An efficient numerical framework for the phase-field crystal equation and its amplitude expansion

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The study of polycrystalline materials requires theoretical and computational techniques enabling multiscale investigations. The phase-field crystal model (PFC) allows for describing crystal lattice properties on diffusive timescales. An amplitude expansion of the PFC model (APFC) focuses on continuous fields varying on length scales larger than the atomic spacing. Thus, it allows for the simulation of larger systems (compared to PFC) still retaining details of the crystal lattice. Fostered by the applications of this approach, we present here an efficient numerical framework to solve both types of equations. In particular, we consider a real space approach exploiting the finite element method. An optimized preconditioner is developed in order to improve the convergence of the linear solver. Moreover, a mesh adaptivity criterion based on the local rotation of the polycrystal in the APFC approach is used. This results in an unprecedented capability of simulating large, three-dimensional systems including the dynamical description of the microstructures in polycrystalline materials together with their dislocation networks. This is joint work with Marco Salvalaglio and Axel Voigt.

References:

[1] S. Praetorius, M. Salvalaglio, and A. Voigt, An efficient numerical framework for the amplitude expansion of the phase-field crystal model, In Model. Sim. Mater. Sci., Vol. 27 (4), pp. 044004, 2019., https://dx.doi.org/10.1088/1361-651X/ab1508

[2] S. Praetorius and A. Voigt, Development and Analysis of a Block-Preconditioner for the Phase-Field Crystal Equation, In SIAM J. Sci. Comp., Vol. 37 (3), pp. B425–B451, 2015., https://dx.doi.org/10.1137/140980375

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