Large-scale and massively parallel phase-field simulations of pattern formations in ternary eutectic alloys

[Extended Abstract]

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ABSTRACT

Various patterns form during directional solidification of ternary eutectic alloys. These macroscopic patterns strongly influences the material properties. To study the influence of the material and process parameters for a wide range of ternary alloys during solidification, simulations are conducted to gain new insights. In this poster, we present the results of massive parallel phase-field simulations on up to 262 144 cores, based on the HPC framework WALBERLA. Results of optimization techniques are shown, starting from the model up to the code level, including buffering strategies and vectorization. The approach comprises systematic node level performance engineering and gains in a speedup of factor 80 compared to the original code. Excellent weak scaling results on the currently largest German supercomputers, SuperMUC, Hornet and Juqueen, are presented. Novel methods like principle component analysis and graph based approaches are applied to compare the computed microstructural patterns with experimental Ag-Al-Cu micrographs.

Categories and Subject Descriptors

I.6.3 [**SIMULATION AND MODELING**]: Applications; J.2 [**PHYSICAL SCIENCES AND ENGINEERING**]: Engineering, Physics; D.2.8 [**SOFTWARE ENGINEERING**]: Metrics—*performance measures*; G.1.6 [**NUMERICAL ANALYSIS**]: Optimization—*Global optimization, Gradient methods*; G.4 [**MATHEMATICAL SOFTWARE**]: *Efficiency, Parallel and vector implementations,Portability*; G.1.8 [**NUMERICAL ANALYSIS**]: Partial Differential Equations —*Finite difference methods*

General Terms

Algorithms, Experimentation, Measurements, Performance

Keywords

Massive Parallel, Phase-Field, Large Scale Simulations, Ternary Eutectic Directional Solidification, Optimization, Vectorization

1. EXTENDED ABSTRACT

Due to a growing demand in the development of improved materials with a defined macroscopic behavior, and the widely adjustable properties of ternary eutectics, these alloys are subject of industrial and scientific research. During directional solidification of ternary eutectics, the melt solidifies in three phases at a defined temperature and concentration, the so-called ternary eutectic point. These solid phases form a wide range of patterns in the microstructure [11, 13], which strongly influence the resulting macroscopic material properties. The formation depends on the various material- and process-parameters, but their influence is not yet fully understood [8, 5, 6].

Phase-field simulations allow the study of pattern formation for a wide range of ternary alloys and to specifically control the solidification process. Therefore we use a thermodynamic consistent phase-field model based on the grand potential functional, including temperature and concentration evolution [4, 10]. This model results in computationally intensive, coupled stencil codes, compared to previously published models [12, 14, 15].

In order to study the pattern formation in representative volume elements (RVE), large scale phase-field simulations are necessary [10]. For this, optimizations on various levels, from the model, over the parameters up to the code level are conducted.

Based on the physical parameters, a frozen temperature assumption is used to model the moving temperature gradient. The 1000 times lower diffusion in the solidified material allows us to use a moving window technique in which only the vicinity of the solidification front needs to be simulated [16]. Through measurements and a Roofline models [17] we could show that the code is compute bound. Therefore we reuse staggered values and gradients by using buffering fields to reduce the calculation time. By only calculating the required terms for each voxel cell, through a classification, the calculation time is further reduced. To fully utilize modern processors, the kernels are explicitly vectorized using vector intrinsics for SSE2, SSE4, AVX, AVX2 and QPX instruction sets. With this systematic node level performance engineering techniques, a speedup of factor 80, compared to the original code, and 25% of the peak performance of a single node is reached on the SuperMUC [2].

To efficiently study large domains, the code is implemented in the highly parallel waLBerla framework [7, 9], where the provided load balancing and communication infrastructure is used. The results show an excellent weak scaling behavior on the three largest German supercomputers [1]: SuperMUC, Hornet and Juqueen.

In order to model the solidification behavior and pattern formation in representative volume elements, large scale phase-field simulations with up to $2420\times2420\times1474$ voxel cells and 84 700 cores are employed [10]. To study the ternary eutectic pattern formation, two datasets were used: A model system and the real system Ag-Al-Cu based on the thermodynamic Calphad database [3]. The Ag-Al-Cu system shows a good visual agreement with experimental micrographs of [8, 5, 6]. Multiple features, similar to the experimental data, such as chain-like structures, chain junctions and ring formations are found in simulations on large scale domains.

To quantify the comparison between experimental and simulated microstructures, we use a novel method based on two point correlations and principle component analysis (PCA) to compare the micrographs and the computed images.

Besides two dimensional micrographs, simulations allow to study the solidification behavior during the growth of the structure in three dimensions. In contrast, only the final microstructure of experiments in 3D can be made visible in a complicated process, using synchrotron tomography at a particle accelerator. In order to understand the microstructure evolution during the growth, such as splitting, merging or termination of the rods and lamellae, a graph based approach is presented to classify the structures.

Indication of a spatially complex pattern, helical spiral growth, is found in experiments of Ag-Al-Cu by [8]. By using systematic parameter studies, the experimental indication could be reproduced using large scale simulations with domain sizes of $800 \times 800 \times 8,000$ voxel cells.

In this poster, we present the workflow from the physical process, the model, the parameters, the node level to inter node optimization resulting in a speedup of factor 80 compared to the original code and an excellent scaling behavior on the largest German supercomputers. With this, we are able to simulate realistic patterns in representative volume elements and to proof experimental observed pattern formations such as spiral growth.

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