COL865: Special Topics in Computer Applications Physics-Based Animation

5 — Time integration

Paper discussions this Thursday

- 1. Selle et al., "A Mass Spring Model for Hair Simulation", 2008
- 2. Liu et al., "Fast Simulation of Mass-Spring Systems", 2013

Lead: me

Your job:

- Read both papers before Thursday's class
- Come prepared with questions, comments, ideas (at least one)

Today

Time integration

- Forward and backward Euler, Runge-Kutta methods, implicit methods, leapfrog and symplectic Euler
- Accuracy and stability analysis
- Reading: Numerical Algorithms Ch. 15



Forward Euler

 $y'(t) = \varphi(t,y(t))$

Choose $t = t_0$, use forward difference $y'(t^0) \approx (y^1 - y^0)/\Delta t$

 $y^1 = y^0 + \varphi(t^0, y^0) \, \Delta t$

Drawbacks:

- Based on first-order accurate discretization of time derivative
- Can be **unstable** if forces are stiff / time step is large

Test problem

Consider a damped harmonic oscillator

$$x^{\prime\prime} = -kx - cx^{\prime}$$

Analytical solution:

$$\begin{aligned} \mathsf{x}(t) &= e^{-ct/2} (a_1 \cos \omega t + a_2 \sin \omega t) \\ \omega &= \sqrt{k - c^2/4} \end{aligned}$$

Forward Euler solutions with different Δt :





Backward Euler

$$(y^1 - y^0) / \Delta t \approx y'(t^1) = \varphi(t^1, y^1)$$
$$y^1 - \varphi(t^1, y^1) \Delta t = y^0$$

Also known as "**implicit Euler**" (vs. FE = explicit Euler)



Accuracy still $O(\Delta t)$, but can take arbitrarily large time steps!

Drawback: Lots of **artificial dissipation**, especially for large Δt

Accuracy and stability analysis

Accuracy analysis

An oversimplified analysis:

(for rigorous version, see Numerical Analysis Ch. 5.2)

Taylor series: $y(t_1) = y(t_0) + y'(t_0) \Delta t + \frac{1}{2} y''(t_0) \Delta t^2 + \cdots$

Forward Euler: $y^1 = y^0 + y'(t_0) \Delta t$

Local error between computed y^1 and true $y(t_1) = O(\Delta t^2)$

Error will accumulate over $O(1/\Delta t)$ time steps, so **global error** is $O(\Delta t)$: forward Euler is first-order accurate

Same analysis for backward Euler: also first-order

Stability

ODE is **stable** if two nearby solutions remain nearby



We want numerical solution of stable ODE to also be stable

- How to determine if an ODE is stable?
- How to determine if a numerical method is stable?

Stability analysis

Consider an **autonomous** linear ODE (RHS independent of *t*)

y′ = **Ay**

Take eigendecomposition, $\mathbf{A} = \mathbf{Q} \wedge \mathbf{Q}^{-1}$ (Λ is diagonal, both \mathbf{Q} and Λ may be complex)

Express **y** in eigenbasis: $\mathbf{z} = \mathbf{Q}^{-1}\mathbf{y}$

 $\mathbf{z}' = \mathbf{\Lambda} \mathbf{z}$

All components of **z** are decoupled!

$$z_1' = \lambda_1 z_1$$
$$z_2' = \lambda_2 z_2$$
$$\vdots$$

Stability analysis in 1 variable



Stability analysis of forward Euler

Forward Euler: $z^1 = (1 + \lambda \Delta t) z^0$

 $\Rightarrow z^n = (1 + \lambda \Delta t)^n \, z^0$

FE solution is stable if $|1 + \lambda \Delta t| \le 1$

 $\lambda \Delta t$ must lie in the **stability region:**

- With larger λ (stiffer springs / more damping), Δt must become smaller to remain in stability region
- If $\operatorname{Re}(\lambda) = 0$ (no damping), forward Euler is not stable for any Δt !



Stability analysis of backward Euler

Backward Euler: $z^1 = (1 - \lambda \Delta t)^{-1} z^0$

 $\Rightarrow z^n = (1 - \lambda \, \Delta t)^{-n} \, z^0$

Stable if $|1 - \lambda \Delta t|^{-1} \le 1...$ Always true if $\operatorname{Re}(\lambda) \le 0!$

BE is **unconditionally stable**, or **A-stable**



Review

For any autonomous linear ODE:

- Forward Euler is stable if $|1 + \lambda \Delta t| \le 1$
- Backward Euler is always stable if ODE is stable

Stability condition must hold for **every** eigenvalue $\lambda_i \dots$ Bad news for FE if even a single extremely stiff force in system

Runge-Kutta methods

Higher-order methods

Recall interpretation of ODE as quadrature:

$$y_1 - y_0 = \int_{t_0}^{t_1} \varphi(t, y(t)) dt$$

Forward Euler = quadrature point at start of interval

$$y^1 = y^0 + \varphi(t^0, y^0) \Delta t$$

Midpoint method = quadrature point at center. But what's $y^{\frac{1}{2}}$? Take **explicit** approximation: FE step of length $\Delta t/2$

$$y^{\frac{1}{2}} = y^{0} + \varphi(t^{0}, y^{0}) \Delta t/2$$
$$y^{1} = y^{0} + \varphi(t^{\frac{1}{2}}, y^{\frac{1}{2}}) \Delta t$$

Explicit midpoint method

 $y^{\frac{1}{2}} = y^{0} + \varphi(t^{0}, y^{0}) \Delta t/2$ $y^{1} = y^{0} + \varphi(t^{\frac{1}{2}}, y^{\frac{1}{2}}) \Delta t$

Second-order accurate

 Even though y^{1/2} is only first-order... why?

Stability region: $|1 + \lambda \Delta t + \frac{1}{2} (\lambda \Delta t)^2| \le 1$







Runge-Kutta methods

Equivalent form:

$$\varphi^{0} = \varphi(t^{0}, y^{0})$$

$$\varphi^{\frac{1}{2}} = \varphi(t^{0} + \frac{1}{2} \Delta t, y^{0} + \frac{1}{2} \varphi^{0} \Delta t)$$

$$y^{1} = y^{0} + \varphi^{\frac{1}{2}} \Delta t$$

Higher-order generalization: Evaluate φ at various quadrature points, chosen using previously evaluated values of φ

$$\varphi_{0} = \varphi(t^{0} + 0 \Delta t, y^{0})$$

$$\varphi_{1} = \varphi(t^{0} + c_{1} \Delta t, y^{0} + (a_{10} \varphi_{0}) \Delta t)$$

$$\varphi_{2} = \varphi(t^{0} + c_{2} \Delta t, y^{0} + (a_{20} \varphi_{0} + a_{21} \varphi_{1}) \Delta t)$$

$$\vdots$$

$$y^{1} = y^{0} + (b_{0} \varphi_{0} + b_{1} \varphi_{1} + b_{2} \varphi_{2} + \cdots) \Delta t$$

RK4: "the" Runge-Kutta method

$$\begin{split} \varphi_{0} &= \varphi(t^{0} + 0 \Delta t, y^{0}) \\ \varphi_{1} &= \varphi(t^{0} + \frac{1}{2} \Delta t, y^{0} + \frac{1}{2} \varphi_{0} \Delta t) \\ \varphi_{2} &= \varphi(t^{0} + \frac{1}{2} \Delta t, y^{0} + \frac{1}{2} \varphi_{1} \Delta t) \\ \varphi_{3} &= \varphi(t^{0} + 1 \Delta t, y^{0} + \varphi_{2} \Delta t) \\ y^{1} &= y^{0} + (\frac{1}{6} \varphi_{0} + \frac{1}{3} \varphi_{1} + \frac{1}{3} \varphi_{2} + \frac{1}{6} \varphi_{3}) \Delta t \end{split}$$

Fourth-order accurate

Reduces to Simpson's rule if $\varphi(t)$ independent of y



Butcher tableaus

Compact way of expressing RK methods

$$\varphi_{0} = \varphi(t^{0} + 0 \Delta t, y^{0})$$

$$\varphi_{1} = \varphi(t^{0} + c_{1} \Delta t, y^{0} + (a_{10} \varphi_{0}) \Delta t)$$

$$\varphi_{2} = \varphi(t^{0} + c_{2} \Delta t, y^{0} + (a_{20} \varphi_{0} + a_{21} \varphi_{1}) \Delta t)$$

$$\vdots$$

$$y^1 = y^0 + (b_0 \varphi_0 + b_1 \varphi_1 + b_2 \varphi_2 + \cdots) \Delta t$$

0				
<i>C</i> ₁	a_{10}			
<i>C</i> ₂	a ₂₁	a ₂₂		
:	•	:	·	
	b_0	b_1	b_2	• • •

Example: RK4

Butcher tableaus

- What is the tableau for explicit midpoint?
- Heun's method is given by the following tableau.
 How does it work?

• What quadrature scheme does it look like?

Implicit methods

Second-order implicit methods

EM, Heun's method: second-order, not unconditionally stable

Instead of approximating future y's, make them **implicit** in y¹

Implicit midpoint:

$$y^{1} = y^{0} + \varphi \left(\frac{t^{0} + t^{1}}{2}, \frac{y^{0} + y^{1}}{2} \right) \Delta t$$

Trapezoidal method:

$$y^{1} = y^{0} + \left(\frac{\varphi(t^{0}, y^{0}) + \varphi(t^{1}, y^{1})}{2}\right) \Delta t$$

Both second-order accurate, equivalent for linear problems

Stability

Implicit midpoint and trapezoidal method are unconditionally stable

Stability region: $\operatorname{Re}(\lambda) \leq 0$

Artificial oscillations for large time steps





L-stability



A-stability: If $\operatorname{Re}(\lambda) \leq 0$, then $|y^1|/|y^0| \leq 1$

L-stability: If $\operatorname{Re}(\lambda) \leq 0$ and $\Delta t \to \infty$, then $|y^1|/|y^0| \to 0$

Backward Euler is L-stable, but implicit midpoint and trapezoidal method are not

BDF2

What if we use **second-order** finite difference approximation of *y*?

- Centered differences is no good. Why?
- Second-order backward differences:

$$y'(t^{n+1}) = (3/2 \, y^{n+1} - 2 \, y^n + 1/2 \, y^{n-1})/\Delta t$$

Second-order accurate, A-stable, L-stable, less dissipative than BE



This is a **multistep method**: uses two previous states y^n and y^{n-1}

Downsides: Needs to be "kickstarted" with one-step method, not good near nonsmooth points (e.g. collisions)

Symplectic methods

Verlet/leapfrog integration

Suppose **f** independent of **v**. Then we can just write $\mathbf{x}'' = \mathbf{M}^{-1} \mathbf{f}(\mathbf{x})$. Apply three-point formula for second derivative:

$$(\mathbf{x}^{n+1} - 2 \mathbf{x}^n + \mathbf{x}^{n-1})/\Delta t^2 = \mathbf{M}^{-1} \mathbf{f}(\mathbf{x}^n)$$

$$\Rightarrow \mathbf{x}^{n+1} = 2 \mathbf{x}^n - \mathbf{x}^{n-1} + \mathbf{M}^{-1} \mathbf{f}(\mathbf{x}^n) \Delta t^2$$

Another interpretation: Let $(\mathbf{x}^n - \mathbf{x}^{n-1})/\Delta t = \mathbf{v}^{n-1/2}$

$$\mathbf{v}^{n+1/2} = \mathbf{v}^{n-1/2} + \mathbf{M}^{-1} \mathbf{f}(\mathbf{x}^n) \Delta t$$
$$\mathbf{x}^{n+1} = \mathbf{x}^n + \mathbf{v}^{n+1/2} \Delta t$$



Also called "leapfrog" integration

Symplectic Euler

Compare forward Euler:

$$\mathbf{v}^{1} = \mathbf{v}^{0} + \mathbf{M}^{-1} \mathbf{f}(\mathbf{x}^{0}, \mathbf{v}^{0}) \Delta t$$
$$\mathbf{x}^{1} = \mathbf{x}^{0} + \mathbf{v}^{0} \Delta t$$

Backward Euler:

 $\mathbf{v}^{1} = \mathbf{v}^{0} + \mathbf{M}^{-1} \mathbf{f}(\mathbf{x}^{1}, \mathbf{v}^{1}) \Delta t$ $\mathbf{x}^{1} = \mathbf{x}^{0} + \mathbf{v}^{1} \Delta t$

Symplectic Euler: implicit in v, explicit in x

 $\mathbf{v}^{1} = \mathbf{v}^{0} + \mathbf{M}^{-1} \mathbf{f}(\mathbf{x}^{0}, \mathbf{v}^{1}) \Delta t$ $\mathbf{x}^{1} = \mathbf{x}^{0} + \mathbf{v}^{1} \Delta t$

Using $f(x^0, v^0)$ is usually good enough — then no solve needed

Symplecticity

"Symplectic" is a technical term with a complicated meaning

In absence of damping, symplectic methods conserve volumes in phase space (even for nonlinear systems!)



[Hairer et al. 2002]

Tend to conserve energy in the long term (**if** they remain stable)

Leapfrog, SE, IM are symplectic



[Stern and Desbrun 2006]

Summary

Summary of integration methods

N	ame	Accuracy	Exp/imp	Stability	Symplectic
Forwa	ard Euler	1st order	explicit	conditional	no
Backward Euler		1st order	implicit	L-stable	no
Explicit Heun'	midpoint, s method	2nd order	explicit	conditional	no
1	RK4	4th order	explicit	conditional	no
Implicit trap	: midpoint, ezoidal	2nd order	implicit	A-stable	IM: yes, TR: no
BDF2		2nd order	implicit	L-stable	no
Leapfrog, symplectic Euler		LF: 2nd, SE: 1st	explicit / semi-implicit	conditional	yes

Summary of integration methods

Which to use?

- Unconditional stability on stiff problems: BE, BDF2
- Long-term energy conservation: SE, IM, TR
- Fast and easy to implement: SE, EM, Heun's
- High-accuracy reference solution for validation: RK4

FE: just don't

Implementation notes

Always try to decouple model and integrator

Model should provide methods to:

- get number of DOFs *n*,
- get/set current state vector $\mathbf{y} \in \mathbb{R}^n$,
- evaluate current time derivative $\boldsymbol{\varphi}(\mathbf{y}) \in \mathbb{R}^n$

Then you can switch integrators as needed, reuse integrator code for different problems, etc.

e.g. Explicit midpoint:

```
y0 = model.getState()
φ0 = model.getDerivative()
model.setState(y0 + φ0 Δt/2)
φh = model.getDerivative()
model.setState(y0 + φh Δt)
```

See Pixar notes for more

For some integrators (BE, SE, ...), may need to provide more:

- get/set current position **x**, velocity $\mathbf{v} \in \mathbb{R}^n$,
- get inertia matrix $\mathbf{M} \in \mathbb{R}^{n \times n}$,
- compute current force $\mathbf{f}(\mathbf{x}, \mathbf{v}) \in \mathbb{R}^n$

Adaptive time stepping

If **f** is changing rapidly, may need to reduce Δt for accuracy/stability. How to know when?

- In numerical analysis: see Burden & Faires Ch. 5.5
- In graphics: problem-dependent time step criteria
 - Collisions not resolved \Rightarrow reduce Δt
 - Continuum mechanics (elasticity, fluids, etc.) ⇒ stability criteria (e.g. CFL condition)

Caveats: Adaptivity is hard to do for BDF2, breaks properties of symplectic methods

Next class

Equation solving and optimization

- Solving systems of equations for implicit methods
- Numerical optimization for robust quasistatic simulation
- Solomon, *Numerical Algorithms*, Ch. 8; Nocedal and Wright, *Numerical Optimization*, Ch. 2, 3

