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PHASE-FIELD-DRIVEN MODEL ADAPTIVITY

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Abstract.

Methods for coupling two compatible models have been developed during the last decade or so to simulate problems for which one may identify a small subregion where the assumptions of a *coarse-scale model* break down and whose physical behavior should rather be described by some *fine-scale* model. Examples of blending techniques to couple continuum models with non-local particle models can be found, for instance, in [1, 2]. The main motivation in using such approaches is that fine-scale models are usually too expensive to be employed in the entire domain Ω due to their small length- and time-scale features and their nonlinear behavior. Therefore, the idea is to use the fine model only in a subdomain $\omega \subset \Omega$, where it is deemed necessary, and the coarse-scale model in the remainder of Ω, except in a layer separating these two within which one imposes a gradual transition, via a so-called weighting or *blending function*, from the fine-scale to the coarse-scale model. More concretely, the blending function has value unity in the region of the fine-scale model, zero in the region of the coarse-scale model, and monotonically varies from unity to zero between these two regions.

Questions that naturally arise are how to quantify the errors incurred by substituting a hybrid model for the fine-scale model and how to choose the domain of the fine-scale

model in an optimal way. Note that errors and optimality should be measured in terms of a quantity of interest $Q = Q(u)$, a functional of the solution u of the problem, that characterizes the goal of the simulations. Goal-oriented adaptivity provides a framework to estimate, and substantially control, these approximation errors. Finding the optimal configuration of the coupled problem can be achieved by considering the blending function as an unknown and determining its optimal shape. We develop here a phase-field formulation to solve for the blending function as the problem drives the solution either to the value one or to the value zero with a smooth, narrow transition in between. In addition, a phase-field model satisfies a gradient flow structure, for which an energy is minimized. By adding to the energy functional the error in the quantity of interest, one can thus determine the evolution of the blending function that drives down the error with respect to the goal.

The phase-field formulation for model blending adaptivity will be explored on a simple problem that couples a fourth-order partial differential equation model (the fine-scale model that incorporates non-local effects) with a second-order partial differential equation model (the coarse-scale model that ignores those non-local effects). In particular, we will present some mathematical properties of the formulation, provide some numerical results, and discuss the viability of the methodology.

REFERENCES

[1] Prudhomme, S., Ben Dhia, H., Bauman, P.T., Elkhodja, N., and Oden, J.T. Computational analysis of modeling error for the coupling of particle and continuum models by the Arlequin method. *Comput. Methods Appl. Mech. and Engrg.* (2008) **197**(41–42):3399—3409.

[2] Seleson, P., Beneddine, S., and Prudhomme S. A force-based coupling scheme for peridynamics and classical elasticity. *Computational Material Science*, (2012) in press.