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Coarse-graining molecular dynamics models using an extended Galerkin method[1]

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I will present a systematic approach to coarse-grain molecular dynamics models for solids. The coarse-grained models are derived by Galerkin projection to a sequence of Krylov subspaces. On the coarsest space, the model corresponds to a finite element discretization of the continuum elasto-dynamics model. On the other hand, the projection to the finest space yields the full molecular dynamics description. The models in between serve as a smooth transition between the two scales. We start with a molecular dynamics (MD) model, $m_i\ddot{\mathbf{x}}_i = -\frac{\partial V}{\partial \mathbf{x_i}}$. First, let Y_0 be the approximation space for the continuum model. By projecting the MD model onto the subspace, we obtain a coarse-grained model, $M\ddot{\mathbf{q}} = F(\mathbf{q})$. Using the Cauchy-Born approximation, this model can be shown to coincide with the finite element representation of the continuum elastodynamics model. This model has limited accuracy near lattice defects. One natural idea is to switch to the MD model in regions surround local defect. As a result, one creates an interface between the continuum and atomistic description, where coupling conditions are needed. Direct coupling methods may involve enforcing constraints or mixing the energy or forces. Such an approach may suffer from large phonon reflections at the interface, and introduce large modeling error. In order to seamlessly couple this model to MD, we successively expand the approximation space to the Krylov spaces, $K_\ell = Y_0 + AY_0 + \cdots + A^\ell Y_0$. Here A is the force constant matrix, computed from the atomistic model. Due to the translational invariance, only a smaller number of such matrices need to be computed. By projecting the MD model onto this new subspace, we obtain an extended system, $M\ddot{\mathbf{q}} = F_0(\mathbf{q}, \boldsymbol{\xi_1}, \cdots, \xi_\ell), \ddot{\boldsymbol{\xi}}_\mathbf{1} = \mathbf{F_1}(\mathbf{q}, \boldsymbol{\xi_1}, \cdots, \xi_\ell), \cdots\cdots, \ddot{\boldsymbol{\xi}}_\ell = \mathbf{F}_\ell(\mathbf{q}, \boldsymbol{\xi_1}, \cdots, \xi_\ell)$. The additional variables ξ_j represent the coefficients in the extended approximation space. Using this systematic approach, one can build a hierarchy of models with increasing accuracy, each of which is a well-posed model. At the top of the hierarchy is the continuum model, represented on a finite element mesh. Then, on the same mesh, we obtain higher order approximations of MD. In the limit $\ell \to N$, the full MD description is recovered.

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