1D Atomistic-to-Continuum Coupling via Optimization

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ABSTRACT

We consider an optimization-based atomistic-to-continuum coupling strategy where the atomistic and continuum displacements and stresses are constrained to agree over some overlap region where both models hold. A simple 1D example illustrates the optimization scheme.

1. Introduction

Multiscale simulations leverage the accuracy of microscale simulations in regions where the physics are rapidly changing while taking advantage of the efficiency of macroscale simulations in the remainder of the domain. We are interested in the case where the computational domain Ω is divided into three disjoint regions: Ω_a, where the physics of the problem are governed only by first principles at the microscale; Ω_c where a macroscale model holds; and Ω_b which is some *bridge region* acting as an interface between the two models.

In the literature, agreement between the two models is achieved mainly through constraining the microscale dynamics based on macroscale information [1] or using Schwarz iteration to guarantee consistency between the models [2]. However, this paper describes an optimization-based coupling strategy which in [3, 4] was applied to two *macroscale* regions, each governed by a different partial differential equation (PDE). The difference in this paper is that optimization over the bridge region is used to couple a microscale atomistic model over $\overline{\Omega}_a \cup \overline{\Omega}_b$ with a macrocale continuum model over $\overline{\Omega}_b \cup \overline{\Omega}_c$.

2. Models

2.1 Atomistic

The division of Ω into the three subdomains is effected in the reference configuration, $\mathbf{X}$. We let $\mathcal{N}_a$ be the set of indices of particles located in $\overline{\Omega}_a / \left(\overline{\Omega}_a \cap \overline{\Omega}_b\right)$, and $\mathcal{N}_b$ be the set of particle indices located in $\overline{\Omega}_b$. The reference position of particle α is denoted by $\mathbf{X}_\alpha$, while its deformed position is given by $\mathbf{x}_\alpha$. Thus $\mathbf{u}_\alpha = \mathbf{x}_\alpha - \mathbf{X}_\alpha$ is the displacement of the α particle.

The force on particle α is assumed local and due only to particles within the ball $\mathcal{B}_\alpha = \{\mathbf{x} \in \Omega : |\mathbf{x} - \mathbf{x}_\alpha| \leq \eta\}$ for some given $\eta \geq 0$. Let $\mathcal{N}_\alpha = \{\beta | \mathbf{x}_\beta \in \mathcal{B}_\alpha, \beta \neq \alpha\}$, i.e. $\mathcal{N}_\alpha$ is the set of indices

corresponding to the particles in $\mathcal{B}_\alpha$, other than the α particle itself. Then, the force on the atomistic particle α due to all the other particles is given by

$$\sum_{\beta \in \mathcal{N}_\alpha} \mathbf{f}_{\alpha,\beta} = 0 \qquad \text{for } \alpha \in \mathcal{N}_a \cup \mathcal{N}_b, \tag{1}$$

where $\mathbf{f}_{\alpha,\beta}$ denotes the force acting on particle α due to particle β.

We do not apply the atomistic model to particles in Ω_c; however, some particles in $\bar{\Omega}_a \cup \bar{\Omega}_b$ depend upon force contributions from particles in Ω_c. When the atomistic displacement of a particle in Ω_c is required, we assume it is equivalent to the continuum displacement, $\mathbf{u}(\mathbf{X})$.

2.2 Continuum Model

The Cauchy stress tensor, $\sigma(\mathbf{X})$, is used to determine the force over the continuum region. At any point $\mathbf{X}$ in the continuum region, we have the force balance

$$\nabla \cdot \sigma + \mathbf{b}_c = 0 \qquad \text{for } \mathbf{X} \in \bar{\Omega}_c \cup \bar{\Omega}_b \tag{2}$$

where $\mathbf{b}_c$ is an externally applied volumetric force. In §4., we assume $\mathbf{b}_c = 0$.

3. Optimization Scheme

Over Ω_b both models hold, so the atomistic and continuum displacements and stresses should agree in the bridge region. The displacement constraint is expressed as

$$\mathbf{u}_\alpha = \mathbf{u}(\mathbf{X}_\alpha) \qquad \text{for all } \alpha \in \mathcal{N}_b. \tag{3}$$

The stress constraint,

$$\sigma_a^\alpha = \sigma(\mathbf{X}_\alpha) \qquad \text{for all } \alpha \in \mathcal{N}_b \tag{4}$$

requires an averaged "atomistic stress", σ_a^α, based on the computed atomistic displacements. This expression is given by

$$\sigma_a^\iota = \frac{1}{2|\Delta_\iota|} \sum_{j \neq i} d_{ij} \left(\mathbf{x}_i - \mathbf{x}_j\right) \otimes \mathbf{f}_{i,j} \tag{5}$$

where the summation runs over all pairs of particles in the domain Ω, and the averaging is performed over the representative volume element, Δ_ι [5]. The weighting function, d_{ij}, is determined by the fraction of $|\mathbf{x}_i - \mathbf{x}_j|$ that overlaps Δ_ι.

We separately solve the atomistic model in Ω_a and the continuum model in Ω_c by specifying the displacements for the two models along Ω_b in such a way that

$$\mathbf{u}(\mathbf{X}) = \mathbf{U}(\mathbf{X}) \qquad \text{for } \mathbf{X} \in \Omega_b \quad \text{and} \quad \mathbf{u}_\alpha = \mathbf{U}(\mathbf{X}_\alpha) \qquad \text{for } \mathbf{X}_\alpha \in \Omega_b \tag{6}$$

for some guess displacement $\mathbf{U}(\cdot)$. Arbitrary choices for $\mathbf{U}(\cdot)$ will not satisfy (4), so the optimal $\mathbf{U}(\cdot)$ is found by solving the optimization problem

$$\min_{\mathbf{U}} \|\sigma_a^\alpha - \sigma(\mathbf{X}_\alpha)\|, \tag{7}$$

where σ_a^α and $\sigma(\mathbf{X})$ are determined from solving Eqns. (1) and (2) separately using the boundary conditions in Eqn. (6).

4. Numerical Example

Region $\Omega = (0,1)$ is divided into Ω_a, Ω_b, and Ω_c. Fig. 1 shows the scenario of interested in this section: $\Omega_a = (0,0.6)$, $\Omega_b = (0.3,0.6)$, and $\Omega_c = (0.3,1)$. The atomistic grid spacing is $s = 0.005$ while the continuum grid spacing is $h = 0.1$. The Δ_ι used here is 0.05.

To test the algorithm described in §3., we consider the nearest-neighbor atomistic force model

$$f_{\alpha,\beta} = 100 \sum_{\beta=\alpha\pm1} \left(\frac{u_\alpha - u_\beta}{s} \right), \tag{8}$$

and a continuum stress model given by

$$\sigma(u) = 100 \frac{\mathrm{d}u}{\mathrm{d}x}. \tag{9}$$

The exact displacement solution is linear from $u(0) = 0$ to $u(1) = 0.01$, which leads to a constant exact stress solution of one over the whole domain. The initial guess for the displacement is exactly zero, and Matlab's `fmincon` function is used to find the optimal solution with objective function and constraint tolerances of 10^{-6}.

The optimal linear displacement and stress are shown in Fig. 1. One can see that the displacement is well-approximated, and the atomistic and continuum stresses agree with the exact solution up to the 4th decimal place. The optimizer reached this solution after six iterations and 868 function calls. The objective function was reduced to 6.6441×10^{-11}, and the maximum constraint value was 7.903×10^{-8}.

5. Summary

We have illustrated a method for coupling atomistic and continuum simulations using optimization. While the numerical example showed only a simple one-dimension problem with nearest-neighbor atomistic interactions, this procedure can be extended to more complicated coupling problems.

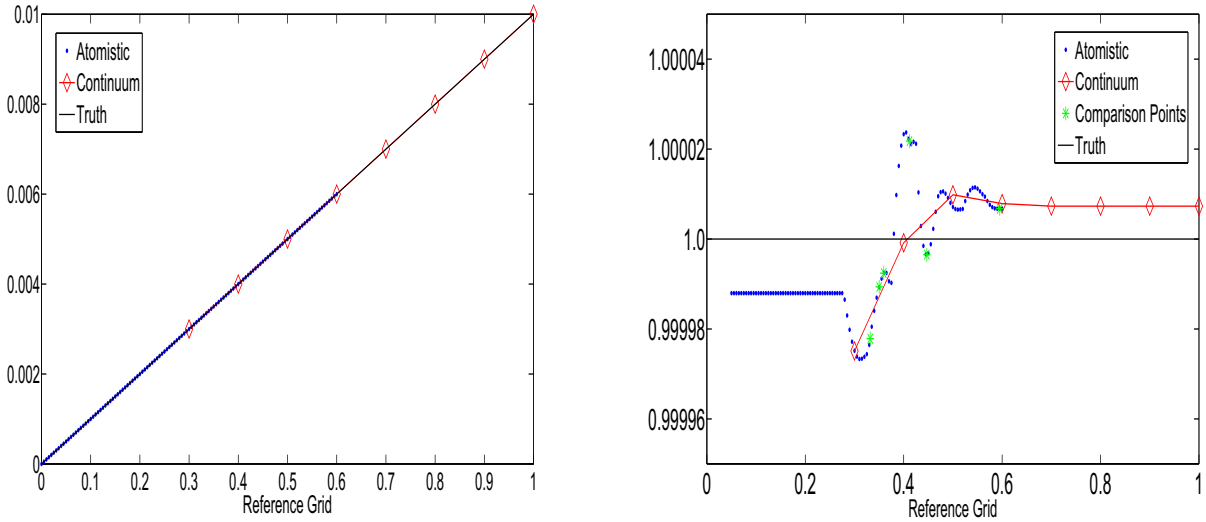

Figure 1: Nearest neighbor interactions, overlap at $[0.3, 0.6]$: displacement (left) and stress (right)

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