

The free energy function is

$$f(\theta_1, \theta_2, \dots, \theta_N) = \frac{1}{4} + \sum_{p=1}^N -\frac{1}{2}\phi_p^2 + \frac{1}{4}\phi_p^4 + \frac{3}{4} \sum_{p=1}^N \sum_{q=1, q \neq p}^N \phi_q^2 \phi_p^2 \quad (1)$$

For two grains the derivatives of the free energy function are below:

$$\frac{\partial f}{\partial \phi_1} = -\phi_1 + \phi_1^3 + 3\phi_1\phi_2^2 \quad \frac{\partial f}{\partial \phi_2} = -\phi_2 + \phi_2^3 + 3\phi_1^2\phi_2 \quad (2)$$

The formulas for more grains follow the same pattern as above. The derivatives are used in the Allen-Cahn Equations for each of N order parameters:

$$\begin{aligned} \frac{\partial \phi_1}{\partial t} &= -M \left(\frac{\partial f}{\partial \phi_1} - 2K\nabla^2 \phi_1 \right) \\ &\dots \\ \frac{\partial \phi_N}{\partial t} &= -M \left(\frac{\partial f}{\partial \phi_N} - 2K\nabla^2 \phi_N \right) \end{aligned} \quad (3)$$

The value of the mobility and gradient energy coefficients are 1 ($M = 1, K = 1$). The simulations are completed with an explicit scheme. The boundary conditions are periodic in both directions. The Laplace operator is done with matrix multiplication. The grid size is 1 and the time step is 0.01. The data is centered about $x = 0$ and $y = 0$.

Planar Boundary Evolution between Two Grains

When two grains are used with step functions as initial conditions, the profiles evolves to the one shown in Figure 1. The periodic boundary conditions result in two intersections of the order parameters. I used 201 mesh points here. The order parameters profiles cross at $\phi_1 = \phi_2 = 0.5$ at equilibrium. The characteristic thickness is 4.46 mesh points based off linear interpolation when 201 mesh points were used. The thickness definition used is the distance covered for the order parameter to go from 0.9 to 0.1.

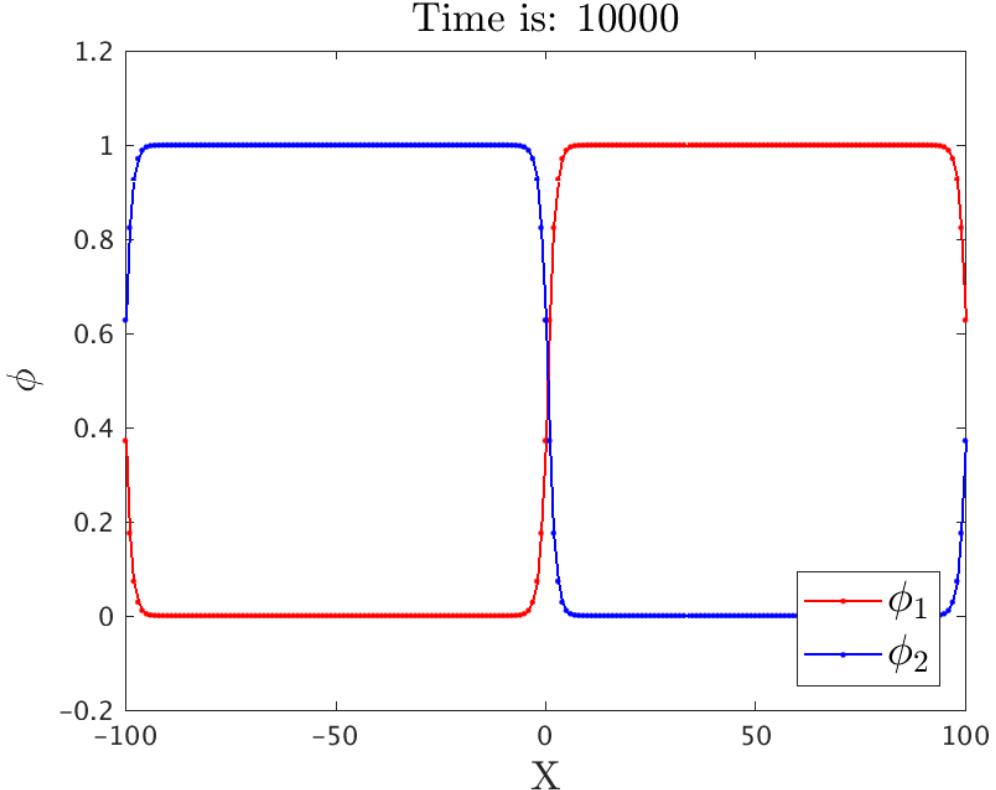


Figure 1: Final Profile with two grains with an initial condition of step functions

Effect of Interface Thickness

In the sharp interface limit, for a circular particle the radius should decrease as $r^2(t) - r^2(0) = -4t$. Starting with a particle radius that is 8 times larger than the thickness of the interface, the Allen-Cahn Simulation was run. The particle radius was taken as the location of the level curve $\phi_1 = \phi_2 = 0.5$. This result is the top-left part of Figure 2. The simulation deviates from the sharp interface limit as the radius goes below 20 and continues to deteriorate. This is because the error propagates as the simulation progresses. This is justified by the top-right part of Figure 2 where the sharp interface limit and the simulation agree well. In order to get a closer look, the simulation was run starting with a particle radius of 10.5 and 5.5 as seen in the bottom part of Figure 2. The simulation matches the sharp interface limit for the early times but it quickly gets worse with increasing simulation time. So the minimum size at which the grain will shrink at a rate given by the sharp interface limit depends on the initial grain size. If

the initial grain radius is 5.5, the limit holds true until about $t = 2$ so the minimum size would be 5. But if the initial grain radius is 36.5 then the limit holds true until the radius goes down to $r = 20$. These same results can also be seen in Figure 3.

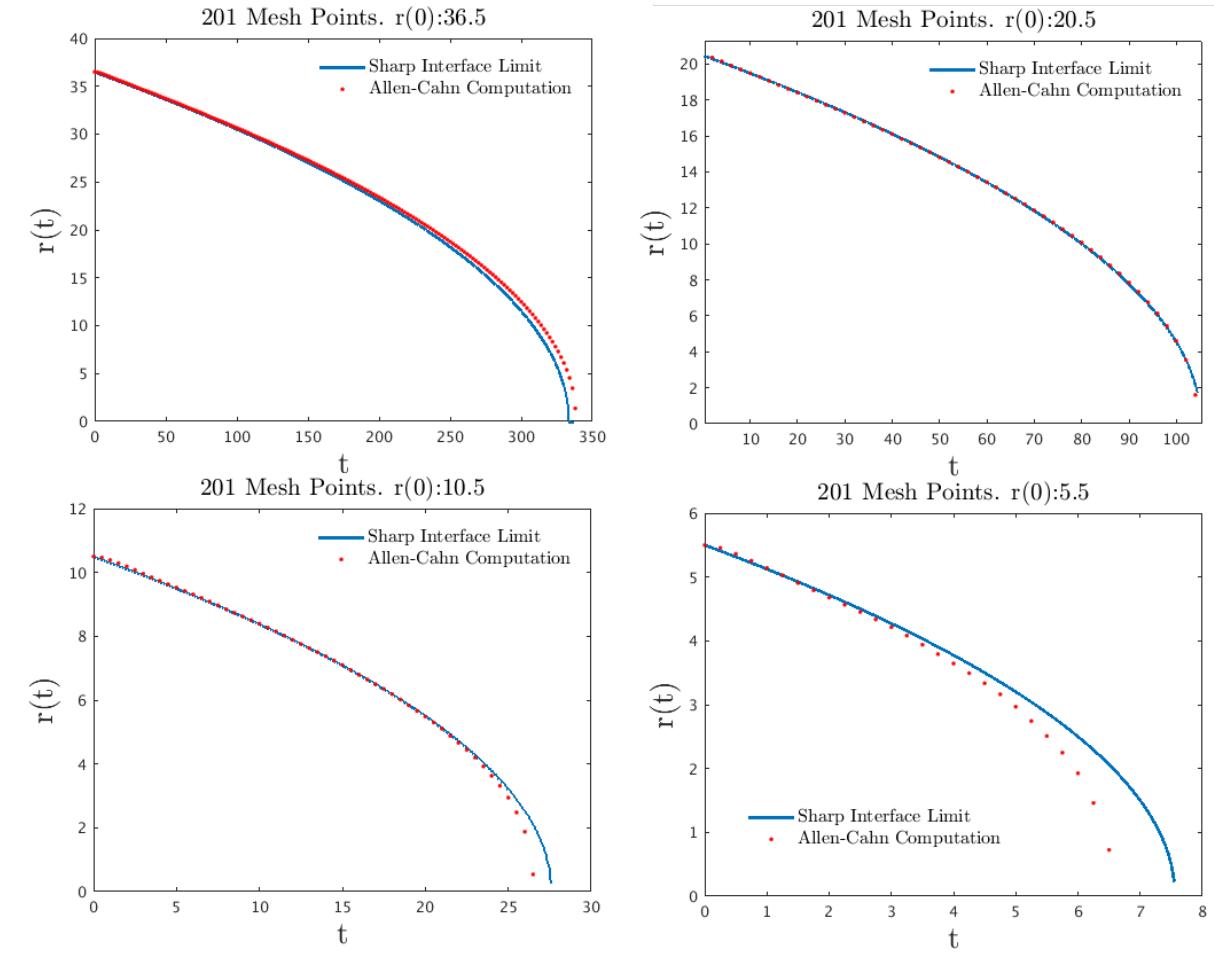


Figure 2: Sharp Interface Limit vs Simulation

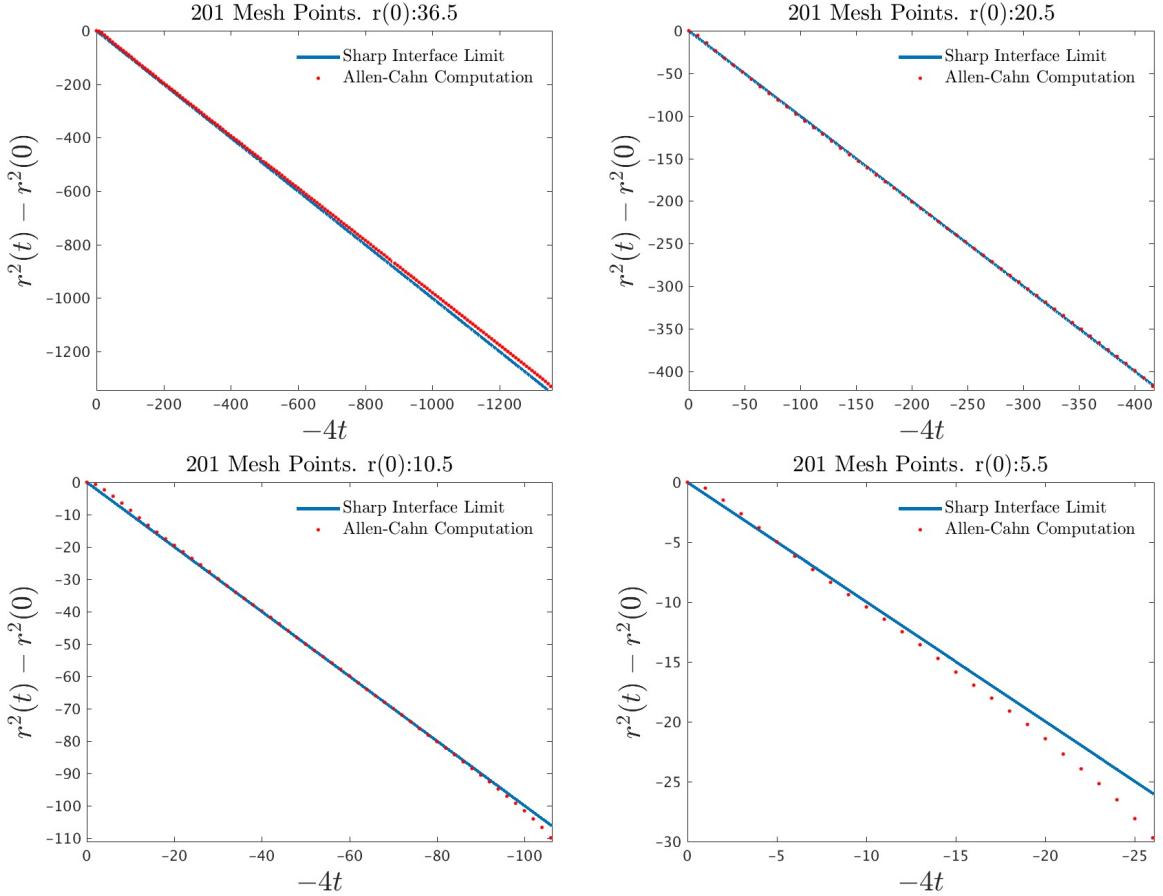


Figure 3: Sharp Interface Limit vs Simulation

Evolution of Grain Structure

Starting with small random noise for each order parameter about $\phi_1 = \phi_2 = \dots = \phi_N = 0$ for $N = 2, 3, 4, 8, 10$ is below in between Figures 4-8 where the plots are of the grain number which is found by taking the area where $\phi_i \geq 0.5$. As N increases, the number of grains increases since more order parameters are present. The small grains disappear, while the large grains grow which is seen for all the N because it is energetically favorable to have less larger grains.

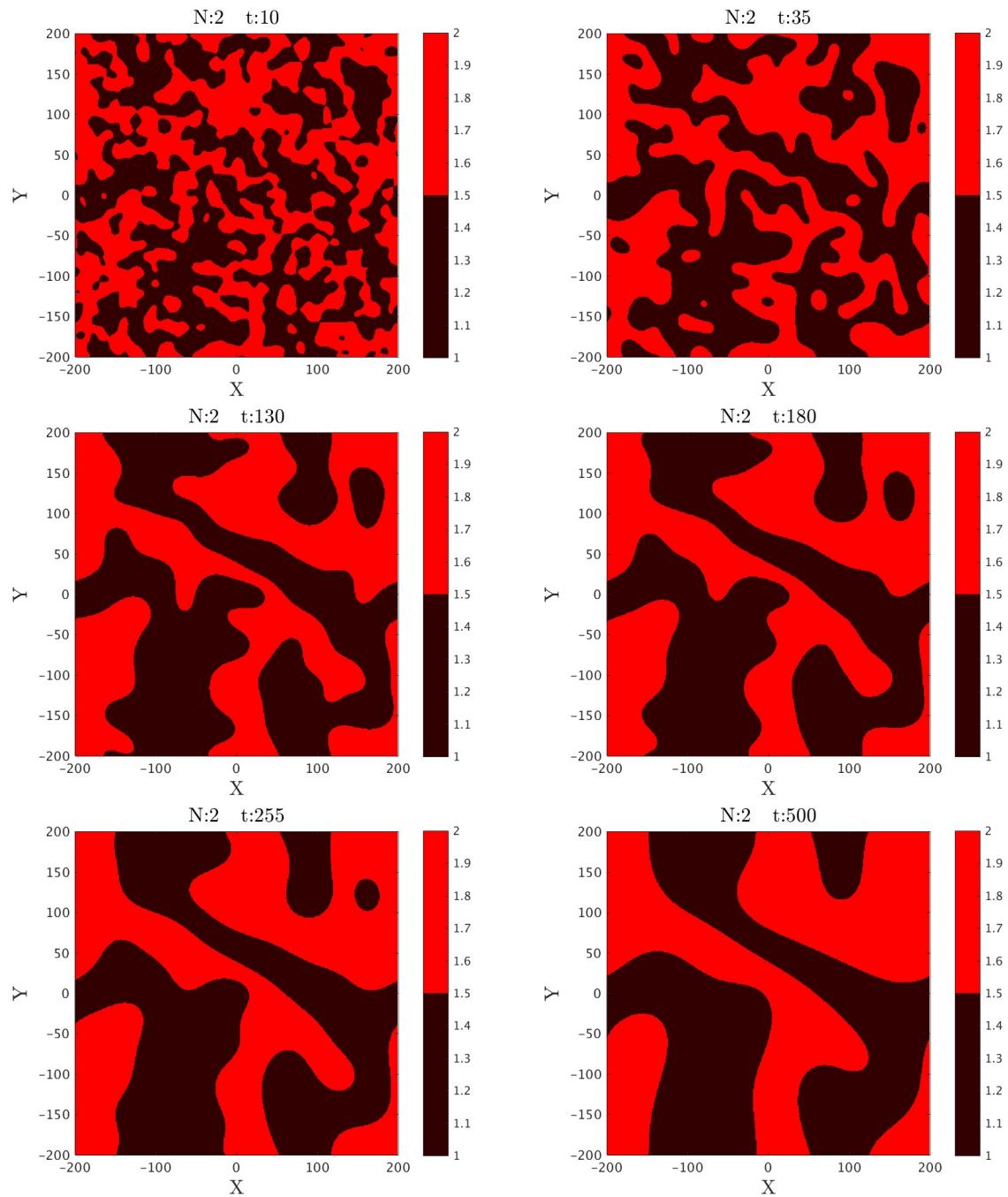


Figure 4: Evolution for $N = 2$

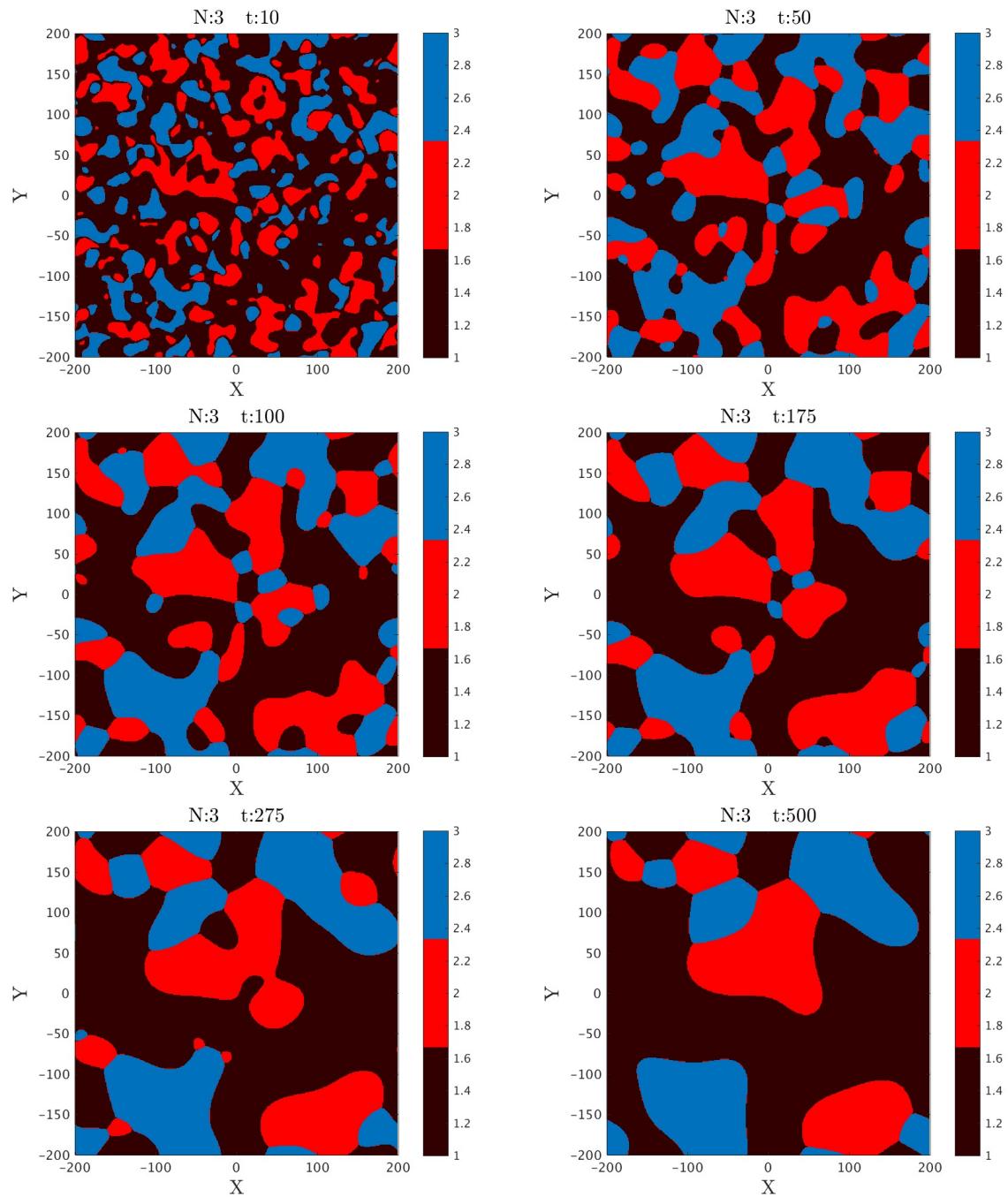


Figure 5: Evolution for $N = 3$

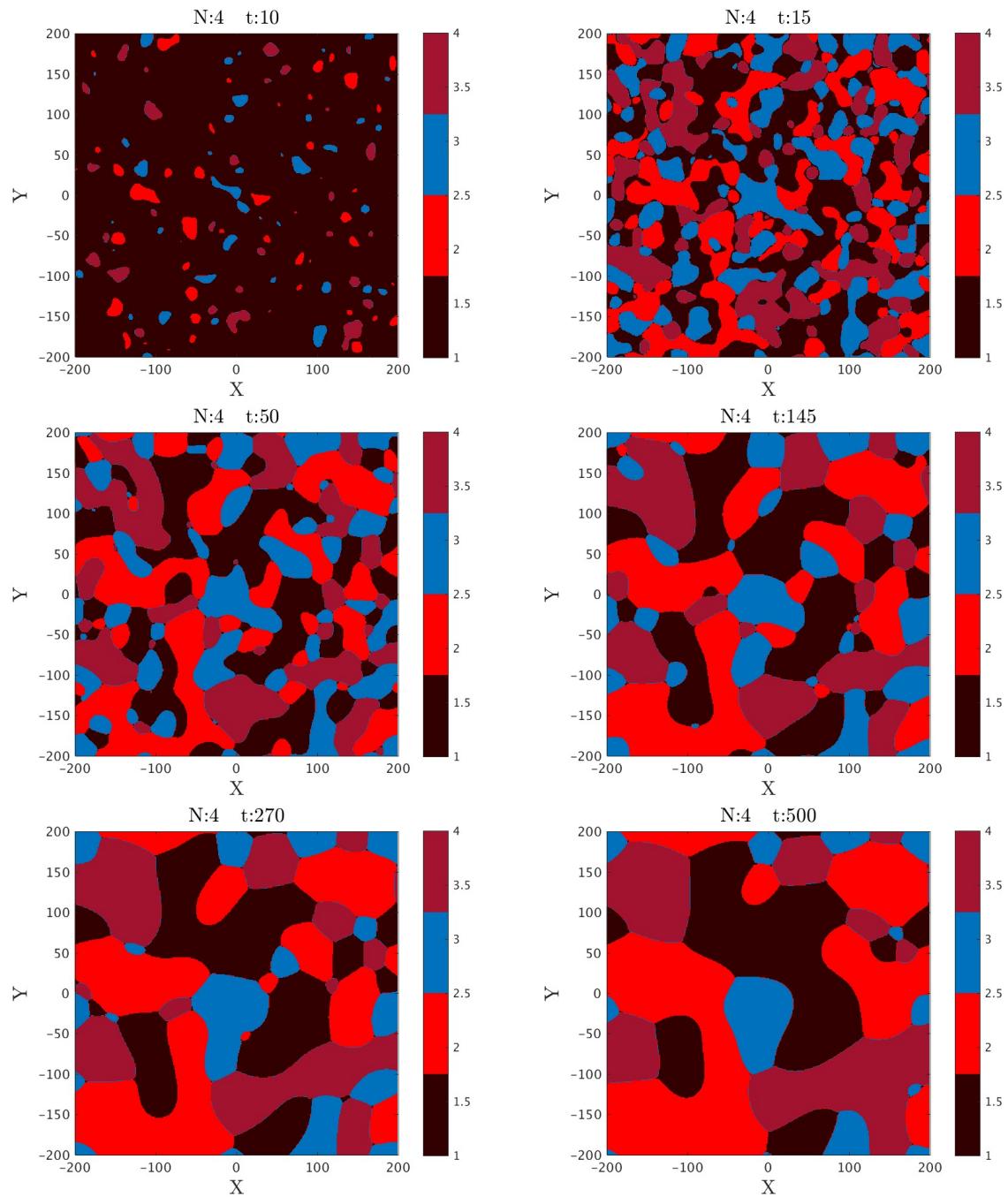


Figure 6: Evolution for $N = 4$

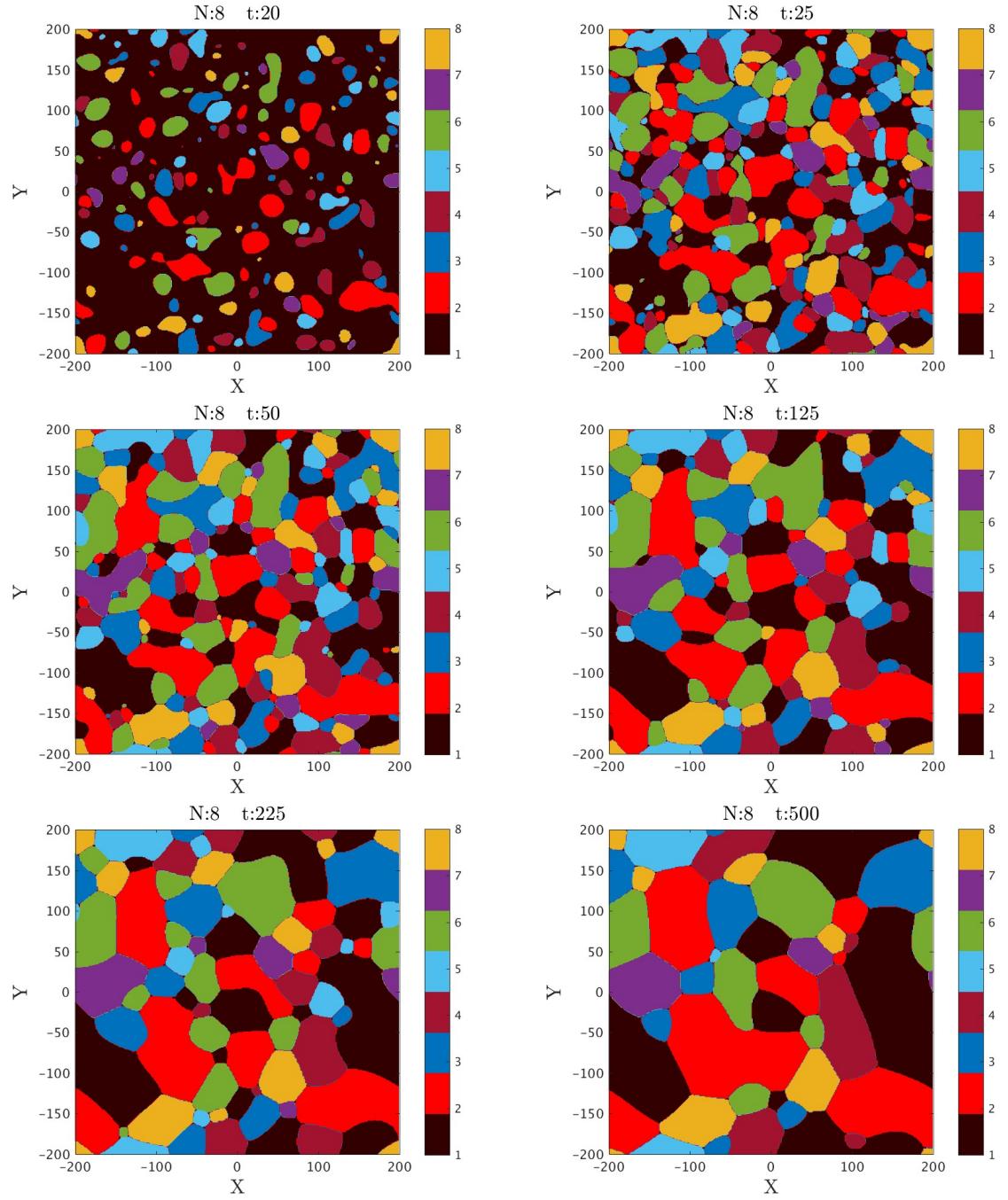


Figure 7: Evolution for $N = 8$

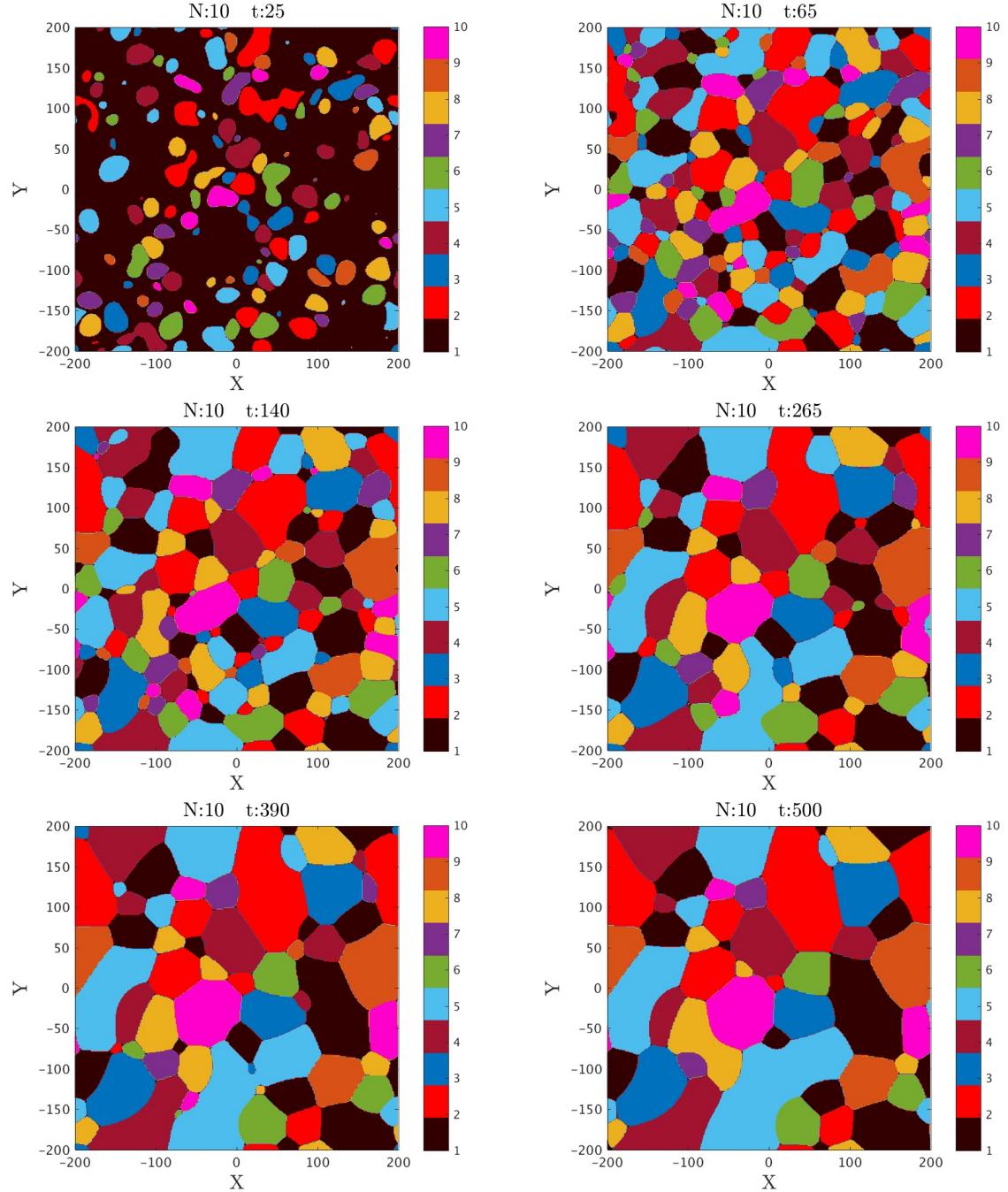


Figure 8: Evolution for $N = 10$

Grain Growth using Phase Field Equations

Starting again with small random noise for $N = 12$, the plot of grain growth is below. This is done by plotting $\sum_{p=1}^N \phi_p^2(\phi_p - 1)^2$ at each mesh point. The simulation shows that small grains disappear and large grains grow as seen in Figure 9. Unstable quadrajunctions are seen in Figure 10 in the top-right of each sub-figure with the colored arrow.

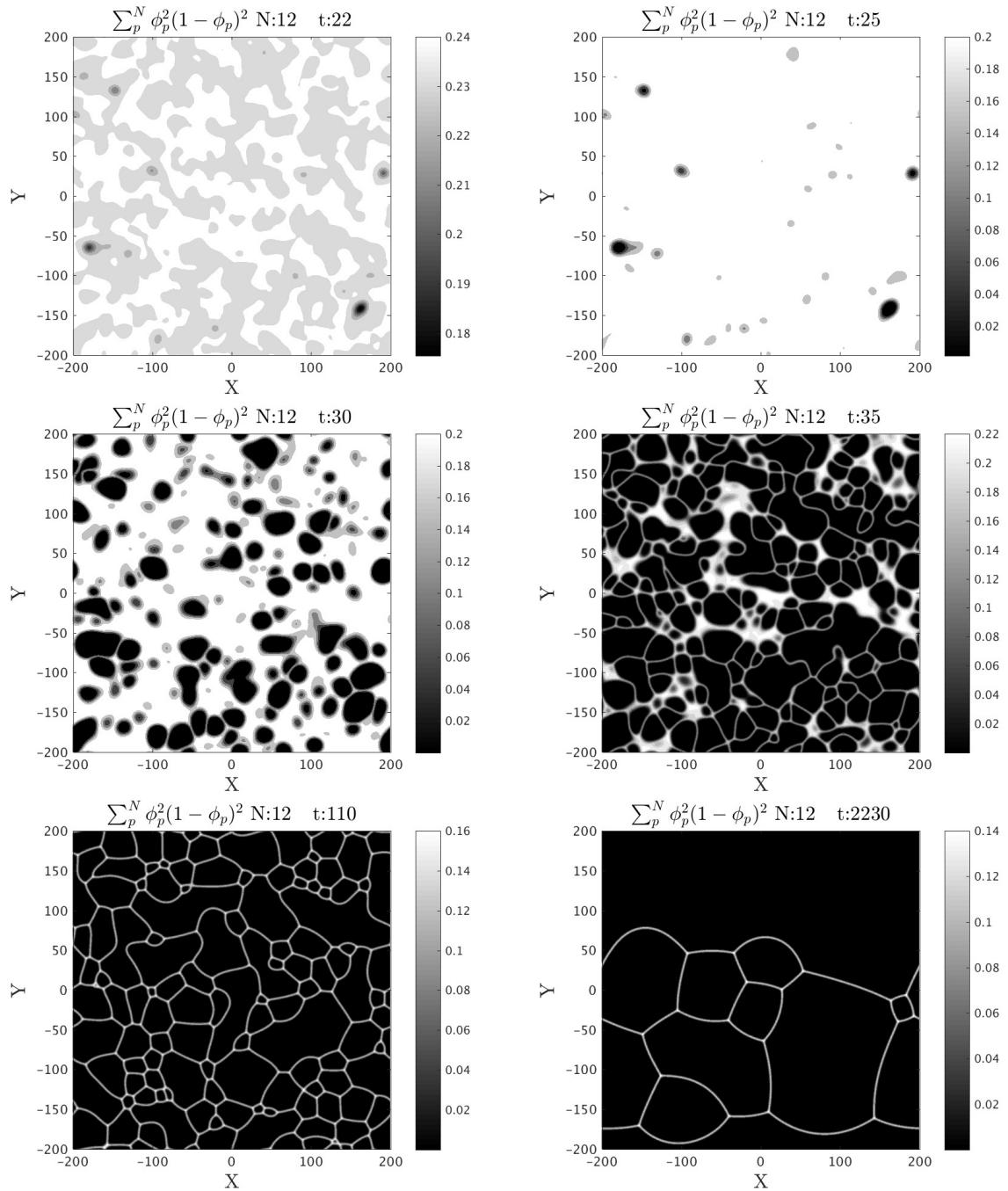


Figure 9: Small grains shrinking and large grains growing

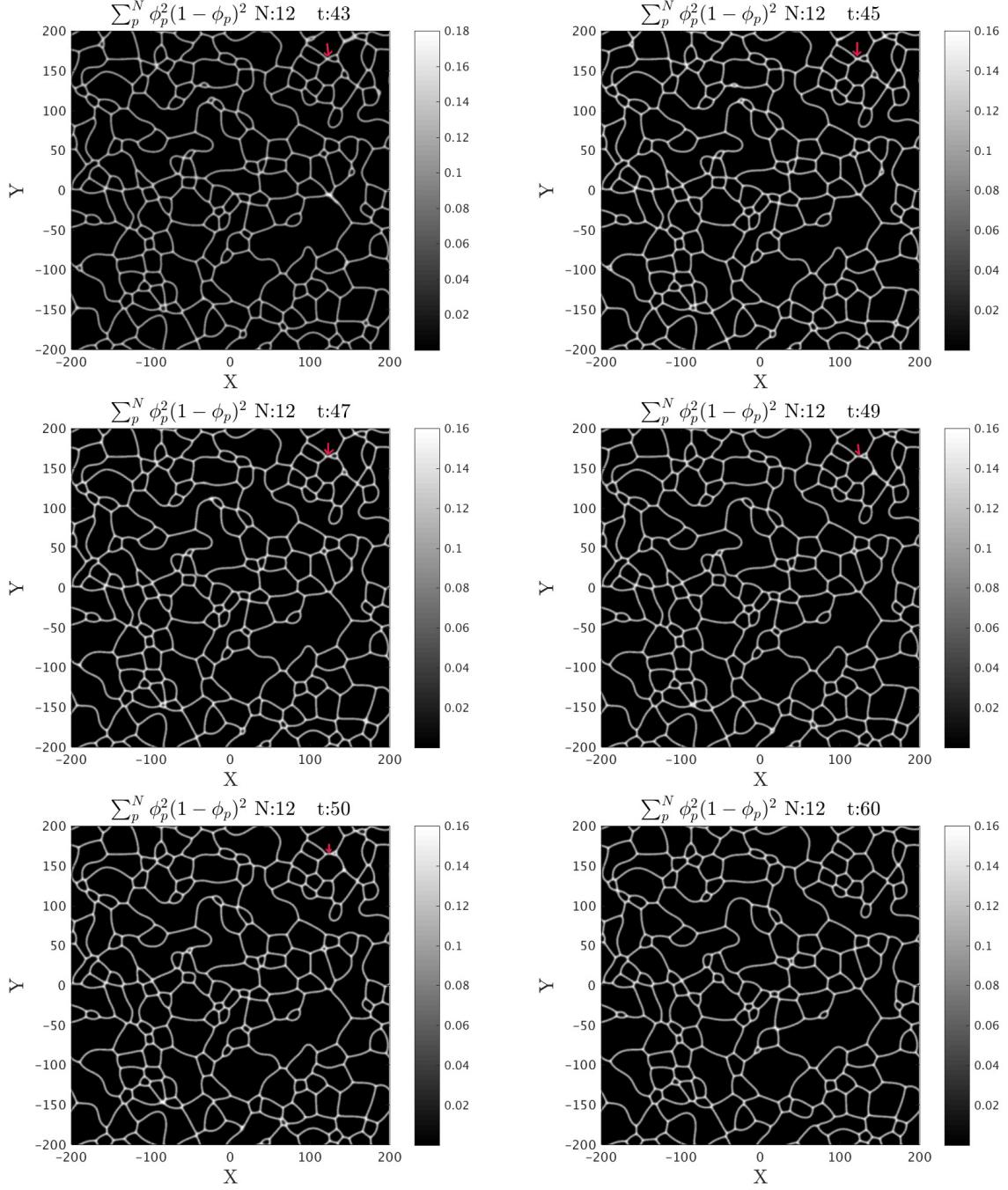


Figure 10: Unstable quadrajunctions

The case of two grains with the same order parameter touching is shown in Figure 11 on the right side. The left side of Figure 11 shows that the grains merge.

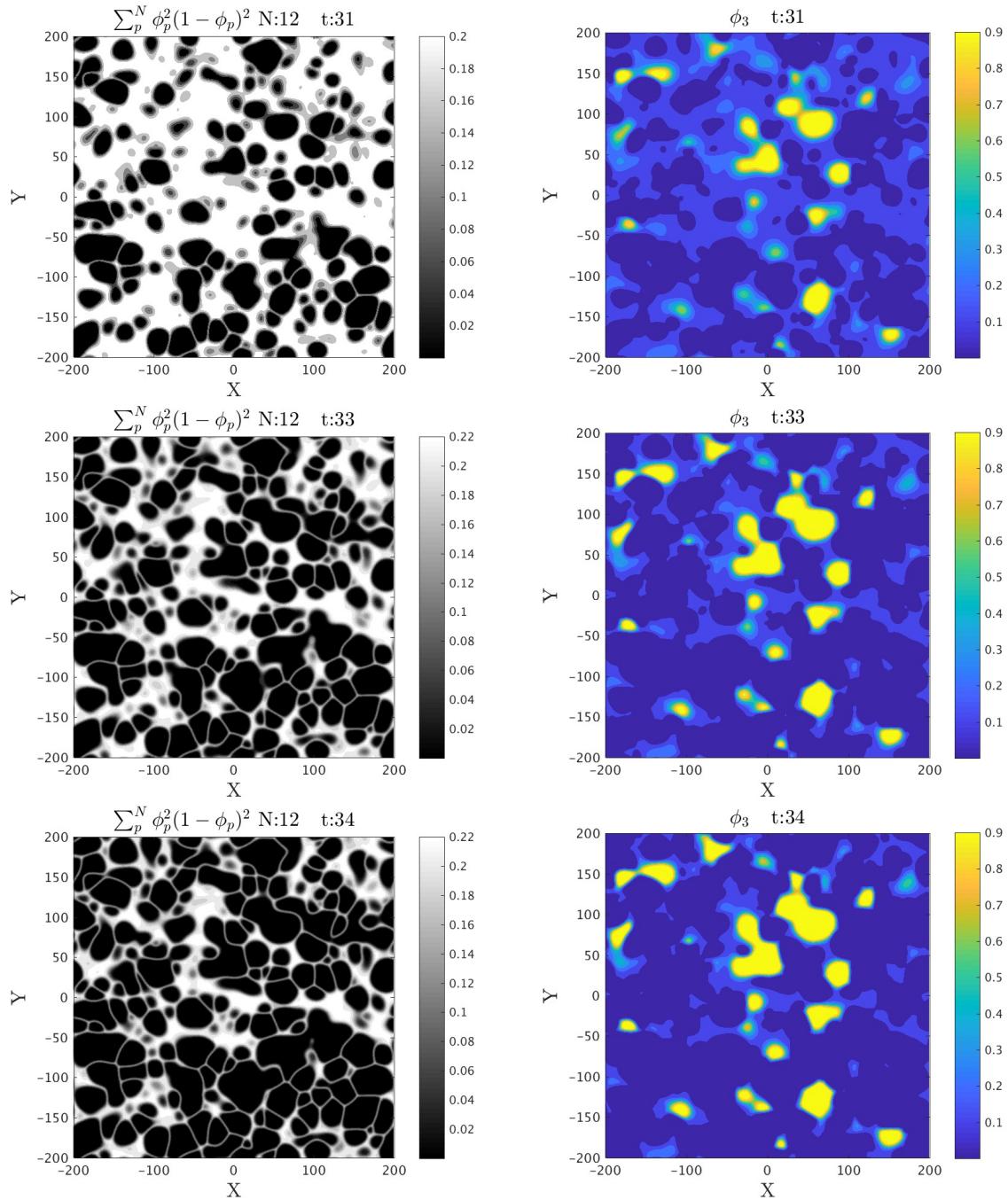


Figure 11: Case of two grains with same order parameter touching