APiE – Molecular Dynamics (MD) for Solids 1D

This 1D exercise is for warm-up and can be skipped (0EC), or the MD for Fluids code can be used and modified. Goal is to set up a linear 1D (one-dimensional) chain. First, generalize your ODE-solver to 2 "particles" or atoms connected by one spring (see APiE-script).

Requirement: Preparation for future programming in 2D:
Using the linear spring model, implement in your solver the interaction force calculation in a function. Do so using vectors, and strictly split the connectivity (neighborhood search) from the force calculation and the latter separate completely from the integration.

Compute forces using the normal vector $\hat{n} = (\vec{x}_i - \vec{x}_j)/|\vec{x}_i - \vec{x}_j|$, and the departure from the equilibrium position length $\delta = |\vec{x}_i - \vec{x}_j| - x_e$. Take care that the signs are correct. Implement the force calculation in a function that receives the two particles and returns the force (scalar in 1D, vector in 2D). Then establish for each particle a loop over all particles it has a spring-connection with (this will be relevant below for the linear chain and later for 2D) and sum up all forces acting on a particle. For each particle pair (i,j), the forces acting on i by j and reverse are related by $f_{i\leftarrow j} = -f_{j\leftarrow i}$.

Note: Make sure that you program modular. Separate variable definition, input, output, force-calculation and integration clearly as different modules – or functions. Write a function for the force-calculation using the methods from above, such that the force calculation appears only once (per particle-pair) in the program. For this implement a loop over particle pairs. Optimization for neighbor-search can be added later.

Display the motion of the pair of particles for some time and also display the total energy and the kinetic and potential fractions. Compare the numerical result to the analytical solutions for contact duration (or oscillation period) and restitution coefficient, without and with dissipation active.

Generalize the program to N particles and implement a linear chain with 11 particles, see Fig. 1 The first and the last particle are connected to a fixed wall. The distance between the particles

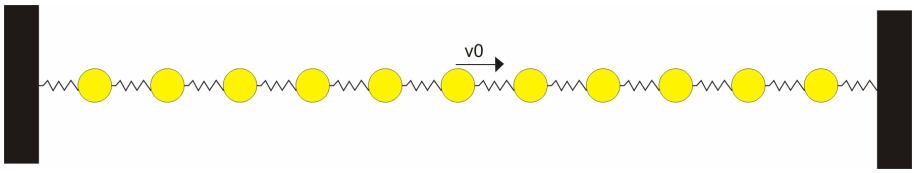

Figure 1: Schematic Linear Chain

is x_e and this is equal to the equilibrium length of the springs. The central particle gets an initial velocity v_0, all the other particles have initial velocity equal to zero. Display the motion of the particles (in a graph).

Visualize the movement of the particles in a movie. Let the color of each particle give a measure of the velocity of the particle.

Hints:
Make sure that you split the force-calculation and the integration (e.g. Verlet or Runge-Kutta) loops. Make sure that you set forces to zero at each new time.

Here an example algorithm (but better also see the script):

Loop 1: integration loop over time ($t_i = t_{i-1} + dt$)

- reset ALL forces ($f_x[.] = 0$)
- **Loop 2:** over all particles (i<N_{max})
  - **Loop 3:** over all contact partners (j<i)
    - distance dist=sqrt((x[i]-x[j])*(x[i]-x[j]))
    - normal n_x=(x[i]-x[j])/dist
    - overlap delta=rad[i]+rad[j]-(x[i]-x[j])*n_x
    - contact-selection (for particles: if delta>0; for solids: if connected?)
      - relative velocity (v_{rel}=-(v_x[i]-v_x[j])*n_x)
      - interaction force (f_x[i]=(k*delta+v*v_{rel})*n_x)
      - partner interaction (f_x[j]=-(k*delta+v*v_{rel})*n_x)
  - **end Loop 3**
- temporary store position (xtmp=x[i])
- integrate (x[i]=2*xtmp-s_x[i]+f_x[i]/m[i]*dt*dt)
- save old position (s_x[i]=xtmp)
- **end Loop 2**
- increase time (t=t+dt)

end Loop 1

end program

APiE Exercise - MDSolids2D (1.0EC)

NEW VERSION January 2017

Consider the 2D spring network as shown below in Figure 2. [This is the generalization of the MD1D assignment, and also can be done directly, but make sure you use the algorithm and detailed instructions given in the MD1D assignment as a guideline. Note that you also can re-use your MD for Fluids code here.]

Setup the code that you have $N_x \times N_y$ particles such that $N \times 1$ provides you back the linear chain (in principle). Use the hints at the end of the 1D section, i.e. use vectors, and do *not* implement a new force calculation for each type of spring, but use one function.

Each spring with masses is equivalent to a truss, as introduced in the finite element part of the APiE-course. Match the stiffness of the springs such that the MD results can be compared to the FEM results. (Alternatively, choose a stiffness k_{MD} and match stress (and moduli) later via: $\sigma_{FEM} = (k_{FEM}/k_{MD})\sigma_{MD}$. In any case explain how the stiffness k_{FEM} and k_{MD} are computed.)

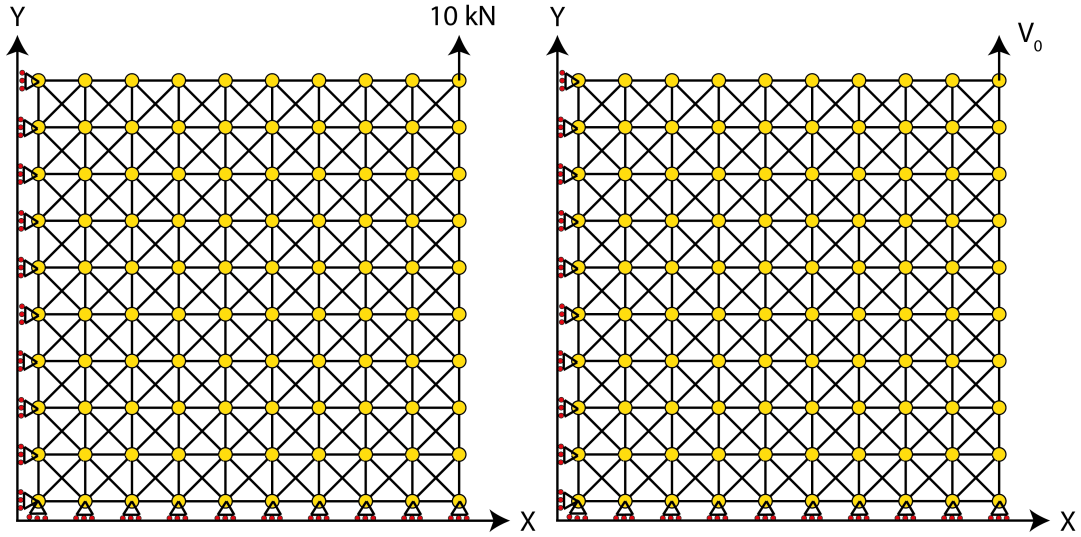

Figure 2: Square Lattice with nearest neighbor bonds and with additional diagonal bonds. The lowermost row of springs is connected to the wall, which can be represented by particles that do not move vertically - they are free to move horizontally. Only the lowermost left particle is fixed (constrained) in both directions! Starting from this, there can be many different further structures developed: For example, remove all diagonal springs and you get a square-lattice. (Left) force boundary condition, and (Right) velocity boundary condition.

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, here, and are connected by linear springs, which can be different (vertical/horizontal vs. diagonal).

- Choose the masses and spring-stiffnesses of the particles such that the mass of the total system is equal to the total mass of the solid and such that the time step can be estimated

conveniently. What is a good time-step for two particles with mass m and stiffness k?

- The horizontal/vertical springs can have different spring constants k as the diagonal springs. Choose the spring constant k_{diag} such that the longer diagonal springs retains correspond to the same Young's modulus when regarding a linear chain (horizontal/vertical as opposed to diagonal). What is k_{diag}/k in that special case? Choose a k_{diag}/k as you like and give arguments for doing so.

- In some cases, the particles have a lot of kinetic energy. Then the MD result has to be relaxed, i.e., the kinetic energy has to be dissipated. Choose a uniform damping coefficients γ such that the horizontal/vertical springs get a restitution coefficient of $r \approx 0.5$, 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.

  The oscillation frequency of the springs is now $\omega = \sqrt{2k/m - (\nu/m)^2}$, the contact duration (momentum exchange time) is $t_c = \pi/\omega$. You should use a time step of order $\Delta t = t_c/50$. (*This should be checked by analytical computation for one pair of particles.*)

  Confirm performance by using larger and smaller time-steps.

Exercise 1 (Implementation+questions above 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, i.e. with and without the diagonal springs in Fig. 2.

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

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.

(a) For example, 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 is the depth of the system. The vertical longitudinal strain is the ratio of change of length to initial vertical length. For this, apply a 1 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 horizontal 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 a horizontal load in the positive (right) direction to all nodes (particles) in the uppermost row of the structures.

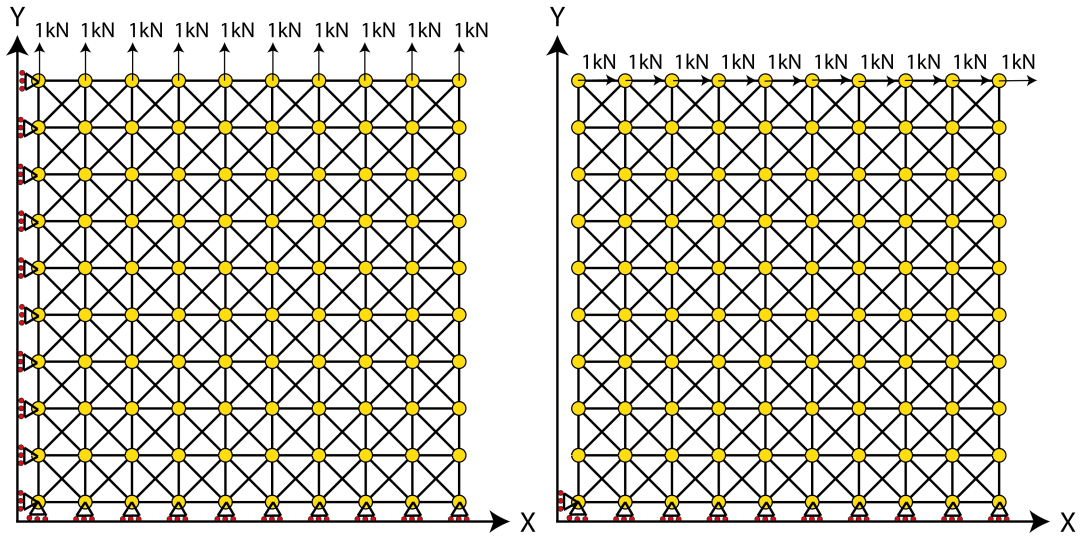

Figure 3: Schematically are shown, the force boundary conditions (Left) for the Young modulus and Poisson, and (Right) for the shear modulus test.

(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 $V_s = L/t_s$. What is your criterion to identify the so-called arrival time? What are other possible criteria? How does the speed compare to the estimate of $t_s = N_s t_c$, where N_s is the number of particles in the respective direction?

(e) For several of 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 to define dissipation? How does it change for different damping coefficients?

How does this change if you add so-called "global" background-damping, i.e., a damping force that is $\vec{f_i} = -\gamma \vec{v_i}$ negative proportional to the velocity of each particle relative to the background.

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: 0.5 EC)

Choose *one* new configuration for both (a) and (b):

(a) Make the packing anisotropic. Either cut some of the springs, e.g. one diagonal direction, or make, e.g., the vertical springs stiffer.

(b) Make the system random. Either randomly vary the spring constants or randomly cut springs out. In the latter case, make sure to relax the system first. What do you observe.

Note that for anisotropic and random systems, one has to measure the Young- and Shear-moduli

as well as Poisson ratio in all directions, since they are not equal anymore.

Perform the same operations and calculations as above. Report and describe the differences.

Exercise 4 (Voluntary extra: 0.5 EC)

Compare your MD and FEM results for the same systems and discuss.