Optimal coupling in a multiscale model

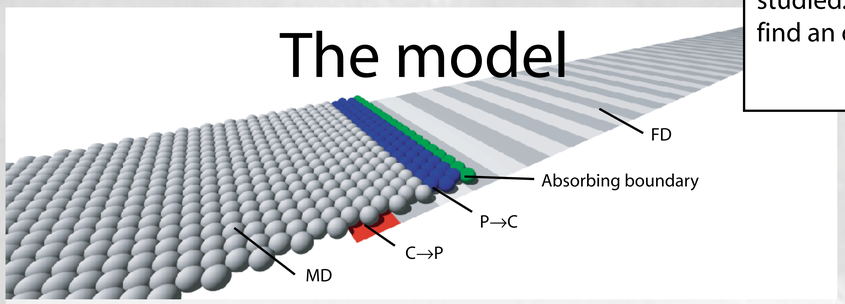
Håkon Enger (PGP), Jens Feder (PGP), Anders Malthe-Sørenssen (PGP), Hans Petter Langtangen (PGP/Simula)

PHYSICS OF GEOLOGICAL PROCESSES

Norwegian Centre of Excellence

We study a multiscale model which is the coupling of a molecular dynamics model with a viscoelastic continuum model. The impact of different coupling strategies on a test problem where a wave propagates through the interface between the different modelling schemes is studied. In particular, the coupling equations are averaged over a time scale which is varied to find an optimal coupling strategy for minimizing nonphysical effects of the interface.

The model



We study a model consisting of an area divided into three sub-areas, one modelled by atomic molecular dynamics (MD), one by a finite difference (FD) scheme, and an "overlap" region between them, which is modelled both by MD and FD. There are two "interfaces" between the different areas. The coupling between MD and FD modelling happens at these interfaces. The outer boundary of the MD simulation, where the boundary condition is imposed from the FD model, is labelled C→P ("continuum to particle"), while the boundary of the FD model is labelled P→C. A sketch of the model is presented above.

Molecular dynamics model

The "small-scale" part of our multiscale model is a 2 or 3 dimensional MD simulation using a Lennard-Jones (LJ) potential,

Finite difference model

The "large-scale" part of the model is a 1- or 2-dimensional FD model of an elastic or viscoelastic medium. The rheology parameters of the model are fitted to be consistent with the MD model.

Coupling

We have tested two different schemes for coupling the two models.
Field coupling: We use the displacement field found in one model at the interface as a boundary condition on the other model.
Force coupling: Here, we determine the (average) force acting in one model and use that as a boundary condition on the other model.

Time averaging

Since the finite difference model is not expected to be valid for small time scales, the coupling scheme may include averaging over several time steps. This time averaging is expected to partly absorb the rapid fluctuations of the MD simulation which should not propagate into the FD model.

Absorbing boundary conditions

At the boundary of the MD model, we must use a scheme to absorb waves travelling out of the system without reflections. We use a special *absorbing boundary condition* adapted for MD at this boundary. The best way to implement such conditions in our model is currently under investigation.

Results

The problem

At the interface between the discrete MD model and the continuum FD model, there may appear unphysical reflections of waves passing from one side to the other. There are three main reasons why this happens:

Rheology matching: If the continuum model has different material properties than the MD model, reflection will occur. We use a best fit of the material parameters to minimize this problem.

Grid size: Waves with smaller wavelength than the grid size can not propagate into the FD model, and may be reflected back into the MD model. We use a set of absorbing boundary conditions at the boundary of the MD model to catch such waves.

Thermal fluctuations: The continuum model is averaged over time as well as space, and thermal fluctuations of the atoms should not propagate into the continuum. We use time averaging in the coupling region to dampen these fluctuations.

The figure on the right shows how well the coupled MD/FD model reproduces a pure MD model in an experiment where a narrow pulse travels from the MD region into the FD region, with a varying time averaging constant τ. We find an optimal time averaging constant at $\tau = 1250\ \Delta t$, where Δt is the time step of the MD model.

We find that *force coupling* combined with time averaging gives superior results to field coupling.

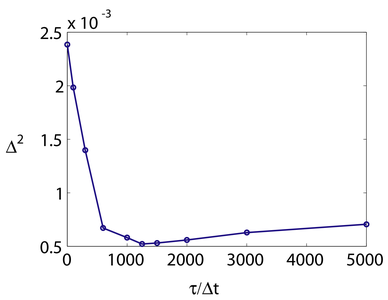
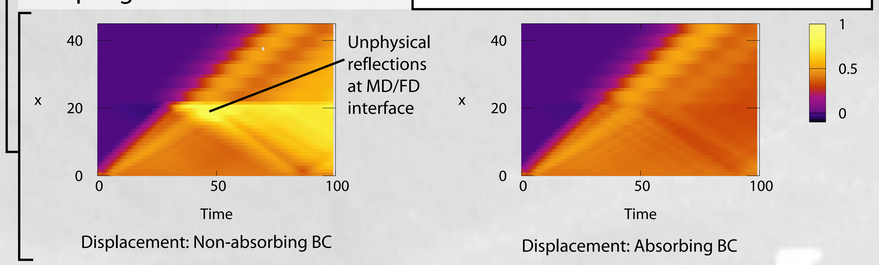
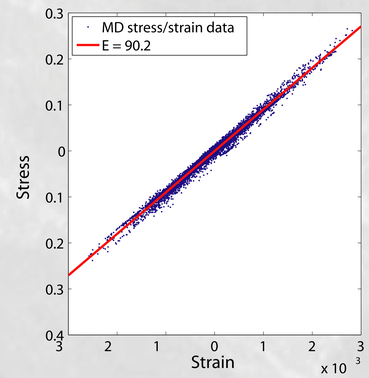


Figure showing deviation between pure MD model and coupled model, at varying time averaging constant. Optimal coupling found near $\tau = 1250\ \Delta t$.





Fitting Young's modulus from observed stress/strain in MD

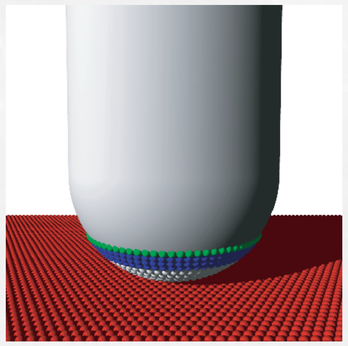
Fit of rheology parameters

To fit parameters in the rheological model used in the FD model, e.g. Young's modulus for linear elasticity, we make a discretization of an MD simulation, computing average displacement at each discrete point in time and space. Differentials are computed as in the FD model, and each point yields a data point (shown in the graph to the left). The points are then fitted to the given model using a least squares method.

Applications

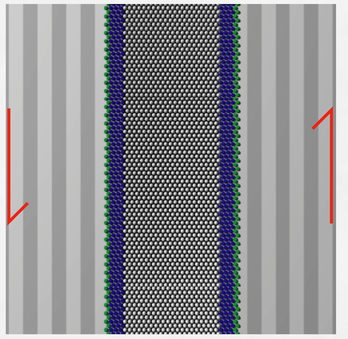
Adhesion and friction

We believe the proposed model is suitable to study adhesion and friction. These phenomena depend both on the atomic structure of the materials in contact[1], and on the larger scale geometry of the objects. Through a multiscale model, both of these dependencies may be studied simultaneously. We currently work on a geometry corresponding to a narrow tip in contact with a plane surface. Other geometries may also be interesting to study with a coupled model. A similar setup has been studied recently in [2].



Shear heating/melting

In a shear heating numerical experiment[3], a slab of material is loaded with a constant shear and released. The initial condition has a small perturbation in temperature along a plane in the material where melting will occur as the elastic energy is released. By modelling the region around this plane with molecular dynamics, the melting process may be studied in more detail.



Before the model may be used in practical applications, it must be thoroughly tested for correctness, accuracy and performance.

References

[1] B. Q. Luan and M. O. Robbins, *Nature* **435** (2005), 929
[2] B. Q. Luan et. al., *Phys. Rev. E* **74** (2006), 046710
[3] S. Bræck and Y. Y. Podlachikov, *Phys. Rev. Lett* **98** (2007), 095504