Dartmouth COSC 89.18/189.02 Computational Methods for Physical Systems, Winter 2019

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Course Notes 1: Mass-Spring Model

1. Spring and Damping Forces

A two-particle mass-spring system consists of a pair of particles i and j, with mass $m_{i(or\ j)}$, position $\vec{x}_{i(or\ j)}$, and velocity $\vec{v}_{i(or\ j)}$ on each particle. The two particles are connected by a spring $s(k_s, k_d, l_0)$, with the spring stiffness coefficient k_s, the damping coefficient k_d, and the rest length l_0.

The total force applied from the spring onto the adjacent particles is composed of two parts: the spring force $\vec{f_s}$ and the damping force $\vec{f_d}$.

The spring force depends on the particle positions only:

$$\vec{f}_i^s = k_s(|\vec{l}_{ij}| - l_0)\vec{n}_{ij} = k_s(|\vec{x}_j - \vec{x}_i| - l_0)\frac{\vec{x}_j - \vec{x}_i}{|\vec{x}_j - \vec{x}_i|} \tag{1.}$$

$$\vec{f}_j^s = -\vec{f}_i$$

The damping force depends on both particle positions and velocities:

$$\vec{f}_i^d = k_d(\vec{v}_{ij} \cdot \vec{n}_{ij})\vec{n}_{ij} = k_d\left((\vec{v}_j - \vec{v}_i) \cdot \frac{\vec{x}_j - \vec{x}_i}{|\vec{x}_j - \vec{x}_i|}\right)\frac{\vec{x}_j - \vec{x}_i}{|\vec{x}_j - \vec{x}_i|} \tag{2.}$$

$$\vec{f}_j^d = -\vec{f}_i$$

The total force from s acting on each particle is calculated as:

$$\vec{f}_i^{total} = \vec{f}_i^s + \vec{f}_i^d \tag{3.}$$

$$\vec{f}_j^{total} = -\vec{f}_i^{total}$$

There are two factors to keep in mind:

- Spring force is conservative, which means it can be written as the negative gradient of some potential energy:

$$\vec{f_s} = -\nabla\phi \tag{4.}$$

  The potential energy for a spring measures how far away the current spring length is from the rest length:

$$\phi = \frac{k_s}{2}(|\vec{l}_{ij}| - l_0)^2 = \frac{k_s}{2}(|\vec{x}_j - \vec{x}_i| - l_0)^2 \tag{5.}$$

- Damping force is dissipative.

2. Time Integration

For a two-particle mass-spring system, the Newton's second law governs the evolution of the particle system:

$$\frac{d}{dt}\begin{pmatrix}\vec{x}\\ \vec{v}\end{pmatrix} = \begin{pmatrix}\vec{v}\\ M^{-1}\vec{f}\end{pmatrix} \tag{6.}$$

with $\vec{x} = \begin{pmatrix}\vec{x}_i\\ \vec{x}_j\end{pmatrix}$, $\vec{v} = \begin{pmatrix}\vec{v}_i\\ \vec{v}_j\end{pmatrix}$, $\vec{f} = \begin{pmatrix}\vec{f}_i\\ \vec{f}_j\end{pmatrix}$, and $M = \begin{pmatrix}M_i & \\ & M_j\end{pmatrix}$. Here we define M_i as a d-dimensional diagonal matrix with m_i as the diagonal entries (M_j is defined in the same way).

For a given time interval Δt from time n to time $n+1$, we approximate the time derivative for $\vec{v}$ (and $\vec{x}$) by finite difference:

$$\frac{d}{dt}\vec{v} = \frac{\vec{v}^{n+1} - \vec{v}^{n}}{\Delta t} \tag{7.}$$

Using this expression to replace the left-hand side of Equation 6, we get:

$$\frac{\vec{x}^{n+1} - \vec{x}^{n}}{\Delta t} = \vec{v} \tag{8.}$$

$$\frac{\vec{v}^{n+1} - \vec{v}^{n}}{\Delta t} = M^{-1}\vec{f}(\vec{x}, \vec{v}) \tag{9.}$$

(Remember that for a spring with both elasticity and damping, $\vec{f}$ is a function of both position and velocity)

2.1 Explicit Euler

If we use the velocity and position in time n to approximate the right hand side of Equation (8) and (9), we will get the explicit Euler time integration scheme:

$$\vec{x}^{n+1} = \vec{x}^{n} + \Delta t\vec{v}^{n} \tag{10.}$$

$$\vec{v}^{n+1} = \vec{v}^{n} + \Delta t M^{-1}\vec{f}(\vec{x}^{n}, \vec{v}^{n}) \tag{11.}$$

The explicit Euler scheme can be converted to a short piece of computation code straightforwardly by updating the position and the velocity of each particle in every time step in sequence.

2.2 Implicit Euler

If we use the velocity and position in time $n+1$ to approximate the right-hand side, we will get the implicit Euler time integration scheme:

$$\vec{x}^{n+1} = \vec{x}^{n} + \Delta t\vec{v}^{n+1} \tag{12.}$$

$$\vec{v}^{n+1} = \vec{v}^{n} + \Delta t M^{-1}\vec{f}(\vec{x}^{n+1}, \vec{v}^{n+1}) \tag{13.}$$

Because $\vec{f}$ is a function of both $\vec{x}$ and $\vec{v}$, we can approximate the value of $\vec{f}$ in time $n+1$ by the Taylor series expanded in time n: (Notice here we ignored the dependency between $\vec{x}$ and $\vec{v}$)

$$\vec{f}(\vec{x}^{n+1},\vec{v}^{n+1}) = \vec{f}(\vec{x}^{n},\vec{v}^{n}) + \Delta\vec{x}\frac{\partial\vec{f}(\vec{x}^{n},\vec{v}^{n})}{\partial\vec{x}^{n}} + \Delta\vec{v}\frac{\partial\vec{f}(\vec{x}^{n},\vec{v}^{n})}{\partial\vec{v}^{n}} + O(\Delta x^2) + O(\Delta v^2) \tag{14.}$$

The two first-order partial derivatives $\partial f/\partial x$ and $\partial f/\partial v$ are Jacobians of the spring force with respect to position and velocity in respective.

We further approximate $\Delta\vec{x} = \Delta t\vec{v}^{n+1}$ and $\Delta\vec{v} = \vec{v}^{n+1} - \vec{v}^{n}$, and substitute Equation (13) into Equation (13):

$$\vec{v}^{n+1} = \vec{v}^{n} + \Delta t M^{-1}\left(\vec{f}(\vec{x}^{n},\vec{v}^{n}) + \Delta t\vec{v}^{n+1}\frac{\partial\vec{f}(\vec{x}^{n},\vec{v}^{n})}{\partial\vec{x}^{n}} + (\vec{v}^{n+1} - \vec{v}^{n})\frac{\partial\vec{f}(\vec{x}^{n},\vec{v}^{n})}{\partial\vec{v}^{n}}\right) \tag{15.}$$

Move all $\vec{v}^{n+1}$ terms to the left-hand side and multiply both sides by M:

$$\left(M - \Delta t\frac{\partial\vec{f}(\vec{x}^{n},\vec{v}^{n})}{\partial\vec{v}^{n}} - \Delta t^2\frac{\partial\vec{f}(\vec{x}^{n},\vec{v}^{n})}{\partial\vec{x}^{n}}\right)\vec{v}^{n+1} = M\vec{v}^{n} + \Delta t\vec{f}^{n} - \Delta t\frac{\partial\vec{f}(\vec{x}^{n},\vec{v}^{n})}{\partial\vec{v}^{n}}\vec{v}^{n} \tag{16.}$$

This is the equation we will use to solve $\vec{v}^{n+1}$ given the position, velocity, and force in time n.

Next, let's compute the two Jacobians.

- For the Jacobian of the total force w.r.t. position, we approximate $\partial\vec{f}/\partial\vec{x} = \partial\vec{f}^{s}/\partial\vec{x}$ (by ignoring the term $\partial\vec{f}^{d}/\partial\vec{x}$ to maintain the symmetry of the system):

$$\frac{\partial\vec{f}_i}{\partial\vec{x}_i} = k_s\left[\left(\frac{l_0}{l} - 1\right)I - \frac{l_0}{l}\vec{x}_{ji}\otimes\vec{x}_{ji}\right] = k_s\left[\left(\frac{l_0}{|\vec{x}_j - \vec{x}_i|} - 1\right)I - \frac{l_0}{|\vec{x}_j - \vec{x}_i|^3}(\vec{x}_j - \vec{x}_i)(\vec{x}_j - \vec{x}_i)^T\right] \tag{17.}$$

  Similarly, we have $\frac{\partial\vec{f}_i}{\partial\vec{x}_j} = -\frac{\partial\vec{f}_i}{\partial\vec{x}_i}$, $\frac{\partial\vec{f}_j}{\partial\vec{x}_j} = \frac{\partial\vec{f}_i}{\partial\vec{x}_i}$, and $\frac{\partial\vec{f}_j}{\partial\vec{x}_i} = -\frac{\partial\vec{f}_j}{\partial\vec{x}_j}$. We then define the four Jacobian matrices as $K_{ii} = \frac{\partial\vec{f}_i}{\partial\vec{x}_i}$, $K_{ij} = \frac{\partial\vec{f}_i}{\partial\vec{x}_j}$, $K_{jj} = \frac{\partial\vec{f}_j}{\partial\vec{x}_j}$, and $K_{ji} = \frac{\partial\vec{f}_j}{\partial\vec{x}_i}$. It is easy to see that $K_{ii} = K_{jj} = -K_{ij} = -Kji$.

- For the Jacobian of the total force w.r.t. velocity, we have $\partial\vec{f}/\partial\vec{v} = \partial\vec{f}^{d}/\partial\vec{v}$ (notice that the spring force is independent from velocity):

$$\frac{\partial\vec{f}_i}{\partial\vec{v}_i} = [Your\ P2\ homework] \tag{18.}$$

  We also define $D_{ii} = \frac{\partial\vec{f}_i}{\partial\vec{v}_i}$, $D_{ij} = \frac{\partial\vec{f}_i}{\partial\vec{v}_j}$, $D_{jj} = \frac{\partial\vec{f}_j}{\partial\vec{v}_j}$, and $D_{ji} = \frac{\partial\vec{f}_j}{\partial v_i}$.

Finally, we rewrite Equation 16 using a matrix form:

$$(M - \Delta tD - \Delta t^2K)\vec{v}^{n+1} = M\vec{v}^{n} + \Delta t\vec{f}^{n} - \Delta tD\vec{v}^{n}, \tag{19.}$$

with $M = \begin{pmatrix} M_i & \\ & M_j \end{pmatrix}$, $D = \begin{pmatrix} Dii & Dij \\ Dji & Djj \end{pmatrix}$ and $K = \begin{pmatrix} Kii & Kij \\ Kji & Kjj \end{pmatrix}$.

This system is read to be solved using any linear sparse solver such as conjugate gradient. We use the states from the previous time step as the initial guess for $\vec{v}^{n+1}$ when solving it iteratively.

A two-particle system can be extended to a multiple-particle one by accumulating D and K for each pair of particles connected by a spring respectively into two global matrices $\widehat{D}$ and $\widehat{K}$.