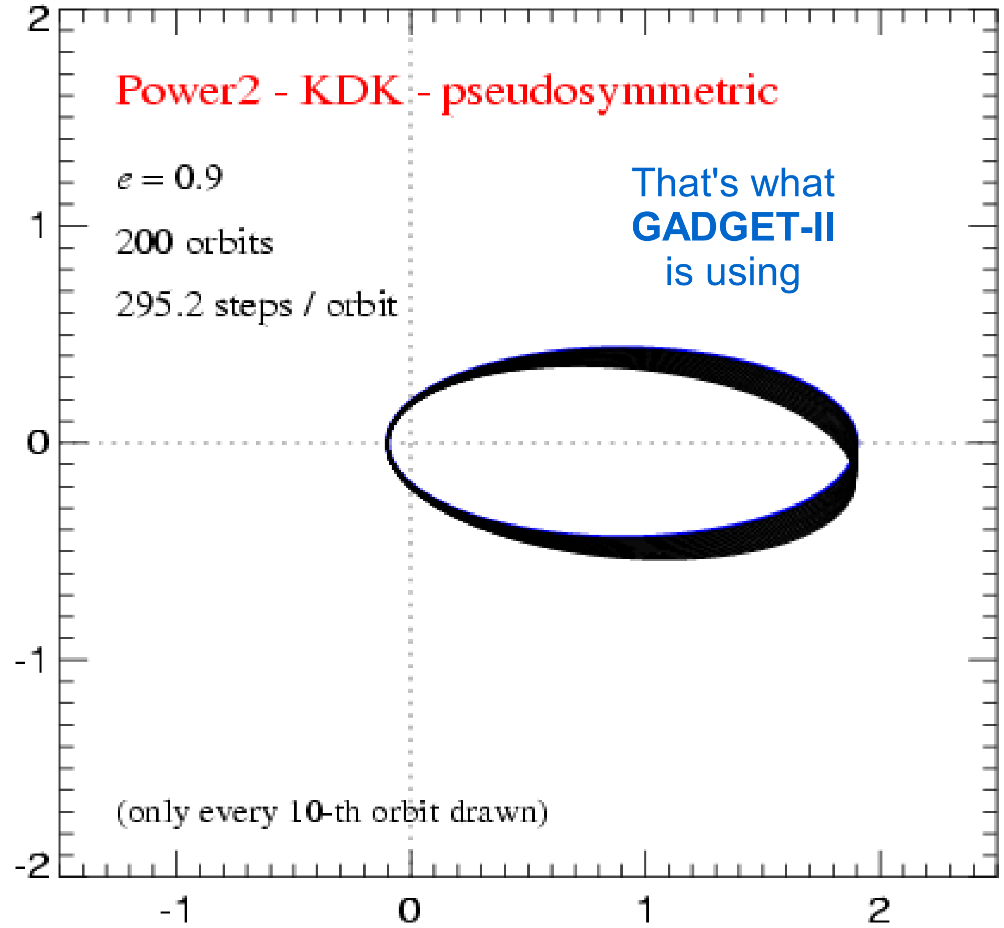
- Force evaluations have to be thrown away in this scheme
- reversibility is only approximatively given
- Requires back-wards drift of system - difficult to combine with SPH

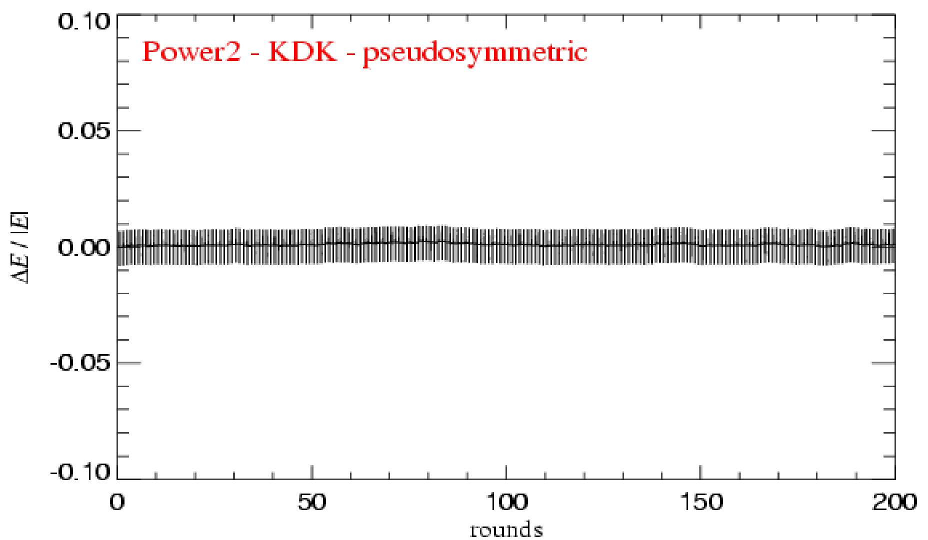
Pseudo-symmetric behaviour can be obtained by making the evolution of the expectation value of the numerical Hamiltonian time reversible

INTEGRATING THE KEPLER PROBLEM

KDK scheme







Gives the best result at a given number of force evaluations.

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

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

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

Choice of timestep

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

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

The force-split can be used to construct a symplectic integrator where long- and short-range forces are treated independently

TIME INTEGRATION FOR LONG AND SHORT-RANGE FORCES

Separate the potential into a long-range and a short-range part:

$$H = \sum_i \frac{\mathbf{p}_i^2}{2m_i a(t)^2} + \frac{1}{2}\sum_{ij} \frac{m_i m_j\, \varphi_{\rm sr}(\mathbf{x}_i - \mathbf{x}_j)}{a(t)} + \frac{1}{2}\sum_{ij} \frac{m_i m_j\, \varphi_{\rm lr}(\mathbf{x}_j - \mathbf{x}_j)}{a(t)}$$

The short-range force can then be evolved in a symplectic way on a smaller timestep than the long range force:

$$\tilde{\mathbf{U}}(\Delta t) = \mathbf{K}_{\rm lr}\left(\frac{\Delta t}{2}\right)\left[\mathbf{K}_{\rm sr}\left(\frac{\Delta t}{2m}\right)\mathbf{D}\left(\frac{\Delta t}{m}\right)\mathbf{K}_{\rm sr}\left(\frac{\Delta t}{2m}\right)\right]^m \mathbf{K}_{\rm lr}\left(\frac{\Delta t}{2}\right)$$