Computational Physics

Mass-spring problems and PDEs

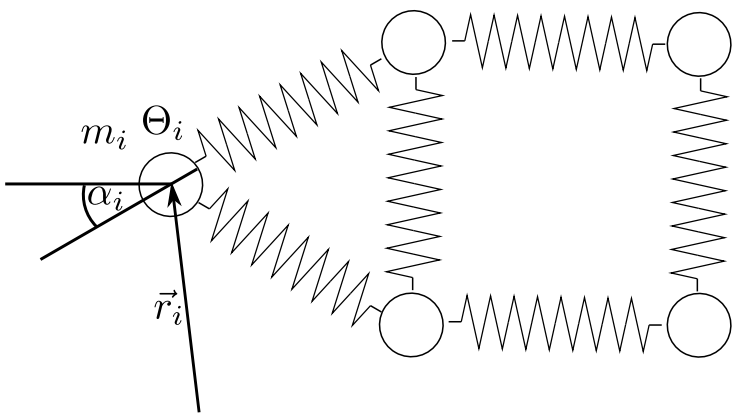
Discrete mass-spring systems

We consider the problem of small masses connected by springs. For simplicity, we only consider two dimensions.

The particles are characterized by

- positions $\mathbf{r}_i$ and momenta $\mathbf{p}_i$
- masses m_i
- orientations α_i and angular momenta J_i
- moments of intertia Θ_i (small)

They are connected by springs.



Models for a spring

The simplest spring creates a linear force if extended (Hookes law):

$$\mathbf{F} = -k\frac{\Delta\mathbf{r}}{|\Delta\mathbf{r}|}(|\Delta\mathbf{r}| - L),$$

where $\Delta\mathbf{r}$ is the vector between its end points, L is its equilibrium length and k the axial stiffness.

Most springs also have a weaker lateral response. It is (to first approximation) proportional to the difference in orientation between a particle and the mean spring orientation:

$$T_i = -\kappa\left(\alpha_i - \tan^{-1}\frac{\Delta r_y}{\Delta r_x}\right).$$

In reality, springs are not linear, but have some higher-order terms, e.g. in axial direction

$$\mathbf{F} = \frac{\Delta\mathbf{r}}{|\Delta\mathbf{r}|}[k_1(|\Delta\mathbf{r}| - L) + k_2(|\Delta\mathbf{r}| - L)^2 + \ldots].$$

Large deformation equations

Writing the equations of motion directly from this is not fun. Instead, it is better to use Hamiltonian or Lagrangian mechanics.

The classical Hamiltonian is the total energy of the system:

$$\mathcal{H} = \underbrace{\sum_i \frac{|\mathbf{p}_i|^2}{2m_i} + \frac{J_i^2}{2\Theta_i}}_{\text{over all particles}} + \underbrace{\sum_i \frac{1}{2}k(|\Delta\mathbf{r}_i| - L_i)^2 + \frac{1}{2}\kappa\left(\alpha_i - \tan^{-1}\frac{\Delta r_{i,y}}{\Delta r_{i,x}}\right)^2}_{\text{over all springs}}$$

This Hamiltonian is only for the simplest spring models.

The equations of motion are then given by the canonic equations:

$$\partial_t \mathbf{r}_i = \frac{\partial \mathcal{H}}{\partial \mathbf{p}_i}, \qquad \partial_t \mathbf{p}_i = -\frac{\partial \mathcal{H}}{\partial \mathbf{r}_i},$$
$$\partial_t \alpha_i = \frac{\partial \mathcal{H}}{\partial J_i}, \qquad \partial_t J_i = -\frac{\partial \mathcal{H}}{\partial \alpha_i}.$$

Lagrangian mechanics allows the inclusion of loss (damping).

Small deformation limit

The large deformation equations are nonlinear: Only time-domain analysis, no frequency-domain.

For frequency-domain: Assume only small deformation around equilibrium

$$\mathbf{r}_i = \mathbf{r}_i^{(\text{eq.})} + \mathbf{u}_i.$$

Axial spring forces depend only on the projection of the displacement on the spring's orientation and they push along this direction:

$$\mathbf{F} = -\mathbf{e}_i^{(o)} k(\Delta\mathbf{u}_i \cdot \mathbf{e}_i^{(o)}),$$

where $\mathbf{e}_i^{(o)}$ is the direction of the spring in equilibrium.

Small deformation limit (cont'd)

For the lateral deformation, we first assume that the particles' orientations remain constant. This simplifies the torque.

For a horizontally oriented spring, we find:

$$T_i = -\kappa \tan^{-1} \frac{\Delta u_y}{\Delta u_x + L} \approx -\kappa \frac{\Delta u_y}{L}.$$

This acts with a lever on the adjacent particles, which then experience a force in y-direction:

$$F_i \approx -\tilde{\kappa} \Delta u_y.$$

For an arbitrarily oriented spring, we must replace u_y with the projection of $\Delta \mathbf{u}$ on a vector $\mathbf{e}_i^{(e)}$ perpendicular to the spring's orientation:

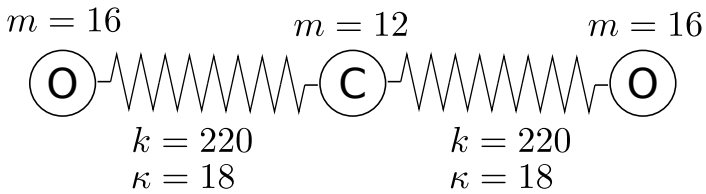
$$F_i \approx -\mathbf{e}_i^{(e)} \tilde{\kappa} (\Delta \mathbf{u} \cdot \mathbf{e}^{(e)}).$$

As a result, the spring's action can be expressed via a matrix K, whose eigenvalues are k and $\tilde{\kappa}$:

$$\mathbf{F}_i = -K \Delta \mathbf{u}_i.$$

Classroom problem: Vibrations of a CO2 molecule

Consider the molecule with annotated masses and spring constants:



Parametrize the molecule by vectors (x_i, y_i) that describe the displacement of the atoms from their equilibrium positions.

- Set up a matrix that models the molecule and find the eigenvalues and corresponding eigenvectors.
- In measurements, one finds absorption bands at frequencies $\nu_1 \approx 7 \times 10^{13}\,\text{Hz}$, $\nu_2 \approx 4 \times 10^{13}\,\text{Hz}$, and $\nu_3 \approx 2 \times 10^{13}\,\text{Hz}$. Identify the corresponding types of oscillations.
- Explain why several eigenvalues are zero. Why is no oscillation experimentally observable at $\nu \approx 1 \times 10^{13}\,\text{Hz}$?
- Modify your program to run a time-domain simulation using a 4th order Runge-Kutta (e.g. *ode45*). Run the program to $t = 100$ with initially one oxygen atom displaced by $(-0.3, 1)$.

Prototypical linear PDEs

For understanding linear ODEs it was sufficient to focus on

$$\partial_t \mathbf{y} = A\mathbf{y},$$

because every linear ODE can be brought to this form.

This is not possible for PDEs.

However, there are a few prototypical ones that represent important classes:

- Advection equation: $\partial_t u + \operatorname{div} \mathbf{j}(u) = 0$ (first order PDEs)
- Laplace equation: $\Delta u = 0$, with $\Delta = \partial_x^2 + \partial_y^2 + \partial_z^2$. (elliptic PDEs)
- Diffusion equation: $\partial_t u - \Delta u = 0$ (parabolic PDEs)
- Wave equation: $\partial_t^2 u - \Delta u = 0$ (hyperbolic PDEs)

The three classes have different types of solutions and typically require different numerical methods.

Dimensionless units

As the example for today we consider the 1d acoustic wave equation

$$\rho_0 \partial_t^2 p(x,t) - \beta^{-1} \partial_x^2 p(x,t) = 0,$$

with equilibrium mass density ρ_0, compressibility β and local pressure p.

First, we transform the problem to dimensionless units, i.e. transform time, space and/or p such that ρ and β disappear.

Absorb factor β^{-1} in the function $p(x,t)$:

$$[\beta\rho_0\partial_t^2 - \partial_x^2] \underbrace{\beta^{-1} p(x,t)}_{\tilde{p}(x,t)} = 0,$$

Introduce new time variable τ (unit of space is still free):

$$t = \sqrt{\beta\rho_0}\tau, \quad \Rightarrow \quad \partial_\tau = \sqrt{\beta\rho_0}\partial_t.$$

$$\Rightarrow \quad [\partial_\tau^2 - \partial_x^2]\tilde{p}(x,t) = 0,$$

Reduction to the advection equation

Elliptic and hyperbolic PDEs can be formally reduced to advection form. We demonstrate this for the wave equation:

$$\partial_t u = -\operatorname{div} \mathbf{j} = -\partial_x j_x - \partial_y j_y - \partial_z j_z, \qquad \partial_t^2 u - \Delta u = 0.$$

The Laplacian is related to the divergence: $\Delta = \operatorname{div} \operatorname{grad}$.

We reformulate:

$$\begin{aligned} \partial_t(\partial_t u) &= \operatorname{div} \operatorname{grad} u = \operatorname{div} \mathbf{j}, \\ \partial_t \mathbf{j} &= \partial_t \operatorname{grad} u = \operatorname{grad}(\partial_t u). \end{aligned}$$

By introducing a vector-valued state vector $\mathbf{U} = [(\partial_t u), j_x, j_y, j_z]^T$, this has the form of the advection equation:

$$\partial_t \begin{pmatrix} (\partial_t u) \\ j_x \\ j_y \\ j_z \end{pmatrix} + \partial_x \begin{pmatrix} j_x \\ (\partial_t u) \\ 0 \\ 0 \end{pmatrix} + \partial_y \begin{pmatrix} j_y \\ 0 \\ (\partial_t u) \\ 0 \end{pmatrix} + \partial_z \begin{pmatrix} j_z \\ 0 \\ 0 \\ (\partial_t u) \end{pmatrix} = 0.$$

How does that look in 1d?

In 1d, this becomes:

$$\partial_t \begin{pmatrix} v \\ w \end{pmatrix} = \partial_x \begin{pmatrix} w \\ v \end{pmatrix} \qquad \text{with} \qquad v = \partial_t p, \quad w = \partial_x p.$$

This is very reminiscent of the harmonic oscillator examples, where leapfrog integration was a good idea:

$$\partial_t \begin{pmatrix} x \\ p \end{pmatrix} = \begin{pmatrix} p \\ -x \end{pmatrix}.$$

Homework

Implement a simple particle-based model for gas dynamics (see problem sheet).