MSE Research Internship: Atomistic Modelling of a 2-D Solid

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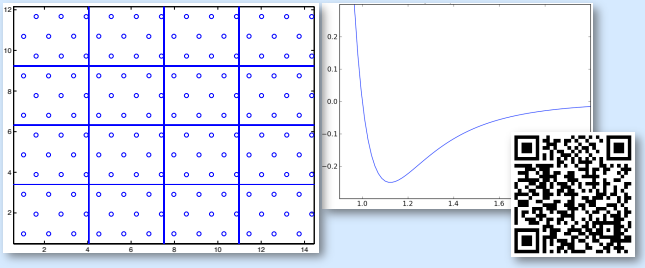
Abstract

•2D model solid: Pairwise Lennard-Jones interaction potential
•Uniform thermodynamic equilibrium
•Non-zero temperature
•***Aim:*** Determination of a stress strain relation by means of simulations on an atomistic

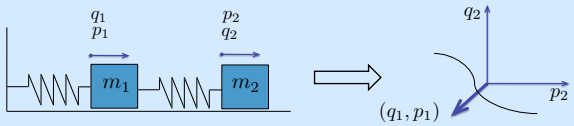


Theoretical Background and Definitions

Phase space:

The phase space is spanned by the degrees of freedom of a dynamical system (2n momenta, 2n position coordinates; n = #atoms)

Example: The phase space of a dynamical system with two masses is spanned by the momenta of the masses and their positions (4-dimensional phase space)



Hamiltonian System:

The solid is modeled as a Hamiltonian System hence each microscopic state corresponds to a unique point/vector in the phase space. The formal representation is the Hamiltonian Function:

$$H(\boldsymbol{q},\boldsymbol{p}) = K_{kin}(\boldsymbol{p}) + V_{pot}(\boldsymbol{q})$$

$$\frac{\partial H}{\partial \boldsymbol{q}} = -\dot{\boldsymbol{p}}$$

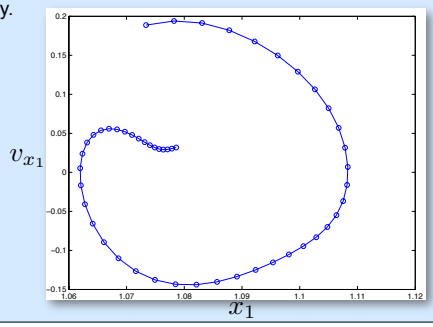
$$\frac{\partial H}{\partial \boldsymbol{p}} = \dot{\boldsymbol{q}}$$

Molecular Dynamics:

The material is modeled by point masses connected with non-linear springs and the dynamics of the system can be described through a system of ordinary differential equation.
Each point in the phase space can be considered as an initial condition and a trajectory in the phase space is computed by solving the ODE numerically. Any macroscopic properties (such as stresses) are obtained by time averaging their microscopic equivalents along the phase space trajectory:

$$\mathcal{F}^{macro} = \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathcal{F}^{micro}(\boldsymbol{q}(t),\boldsymbol{p}(t))dt$$

The figure below displays the x_1 and v_{x_1} component of the phase space trajectory.



Canonical ensemble:

The canonical ensemble is a probability density function that describes the likelihood of the possible states of a Hamiltonian system at a certain temperature T.

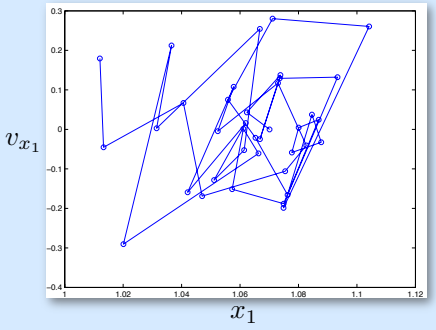
$$\rho(\boldsymbol{q},\boldsymbol{p}) = \frac{1}{Z} e^{\frac{-H(\boldsymbol{q},\boldsymbol{p})}{k_B T}}$$

Monte Carlo:

Instead of computing a trajectory in phase space one can produce samples by means of a Markov Chain Monte Carlo method that (in the limit) correspond to the canonical ensemble. The averaging is then done over all the samples and not over time.

$$\mathcal{F}^{macro} = \int_\Gamma \mathcal{F}^{micro}(\boldsymbol{q},\boldsymbol{p})\rho(\boldsymbol{q},\boldsymbol{p})d\boldsymbol{q}d\boldsymbol{p} \approx \frac{1}{M}\sum_i^M \mathcal{F}^{micro}(\boldsymbol{q}_i,\boldsymbol{p}_i)$$

The figure below displays the x_1 and v_{x_1} components of the state vectors generated with a hybrid MCMC method.

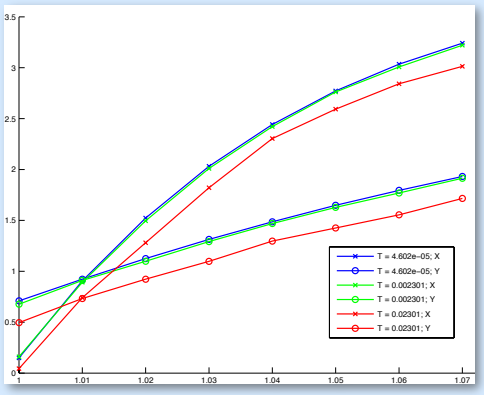


Methods

Hybrid Markov Chain Monte Carlo: The idea behind the Hybrid MCMC is to combine the molecular dynamics approach (deterministic) and the Monte Carlo approach (probabilistic). This means the the MD is used to find new proposals (points in the phase space) that (in the limit) correspond to the Canonical Ensemble.

Results

The simulations were carried out on the 2D model for three different temperatures introducing an uniaxial deformation in x-direction and measuring the resulting stresses in x-direction (-x-) and y-direction (-o-).
As can be seen in the plot below reasonable stress-strain-relations could be established.



@ lowest temperature	T_1:	blue lines
@ medium temperature	$T_2 = 50*T_1$:	green lines
@ highest temperature	$T_3 = 500*T_1$:	red lines

References: - J.H. Weiner; 'Statistical Mechanics of Elasticity'
- D. C. Rapaport; 'The Art of Molecular Dynamics Simulation'
- P. S. Koutsourelakis; 'Atomistic Modeling of Materials' – lecture notes
- M . N. Radford MCMC using Hamiltonian dynamics