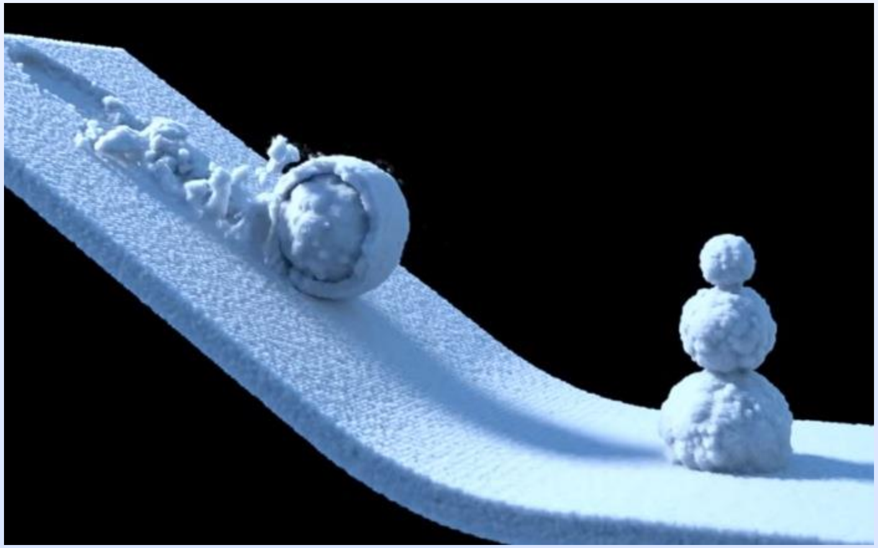
Particle Systems & Time Integration

But first…

Office hours Wed @ 3pm, Smith Hall 232

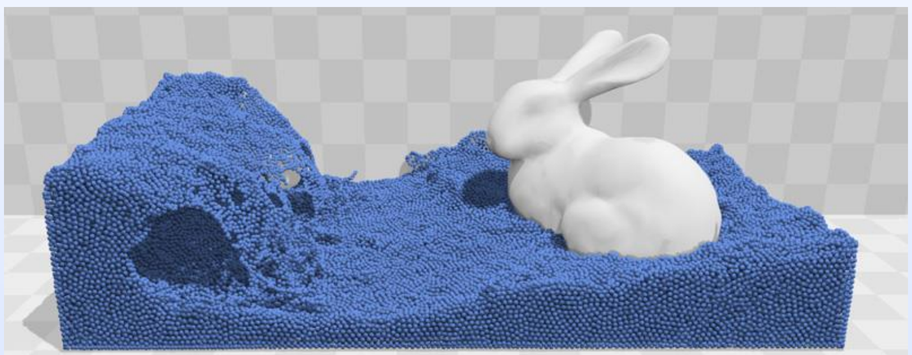
Particle Systems

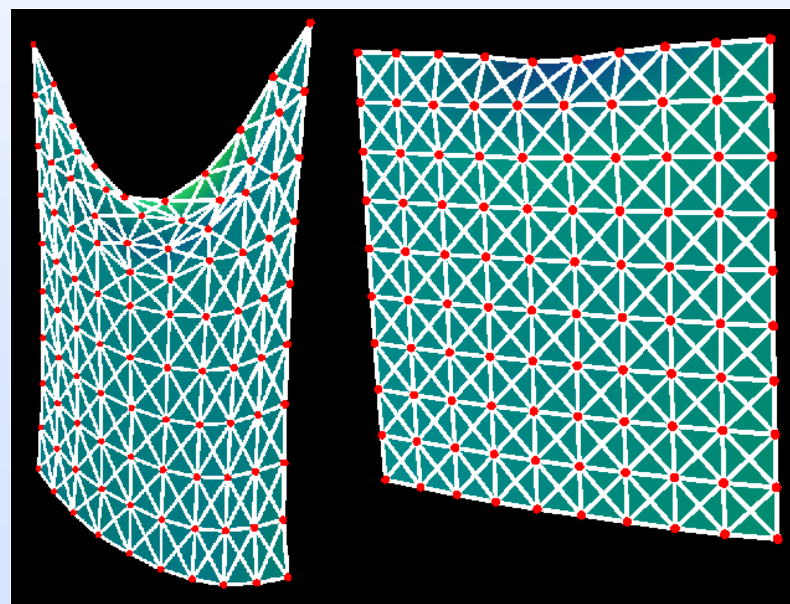
- Some dynamical systems can be naturally described as many small particles



Particle Systems

- Others are more difficult to get a handle on, but may still be approximated through particle systems





Particle Basics

- Each particle has a position
  - perhaps other attributes too: orientation, age, color, velocity, temperature, radius, …
  - Call the state **q** (aka generalized coordinates)
- Seed randomly somewhere at start
  - Maybe some created each frame
- Move (evolve state **q**) each frame according to some formula
- Eventually “die” when some condition met

Particle Basics

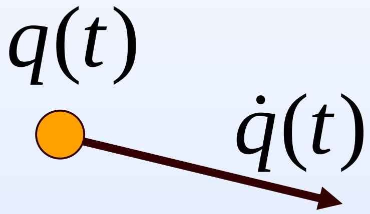
- But let's start with a 1D particle…

$$q(t)$$

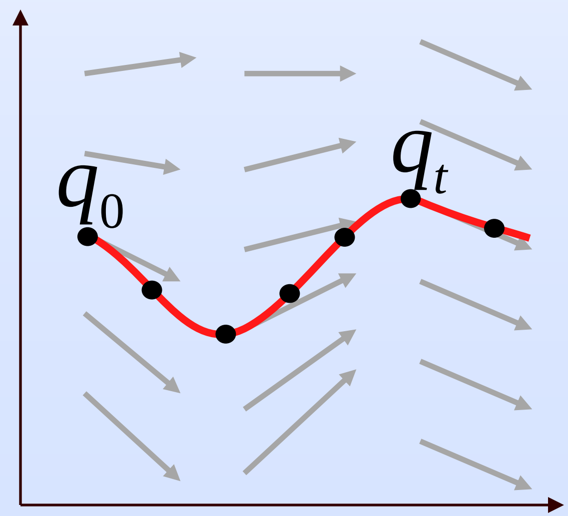
Motion

- An ordinary differential equation (ODE) describes how the particle's state changes through time:

$$\dot{q}(t) = \frac{dq}{dt}(t) = v(q,t)$$



- ODE defines a vector field in state-space. The function we seek, **q**(t), must be solved for
- In general, analytic solutions hopeless
- Need to solve numerically starting from an initial configuration $\mathbf{q}_0$ (= **q**(t=0))
- Main idea: approximate the derivative and discretize in time



Forward Euler

- Simplest method:

$$q_{n+1} = q_n + \Delta t v(q_n, t_n)$$

- First order accurate:
  - Global error accumulated over fixed time interval is O(Δt)
  - Thus it converges to the right answer
- But want error to be small

Forward Euler Accuracy

- Obvious approach: make Δt small
- But then need more time steps - expensive
  - also note - O(1) error made in modeling
  - even if numerical error was 0, still wrong!
  - need to validate against experiments
- Smaller time steps == better, but if we wanted fastest sim possible, how large could we go?

Forward Euler Stability

- The Test Equation

$$\frac{dq}{dt} = aq, a \in \mathbb{C}$$

- Linear ODE, known analytic solution $q(t) = e^{at}$
  - What does it look like?

The Test Equation

- Gives a rough picture of the stability of a method
  - ‘a’ will in general represent eigenvalues of Jacobian (first-order approximation to nonlinear ODEs)

$$v(q,t) \approx v(q^*,t^*) + \underbrace{\frac{\partial v}{\partial q}\cdot(q-q^*)}_{Aq} + \frac{\partial v}{\partial t}\cdot(t-t^*)$$

  - Nonlinear effects can definitely cause problems
  - Even with linear problems, what follows assumes constant time steps - varying (but supposedly stable) steps can induce instability
    - see J. P. Wright, “Numerical instability due to varying time steps…”, JCP 1998

Using the Test Equation

- Forward Euler on test equation is

$$q_{n+1} = q_n + \Delta t a q_n$$

- Solving gives

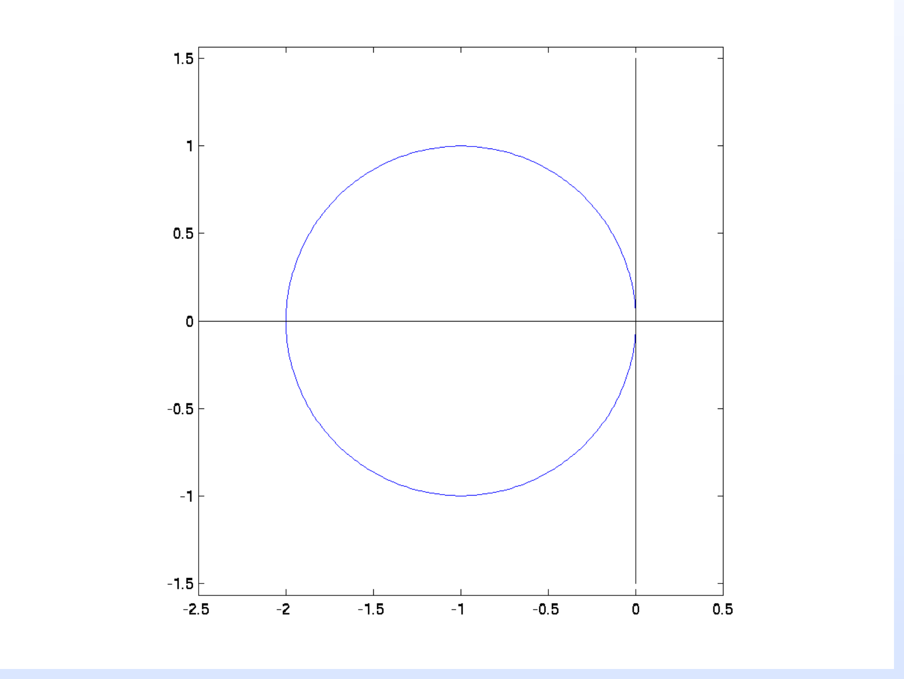
$$q_n = \left(1 + a\Delta t\right)^n q_0$$

- So for stability, need

$$\left|1 + a\Delta t\right| < 1$$

Stability Region

- Can plot all the values of $a\Delta t$ on the complex plane where F.E. is stable:



- Big problem with Forward Euler: not very stable

Real Eigenvalue

- Say eigenvalue is real (and negative)
  - Corresponds to a damping motion, smoothly coming to a halt
- Then need:

$$\Delta t < \frac{2}{|a|}$$

- Is this bad?
  - If ‘a’ is big, could mean small time steps needed for stability (aka stiff problem)

Imaginary Eigenvalue

- If eigenvalue is pure imaginary (oscillatory or rotational motion), cannot make Δt small enough

- Forward Euler unconditionally unstable for these kinds of problems!

- Need to look at other methods

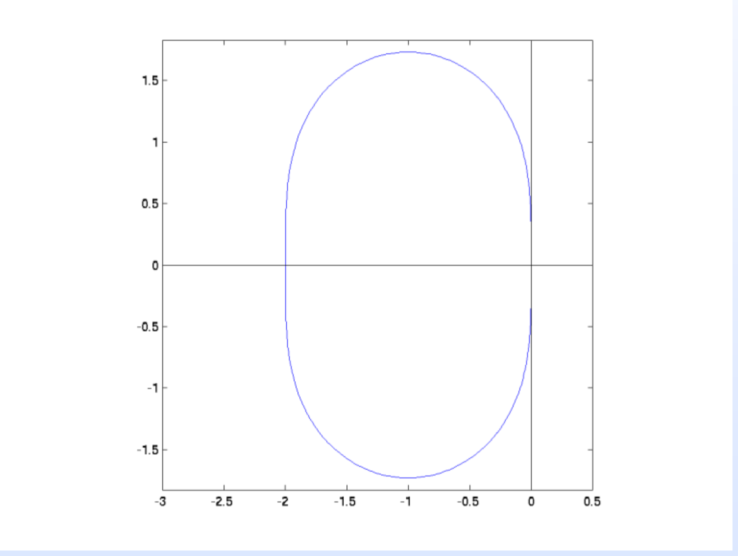
Runge-Kutta Methods

- Also “explicit”
  - next q is an explicit function of previous
- But evaluate v at a few locations to get a better estimate of next q
- E.g. midpoint method (RK2)

$$q_{n+\frac{1}{2}} = q_n + \tfrac{1}{2}\Delta t v(q_n, t_n)$$
$$q_{n+1} = q_n + \Delta t v(q_{n+\frac{1}{2}}, t_{n+\frac{1}{2}})$$

Midpoint RK2

- Second order: error is $O(\Delta t^2)$
- Larger stability region:



- But still not stable on imaginary axis

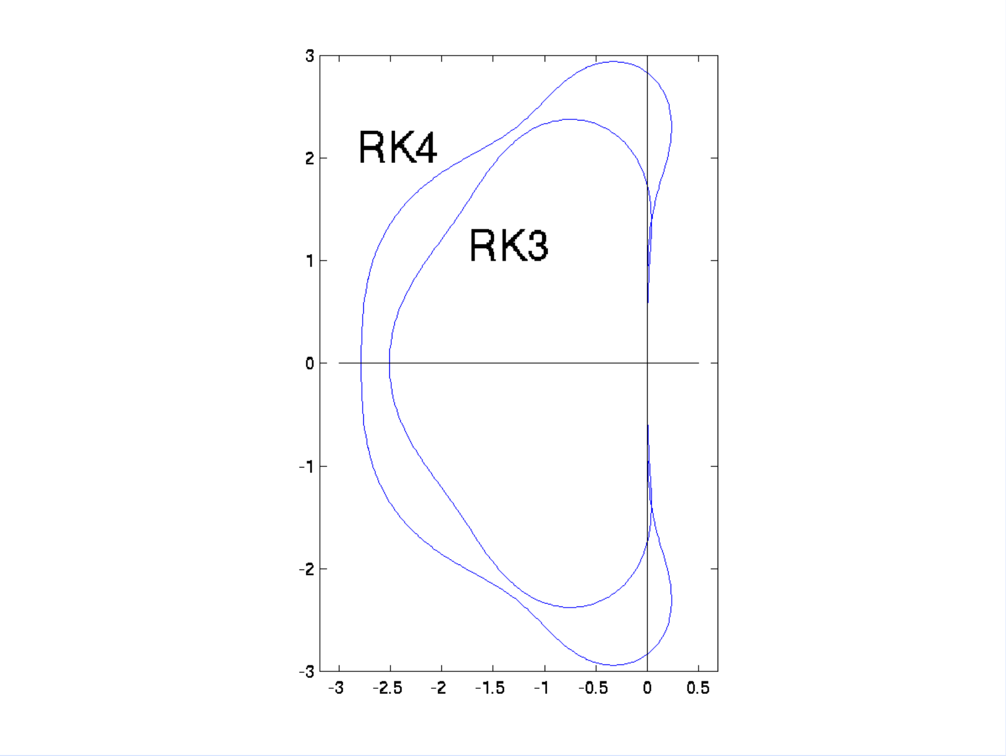
RK4

- Often most bang for the buck
- Combination of Forward Euler steps and averaging

$$
\begin{aligned}
v_1 &= v\left(q_n, t_n\right) \\
v_2 &= v\left(q_n + \tfrac{1}{2}\Delta t v_1, t_{n+1/2}\right) \\
v_3 &= v\left(q_n + \tfrac{1}{2}\Delta t v_2, t_{n+1/2}\right) \\
v_4 &= v\left(q_n + \Delta t v_3, t_{n+1}\right) \\
q_{n+1} &= q_n + \Delta t\left(\tfrac{1}{6}v_1 + \tfrac{2}{6}v_2 + \tfrac{2}{6}v_3 + \tfrac{1}{6}v_4\right)
\end{aligned}
$$

Higher Order Runge-Kutta

- RK3 and up naturally include part of the imaginary axis



Implicit Methods

Backward Euler

- The simplest implicit method:

$$q_{n+1} = q_n + \Delta t v\left(q_{n+1}, t_{n+1}\right)$$

- the next x **implicitly** defined since it appears in derivative
  - Need to solve equations to figure it out

- First order accurate

- We'll come back to it later for a general formulation!

Backward Euler Stability

- Test equation shows stable when $|1 - a\Delta t| > 1$
- This includes everything except a circle in the positive real-part half-plane. *Unconditionally stable* for linear ODEs.
- It's stable even when the physics is unstable!
- This is the biggest problem: damps out motion unrealistically

Trapezoidal Rule

- Can improve by going to second order:

$$q_{n+1} = q_n + \Delta t\left(\tfrac{1}{2}v(q_n, t_n) + \tfrac{1}{2}v(q_{n+1}, t_{n+1})\right)$$

- This is actually just a half step of F.E., followed by a half step of B.E.
  - F.E. is under-stable, B.E. is over-stable, the combination is **just right**
- Stability region is the left half of the plane: **exactly** the same as the underlying ODE!
- Really good for pure rotation (doesn’t amplify or damp)

What to ask for from a numerical integrator?

- No one “best” integrator – pick the right tool for the job!
- Many different integrators because there are many notions of “good”
  - Convergence/accuracy
  - Stability
  - Computational Efficiency
  - Monotonicity
  - …

Monotonicity

- Test equation with real, negative λ
  - True solution is $x(t)=x_0e^{\lambda t}$, which smoothly decays to zero, doesn't change sign (**monotone**)
- Forward Euler at stability limit:
  - $x=x_0, \; -x_0, \; x_0, \; -x_0, \ldots$
- Not smooth, oscillating sign, no good!
- So monotonicity limit stricter than stability

Monotonicity

- Backward Euler is unconditionally monotone
  - No problems with oscillation, just too much damping
- Trapezoidal Rule can suffer though, because of that half-step of F.E.
  - could get ugly oscillation instead of smooth damping
  - for some nonlinear problems, possible to hit instability

Summary 1

- Need to move particles in velocity field according to underlying ODE
- Forward Euler
  - Simple, first choice unless problem has oscillations/rotations
- Runge-Kutta is better, but requires more evaluations
  - RK4 general purpose workhorse

Summary 2

- If stability limit is a problem, look at implicit methods
  - e.g. explicit time steps are way too small
- Trapezoidal Rule
  - If monotonicity isn't a problem
- Backward Euler
  - Almost always works, but may over-damp!