APiE Exercise - MDSolids2D

Consider the 2D spring network as shown in APiE Exercise `MDSolids1D` and below in Figure 1. (Each spring with masses is equivalent to a truss, as introduced later in the finite element part of the APiE-course.)

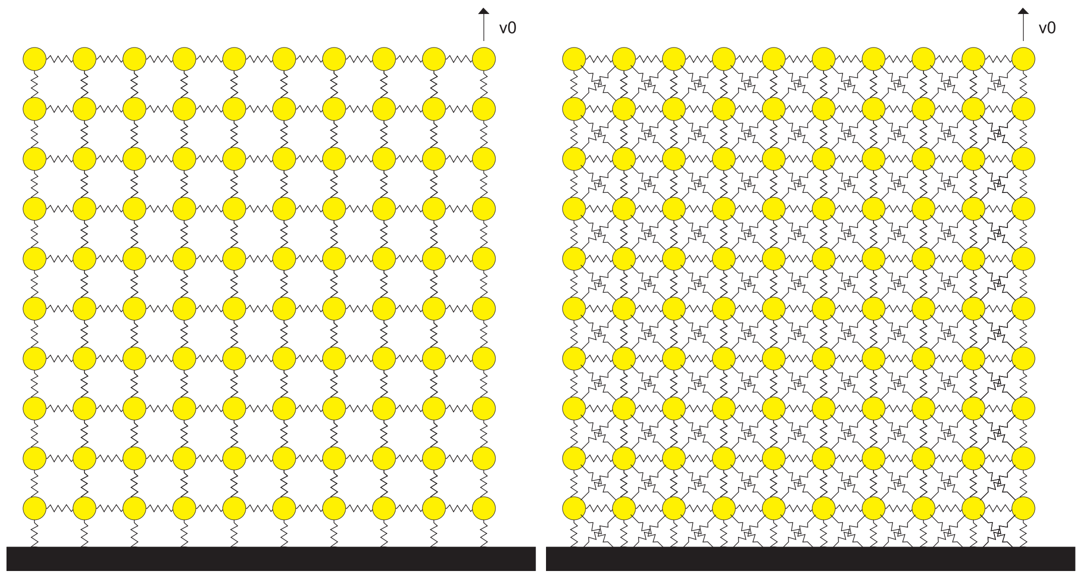

Figure 3: Square Lattice (Left) with nearest neighbor bonds and (Right) with additional diagonal bonds. The lowermost row of springs is connected to the wall, which can be represented by particles that do not move vertically - they are free to move horizontally. Only the lowermost left particle is fixed (constrained) in both directions!

We will now simulate a truss-network, i.e., a mass-spring network, which represents a 2D-solid, by a Molecular Dynamics (MD) simulation. Particles/atoms all have equal mass and are connected by linear springs. (This system will also be solved in the FEM part of the APiE course).

- Choose the mass of the particles such that the mass of the total system is equal to the total mass of the truss-elements (springs) in the (diagonal-network) FEM simulation.

  The parameters used in the FEM exercise are given here: Each truss/spring has a cross-sectional area $A = 0.0031\,m^2$, density $\rho = 7800\,kg/m^2$, and length 1 m (horizontal and vertical) resp. $\sqrt{2}$ m (diagonal). Then the total mass is

  $$[(2 \cdot 9 \cdot 10) \cdot L_0 + 2 \cdot 9^2 \cdot \sqrt{2} L_0] \cdot A \cdot \rho = 9892.1\,\mathrm{kg}$$

  Thus, each particle weighs $m = 98.921\,kg$. Verify this calculation.

- Choose the spring constant k such that the spring retains its Young's modulus of $E = \frac{F/A}{\Delta L/L} = 210$ GPa. Note: The diagonal springs have different constants than the vertical and horizontal springs.

  The Young's modulus satisfies $E = \frac{FL}{A\Delta L}$. A linear spring satisfies $F = k\Delta L$. Thus, $k = \frac{EA}{L} = 6.5100\ 10^8$ N/m for horizontal and vertical springs, $k = 4.6033\ 10^8$ N/m for diagonal springs. Verify this calculation.

- In some cases, the MD result has to be relaxed, i.e., the kinetic energy has to be dissipated. Then, choose a uniform damping coefficients $\gamma = 65020$ kg/s such that the horizontal/vertical springs have a restitution coefficient of $\epsilon = 0.5$, where the restitution coefficient is defined as the velocity after a half-period of the damped harmonic oscillator, divided by the initial velocity. Give the analytical solution for a mass-spring system from the `ODE` exercise, and for a two particle system from the `MDSolids1D` exercise.

  The oscillation frequency of the springs is now $\omega = \sqrt{2k/m - (\nu/m)^2}$, the collision time is $t_c = \pi/\omega$. You should use a time step of $\Delta t = t_c/50$.

Exercise 1 (Implementation 5 pts. + animation 2 pts.)

When the structures are implemented in the 2D MD code, give an initial velocity to the upper right particle and animate the motion in a movie. Explain the differences/similarities in the reaction of the two structures.

Exercise 2 (Moduli and sound-speed measurement 3 pts.)

This question is equal to the `FEM` *exercise, only here we use MD.*

Using MD simulations, obtain the results for the Young's modulus E_{struc}, the shear modulus G_{struc}, the Poisson ratio ν_{struc} and sound speed V_s of the bulk structure – and compare them to the finite element simulation results (when they are available later). For more details see the script.

(a) The Young's modulus is defined as the ratio of longitudinal stress and strain, $E_{struc} = \frac{F_y/d/L_x}{\Delta L_y/L_y}$, where F_y is the total vertical force on all top-row particles (nodes), and $d = 1\,\text{m}$ is the depth of the system (not visible in 2D). The vertical longitudinal strain is the ratio of change of length to initial vertical length. Apply 10 kN vertical load in the positive (up) direction to all nodes (particles) in the uppermost row of the structures.

(b) From the same simulation, the Poisson-ratio can be measured as the ratio of (changes of) horizontal to vertical lengths $\nu_{struct} = \frac{\Delta L_x}{\Delta L_y}$.

(c) The shear modulus is defined as the ratio of shear-stress and -strain, $G_{struc} = \frac{F_x/d/L_x}{\Delta L_x/L_y}$, where F_x is the total horiontal force on all top-row particles (nodes). The shear-strain is the ratio of change of horizontal position to the vertical height. For this, apply 10 kN horizontal load in the positive (right) direction to all nodes (particles) in the uppermost row of the structures.

(d) Estimate the speed of sound (roughly) in the structure by observing the time t_s it takes for the applied force at the top (or the applied initial velocity from Ex.1) to become visible at the bottom. The speed can then be computed as $V_s = L/t_s$.

For the tests, plot the kinetic to potential energy ratio as a function of time. How long does is it take until the kinetic energy is dissipated? Which criterion did you use? How does it change for different damping coefficients?

After each relaxation, check that the displacement at the left and right is “homogeneous”, i.e., the left and right nodes are aligned on a line. Discuss your observations.

Exercise 3 (Voluntary extra: 4 pts.)

Make the packing anisotropic. Either cut one of the diagonal springs, or make, e.g., the vertical springs stiffer. Perform the same operations and calculations as above. Report and describe the differences.