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Large-Scale Simulations of Grain Boundary Motion in Polycrystals

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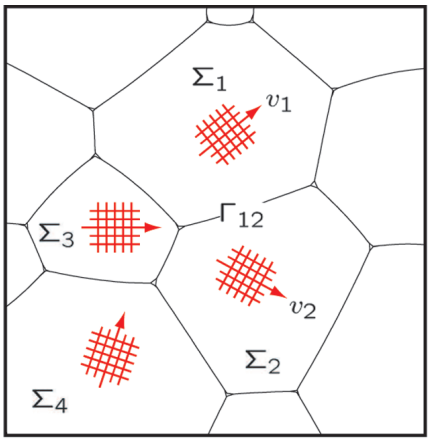


Schematic of a grain network.

Many common materials, including most metals and ceramics, are polycrystalline: They are composed of tiny crystallites—often called grains—that are differentiated from their neighbors by differences in orientation. The grain structure of a polycrystalline material affects its physical properties, such as fracture strength and conductivity. Accordingly, simulating how the network of grains evolves under manufacturing processes, such as annealing (heat treatment), is of great interest. Annealing leads, for example, to coarsening of the grain network: Certain grains grow at the expense of others, leaving fewer and thus larger grains on average.

Many numerical techniques, including Monte Carlo, front tracking, and phase-field methods, have been used in simulations of this important phenomenon. Some of these methods, such as front tracking, can be very accurate in 2D but awkward in 3D simulations because of the variety of topological changes that inevitably take place during the coarsening process. In my talk at the SIAM Materials Science meeting in May, drawing on recent joint work with Matt Elsey and Peter Smereka [4,5], I described new, level set-based algorithms that have allowed us to carry out fully resolved 3D simulations with very large numbers of grains on modest hardware.

Mathematically, we can represent a polycrystalline material as a partitioning of the volume D it occupies into connected, pairwise disjoint regions (grains) $\Sigma_1, \ldots, \Sigma_N$:

$$D = \bigcup_{j=1}^{N} \bar{\Sigma}_j \text{ with } \Sigma_i \cap \Sigma_j = \varnothing \text{ for all } i \neq j. \tag{1}$$

According to a well-known model of Mullins [13], when a material is annealed, its grain network evolves by gradient flow to decrease an interfacial energy of the form

$$E = \sum_{i<j} \int_{\Gamma_{ij}} \sigma(v_i, v_j, n_{ij})\, dS, \tag{2}$$

where Γ_{ij} represents the interface between Σ_i and Σ_j, v_i is a vector describing the crystallographic orientation of Σ_i, and n_{ij} is the unit normal along Γ_{ij}. Although the energy density σ typically depends not only on the misorientation between the grains on either side, but also on the normal to the interface, a much simplified version of the model, with $\sigma = 1$ everywhere, is thought to capture certain important aspects of the grain network dynamics; the energy then becomes

$$E = \frac{1}{2} \sum_{j=1}^{N} \mathrm{Per}(\Sigma_j). \tag{3}$$

Gradient descent for (3) in L^2 leads to the normal speed

$$v_n = \kappa \tag{4}$$

along faces of grains; here κ denotes mean curvature. Along triple curves, where more than two grains meet, natural boundary conditions known as Herring angle conditions [8] hold; they stipulate

$$n_{ij} \cdot n_{jk} = n_{jk} \cdot n_{ki} = n_{ki} \cdot n_{ij} = -\frac{1}{2} \tag{5}$$

along any triple curve formed by the meeting of three distinct grains $\Sigma_i, \Sigma_j, \Sigma_k$, so that all angles formed along the triple curve are 120°.

A correct numerical method needs to impose both (4) and (5). Ours is motivated by an old idea of Merriman, Bence, and Osher called threshold dynamics [12] (see also [15]). The idea is to generate geometric motions of interfaces by representing sets through their characteristic functions and by alternating two very simple operations on them: convolution with a symmetric kernel and thresholding. We had previously found [7] this strategy to be very efficient (though not so accurate) in the context of image processing, where a partitioning problem much like (1) and (3) arises in simplified versions [3] of a famous image segmentation model of Mumford and Shah [14].

In [6], we noted that poor accuracy of threshold dynamics on uniform grids can be rectified by representing sets with their signed distance functions instead; convolution and the construction of the signed distance function (rather than thresholding) are then alternated to generate the desired geometric flow. As there are fast algorithms for constructing signed distance functions (e.g., [16]), the favorable overall complexity of the

original algorithm is maintained. In applications to grain boundary motion, the aim is to represent and track hundreds of thousands of grains; doing so individually would be prohibitively expensive. The first step of our algorithm is therefore to group the grains into families $\Xi_1, \ldots, \Xi_M$, with $M \ll N$, as follows:

$$\Xi_i = \cup \Sigma_j \text{ so that if } \Sigma_j \subset \Xi_i,$$
$$\text{then } \operatorname{dist}(\Sigma_j, \Xi_i \setminus \Sigma_j) > \varepsilon.$$

In words, individual grains constitute connected components of a family, and are separated from their siblings by a distance of at least ε. Our algorithm for simulating normal grain growth then proceeds as follows to generate a discrete (in time) approximation to the flow, with time step size δt:

1. Construct the signed distance function $d_j^n(x)$ for each family Ξ_j^n of grains:

$$d_j^n(x) = \begin{cases} \operatorname{dist}(x, \Xi_j^n) \text{ if } x \in \Xi_j^n, \\ -\operatorname{dist}(x, \Xi_j^n) \text{ if } x \notin \Xi_j^n. \end{cases}$$

2. Form the convolutions

$$C_j(x) = d_j^n * G_{\delta t},$$
$$\text{where } G_t(x) = \frac{1}{(4\pi t)^{3/2}} e^{-\frac{|x|^2}{4t}}.$$

3. Let the families compete for grid points:

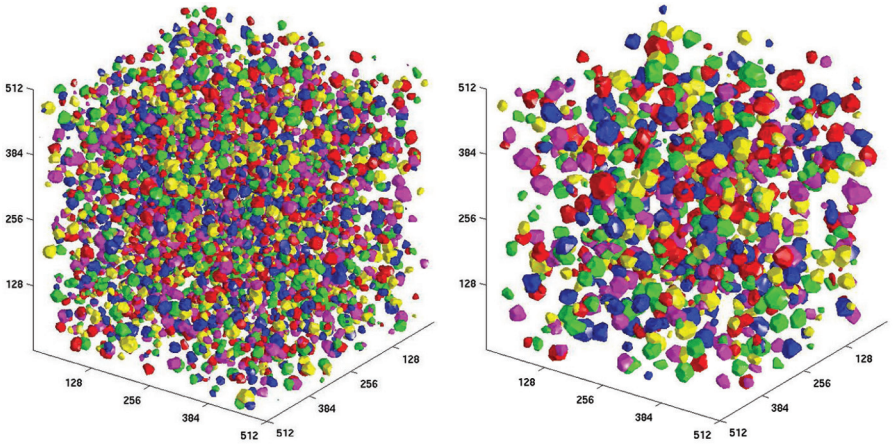
$$L_j(x) = C_j(x) - \max_{i \neq j} C_i(x).$$

In words, whichever family has the largest convolution at a point $x \in D$ will claim that point for itself at the next time step.

4. Grain flipping: The grain families at the new time step $t = (n + 1)\delta t$ are given by:

$$\Xi_j^{n+1} = \{x : L_j(x) > 0\}.$$

If any connected component (grain) Σ of a family Ξ_j^{n+1} is too close to its siblings, move it to another family.



Left: A few families of grains from an initial condition of more than 130,000 grains. Right: After 300 time steps in the simulation, about 14,000 grains remain. (Only some of the grains are shown for visualization purposes.)

A few individual grains from the simulation shown above.

This algorithm is close to, but different from, the algorithms in [12] for multiple junctions. It is unconditionally stable, allowing arbitrarily large time steps constrained only by accuracy considerations. It also achieves good accuracy on uniform grids.

Important statistical measures of grain networks include normalized grain size distribution and such topological characterizations as the number of faces per grain. For verification purposes, we carried out large-scale, 2D grain growth simulations and compared these measures with those of [9,11], in which careful front tracking-based simulations in 2D are reported; we found good agreement. The next natural challenge is to adapt our numerical methods to the simulation of motion under the more realistic energy

$$E = \sum_{i<j} \int_{\Gamma_{ij}} \sigma(v_i, v_j)\, dS,$$

which is intermediate between (2) and (3). It leads to weighted mean curvature motion along faces of grains and a modified angle condition along triple curves. This level of generality is essential for simulating, say, the evolution of grain boundary character distribution [10], which measures the relative frequency of a given misorientation along grain boundaries. There are 2D simulations and reduced theories [1,2] for this important measure (as discussed, in fact, by Maria Emelianenko and Yekaterina Epshteyn in minisympo-

sium talks at the SIAM meeting, and explained in greater detail by Richard Sharp); their results will provide a check of our numerics. Of course, the real benefit of our algorithms will once again come in detailed 3D simulations.

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Additional coverage of the 2010 SIAM conference on materials science—the first official activity of the recently created SIAG on Mathematical Aspects of Materials Science—can be found in the July/August and September issues of SIAM News*; one further article, on thin-film deposition, will appear in an upcoming issue.*