MAE 510 – NUMERICAL METHODS FOR MOVING INTERFACES

SPRING 2016 – HW #2

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SUBMITTED BY

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Introduction:

Phase field method is a diffuse interface method widely used by the material science community. Phase field method comes in two types and in both types the phase is represented by a single function, ϕ. This function, ϕ takes values between two states and each state represents a different phase. Between regions ϕ=0 and ϕ=1, is a smooth transition where the interface is located. This transition zone is a mix of both the phases. The first type of the Phase Field Method is the Cahn-Hilliard Formulation where the function ϕ represents a conserved phase field variable. This formulation leads to the Cahn-Hilliard equation. The second type is the Allen-Cahn formulation. In this type, the variable ϕ is an artificial order parameter and is not conserved. This formulation leads to Allen-Cahn equation.

Cahn-Hilliard phase field model was used to investigate the decomposition of a two-dimensional domain. The total energy density of the domain is given by

$$f = g(\phi) + \frac{1}{2}\alpha\nabla\phi \cdot \nabla\phi \qquad (1)$$

where α is a constant, ϕ is the phase field variable, and $g(\phi)$ is the mixing energy. The chemical potential is given as

$$\mu = g'(\phi) - \alpha\nabla^2\phi \qquad (2)$$

In the Cahn-Hilliard formulation, the evolution of the phase field variable is given by

$$\frac{\partial\phi}{\partial t} = \nabla^2\phi \qquad (3)$$

In the current problem, the mixing solution is given by

$$g(\phi) = 16\beta(\phi - 1)^2\phi^2 \qquad (4)$$

and the constant parameters were fixed as α=10 and β=1.

A square domain of 128 x 128 size was used to simulate the formulation. The grid spacing was kept unity on both the axes. Second-order finite central difference methods were used to compute the derivaties.

Three average concentrations were considered to simulate the formulation and compare the results of each formulation. For each concentration the initial phase field used was a random perturbation with a magnitude of ±0.01. For each concentration, three separate simulations were performed to compare the results. All the simulations were performed for t=0 to t=500 time. The time step used was $dt=2\times10^{-3}$. Thus total 250,000 simulations were performed per simulation.

For each simulation, three plots were generated. The evolution of the phase field variable was plotted and compared for different times t=0, 4, 10, 50, 200, 500. Thus each phase field variable plot includes 6 sub-plots showing the decomposition of the two-dimensional domain. Further, in the second plot, interfacial energy, mixing energy and total energy as function of time were plotted. This plot was used to study the decrease rate of the energy. In the third plot, characteristic length as a function of time was generated. Similar to second plot, the third plot was used to study the increase rates of the characteristic lengths.

MATLAB code was developed to simulate and plot the results. The code is included in the Appendix.

Cahn-Hilliard Formulation:

The Cahn-Hilliard equation is the equation that describes the process of phase separation. In Eq. 1, the total energy was defined. This total energy comprises of mixing energy and interfacial energy. Mixing energy is already defined by Eq. 4 and is denoted by $g(\phi)$. The remaining term in the Eq. 1 is called Interfacial Energy. The motion of the interface is governed by the free energy density function, $f(\phi, \nabla\phi)$. By applying the Taylor Series expansion to this function and simplifying yields Eq. 1. In Eq. 1, the concentration ϕ is a conserved value. Thus, it varies according to Fick's Law

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot J$$

where J is the flux. This flux is assumed to be from regions of high energy potential to low with some motility M.

$$J = -M\nabla\mu$$

Thus we get the Cahn-Hilliard Equation given as

$$\frac{\partial \phi}{\partial t} = \nabla \cdot (M\nabla\mu) = \nabla \cdot (M\nabla(\tilde{f}'(\phi) - \alpha\nabla^2\phi))$$

This is a fourth order, non-linear partial differential equation and M controls the anisotropic motility and the overall speed of the evolution. The parameter α controls the width of the transition zone.

Simulation Results:

For each simulation, the value of phase field variable was distributed randomly over the grid nodes by keeping the magnitude ±0.01 with respect to the average concentration, As the values are randomly distributed, three simulations were carried out for each concentration value to see if the results achieved are uniform and reliable. Thus, total 9 simulations were carried out. Each simulation was performed from time t=0 to t=500. The time step was maintained at $dt=2x10^{-3}$. As discussed earlier, the Cahn-Hilliard formulation leads to an equation which is fourth order non-linear PDE. To solve this PDE, second order central difference scheme was utilized. This can be referred in the Appendix. From each simulation, the phase field variable plot was generated to study the evolution of the domain. The energy decomposition and characteristic length increase were studied and compared with other average concentrations. Below are the results obtained from the simulations and discussion.

Average Concentration ϕ=0.3, Simulation 1:

Initially, the average concentration was taken as 0.3. As mentioned earlier, the magnitude of ±0.01 was used to distribute the random values over the square domain. Thus, the minimum value allotted was 0.29 and the maximum value was 0.31. The plot for phase field variable was generated at 6 different time value, 0, 4, 10, 50, 200, 500. The plot obtained is as in Fig. 1. It can be observed from the plot that at time t=0, the two-dimensional domain is randomly distributed with values of concentration at each node. The two domains are well mixed here. We can observe this closely with yellow and blue particles. As time progresses, we can observe that the particles (yellow) have started to evolve and the smaller particles are getting decomposed and the merged with larger particles. At t=4 we can see the merging of the particles. At t=10, we can observe that the particles are evolving further and increasing in size. At t=50 we can observe that gradually the number of small sized particles reducing and the bigger particles growing in number. At t=200, there are very few small particles remaining, and the larger particles are further merging to grow more. At t=500, all the smaller particles have merged or decomposed and formed in larger particles. We can see that gradually the domain which was initially well mixed has started to separate into two distinct domains. It can be observed that the domain with yellow color has coarsened over time and thus the energy is reduced. It can be observed in Fig. 2 the total energy has decreased and it can be seen from the two expected lines that the rate of decrease of energy is between $t^{1/4}$ and $t^{1/3}$. In Fig. 3 we have generated a

plot for characteristic length of the domain r_c. The characteristic length of domain is the ratio of the total area of the domain and the total interfacial length. The total area is the sum of the phase field variable. The total interfacial length is the sum of the phase field gradient magnitude. This plot was generated to study the growth rate of the interface. It is expected that the characteristic length grows at a rate between $t^{1/4}$ and $t^{1/3}$. However, in case of concentration value 0.3, the characteristic length has not increased in the expected range of rate.

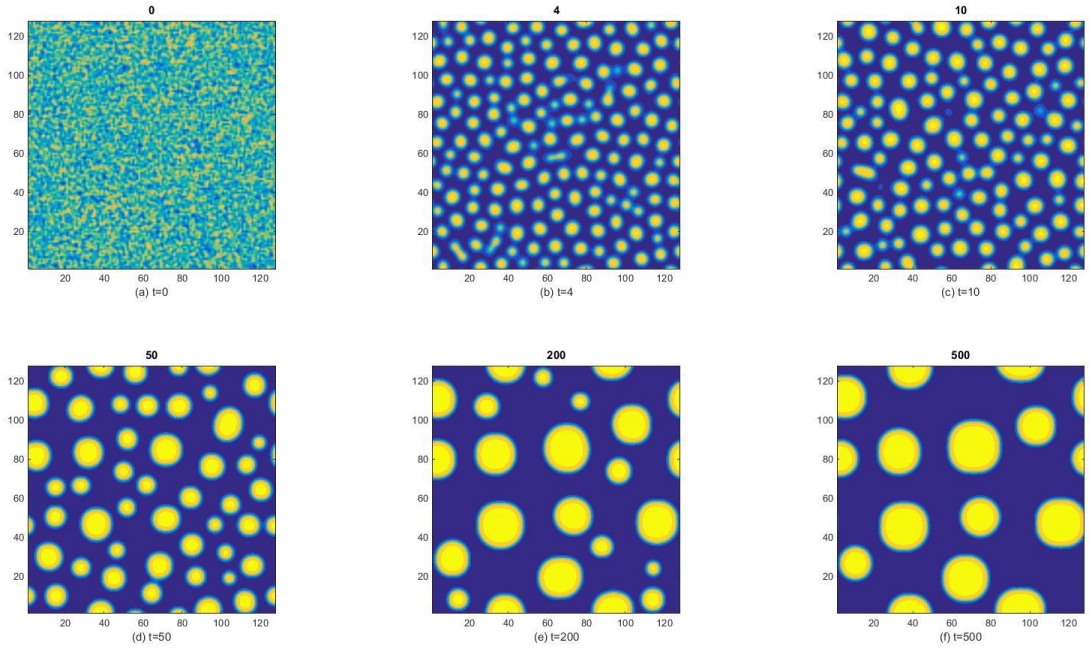

Figure 1 Simulation 1- Evolution with an average concentration of 0.3

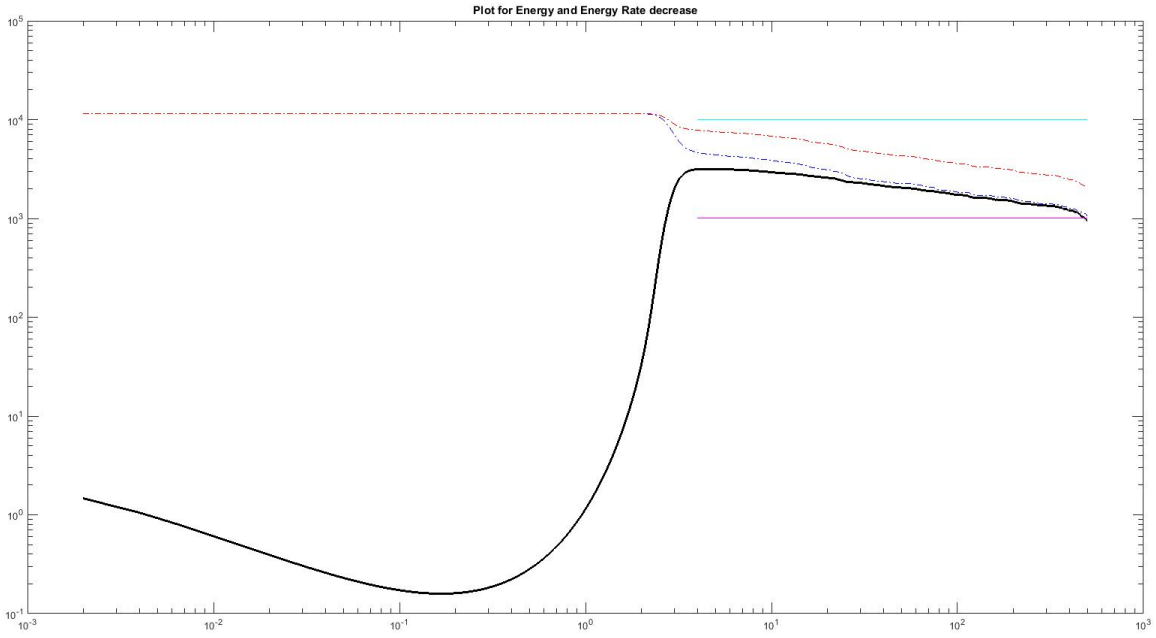

Figure 2 Simulation 1- Interfacial, Mixing and Total Energy as function of time for an average concentration of 0.3

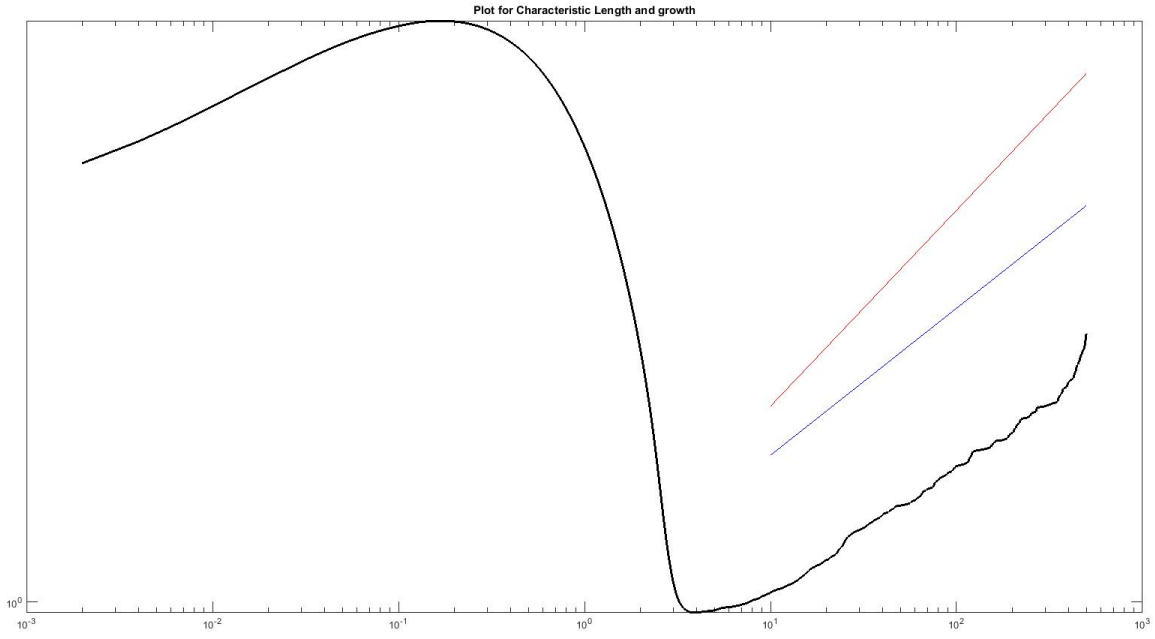

Figure 3 Simulation 1- Characteristic Length as function of time for an average concentration of 0.3

Average Concentration ϕ=0.3, Simulation 2:

With keeping the same parameters as in Case 1, same simulation was performed again and same plots were generated. As seen from Fig. 4, the domains are well mixed at t=0. As time advances, at t=4 we can observe that the domains have started separating with the particles growing in size and merging together. Similar to Simulation 1, as time advance the particles grow in size and the interface evolves coarsening one domain and separating it from the other. At t=500, we observe similar phenomenon as in Simulation 1 that the small particles have coarsened and larger particles are formed. In Fig. 5 we can again observe that the energy decreases at a rate between $t^{1/4}$ and $t^{1/3}$. Similar increase rate is observed for characteristic length from Fig. 6.

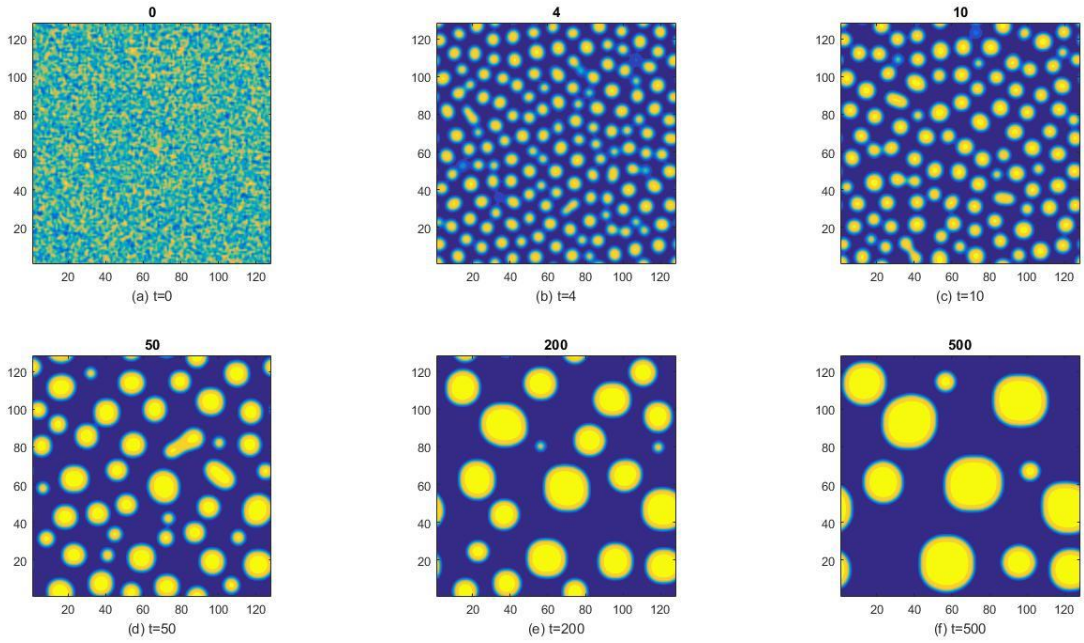

Figure 4 Simulation 2- Evolution with an average concentration of 0.3

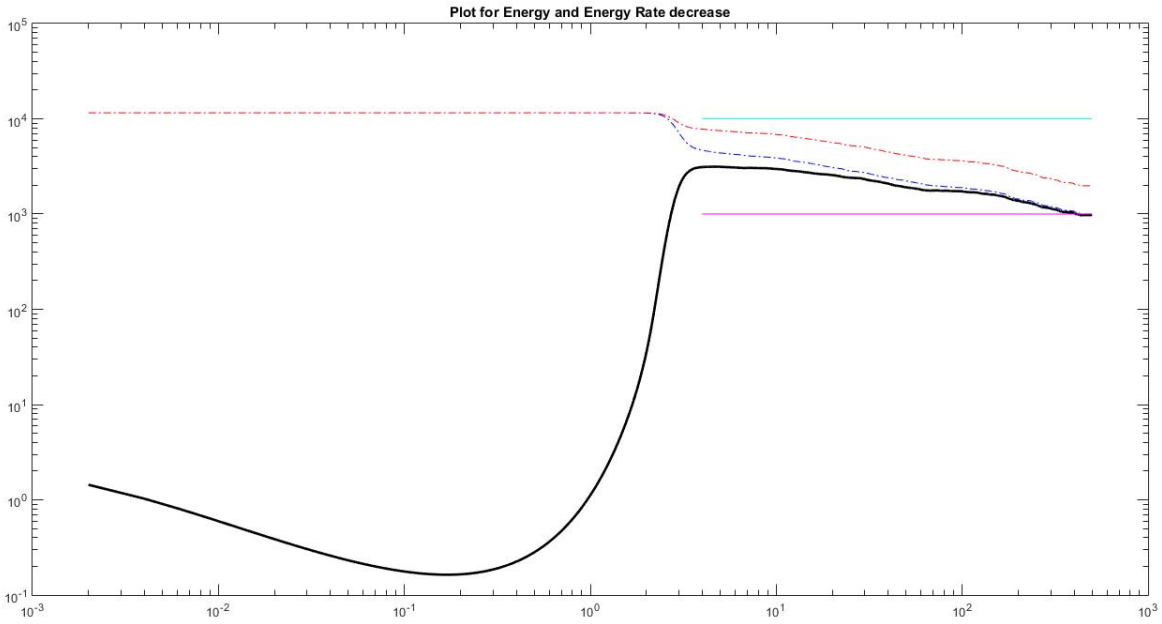

Figure 5 Simulation 2- Interfacial, Mixing and Total Energy as function of time for an average concentration of 0.3

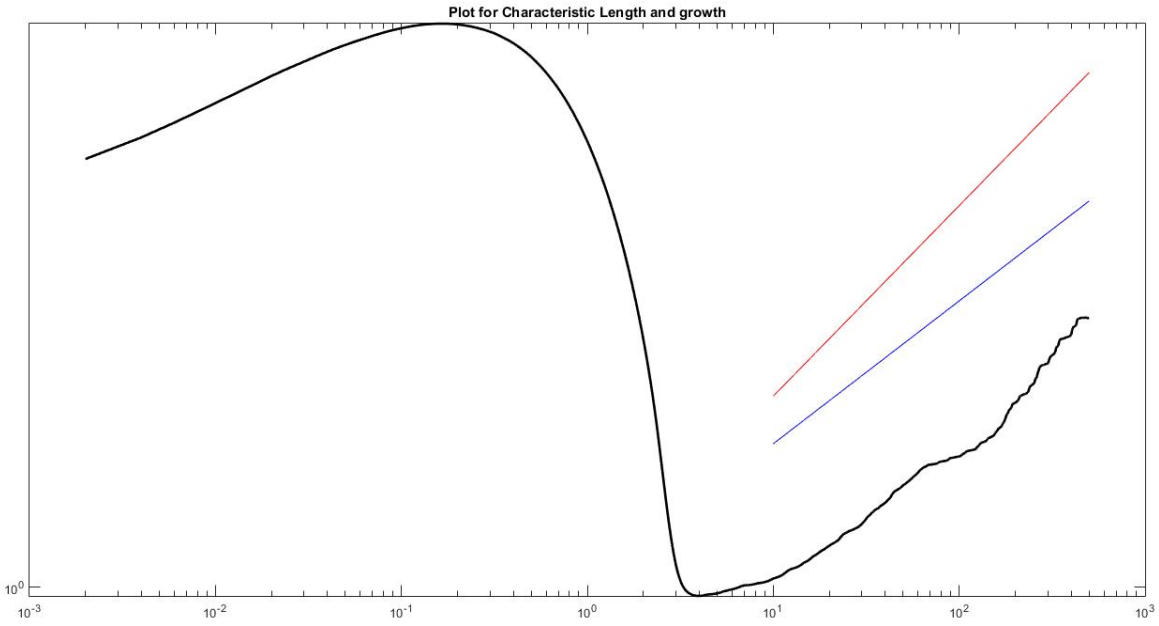

Figure 6 Simulation 2- Characteristic Length as function of time for an average concentration of 0.3

Average Concentration ϕ=0.3, Simulation 3:

As in simulation 1 and 2, simulation 3 was performed with same parameters. Results obtained are as in Fig. 7-9. It can be observed from these plots that the results are similar to that in case of Simulation 1 and 2.

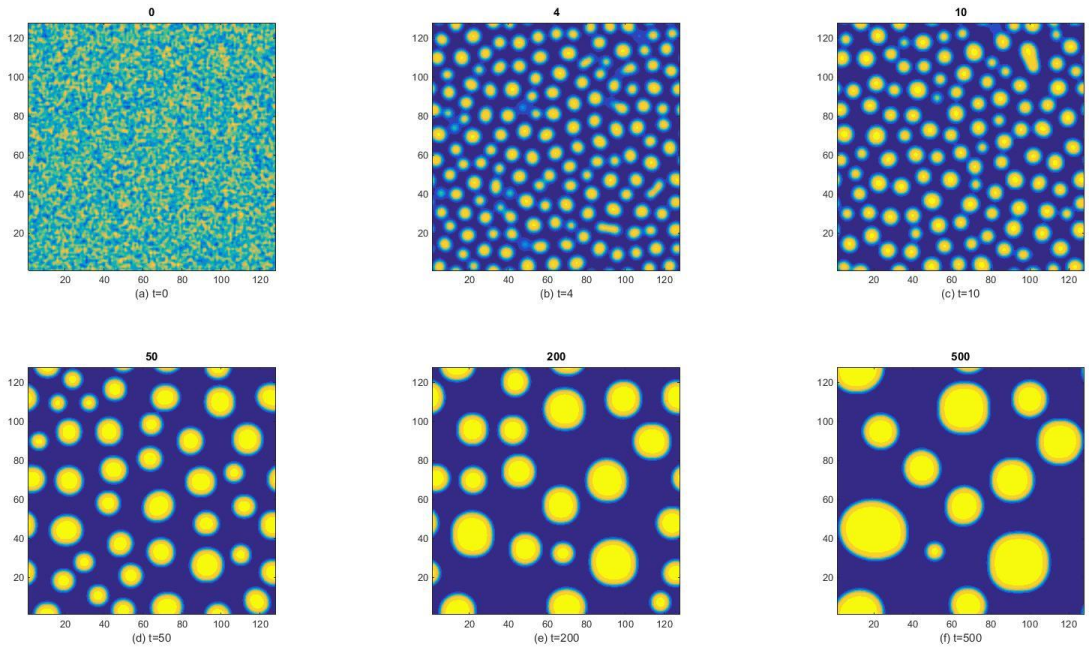

Figure 7 Simulation 3- Evolution with an average concentration of 0.3

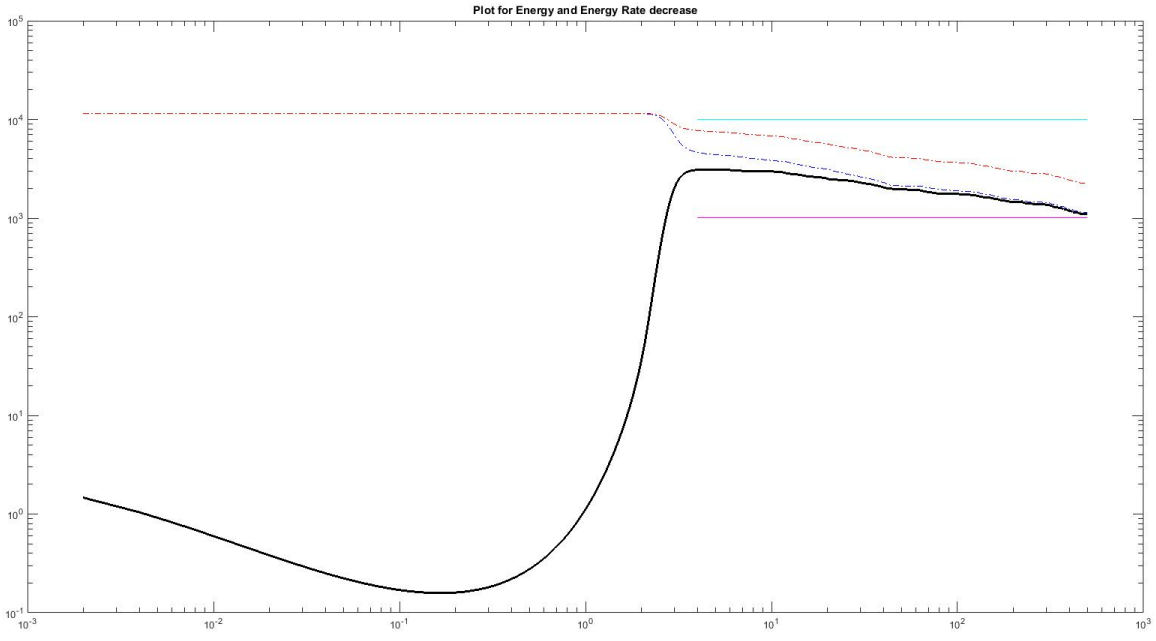

Figure 8 Simulation 3- Interfacial, Mixing and Total Energy as function of time for an average concentration of 0.3

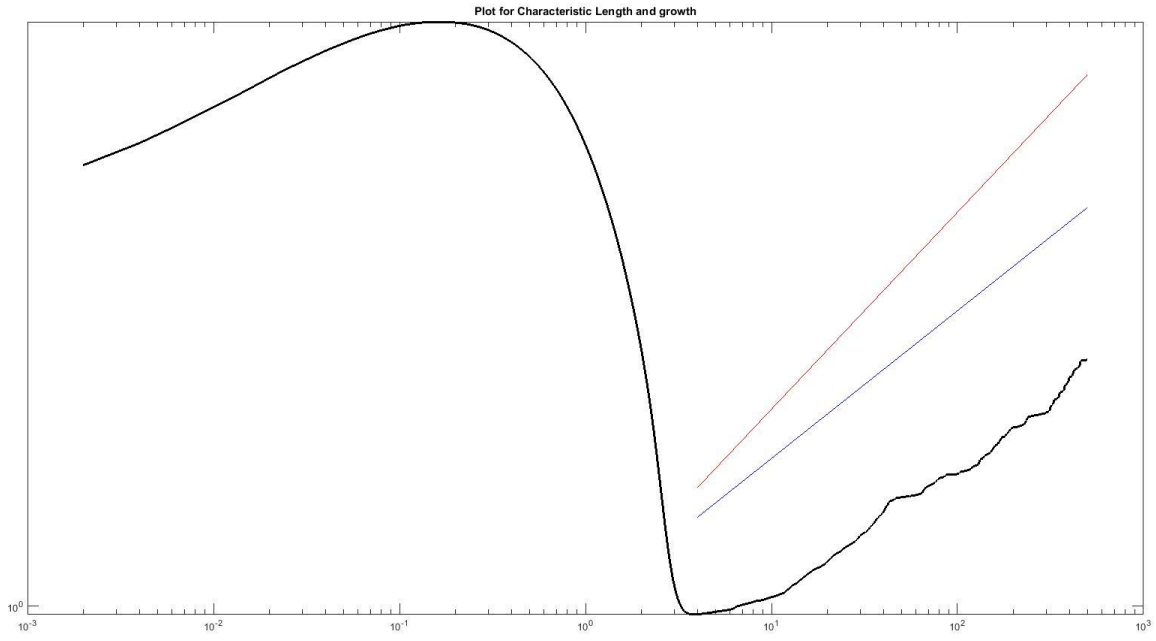

Figure 9 Simulation 3- Characteristic Length as function of time for an average concentration of 0.3

Average Concentration ϕ=0.5, Simulation 1:

Now the average value of concentration is changed from 0.3 to 0.5. As the magnitude value is ±0.01, the domain is distributed with random values between 0.49 and 0.51. Similar to Case 1, again 3 plots were generated for each simulation for Phase field variable, energy and characteristic lengths. The phase field evolution was plotted at t=0, 4, 10, 50, 200, 500. It can be observed in Fig. 10 that the domains are well mixed at t=0. As time advances, the domain starts to evolve and start separating from each other. Unlike in Case 1, here the yellow color domain does not evolve in particles. Rather it evolves with merging with all the surrounding particles and forming a surface. This grows as time advances and the particles which are not merged merge with smaller particles as can be seen at t=200 and t=500. Thus, here the domains separate in a different way as compared to Case 1 with average concentration of 0.3. From Fig. 11 we can observe that energy decreases at the rate between $t^{1/4}$ and $t^{1/3}$ as in Case 1. However, in Fig. 12 we can see that now the characteristic length has a growth rate which is between $t^{1/4}$ and $t^{1/3}$.

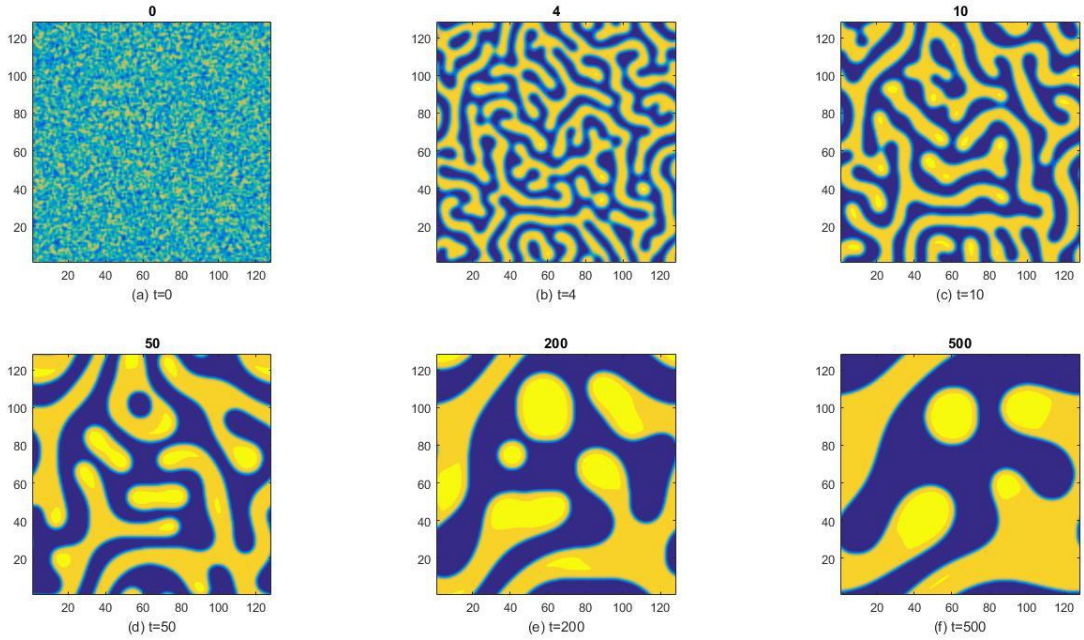

Figure 10 Simulation 1- Evolution with an average concentration of 0.5

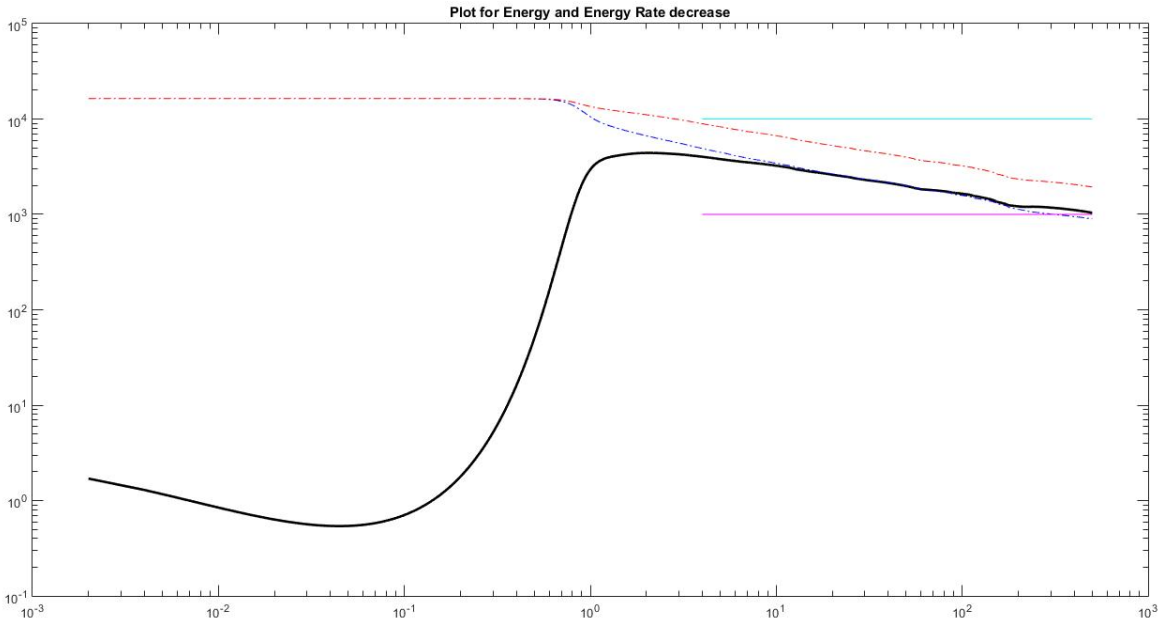

Figure 11 Simulation 1- Interfacial, Mixing and Total Energy as function of time for an average concentration of 0.5

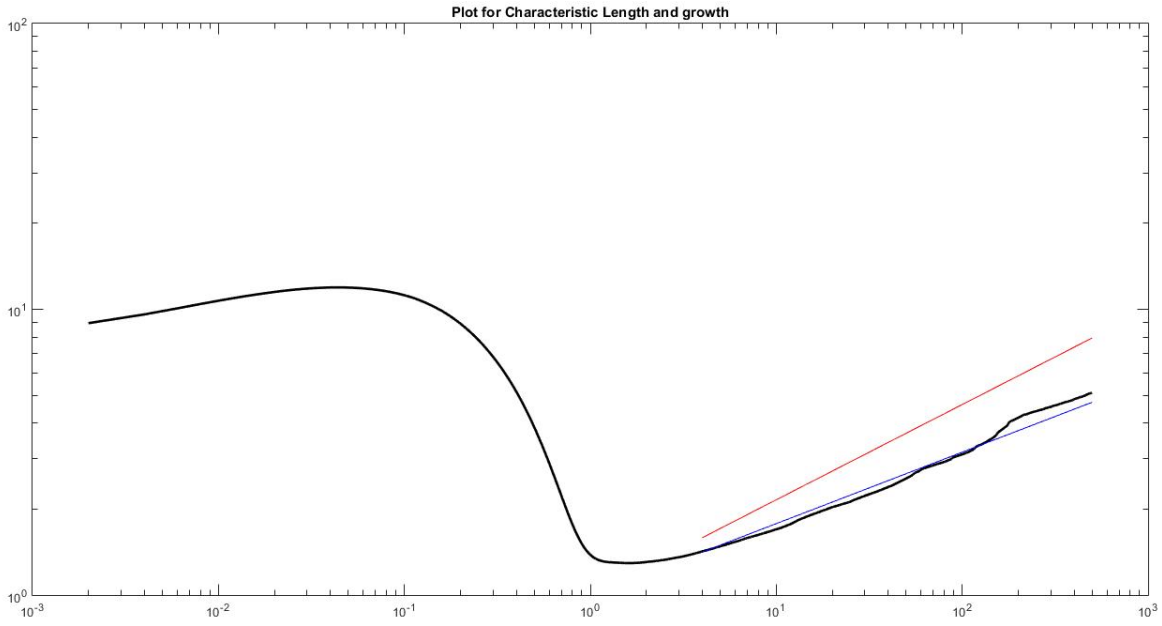

Figure 12 Simulation 1- Characteristic Length as function of time for an average concentration of 0.5

Average Concentration ϕ=0.5, Simulation 2 and 3:

Now similar to Case 1 with an average concentration of 0.3, we have performed 3 simulations in case 2 with a n average concentration of 0.5. The same 3 plots were generated in all 3 simulations for case 2. These results are shown in Fig. 13-18. It can be seen from these figures that the domains behave similar to Simulation 1 above. The domains get separated from each other by forming surfaces and the small particles which do not merge initially, merge with the larger surfaces as time advances. Ultimately, the domain separates as the interface

coarsens and decomposes. Thus the energy decreases and it can be seen that the decrease rate is in between $t^{1/4}$ and $t^{1/3}$. It is also observed that the characteristic length decreases at a rate between $t^{1/4}$ and $t^{1/3}$.

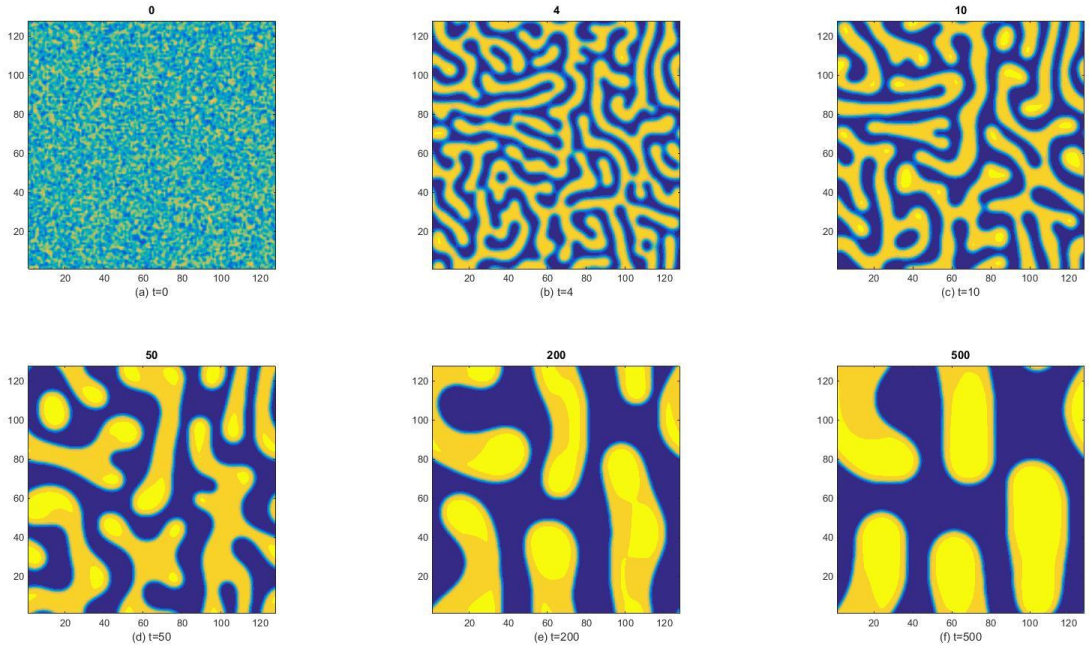

Figure 13 Simulation 2- Evolution with an average concentration of 0.5

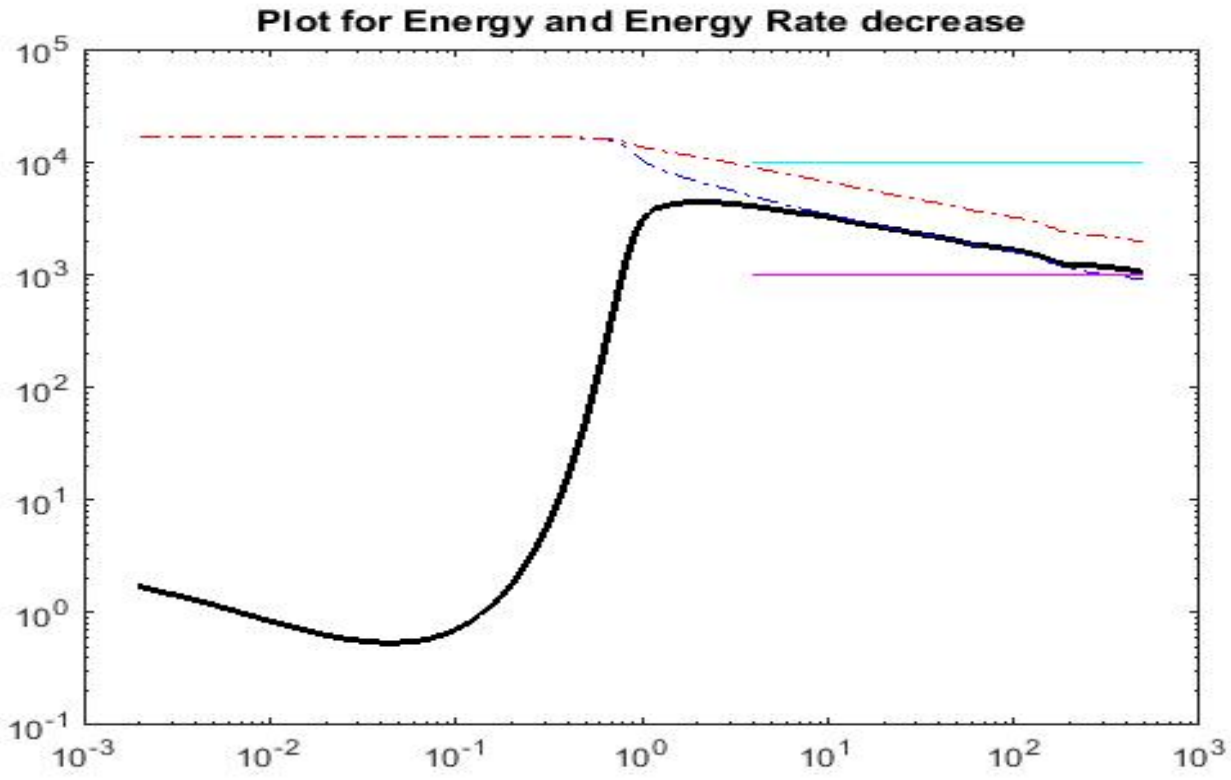

Figure 14 Simulation 2- Interfacial, Mixing and Total Energy as function of time for an average concentration of 0.5

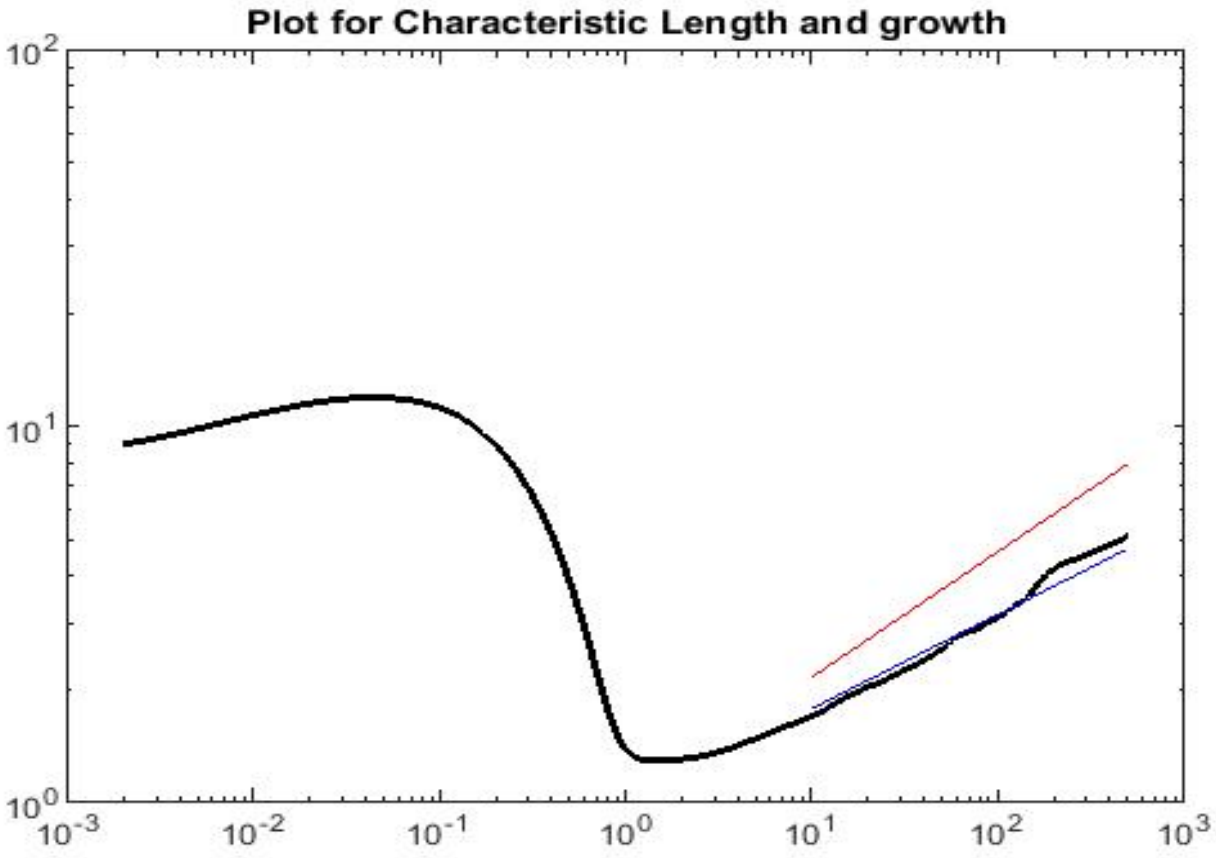

Figure 15 Simulation 2- Characteristic Length as function of time for an average concentration of 0.5

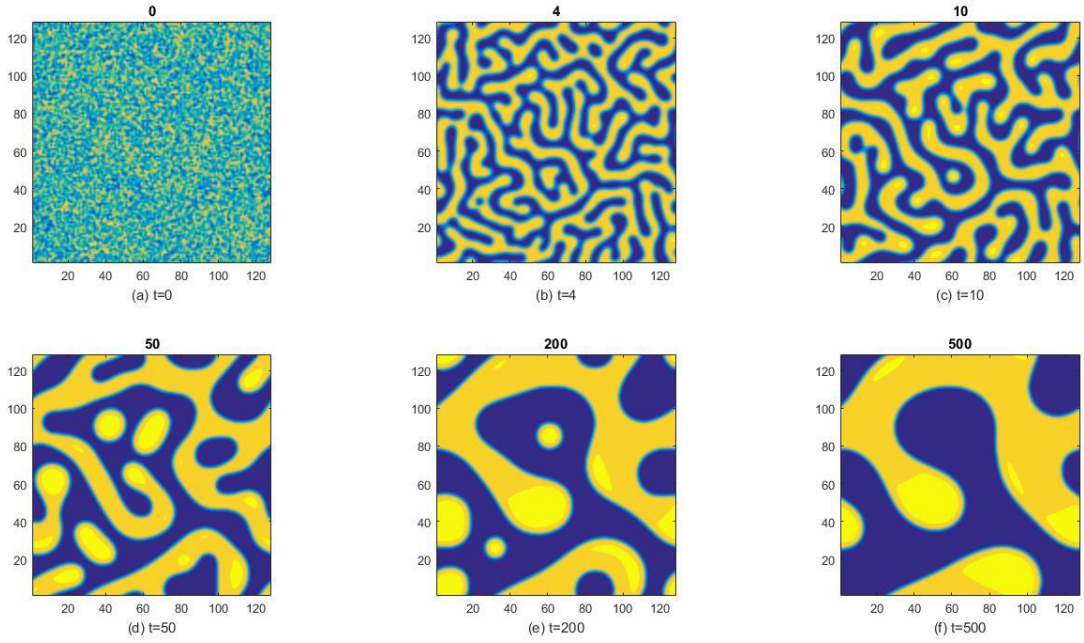

Figure 16 Simulation 3- Evolution with an average concentration of 0.5

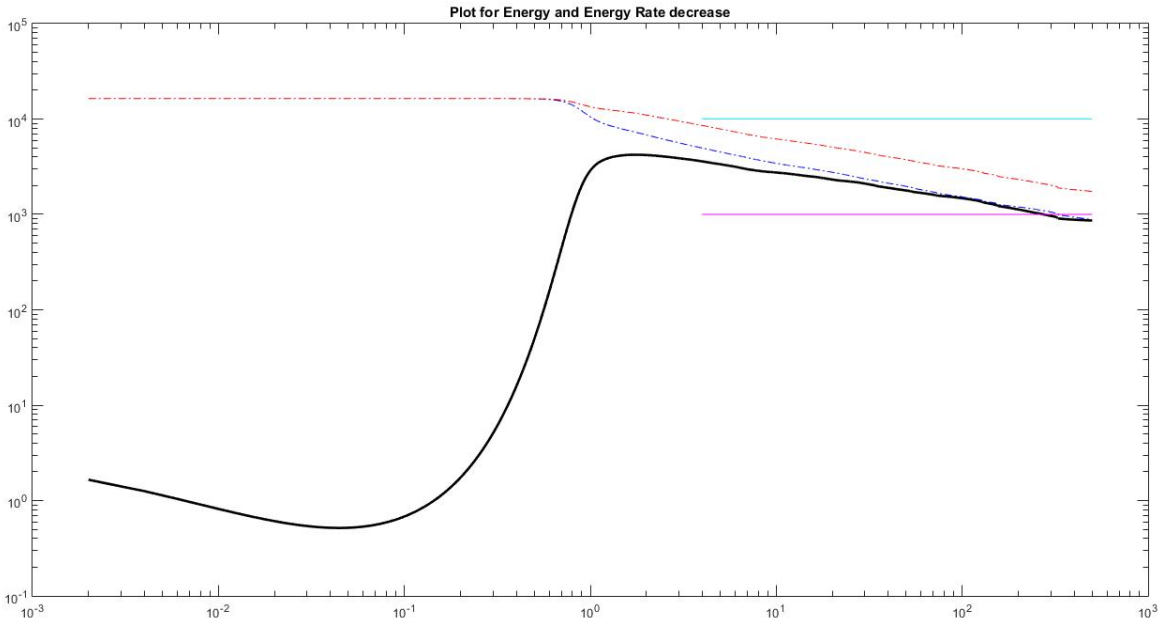

Figure 17 Simulation 3- Interfacial, Mixing and Total Energy as function of time for an average concentration of 0.5

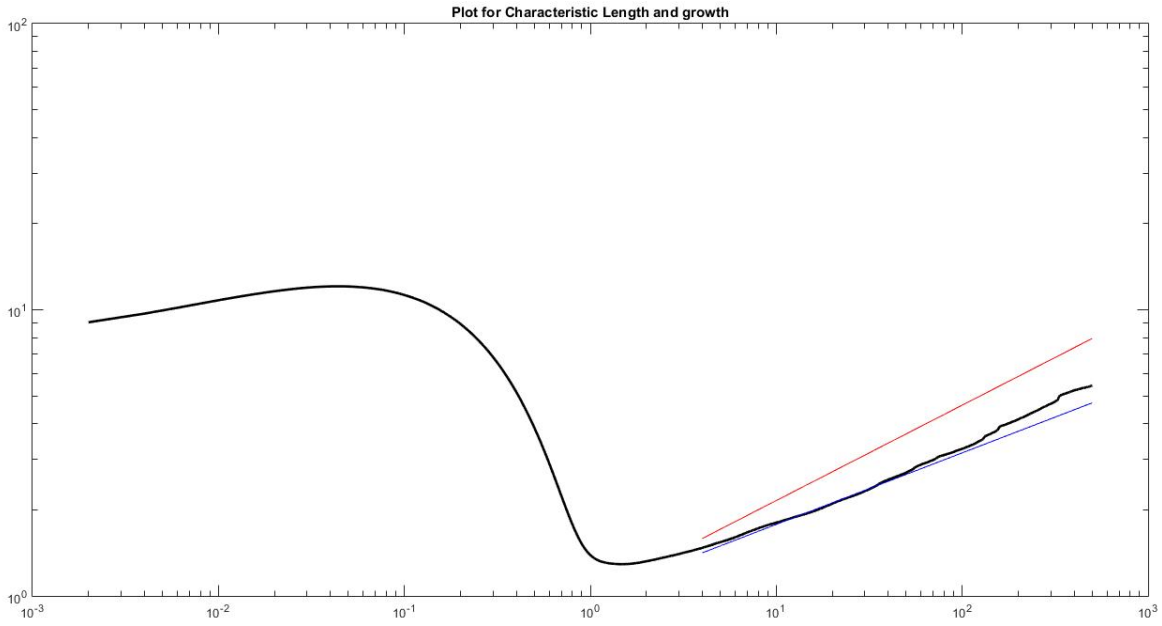

Figure 18 Simulation 3- Characteristic Length as function of time for an average concentration of 0.5

We can see that the domain separation is faster in case of average concentration 0.5 as compared to concentration 0.3.

Average Concentration ϕ=0.7, Simulation 1, 2 and 3:

This is Case 3 of the problem. In this case, the value of average concentration is taken as 0.7. The concentration is randomly distributed over the grid with minimum value 0.69 and maximum value 0.71. Same plots were generated as in Case 1 and 2. It can be observed from Fig. 19 the both domains are well mixed at t=0. As time advances we can see that as the concentration is now increased, the domain distribution has inverted. Now we have yellow domain at the background and the blue domain is separating from the yellow domain. We can also observe from Fig. 19 that the separation is similar to the case with the average concentration 0.3. Initially, as time advances, the blue particles start merging and the smaller particles coarsening, Slowly the domain evolves with particles increasing in size and small particles decomposing. It can be observed that at t=500 the smaller particle has disappeared by merging and larger sized particles are formed. Figure 20 shows the plot for energy and we can see that in this case also the energy decreases at a rate between $t^{1/4}$ and $t^{1/3}$. Figure 21 is the plot for Characteristic length which again increases at a rate between $t^{1/4}$ and $t^{1/3}$. Similar results were plotted two more times as can be seen in Fig. 22-27. We can observe that in all 3 simulations the results are similar.

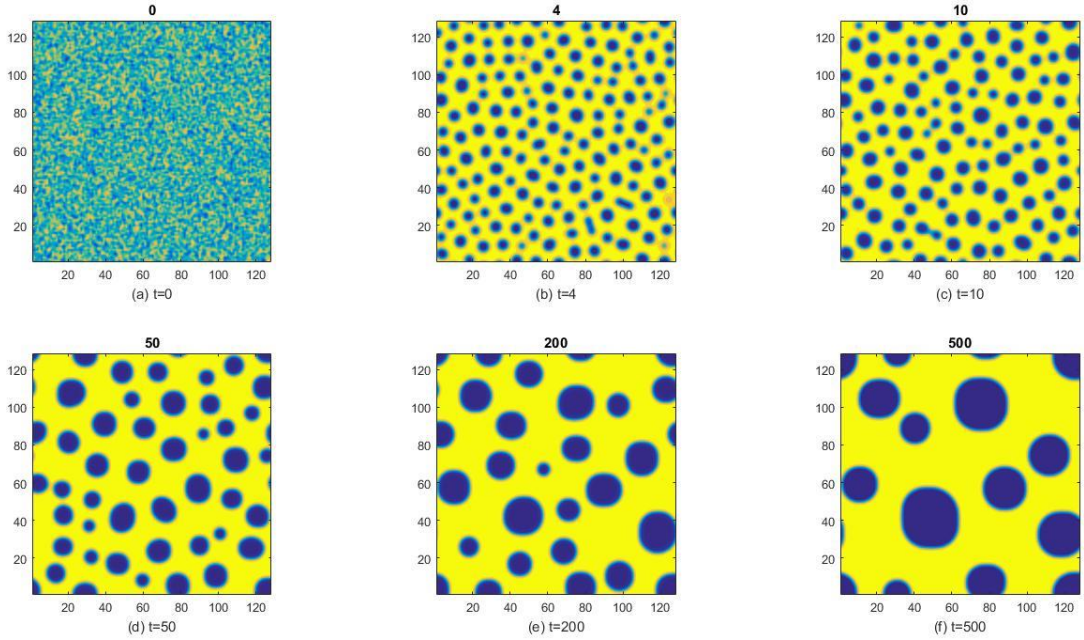

Figure 19 Simulation 1- Evolution with an average concentration of 0.7

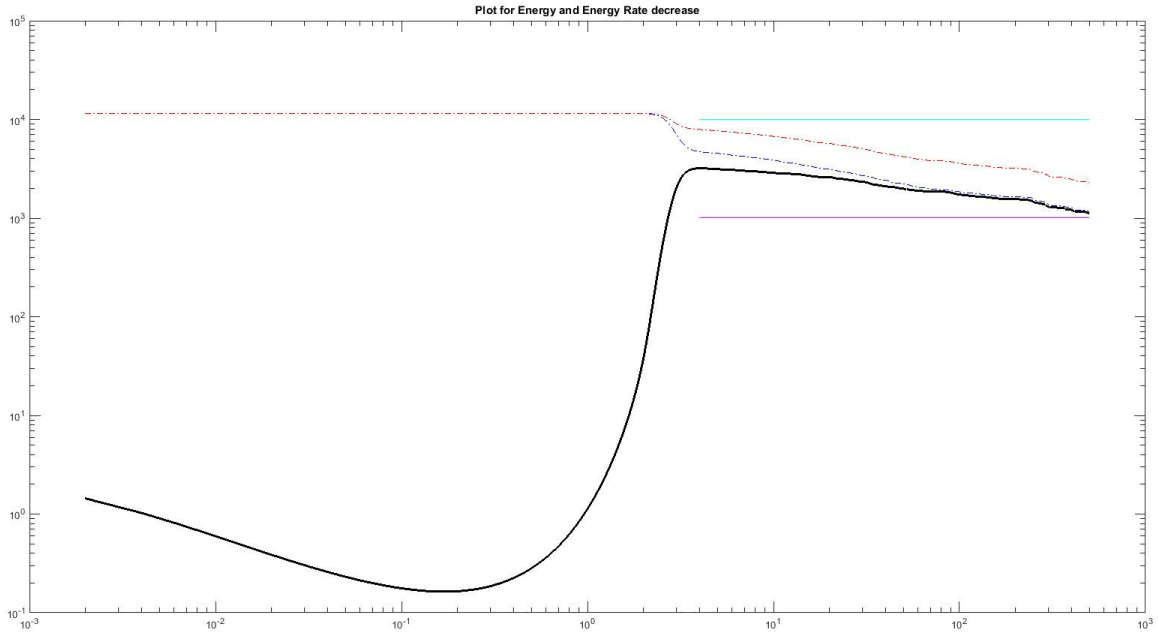

Figure 20 Simulation 1- Interfacial, Mixing and Total Energy as function of time for an average concentration of 0.7

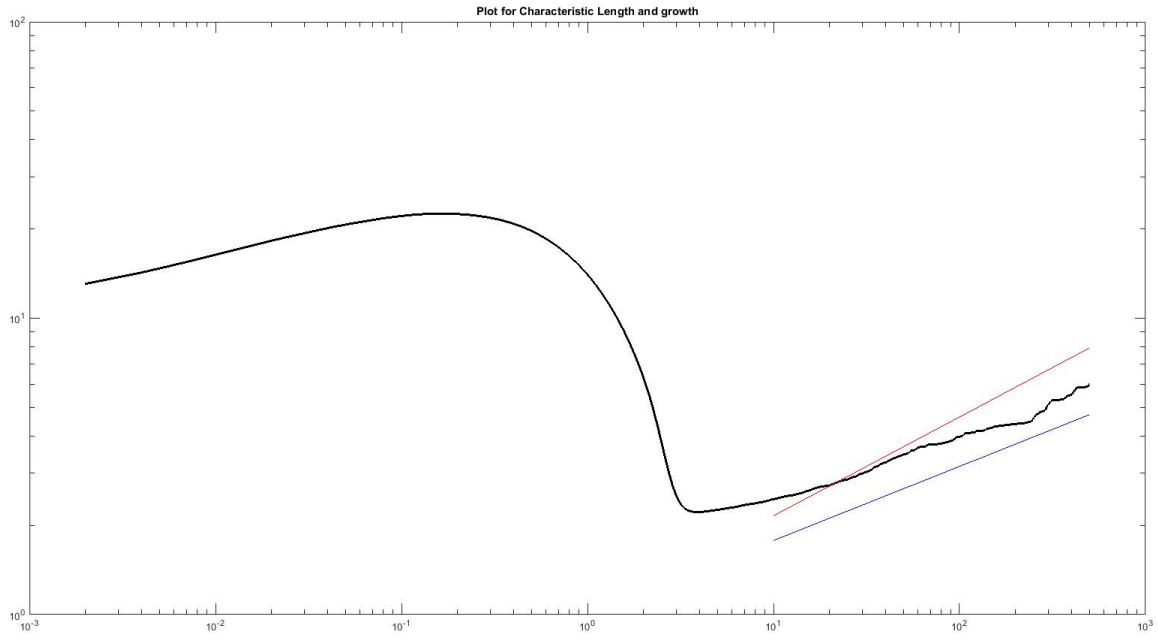

Figure 21 Simulation 1- Characteristic Length as function of time for an average concentration of 0.7

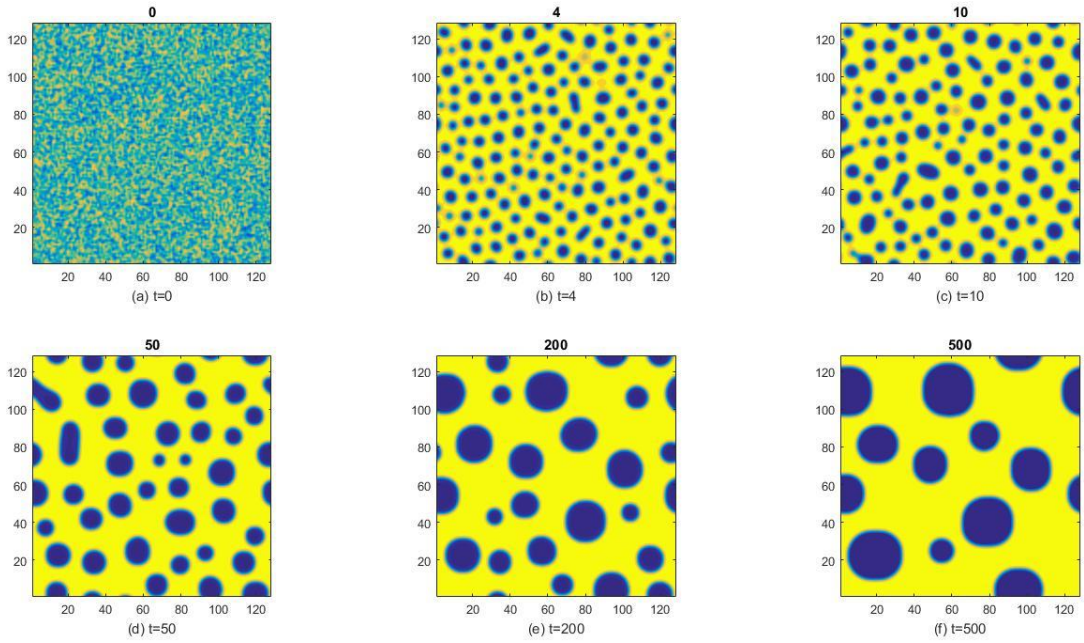

Figure 22 Simulation 2- Evolution with an average concentration of 0.7

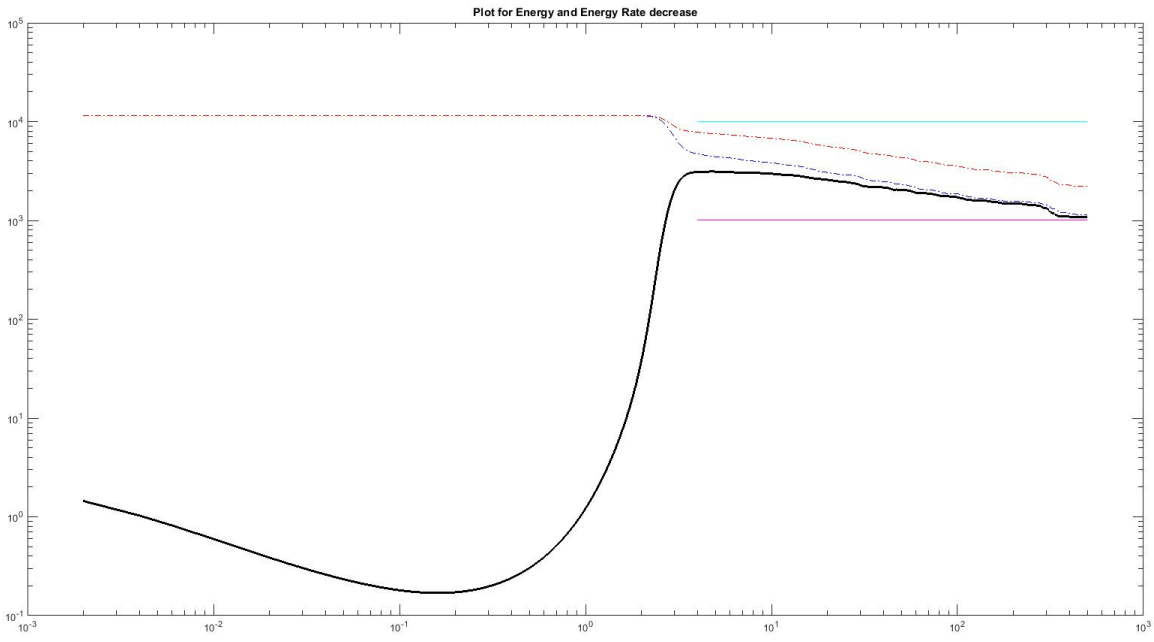

Figure 23 Simulation 2- Interfacial, Mixing and Total Energy as function of time for an average concentration of 0.7

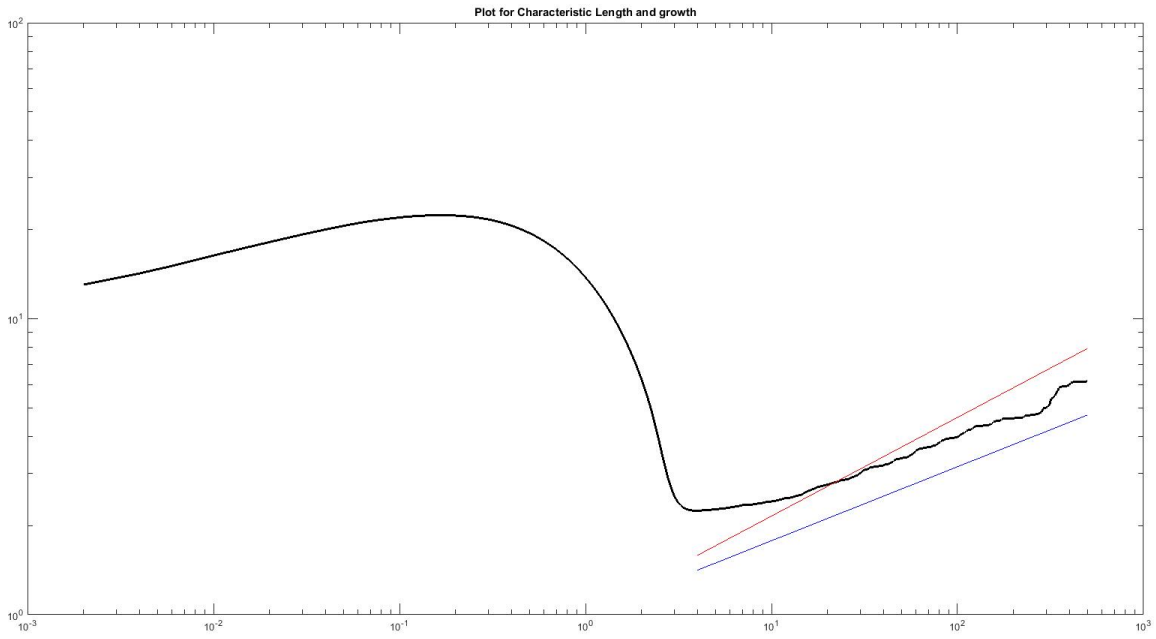

Figure 24 Simulation 2- Characteristic Length as function of time for an average concentration of 0.7

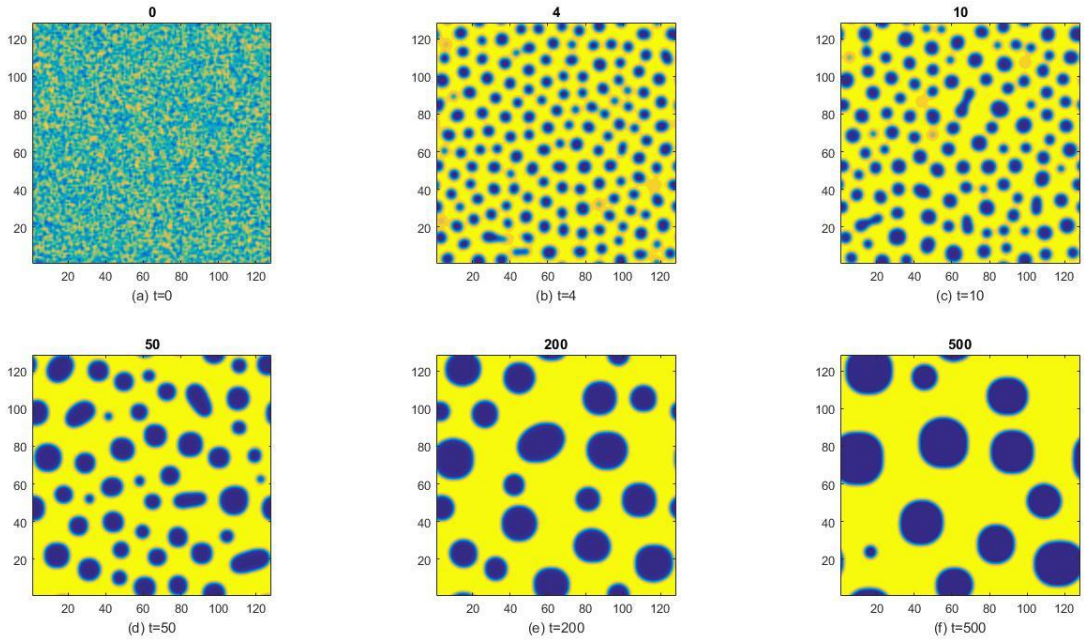

Figure 25 Simulation 3- Evolution with an average concentration of 0.7

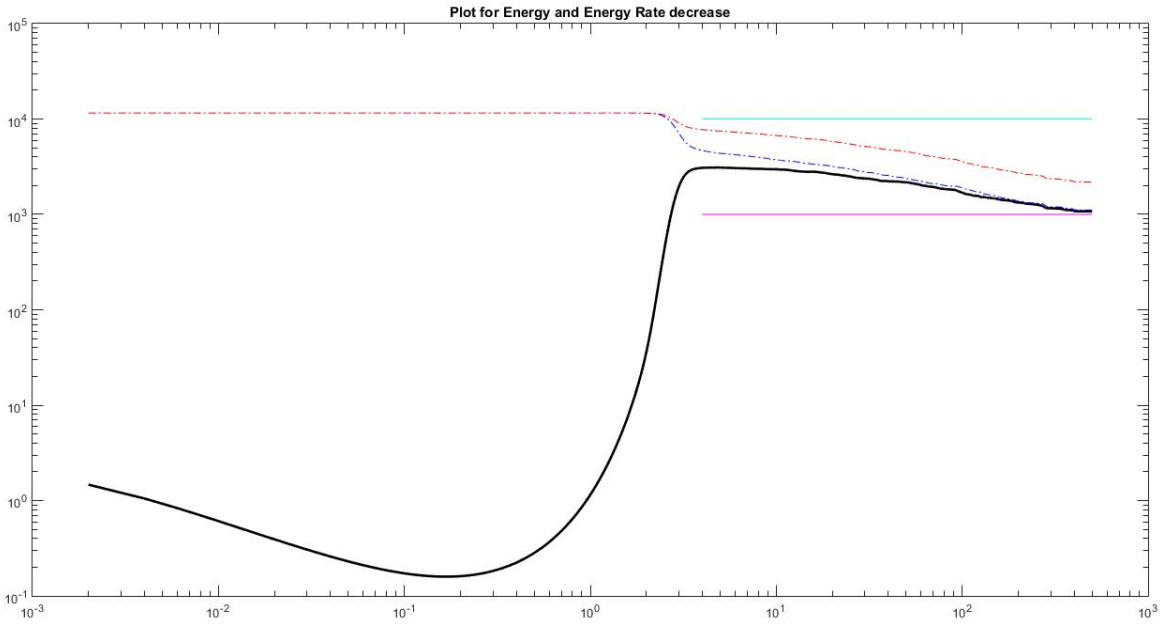

Figure 26 Simulation 3- Interfacial, Mixing and Total Energy as function of time for an average concentration of 0.7

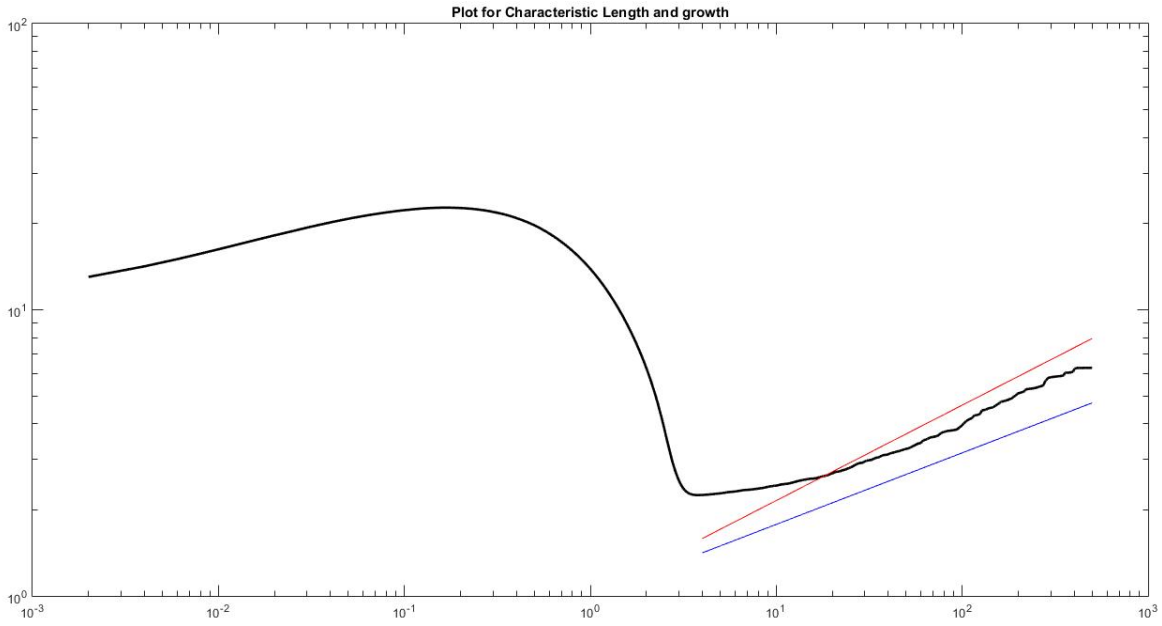

Figure 27 Simulation 3- Characteristic Length as function of time for an average concentration of 0.7

Conclusion:

Cahn-Hilliard Phase Field formulation was used to study the decomposition of a two-dimensional domain. Three average concentrations were considered to study the separation of domains from each other when they are initially well mixed. The simulations were run from t=0 to t=500 with a time step of $dt=2x10^{-3}$. 9 such simulations were performed with 3 each per average concentration value. The values of average concentration were taken as 0.3, 0.5 and 0.7. The magnitude of these concentrations was ±0.1. The domain was square with size range $[1, 128]^2$.

The grid spacing was unity in both directions. Second-order central finite difference method was used to formulate the solution. The phase field variable was plotted at 6 different times to study its evolution and separation of the two well mixed domains. It is observed that the domain coarsens thus decreasing the energy at a rate between $t^{1/4}$ and $t^{1/3}$. It is also observed that the characteristic length of the domain increases at a rate between $t^{1/4}$ and $t^{1/3}$. The source code to simulate the formulation was developed in MATLAB and is attached in the Appendix.

References:

1. Class Notes by Dr. Salac
2. Printed Notes by Dr. Salac.
3. http://www.mathworks.com/help/matlab/

Appendix:

MATLAB Source Code:

```
clear all; close all; clc;
imax=128; jmax=128;
hx=1; hy=1;
dx=hx; dy=hy;
a=10; b=1;
dt=2*10^-3;
tmax=500;
t=tmax/dt;
m=0:dt:tmax-dt;
%Initialization
phi=[0.49,0.51];
phi=(phi(2)-phi(1)).*rand(128,128)+phi(1);
% mesh(phi); contour(phi);

%Running the simulation
for k=1:t;

    %Finding out the Laplacians of phi
    for j=1:jmax
        for i=2:imax-1
            d2phi_x(i,j)=(phi(i+1,j)-2*phi(i,j)+phi(i-1,j))/dx^2;
        end
        d2phi_x(1,j)=(phi(2,j)-2*phi(1,j)+phi(imax,j))/(dx^2);
        d2phi_x(imax,j)=(phi(1,j)-2*phi(imax,j)+phi(imax-1,j))/dx^2;
    end

    for i=1:imax
        for j=2:jmax-1
            d2phi_y(i,j)=(phi(i,j+1)-2*phi(i,j)+phi(i,j-1))/dy^2;
        end
        d2phi_y(i,1)=(phi(i,2)-2*phi(i,1)+phi(i,jmax))/dy^2;
        d2phi_y(i,jmax)=(phi(i,1)-2*phi(i,jmax)+phi(i,jmax-1))/dy^2;
    end

    %Finding out the g'(phi) values
    for j=1:jmax
        for i=1:imax
            gdashphi(i,j)=32*b*(2*phi(i,j).^3-3*phi(i,j).^2+phi(i,j));
        end
    end

    %Finding value of mu
    for j=1:jmax
        for i=1:imax
            mu(i,j)=gdashphi(i,j)-a.*(d2phi_x(i,j)+d2phi_y(i,j));
        end
    end

    %Finding laplacian of mu
    for j=1:jmax
        for i=2:imax-1
            d2mu_x(i,j)=(mu(i+1,j)-2*mu(i,j)+mu(i-1,j))/dx^2;
        end
        d2mu_x(1,j)=(mu(2,j)-2*mu(1,j)+mu(imax,j))/dx^2;
        d2mu_x(imax,j)=(mu(1,j)-2*mu(imax,j)+mu(imax-1,j))/dx^2;
```

```
end

for i=1:imax
    for j=2:jmax-1
        d2mu_y(i,j)=(mu(i,j+1)-2*mu(i,j)+mu(i,j-1))/dy^2;
    end
    d2mu_y(i,1)=(mu(i,2)-2*mu(i,1)+mu(i,jmax))/dy^2;
    d2mu_y(i,jmax)=(mu(i,1)-2*mu(i,jmax)+mu(i,jmax-1))/dy^2;
end

%Finding out the new phi values
for j=1:jmax
    for i=1:imax
        new_phi(i,j)=phi(i,j)+dt.*(d2mu_x(i,j)+d2mu_y(i,j));
    end
end

%Calculation of Interfacial energy, Mixing Energy and Total Energy

%Finding out the divergence of phi
for j=1:jmax
    for i=2:imax-1
        dphi_x(i,j)=(phi(i+1,j)-phi(i-1,j))/(2*dx);
    end
    dphi_x(1,j)=(phi(2,j)-phi(imax,j))/(2*dx);
    dphi_x(imax,j)=(phi(1,j)-phi(imax-1,j))/(2*dx);
end

for i=1:imax
    for j=2:jmax-1
        dphi_y(i,j)=(phi(i,j+1)-phi(i,j-1))/(2*dy);
    end
    dphi_y(i,1)=(phi(i,2)-phi(i,jmax))/(2*dy);
    dphi_y(i,jmax)=(phi(i,1)-phi(i,jmax-1))/(2*dy);
end

for j=1:jmax
    for i=1:imax
        div_phi(i,j)=dphi_x(i,j)+dphi_y(i,j);
    end
end
IE(k)=0; ME(k)=0; TE(k)=0; int_area(k)=0; int_length(k)=0;

for j=1:jmax
    for i=1:imax
        IE(k)=IE(k)+0.5*a.*(div_phi(i,j)*div_phi(i,j));
        ME(k)=ME(k)+16*b.*((phi(i,j)-1).^2).*(phi(i,j)).^2;
        TE(k)=TE(k)+0.5*a.*(div_phi(i,j)*div_phi(i,j))+...
            16*b.*((phi(i,j)-1).^2).*(phi(i,j)).^2;
        int_area(k)=int_area(k)+phi(i,j);
        int_length(k)=int_length(k)+abs(sqrt(div_phi(i,j)));
    end
end


%Characteristic Length
rc(k)=int_area(k)/int_length(k);

phi=new_phi;
```

```
    %Plotting the results for phase field
    figure(1);
    if k*dt==0.002
        subplot(2,3,1)
        axis square
        [hC hC]=contourf(phi);
        set(hC,'LineStyle','none');
        daspect([1 1 1]);
        xlabel('(a) t=0');
        title(k*dt);
    end
    if k*dt==4
        subplot(2,3,2)
        axis square
        [hC hC]=contourf(phi);
        set(hC,'LineStyle','none');
        daspect([1 1 1]);
        xlabel('(b) t=4');
        title(k*dt);
    end
    if k*dt==10
        subplot(2,3,3)
        axis square
        [hC hC]=contourf(phi);
        set(hC,'LineStyle','none');
        daspect([1 1 1]);
        xlabel('(c) t=10');
        title(k*dt);
    end
    if k*dt==50
        subplot(2,3,4)
        axis square
        [hC hC]=contourf(phi);
        set(hC,'LineStyle','none');
        daspect([1 1 1]);
        xlabel('(d) t=50');
        title(k*dt);
    end
    if k*dt==200
        subplot(2,3,5)
        axis square
        [hC hC]=contourf(phi);
        set(hC,'LineStyle','none');
        daspect([1 1 1]);
        xlabel('(e) t=200');
        title(k*dt);
    end
    if k*dt==500
        subplot(2,3,6)
        axis square
        [hC hC]=contourf(phi);
        set(hC,'LineStyle','none');
        daspect([1 1 1]);
        xlabel('(f) t=500');
        title(k*dt);
    end
end

figure(2);
loglog(m,IE,'-k','LineWidth',2);
```

```
hold on
loglog(m,ME,'-.b');
loglog(m,TE,'-.r');
%Including t^(-1/3) and t^(-1/4) lines in the plot
q=4:dt:tmax;
t_4=(q).^(-1/4)+10000;
t_3=(q).^(-1/3)+1000;
loglog(q,t_4,'-c');
loglog(q,t_3,'m');
title('Plot for Energy and Energy Rate decrease');
hold off;

figure(3);
loglog(m,rc,'-k','LineWidth',2);
hold on
w=4:dt:tmax;
tc_4=(w).^(1/4);
tc_3=(w).^(1/3);
loglog(w,tc_4,'-b');
loglog(w,tc_3,'-r');
title('Plot for Characteristic Length and growth');
hold off;
```