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Three-dimensional phase field simulations of grain growth in materials containing finely dispersed second-phase particles

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Phase field modelling has proven to be a versatile tool for simulating microstructural evolution phenomena, such as grain growth in polycrystalline materials. However, the computational requirements of a phase field model impose strong limitations on the number of phase field variables employed in a practical implementation. In this paper, a bounding box algorithm is proposed allowing the use of a large number of phase field variables without excessive computational requirements.

1 Introduction

The microstructure of materials is often composed of multiple grains with different crystallographic orientations. Since many material properties depend on the microstructure, the study of the evolution of these grains is technologically important. Computer simulations are essential, since they allow to study the roles of different parameters separately, which is impossible in experimental studies. Furthermore, three-dimensional simulation results provide more insight in microstructural evolution than two-dimensional microscopic images of cross-sections of a material.

Phase field modelling is a versatile tool for simulating microstructural evolution phenomena. It allows to predict the evolution of complex morphologies with different thermodynamic driving forces. In [1], a phase field model is used to model the microstructure of a single-phase material by a set of non-conserved phase field variables that distinguish the different crystallographic orientations of the grains. Inside a grain, one phase field variable takes a nonzero equilibrium value, 1 or -1, while the other variables assume values close to zero. Across the grain boundaries, the corresponding phase field variables vary continuously to their equilibrium value in the neighboring grains. An extension of the model was presented in [2, 3], to simulate grain growth in the presence of second-phase particles which do not evolve over time. Unfortunately, realistic three-dimensional grain growth simulations with this phase field model demand significant amounts of computation power.

This paper presents a bounding box algorithm, that exploits the observation that only a few crystallographic orientations are active at a given location in a microstructure. The algorithm is designed for use with semi-implicit time integration methods and in the context of the grain growth model of [1, 2, 3]. However, it can be applied to other cases as well. Thanks to the object-oriented design, the algorithm can easily be extended to more complex phase field models and has definite advantages in post-processing.

2 Phase Field Model and Discretization

According to [1], the microstructure of a single-phase material is represented by a set of phase field variables $\eta_1(\mathbf{r},t)$, $\eta_2(\mathbf{r},t)$, …, $\eta_p(\mathbf{r},t)$ that are continuous functions of the spatial coordinates and time. Their evolution is governed by the equations

$$\frac{\partial \eta_i}{\partial t} = L\Big(\kappa\nabla^2\eta_i - \eta_i^3 + \eta_i - 2\eta_i(\sum_{j\neq i}^{p}\eta_j^2 + \phi^2)\Big), \qquad i = 1,\ldots,p. \tag{1}$$

In [2, 3], the parameter ϕ is added to include small incoherent second-phase particles with constant properties. This parameter equals 1 inside a particle and 0 elsewhere and remains constant over time. For isotropic grain boundary energy and mobility the coefficients κ and L are constants. Periodic boundary conditions are applied.

To solve the equations (1), the spatial derivative is discretized with second order central differences and the time derivative with a first order semi-implicit scheme [4]. By treating the diffusion part of (1) implicitly and the reaction part explicitly, this scheme allows the use of a large time step without the need to solve one large coupled system of equations.

3 Bounding Box Algorithm

A phase field variable η_i is *active* at a grid point $\mathbf{r}$ when $|\eta_i(\mathbf{r})| > \epsilon$, with ϵ a small positive value. In the interior of a grain, only one phase field variable is active. Near grain boundaries, only the phase field variables corresponding to the neighboring

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grains are active. We define a *grain region* $\hat{G}_{i,k}$ as the set $\hat{G}_{i,k} = \{(\mathbf{r}, \eta_i(\mathbf{r})) : |\eta_i(\mathbf{r})| > \epsilon$ and $\mathbf{r}$ are connected$\}$. The index k ranges from 1 to n_i, the number of grain regions associated with η_i. To take periodic boundary conditions into account, the grain regions are allowed to wrap around the grid boundaries. Also, the grain regions can overlap, which allows them to interact. For each $\hat{G}_{i,k}$, a bounding box is established as the smallest cuboid grid part containing its grid points $\mathbf{r}$. The set $\hat{B}_{i,k}$ is now defined as $\hat{B}_{i,k} = \{(\mathbf{r}, \eta_i(\mathbf{r})) : \mathbf{r}$ lies inside the bounding box of $\hat{G}_{i,k}\}$.

The bounding box algorithm proceeds in two steps. In the *preprocessing step*, first, for every phase field variable η_i, the grain regions $\hat{G}_{i,k}$ are located. Second, the corresponding bounding boxes and sets $\hat{B}_{i,k}$ are determined. Finally, a grain region numbering is performed in which a one to one mapping between grain regions and phase field variables is established. Every grain region $\hat{G}_{i,k}$ is rewritten as G_l, a grain region corresponding to a unique new phase field variable, η_l, with l ranging from 1 to q, the total number of grain regions and $q = \sum_{i=1}^{p} n_i$. The bounding box information of the set B_l is copied from $\hat{B}_{i,k}$. The renumbering of grain regions is allowed, since the actual value of the grain orientation does not play a role in equations (1). Thanks to the assignment of unique phase field variables to every grain region, grain growth simulations with the bounding box algorithm are coalescence-free. In the *computation step*, the microstructural evolution is simulated. Within each time step, for every set B_l, the solution of the equation (1) is computed. Next, the algorithm checks whether the grain region G_l has shrunk or grown, and updates the bounding box and B_l accordingly.

To allow for easy extension to more complex phase field models, the bounding box data structure was designed following the object-oriented methodology. This object-oriented approach can save significant time of post-processing, since e.g. the number of grains and their location is known throughout a simulation.

4 Results

The memory requirements of the bounding box data structure are significantly lower than those of a conventional grid-based data structure. The requirements of the latter equal the number of phase field variables multiplied by the grid size. The requirements of the bounding box data structure are determined by the number of active phase field variables per grid point and equal the number of phase field values included in the sets B_l. Simulations showed that at each time point approximately 7 phase field variables are active at every grid point. The computational requirements of the bounding box algorithm thus depend on the system size and not on the number of phase field variables.

To validate the bounding box algorithm, which solves the equations (1) locally, a parallel implementation of a conventional grid-based algorithm, solving the equations globally, was made based on the scheme proposed in [5]. The computational requirements of this algorithm are constant in time, whereas the bounding box algorithm requires fewer resources as simulation time progresses and the mean grain size increases. For a simulation on a $256 \times 256 \times 256$ grid with $p = 100$, the global algorithm required 20 processors, in contrast to the bounding box algorithm which could be executed on a single processor.

5 Conclusion

In this paper, a sparse bounding box algorithm is presented to perform efficient phase field simulations of three-dimensional grain growth. The algorithm only solves the phase field equations locally, inside bounding boxes delimiting regions of activity. Furthermore, because of the object-oriented design, the bounding box algorithm is extendible to more complex models and has advantages in post-processing. The computational requirements of the bounding box algorithm depend on the system size and not on the number of involved phase field variables. In combination with the one to one mapping between grains and phase field variables, this allows to perform coalescence-free simulations of grain growth without the excessive use of resources associated with conventional grid-based methods. We believe that the bounding box algorithm will enable simulations with realistic materials and provide more insight in microstructural evolution.

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