Numerical solutions of classical equations of motion

Newton's laws govern the dynamics of

- Solar systems, galaxies,...
- Molecules in liquids, gases; often good approximation
  - quantum mechanics gives potentials
  - large (and even rather small) molecules move almost classically if the density is not too high
- "Everything that moves"

Almost no "real" systems can be solved analytically

- **Numerical integration of equations of motion**

One-dimensional motion

➢ A single "point particle" at x(t)

Equation of motion

$$\ddot{x}(t) = \frac{1}{m} F[x(t), \dot{x}(t), t]$$

Notation: velocity: $v(t) = \dot{x}(t)$

acceleration: $a(t) = \ddot{x}(t)$

Forces from: potential, damping (friction), driving (can be mix)

Rewrite second-order diff. eqv. as coupled first-order:

$$\dot{x}(t) = v(t)$$

$$\dot{v}(t) = a[x(t), v(t), t)]$$

Discretized time axis

$$t = t_0, t_1, \ldots, t_N, \quad t_{n+1} - t_n = \Delta_t$$

Start from given initial conditions: $v = v_0, \; x = x_0$

Simplest integration method: **Euler forward algorithm**

$$x_{n+1} = x_n + \Delta_t v_n$$
$$v_{n+1} = v_n + \Delta_t a_n$$

Step error: $O(\Delta_t^2)$

Fortran 90 implementations:

```
do i=1,nt
   t0=dt*(i-1)
   x1=x0+dt*v0
   v1=v0+dt*acc(x0,v0,t0)
   x0=x1; v0=v1
enddo
```

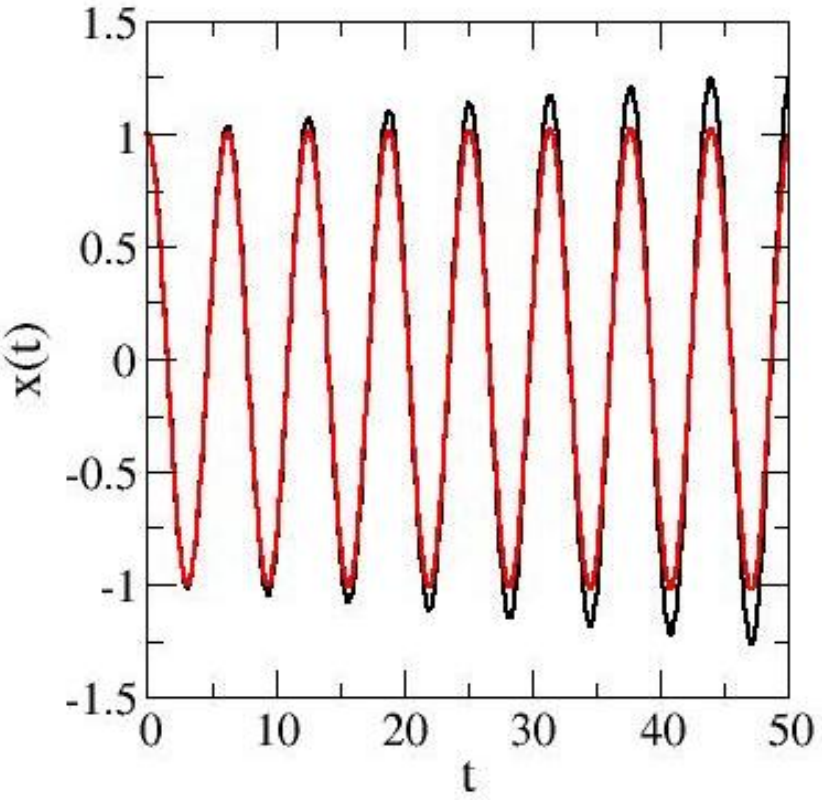
```
do i=1,nt
   t=dt*(i-1)
   a=acc(x,v,t)
   x=x+dt*v
   v=v+dt*a
enddo
```

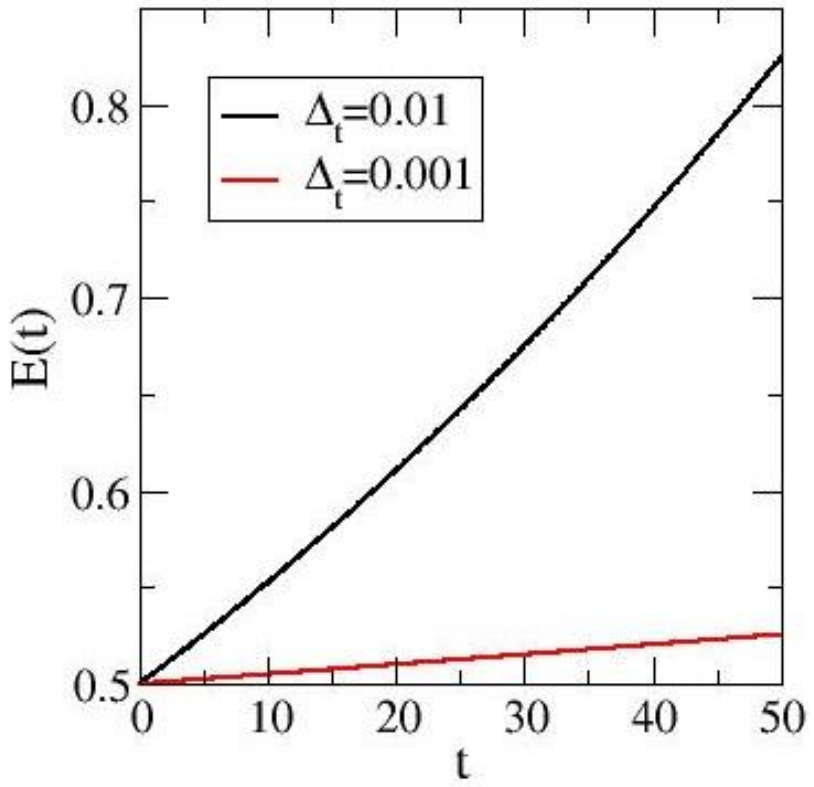
- Euler is not a very good algorithm in practice
- Energy error unbounded (can diverge)
- Algorithms with better precision almost as simple

Illustration of Euler algorithm: Harmonic oscillator

$$E = \frac{1}{2}kx^2 + \frac{1}{2}mv^2 \qquad \text{(F = -kx)}$$

Integrated equations of motion for k=m=1; $\Delta_t = 0.01,\ 0.001$





Leapfrog algorithm (no damping)

Taylor expand x(t) to second order in time step

$$x(t_n + \Delta_t) = x(t_n) + \Delta_t v(t_n) + \frac{1}{2}\Delta_t^2 a(x_n, t_n) + O(\Delta_t^3).$$

Contains velocity at "half step": $v(t_n) + \frac{1}{2}\Delta_t a(x_n, t_n) = v(t_{n+1/2})$

Substituting this gives

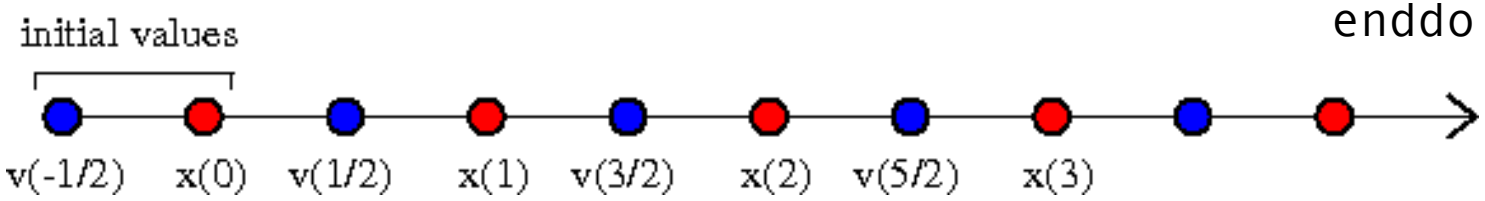
$$x(t_n + \Delta_t) = x(t_n) + \Delta_t v(t_n + \Delta_t/2) + O(\Delta_t^3)$$

Use similar form for v propagation: Leapfrog algorithm

$$v_{n+1/2} = v_{n-1/2} + \Delta_t a_n$$

$$x_{n+1} = x_n + \Delta_t v_{n+1/2}$$

```
do i=1,nt
   t=dt*(i-1)
   a=acc(x,v,t)
   v=v+dt*a
   x=x+dt*v
enddo
```



Starting velocity from: $v_{-1/2} = v_0 - a_0\Delta_t/2$

What is the step error in the leapfrog algorithm?

- Might expect: $O(\Delta_t^3)$
- Actually: $O(\Delta_t^4)$
- Can be easily seen in a different derivation

The Verlet algorithm

Start from two Taylor expansions: $x(t_n \pm \Delta_t)$

$$x_{n+1} = x_n + \Delta_t v_n + \frac{1}{2}\Delta_t^2 a_n + \frac{1}{6}\Delta_t^3 \dot{a}_n + O(\Delta_t^4)$$

$$x_{n-1} = x_n - \Delta_t v_n + \frac{1}{2}\Delta_t^2 a_n - \frac{1}{6}\Delta_t^3 \dot{a}_n + O(\Delta_t^4)$$

Adding these gives the so-called Verlet algorithm

$$x_{n+1} = 2x_n - x_{n-1} + \Delta_t^2 a_n + O(\Delta_t^4)$$

Velocity defined by: $v_{n-1/2} = (x_n - x_{n-1})/\Delta_t$

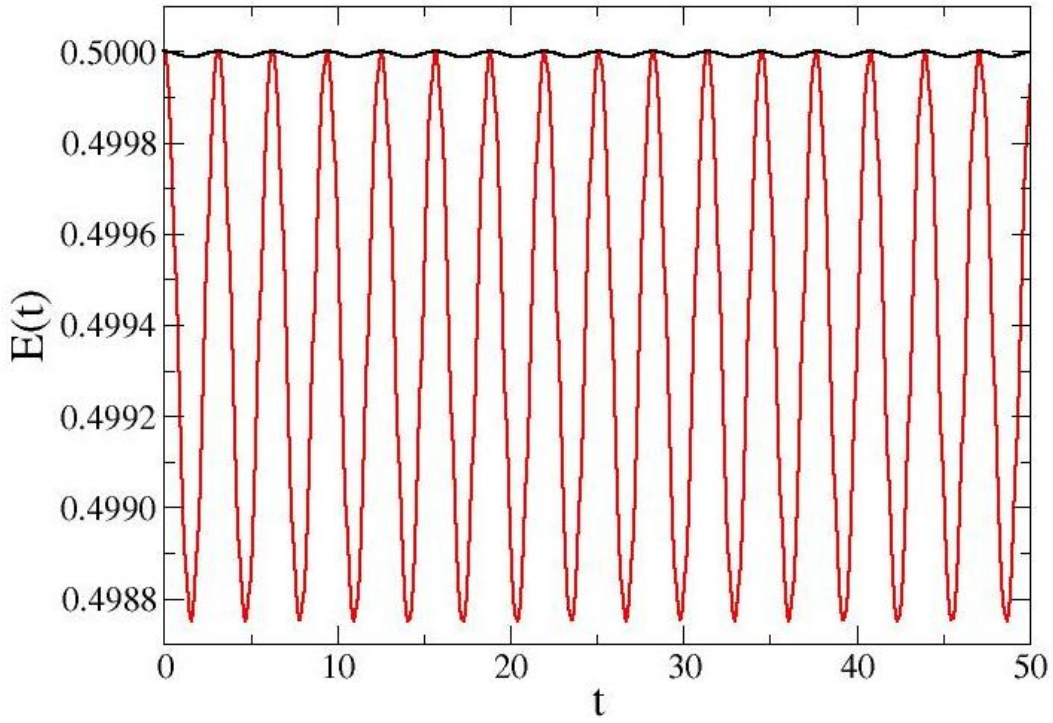
$$x_{n+1} = x_n + \Delta_t(v_{n-1/2} + \Delta_t a_n) + O(\Delta_t^4)$$

Same as leapfrog, since $v_{n-1/2} + \Delta_t a_n = v_{n+1/2}$

Properties of Verlet/leapfrog algorithm

- Time reversal symmetry (check for round-off errors)
- Errors bounded for periodic motion (time-reversal)
- High accuracy with little computational effort

Illustration: Harmonic oscillator (k=m=1), $\Delta_t = 0.1, 0.01$



Code almost identical to Euler (swicth 2lines!)

```
do i=1,nt
   t=dt*(i-1)
   a=acc(x,t)
   v=v+dt*a
   x=x+dt*v
enddo
```

Remember, initialize v at the half-step -dt/2!

Two equivalent Verlet/leapfrog methods

Verlet:

$$x_{n+1} = 2x_n - x_{n-1} + \Delta_t^2 a_n + O(\Delta_t^4)$$

Leapfrog:

$$v_{n+1/2} = v_{n-1/2} + \Delta_t a_n$$

$$x_{n+1} = x_n + \Delta_t v_{n+1/2}$$

Error build-up in Verlet/leapfrog method

Error in x after N steps, time $T = t_N - t_0 = N\Delta_t$

Difference between numerical and exact solution: $x_n = x_n^{\rm ex} + \delta_n$

Inserting this in Verlet equation

$$x_{n+1} = 2x_n - x_{n-1} + \Delta_t^2 a_n + O(\Delta_t^4)$$

gives

$$\delta_{n-1} - 2\delta_n + \delta_{n+1} = -(x_{n-1}^{\rm ex} - 2x_n^{\rm ex} + x_{n+1}^{\rm ex}) + \Delta_t^2 a_n + O(\Delta_t^4).$$

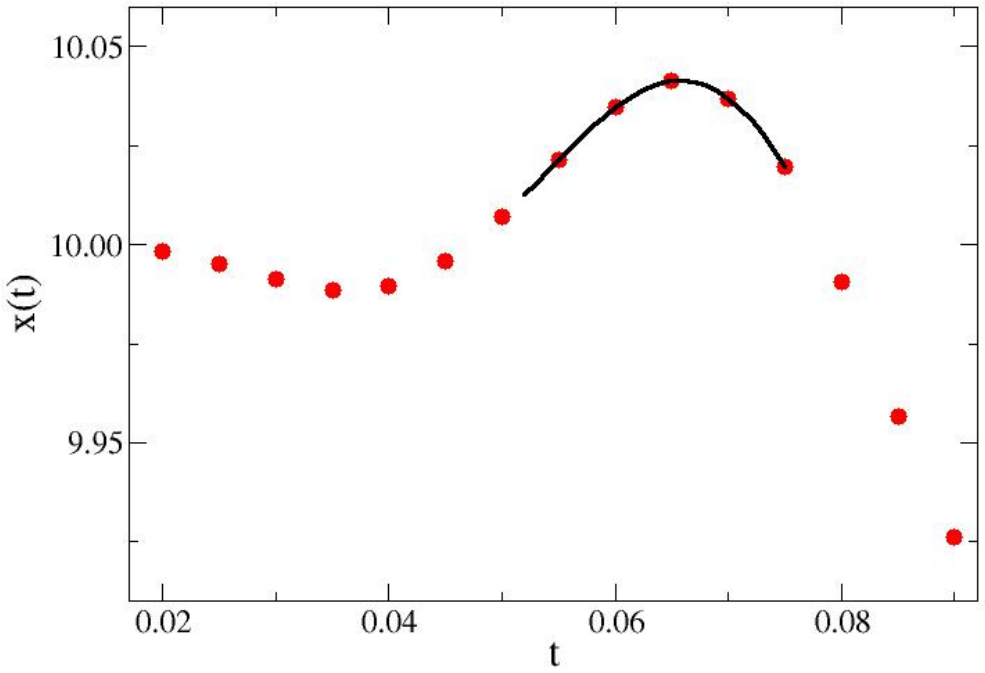
Discretized second derivative:

$$\frac{d^2 f(t_n)}{dt^2} = \frac{d}{dt}\frac{1}{\Delta_t}[f(t_{n+1/2}) - f(t_{n-1/2})] = \frac{1}{\Delta_t^2}(f_{n-1} - 2f_n + f_{n+1})$$

The equation of motion for the error is thus:

$$\ddot{\delta}(t_n) = -\ddot{x}^{\rm ex}(t_n) + a(t_n) + O(\Delta_t^2)$$

$$\ddot{\delta}(t_n) = -\ddot{x}^{\mathrm{ex}}(t_n) + a(t_n) + O(\Delta_t^2)$$



Assume smoothness on scale of time-step, use continuum derivative (imagine a high-order interpolating polynomial between points)

Exact solution satisfies: $\ddot{x}^{\mathrm{ex}}(t_n) = a(t_n)$

We are thus left with: $\ddot{\delta}(t_n) \sim \Delta_t^2$

Integrate to obtain error after time T:

Worst case: no error cancellations (same sign for all n):

$$\delta(T) = \int_0^T dt \dot{\delta}(t) = \int_0^T dt \int_0^t dt' \ddot{\delta}(t') \sim T^2 \Delta_t^2$$