Intoduction to Optimization (Part 2)

Computer Graphics
CMU 15-462/15-662

Last week we talked about how to set up optimization problems and determine whether they could be solved.

How do we solve optimization problems in general?

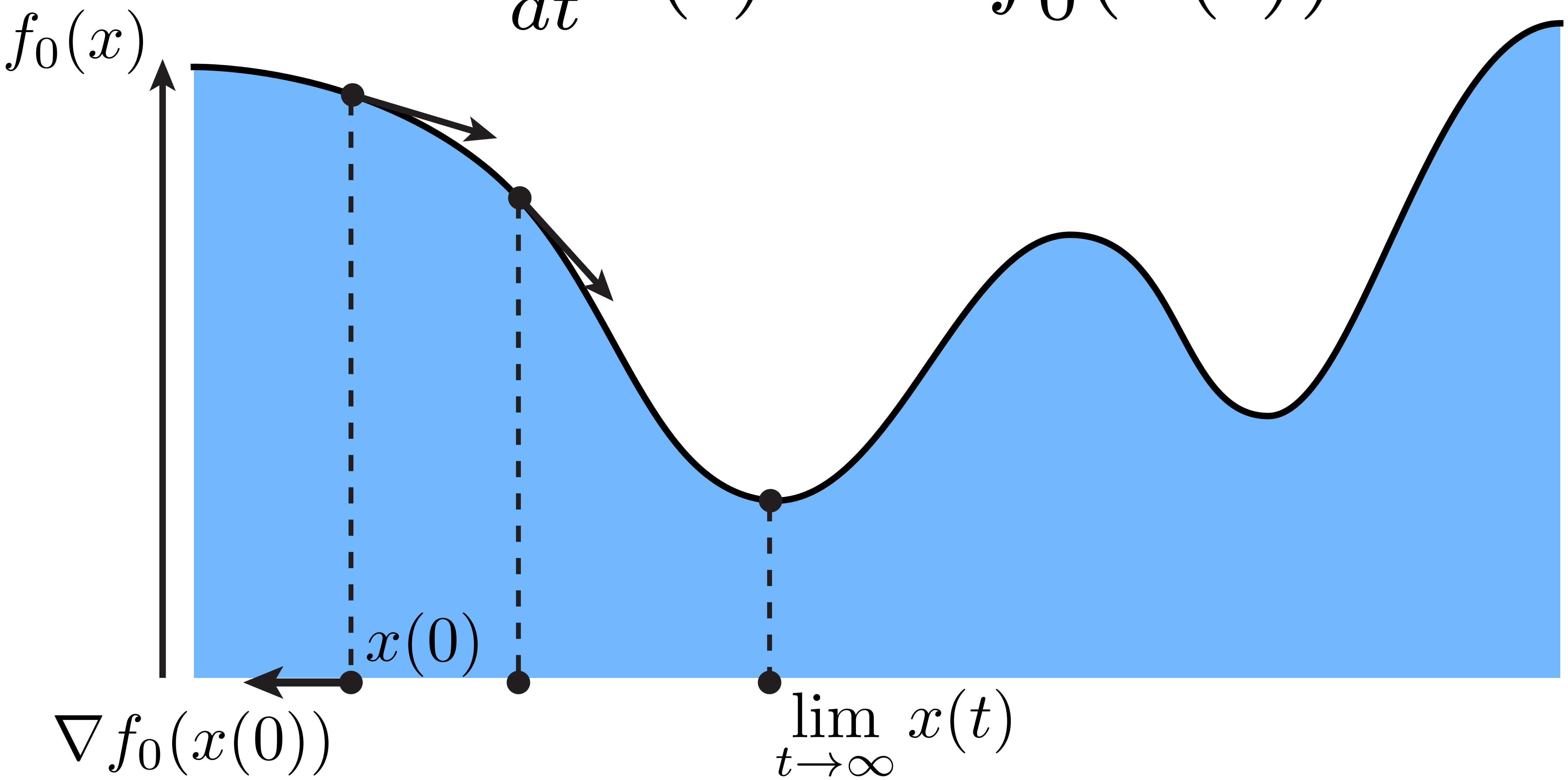
Descent Methods

An idea as old as the hills:

Gradient Descent (1D)

- Basic idea: follow the gradient "downhill" until it's zero
- (Zero gradient was our 1st-order optimality condition)

$$\frac{d}{dt}x(t) = -f_0'(x(t))$$

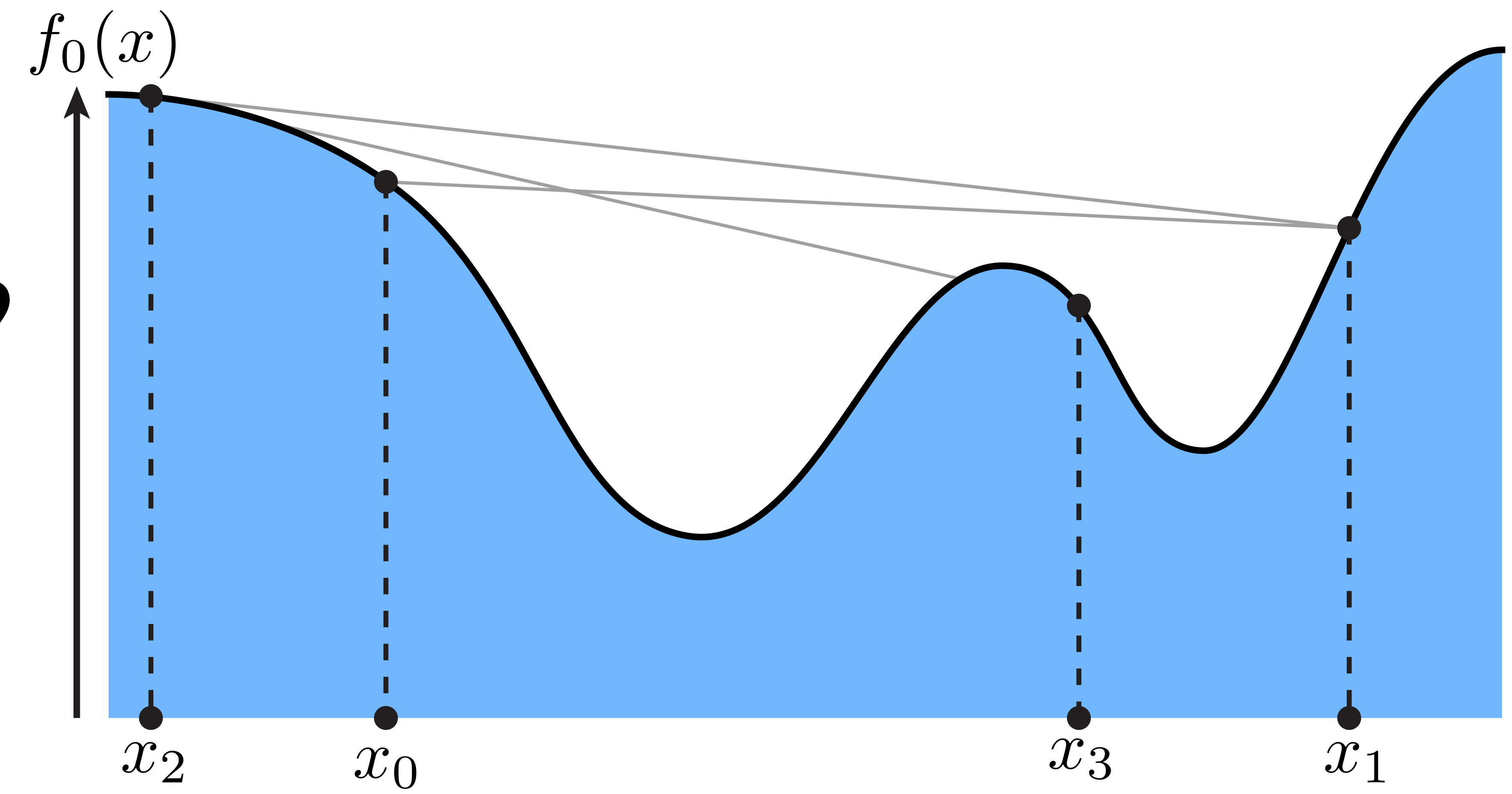


- Do we always end up at a (global) minimum?
- How do we compute gradient descent in practice?

Gradient Descent Algorithm (1D)

- Did you notice that gradient descent equation is an ODE?
- Q: How do we solve it numerically? $\frac{d}{dt}x(t) = -f_0'(x(t))$
- One way: forward Euler:

$$x_{k+1} = x_k + \tau f_0'(x_k)$$



- Q: How do we pick the time step?
- If we're not careful, we'll go zipping all over the place; won't make any progress.
- Basic idea: use "step control" to determine step size based on value of objective & derivatives.
- A careful strategy (e.g., Armijo-Wolfe) can guarantee convergence at least to a local minimum.
- For now we will do something simpler: make τ really small!

Gradient Descent Algorithm (nD)

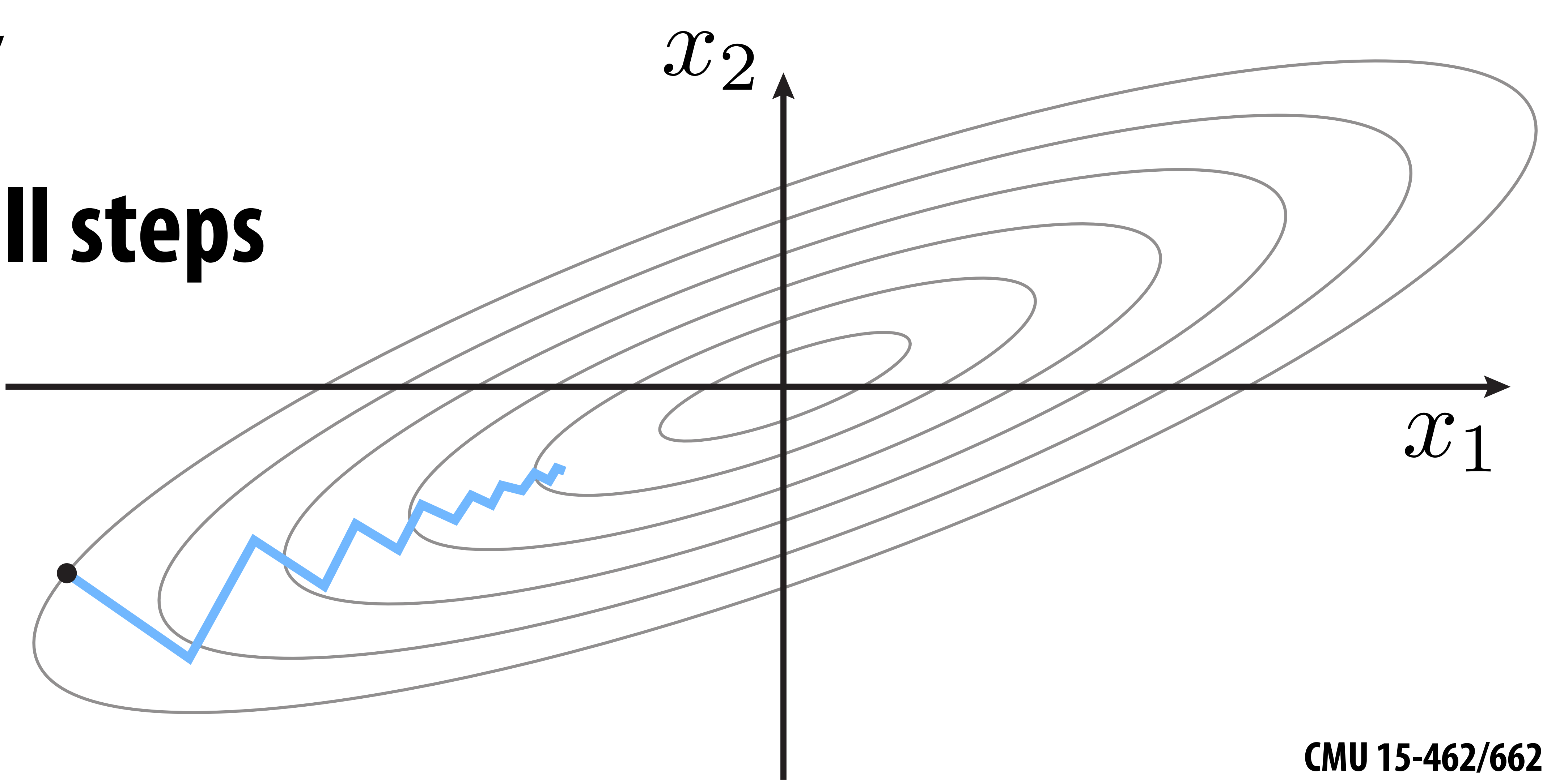
- **Q: How do we write gradient descent equation in general?**

$$\frac{d}{dt}x(t) = -\nabla f_0(x(t))$$

- **Q: What's the corresponding discrete update?**

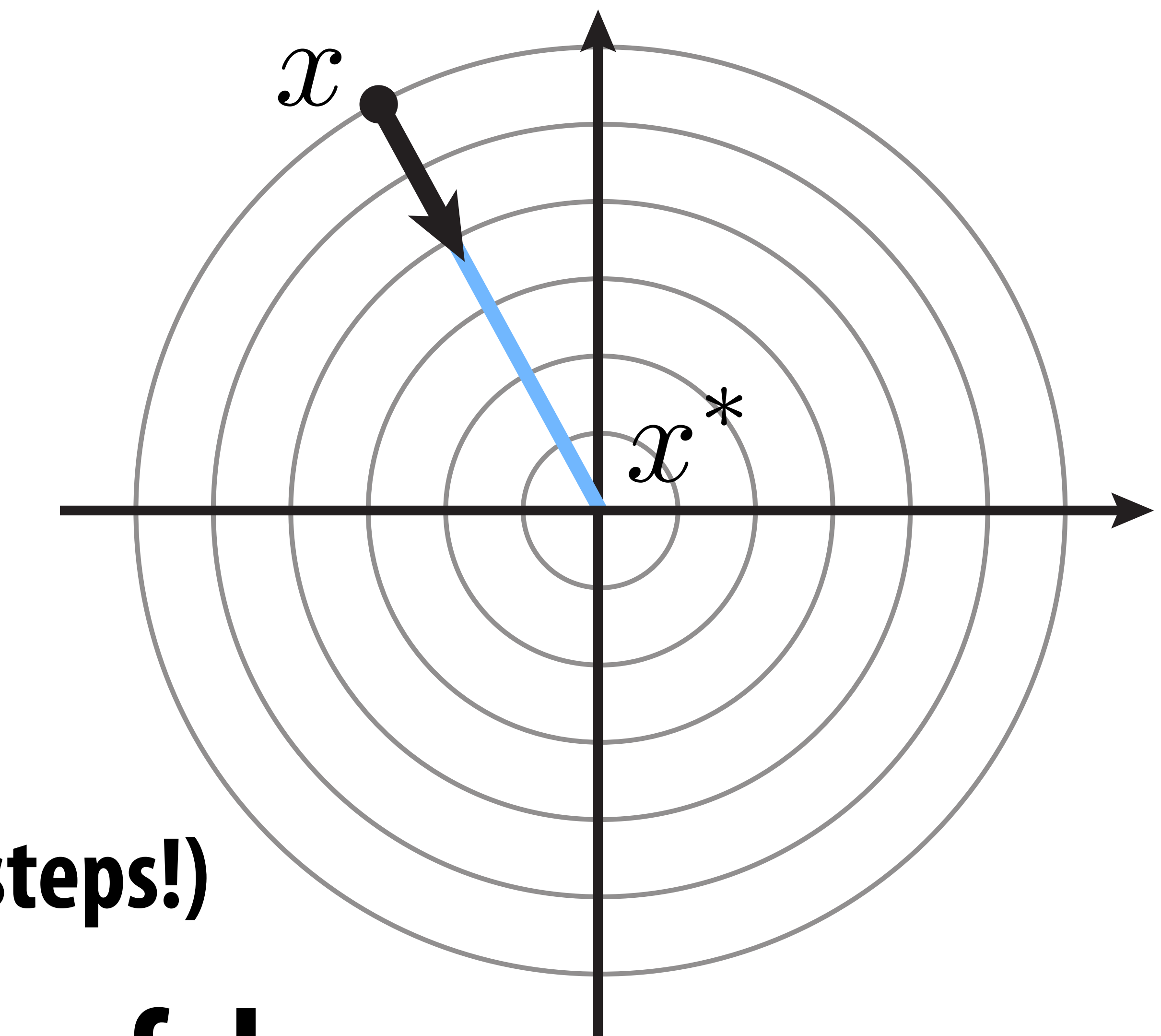
$$x_{k+1} = x_k - \tau \nabla f_0(x_k)$$

- **Basic challenge in nD:**
  - **solution can "oscillate"**
  - **takes many, many small steps**
  - **very slow to converge**



Higher Order Descent

- **General idea: apply a coordinate transformation so that the local energy landscape looks more like a "round bowl"**
- **Gradient now points directly toward nearby minimizer**
- **Most basic strategy: Newton's method:**



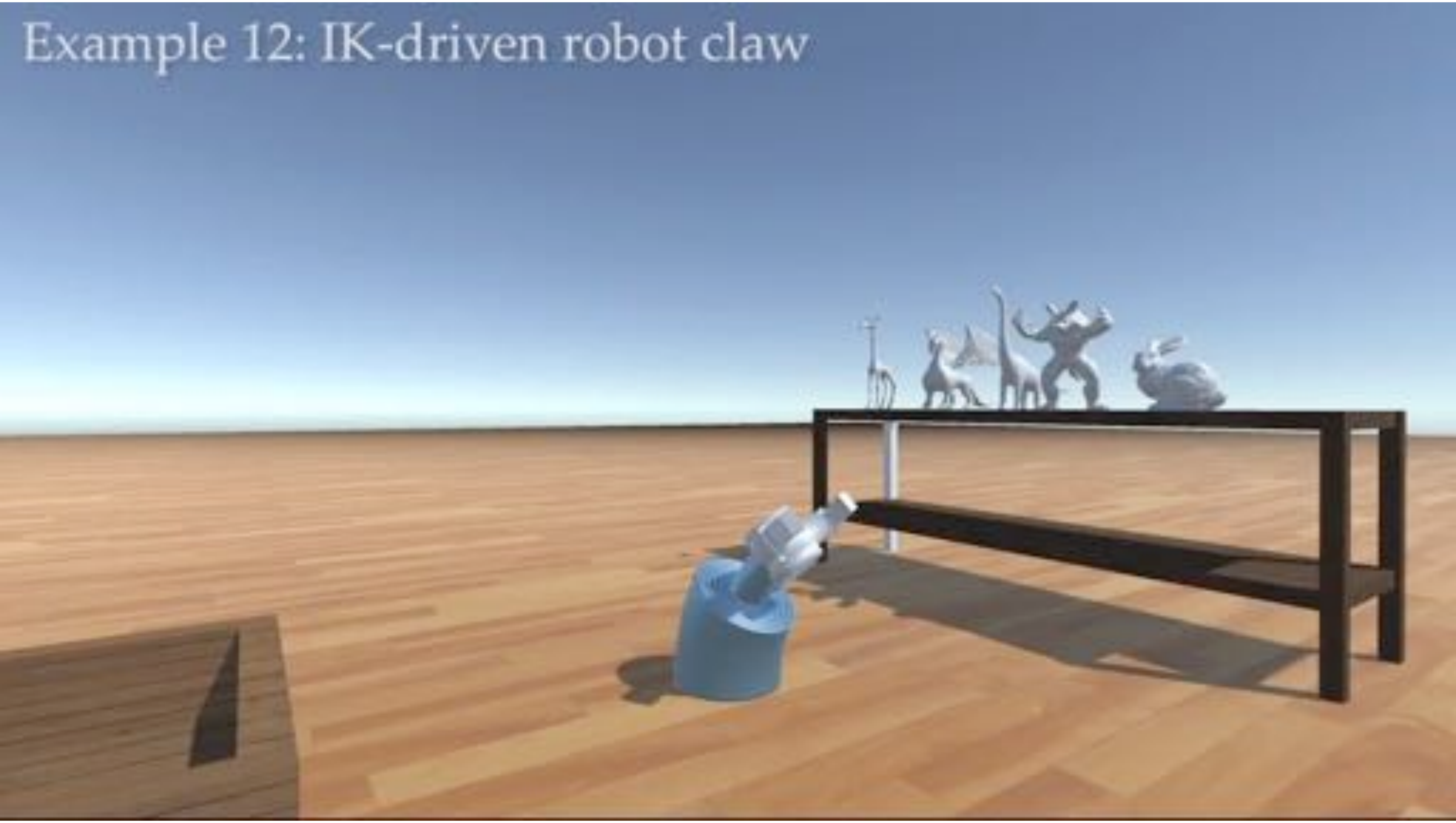
gradient

$$x_{k+1} = x_k - \tau(\nabla^2 f_0(x_k))^{-1} \nabla f_0(x_k)$$

Hessian inverse

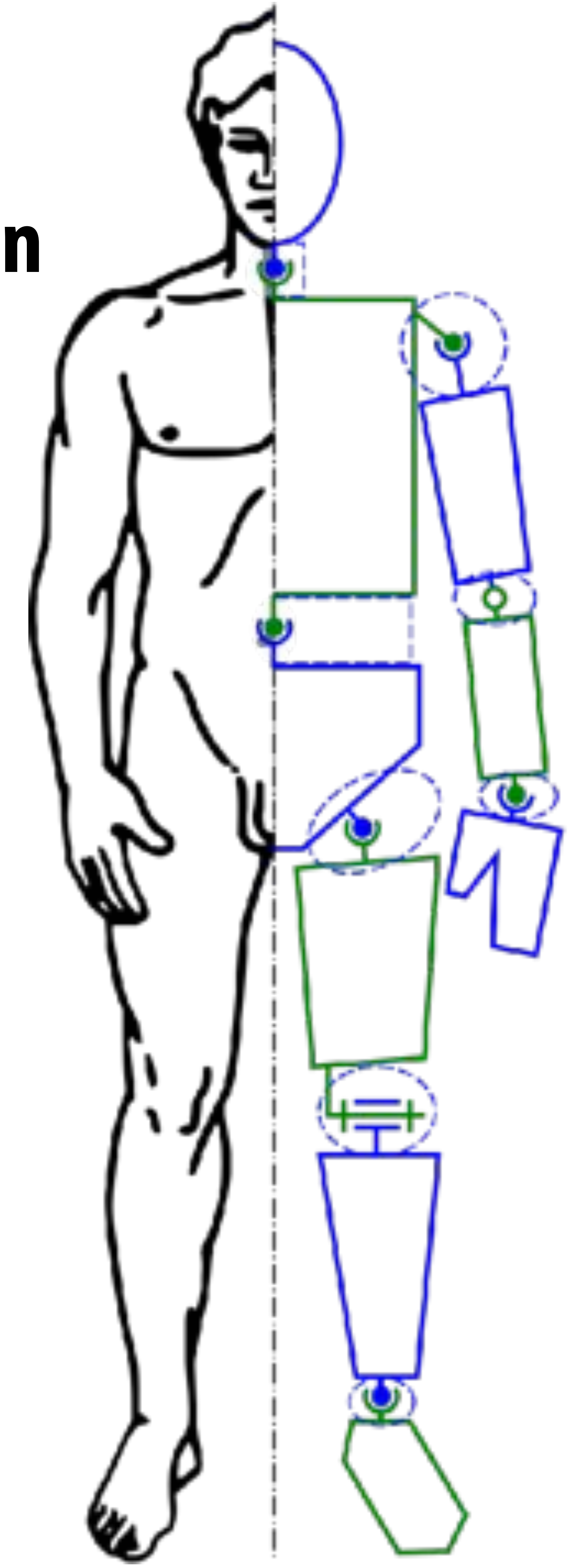
- **Great for convex problems (even proofs about # of steps!)**
- **For nonconvex problems, need to be more careful**
- **In general, nonconvex optimization is a BLACK ART**
- **Meta-strategy: try lots of solvers, see what works!**
  - **quasi-Newton, trust region, L-BFGS, ...**

Example: Inverse Kinematics

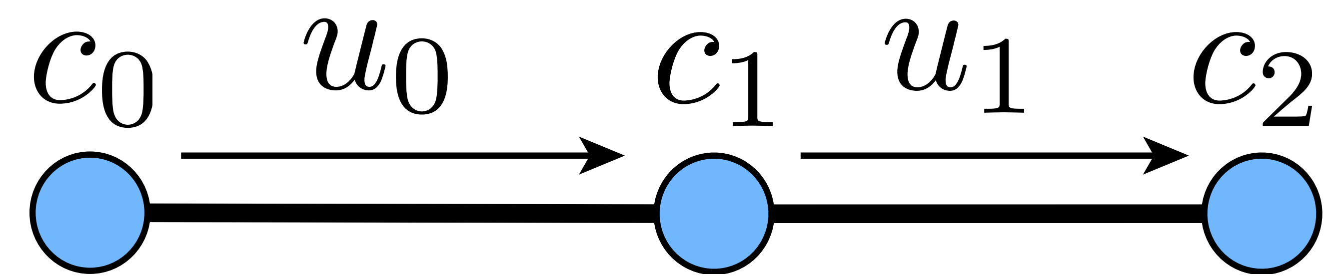


Forward Kinematics

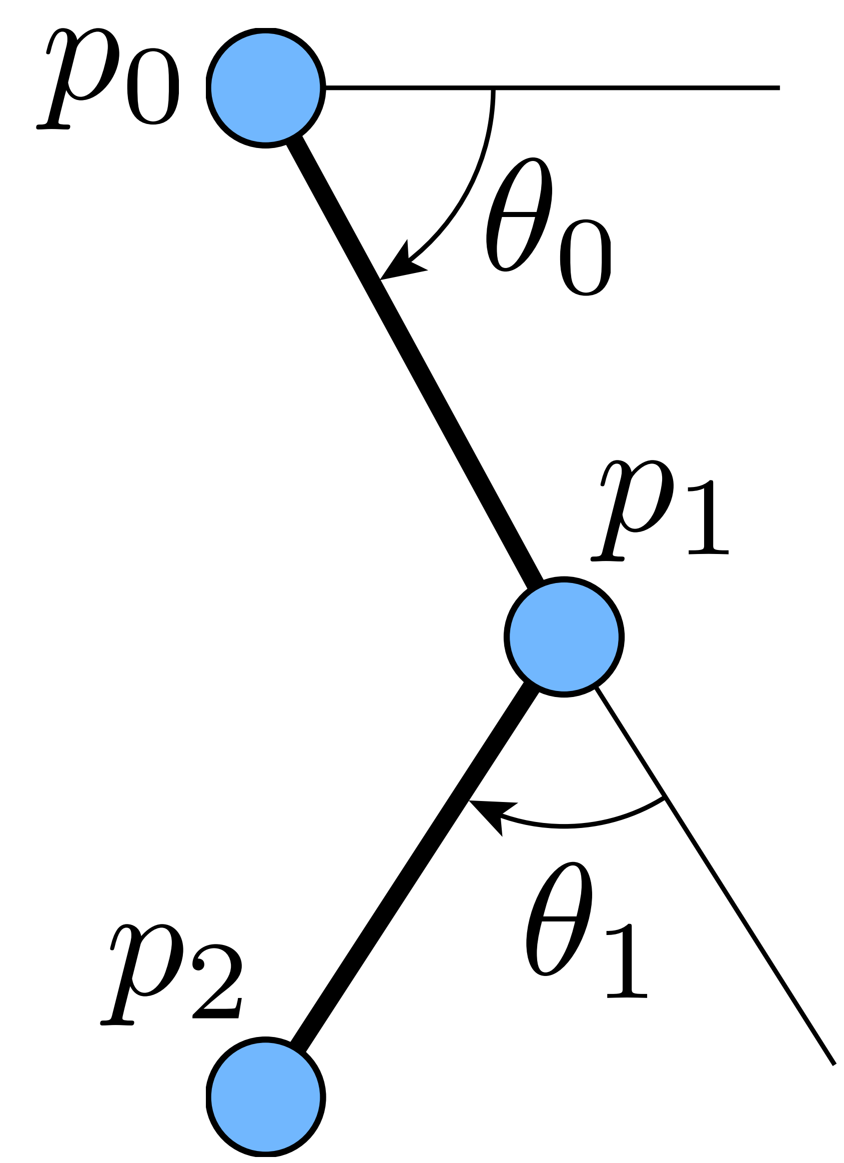
- Many systems well-described by a kinematic chain
  - collection of rigid bodies, connected by joints
  - joints have various behaviors (ball, piston, ...)
  - also have constraints (e.g., range of angles)
  - hierarchical structure (body→leg→foot)
- In animation, often called a rig
- How do we specify the configuration of a "rig"?
  - One way: artist sets each joint individually
  - Another way: ...optimization!



Simple Kinematic Chain



- **Consider a simple path-like chain in 2D**
- **Q: How do we write p_1 in terms of the root position p_0, angles, & vectors $u := c_{i+1}-c_i$?**



$$p_1 = p_0 + \begin{bmatrix} \cos\theta_0 & \sin\theta_0 \\ -\sin\theta_0 & \cos\theta_0 \end{bmatrix} u_0$$

- **(For brevity, can use complex numbers:)**

$$p_1 = p_0 + e^{\imath\theta_0} u_0$$

- **Q: How about p_2?**

$$p_2 = p_0 + e^{\imath\theta_0} u_0 + e^{\imath\theta_0} e^{\imath\theta_1} u_1$$

Simple IK Algorithm

- **Basic idea behind our IK algorithm:**
  - **write down distance between final point and "target"**
  - **compute gradient with respect to angles**
  - **apply gradient descent**
- **Objective?**

$$f_0(\theta) = \frac{1}{2}|\tilde{p}_n - p_n|^2$$

- **Constraints?**
  - **None! The joint angle can take any value.**
  - **Though we could limit joint angles (for instance)**

Physically-Based Animation and PDEs

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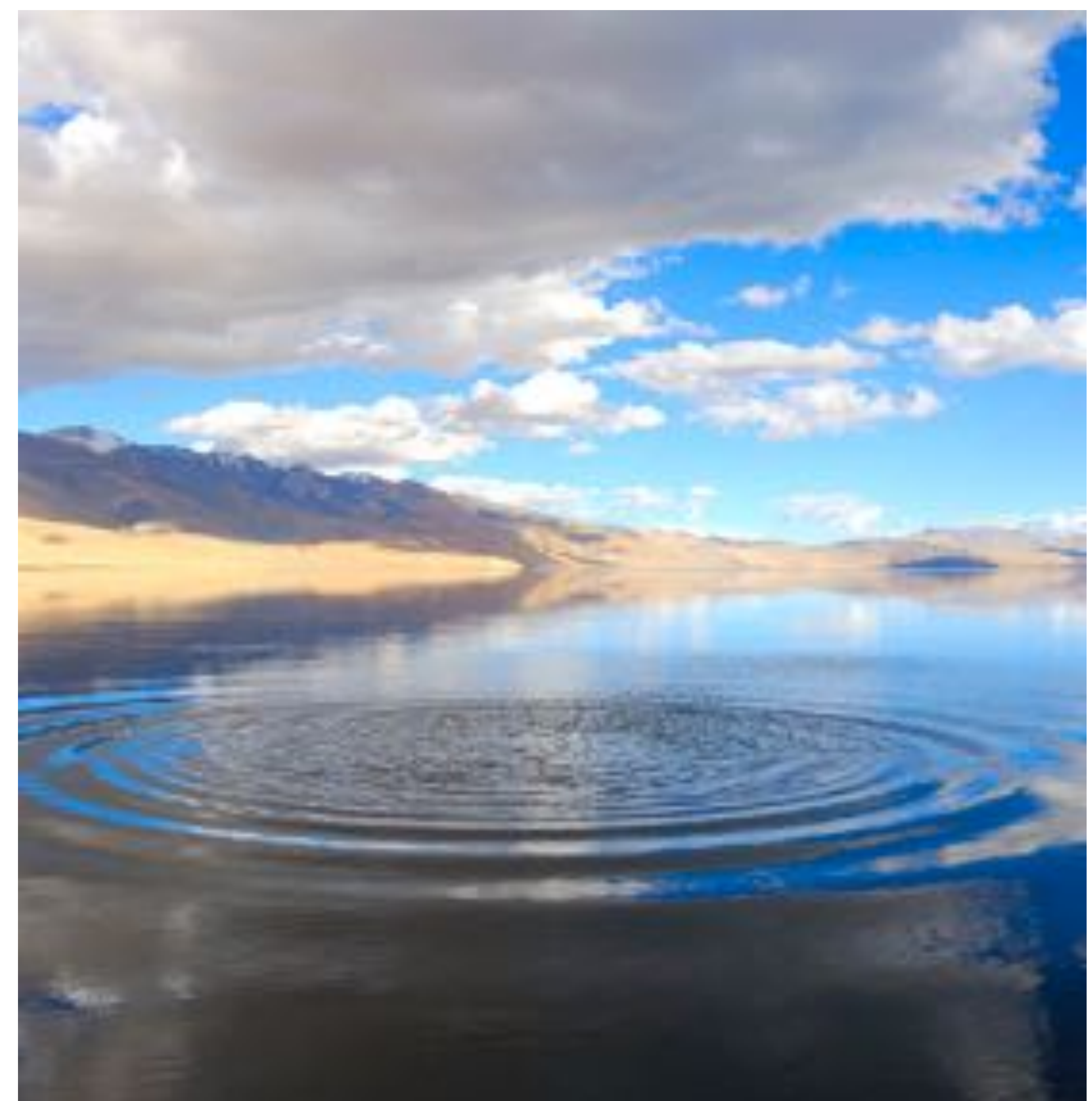
Partial Differential Equations (PDEs)

- ODE: Implicitly describe function in terms of its time derivatives
- Like any implicit description, have to solve for actual function
- PDE: Also include space derivatives in description

ODE—rock flies through air

PDE—rock lands in pond



To make a long story short...

- **Solving ODE looks like "add a little velocity each time"**

$$q_{k+1} = q_k + \tau f(q)$$

- **Solving a PDE looks like "take weighted combination of neighbors to get velocity (...and add a little velocity each time)"**

	1	
1	-4	1
	1	

$f(q)$

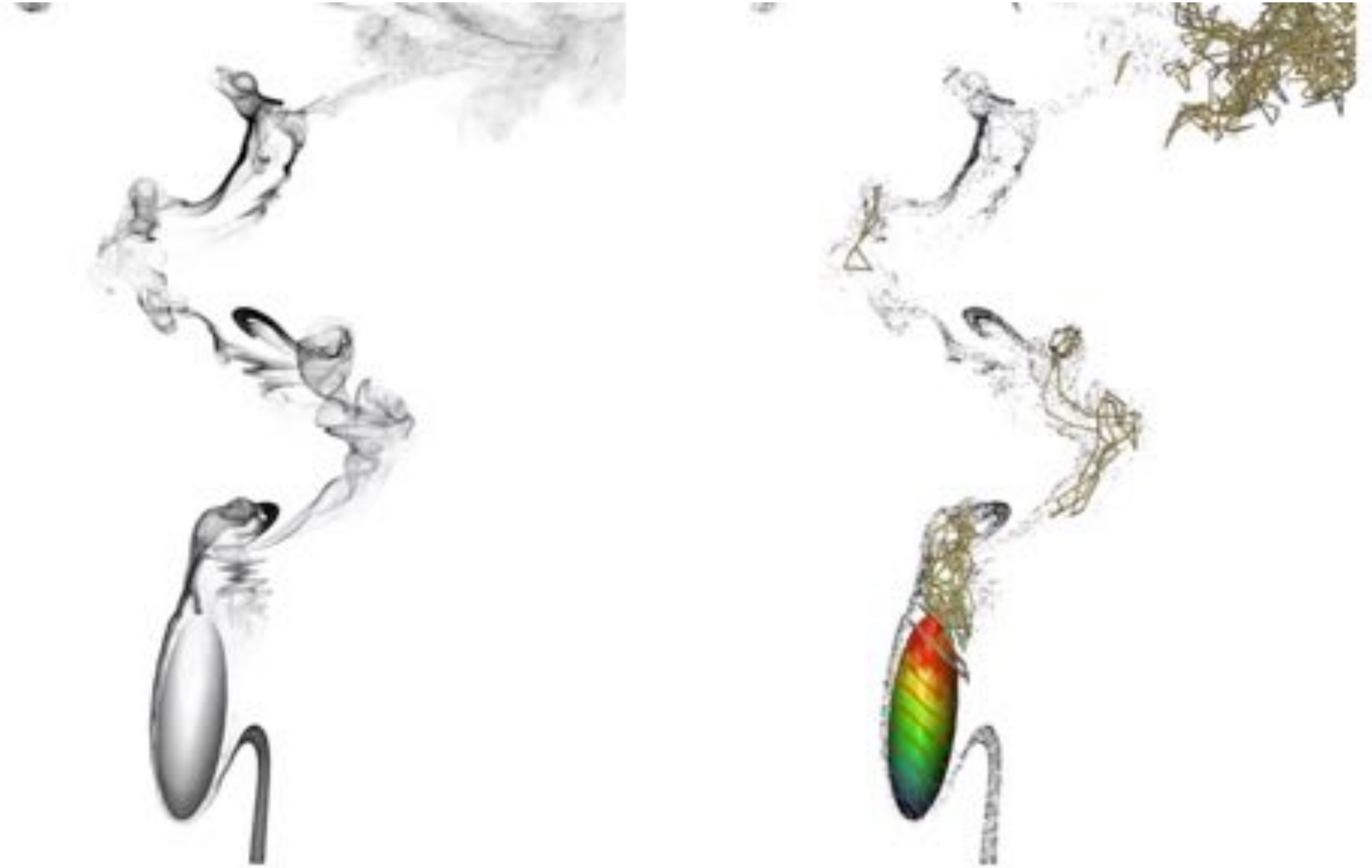
$$q_{k+1} = q_k + \tau f(q)$$

...obviously there is a lot more to say here!

Liquid Simulation in Graphics

Losasso, F., Shinar, T. Selle, A. and Fedkiw, R., "Multiple Interacting Liquids"

Smoke Simulation in Graphics

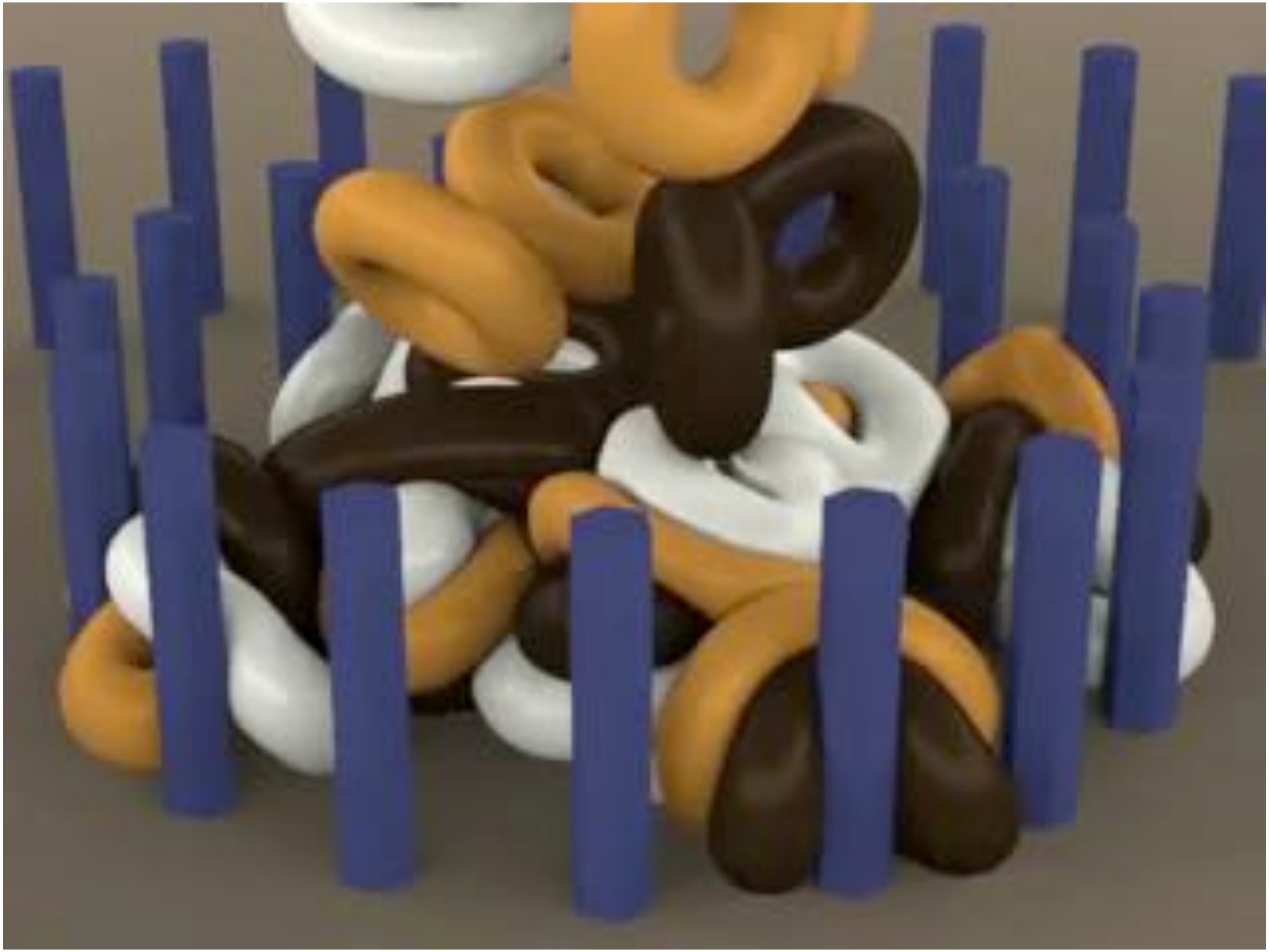


S. Weißmann, U. Pinkall. "Filament-based smoke with vortex shedding and variational reconnection"

Cloth Simulation in Graphics

Zhili Chen, Renguo Feng and Huamin Wang, “Modeling friction and air effects between cloth and deformable bodies”

Elasticity in Graphics

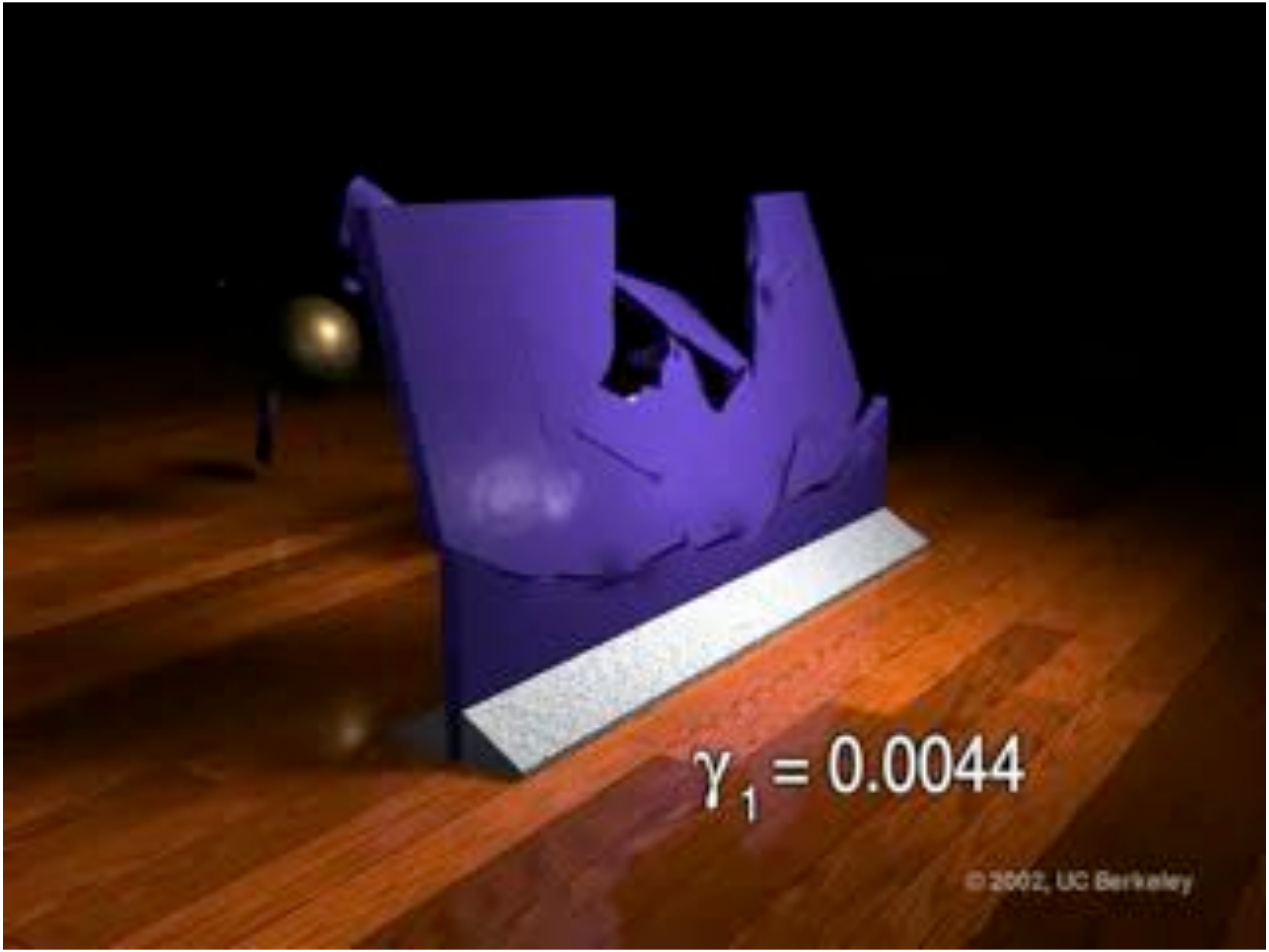


Irving, G., Schroeder, C. and Fedkiw, R., "Volume Conserving Finite Element Simulation of Deformable Models"

Hair Simulation in Graphics

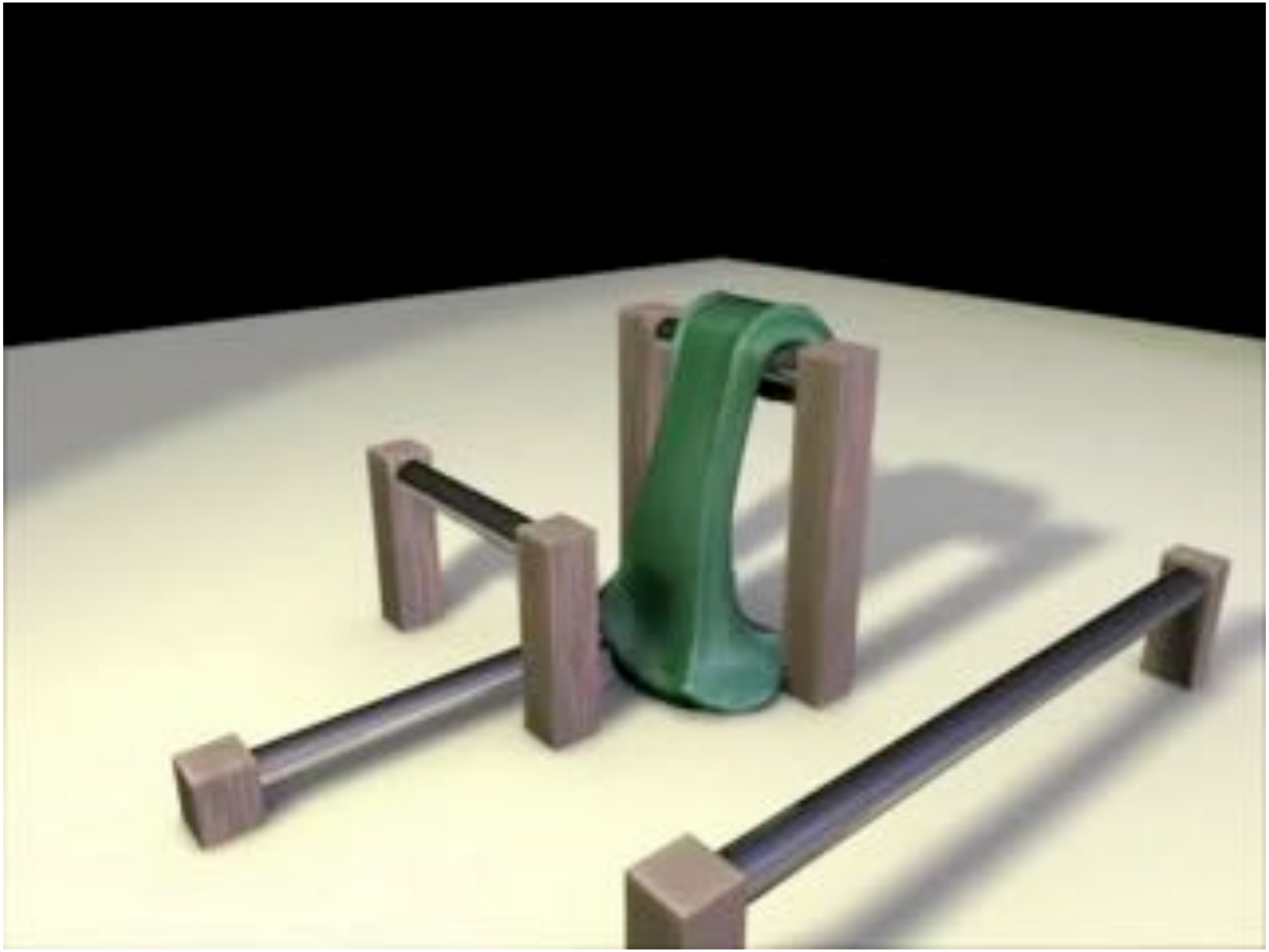
Danny M. Kaufman, Rasmus Tamstorf, Breannan Smith, Jean-Marie Aubry, Eitan Grinspun, "Adaptive Nonlinearity for Collisions in Complex Rod Assemblies"

Fracture in Graphics



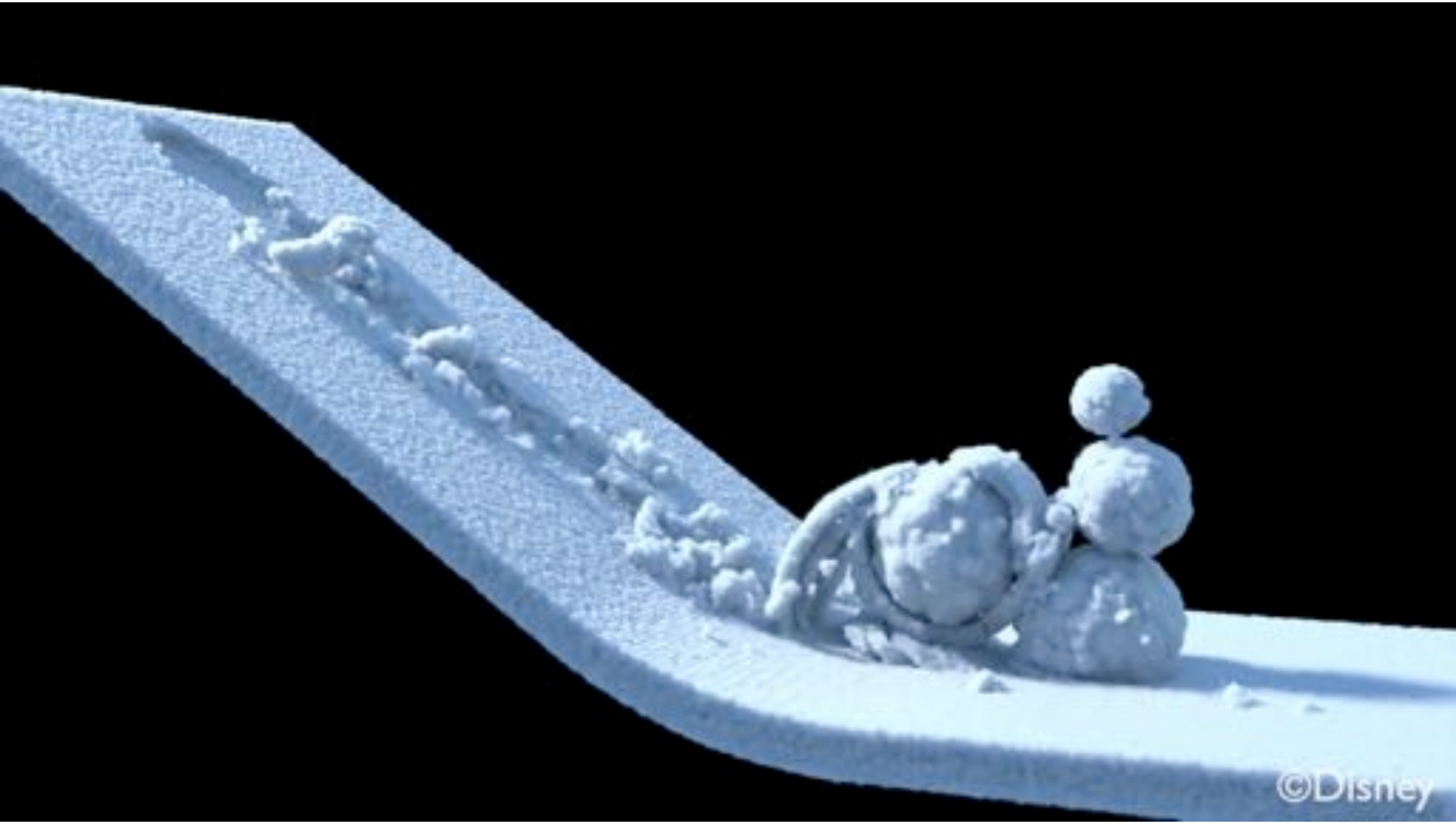
James F. O'Brien, Adam Bargteil, Jessica Hodgins, “Graphical Modeling and Animation of Ductile Fracture”

Viscoelasticity in Graphics



Chris Wojtan, Greg Turk, "Fast Viscoelastic Behavior with Thin Features"

Snow Simulation in Graphics



Alexey Stomakhin, Craig Schroeder, Lawrence Chai, Joseph Teran, Andrew Selle, “A Material Point Method For Snow Simulation”

Definition of a PDE

- **Want to solve for a function of time and space**

$$\underset{\text{time}}{} \quad u(t, x) \quad \underset{\text{space}}{}$$

time space

- **Function given implicitly in terms of derivatives:**

$$\dot{u}, \ddot{u}, \frac{d}{dt^3}u, \frac{d}{dt^4}u, \ldots$$

any combination of time derivatives

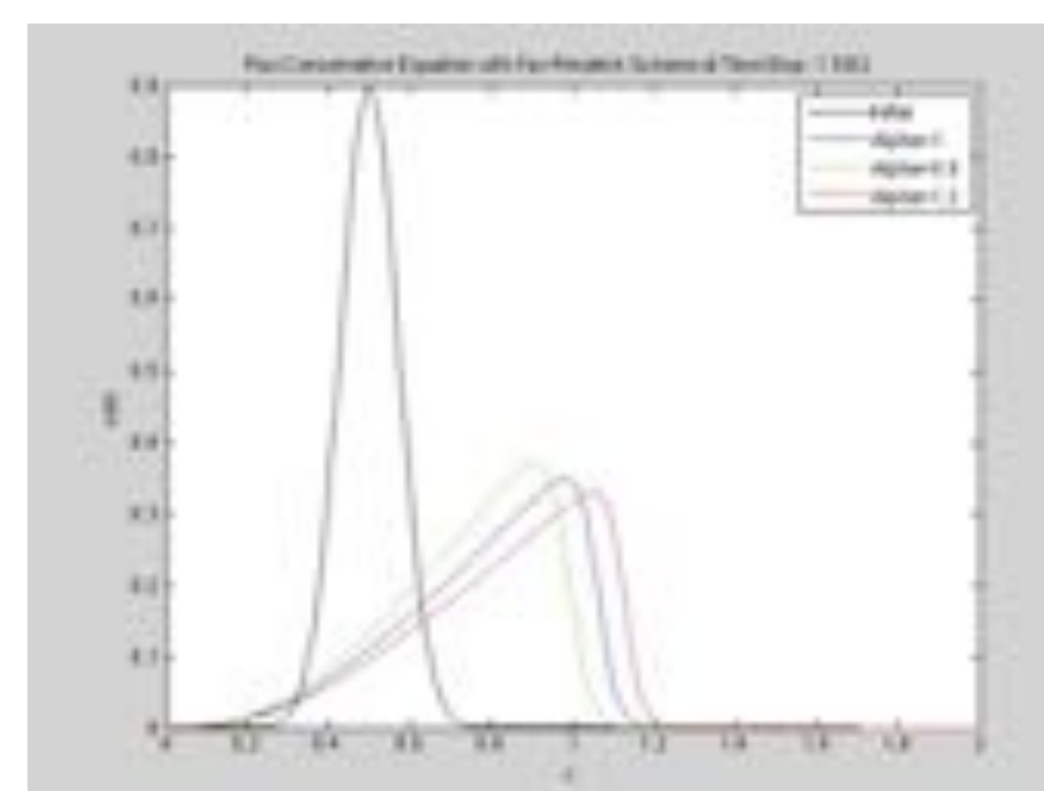
$$\frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, \frac{\partial^2 u}{\partial x_1 \partial x_2}, \frac{\partial^m + nu}{\partial x_i^m \partial x_j^n}, \ldots$$

plus any combination of space derivatives

- **Example:**

$$\dot{u} + uu' = au''$$

(Burgers' equation)



Anatomy of a PDE

- **Linear vs. nonlinear: how are derivatives combined?**

nonlinear!

$$\dot{u} + uu' = au''$$

(Burgers' equation)

$$\dot{u} = au''$$

(diffusion equation)

- **Order: how many derivatives in space & time?**

1st order in time

2nd order in space

$$\dot{u} + uu' = au''$$

(Burgers' equation)

2nd order in time

2nd order in space

$$\ddot{u} = au''$$

(wave equation)

- **Nonlinear / higher order $\Rightarrow$ HARDER TO SOLVE!**

Model Equations

- **Fundamental behavior of many important PDEs is well-captured by three model linear equations:**

Solve numerically?

"Laplacian" (more later!)

LAPLACE EQUATION ("ELLIPTIC") $\Delta u = 0$

"what's the smoothest function interpolating the given boundary data"

HEAT EQUATION ("PARABOLIC") $\dot{u} = \Delta u$

"how does an initial distribution of heat spread out over time?"

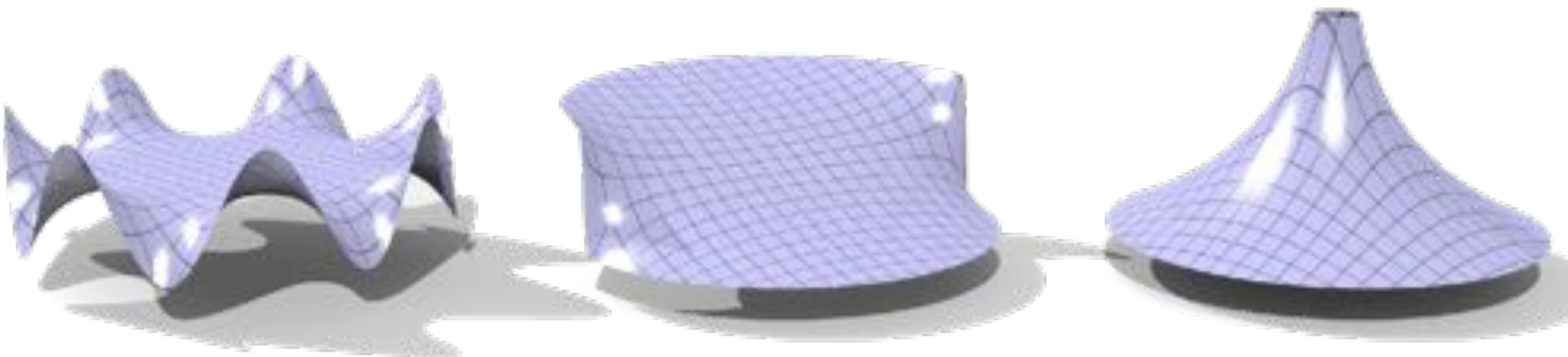
WAVE EQUATION ("HYPERBOLIC") $\ddot{u} = \Delta u$

"if you throw a rock into a pond, how does the wavefront evolve over time?"

[NONLINEAR + HYPERBOLIC + HIGH-ORDER]

Elliptic PDEs / Laplace Equation

- "What's the smoothest function interpolating the given boundary data?"

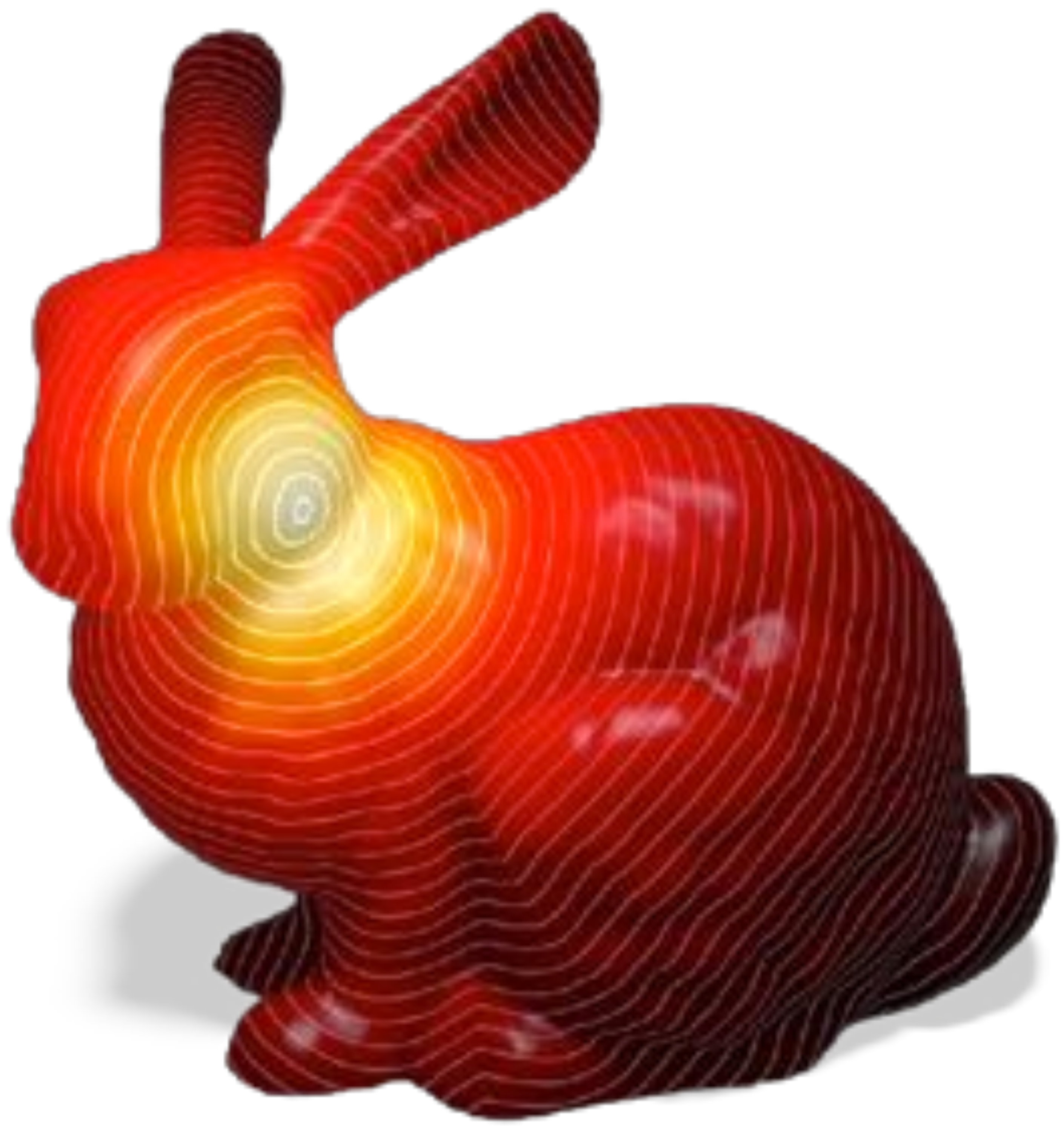


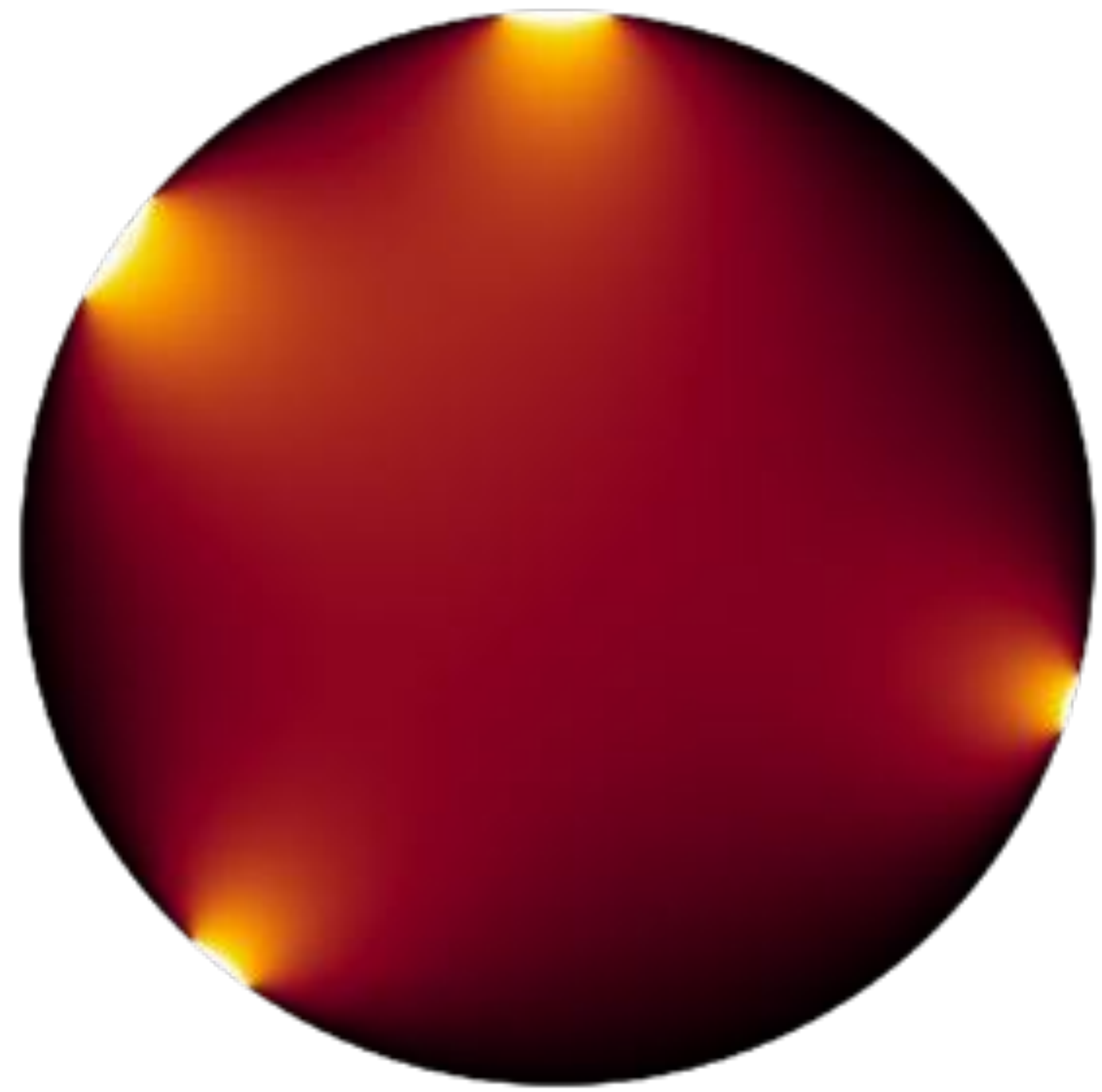
- Conceptually: each value is at the average of its "neighbors"
- Roughly speaking, why is it easier to solve?
- Very robust to errors: just keep averaging with neighbors!

Image from Solomon, Crane, Vouga, "Laplace-Beltrami: The Swiss Army Knife of Geometry Processing"

Parabolic PDEs / Heat Equation

- "How does an initial distribution of heat spread out over time?"





- After a long time, solution is same as Laplace equation!
- Models damping / viscosity in many physical systems

Hyperbolic PDEs / Wave Equation

- "If you throw a rock into a pond, how does the wavefront evolve over time?"

- Errors made at the beginning will persist for a long time! (hard)

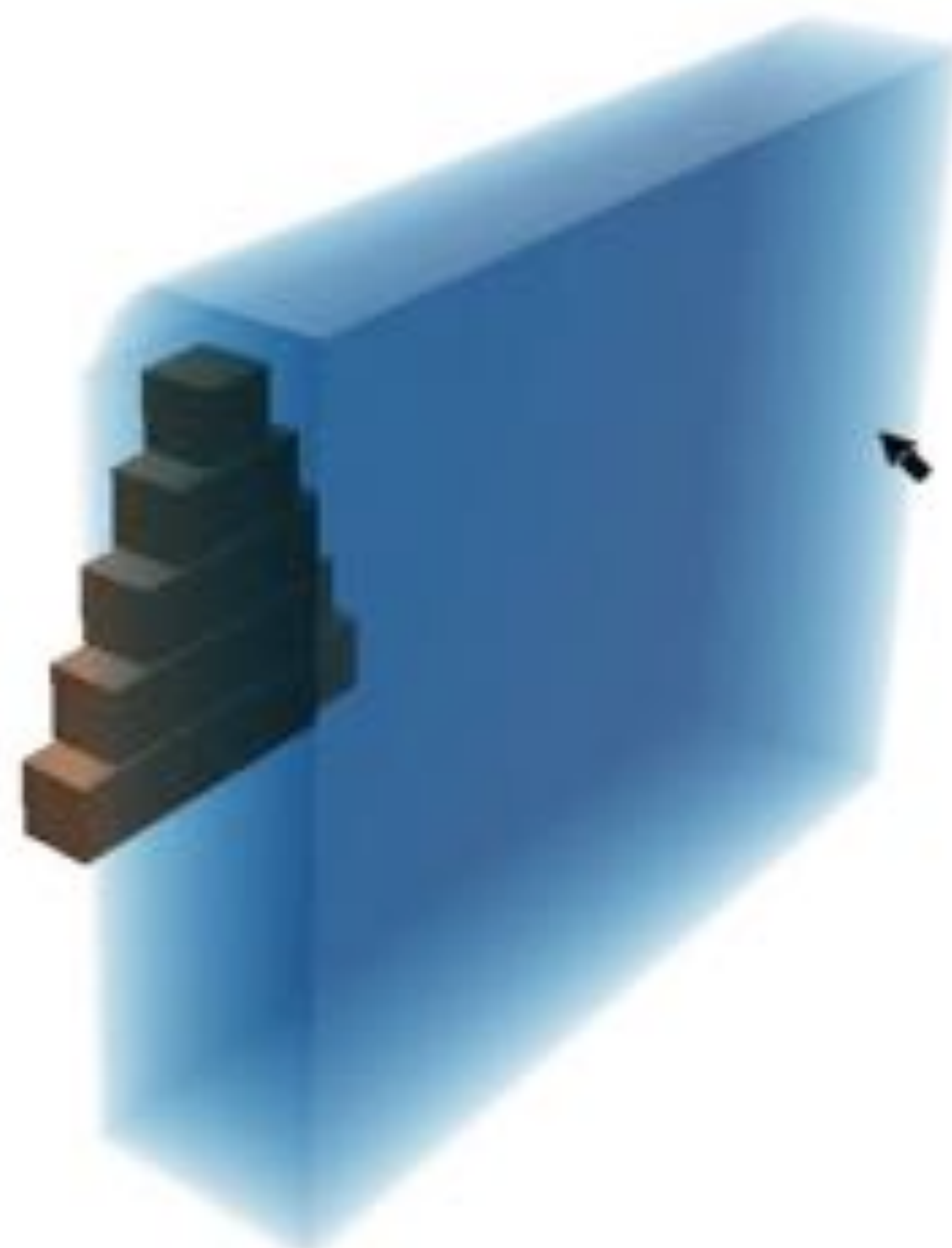
How did we do that?

Numerical Solution of PDEs—Overview

- Like ODEs, many interesting PDEs are difficult/impossible to solve analytically—especially if we want to incorporate data (e.g., user interaction)
- Must instead use numerical integration
- Basic strategy:
  - pick a time discretization (forward Euler, backward Euler...)
  - pick a spatial discretization (TODAY)
  - as with ODEs, run a time-stepping algorithm
- Historically, very expensive—only for "hero shots" in movies
- Computers are ever faster...
- More & more use of PDEs in games, interactive tools, ...

Real Time PDE-Based Simulation (Fire)

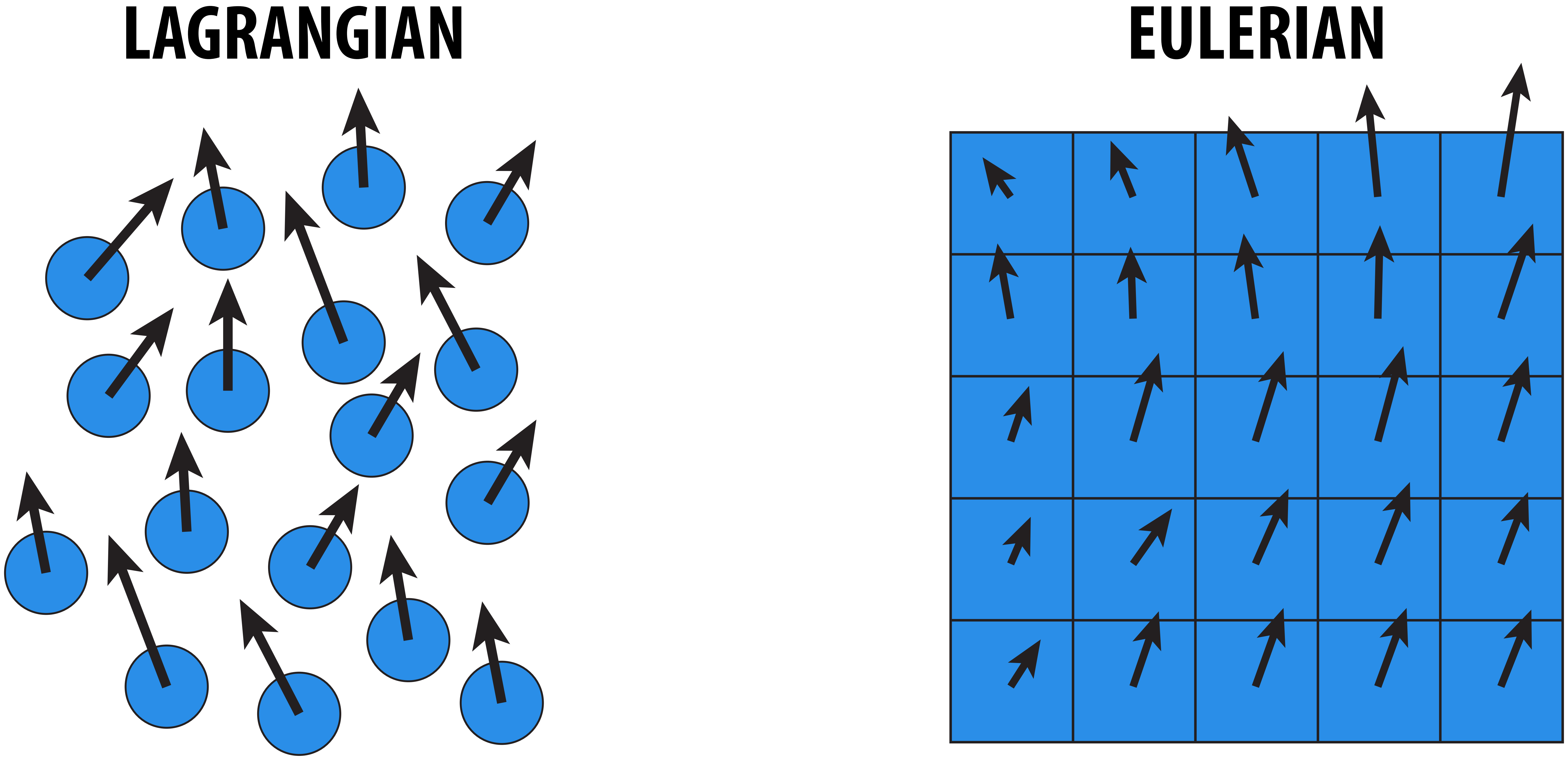
Real Time PDE-Based Simulation (Water)



Nuttapong Chentanez, Matthias Müller, “Real-time Eulerian water simulation using a restricted tall cell grid”

Lagrangian vs. Euler

- Two basic ways to discretize space: Lagrangian & Eulerian
- E.g., suppose we want to encode the motion of a fluid

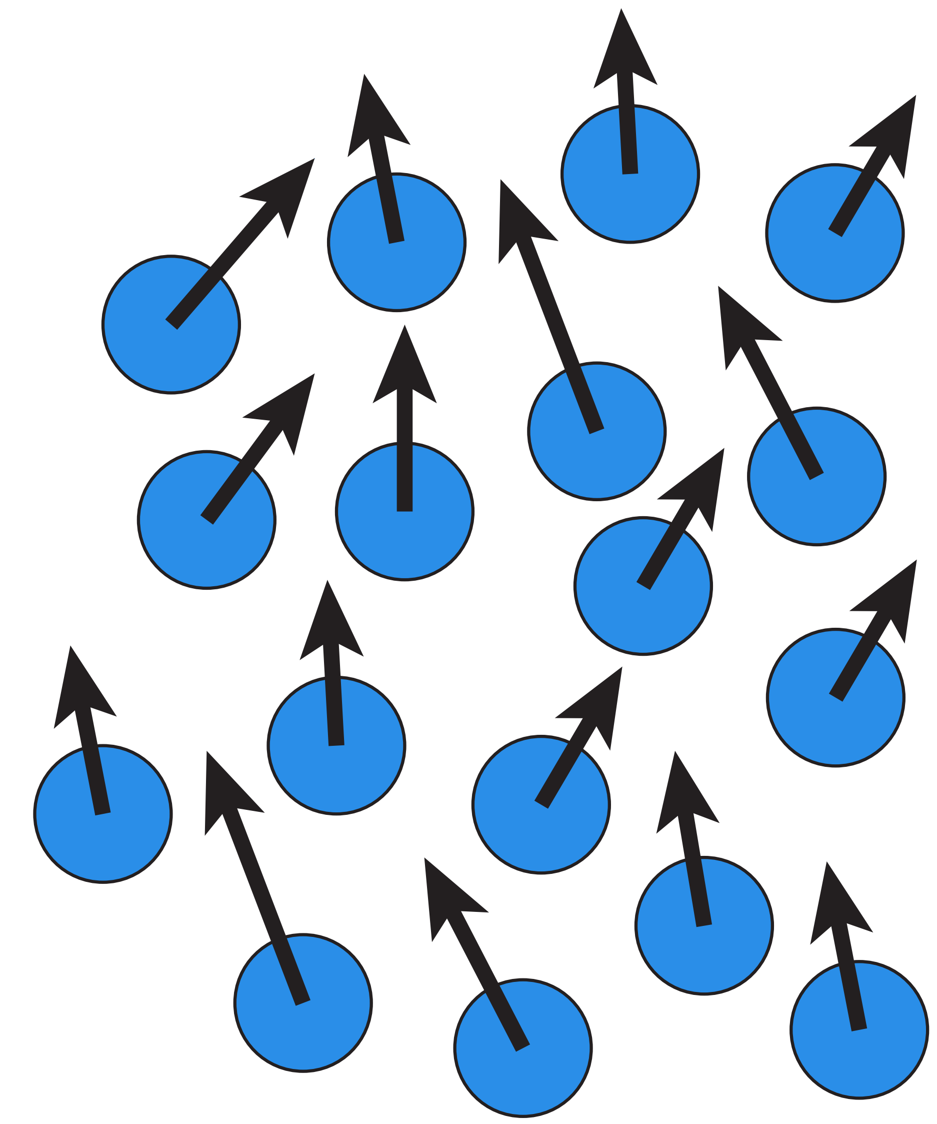


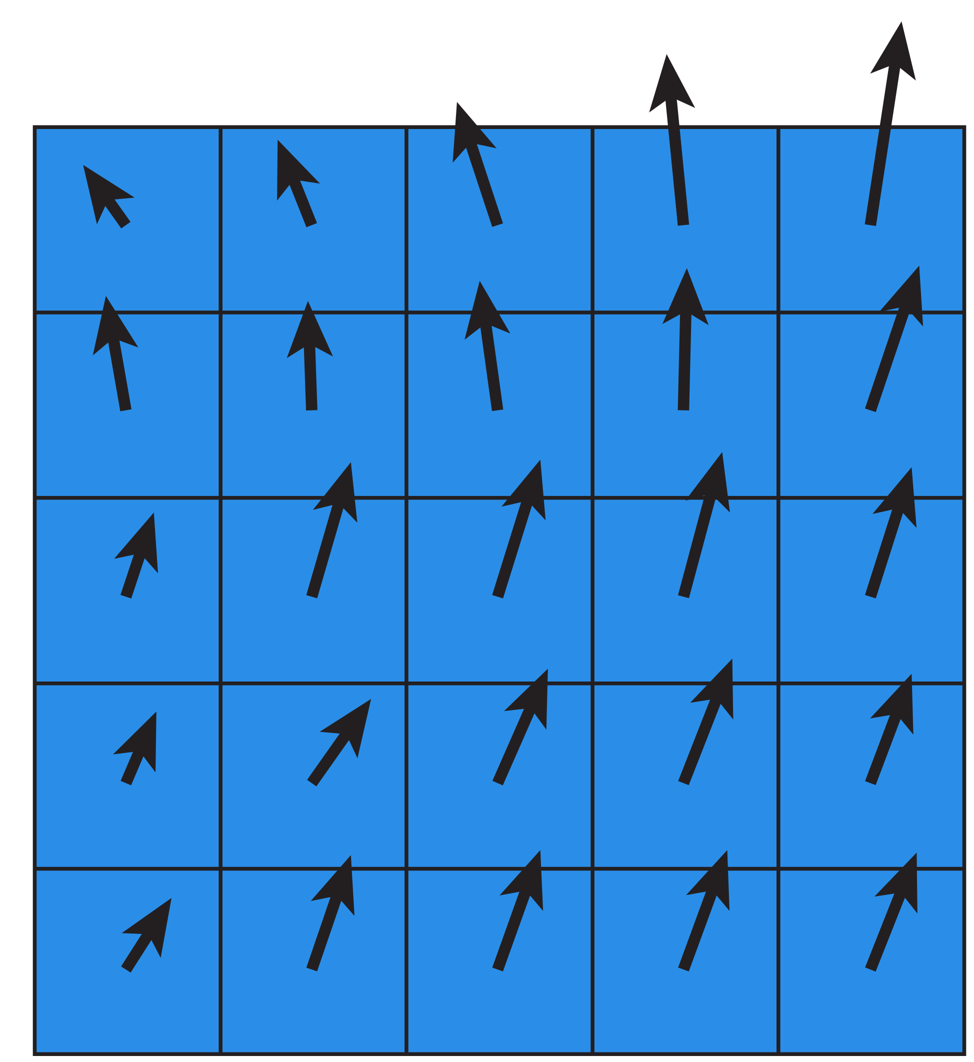
track position & velocity of moving particles

track velocity (or flux) at fixed grid locations

Lagrangian vs. Eulerian—Trade-Offs

- **Lagrangian**
  - conceptually easy (like polygon soup!)
  - resolution/domain not limited by grid
  - good particle distribution can be tough
  - finding neighbors can be expensive
- **Eulerian**
  - fast, regular computation
  - easy to represent, e.g., smooth surfaces
  - simulation “trapped” in grid
  - grid causes “numerical diffusion” (blur)
  - need to understand PDEs (but you will!)





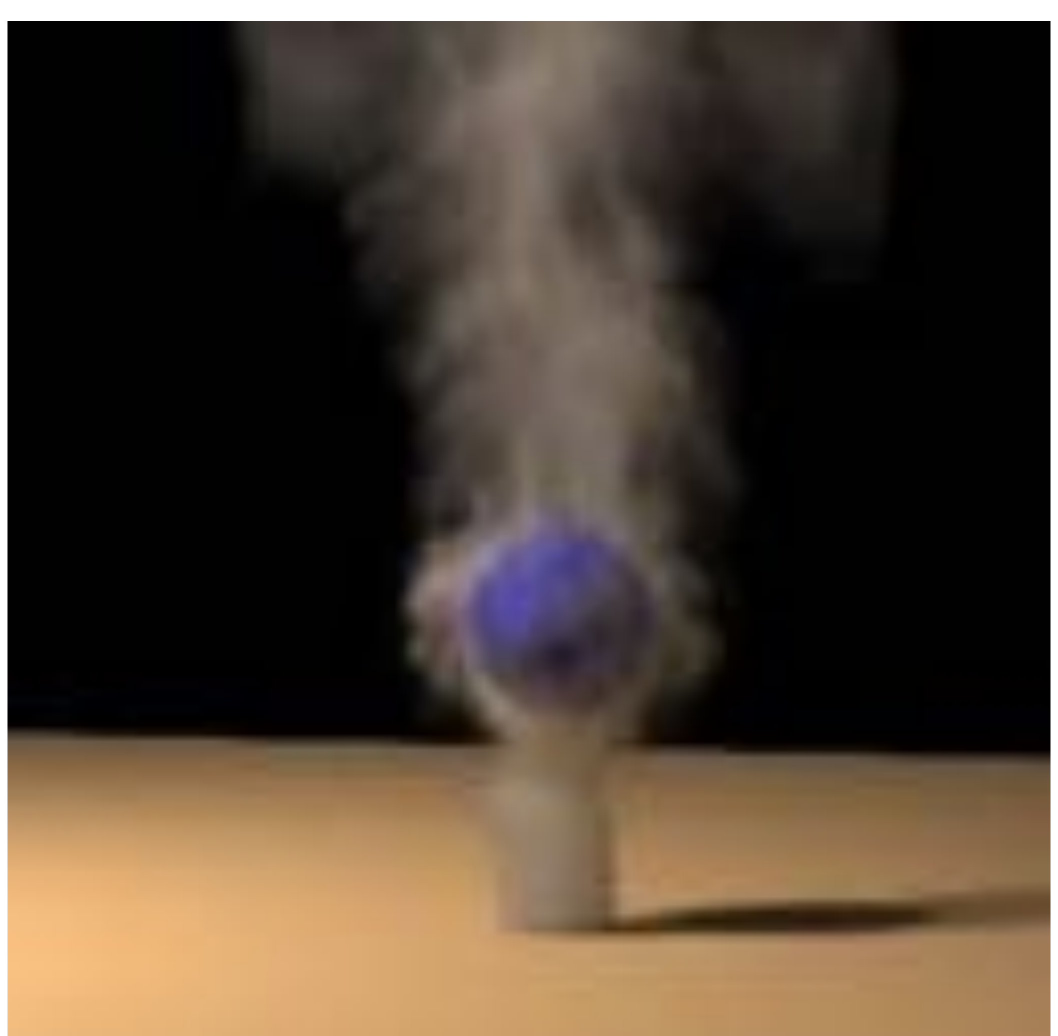
Mixing Lagrangian & Eulerian

- Of course, no reason you have to choose just one!
- Many modern methods mix Lagrangian & Eulerian:
  - PIC/FLIP, particle level sets, mesh-based surface tracking, Voronoi-based, arbitrary Lagrangian-Eulerian (ALE), ...
- Pick the right tool for the job!

Maya Bifrost

Aside: Which Quantity Do We Solve For?

- Many PDEs have mathematically equivalent formulations in terms of different quantities
- E.g., incompressible fluids:
  - velocity—how fast is each particle moving?
  - vorticity—how fast is fluid "spinning" at each point?
- Computationally, can make a big difference
- Pick the right tool for the job!



Ok, but we're getting way ahead of ourselves. How do we solve easy PDEs?

Numerical PDEs—Basic Strategy

Richard Courant

- Pick PDE formulation
  - Which quantity do we want to solve for?
  - E.g., velocity or vorticity?
- Pick spatial discretization
  - How do we approximate derivatives in space?
- Pick time discretization
  - How do we approximate derivatives in time?
  - When do we evaluate forces?
  - Forward Euler, backward Euler, symplectic Euler, ...
- Finally, we have an update rule
- Repeatedly solve to generate an animation

The Laplace Operator

- All of our model equations used the Laplace operator
- Different conventions for symbol:

Δ same symbol used for "change"

∇^2 same symbol used for Hessian!

- Unbelievably important object showing up everywhere across physics, geometry, signal processing, ...
- Ok, but what does it mean?
- Differential operator: eats a function, spits out its "2nd derivative"
- What does that mean for a function u: $R^n \rightarrow R$?
  - divergence of gradient
  - sum of second derivatives

$$\Delta u = \underbrace{\nabla}_{\text{div}} \cdot \underbrace{\nabla}_{\text{grad}} u$$

$$\Delta u = \frac{\partial u^2}{\partial x_1^2} + \cdots + \frac{\partial u^2}{\partial x_n^2}$$

Discretizing the Laplacian

- How do we approximate the Laplacian?
- Depends on discretization (Eulerian, Lagrangian, grid, mesh, ...)
- Two extremely common ways in graphics:

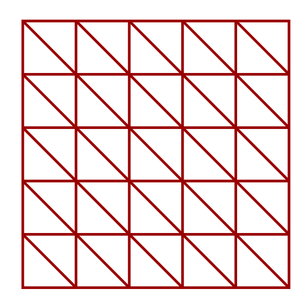
GRID

h

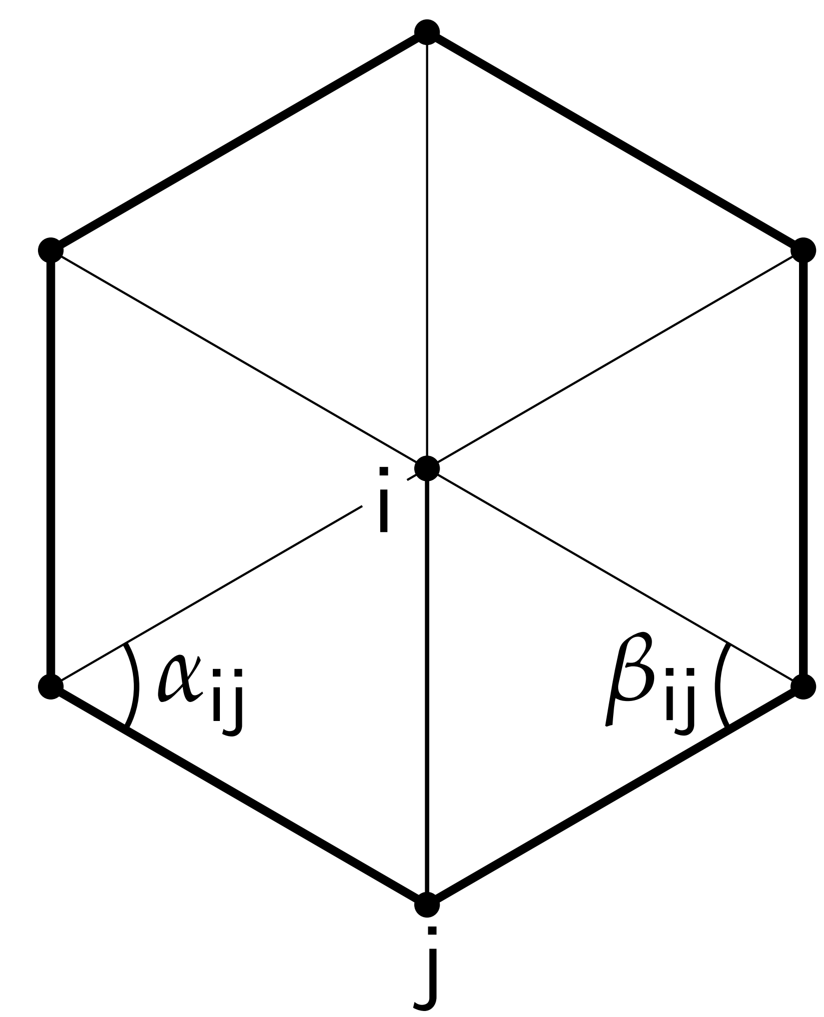
	1	
1	-4	1
	1	

$$\frac{4u_{ij} - u_{i+1,j} - u_{i-1,j} - u_{i,j+1} - u_{i,j-1}}{h^2}$$

(actually, this becomes that)



TRIANGLE MESH



$$\frac{1}{2}\sum_j (\cot\alpha_{ij} + \cot\beta_{ij})(u_j - u_i)$$

- Also not too hard on point clouds, polygon meshes, ...

Numerically Solving the Laplace Equation

- **Want to solve $\Delta u = 0$**
- **Plug in one of our discretizations, e.g.,**

	c	
d	a	b
	e	

$$\frac{4a - b - c - d - e}{h} = 0$$

$$\iff \quad a = \frac{1}{4}(b + c + d + e)$$

- **Oh: if we have a solution, then each value must be the average of the neighboring values.**
- **How do we solve this?**
- **One idea: keep averaging with neighbors! ("Jacobi method")**
- **Correct, but slow. Much better to use modern linear solver**

Solving the Heat Equation

- **Back to our three model equations, want to solve heat eqn.**

$$\dot{u} = \Delta u$$

- **Just saw how to discretize Laplacian**
- **Also know how to do time (forward Euler, backward Euler, ...)**
- **E.g., forward Euler:**

$$u^{k+1} = u^k + \Delta u^k$$

- **Q: On a grid, what's our overall update now at $u_{i,j}$?**

$$u_{i,j}^{k+1} = u^k + \tfrac{\tau}{h^2}(4u_{i,j}^k - u_{i+1,j}^k - u_{i-1,j}^k - u_{i,j+1}^k - u_{i,j-1}^k)$$

- **Not hard to implement! Loop over grid, add up some neighbors.**

Solving the Wave Equation

- **Finally, wave equation:**

$$\ddot{u} = \Delta u$$

- **Not much different; now have 2nd derivative in time**
- **By now we've learned two different techniques:**
  - **Convert to two 1st order (in time) equations:**

$$\dot{u} = v, \quad \dot{v} = \Delta u$$

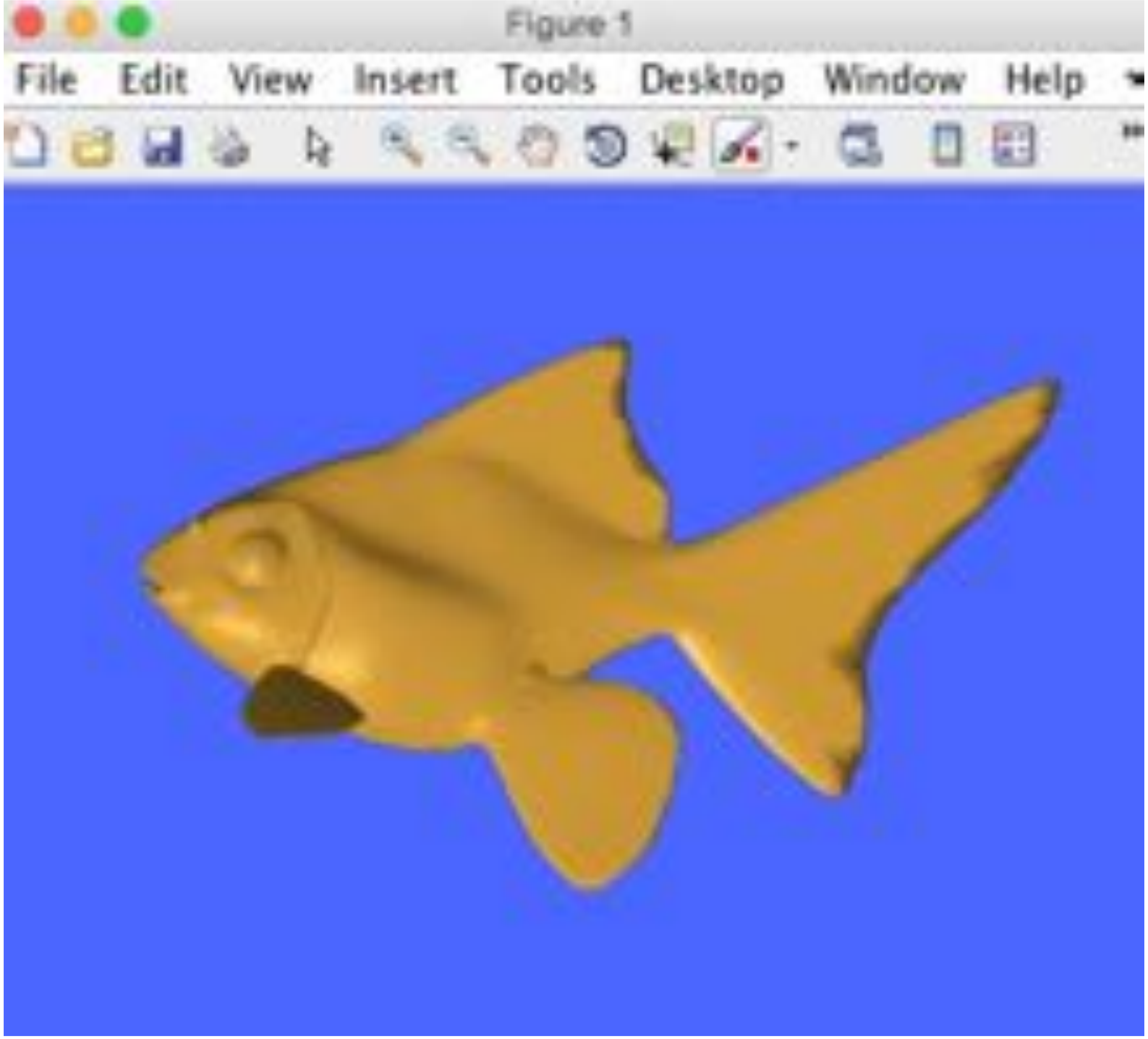
  - **Or, use centered difference (like Laplace) in time:**

$$\frac{u^{k+1} - 2u^k + u^{k-1}}{\tau^2} = \Delta u^k$$

- **Plus all our choices about how to discretize Laplacian.**
- **So many choices! And many, many (many) more we didn't discuss.**

Wave Equation on a Triangle Mesh

Credit: Alec Jacobson (http://www.alecjacobson.com/weblog/?p=4363)

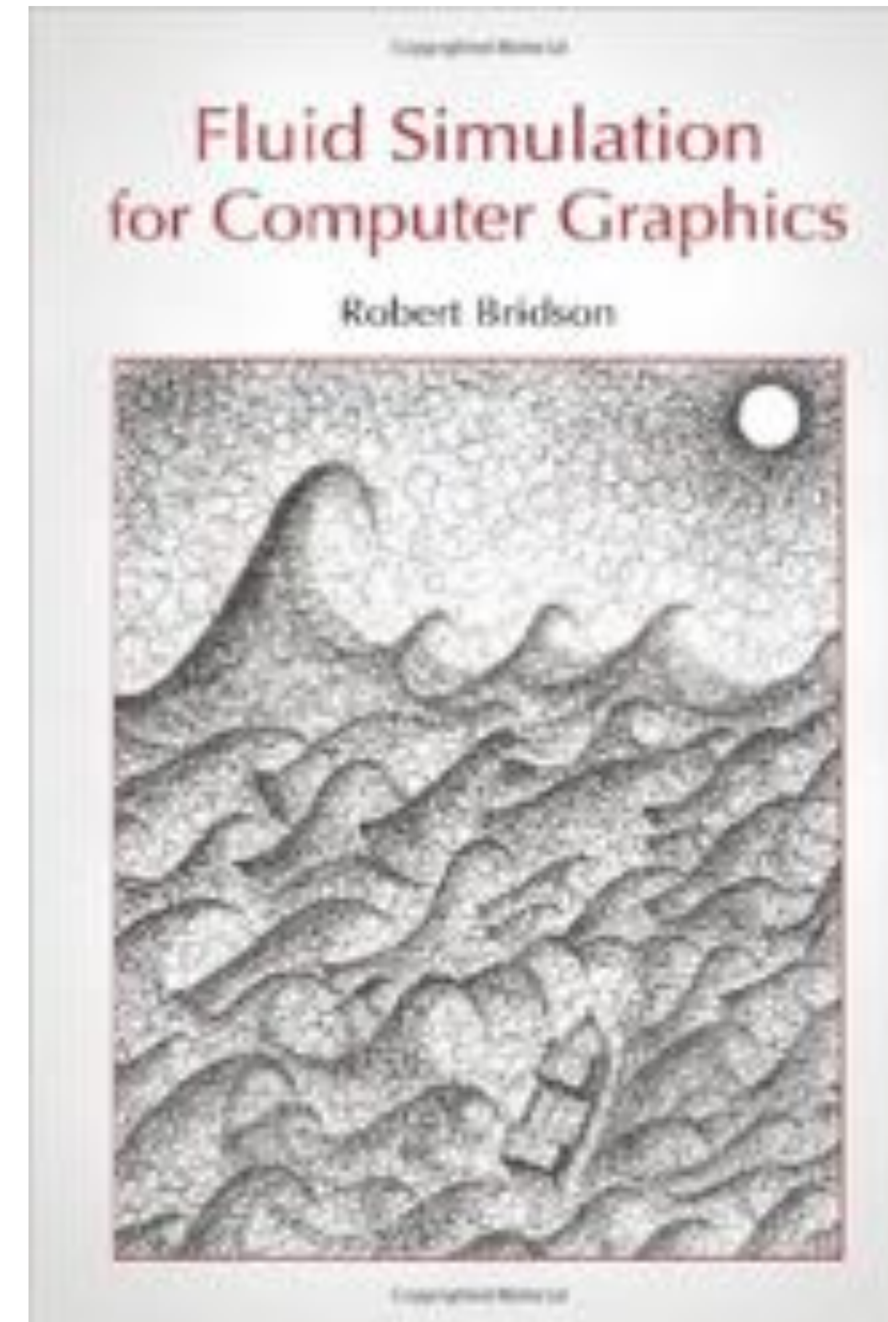


Also: http://www.adultswim.com/etcetera/elastic-man/

Wait, what about all those cool fluids and stuff?

Want to Know More?

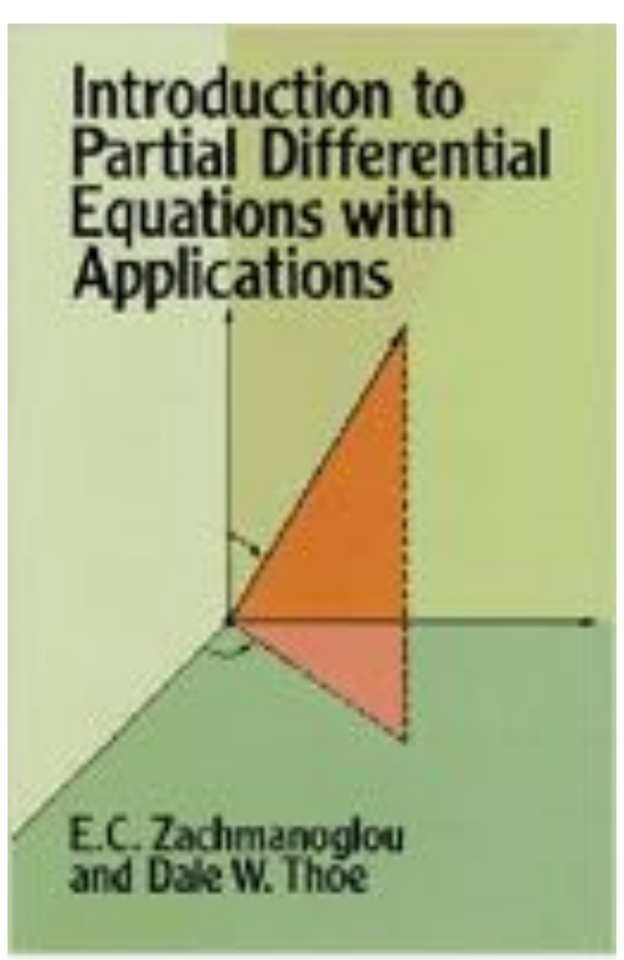
- There are some good books:

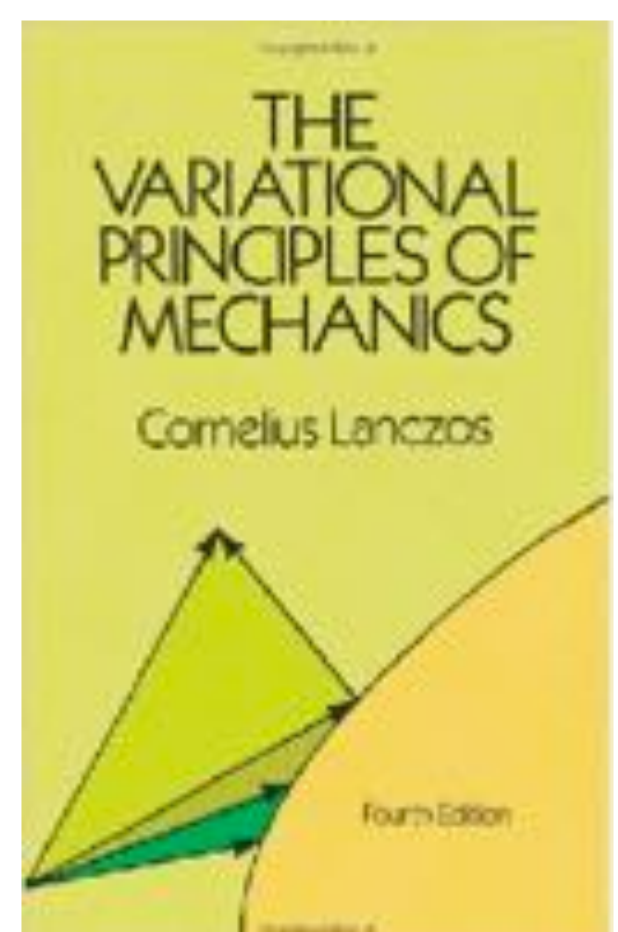


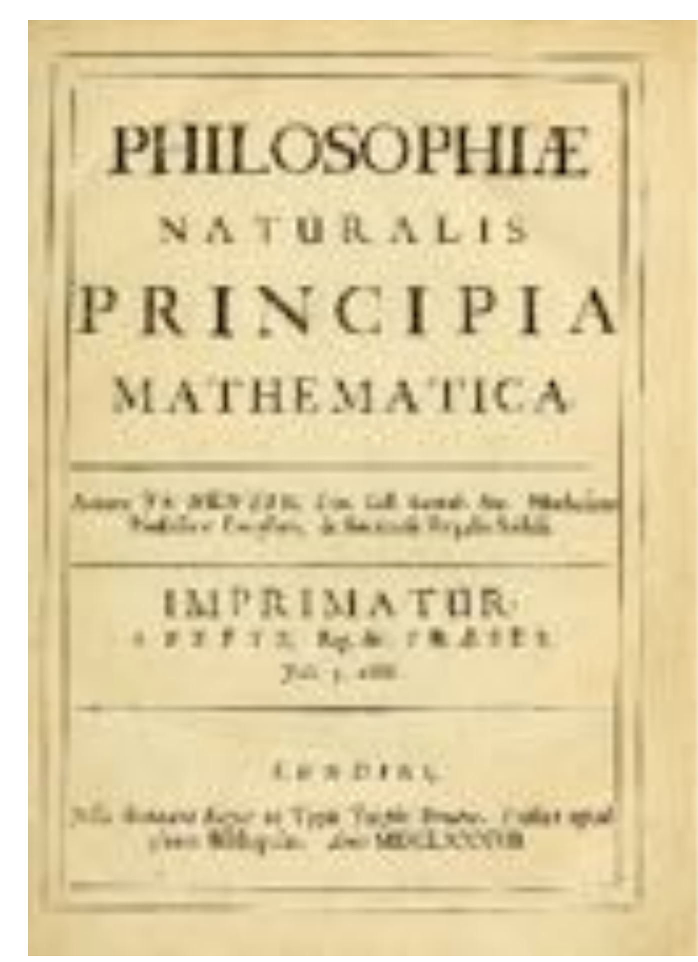
- And papers:

http://www.physicsbasedanimation.com/

- Also, what did the folks who wrote these books & papers read?







Also not covered: solving linear equations