Integration

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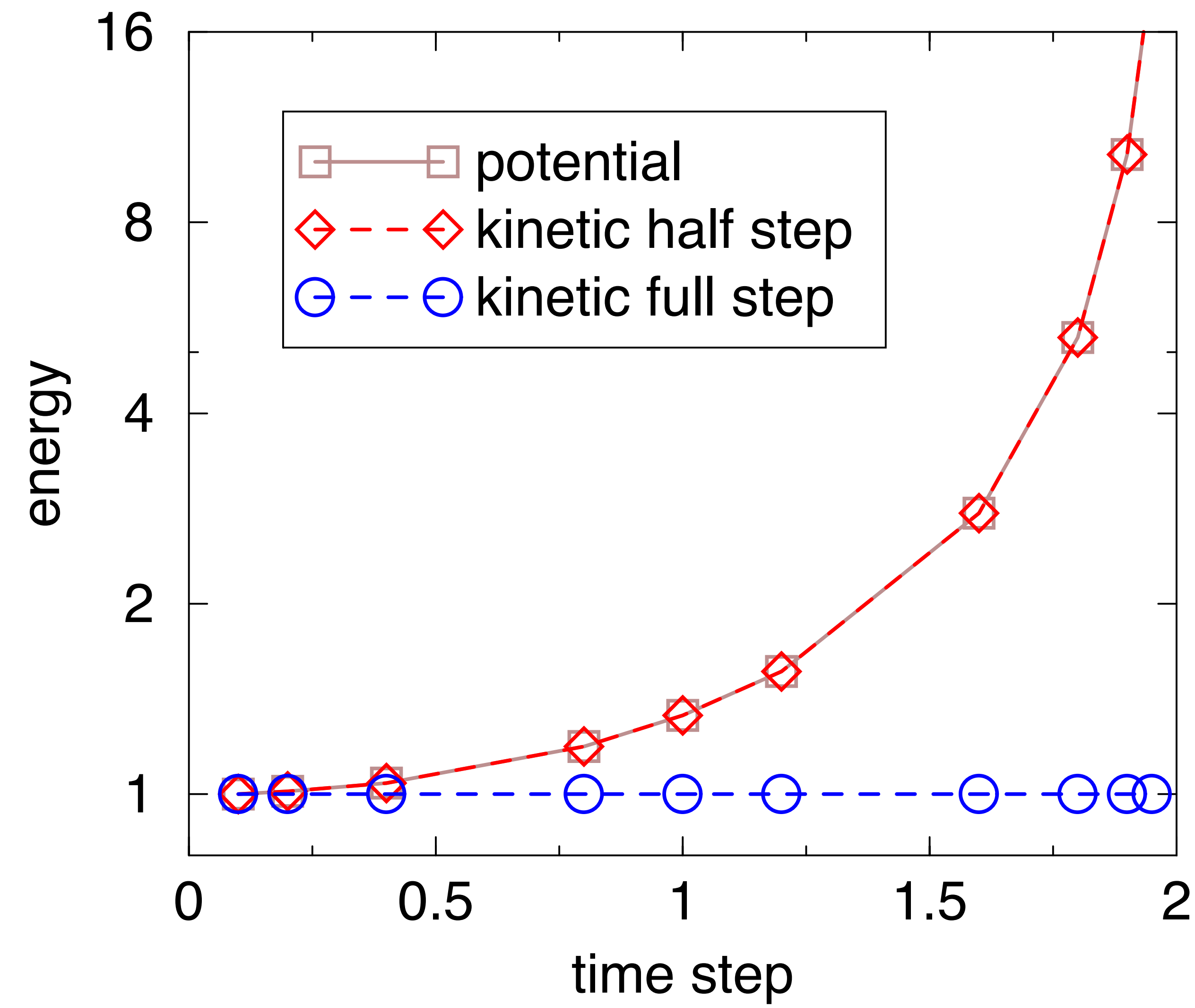
Integration of harmonic oscillator

$$\text{period} = 2\pi\sqrt{\frac{m}{k}}$$

- k and the temperature T determine the sampling of x (here T is related with v_0)
- The time scales as $\sqrt{m}$
  - Some people don't realize this
    - I have seen papers where people scale masses and accelerate MD!

Energy comparisons

- Euler not stable
- VV & LF very stable
- Euler not reversible
- VV+LF symplectic
- Largest timestep: 2
  - This is 3.14 steps per period!!!
- Advantage: great stability!
- Disadvantage: too (?) great stability



The kinetic energy is LF and VV

- With the same initial conditions LF and VV produce the same trajectory sequence x_i
- $v_i = (v_{i-1/2} + v_{i+1/2})/2$
- $K = 1/2\ m\ v^2$
- unless equal: $v_i^2 < [(v_{i-1/2} + v_{i+1/2})/2]^2$
- The LF velocity are the “real” steps in the trajectory
  - LF <K> should be close to <U>
  - VV <K> might underestimate <U>

Integrator exercise conclusions

- Not considering v, LF and VV are identical
- LF gives a good K
- VV has x and v at the same time
  - but with VV you can also do half steps for v and get the better K
- Use whatever you want, but be aware of the K issue with VV

Symplectic integration

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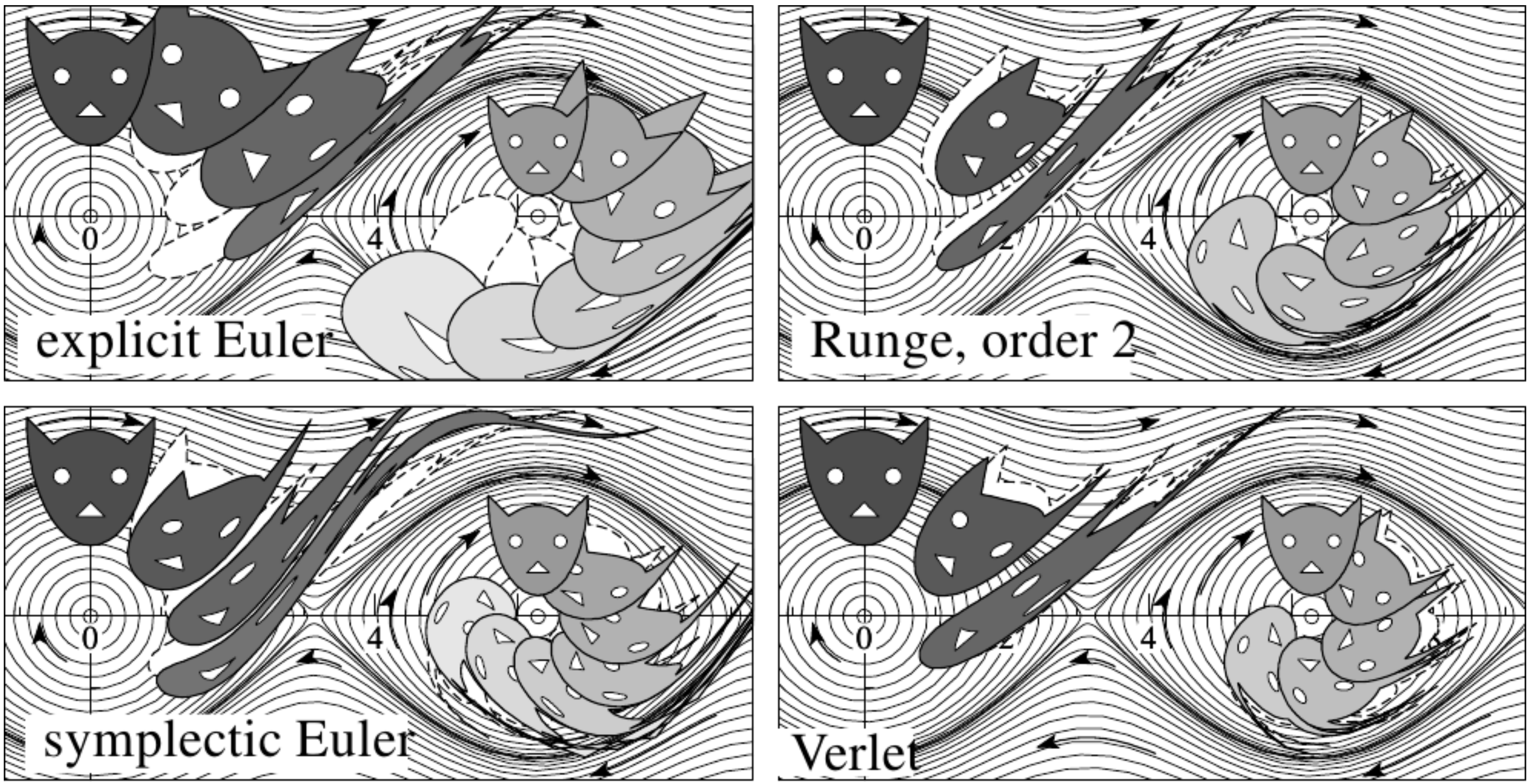
Why do some methods conserve energy?

- The Hamiltonian formulation of classical mechanics is based on the observation that
$$F = ma \ , \ p = mv \Rightarrow \dot{p} = -\frac{\partial H}{\partial x} \ , \ \dot{x} = \frac{\partial H}{\partial p}$$
where $H = \frac{p^2}{2m} + V(x)$ is called the Hamilton function and gives the total energy
- Symplectic means "area preserving", so that the area element $dA = |dxdp|$ is unchanged under the map $(x,p) \to (x',p')$ which gives
$$dA' = \left| \left(\frac{\partial x'}{\partial x}\hat{x} + \frac{\partial p'}{\partial x}\hat{p} \right) dx \times \left(\frac{\partial x'}{\partial p}\hat{x} + \frac{\partial p'}{\partial p}\hat{p} \right) dp \right| = |J|\, dA \ \Rightarrow \ dA' = dA \text{ if the Jacobian } J = \begin{pmatrix} \frac{\partial x'}{\partial x} & \frac{\partial x'}{\partial p} \\ \frac{\partial p'}{\partial x} & \frac{\partial p'}{\partial p} \end{pmatrix} = 1$$
- This prevents the coordinates and momenta from running away, and as a consequence it is possible to show that a slightly perturbed energy is conserved
- Example: Euler-Cromer is symplectic since $J = \begin{pmatrix} 1 & 0 \\ \frac{\partial F}{\partial x}\Delta t & 1 \end{pmatrix} = 1$
- Verlet and leapfrog are also symplectic
- Euler and Runge-Kutta are not symplectic
- Higher order symplectic methods can be constructed systematically

Symplectic integrators: area preserving



integration of pendulum motion

Trotter decomposition

A system of coupled, first-order differential eq. can be evolved from time t=0 to time t by applying the evolution operator where L is the Liouville operator, and Γ is he multidim. vector of indep. variables (x & v)

$$\Gamma(t) = \exp(iLt)\Gamma(0)$$
$$iL = \dot{\Gamma} \cdot \nabla_{\Gamma},$$

Apply P times:

$$\Gamma(t) = \prod_{i=1}^{P} \exp(iL\Delta t)\Gamma(0)$$

For NVE dynamics:

$$iL = \sum_{i=1}^{N} \mathbf{v}_i \cdot \nabla_{\mathbf{r}_i} + \sum_{i=1}^{N} \frac{1}{m_i}\mathbf{F}(r_i) \cdot \nabla_{\mathbf{v}_i}\,.$$

This can be split:

$$iL_1 = \sum_{i=1}^{N} \frac{1}{m_i}\mathbf{F}(r_i) \cdot \nabla_{\mathbf{v}_i}$$
$$iL_2 = \sum_{i=1}^{N} \mathbf{v}_i \cdot \nabla_{\mathbf{r}_i}$$

Short time approx:

$$\exp(iL\Delta t) = \exp(iL_2\frac{1}{2}\Delta t)\exp(iL_1\Delta t)\exp(iL_2\frac{1}{2}\Delta t) + \mathcal{O}(\Delta t^3)\,.$$

Multiple time-stepping

- Liouville operator for time reversible integration: see section 4.3.3 of Frenkel & Smit
- Liouville and multiple time-stepping: see section 15.3 of Frenkel & Smit
- Sympletic multiple time-stepping:
  - Split forces into a set of fast & set of slow changing
  - Integrate x as usual
  - $$\begin{aligned}\text{every n steps}: \quad & v_{i+1/2} = v_{i-1/2} + \frac{\Delta t}{m}(F_{\text{fast}} + n\,F_{\text{slow}}) \\ \text{other steps}: \quad & v_{i+1/2} = v_{i-1/2} + \frac{\Delta t}{m}F_{\text{fast}}\end{aligned}$$