MEUMAPPS-SS Overview

MEUMAPPS-SS (Microstructure Evolution Using Massively Parallel Phase-field Simulation for Solid State is a phase field code developed at the Oak Ridge National Laboratory. The motivation for developing the code is to take advantage of the Oak Ridge Leadership Class (OLCF) computing capabilities to simulate solid-state phase transformations in structural alloys under the thermal conditions encountered during powder-bed based additive manufacturing (AM) processes, as well during post-process annealing of as-solidified microstructures obtained during laser-based AM processes especially in precipitation-hardenable alloys such as the Ni-base superalloy 718. The code is constantly undergoing both physics and computational enhancement and will be released as future versions as and when sufficient progress is achieved in either front.

The salient aspects of the code that make it attractive for use in advanced processing are:

(1) ability to handle simultaneous nucleation and growth of multiple phases
(2) variable phase and composition-dependent species mobility (under testing)
(3) coupling with multi-component alloy thermodynamics using analytical fits to the Calphad free energies of both stable and metastable phases, and
(4) handle systems with extreme elastic inhomogeneity.

The phase field model used in MEUMAPP-SS is an extension of the Kim-Kim-Suzuki (KKS) model [1] to multi-component, multi-phase alloys. The strategy for multi-phase alloys is based on the approach by Zhou et al. [2]. Linking thermodynamic properties of multi-component alloys to the phase field code is obtained through polynomial fits to the free energies of phases using thermodynamic databases such as ThermoCalc™. Elastic energy arising from transformation strains are calculated using a modification to the approach of Hu and Chen [3]. The governing equations, time-dependent Ginzburg-Landau (TDGL) equations, and the multi-component diffusion equation, are solved using a semi-implicit Fourier spectral method, as commonly implemented in phase field codes [4]. However, in MEUMAPPS-SS we use a parallel Fast Fourier Transformations (FFT) package, P3DFFT developed by Pekurovsky [5] in order to achieve significant massively parallel speed-up using Message Passing Interface (MPI) protocol. Nucleation is achieved by resorting to several options ranging from single nucleus – single variant to multiple nuclei – multiple variant. A composite nucleus strategy is used to allow natural variant selection as influenced by the internal strain fields of pre-existing crystallographic variants or externally imposed strain fields [6].

The parallel performance of the code has been tested using the Titan supercomputer at ORNL. Figure 1 shows the strong scaling performance using a test problem that involved the calculation of the elastic energy. The code has been used to simulate $\beta \rightarrow \alpha$ transformation in Ti-6Al-4V using a pseudo-binary approximation [6], Ni-base superalloys 625 and 718 using pseudo-ternary surrogate alloys Ni-Mo-Nb [7] and Ni-Fe-Nb [8]. The precipitation of the delta phase due to Nb enrichment in the interdendritic areas of Ni-base alloy 625 obtained using a Ni-Al-Nb pseudo-ternary alloy is shown in Figure 2. The simulations were carried out in Summitdev using 640 CPUs and 128 GPUs using OpenACC.

References

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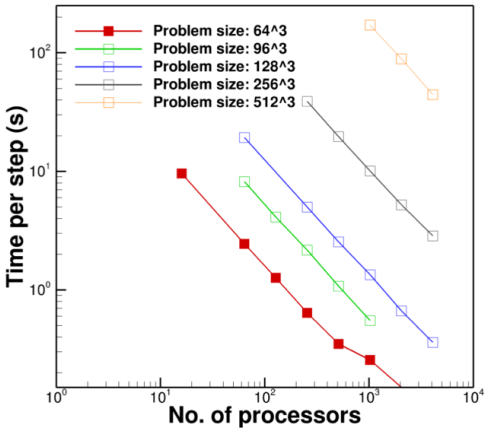

Figure 1. Strong scaling of MEUMAPPS-SS in Titan for a test problem involving the growth of BCC precipitate from a HCP matrix in Ti-6Al-4V alloy

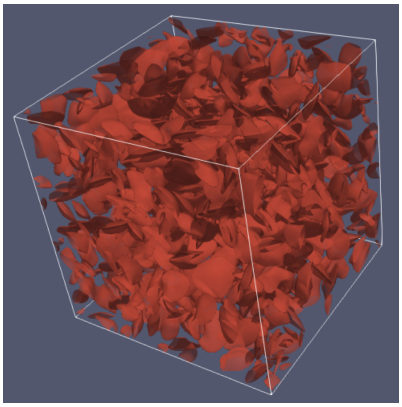

Figure 2. Precipitation of 12 variants of the delta phase in alloy 625 in simulation volume of 320 x 320 x320.