Time integration issues
Time integration methods

Want to numerically integrate an ordinary differential equation (ODE)

\[ \dot{y} = f(y) \]

Note: \( y \) can be a vector

**Example:** Simple pendulum

\[ \ddot{\alpha} = -\frac{g}{l} \sin \alpha \]

\[ y_0 \equiv \alpha \quad y_1 \equiv \dot{\alpha} \]

\[ \dot{y} = f(y) = \begin{pmatrix} y_1 \\ -\frac{g}{l} \sin y_0 \end{pmatrix} \]

A numerical approximation to the ODE is a set of values 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 \( O(\Delta t^2) \), 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 \( y_{n+1} \)
Implicit mid-point rule

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

- 2\textsuperscript{nd} order accurate
- Time-symmetric, in fact \textbf{symplectic}
- But still implicit...

Runge-Kutta methods

whole class of integration methods

2\textsuperscript{nd} order accurate

\[
\begin{align*}
    k_1 &= f(y_n) \\
    k_2 &= f(y_n + k_1 \Delta t) \\
    y_{n+1} &= y_n + \left( \frac{k_1 + k_2}{2} \right) \Delta t
\end{align*}
\]

4\textsuperscript{th} order accurate.

\[
\begin{align*}
    k_1 &= f(y_n, t_n) \\
    k_2 &= f(y_n + k_1 \Delta t/2, t_n + \Delta t/2) \\
    k_3 &= f(y_n + k_2 \Delta t/2, t_n + \Delta t/2) \\
    k_4 &= f(y_n + k_3 \Delta t/2, t_n + \Delta t) \\
    y_{n+1} &= y_n + \left( \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} \right) \Delta t
\end{align*}
\]
The Leapfrog

For a second order ODE: \[ \ddot{x} = f(x) \]

<table>
<thead>
<tr>
<th>“Drift-Kick-Drift” version</th>
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</tr>
</thead>
<tbody>
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<td>(x_{n+\frac{1}{2}}) = (x_n + v_n \frac{\Delta t}{2})</td>
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- \(2^{\text{nd}}\) order accurate
- symplectic
- can be rewritten into time-centred formulation
The leapfrog is behaving much better than one might expect...

INTEGRATING THE KEPLER PROBLEM

\[ \Delta E / E = \begin{cases} \text{fourth-order Runge-Kutta} \\ \text{Leapfrog (fixed stepsize)} \end{cases} \]

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

fourth-order Runge-Kutta
\[ e = 0.9 \]
200 orbits
502.8 steps / orbit
2011.0 forces / orbit

(only every 10-th orbit drawn)

Leapfrog (fixed stepsize)
\[ e = 0.9 \]
200 orbits
2010.6 steps / orbit

(only every 10-th orbit drawn)
When compared with an integrator of the same order, the leapfrog is highly superior.

INTEGRATING THE KEPLER PROBLEM

(second-order Runge-Kutta)

e = 0.9
51 orbits
2784.6 steps/orbit
5569.2 forces/orbit

(only every 10-th orbit drawn)

Leapfrog (fixed stepsizes)

e = 0.9
200 orbits
2010.6 steps/orbit

(only every 10-th orbit drawn)
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

\[ H(p_1, \ldots, p_n, x_1, \ldots, x_n) = \sum_i \frac{p_i^2}{2m_i} + \frac{1}{2} \sum_{ij} m_i m_j \phi(x_i - x_j) \]

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 \textit{canonical} transformation. Such integration schemes are called \textit{symplectic}.

Poisson bracket

\[ \{A, B\} \equiv \sum_i \left( \frac{\partial A}{\partial x_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial x_i} \right) \]

Hamilton's equations

\[ \frac{dx_i}{dt} = \{x_i, H\} \]
\[ \frac{dp_i}{dt} = \{p_i, H\} \]

Hamilton operator

\[ Hf \equiv \{f, H\} \]

System state vector

\[ |t\rangle \equiv |x_1(t), \ldots, x_n(t), p_1(t), \ldots, p_n(t), t\rangle \]

Time evolution operator

\[ |t_1\rangle = U(t_1, t_0) \ |t_0\rangle \]
\[ U(t + \Delta t, t) = \exp \left( \int_t^{t+\Delta t} H \ dt \right) \]

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**

\[ D(\Delta t) \equiv \exp \left( \int_t^{t+\Delta t} dt \, H_{\text{kin}} \right) = \begin{cases} p_i & \mapsto p_i \\ x_i & \mapsto x_i + \frac{p_i}{m_i} \Delta t \end{cases} \]

\[ K(\Delta t) = \exp \left( \int_t^{t+\Delta t} dt \, H_{\text{pot}} \right) = \begin{cases} x_i & \mapsto x_i \\ p_i & \mapsto p_i - \sum_j m_i m_j \frac{\partial \phi(x_{ij})}{\partial x_i} \Delta t \end{cases} \]

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

**The Leapfrog**

Drift-Kick-Drift:

\[ \tilde{U}(\Delta t) = D \left( \frac{\Delta t}{2} \right) \ K(\Delta t) \ D \left( \frac{\Delta t}{2} \right) \]

Kick-Drift-Kick:

\[ \tilde{U}(\Delta t) = K \left( \frac{\Delta t}{2} \right) \ D(\Delta t) \ K \left( \frac{\Delta t}{2} \right) \]

**Hamiltonian of the numerical system:**

\[ \tilde{H} = H + H_{\text{err}} \quad H_{\text{err}} = \frac{\Delta t^2}{12} \left\{ \left\{ H_{\text{kin}}, H_{\text{pot}} \right\} , H_{\text{kin}} + \frac{1}{2} H_{\text{pot}} \right\} + \mathcal{O}(\Delta t^3) \]
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 TIME STEP**

### DKD

- **Δt**
- **Forwards** and **backwards** arrows indicate direction of progression.
- **Asymmetry** is depicted between steps.

### KDK

- **Δt**
- **Forwards** and **backwards** arrows indicate direction of progression.
- **Asymmetry** is depicted between steps.
The key for obtaining better long-term behaviour is to make the choice of timestep time-reversible.

INTEGRATING THE KEPLER PROBLEM

\[ \Delta t_1 + \Delta t_2 = f(a, v) \]
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

That's what PKDGRAV (presumably) uses
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

\[
p (\text{change step}) = 1 - \frac{\Delta t_c}{\Delta t}
\]

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 \( p = a^2 \dot{x} \)

\[
H(p_1, \ldots, p_n, x_1, \ldots, x_n, t) = \sum_i \frac{p_i^2}{2m_i a(t)^2} + \frac{1}{2} \sum_{ij} m_i m_j \phi(x_i - x_j)
\]

Drift- and Kick operators

\[
D(t + \Delta t, t) = \exp \left( \int_t^{t+\Delta t} dt \, H_{\text{kin}} \right) = \begin{cases} 
  p_i &\mapsto p_i \\
  x_i &\mapsto x_i + \frac{p_i}{m_i} \int_t^{t+\Delta t} \frac{dt}{a(t)}
\end{cases}
\]

\[
K(t + \Delta t, t) = \exp \left( \int_t^{t+\Delta t} dt \, H_{\text{pot}} \right) = \begin{cases} 
  x_i &\mapsto x_i \\
  p_i &\mapsto p_i - \sum_j m_i m_j \frac{\partial \phi(x_{ij})}{\partial x_i} \int_t^{t+\Delta t} \frac{dt}{a(t)}
\end{cases}
\]

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:

\[
H = \sum_i \frac{p_i^2}{2m_i a(t)^2} + \frac{1}{2} \sum_{ij} m_i m_j \varphi_{sr}(x_i - x_j) a(t) + \frac{1}{2} \sum_{ij} m_i m_j \varphi_{lr}(x_j - x_j) a(t)
\]

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

\[
\tilde{U}(\Delta t) = K_{lr} \left( \frac{\Delta t}{2} \right) \left[ K_{sr} \left( \frac{\Delta t}{2m} \right) D \left( \frac{\Delta t}{m} \right) K_{sr} \left( \frac{\Delta t}{2m} \right) \right]^m K_{lr} \left( \frac{\Delta t}{2} \right)
\]