

# Optimization-based Atomistic-to-Continuum Coupling

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Multiscale simulations are able to leverage the accuracy of the microscale simulation in regions of the domain where the physics are rapidly changing while taking advantage of the efficiency of the macroscale simulations in the remainder of the domain. We are interested in the case where the microscale and macroscale are combined via a *domain decomposition* strategy. In particular the computational domain  $\Omega$  is divided into three disjoint regions:  $\Omega_a$ , where the physics of the problem are governed only by first principles at the microscale;  $\Omega_c$  where the physics can be described by a macroscale model; and  $\Omega_b$  which is some *bridge region* acting as an interface between the two models.

The difficulty arises in this bridge region, where the solution provided by the macroscale model must agree with the microscale solution. In the literature, this model coupling has been achieved mainly through constraining the microscale dynamics based on current macroscale information [4, 5] or using Schwarz iteration to guarantee consistency between the models [3]. However, this poster describes an optimization-based coupling strategy originally applied in [1, 2] to two *macroscale* regions, each governed by a different partial differential equation (PDE). In the multiscale case, this strategy uses a stress-based objective function constrained by the values of displacement and stress to seek agreement between a microscale molecular statics model and a macroscale PDE over the bridge region. Supporting results are provided for a number of atomistic force models.

## References

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