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### Interacting particles give us much more interesting dynamics...



- For each particle *i*, compute total force  $f_i(t)$
- For each particle *i*, compute new state

mathematically:

We can easily implement this with time stepping:

$$\mathbf{v}_i(t + \Delta t) = \mathbf{v}_i(t) + m_i^{-1} \mathbf{f}_i(t) \Delta t$$
  
$$\mathbf{x}_i(t + \Delta t) = \mathbf{x}_i(t) + \mathbf{v}_i(t + \Delta t) \Delta t$$

- But this may be a bit inconvenient to analyze
- Each  $f_i(t)$  could depend on  $x_1(t)$ ,  $v_1(t)$ ,  $x_2(t)$ ,  $v_2(t)$ , ...

Simpler with generalized coordinates:



Now we're solving for the evolution of a single (though 3*n*-dimensional!) vector

# Example: A small mass-spring system

$$\begin{bmatrix} \mathbf{f}_{1}(t, \mathbf{q}, \mathbf{v}) \\ \mathbf{f}_{2}(t, \mathbf{q}, \mathbf{v}) \\ \vdots \\ \mathbf{f}_{6}(t, \mathbf{q}, \mathbf{v}) \end{bmatrix} = \begin{bmatrix} \mathbf{f}_{12} + \mathbf{f}_{15} \\ \mathbf{f}_{21} + \mathbf{f}_{23} + \mathbf{f}_{25} \\ \vdots \\ \mathbf{f}_{64} \end{bmatrix}$$

Force due to spring between particles 2 and 3:

(of course,  $f_{32} = -f_{23}$ )

Total force on system =  $\sum$  force due to each spring





Per-particle formulation:

$$\frac{\mathrm{d}^2 \mathbf{x}_i(t)}{\mathrm{d}t^2} = m_i^{-1} \mathbf{f}_i(t, \ldots) \quad \forall i = 1, 2, \ldots$$

$$\mathbf{v}_{i}(t + \Delta t) = \mathbf{v}_{i}(t) + m_{i}^{-1}\mathbf{f}_{i}(t, \ldots) \Delta t \quad \forall i = 1, 2, \ldots \qquad \mathbf{v}(t + \mathbf{x}_{i}(t + \Delta t)) = \mathbf{x}_{i}(t) + \mathbf{v}_{i}(t + \Delta t) \Delta t \quad \forall i = 1, 2, \ldots \qquad \mathbf{q}(t + \Delta t)$$

Careful not to update  $\mathbf{x}_1$ ,  $\mathbf{v}_1$  before computing  $\mathbf{f}_2$ , in case it depends on them

Generalized coordinates:

$$\frac{\mathrm{d}^2 \mathbf{q}(t)}{\mathrm{d}t^2} = \mathbf{M}^{-1} \mathbf{f}(t, \mathbf{q}, \mathbf{v})$$

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

Simple! And generalizes to other things (e.g. rigid bodies) with few changes

# Mass-spring systems









Selle et al. 2008



Recall springs in 1 dimension from physics classes. Hooke's law: force is proportional to displacement  $F = -k x = -k (\ell - \ell_0)$ 

Potential energy:

$$U = \frac{1}{2} k (\ell - \ell_0)^2$$

In fact  $F = -dU/d\ell$ 





Let's first define the potential:

Then  $\mathbf{f}_{ij} = -\partial U / \partial \mathbf{x}_i \Rightarrow$ 

 $f_{ii} = -k (||x_i| -$ 

Similarly  $\mathbf{f}_{ii} = -\partial U / \partial \mathbf{x}_i$  (but it's also just  $-\mathbf{f}_{ii}$ )

**Exercise:** 1. Derive this expression from  $-\partial U/\partial \mathbf{x}_i$ . 2. (Optional) Look for high-level steps so you don't have to differentiate componentwise.

In 3D, suppose a spring connects particles i and j. What should be the force  $f_{ij}$  on i due to j?

 $U = \frac{1}{2} k (||\mathbf{x}_i - \mathbf{x}_i|| - \ell_0)^2$ 

$$k \left( \|\mathbf{x}_{i} - \mathbf{x}_{j}\| - \ell_{0} \right) \frac{\mathbf{x}_{i} - \mathbf{x}_{j}}{\|\mathbf{x}_{i} - \mathbf{x}_{j}\|}$$
$$= -k \left( \|\mathbf{x}_{ij}\| - \ell_{0} \right) \mathbf{\hat{x}}_{ij}$$





Suppose I model a stretchy rope (e.g. a rubber band) as a spring of stiffness k.

Now I want to allow it bend, so I replace it with two springs of half the length. What should be the stiffness of these springs to get the same stretchiness?



## **Puzzle:**



Different "resolutions" have different absolute change in length...

but same relative length change! This is called strain

$$\varepsilon = \frac{\Delta l}{l_0} = \frac{\|\mathbf{x}_i - \mathbf{x}_j\|}{l_0} - 1$$

For more consistent behaviour, define spring force in terms of strain:



 $U = \frac{1}{2} k \ell_0 \varepsilon^2$ 

 $\mathbf{f}_{ii} = -k \, \boldsymbol{\varepsilon} \, \hat{\mathbf{x}}_{ii}$ 



Problem: Real springs dissipate energy and don't keep oscillating forever!

**Bad idea**: Just add a force that opposes all velocities

$$\mathbf{f}_i = -k_d \, \mathbf{v}_i$$

Sometimes called "ether drag"

- Particles look like they're suspended in a viscous medium
- Should a rusty spring fall slower than a clean spring?

**Good idea**: Only oppose relative velocities along the spring

$$\mathbf{f}_{ij} = -k_d \left( \frac{\mathbf{v}_i - \mathbf{v}_j}{l_0} \cdot \hat{\mathbf{x}}_{ij} \right) \hat{\mathbf{x}}_{ij}$$



Time

Force due to a spring, finally:

where

• Strain 
$$\varepsilon = \frac{\|\mathbf{x}_i - \mathbf{x}_j\|}{l_0} - 1$$
  
• Strain rate  $\dot{\varepsilon} = \frac{\mathrm{d}\varepsilon}{\mathrm{d}t} = \frac{\mathbf{v}_i - \mathbf{v}_j}{l_0} \cdot \hat{\mathbf{x}}_{ij}$ 

- Spring constant  $k_s \ge 0$
- Damping constant  $k_d \ge 0$



• Structural springs



- Structural springs
- Shear springs



- Structural springs
- Shear springs
- Bending springs



- Structural springs
- Shear springs
- Bending springs







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Here's a problem you'll encounter:

Sometimes your simulation blows up for no apparent reason!

Why?





# Time integration

# We have an ordinary differential equation $\label{eq:quation} \ddot{\mathbf{q}} = \mathbf{N}$

- and are trying to solve an initial value problem: Given  $\mathbf{q}(0)$ ,  $\dot{\mathbf{q}}(0)$ , find  $\mathbf{q}(t)$ ,  $\dot{\mathbf{q}}(t)$  for t > 0.
- Let's start by understanding this for a simple 1st-order ODE:  $\dot{x}(t) = \phi(t, x(t))$
- Like a leaf in a river: if you are at position x at time t, your velocity is  $\phi(t, x)$

 $\ddot{\mathbf{q}} = \mathbf{M}^{-1} \mathbf{f}(t, \mathbf{q}, \dot{\mathbf{q}})$ 





Witkin & Bara ff 2001

Taylor series:  $x(t + \Delta t) = x(t) + \dot{x}(t) \Delta t + O(\Delta t^2)$  $\dot{x}(t) = \phi(t, x(t)), so$ 

where  $t_n = n \Delta t$ , and  $x_n = \text{computed estimate of } x(t_n)$ 

This is called the (forward) Euler method

Idea: measure your current velocity  $\phi(t_n, x_n)$ , then just move forward with that velocity for time  $\Delta t$ 

Error in each time step:  $O(\Delta t^2)$ Error in solution at fixed time  $T = O(\Delta t)$ : first-order accurate

 $x_{n+1} = x_n + \phi(t_n, x_n) \Delta t$ 





Suppose the ODE is  $\dot{x} = a x$ .

- Exact solution:  $x(t) = \exp(a t) x(0)$
- FE solution:  $x_{n+1} = x_n + a x_n \Delta t = (1 + a \Delta t) x_n$

For any *a* < 0, exact solution decays smoothly. But if  $|a \Delta t| > 2$ , FE solution diverges!

If a is imaginary, exact solution moves in a circle. But for any  $\Delta t$ , FE solution spirals outward!







## What does this mean in practice?

- The problem is not accuracy (error after *n* steps) but stability (whether  $|x_n|$  stays bounded)
- When forces vary rapidly with x,  $\Delta t$  needs to be much smaller
- **Rule of thumb:** If time scale of decay / oscillations  $\ll \Delta t$ , expect problems!

Not good: if we have even a single stiff spring in the system ( $k_s$  or  $k_d$  very large), we will have to take tiny time steps







