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MULTISCALE MODELING AND SIMULATION OF GRAIN BOUNDARY EVOLUTION

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Abstract

In this paper we discuss modeling and simulation of two dimensional grain boundary evolution at different scales, with emphasis on their relations. The motivation is the need to reduce the high computational complexity of detailed models on one hand, and the additional physical insight offered by multiscale representations on the other hand. Both are essential to our understanding of polycrystalline materials, facilitating the construction of new tools with predictive capabilities. The smallest scale model in this study is a Monte-Carlo Potts model which is followed by a curvature driven model, governed by the Mullins Equation together with the Herring Condition at triple junctions. Spatial coarse-graining results in a model that uses representation of the grain boundaries in terms of their end points and a constant curvature, that is able to capture size distribution function quite accurately at a fraction of the cost. Temporal coarse graining, in which grains are represented in terms of area and number of sides, is governed by a stochastic process, offering new statistical quantities that characterize evolution of large networks. The models are studied from coarse graining view point, facilitating the construction of tools with predictive capabilities which are essential for engineering applications.

1 INTRODUCTION

Most technologically useful materials arise as polycrystalline microstructures, composed of myriads of small crystallites, called grains, separated by their interfaces, called grain boundaries. The orientations and arrangements of the grains and their network of boundaries are implicated in many properties across wide scales, for example, functional properties, like conductivity in microprocessors, and lifetime properties, like fracture toughness in structures.

In this paper we discuss modeling and simulation of grain growth at several scales. The most commonly used computer simulation model of grain growth is the Monte-Carlo (MC) model. In fact, the model has been applied to the study of a variety of subcontinuum processes, such as grain growth in one phase, two phase, directional grain growth, recrystallization, etc. Monte-Carlo model exploits a random scheme aimed at reducing the Hamiltonian of the system associated with the grain interfaces. Another approach uses as a starting point a mesoscale description of grain boundary evolution in using partial differential equations (PDE). These are the Mullins Equation of curvature driven growth with the Herring Condition at triple junctions. Detailed simulation using a large number of grains, that is required for good statistical analysis, is computationally expensive either by MC or PDE based models. Thus, coarse graining techniques are essential for dealing with questions of engineering significance. In addition, we are faced with more basic questions regarding such large interacting networks of grains or grain boundaries. These include the question of predictability in these systems and the role of simulation in determining robust statistical properties.

Although the MC and PDE models are defined in a very different manner, especially in that one is stochastic and the other is deterministic, an extensive comparison of the two models [14] has revealed that in the large scale limit, the Monte-Carlo model approaches the PDE model both for the behavior of individual grains, and for the evolution of the size distribution functions. More specifically, as the underlying lattice used by the Monte-Carlo model is refined

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or equivalently as the microstructure coarsens, the behavior of the MC approaches the curvature driven growth defined by the Mullins Equation and the Herring Condition. Thus, the PDE model can be viewed as the large scale limit of MC.

The computational complexity of these detailed models gave rise to investigation of more efficient representation that is useful in the study of the size distribution function. We have approached the problem from two different directions leading to two classes of models. The first involves a coarse representation of grain boundaries (GB) involving only their end points, which are also triple junctions, and a single curvature variable per GB. The model is governed by a system of ODEs instead of PDEs as the original model, and its computational complexity is by far smaller, yet its results are very close to the full detailed model.

The other approach involves a temporal coarsening and it is motivated by observations made on the behavior of grains in the PDE model at large time scales. Following the evolution of single grains we have found that their dynamics can be viewed as a combination of a deterministic growth (or decay) of grain size (following the n-6 rule), together with a stochastic behavior governing the number of edges. Two events in the evolution of a grain, in two dimension, call for a stochastic description. The first is edge flipping and the second is the disappearance of small grains. Statistical analysis on large samples of grains revealed possible rules governing the stochastic process. This led us to consider models that describe grains in terms of area and number of edges, where the network connectivity is omitted, and its implication on the evolution is replaced by a stochastic description. The stochastic model (SM) is valid at scales comparable to the average time interval between events (flipping and disappearance) and is limited to studying grain size and number of edges, and may not address important questions such as texture, and grain boundary characterization. However, it serves us as an important exercise in coarse graining, and the lessons learned from it can be applied to more general questions in grain growth. Probabilities used in this model are computed by simulation of detailed model, which in our case was the PDE based model. The stochastic model is significantly less expensive than any of the detailed models, MC or PDE curvature driven models, therefore allowing the simulation of much larger number of grains leading to more accurate statistical properties. At a higher level than the stochastic model, we are dealing with probability densities, describing ensemble of large grains. Evolution equations for distribution of grain size and number of edges can be easily derived. While the vertex model, which we view as a spatial coarse graining model, still posses information regarding configuration of grains, angles at triple junctions, etc., the stochastic model has only statistical properties.

There are many open questions regarding the relation between the models. Do the statistics of critical events in the vertex model follow that of the PDE model? Do the MC model and the PDE model have the same statistics in terms of critical events? Furthermore, common distribution functions studied in material sciences, such as, size distribution, texture, and grain boundary characterization are only a few of the statistical properties that characterize these complex networks of evolving grains and grain boundaries. The study of multiscale modeling in this context allows a more detailed understanding of these complex models, and further insight into predictability issues in such large systems.

Numerical results are given and compared for the different models. In all models we focus on constant mobility and energy, which is the simplest case on which we can explain the processes and demonstrate the ideas.

2 MONTE-CARLO (MC) MODEL

In MC simulation [1] [13], the microstructure is mapped onto a discrete lattice and each lattice site i is assigned a spin number S_i. The GB is defined to lie between sites of different orientations and the Hamiltonian describing the grain boundary energy is

$$H = -J \sum_{<i,j>} (\delta_{S_i S_j} - 1) \tag{1}$$

where the sum $< i, j >$ is over all pairs of nearest neighbor sites and δ is the Kronecker delta. The kinetics of the boundary motion are simulated by employing a Monte-Carlo technique. A lattice site i and a new trial orientation S_i^* are chosen at random where the transition probability is given by

$$P(S_i \rightarrow S_i^*) = \begin{cases} e^{-\Delta H/k_B T} & \Delta H > 0 \\ 1 & \Delta H \leq 0 \end{cases} \tag{2}$$

ΔH being the change of energy caused by the change in orientation, k_B is the Boltzmann constant, and T is the temperature.

An attractive feature of the MC model is its simplicity, especially with regard to topological events including grain boundary flipping and grain disappearance, which are automatically performed without introducing extra mechanisms. However, the fact that the underlying lattice discretizes the grain interiors as well as the GBs places high memory and CPU requirements. In practice, an accelerated MC algorithm called N-Fold Way is often used [5].

3 PDE MODEL

The partial differential equation (PDE) model used here [7] [8] [9] is a boundary tracking model, that does not require discretizing grains, but only their boundaries. It offers an attractive alternative to MC models since it deals with quantities of lower dimension. It is based on surface energy density function $\sigma(\theta, \alpha)$, where α is the mismatch angle between neighboring grains, and θ defines the normal by $\mathbf{n} = (\cos\theta, \sin\theta)$. The model is curvature driven and is given by the Mullins Equation,

$$v_n = \mu\left(\frac{d^2\sigma}{d\theta^2} + \sigma\right)\kappa \tag{3}$$

that governs the evolution of each grain boundary, where κ is the curvature. In this equation μ is the mobility of the GB. These equations are supplemented with a boundary condition at triple junction, the Herring Condition,

$$\sum_{j=1}^{3}\left(\frac{d\sigma^j}{d\theta}\mathbf{n}_j + \sigma^j\mathbf{b}_j\right) = 0. \tag{4}$$

where $\mathbf{n}_j$, $\mathbf{b}_j$ are the unit normal and tangential vectors at the triple junction. One derivation of these equations is based on the total GB energy,

$$E(t) = \sum_{k=1}^{K}\int_0^1 \sigma^k(\theta^k(s,t), \alpha^k)|l^k(s,t)|ds, \tag{5}$$

where $l^k = \frac{d\xi^k}{ds}$. This energy is equal to the amount of work required to create an infinitesimal amount of new surface. It can be shown that equation (3) with boundary condition (4), can be seen as a steepest descent direction for the total energy. This also forms the basis of our discretization scheme.

Using the notation

$$T = \frac{d\sigma}{d\theta}\mathbf{n} + \sigma\mathbf{b} \tag{6}$$

the discrete evolution equation are given by,

$$v_j^k(t) = \frac{2\mu_j^k}{|x_{j+1}^k - x_{j-1}^k|}(T^{k,j+1/2} - T^{k,j-1/2}), \tag{7}$$

where the index j refers to grain boundary, and k refers to a node on this GB. The scaling $2/|x_{j+1}^k - x_{j-1}^k|$ makes the correspondence to the continuous velocity obvious. These equations are supplemented by an approximation of the Herring Condition. The evolution is done in two steps: the first evolves all nodes corresponding to GB internal points, and the second moves the triple junctions according to the Herring Condition.

3.1 Critical Events

Equations (3),(4) are valid as long as the network connectivity is unchanged. During the evolution there are instances where grains or grain boundaries disappear. We refer to these as critical events where we perform network connectivity changes that are consistent with energy dissipation.

Grain boundary flipping: When the length of a grain boundary becomes 0, it disappears, and its two triple junctions become one quadruple-junction, a point where four grain boundaries meet. Triple junctions are typically the only stable junctions, and therefore the quadruple-junction instantly splits into two new triple junctions connected by an infinitesimally small new grain boundary. The split is consistent with decreasing of energy, maintaining the dissipative quality of the evolution. The edge flipping event is shown in figure (1).

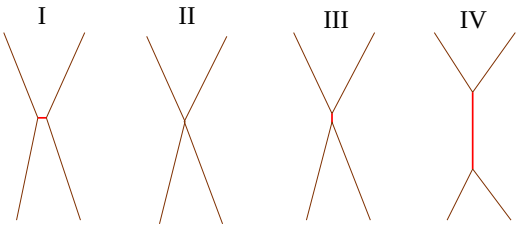

Figure 1: Edge flipping event

Grain disappearance: As a small grain shrinks, it eventually becomes a point at which three, four or five grain boundaries meet, see figure (2). This applies to grains with 3, 4 or 5 edges. The area of a grain with six or more grain boundaries does not decrease as follows from the Von Neumann-Mullins $(n-6)$ rule [10],

$$\frac{d}{dt}A(t) = \frac{\pi}{3}\sigma\mu(n-6), \tag{8}$$

which holds for a curvature-driven system with constant energy σ, and constant mobility μ, and that satisfies the Herring Condition at triple junctions.

The newly formed multi-junction instantly splits into triple junctions, one after the other (quadruple junctions split into two triple junctions, the junctions with five incoming grain boundaries first split into a triple junction and a quadruple junction, and the latter immediately splits into two triple junctions). The choice of the order in splitting the edges is done in a way compatible with steepest descent for the energy.

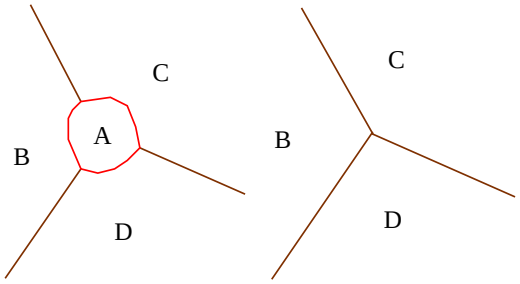

Figure 2: Grain disappearance event

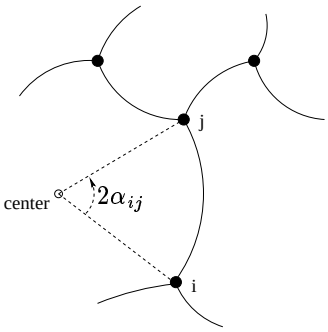

Figure 3: The circular GB connecting vertices i and j is parametrized by its half-angle α_{ij}.

4 VERTEX MODEL (VM)

The computational complexity of the above described models and the fact that only statistical information is required suggests looking at coarse grained models. A natural simplification of grain boundaries is to represent GB in terms of end points, the triple junctions, as well as one parameter for curvature. This brings us to a family of models called vertex models which have an extensive literature. Here we focus on a particular model that we have developed and that fits within the context of coarse graining of the detailed models described before. In this model [15], GBs form circular arcs. The GB connecting vertices i and j is parametrized by its half-angle α_{ij} (see figure 3). By definition, we have $\alpha_{ij} = -\alpha_{ji}$.

Similar to the PDE model, the proposed vertex algorithm is divided into two alternating steps: moving vertices and moving GBs. In the vertex step, instead of solving the Herring Condition which imposes a nonlocal effect on the grain boundaries, we impose a vertex motion defined by line tensions,

$$v_i = -\lambda \sum_j^{(i)} \mathcal{R}_{\alpha_{ji}} \left(\frac{r_{ij}}{|r_{ij}|} \right), \qquad (9)$$

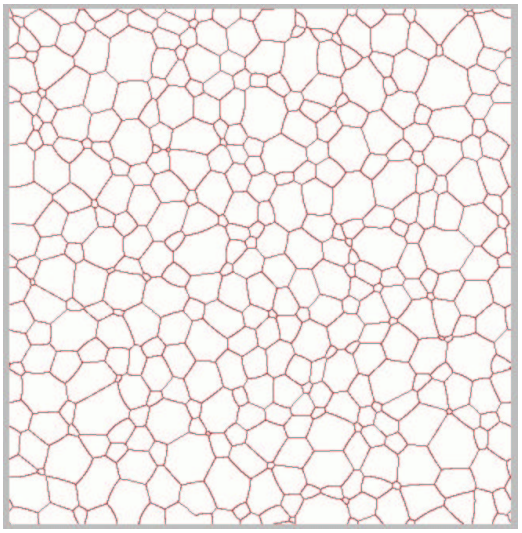

Figure 4: A domain pattern in the simulation of VM. $\lambda = 20$. $\mu = 1$.

where λ is the vertex mobility and $\mathcal{R}_{\alpha_{ji}}$ is the linear operator that rotates a vector by α_{ji}. This model, in addition to being a coarse-graining of the PDE model can be viewed as an extension of the Soares et al. vertex model [12] that allows only straight edges. Equation (9) is integrated using the forward Euler method. The new GB is obtained by interpolating a circle to the fixed midpoint of the old arc and the two new vertices.

In the GB step, the vertices are fixed and the displacement of the GB is determined from moving the midpoint of the arc by the Mullins Equation of curvature driven growth. Denoting the velocity of the midpoint of the GB connecting vertices i and j by v_{ij}^m, and using the fact that the radius of curvature is $|r_{ij}|/2\sin\alpha_{ij}$, we get,

$$v_{ij}^m = \mu \frac{2\sin\alpha_{ij}}{|r_{ij}|} n_{ij}^m, \qquad (10)$$

where μ is the boundary mobility and n_{ij}^m is the normal to the circular GB at the midpoint. By symmetry, $n_{ij}^m = -R_{\pi/2}(\frac{r_{ij}}{|r_{ij}|})$. Finally, like all models that employ the grain boundaries as a fundamental data structure, the equations of motion have to be supplemented with the two topological events: grain boundary flipping and grain disappearance.

Figure 4 shows microstructure configuration produced by VM with the vertex mobility $\lambda = 20$ and the boundary mobility $\mu = 1$. The configuration is practically indistinguishable from those obtained from the PDE model.

As the time step Δt goes to zero, the above discrete

model approaches a system of ODEs governing the evolution of r_i and α_{ij}. In addition to the governing equation for r_i simply defined by (9), one can deduce the governing equation for α_{ij} by differentiating the geometric relation implied by the circular GB shapes,

$$\cos\alpha_{ij} = \frac{r - r_i}{|r - r_i|} \cdot \frac{r_j - r}{|r_j - r|}. \tag{11}$$

and obtain,

$$\begin{aligned} \dot{\alpha}_{ij} \quad = \quad & \frac{1}{|r_{ij}|}[-\frac{4\mu \sin\alpha_{ij}(1+\cos\alpha_{ij})}{|r_{ij}|} - \\ & (\dot{r}_i + \dot{r}_j) \cdot \mathcal{R}_{\frac{\pi}{2}} \left(\frac{r_{ij}}{|r_{ij}|}\right)(1+\cos\alpha_{ij}) - \\ & \dot{r}_{ij} \cdot \frac{r_{ij}}{|r_{ij}|}\sin\alpha_{ij}]. \end{aligned} \tag{12}$$

Such an analytical form opens the door for mathematical analysis. It also has immediate numerical implications. For example, the algorithm described above can be rewritten in terms of solving the differential system simultaneously for both r_i and α_{ij} using standard higher order ODE schemes such as the fourth order Runge-Kutta method.

Vertex models in general have been developed with a primary goal to relax the high CPU and memory requirements of the more detailed simulation models. In comparison with the Soares et al. model, our system has one more equation for the additional parameter α_{ij} per GB and thus the extra computational load is minimal. In fact, the present vertex model is about 10 to 100 times faster than the PDE model depending on the accuracy requirement on the PDE model.

5 STOCHASTIC MODEL (SM)

Physical and engineering questions regarding grain growth involve distribution functions, and actual grain configurations is of less significance with respect to material properties. This calls for models that describe directly the evolution of quantity of interest such as texture, grain boundary characterization, size distribution, etc. This, however, is a hard task which we approach by considering the formulation of a stochastic process describing grain growth on large time scales. Grain size distribution is accessible experimentally, and allows for calibration of models, and is thus the focus here.

The model described in this section allows us to accelerate computationally expensive algorithm on one hand, and to gain new insight into mesoscale processes. The model is build on the detailed PDE model, using statistical analysis. It sheds new light on the details of grains evolution in terms of their area and number of facets. It can be viewed as a temporal coarse graining of the PDE model and its motivation goes back to the goal of simulation, being statistical in nature.

The main observation that led to the construction of the stochastic process describing grain size distribution is the following. Single grain evolution follows a deterministic evolution for a while, the $(n-6)$ rule, which is interrupted at certain times that seem random, by a change in the number of edges as a result of critical events. A stochastic process is constructed for time scale of the order of the mean time between critical events, which is significantly larger than the time scale used in the PDE, the MC, or the Vertex Models. The full process involves a deterministic behavior following the $n-6$ rule, for isotropic energy and mobility, together with a random events related to flipping edges, or disappearance of grains. As a result of the critical events some grains may lose edges, while others may gain edges. Although we have used the detailed PDE model to build the stochastic model, other detailed models could as well serve that purpose. Since in the stochastic model there is no network connectivity the details of the critical events must be done with some care.

Grain boundary flipping: In this event two grains lose an edge and two grains gain an edge, see figure 1. Using the PDE model we collect statistics regarding this event. The simulation time in the PDE model to collect this statistics is not very large, compared to a full simulation, say to reach self-similarity in the size distribution function.

Simulation with the detailed PDE model reveals that the probability that a grain with n edges will lose an edge due to flipping in a short time interval, is proportional to the interval length, and inversely proportional to some power of the average area.

Grain disappearance: As a small grain shrinks, it eventually becomes a point at which three, four or five grain boundaries meet. The disappearance of a grain causes several other grains to lose or gain edges.

- If a 3-edge grain disappears, then three grains lose an edge.
- If a 4-edge grain disappears, then two grains lose an edge.
- If a 5-edge grain disappears, then one grain gain an edge, and two grains lose an edge.

The event of a grain disappearing is a direct result of its size shrinking to zero, so we do not regard it as a random event. Its effect on other grains is considered as random. As in the flipping event, the grains

that gain, or lose an edge, are selected according a probability computed from the PDE model.

Implementation. We begin in this model with N grains where each has an area denoted by $A_j, \quad j = 1, \ldots, N$, and number of edges denoted by $n_j, \quad j = 1, \ldots, N$. Note than N changes during simulation, due to grain disappearance.

`Grain disappearance:` Let D_n be the total number of grains having n edges that have disappeared in the last time step. The total number of grains that lose edges as a result of these disappearance events is $D = 3D_3 + 2D_4 + D_5$, (discussion above). Let $p_n^D, \quad n = 4, 5, \ldots$ be the fraction of the n-edge grains that will lose an edge. The probability p_n^D can be interpreted as a conditional probability that an n-edge grain loses an edge, given that an edge was lost in the system, and have $\sum_{n \geq 4} p_n^D = 1$. We pick randomly $p_n^D D$ grains from the n-edge population and reduce the number of edges of each by 1, this is done for $n = 4, 5, \ldots$. The numbers p_n^D are calculated from the detailed PDE model.

`Edge flipping:` This event is governed by a set of probabilities q_n that a grain with n-edges loses an edge, during a prescribed time interval. Let M_n be the total number of n-edge grains. We choose randomly $q_n M_n$ grains out of the n-edge population, for $n = 4, 5, \ldots$, and reduce their number of edges by 1. The total number of grains that have lost edges by this process is $M = \sum_{n \geq 3} q_n M_n$, and this is the same number of grains that gain edges due to flipping. This is done according to a fixed proportion as in the disappearance case. Let p_n^F be the fraction of n-edge grains that will gain an edge due to flipping. Again this quantity can be interpreted as the conditional probability that an n-edge grain gains an edge due to flipping, given that a flipping occurred. We implement this by picking $M p_n^F$ grains from the n-edge population and increase their number of edges by 1, and do it for $n = 3, \ldots$.

Again, the number P_n^F are calculated using the PDE model. To summarize, the algorithm is performed in three steps,

1. $A_j(t + \triangle t) = A_j(t) + \alpha(n_j(t) - 6)\triangle t$
2. Perform Grain disappearing events
3. Perform grain flipping events

6 SIMULATION RESULTS

6.1 PDE vs. MC

We have carried out an extensive comparison of the PDE and MC for the isotropic case of grain boundary energy and mobility [14]. For the MC simulations, we use a triangular lattice, and we choose a low temperature T such that $k_B T/J = 0.1$ in order to prevent grains nucleation. The total number of different spins Q is set to 100. It is shown that the Von Neumann-Mullins $(n-6)$ rule is approached by individual MC grains in an average sense and also as the underlying lattice gets finer. It is also argued that the relative grain size distribution (the distribution of the relative grain area $x = A/ < A >$ where A is the grain area and $< A >$ is the mean grain area) of the MC model approaches that of the PDE model as the microstructure evolves, or equivalently, as the lattice becomes finer. A comparison of the scaling size distributions generated by the two models is shown in figure 5. Since they are practically indistinguishable from each other, we will only use the PDE model for the comparative study of the coarse grained models discussed later.

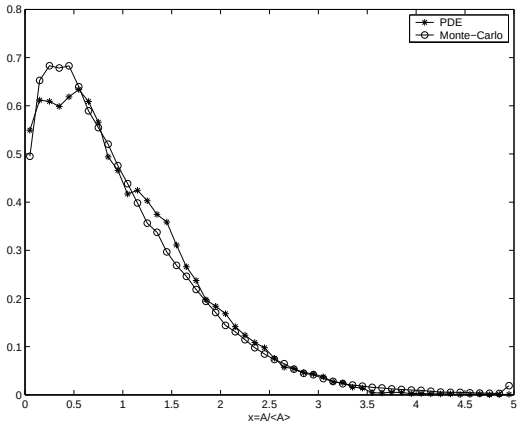

Figure 5: Self-similar relative grain size distributions in PDE and MC simulations.

6.2 SM vs. PDE

We have performed simulation of the PDE model in order to define the probabilities P_n^D, q_n, P_n^F, required for the simulation of the stochastic model (SM). These probabilities are not time invariant, as was assumed by Fradkov et. al. [2] [3] [4]. This is expected since the disappearance event for example, becomes less frequent as the average area increases. Similar observation holds for edge flipping.

Simulations with the stochastic model were compared to the PDE model. The size distribution comparison is shown in figure 6. This shows good agreement of the two models. Edge distribution compari-

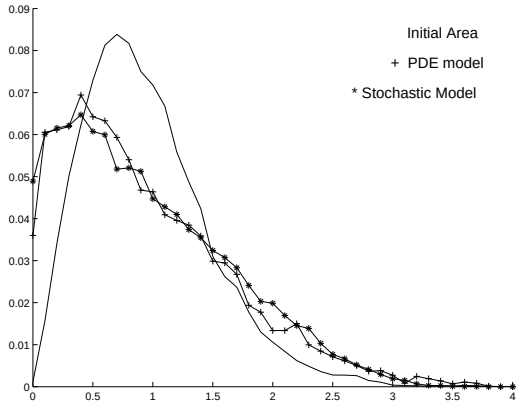

Figure 6: Area

son is shown in figure 7. The agreement here is not as good as for the area distribution and will be studied further elsewhere.

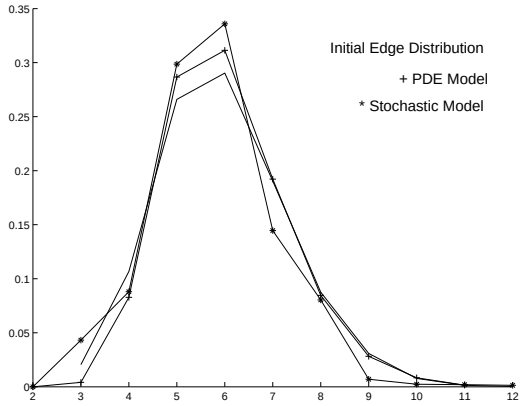

Figure 7: Edge distribution

6.3 VM vs. PDE

In order to study how well the coarse grained representation used in the vertex model is able to maintain certain statistics of the more detailed PDE model, we carried out computer simulations of VM with different ratios of the vertex mobility λ and the boundary mobility μ. We choose the Voronoi digram as the initial state and use the periodic boundary condition to minimize finite size effects. The boundary mobility μ is set to 1 in all simulations and the vertex mobility λ varies. We first present results for $\lambda = 20$. Simulations revealed that the grain size statistics hardly change as λ is larger than 10, we picked $\lambda = 20$ to represent the large vertex mobility limit.

With $\lambda = 20$, we find that not only the mean grain area in VM simulations grows linearly with a similar rate to the PDE model, but the equilibrium relative grain size distributions obtained from the two models are also in excellent agreement as can be seen in figure 8. A significant result is that the dependence of the mean curvature on time in the VM simulations fits the PDE model well, see figure 9. The mean curvature is defined as the average of interfacial curvatures (in absolute value) weighted by arc lengths, i.e.

$$\bar{\kappa} = \frac{\sum \int_{\Gamma_{ij}} |\kappa| \; ds}{\sum \int_{\Gamma_{ij}} 1 \; ds}, \tag{13}$$

where s is the arc length parameter and the sum is taken over all GBs. Under the constant curvature assumption of VM, (13) reduces to,

$$\bar{\kappa} = \frac{\sum 2|\alpha_{ij}|}{\sum |r_{ij}|\alpha_{ij}/\sin\alpha_{ij}}. \tag{14}$$

The excellent agreement of $\bar{\kappa}$ between VM and the PDE model indicates that the constant curvature assumption is able to capture overall how curved the grain network evolves. Apparently, this cannot be achieved with vertex models assuming straight interfaces, such as the Soares et al. model and the Kawasaki et al. models [6].

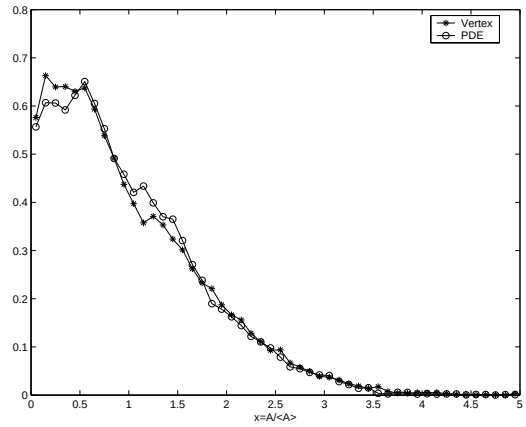

Figure 8: Comparison of the equilibrium size distributions generated by simulating the proposed vertex model and the PDE model.

In addition to achieving higher computational efficiency, the VM obtained from coarsening the PDE model offers a user-controlled parameter λ/μ that facilitates convenient investigation of the relationship between two types of kinetics, the vertex kinetics and the boundary kinetics. Their relationship has been

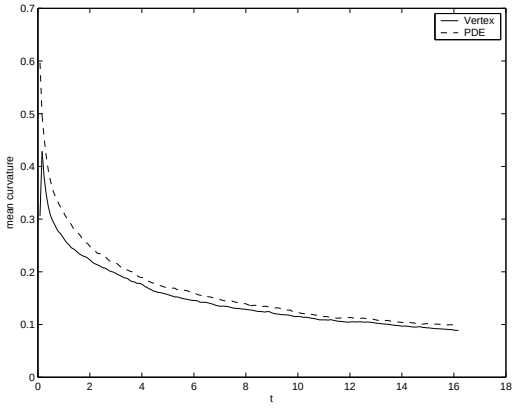

Figure 9: Mean curvature $\bar{\kappa}$ plotted as a function of time in the VM simulation. It agrees very well with $\bar{\kappa}$ in the PDE simulation (dashed curve).

discussed in [11], where the influence of vertex drag on the boundary motion is investigated for a symmetric grain boundary system with only one triple junction, and in [2] [3], where a qualitative criterion for estimating the relative strength of vertex drag is given for general grain networks. The present vertex model combining the two types of kinetics provides an opportunity to understand their relation from the perspective of grain growth statistics.

To illuminate the effect of different ratios λ/μ, we present the relative grain size distributions obtained from simulations for $\lambda = 1, 2, 5, 20$ respectively. The simulations all start from the same initial Voronoi diagram of 25600 cells. The metastable distributions are taken when approximately 90% of the grains dissapeared as a result of coarsening. In this time regime the mean grain area depends linearly on time, for all the above choices of λ. The distributions are plotted in figure 10 together with that of the Soares et al. model that represents the small vertex mobility limit $\lambda \to 0$. It is observed that as λ decreases, the spike of distribution around 0 becomes sharper, approaching the highly peaked distribution of the Soares et al. model. On the other hand, as λ increases, the distribution flattens out around 0, approaching the typical grain size distribution of the PDE curvature driven grain growth.

To summarize, for small λ, the GB motion is dragged by the slowly moving vertices and the system is dominated by the vertex kinetics, which favors relatively small grains. For large λ, the system is dominated by the curvature driven boundary motion, vertices merely trying to establish the thermodynamic equilibrium angles. Thus, the relative grain size distribution is similar to that in the PDE model. A range of metastable relative grain size distributions are obtained for intermediate values of λ.

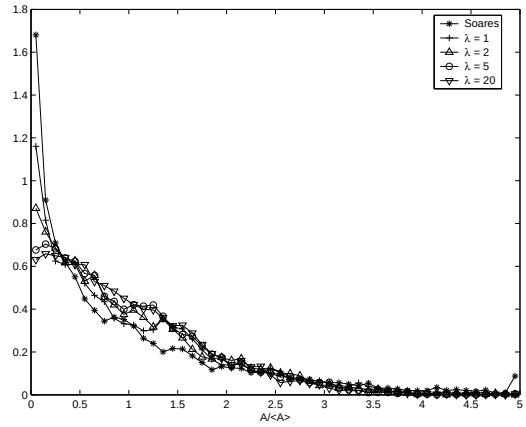

Figure 10: Metastable relative grain size distributions obtained from simulating VM for different choices of the vertex mobility λ.

7 DISCUSSION

The paper discusses a sequence of models for studying grain growth from thermodynamically and kinetically detailed models to coarse grained models. We have applied temporal as well as spatial coarse graining, leading to very different models that capture different aspects of the system behavior. In addition to acceleration of computationally expensive methods, these coarse grained models offer new insights into mechanisms at the mesoscale. There are challenging questions in coarse graining of such system that aim at understanding texture and grain boundary characterization. This work has focused on the simplest distribution function, and the most studied one, the size distribution. However, the methodology applied is general and we expect that study to pave the road to further investigation using coarse graining ideas aiming at particular distribution functions, e.g., texture and grain boundary characterization.

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