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Large Scale Simulations of Grain Boundary Motion in Polycrystals

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Many common materials, such as most metals and ceramics, are polycrystalline: They are composed of tiny crystallites – often called *grains* – that are differentiated from their neighbors by differing 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 evolve under manufacturing processes such as annealing (heat treatment) is of great interest. For example, annealing leads to coarsening of the grain network, whereby 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 due to 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) $\Sigma_1, \ldots, \Sigma_N$:

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

According to a well-known model due to 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

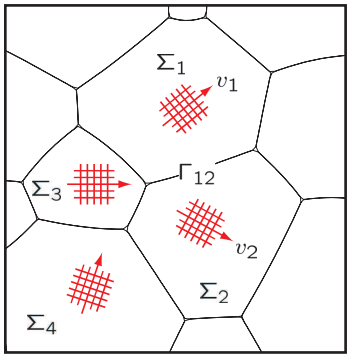

Figure 1: Schematic of a grain network.

simplified version of the model, with $\sigma = 1$ everywhere, is thought to already 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 three 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 Σ_i, Σ_j, Σ_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 due to Merriman, Bence, and Osher called threshold dynamics [12] (see also [15]). This idea generates 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) & (3) arises in simplified versions [3] of a famous *image segmentation* model due to Mumford and Shah [14]. In [6], we noted that poor accuracy of threshold dynamics on uniform grids can be rectified by representing sets through their signed distance functions instead; one then alternates convolution and the construction of the signed distance function (instead of thresholding) 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, one would like to represent and track hundreds of thousands of grains; doing so individually would be prohibitive. 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

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

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.

The algorithm given above 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 topological characterizations such 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] where careful front tracking based simulations in 2D are reported; we found good agreement.

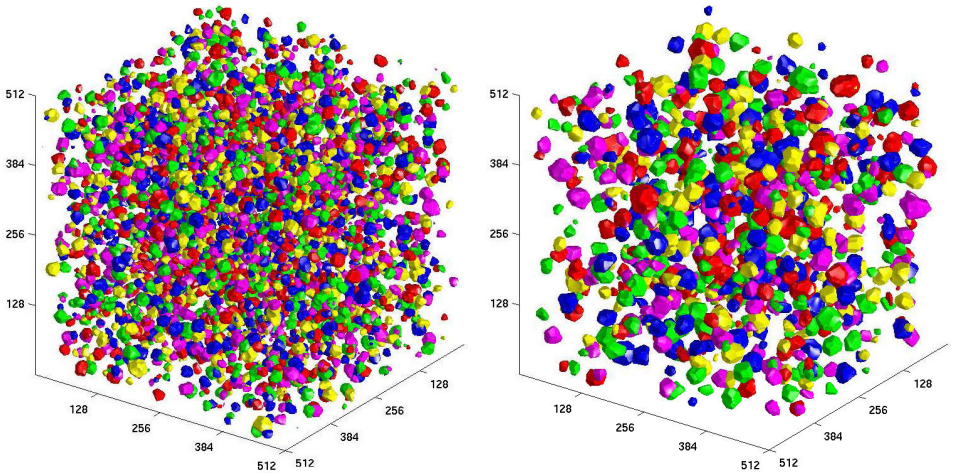

Figure 2: Left: A few families of grains from an initial condition containing over 130,000. Right: Grains from the simulation after 300 time steps; about 14,000 remain. Only some of the grains are shown for visualization purposes.

Figure 3: A few individual grains from the simulation shown in Figure 2.

The next natural challenge is to adapt our numerical methods to simulating 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 e.g. 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 (in fact, two minisymposium talks at the SIAM meeting, one by Maria Emelianenko and the other by Yekaterina Epshteyn, discussed this); they will provide a check of our numerics. Of course, the real benefit of our algorithms will once again be in detailed 3D simulations.

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