Eigenstrain-based Reduced Order Homogenization Models for Polycrystal Plasticity: Addressing Scalability

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ABSTRACT

We propose a highly scalable reduced order multiscale computational framework for modeling the plastic deformation in polycrystalline materials. The proposed approach is based on the eigenstrain-based reduced order homogenization model (EHM) [1] for polycrystalline materials, which has been recently developed by the authors [2]. EHM operates in a computational homogenization setting, which takes the concept of transformation field theory [3] that pre-computes certain microscale information (e.g. localization and concentration tensors) by evaluating linear elastic microscale problems and considers piece-wise constant inelastic response within partitions (e.g., grains) of the microstructure. By this approach, a significant reduction in computational cost is achieved, compared with classical computational homogenization approaches that employ crystal plasticity finite element (CPFE) simulation to describe the microscale response.

While EHM provides approximately two orders of magnitude efficiency compared with CPFE for middle-sized microstructure, its efficiency degrades as microstructure size increases. A grain-cluster accelerated, sparse and scalable reduced order homogenization model (sparse EHM) has been developed to address this issue for computationally efficient multiscale analysis of complex polycrystalline microstructure. The acceleration is achieved by introducing sparsity into the linearized reduced order system through selectively considering the interactions between grains based on the idea of grain clustering. The proposed approach results in a hierarchy of reduced models that recovers full EHM, when full range of interactions is considered, and recovers the Taylor model, when all inter-grain interactions are neglected. The resulting sparse system is solved efficiently using both direct and iterative sparse solvers, both of which show significant efficiency improvements compared to the full EHM. A layer-by-layer neighbor grain clustering scheme is proposed and implemented to define ranges of grain interactions. Performance of the proposed approach is evaluated by comparing the results against the original full EHM and CPFE simulations.

REFERENCES

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