An example of an implicit Euler implementation

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1 Setting

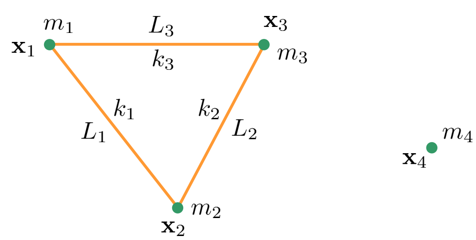

Figure 1: Example setting with four particles and three springs.

Fig. 1 illustrates an example with four particles at positions $\mathbf{x}_{1..4}$ with masses $m_{1..4}$ and three springs with rest lengths $L_{1..3}$ and stiffness constants $k_{1..3}$. Gravity $\mathbf{g}$, other accelerations $\mathbf{a}_i^{\text{other}}$ that do not depend on positions, e.g. damping of relative velocities, and spring forces $\mathbf{F}_i^{\text{spring}}$ are considered at particles. E.g., the acceleration $\mathbf{a}_1^t$ at particle $\mathbf{x}_1^t$ at time t is computed as

$$\mathbf{a}_1^t = \mathbf{g} + \mathbf{a}_1^{\text{other},t} + \frac{1}{m_1}\mathbf{F}_1^{\text{spring},t} \quad (1)$$

with

$$\mathbf{F}_1^{\text{spring},t} = k_1\left(\mathbf{x}_2^t - \mathbf{x}_1^t - L_1\frac{\mathbf{x}_2^t - \mathbf{x}_1^t}{|\mathbf{x}_2^t - \mathbf{x}_1^t|}\right) + k_3\left(\mathbf{x}_3^t - \mathbf{x}_1^t - L_3\frac{\mathbf{x}_3^t - \mathbf{x}_1^t}{|\mathbf{x}_3^t - \mathbf{x}_1^t|}\right). \quad (2)$$

Note that $\mathbf{x}_j^t - \mathbf{x}_i^t - L_k\frac{\mathbf{x}_j^t - \mathbf{x}_i^t}{|\mathbf{x}_j^t - \mathbf{x}_i^t|} = (|\mathbf{x}_j^t - \mathbf{x}_i^t| - L_k)\frac{\mathbf{x}_j^t - \mathbf{x}_i^t}{|\mathbf{x}_j^t - \mathbf{x}_i^t|}$.

2 Formulation

Implicit Euler computes velocities $\mathbf{v}_i^{t+h}$ at the next timestep $t+h$ by solving a linear system. The computed velocities are used to update the particle positions with $\mathbf{x}_i^{t+h} = \mathbf{x}_i^t + h\mathbf{v}_i^{t+h}$. The implicit formulation for the velocity computation according to Euler would be

$$\mathbf{v}_i^{t+h} = \mathbf{v}_i^t + h(\mathbf{g} + \mathbf{a}_i^{\text{other},t+h} + \frac{1}{m_i}\mathbf{F}_i^{\text{spring},t+h}). \tag{3}$$

This is typically considered as too complex and the following formulation is solved instead:

$$\mathbf{v}_i^{t+h} = \mathbf{v}_i^t + h(\mathbf{g} + \mathbf{a}_i^{\text{other},t}) + h\frac{1}{m_i}\mathbf{F}_i^{\text{spring},t+h}. \tag{4}$$

The term $\mathbf{v}_i^* = \mathbf{v}_i^t + h(\mathbf{g} + \mathbf{a}_i^{\text{other},t})$ is explicitly computed and referred to as predicted velocity. Instead of Eq. 4, the following formulation is solved:

$$\begin{aligned} \mathbf{v}_i^{t+h} &= \mathbf{v}_i^* + h\frac{1}{m_i}\mathbf{F}_i^{\text{spring},t+h} \\ m_i\mathbf{v}_i^{t+h} &= m_i\mathbf{v}_i^* + h\mathbf{F}_i^{\text{spring},t+h}. \end{aligned} \tag{5}$$

We now consider vectors that represent all particles, e.g.

$$\mathbf{x}^t = \begin{pmatrix} \mathbf{x}_1^t \\ \mathbf{x}_2^t \\ \mathbf{x}_3^t \\ \mathbf{x}_4^t \end{pmatrix} \quad \mathbf{v}^t = \begin{pmatrix} \mathbf{v}_1^t \\ \mathbf{v}_2^t \\ \mathbf{v}_3^t \\ \mathbf{v}_4^t \end{pmatrix} \quad \mathbf{F}^{\text{spring},t} = \begin{pmatrix} \mathbf{F}_1^{\text{spring},t} \\ \mathbf{F}_2^{\text{spring},t} \\ \mathbf{F}_3^{\text{spring},t} \\ \mathbf{F}_4^{\text{spring},t} \end{pmatrix} \tag{6}$$

Eq. 5 can now be written for the entire particle set:

$$\mathbf{M}\mathbf{v}^{t+h} = \mathbf{M}\mathbf{v}^* + h\mathbf{F}^{\text{spring},t+h} \tag{7}$$

with

$$\mathbf{M} = \begin{pmatrix} m_1 & 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & m_1 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & m_1 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & m_2 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & m_2 & 0 & \dots \\ 0 & 0 & 0 & 0 & 0 & m_2 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix} \tag{8}$$

of size 12×12 for our example setting.

3 Linearization

The formulation

$$\mathbf{M}\mathbf{v}^{t+h} = \mathbf{M}\mathbf{v}^* + h\mathbf{F}^{\text{spring},t+h} \tag{9}$$

is replaced by the approximation

$$\mathbf{M}\mathbf{v}^{t+h} = \mathbf{M}\mathbf{v}^* + h\mathbf{F}^{\text{spring},t} + h\mathbf{J}^t(\mathbf{x}^{t+h} - \mathbf{x}^t) \tag{10}$$

with $\mathbf{J}^t$ being a Jacobi matrix that represents all partial derivatives of all spring forces with respect to all positions. This linearization of the forces and the fact that $\mathbf{x}^{t+h} - \mathbf{x}^t = h\mathbf{v}^{t+h}$ results in a linear system with unknown velocities $\mathbf{v}^{t+h}$:

$$\begin{aligned} \mathbf{M}\mathbf{v}^{t+h} &= \mathbf{M}\mathbf{v}^* + h\mathbf{F}^{\text{spring},t} + h\mathbf{J}^t h\mathbf{v}^{t+h} \\ (\mathbf{M} - h^2\mathbf{J}^t)\mathbf{v}^{t+h} &= \mathbf{M}\mathbf{v}^* + h\mathbf{F}^{\text{spring},t} \end{aligned} \tag{11}$$

We omit the time index for quantities at time t to improve readability. We also replace $\mathbf{F}^{\text{spring}}$ with $\mathbf{F}$.

$$(\mathbf{M} - h^2\mathbf{J})\mathbf{v}^{t+h} = \mathbf{M}\mathbf{v}^* + h\mathbf{F} \tag{12}$$

4 The Jacobi matrix

The Jacobi matrix consists of submatrices $\mathbf{J}_{i,j}$ of size 3×3. In our example setting, we have

$$\mathbf{J} = \begin{pmatrix} \mathbf{J}_{1,1} & \mathbf{J}_{1,2} & \mathbf{J}_{1,3} & \mathbf{J}_{1,4} \\ \mathbf{J}_{2,1} & \mathbf{J}_{2,2} & \mathbf{J}_{2,3} & \mathbf{J}_{2,4} \\ \mathbf{J}_{3,1} & \mathbf{J}_{3,2} & \mathbf{J}_{3,3} & \mathbf{J}_{3,4} \\ \mathbf{J}_{4,1} & \mathbf{J}_{4,2} & \mathbf{J}_{4,3} & \mathbf{J}_{4,4} \end{pmatrix} \tag{13}$$

Each submatrix $\mathbf{J}_{i,j}$ encodes the spatial derivative of the force $\mathbf{F}_i$ with respect to the position $\mathbf{x}_j$, i.e. the dependency of $\mathbf{F}_i$ from $\mathbf{x}_j$. $\mathbf{J}_{i,j}$ encodes, how the force $\mathbf{F}_i$ changes due a small displacement of $\mathbf{x}_j$.

If a force $\mathbf{F}_i$ does not depend from a position $\mathbf{x}_j$, the respective derivative $\mathbf{J}_{i,j}$ is zero. In our example, the force $\mathbf{F}_4 = m_4\mathbf{g} + m_4\mathbf{a}_4^{\text{other}}$ does not depend on any of the positions $\mathbf{x}_{1..4}$. I.e., $\mathbf{J}_{4,1..4} = \mathbf{0}$. Further, the forces $\mathbf{F}_{1..3}$ do not depend on position $\mathbf{x}_4$. Thus, $\mathbf{J}_{1..3,4} = \mathbf{0}$. The forces $\mathbf{F}_{1..3}$ depend on positions $\mathbf{x}_{1..3}$. So, $\mathbf{J}_{1..3,1..3}$ have to be computed. The Jacobian in our example has the following structure:

$$\mathbf{J} = \begin{pmatrix} \mathbf{J}_{1,1} & \mathbf{J}_{1,2} & \mathbf{J}_{1,3} & \mathbf{0} \\ \mathbf{J}_{2,1} & \mathbf{J}_{2,2} & \mathbf{J}_{2,3} & \mathbf{0} \\ \mathbf{J}_{3,1} & \mathbf{J}_{3,2} & \mathbf{J}_{3,3} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \tag{14}$$

4.1 Spring forces

The spring forces at the particles are

$$\begin{aligned}
\mathbf{F}_1 &= \frac{k_1}{L_1}\left(\mathbf{x}_2 - \mathbf{x}_1 - L_1\frac{\mathbf{x}_2 - \mathbf{x}_1}{|\mathbf{x}_2 - \mathbf{x}_1|}\right) + \frac{k_3}{L_3}\left(\mathbf{x}_3 - \mathbf{x}_1 - L_3\frac{\mathbf{x}_3 - \mathbf{x}_1}{|\mathbf{x}_3 - \mathbf{x}_1|}\right) \\
\mathbf{F}_2 &= -\frac{k_1}{L_1}\left(\mathbf{x}_2 - \mathbf{x}_1 - L_1\frac{\mathbf{x}_2 - \mathbf{x}_1}{|\mathbf{x}_2 - \mathbf{x}_1|}\right) + \frac{k_2}{L_2}\left(\mathbf{x}_3 - \mathbf{x}_2 - L_2\frac{\mathbf{x}_3 - \mathbf{x}_2}{|\mathbf{x}_3 - \mathbf{x}_2|}\right) \\
\mathbf{F}_3 &= -\frac{k_2}{L_2}\left(\mathbf{x}_3 - \mathbf{x}_2 - L_2\frac{\mathbf{x}_3 - \mathbf{x}_2}{|\mathbf{x}_3 - \mathbf{x}_2|}\right) - \frac{k_3}{L_3}\left(\mathbf{x}_3 - \mathbf{x}_1 - L_3\frac{\mathbf{x}_3 - \mathbf{x}_1}{|\mathbf{x}_3 - \mathbf{x}_1|}\right)
\end{aligned} \tag{15}$$

Each particle is connected to two springs. If we have a spring k that connects two particles i and j, the force at particle i can be denoted as $\mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_j)$. E.g.,

$$\begin{aligned}
\mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2) &= \frac{k_1}{L_1}(\mathbf{x}_2 - \mathbf{x}_1 - L_1\frac{\mathbf{x}_2 - \mathbf{x}_1}{|\mathbf{x}_2 - \mathbf{x}_1|}) \\
\mathbf{f}_2(\mathbf{x}_2 \leftarrow \mathbf{x}_3) &= \frac{k_2}{L_2}(\mathbf{x}_3 - \mathbf{x}_2 - L_2\frac{\mathbf{x}_3 - \mathbf{x}_2}{|\mathbf{x}_3 - \mathbf{x}_2|}) \\
\mathbf{f}_3(\mathbf{x}_1 \leftarrow \mathbf{x}_3) &= \frac{k_3}{L_3}(\mathbf{x}_3 - \mathbf{x}_1 - L_3\frac{\mathbf{x}_3 - \mathbf{x}_1}{|\mathbf{x}_3 - \mathbf{x}_1|})
\end{aligned} \tag{16}$$

The spring forces are symmetric and sum up to zero, i.e.

$$\mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_j) = -\mathbf{f}_k(\mathbf{x}_j \leftarrow \mathbf{x}_i). \tag{17}$$

The spring forces at the three particles can now be written as

$$\begin{aligned}
\mathbf{F}_1 &= \mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2) + \mathbf{f}_3(\mathbf{x}_1 \leftarrow \mathbf{x}_3) \\
\mathbf{F}_2 &= \mathbf{f}_1(\mathbf{x}_2 \leftarrow \mathbf{x}_1) + \mathbf{f}_2(\mathbf{x}_2 \leftarrow \mathbf{x}_3) = -\mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2) + \mathbf{f}_2(\mathbf{x}_2 \leftarrow \mathbf{x}_3) \\
\mathbf{F}_3 &= \mathbf{f}_2(\mathbf{x}_3 \leftarrow \mathbf{x}_2) + \mathbf{f}_3(\mathbf{x}_3 \leftarrow \mathbf{x}_1) = -\mathbf{f}_2(\mathbf{x}_2 \leftarrow \mathbf{x}_3) - \mathbf{f}_3(\mathbf{x}_1 \leftarrow \mathbf{x}_3).
\end{aligned} \tag{18}$$

Due to the symmetry, one force computation is sufficient to assemble the overall forces at particles.

4.2 Spatial derivatives of spring forces

We consider force $\mathbf{F}_1$ at particle $\mathbf{x}_1$. We have to compute the spatial derivatives of $\mathbf{F}_1 = (F_{1,x}, F_{1,y}, F_{1,z})^{\mathrm{T}}$ with respect to positions $\mathbf{x}_{1..3} = (x_{1..3,x}, x_{1..3,y}, x_{1..3,z})^{\mathrm{T}}$.

I.e.

$$\mathbf{J}_{1,1} = \begin{pmatrix} \frac{\partial F_{1,x}}{\partial x_{1,x}} & \frac{\partial F_{1,x}}{\partial x_{1,y}} & \frac{\partial F_{1,x}}{\partial x_{1,z}} \\ \frac{\partial F_{1,y}}{\partial x_{1,x}} & \frac{\partial F_{1,y}}{\partial x_{1,y}} & \frac{\partial F_{1,y}}{\partial x_{1,z}} \\ \frac{\partial F_{1,z}}{\partial x_{1,x}} & \frac{\partial F_{1,z}}{\partial x_{1,y}} & \frac{\partial F_{1,z}}{\partial x_{1,z}} \end{pmatrix} \mathbf{J}_{1,2} = \begin{pmatrix} \frac{\partial F_{1,x}}{\partial x_{2,x}} & \frac{\partial F_{1,x}}{\partial x_{2,y}} & \frac{\partial F_{1,x}}{\partial x_{2,z}} \\ \frac{\partial F_{1,y}}{\partial x_{2,x}} & \frac{\partial F_{1,y}}{\partial x_{2,y}} & \frac{\partial F_{1,y}}{\partial x_{2,z}} \\ \frac{\partial F_{1,z}}{\partial x_{2,x}} & \frac{\partial F_{1,z}}{\partial x_{2,y}} & \frac{\partial F_{1,z}}{\partial x_{2,z}} \end{pmatrix} \mathbf{J}_{1,3} = \dots \quad (19)$$

The matrices can also be rewritten using $\mathbf{f}$ instead of $\mathbf{F}$. E.g.,

$$\begin{aligned} \mathbf{J}_{1,1} &= \begin{pmatrix} \frac{\partial f_{1,x}}{\partial x_{1,x}} & \frac{\partial f_{1,x}}{\partial x_{1,y}} & \frac{\partial f_{1,x}}{\partial x_{1,z}} \\ \frac{\partial f_{1,y}}{\partial x_{1,x}} & \frac{\partial f_{1,y}}{\partial x_{1,y}} & \frac{\partial f_{1,y}}{\partial x_{1,z}} \\ \frac{\partial f_{1,z}}{\partial x_{1,x}} & \frac{\partial f_{1,z}}{\partial x_{1,y}} & \frac{\partial f_{1,z}}{\partial x_{1,z}} \end{pmatrix} + \begin{pmatrix} \frac{\partial f_{3,x}}{\partial x_{1,x}} & \frac{\partial f_{3,x}}{\partial x_{1,y}} & \frac{\partial f_{3,x}}{\partial x_{1,z}} \\ \frac{\partial f_{3,y}}{\partial x_{1,x}} & \frac{\partial f_{3,y}}{\partial x_{1,y}} & \frac{\partial f_{3,y}}{\partial x_{1,z}} \\ \frac{\partial f_{3,z}}{\partial x_{1,x}} & \frac{\partial f_{3,z}}{\partial x_{1,y}} & \frac{\partial f_{3,z}}{\partial x_{1,z}} \end{pmatrix} \\ &= \frac{\partial \mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2)}{\partial \mathbf{x}_1} + \frac{\partial \mathbf{f}_3(\mathbf{x}_1 \leftarrow \mathbf{x}_3)}{\partial \mathbf{x}_1} \end{aligned} \quad (20)$$

and

$$\begin{aligned} \mathbf{J}_{1,2} &= \frac{\partial \mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2)}{\partial \mathbf{x}_2} + \frac{\partial \mathbf{f}_3(\mathbf{x}_1 \leftarrow \mathbf{x}_3)}{\partial \mathbf{x}_2} \\ \mathbf{J}_{1,3} &= \frac{\partial \mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2)}{\partial \mathbf{x}_3} + \frac{\partial \mathbf{f}_3(\mathbf{x}_1 \leftarrow \mathbf{x}_3)}{\partial \mathbf{x}_3}. \end{aligned} \quad (21)$$

We have already discussed that $\mathbf{J}_{1,4} = \mathbf{0}$, because there is no spring between particles 1 and 4. This fact can also be seen from

$$\mathbf{J}_{1,4} = \frac{\partial \mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2)}{\partial \mathbf{x}_4} + \frac{\partial \mathbf{f}_3(\mathbf{x}_1 \leftarrow \mathbf{x}_3)}{\partial \mathbf{x}_4} = \mathbf{0} \quad (22)$$

as the forces $\mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2)$ and $\mathbf{f}_3(\mathbf{x}_1 \leftarrow \mathbf{x}_3)$ do not depend on $\mathbf{x}_4$. The same argument can be used to see that $\mathbf{J}_{1,2}$ and $\mathbf{J}_{1,3}$ simplify to

$$\begin{aligned} \mathbf{J}_{1,2} &= \frac{\partial \mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2)}{\partial \mathbf{x}_2} \\ \mathbf{J}_{1,3} &= \frac{\partial \mathbf{f}_3(\mathbf{x}_1 \leftarrow \mathbf{x}_3)}{\partial \mathbf{x}_3}. \end{aligned} \quad (23)$$

Generally,

$$\mathbf{J}_{i,j} = \sum_k \frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_m)}{\partial \mathbf{x}_j}. \quad (24)$$

We sum over all springs k that are connected to particle i. If a spring k connects particles i and m and $j \neq i$ and $j \neq m$, then $\frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_m)}{\partial \mathbf{x}_j} = \mathbf{0}$.

4.3 Derivative of $\mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2)$ with respect to $\mathbf{x}_1$

The components of $\mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2)$ are

$$
\begin{aligned}
f_{1,x} &= \frac{k_1}{L_1}\left(x_{2,x} - x_{1,x} - L_1 \frac{x_{2,x} - x_{1,x}}{\sqrt{(x_{2,x} - x_{1,x})^2 + (x_{2,y} - x_{1,y})^2 + (x_{2,z} - x_{1,z})^2}}\right) \\
f_{1,y} &= \frac{k_1}{L_1}\left(x_{2,y} - x_{1,y} - L_1 \frac{x_{2,y} - x_{1,y}}{\sqrt{(x_{2,x} - x_{1,x})^2 + (x_{2,y} - x_{1,y})^2 + (x_{2,z} - x_{1,z})^2}}\right) \\
f_{1,z} &= \frac{k_1}{L_1}\left(x_{2,z} - x_{1,z} - L_1 \frac{x_{2,z} - x_{1,z}}{\sqrt{(x_{2,x} - x_{1,x})^2 + (x_{2,y} - x_{1,y})^2 + (x_{2,z} - x_{1,z})^2}}\right).
\end{aligned}
\tag{25}
$$

We define

$$
l_{i,j} = \sqrt{(x_{j,x} - x_{i,x})^2 + (x_{j,y} - x_{i,y})^2 + (x_{j,z} - x_{i,z})^2} \tag{26}
$$

and the partial derivatives of $\mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2)$ with respect to $\mathbf{x}_1$ can be written as

$$
\begin{aligned}
\frac{\partial f_{1,x}}{\partial x_{1,x}} &= \frac{k_1}{L_1}\left(-1 + \frac{L_1}{l_{1,2}}\left(1 - \frac{(x_{2,x} - x_{1,x})(x_{2,x} - x_{1,x})}{(l_{1,2})^2}\right)\right) \\
\frac{\partial f_{1,x}}{\partial x_{1,y}} &= \frac{k_1}{L_1}\left(0 + \frac{L_1}{l_{1,2}}\left(0 - \frac{(x_{2,x} - x_{1,x})(x_{2,y} - x_{1,y})}{(l_{1,2})^2}\right)\right) \\
\frac{\partial f_{1,x}}{\partial x_{1,z}} &= \frac{k_1}{L_1}\left(0 + \frac{L_1}{l_{1,2}}\left(0 - \frac{(x_{2,x} - x_{1,x})(x_{2,z} - x_{1,z})}{(l_{1,2})^2}\right)\right) \\
\frac{\partial f_{1,y}}{\partial x_{1,x}} &= \frac{k_1}{L_1}\left(0 + \frac{L_1}{l_{1,2}}\left(0 - \frac{(x_{2,y} - x_{1,y})(x_{2,x} - x_{1,x})}{(l_{1,2})^2}\right)\right) \\
\frac{\partial f_{1,y}}{\partial x_{1,y}} &= \frac{k_1}{L_1}\left(-1 + \frac{L_1}{l_{1,2}}\left(1 - \frac{(x_{2,y} - x_{1,y})(x_{2,y} - x_{1,y})}{(l_{1,2})^2}\right)\right) \\
\frac{\partial f_{1,y}}{\partial x_{1,z}} &= \frac{k_1}{L_1}\left(0 + \frac{L_1}{l_{1,2}}\left(0 - \frac{(x_{2,y} - x_{1,y})(x_{2,z} - x_{1,z})}{(l_{1,2})^2}\right)\right) \\
\frac{\partial f_{1,z}}{\partial x_{1,x}} &= \frac{k_1}{L_1}\left(0 + \frac{L_1}{l_{1,2}}\left(0 - \frac{(x_{2,z} - x_{1,z})(x_{2,x} - x_{1,x})}{(l_{1,2})^2}\right)\right) \\
\frac{\partial f_{1,z}}{\partial x_{1,y}} &= \frac{k_1}{L_1}\left(0 + \frac{L_1}{l_{1,2}}\left(0 - \frac{(x_{2,z} - x_{1,z})(x_{2,y} - x_{1,y})}{(l_{1,2})^2}\right)\right) \\
\frac{\partial f_{1,z}}{\partial x_{1,z}} &= \frac{k_1}{L_1}\left(-1 + \frac{L_1}{l_{1,2}}\left(1 - \frac{(x_{2,z} - x_{1,z})(x_{2,z} - x_{1,z})}{(l_{1,2})^2}\right)\right).
\end{aligned}
\tag{27}
$$

Finally, we have

$$
\begin{aligned}
\frac{\partial \mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2)}{\partial \mathbf{x}_1} &= \begin{pmatrix} \frac{\partial f_{1,x}}{\partial x_{1,x}} & \frac{\partial f_{1,x}}{\partial x_{1,y}} & \frac{\partial f_{1,x}}{\partial x_{1,z}} \\ \frac{\partial f_{1,y}}{\partial x_{1,x}} & \frac{\partial f_{1,y}}{\partial x_{1,y}} & \frac{\partial f_{1,y}}{\partial x_{1,z}} \\ \frac{\partial f_{1,z}}{\partial x_{1,x}} & \frac{\partial f_{1,z}}{\partial x_{1,y}} & \frac{\partial f_{1,z}}{\partial x_{1,z}} \end{pmatrix} \\
&= \frac{k_1}{L_1}\left(-\mathbf{I} + \frac{L_1}{\|\mathbf{x}_2 - \mathbf{x}_1\|}\left(\mathbf{I} - \frac{(\mathbf{x}_2 - \mathbf{x}_1)(\mathbf{x}_2 - \mathbf{x}_1)^{\mathrm{T}}}{\|\mathbf{x}_2 - \mathbf{x}_1\|^2}\right)\right) \qquad (28)
\end{aligned}
$$

4.4 Assembly of J

It is sufficient to compute one 3×3 Jacobian per spring, i.e. 3 Jacobians in our example.

$$
\begin{aligned}
\frac{\partial \mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2)}{\partial \mathbf{x}_1} &= \frac{k_1}{L_1}\left(-\mathbf{I} + \frac{L_1}{\|\mathbf{x}_2 - \mathbf{x}_1\|}\left(\mathbf{I} - \frac{(\mathbf{x}_2 - \mathbf{x}_1)(\mathbf{x}_2 - \mathbf{x}_1)^{\mathrm{T}}}{\|\mathbf{x}_2 - \mathbf{x}_1\|^2}\right)\right) \\
\frac{\partial \mathbf{f}_2(\mathbf{x}_2 \leftarrow \mathbf{x}_3)}{\partial \mathbf{x}_2} &= \frac{k_2}{L_2}\left(-\mathbf{I} + \frac{L_2}{\|\mathbf{x}_3 - \mathbf{x}_2\|}\left(\mathbf{I} - \frac{(\mathbf{x}_3 - \mathbf{x}_2)(\mathbf{x}_3 - \mathbf{x}_2)^{\mathrm{T}}}{\|\mathbf{x}_3 - \mathbf{x}_2\|^2}\right)\right) \\
\frac{\partial \mathbf{f}_3(\mathbf{x}_1 \leftarrow \mathbf{x}_3)}{\partial \mathbf{x}_1} &= \frac{k_3}{L_3}\left(-\mathbf{I} + \frac{L_3}{\|\mathbf{x}_3 - \mathbf{x}_1\|}\left(\mathbf{I} - \frac{(\mathbf{x}_3 - \mathbf{x}_1)(\mathbf{x}_3 - \mathbf{x}_1)^{\mathrm{T}}}{\|\mathbf{x}_3 - \mathbf{x}_1\|^2}\right)\right) \qquad (29)
\end{aligned}
$$

All submatrices $\mathbf{J}_{i,j}$ can be assembled from these three Jacobians. If a spring k connects particles i and j, we have

$$
\frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_j)}{\partial \mathbf{x}_i} = \frac{\partial \mathbf{f}_k(\mathbf{x}_j \leftarrow \mathbf{x}_i)}{\partial \mathbf{x}_j} = -\frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_j)}{\partial \mathbf{x}_j} = -\frac{\partial \mathbf{f}_k(\mathbf{x}_j \leftarrow \mathbf{x}_i)}{\partial \mathbf{x}_i} \qquad (30)
$$

Again, each submatrix $\mathbf{J}_{i,j}$ is computed by summing up contributions from all springs k that are connected to particle i:

$$
\mathbf{J}_{i,j} = \sum_k \frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_m)}{\partial \mathbf{x}_j}. \qquad (31)
$$

We sum over all springs k that are connected to particle i. If $i = j$, we have

$$
\mathbf{J}_{i,i} = \sum_k \frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_m)}{\partial \mathbf{x}_i}. \qquad (32)
$$

In this case, the sum contains as many elements as there are springs connected to particle i. If no spring is connected to particle i, e.g., particle 4 in our example, we have $\mathbf{J}_{i,i} = \mathbf{0}$. If $i \neq j$, we have $\mathbf{J}_{i,j} = \mathbf{0}$, if there is no spring between i and j. If there is one spring, we have

$$
\mathbf{J}_{i,j} = \frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_j)}{\partial \mathbf{x}_j}. \qquad (33)
$$

4.5 The final J

We define

$$\begin{aligned}
\mathbf{S}_1 &= \frac{\partial \mathbf{f}_1(\mathbf{x}_1 \leftarrow \mathbf{x}_2)}{\partial \mathbf{x}_1} \\
\mathbf{S}_2 &= \frac{\partial \mathbf{f}_2(\mathbf{x}_2 \leftarrow \mathbf{x}_3)}{\partial \mathbf{x}_2} \\
\mathbf{S}_3 &= \frac{\partial \mathbf{f}_3(\mathbf{x}_1 \leftarrow \mathbf{x}_3)}{\partial \mathbf{x}_1}
\end{aligned} \tag{34}$$

and we remember

$$\mathbf{S}_k = \frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_j)}{\partial \mathbf{x}_i} = \frac{\partial \mathbf{f}_k(\mathbf{x}_j \leftarrow \mathbf{x}_i)}{\partial \mathbf{x}_j} = -\frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_j)}{\partial \mathbf{x}_j} = -\frac{\partial \mathbf{f}_k(\mathbf{x}_j \leftarrow \mathbf{x}_i)}{\partial \mathbf{x}_i} \tag{35}$$

The final form of our exemplary Jacobian $\mathbf{J}$ is now

$$\mathbf{J} = \begin{pmatrix} \mathbf{S}_1 + \mathbf{S}_3 & -\mathbf{S}_1 & -\mathbf{S}_3 & \mathbf{0} \\ -\mathbf{S}_1 & \mathbf{S}_1 + \mathbf{S}_2 & -\mathbf{S}_2 & \mathbf{0} \\ -\mathbf{S}_3 & -\mathbf{S}_2 & \mathbf{S}_2 + \mathbf{S}_3 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \tag{36}$$

Each spring influences forces at two particles and depends on two particle positions. Thus, $\mathbf{S}_i$ occurs four times in $\mathbf{J}$ for a spring i.

4.6 The final system

Our system

$$\underbrace{\left(\mathbf{M} - h^2\mathbf{J}\right)}_{\mathbf{A}} \mathbf{v}^{t+h} = \underbrace{\mathbf{M}\mathbf{v}^* + h\mathbf{F}}_{\mathbf{s}} \tag{37}$$

represents four particles and can be written as $\mathbf{A}\mathbf{v}^{t+h} = \mathbf{s}$ or

$$\begin{aligned}
&\begin{pmatrix} \mathbf{M}_1 - h^2\mathbf{J}_{1,1} & -h^2\mathbf{J}_{1,2} & -h^2\mathbf{J}_{1,3} & -h^2\mathbf{J}_{1,4} \\ -h^2\mathbf{J}_{2,1} & \mathbf{M}_2 - h^2\mathbf{J}_{2,2} & -h^2\mathbf{J}_{2,3} & -h^2\mathbf{J}_{2,4} \\ -h^2\mathbf{J}_{3,1} & -h^2\mathbf{J}_{3,2} & \mathbf{M}_3 - h^2\mathbf{J}_{3,3} & -h^2\mathbf{J}_{3,4} \\ -h^2\mathbf{J}_{4,1} & -h^2\mathbf{J}_{4,2} & -h^2\mathbf{J}_{4,3} & \mathbf{M}_4 - h^2\mathbf{J}_{4,4} \end{pmatrix} \begin{pmatrix} \mathbf{v}_1^{t+h} \\ \mathbf{v}_2^{t+h} \\ \mathbf{v}_3^{t+h} \\ \mathbf{v}_4^{t+h} \end{pmatrix} \\
&\qquad = \begin{pmatrix} \mathbf{M}_1\mathbf{v}_1^* \\ \mathbf{M}_2\mathbf{v}_2^* \\ \mathbf{M}_3\mathbf{v}_3^* \\ \mathbf{M}_4\mathbf{v}_4^* \end{pmatrix} + \begin{pmatrix} h\mathbf{F}_1 \\ h\mathbf{F}_2 \\ h\mathbf{F}_3 \\ h\mathbf{F}_4 \end{pmatrix}
\end{aligned} \tag{38}$$

with

$$\mathbf{M}_i = \begin{pmatrix} m_i & 0 & 0 \\ 0 & m_i & 0 \\ 0 & 0 & m_i \end{pmatrix} \tag{39}$$

or

$$\begin{pmatrix} \mathbf{A}_{1,1} & \mathbf{A}_{1,2} & \mathbf{A}_{1,3} & \mathbf{A}_{1,4} \\ \mathbf{A}_{2,1} & \mathbf{A}_{2,2} & \mathbf{A}_{2,3} & \mathbf{A}_{2,4} \\ \mathbf{A}_{3,1} & \mathbf{A}_{3,2} & \mathbf{A}_{3,3} & \mathbf{A}_{3,4} \\ \mathbf{A}_{4,1} & \mathbf{A}_{4,2} & \mathbf{A}_{4,3} & \mathbf{A}_{4,4} \end{pmatrix} \begin{pmatrix} \mathbf{v}_1^{t+h} \\ \mathbf{v}_2^{t+h} \\ \mathbf{v}_3^{t+h} \\ \mathbf{v}_4^{t+h} \end{pmatrix} = \begin{pmatrix} \mathbf{s}_1 \\ \mathbf{s}_2 \\ \mathbf{s}_3 \\ \mathbf{s}_4 \end{pmatrix} \tag{40}$$

4.7 Jacobi solver

The Jacobi update is

$$\mathbf{v}^{l+1} = \mathbf{v}^l + \omega \mathbf{D}^{-1}(\mathbf{s} - \mathbf{A}\mathbf{v}^l) \tag{41}$$

with l being the iteration count, $0 < \omega \leq 0.5$ being a coefficient and $\mathbf{D}$ being a matrix with the diagonal elements of $\mathbf{A}$. This update can be written as

$$\begin{pmatrix} \mathbf{v}_1^{l+1} \\ \mathbf{v}_2^{l+1} \\ \mathbf{v}_3^{l+1} \\ \mathbf{v}_4^{l+1} \end{pmatrix} = \begin{pmatrix} \mathbf{v}_1^{l} \\ \mathbf{v}_2^{l} \\ \mathbf{v}_3^{l} \\ \mathbf{v}_4^{l} \end{pmatrix} +$$
$$\omega \begin{pmatrix} \mathbf{D}_1 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{D}_2 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{D}_3 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{D}_4 \end{pmatrix}^{-1} \left(\begin{pmatrix} \mathbf{s}_1 \\ \mathbf{s}_2 \\ \mathbf{s}_3 \\ \mathbf{s}_4 \end{pmatrix} - \begin{pmatrix} \mathbf{A}_{1,1} & \mathbf{A}_{1,2} & \mathbf{A}_{1,3} & \mathbf{A}_{1,4} \\ \mathbf{A}_{2,1} & \mathbf{A}_{2,2} & \mathbf{A}_{2,3} & \mathbf{A}_{2,4} \\ \mathbf{A}_{3,1} & \mathbf{A}_{3,2} & \mathbf{A}_{3,3} & \mathbf{A}_{3,4} \\ \mathbf{A}_{4,1} & \mathbf{A}_{4,2} & \mathbf{A}_{4,3} & \mathbf{A}_{4,4} \end{pmatrix} \begin{pmatrix} \mathbf{v}_1^{l} \\ \mathbf{v}_2^{l} \\ \mathbf{v}_3^{l} \\ \mathbf{v}_4^{l} \end{pmatrix} \right) \tag{42}$$

with $\mathbf{D}_i$ representing the diagonal elements of $\mathbf{A}_{i,i}$. The update could be implemented on a per particle basis, i.e.:

$$\mathbf{v}_i^{l+1} = \mathbf{v}_i^l + \omega \mathbf{D}_i^{-1} \left(\mathbf{s}_i - \sum_{j=1..4} \mathbf{A}_{i,j} \mathbf{v}_j^l \right) \tag{43}$$

This requires to represent $\mathbf{A}_{i,j}$. As $\mathbf{A}$ is sparsely filled in larger practical scenarios, $\mathbf{A}_{i,j} = \mathbf{0}$ for many i and j. Alternatively,

$$\begin{pmatrix} \mathbf{A}_{1,1} & \mathbf{A}_{1,2} & \mathbf{A}_{1,3} & \mathbf{A}_{1,4} \\ \mathbf{A}_{2,1} & \mathbf{A}_{2,2} & \mathbf{A}_{2,3} & \mathbf{A}_{2,4} \\ \mathbf{A}_{3,1} & \mathbf{A}_{3,2} & \mathbf{A}_{3,3} & \mathbf{A}_{3,4} \\ \mathbf{A}_{4,1} & \mathbf{A}_{4,2} & \mathbf{A}_{4,3} & \mathbf{A}_{4,4} \end{pmatrix} \begin{pmatrix} \mathbf{v}_1^{l} \\ \mathbf{v}_2^{l} \\ \mathbf{v}_3^{l} \\ \mathbf{v}_4^{l} \end{pmatrix} = \begin{pmatrix} \mathbf{t}_1 \\ \mathbf{t}_2 \\ \mathbf{t}_3 \\ \mathbf{t}_4 \end{pmatrix} \tag{44}$$

could be implemented by collecting the contributions from particles and springs. In our example,

$$\mathbf{A} = \begin{pmatrix} \mathbf{M}_1 & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_2 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{M}_3 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{M}_4 \end{pmatrix} - h^2 \begin{pmatrix} \mathbf{S}_1 + \mathbf{S}_3 & -\mathbf{S}_1 & -\mathbf{S}_3 & \mathbf{0} \\ -\mathbf{S}_1 & \mathbf{S}_1 + \mathbf{S}_2 & -\mathbf{S}_2 & \mathbf{0} \\ -\mathbf{S}_3 & -\mathbf{S}_2 & \mathbf{S}_2 + \mathbf{S}_3 & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{pmatrix} \tag{45}$$

Initialization: Set $\mathbf{t}_i = \mathbf{0}$ for all particles i. For all springs k, compute $\mathbf{S}_k = \frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_j)}{\partial \mathbf{x}_i}$ with i and j being the two particles of spring k.

Iterate over particles i: Compute $\mathbf{t}_i += \mathbf{M}_i \mathbf{v}_i^l = m_i \mathbf{v}_i^l$.

Iterate over springs k: Spring k contributes to forces i and j and connects particles i and j corresponding to four contributions in matrix $\mathbf{J}$:

$$\mathbf{S}_k = \frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_j)}{\partial \mathbf{x}_i} = \frac{\partial \mathbf{f}_k(\mathbf{x}_j \leftarrow \mathbf{x}_i)}{\partial \mathbf{x}_j} = -\frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_j)}{\partial \mathbf{x}_j} = -\frac{\partial \mathbf{f}_k(\mathbf{x}_j \leftarrow \mathbf{x}_i)}{\partial \mathbf{x}_i} \tag{46}$$

Compute

$$\begin{aligned} \mathbf{t}_i += & -h^2 \left(\frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_j)}{\partial \mathbf{x}_i} \mathbf{v}_i^l + \frac{\partial \mathbf{f}_k(\mathbf{x}_i \leftarrow \mathbf{x}_j)}{\partial \mathbf{x}_j} \mathbf{v}_j^l \right) \\ = & -h^2 \left(\mathbf{S}_k \mathbf{v}_i^l - \mathbf{S}_k \mathbf{v}_j^l \right) = -h^2 \mathbf{S}_k \left(\mathbf{v}_i^l - \mathbf{v}_j^l \right) \\ \mathbf{t}_j += & -h^2 \left(\frac{\partial \mathbf{f}_k(\mathbf{x}_j \leftarrow \mathbf{x}_i)}{\partial \mathbf{x}_i} \mathbf{v}_i^l + \frac{\partial \mathbf{f}_k(\mathbf{x}_j \leftarrow \mathbf{x}_i)}{\partial \mathbf{x}_j} \mathbf{v}_j^l \right) \\ = & -h^2 \left(-\mathbf{S}_k \mathbf{v}_i^l + \mathbf{S}_k \mathbf{v}_j^l \right) = -h^2 \mathbf{S}_k \left(\mathbf{v}_j^l - \mathbf{v}_i^l \right) \end{aligned} \tag{47}$$

Iterate over particles i: Compute

$$\mathbf{v}_i^{l+1} = \mathbf{v}_i^l + \omega \mathbf{D}_i^{-1} (\mathbf{s}_i - \mathbf{t}_i) \tag{48}$$

Note: Matrix $\mathbf{D}_i$ contains the three diagonal elements a_{11}, a_{22}, a_{33}, of $\mathbf{A}_{i,i}$. I.e.,

$$\mathbf{D}_i^{-1} = \begin{pmatrix} \frac{1}{a_{11}} & 0 & 0 \\ 0 & \frac{1}{a_{22}} & 0 \\ 0 & 0 & \frac{1}{a_{33}} \end{pmatrix} \tag{49}$$

These values can be precomputed and stored at particles.