Chapter 6

Conclusions and Future Work

This thesis examines cell structures that change over time, primarily through curvature flow. Chapter 1 is an informal introduction to the topics of cell structures and dynamic cell structures. There we considered the concepts of an evolving cell structure, steady state, and universal steady state, which is associated to a particular dynamic imposed on evolving cell structures.

In Chapter 2 we simulated one-dimensional cell structures that evolve under a variety of dynamics. Although a relatively simple, this sort of work does not seem to have been previously. In this chapter we provide experimental evidence of the existence of steady states and universal steady states for one-dimensional cell structures that evolve under a variety of dynamics. We report coarsening rates and long-time behavior of these systems.

This area looks promising in terms of future work. The system itself is quite simple compared with systems in higher dimensions. There is hope that some problems in this area can be answered analytically, perhaps benefitting from insight gleaned from simulation results. In this chapter we considered only deterministic dynamics which only considered very local features in determining the motion of each boundary point. In future work we might consider both allowing non-local calculations as well as stochastic components of the motions.

In Chapter 3 we consider two-dimensional cell structures that evolve through curvature flow. We develop a method for simulating such systems that satisfies the von Neumann-Mullins relation with error of order $O(\Delta t)^2$, where $\Delta t$ is the time-step. This surpasses in accuracy previous methods used for modeling two-dimensional isotropic grain growth. This method allows us to model very large systems and obtain accurate statistics about the steady state.

We have considered only isotropic systems, in which the boundary mobility and surface tension
are uniform throughout the system. Real systems, however, are often anisotropic and this must be considered in modeling any real problem. Future work might focus on generalizing the work here for these cases. Another direction of research might consider two-dimensional cell structures that evolve in various other manners. For example, the evolution of dry foams through gas diffusion through cell boundaries shares much in common with coarsening in polycrystalline materials, though it is different in substantial ways. The list of events that can occur throughout the evolution of such a structure appears to be different, as is the long-time steady state such a system reaches. Future work might consider a more general framework of two-dimensional dynamical cell structures.

In Chapter 4 we consider three-dimensional cell structures that evolve through mean curvature flow. We develop a method for simulating such systems that satisfies the MacPherson-Srolovitz relation with error of order $O(\Delta t)^2$, where $\Delta t$ is the time-step; it is difficult to compare this with previous models as calculations of this error have not been reported. The method also allows us to compute important geometric and topological statistics of steady state structures much larger than have been previously reported. We find that the evolution of a three-dimensional cell structures can be captured by five basic topological changes; from our simulations it appears that more complex topological transformations can be composed of combinations of these five. We also develop in this chapter a method to characterize the combinatorial structure of individual grains. This allows us to investigate more detailed questions about what sort of grains appear in structures that have been formed through a mean curvature flow coarsening process. We observed that grain growth structures tend to have more symmetric grains (in both a geometric and combinatorial sense) than cells in a certain type of Voronoi construction.

The work in this chapter has been limited in a number of important ways. First, the discretization used here is not ideal. Faces in our simulations are triangulated by placing one node in the center and many nodes around the face boundary. This is not ideal because even in the most refined version of this method, triangles will remain large in at least one linear dimension. A more ideal discretization of the surfaces involves using equiaxed triangles to represent the surface. This would allow for arbitrarily small triangles, which would allow more accurate representation of the surfaces. In particular, it would allow us to measure important quantities of interest that are unavailable to us now, or else are available with only poor accuracy. One example is the total Gaussian curvature over the faces, a quantity that will suffer from poor accuracy using the current method. The reason that this has not been implemented here has mainly been the complexity of implementing such a representation. The triangulations we use here were considerably easier to implement. Although we think the impact of this choice of discretization is small, it is not clear what differences it makes.
to both the evolution of the system and to its long-time steady state. In future work we hope to rewrite the code in a way that will allow this superior representation to be utilized.

Another limitation of the three-dimensional code as developed here is its restriction to the isotropic case. This idealized model of grain growth fails to account for anisotropy in the grain boundary surface tension and mobility in real systems. In real polycrystalline materials, the orientation nature of individual grains leads to surface energies and mobilities that depend strongly on the way in which two neighboring grains are aligned and “misaligned” from one another. Although this anisotropy certainly effects the local laws of grain growth, it is not clear how this affects the long-time steady state of a typical material. Future work in modeling grain growth will need to eventually accurately account for these anisotropic conditions.

Another future direction worth pursuing is connected to complicated combinatorial nature of the individual cells. In the thesis itself we described a way to completely characterize the combinatorial structure of individual cells. We might consider using this to help us understand how individual grains evolve over time. For example, is there a “typical” trajectory that a certain kind of grain can be expected to travel? Do global properties such as the relative frequencies of basic topological transitions tell us something about the likelihood of finding grains with certain combinatorial structures? What can both of these tell us about the more global structure we might expect to see in typical grain growth structures?

In Chapter 5 we compare grain growth in different dimensions, focusing primarily on two and three dimensions. We use the opportunity to report results of large steady state structures. We also report statistics of two-dimensional cross-sections of three-dimensional structures. We observe that grain volumes in three-dimensional systems appear to be exponentially distributed, something we observe in some one-dimensional systems but which we do not observe in two-dimensional systems.