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Highly Efficient Parallel Multigrid Solver For Large-Scale Simulation of Grain Growth Using the Structural Phase Field Crystal Model ZHEN GUAN, University of California, Irvine, DMITRY PEKUROVSKY, San Diego Supercomputer Center, JASON LUCE, KATSUYO THORNTON, University of Michigan, JOHN LOWENGRUB, University of California, Irvine — The structural phase field crystal (XPFC) model can be used to model grain growth in polycrystalline materials at diffusive time-scales while maintaining atomic scale resolution. However, the governing equation of the XPFC model is an integral-partial-differential-equation (IPDE), which poses challenges in implementation onto high performance computing (HPC) platforms. In collaboration with the XSEDE Extended Collaborative Support Service, we developed a distributed memory HPC solver for the XPFC model, which combines parallel multigrid and P3DFFT. The performance benchmarking on the Stampede supercomputer indicates near linear strong and weak scaling for both multigrid and transfer time between multigrid and FFT modules up to 1024 cores. Scalability of the FFT module begins to decline at 128 cores, but it is sufficient for the type of problem we will be examining. We have demonstrated simulations using 1024 cores, and we expect to achieve 4096 cores and beyond. Ongoing work involves optimization of MPI/OpenMP-based codes for the Intel KNL Many-Core Architecture. This optimizes the code for coming pre-exascale systems, in particular many-core systems such as Stampede 2.0 and Cori 2 at NERSC, without sacrificing efficiency on other general HPC systems.

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