A DATA-DRIVEN CONTINUUM MODEL FOR UPSCALING NOISY MOLECULAR DYNAMICS DISPLACEMENTS

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ABSTRACT

Nonlocal models, including peridynamics, often use integral operators that embed length-scales in their definition. However, the integrands in these operators are difficult to define from the data that are typically available for a given physical system, such as laboratory mechanical property tests. In contrast, molecular dynamics (MD) does not require these integrands, but it suffers from computational limitations in the length and time scales it can address. To combine the strengths of both methods and to obtain a coarse-grained, homogenized continuum model that efficiently and accurately captures materials' behavior, we propose a learning framework to extract, from MD data, an optimal Linear Peridynamic Solid (LPS) model as a surrogate for MD displacements. To maximize the accuracy of the learnt model we allow the peridynamic influence function to be partially negative, while preserving the well-posedness of the resulting model. Our framework guarantees that the resulting model is mathematically well-posed, physically consistent, robust to noise, and that it generalizes well to settings that are different from the ones used during training. We illustrate the efficacy of the proposed approach with several numerical tests for single layer graphene. Our two-dimensional tests show the robustness of the proposed algorithm on validation data sets that include thermal noise, different domain shapes and external loadings, and discretizations substantially different from the ones used for training.