

**SOFTWARE DESIGN FOR MULTISCALE
ENGINEERING SIMULATION**

By

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Abstract

This work explores several aspects of software design for multiscale simulation. First, we provide an introduction to multiscale simulation, including a high-level, abstract view. We illustrate that existing single-scale simulation software can be utilized as components of multiscale simulation. We provide an example of refactoring a particular single-scale software, LAMMPS, to transform it into an effective component in multiscale software. We detail the construction of a sparse data structure to represent polycrystals and demonstrate how this structure can be used to implement a computationally-efficient approximate relaxation algorithm. Finally, we suggest directions for future research.