Chapter 6

Ternary Cahn-Hilliard system

We consider a second-order conservative multigrid method for the ternary Cahn-Hilliard system of a model for phase separation in a ternary mixture. We prove stability of the numerical solution for a sufficiently small time step and convergence to the solution of the associated continuous problem. We perform a linear stability analysis of the system, demonstrate the second-order accuracy of the numerical scheme, and describe some numerical experiments.

6.1 Governing equations

The purpose of this chapter is to consider a conservative nonlinear multigrid method of the ternary Cahn-Hilliard (**C-H**) system for three component mixture, occupying a domain $\Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$. It is concerned with finding the vector pair $\{\mathbf{c}(\mathbf{x}, t),\ \boldsymbol{\mu}(\mathbf{x}, t)\} \in \mathbb{R}^2 \times \mathbb{R}^2$ for $\mathbf{x} \in \Omega$ and $t > 0$ solving the system of non-linear diffusion equations given by

$$\frac{\partial \mathbf{c}}{\partial t} = \nabla \cdot (M(\mathbf{c})\nabla \boldsymbol{\mu}), \quad (\mathbf{x}, t) \in \Omega \times (0, T) \tag{6.1.1}$$

$$\boldsymbol{\mu} = \mathbf{f}(\mathbf{c}) - \boldsymbol{\Gamma}\Delta\mathbf{c}, \tag{6.1.2}$$

$$\text{where } \mathbf{f}(\mathbf{c})_i = \frac{\partial F(\mathbf{c})}{\partial c_i}, \quad M(\mathbf{c}) = \sum_{i<j}^{3} c_i c_j, \tag{6.1.3}$$

$$\boldsymbol{\Gamma} = \begin{pmatrix} \epsilon_1^2 + \epsilon_3^2 & \epsilon_3^2 \\ \epsilon_3^2 & \epsilon_2^2 + \epsilon_3^2 \end{pmatrix} \in \mathbb{R}^2 \times \mathbb{R}^2$$

The typical boundary conditions for the ternary (**C-H**) system are the zero Neumann boundary conditions

$$\frac{\partial \mathbf{c}}{\partial n} = \frac{\partial \boldsymbol{\mu}}{\partial n} = \mathbf{0} \quad \text{on } \partial\Omega \times (0,T) \tag{6.1.4}$$

$$\mathbf{c}(\mathbf{x},0) = \mathbf{c}^0(\mathbf{x}) \quad \text{in } \Omega$$

We only solve equations of c_1 and c_2 since $c_1 + c_2 + c_3 = 1,$ i.e., $\mathbf{c} = (c_1, c_2),\ \boldsymbol{\mu} = (\mu_1, \mu_2).$

Two important aspects of the ternary (**C-H**) problem in the case of zero Neumann boundary conditions are the conservation of the average $\frac{1}{|\Omega|}\int_\Omega \mathbf{c}(\mathbf{x},t)d\mathbf{x}$, and the existence of a Lyapunov function $\mathcal{E}(\mathbf{c})$

$$\mathcal{E}(\mathbf{c}) = \int_\Omega \left[F(\mathbf{c}) + \sum_{i=1}^{3} \frac{\epsilon_i^2}{2} |\nabla c_i|^2 \right] d\mathbf{x} \tag{6.1.5}$$

so that

$$\frac{d}{dt}\mathcal{E}(\mathbf{c}) = -\int_\Omega |\nabla \boldsymbol{\mu}|^2 d\mathbf{x}.$$

The Cahn-Hilliard equation is a continuum model for phase separation in binary systems. An extension to this model for ideal mixtures with more than two components was proposed by Morral and Cahn [95]. And ternary numerical experiments were performed by a couple of authors [14], [37], and [51].

6.2 Numerical analysis

We shall first discretize the ternary (**C-H**) system (6.1.1) and (6.1.2) in space. Let $[a,b]$ and $[c,d]$ be partitioned by

$$a = x_{\frac{1}{2}} < x_{1+\frac{1}{2}} < \cdots < x_{N_x-1+\frac{1}{2}} < x_{N_x+\frac{1}{2}} = b,$$

$$c = y_{\frac{1}{2}} < y_{1+\frac{1}{2}} < \cdots < y_{N_x-1+\frac{1}{2}} < y_{N_y+\frac{1}{2}} = d$$

so that the cells

$$I_{ij} = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \times [y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}], \quad 1 \le i \le N_x,\ 1 \le j \le N_y$$

cover $\Omega = [a,b] \times [c,d]$. We denote

$$\Delta x_i = x_{i+\frac{1}{2}} - x_{i-\frac{1}{2}}, \qquad \Delta y_j = y_{j+\frac{1}{2}} - y_{j-\frac{1}{2}}$$

and, for simplicity, we assume the above partitions are uniform in both directions, that is

$$\Delta x_i = \Delta y_j = h \quad \text{for } 1 \le i \le N_x, \quad 1 \le j \le N_y$$

where $h = (b-a)/N_x = (d-c)/N_y$. Therefore, $x_{i+\frac{1}{2}}$ and $y_{j+\frac{1}{2}}$ can be represented as follows:

$$x_{i+\frac{1}{2}} = a + ih, \qquad y_{j+\frac{1}{2}} = c + jh.$$

We denote by $\Omega_h = \{(x_i, y_j) : 1 \le i \le N_x,\ \ 1 \le j \le N_y\}$ set of cell centered points (x_i, y_j) where

$$x_i = \frac{1}{2}(x_{i-\frac{1}{2}} + x_{i+\frac{1}{2}}), \quad y_j = \frac{1}{2}(y_{j-\frac{1}{2}} + y_{j+\frac{1}{2}}).$$

For Neumann boundary value problems, it is natural to compute numerical solutions at cell centers. Let $\mathbf{c}_{ij}$ and $\boldsymbol{\mu}_{ij}$ be approximations of $\mathbf{c}(x_i, y_j)$ and $\boldsymbol{\mu}(x_i, y_j)$. We first implement the zero Neumann boundary condition (6.1.4) by requiring that

$$D_x\mathbf{c}_{i-\frac{1}{2},j} = 0 \quad \text{for } i = 0, \qquad D_x\mathbf{c}_{i+\frac{1}{2},j} = 0 \quad \text{for } i = N_x,$$
$$D_y\mathbf{c}_{i,j-\frac{1}{2}} = 0 \quad \text{for } j = 0, \qquad D_y\mathbf{c}_{i,j+\frac{1}{2}} = 0 \quad \text{for } j = N_y,$$

where the discrete differentiation operators are

$$D_x\mathbf{c}_{i+\frac{1}{2},j} = \frac{1}{h}(\mathbf{c}_{i+1,j} - \mathbf{c}_{i,j}), \quad D_y\mathbf{c}_{i,j+\frac{1}{2}} = \frac{1}{h}(\mathbf{c}_{i,j+1} - \mathbf{c}_{i,j}).$$

We then define the discrete Laplacian by

$$\Delta_d\mathbf{c}_{ij} = \frac{1}{h}(D_x\mathbf{c}_{i+\frac{1}{2},j} - D_x\mathbf{c}_{i-\frac{1}{2},j}) + \frac{1}{h}(D_y\mathbf{c}_{i,j+\frac{1}{2}} - D_y\mathbf{c}_{i,j-\frac{1}{2}}),$$

and the discrete L^2 inner product by

$$(\mathbf{c}, \mathbf{d})_h = h^2 \sum_{i=1}^{N_x}\sum_{j=1}^{N_y}(c_{1ij}d_{1ij} + c_{2ij}d_{2ij}). \tag{6.2.6}$$

For a grid function $\mathbf{c}$ defined at cell centers, $D_x\mathbf{c}$ and $D_y\mathbf{c}$ are defined at cell-edges, and we use the following notation

$$\nabla_d^e\mathbf{c}_{ij} = (D_x\mathbf{c}_{i+\frac{1}{2},j}, D_y\mathbf{c}_{i,j+\frac{1}{2}}),$$

to represent the discrete gradient of $\mathbf{c}$. We can define an inner product for $\nabla_d^e\mathbf{c}$ on the staggered grid by

$$\begin{aligned}(\nabla_d^e\mathbf{c}, \nabla_d^e\mathbf{d})_h \quad = \quad & h^2[\sum_{i=0}^{N_x}\sum_{j=1}^{N_y}(D_xc_{1_{i+\frac{1}{2},j}}D_xd_{1_{i+\frac{1}{2},j}} + D_xc_{2_{i+\frac{1}{2},j}}D_xd_{2_{i+\frac{1}{2},j}}) \\ & + \sum_{i=1}^{N_x}\sum_{j=0}^{N_y}(D_yc_{1_{i,j+\frac{1}{2}}}D_yd_{1_{i,j+\frac{1}{2}}} + D_yc_{2_{i,j+\frac{1}{2}}}D_yd_{2_{i,j+\frac{1}{2}}})].\end{aligned} \tag{6.2.7}$$

We also define discrete norms associated with (6.2.6) and (6.2.7) as

$$\|\mathbf{c}\|^2 = (\mathbf{c}, \mathbf{c})_h, \qquad |\mathbf{c}|_{e,1}^2 = (\nabla_d^e\mathbf{c}, \nabla_d^e\mathbf{c})_e.$$

The time-continuous, space-discrete system that corresponds to (6.1.1-6.1.2) is

$$\frac{d}{dt}\mathbf{c}_{ij} = \Delta_d \boldsymbol{\mu}_{ij}, \quad \boldsymbol{\mu}_{ij} = \mathbf{f}(\mathbf{c}_{ij}) - \Gamma_\epsilon \Delta_d \mathbf{c}_{ij}, \tag{6.2.8}$$

where $\mathbf{f}(\mathbf{c}_{ij})$ is defined in (6.1.3) and boundary conditions are implemented using (6.1.4). It is easy to see that this discretization is second order accurate in space and that mass is conserved identically. The scheme also has an energy functional given by the discretization of (6.1.5). Here, we assume $\epsilon_1 = \epsilon_2 = \epsilon_3 \equiv \epsilon$ and $M(\mathbf{c}) \equiv 1$ and for simplicity, we use the following notations

$$\mathbf{f} \equiv (\frac{\partial F}{\partial c_1}, \frac{\partial F}{\partial c_2}), \quad \mathbf{f}(\mathbf{c}_{ij}^n) \equiv (\frac{\partial F}{\partial c_1}(\mathbf{c}_{ij}^n), \frac{\partial F}{\partial c_2}(\mathbf{c}_{ij}^n))$$

and

$$\mathbf{\Gamma}_\epsilon \equiv \begin{pmatrix} 2\epsilon^2 & \epsilon^2 \\ \epsilon^2 & 2\epsilon^2 \end{pmatrix} \in \mathbb{R}^2 \times \mathbb{R}^2.$$

We discretize (6.2.8) in time by the Crank-Nicholson algorithm:

$$\frac{\mathbf{c}_{ij}^{n+1} - \mathbf{c}_{ij}^n}{\Delta t} = \frac{1}{2}\Delta_d \boldsymbol{\mu}_{ij}^{n+\frac{1}{2}} \tag{6.2.9}$$

$$\boldsymbol{\mu}_{ij}^{n+\frac{1}{2}} = \frac{1}{2}(\mathbf{f}(\mathbf{c}_{ij}^{n+1}) + \mathbf{f}(\mathbf{c}_{ij}^n)) - \frac{1}{2}\mathbf{\Gamma}_\epsilon \Delta_d(\mathbf{c}_{ij}^{n+1} + \mathbf{c}_{ij}^n), \tag{6.2.10}$$

where $\mathbf{f}(\mathbf{c}) = \nabla F(\mathbf{c})$ and the free energy $F(\mathbf{c})$ is defined as follows:

$$F(\mathbf{c}) = \frac{1}{4}[c_1^2 c_2^2 + c_2^2(1 - c_1 - c_2)^2 + (1 - c_1 - c_2)^2 c_1^2].$$

2.A Stability and convergence

In this subsection, we establish mass conservation and stability estimate of a discrete energy functional. Moreover, we demonstrate the convergence of the scheme at a fixed time. Next lemma shows the mass conservation.

Lemma 6.1. *If* $\{\mathbf{c}^{n+1}, \boldsymbol{\mu}^{n+\frac{1}{2}}\}$ *is the solution of (6.2.9) Then*

$$(\mathbf{c}^{n+1}, 1)_h = (\mathbf{c}^n, 1)_h.$$

Proof. It is straightforward by using summation by parts. Indeed,

$$\begin{aligned} (\mathbf{c}^{n+1}, 1)_h &= (\mathbf{c}^n + \Delta t \Delta_d \boldsymbol{\mu}^{n+\frac{1}{2}}, 1)_h \\ &= (\mathbf{c}^n, 1)_h + (\Delta t \Delta_d \boldsymbol{\mu}^{n+\frac{1}{2}}, 1)_h = (\mathbf{c}^n, 1)_h. \end{aligned}$$

This completes the proof. □

The discrete energy functional is given by

$$\mathcal{E}(\mathbf{c}^n) = (F(\mathbf{c}^n), 1)_h + \frac{\epsilon^2}{2} \left\|\nabla_d^e \mathbf{c}^n\right\|_m^2, \tag{6.2.11}$$

where

$$\begin{aligned} \left\|\nabla_d^e \mathbf{c}^n\right\|_m^2 &= |\mathbf{c}_1^n|_{e,1}^2 + |\mathbf{c}_2^n|_{e,1}^2 + |1 - \mathbf{c}_1^n - \mathbf{c}_2^n|_{e,1}^2 \\ &= 2|\mathbf{c}_1^n|_{e,1}^2 + 2|\mathbf{c}_2^n|_{e,1}^2 + 2(\nabla_d^e \mathbf{c}_1^n, \nabla_d^e \mathbf{c}_2^n). \end{aligned}$$

Theorem 6.1. *Suppose that* $0 \le c_1^k,\ c_2^k \le 1$ *for all* k. *Under the same assumptions in Lemma 6.1, there exists an absolute constant* C *depending only on* Ω *such that if*

$$\Delta t < \frac{h^2}{2C\left\|D^2 F\right\|_{L^\infty}},$$

then

$$\mathcal{E}(\mathbf{c}^{n+1}) - \mathcal{E}(\mathbf{c}^n) \le -\Delta t|\boldsymbol{\mu}^{n+\frac{1}{2}}|_{e,1}^2 (1 - \frac{C\left\|D^2 F\right\|_{L^\infty} \Delta t}{h^2}).$$

Proof. First, multiplying $\boldsymbol{\mu}^{n+\frac{1}{2}}$ and $\mathbf{c}^{n+1} - \mathbf{c}^n$ to (6.2.9) and (6.2.10), we obtain the following two identities:

$$(\mathbf{c}^{n+1} - \mathbf{c}^n, \boldsymbol{\mu}^{n+\frac{1}{2}})_h + \Delta t|\boldsymbol{\mu}^{n+\frac{1}{2}}|_{e,1}^2 = 0, \tag{6.2.12}$$

$$(\boldsymbol{\mu}^{n+\frac{1}{2}}, \mathbf{c}^{n+1} - \mathbf{c}^n)_h = \frac{1}{2}(\mathbf{f}(\mathbf{c}^{n+1}) + \mathbf{f}(\mathbf{c}^n),\ \mathbf{c}^{n+1} - \mathbf{c}^n)_h + \frac{\epsilon^2}{2}(\left\|\nabla_d^e \mathbf{c}^{n+1}\right\|_m^2 - \left\|\nabla_d^e \mathbf{c}^n\right\|_m^2).$$

Since the first one is straightforward, the details are omitted. Thus we need to verify only the second one. Indeed,

$$\begin{aligned} (\boldsymbol{\mu}^{n+\frac{1}{2}}, \mathbf{c}^{n+1} - \mathbf{c}^n)_h &= \frac{1}{2}(\mathbf{f}(\mathbf{c}^{n+1}) + \mathbf{f}(\mathbf{c}^n) - \boldsymbol{\Gamma}_\epsilon(\Delta_d \mathbf{c}^{n+1} + \Delta_d \mathbf{c}^n), \mathbf{c}^{n+1} - \mathbf{c}^n)_h \\ &= \frac{1}{2}(\mathbf{f}(\mathbf{c}^{n+1}) + \mathbf{f}(\mathbf{c}^n),\ \mathbf{c}^{n+1} - \mathbf{c}^n)_h - \frac{1}{2}(\boldsymbol{\Gamma}_\epsilon(\Delta_d \mathbf{c}^{n+1} + \Delta_d \mathbf{c}^n), \mathbf{c}^{n+1} - \mathbf{c}^n)_h. \end{aligned}$$

The second one in the right side is calculated as follows:

$$(\boldsymbol{\Gamma}_\epsilon(\Delta_d \mathbf{c}^{n+1} + \Delta_d \mathbf{c}^n), \mathbf{c}^{n+1} - \mathbf{c}^n)$$

$$= \begin{pmatrix} 2\epsilon^2 & \epsilon^2 \\ \epsilon^2 & 2\epsilon^2 \end{pmatrix} \begin{pmatrix} \Delta_d {c_1}^{n+1} + \Delta_d {c_1}^n \\ \Delta_d {c_2}^{n+1} + \Delta_d {c_2}^n \end{pmatrix} \cdot \begin{pmatrix} {c_1}^{n+1} - {c_1}^n \\ {c_2}^{n+1} - {c_2}^n \end{pmatrix}$$

$$= -2\epsilon^2(|\mathbf{c}^{n+1}|_{e,1}^2 - |\mathbf{c}^n|_{e,1}^2) - 2\epsilon^2(\nabla_d^e {c_2}^{n+1}, \nabla_d^e {c_1}^{n+1}) + 2\epsilon^2(\nabla_d^e {c_2}^n, \nabla_d^e {c_1}^n)$$

$$= -2\epsilon^2(|\mathbf{c}^{n+1}|_{e,1}^2 + (\nabla_d^e {c_2}^{n+1}, \nabla_d^e {c_1}^{n+1})) + 2\epsilon^2(|\mathbf{c}^n|_{e,1}^2 + (\nabla_d^e {c_2}^n, \nabla_d^e {c_1}^n)).$$

This completes the second assertion above. Next, using our scheme (6.2.9) and (6.2.10), we also have the following estimates.

$$\left\|\mathbf{c}^{n+1}-\mathbf{c}^n\right\|^2 \leq \frac{C|\Delta t|^2}{h^2}|\boldsymbol{\mu}^{n+\frac{1}{2}}|_{e,1}^2 \tag{6.2.13}$$

$$|\mathbf{c}^{n+1}-\mathbf{c}^n|_{e,1}^2 \leq \frac{C|\Delta t|^2}{h^4}|\boldsymbol{\mu}^{n+\frac{1}{2}}|_{e,1}^2,$$

where C depends on Ω. Indeed, multiplying $\mathbf{c}^{n+1}-\mathbf{c}^n$ to (6.2.9) and the Hölder inequality, we obtain

$$\left\|\mathbf{c}^{n+1}-\mathbf{c}^n\right\|^2 \leq \Delta t|\boldsymbol{\mu}^{n+\frac{1}{2}}|_{e,1}|\mathbf{c}^{n+1}-\mathbf{c}^n|_{e,1}.$$

On the other hand, the following inequality can be easily verified

$$|\mathbf{c}^{n+1}-\mathbf{c}^n|_{e,1}^2 \leq \frac{C}{h^2}\left\|\mathbf{c}^{n+1}-\mathbf{c}^n\right\|^2.$$

Combining the above inequalities, we get

$$\left\|\mathbf{c}^{n+1}-\mathbf{c}^n\right\| \leq \frac{C\Delta t}{h}|\boldsymbol{\mu}^{n+\frac{1}{2}}|_{e,1}.$$

The second estimate is easy consequence of first one. Indeed,

$$|\mathbf{c}^{n+1}-\mathbf{c}^n|_{e,1}^2 \leq \frac{C}{h^2}\left\|\mathbf{c}^{n+1}-\mathbf{c}^n\right\|^2 \leq \frac{C\Delta t^2}{h^4}|\boldsymbol{\mu}^{n+\frac{1}{2}}|_{e,1}^2.$$

Now we consider

$$\begin{aligned}
\mathcal{E}(\mathbf{c}^{n+1})-\mathcal{E}(\mathbf{c}^n) &= (F(\mathbf{c}^{n+1})-F(\mathbf{c}^n),1)_h+\frac{\epsilon^2}{2}(\left\|\nabla\mathbf{c}^{n+1}\right\|_m^2-\|\nabla\mathbf{c}^n\|_m^2) \\
&= (F(\mathbf{c}^{n+1})-F(\mathbf{c}^n),1)_h+(\boldsymbol{\mu}^{n+\frac{1}{2}},\mathbf{c}^{n+1}-\mathbf{c}^n)_h \\
&\quad -\frac{1}{2}(\mathbf{f}(\mathbf{c}^{n+1})+\mathbf{f}(\mathbf{c}^n),\mathbf{c}^{n+1}-\mathbf{c}^n)_h \\
&= (F(\mathbf{c}^{n+1})-F(\mathbf{c}^n),1)_h-\frac{1}{2}(\mathbf{f}(\mathbf{c}^{n+1}) \\
&\quad +\mathbf{f}(\mathbf{c}^n),\mathbf{c}^{n+1}-\mathbf{c}^n)_h-\Delta t|\nabla\boldsymbol{\mu}^{n+\frac{1}{2}}|^2,
\end{aligned}$$

where we used the identities (6.2.12) and (6.2.13). Since F is differentiable, the first term in right-side is estimated as follows:

$$F(\mathbf{c}^{n+1})-F(\mathbf{c}^n)=\frac{F(\tilde{c}_1^n,c_2^{n+1})}{\partial c_1}(c_1^{n+1}-c_1^n)+\frac{F(c_1^n,\tilde{c}_2^n)}{\partial c_2}(c_2^{n+1}-c_2^n)$$

$$=(\frac{F(\tilde{c}_1^n,c_2^{n+1})}{\partial c_1},\frac{F(c_1^n,\tilde{c}_2^n)}{\partial c_2})\cdot(\mathbf{c}^{n+1}-\mathbf{c}^n),$$

where $\tilde{c}_1^n$ and $\tilde{c}_2^n$ are numbers between c_1^n and c_1^{n+1}, and c_2^n and c_2^{n+1}, respectively. Therefore, using the identity above, we have

$$\left|(F(\mathbf{c}^{n+1})-F(\mathbf{c}^n),1)_h-\frac{1}{2}(\mathbf{f}(\mathbf{c}^{n+1})+\mathbf{f}(\mathbf{c}^n),\ \mathbf{c}^{n+1}-\mathbf{c}^n)_h\right|$$

$$\leq 2 \left\| D^2 F \right\|_{L^\infty} \left\| \mathbf{c}^{n+1} - \mathbf{c}^n \right\|^2 .$$

Putting above inequalities together, we obtain

$$\begin{aligned}
\mathcal{E}(\mathbf{c}^{n+1}) - \mathcal{E}(\mathbf{c}^n) &\leq -\Delta t |\boldsymbol{\mu}^{n+\frac{1}{2}}|_{e,1}^2 + 2 \left\| D^2 F \right\|_{L^\infty} \left\| \mathbf{c}^{n+1} - \mathbf{c}^n \right\|^2 \\
&\leq -\Delta t |\boldsymbol{\mu}^{n+\frac{1}{2}}|_{e,1}^2 + \frac{C \left\| D^2 F \right\|_{L^\infty} |\Delta t|^2}{h^2} |\boldsymbol{\mu}^{n+\frac{1}{2}}|_{e,1}^2 \\
&\leq -\Delta t |\boldsymbol{\mu}^{n+\frac{1}{2}}|_{e,1}^2 (1 - \frac{C \left\| D^2 F \right\|_{L^\infty} \Delta t}{h^2}),
\end{aligned}$$

where we used the estimate (6.2.13). If we take Δt sufficiently small such that it satisfies

$$1 - \frac{C \left\| D^2 F \right\|_{L^\infty} \Delta t}{h^2} > 0$$

(For example, we may take $\Delta t = h^2/[2C \left\| D^2 F \right\|_{L^\infty}]$), then the right side is negative. This completes the proof. □

Since discrete energy is bounded, it can be easily seen that a numeric solution $\mathbf{c}^n$ is bounded in L^2.

Next we demonstrate the convergence of the scheme at a fixed time. Let $\mathbf{C}^n = (C_1^n, C_2^n)$ and $\mathbf{c}^n = (c_1^n, c_2^n)$ be analytic and numerical solution, respectively and we denote $\mathbf{e}^n = \mathbf{C}^n - \mathbf{c}^n$. Then we have the following error estimate.

Theorem 6.2. *Suppose $\mathbf{C}^n$ is smooth. Then there exists a constant K such that the following error estimate holds:*

$$\|\mathbf{e}^n\| \leq K(h^2 + \Delta t^2). \tag{6.2.14}$$

Proof. Using the numerical scheme, we obtain

$$\begin{aligned}
\partial_t \mathbf{e}^m + \boldsymbol{\Gamma}_\epsilon \Delta_d^2 \mathbf{e}^{m+\frac{1}{2}} &= \partial_t \mathbf{u}^m + \boldsymbol{\Gamma}_\epsilon \Delta_d^2 \mathbf{u}^{m+\frac{1}{2}} - \frac{1}{2} \Delta_d (\mathbf{f}(\mathbf{c}^m) + \mathbf{f}(\mathbf{c}^{m+1})) \\
&= \mathbf{u}_t(t_{m+\frac{1}{2}}) + \boldsymbol{\Gamma}_\epsilon \Delta^2 \mathbf{u}(t_{m+\frac{1}{2}}) - \frac{1}{2} \Delta_d (\mathbf{f}(\mathbf{c}^m) + \mathbf{f}(\mathbf{c}^{m+1})) + O(h^2 + \Delta t^2) \\
&= \Delta \mathbf{f}(\mathbf{u}^{m+\frac{1}{2}}) - \frac{1}{2} \Delta_d (\mathbf{f}(\mathbf{c}^m) + \mathbf{f}(\mathbf{c}^{m+1})) + O(h^2 + \Delta t^2) \\
&= \Delta_d \mathbf{f}(\mathbf{u}^{m+\frac{1}{2}}) - \frac{1}{2} \Delta_d (\mathbf{f}(\mathbf{c}^m) + \mathbf{f}(\mathbf{c}^{m+1})) + O(h^2 + \Delta t^2) \\
&= \Delta_d \mathbf{f}(\mathbf{u}^{m+\frac{1}{2}}) - \Delta_d \mathbf{f}(\mathbf{c}^{m+\frac{1}{2}}) + \Delta_d \mathbf{f}(\mathbf{c}^{m+\frac{1}{2}}) - \frac{1}{2} \Delta_d (\mathbf{f}(\mathbf{c}^m) + \mathbf{f}(\mathbf{c}^{m+1})) \\
&\quad + O(h^2 + \Delta t^2).
\end{aligned}$$

For convenience, we denote

$$A \equiv \mathbf{f}(\mathbf{u}^{m+\frac{1}{2}}) - \mathbf{f}(\mathbf{c}^{m+\frac{1}{2}}), \quad B \equiv \mathbf{f}(\mathbf{c}^{m+\frac{1}{2}}) - \frac{1}{2} (\mathbf{f}(\mathbf{c}^m) + \mathbf{f}(\mathbf{c}^{m+1})).$$

Forming the inner product with $\mathbf{e}^{m+\frac{1}{2}}$ and using summation by parts and Young's inequality, we have

$$\begin{aligned} \frac{1}{2}\partial_t \|\mathbf{e}^m\|^2 + \epsilon^2 \left\|\Delta_d \mathbf{e}^{m+\frac{1}{2}}\right\|^2 &\leq (A, \Delta_d \mathbf{e}^{m+\frac{1}{2}})_h + (B, \Delta_d \mathbf{e}^{m+\frac{1}{2}})_h \\ &\quad + K(h^4 + \Delta t^4) + \left\|\mathbf{e}^{m+\frac{1}{2}}\right\|^2, \end{aligned} \tag{6.2.15}$$

where we used

$$\epsilon^2 \left\|\Delta_d \mathbf{e}^{m+\frac{1}{2}}\right\|^2 \leq (\mathbf{\Gamma}_\epsilon \Delta_d \mathbf{e}^{m+\frac{1}{2}}, \Delta_d \mathbf{e}^{m+\frac{1}{2}}).$$

We first consider the first term of the right side of (6.2.15). Since $\|\mathbf{u}^n\|_\infty$ and $\|\mathbf{c}^n\|_\infty$ are bounded, it can be easily seen that $|A| \leq K|\mathbf{e}^{m+\frac{1}{2}}|$. Therefore, we obtain

$$(A, \Delta_d \mathbf{e}^{m+\frac{1}{2}}) \leq K(|\mathbf{e}^{m+\frac{1}{2}}|, |\Delta_d \mathbf{e}^{m+\frac{1}{2}}|) \leq K \left\|\mathbf{e}^{m+\frac{1}{2}}\right\|^2 + \frac{\epsilon^2}{4} \left\|\Delta_d \mathbf{e}^{m+\frac{1}{2}}\right\|^2.$$

It remains to estimate the second term. With similar computations as the first term, we obtain

$$|B| \leq K|\mathbf{c}^{m+1} - \mathbf{c}^m|^2,$$

where C again depends on upper bounds of smooth and numerical solutions. Using the factorization and Young's inequality, we get

$$\begin{aligned} (B, \Delta_d \mathbf{e}^{m+\frac{1}{2}}) &\leq K\|B\|^2 + \frac{\epsilon^2}{4} \left\|\Delta_d \mathbf{e}^{m+\frac{1}{2}}\right\|^2 \\ &\leq K \left\|(\mathbf{c}^{m+1} - \mathbf{c}^m)^2\right\|^2 + \frac{\epsilon^2}{4} \left\|\Delta_d \mathbf{e}^{m+\frac{1}{2}}\right\|^2. \end{aligned}$$

Next step is to estimate $\left\|(\mathbf{c}^{m+1} - \mathbf{c}^m)^2\right\|^2$. Adding and subtracting the analytic solution, we have

$$\left\|(\mathbf{c}^{m+1} - \mathbf{c}^m)^2\right\|^2 \leq K(\left\|\mathbf{e}^{m+1} - \mathbf{e}^m\right\|^2 + \left\|(\mathbf{u}^{m+1} - \mathbf{u}^m)^2\right\|^2),$$

where the fact is again used that numeric and analytic solutions are bounded. Since analytic solution u is smooth, the second term is estimated as follows:

$$\left\|(\mathbf{u}^{m+1} - \mathbf{u}^m)^2\right\|^2 \leq K(\Delta t)^4 \|\mathbf{u}_t\|_\infty^4.$$

Summing up all estimates above, we obtain

$$(B, \Delta_d \mathbf{e}^{m+\frac{1}{2}}) \leq K \left\|\mathbf{e}^{m+1} - \mathbf{e}^m\right\|^2 + \frac{\epsilon^2}{4} \left\|\Delta_d \mathbf{e}^{m+\frac{1}{2}}\right\|^2 + K(h^4 + \Delta t^4),$$

and therefore,

$$\begin{aligned} \frac{1}{2}\partial_t \|\mathbf{e}^m\|^2 + \epsilon^2 \left\|\Delta_d \mathbf{e}^{m+\frac{1}{2}}\right\|^2 &\leq K \left\|\mathbf{e}^{m+\frac{1}{2}}\right\|^2 + \frac{\epsilon^2}{2} \left\|\Delta_d \mathbf{e}^{m+\frac{1}{2}}\right\|^2 \\ &\quad + K\left\|\mathbf{e}^{m+1} - \mathbf{e}^m\right\|^2 + K(h^4 + \Delta t^4). \end{aligned} \tag{6.2.16}$$

Subtracting $\frac{\epsilon^2}{2}\left\|\Delta_d \mathbf{e}^{m+\frac{1}{2}}\right\|^2$ and multiplying 2 to both sides in (6.2.16), we obtain

$$\begin{aligned} \partial_t \left\|\mathbf{e}^m\right\|^2 + \epsilon^2 \left\|\Delta_d \mathbf{e}^{m+\frac{1}{2}}\right\|^2 &\le K\left\|\mathbf{e}^{m+\frac{1}{2}}\right\|^2 + K\left\|\mathbf{e}^{m+1} - \mathbf{e}^m\right\|^2 \\ &\quad + K(h^4 + \Delta t^4). \end{aligned}$$

Dropping $\epsilon^2\left\|\Delta_d \mathbf{e}^{m+\frac{1}{2}}\right\|^2$ and summing up from 0 to $n-1$, we have

$$\begin{aligned} \frac{\left\|\mathbf{e}^n\right\|^2}{\Delta t} &\le \sum_{m=0}^{n-1}[K\left\|\mathbf{e}^{m+\frac{1}{2}}\right\|^2 + K\left\|\mathbf{e}^{m+1} - \mathbf{e}^m\right\|^2 + K(h^4 + \Delta t^4)] \\ &\le \sum_{m=0}^{n-1}[K\left\|\mathbf{e}^{m+1}\right\|^2 + K\left\|\mathbf{e}^m\right\|^2 + K(h^4 + \Delta t^4)] \\ &= 2K\sum_{m=0}^{n-1}\left\|\mathbf{e}^m\right\|^2 + K\left\|\mathbf{e}^n\right\|^2 + Kn(h^4 + \Delta t^4). \end{aligned}$$

Multiplying Δt to both sides and simplifying it, we obtain

$$\begin{aligned} (1 - K\Delta t)\left\|\mathbf{e}^n\right\|^2 &\le K\Delta t\sum_{m=0}^{n-1}\left\|\mathbf{e}^m\right\|^2 + K(n\Delta t)(h^4 + \Delta t^4) \\ &\le K\Delta t\sum_{m=0}^{n-1}\left\|\mathbf{e}^m\right\|^2 + KT(h^4 + \Delta t^4) \end{aligned}$$

where we used the fact that $n\Delta t \le T$. Since Δt can be chosen such that $1 - K\Delta t > 0$, according to discrete version of Gronwall's inequality, we obtain $\|\mathbf{e}^n\| \le K(h^2 + \Delta t^2)$. This completes the proof. $\square$

6.3 Solution of the system

In this section, we develop a nonlinear Full Approximation Storage (**FAS**) multigrid method to solve the nonlinear discrete system at the implicit time level. The fundamental idea of the nonlinear multigrid is analogous to the linear case. First, the errors to the solution have to be smoothed so that they can be approximated on a coarser grid. An analog of the linear defect equation is transformed to the coarse grid. The coarse grid corrections are interpolated back to the fine grid, where the errors are again smoothed. However, because the system is nonlinear formally we do not work with the errors, but rather with full approximations to the discrete solution on the coarse grid. The nonlinearity is treated using one step of Newton's iteration and a pointwise Gauss-Seidel relaxation scheme is used as the smoother in the multigrid method. See the reference text [125] for additional details and background.

3.A Smoothing operator

We discretize the ternary (**C-H**) system by Crank-Nicholson in time and a centered difference in space discretizations, and solve the resulting system of second order equations. Here, we present a 3D space discretization, 1D and 2D are straightforward. For clarity, let $c = c_1, d = c_2, \mu = \mu_1$ and $\nu = \mu_2$, then

$$\frac{c_{ijk}^{n+1} - c_{ijk}^{n}}{\Delta t} = \Delta_d \mu_{ijk}^{n+\frac{1}{2}}, \tag{6.3.17}$$

$$\begin{aligned} \mu_{ijk}^{n+\frac{1}{2}} &= \frac{1}{2}[\frac{\partial F}{\partial c}(c_{ijk}^{n+1}, d_{ijk}^{n+1}) + \frac{\partial F}{\partial c}(c_{ijk}^{n}, d_{ijk}^{n})] \\ &\quad -\frac{\epsilon_1^2 + \epsilon_3^2}{2}\Delta_d(c_{ijk}^{n+1} + c_{ijk}^{n}) - \frac{\epsilon_3^2}{2}\Delta_d(d_{ijk}^{n+1} + d_{ijk}^{n}). \end{aligned} \tag{6.3.18}$$

After applying the standard discrete Laplacian operator to (6.3.17), we get

$$\begin{gathered} \frac{c_{ijk}^{n+1}}{\Delta t} - (\frac{\mu_{i+1,jk}^{n+\frac{1}{2}} - 2\mu_{ijk}^{n+\frac{1}{2}} + \mu_{i-1,jk}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{\mu_{i,j+1,k}^{n+\frac{1}{2}} - 2\mu_{ijk}^{n+\frac{1}{2}} + \mu_{i,j-1,k}^{n+\frac{1}{2}}}{\Delta y^2} \\ + \frac{\mu_{ij,k+1}^{n+\frac{1}{2}} - 2\mu_{ijk}^{n+\frac{1}{2}} + \mu_{ij,k-1}^{n+\frac{1}{2}}}{\Delta z^2}) = \frac{c_{ijk}^{n}}{\Delta t} \end{gathered}$$

$$\begin{gathered} \frac{c_{ijk}^{n+1}}{\Delta t} + (\frac{2}{\Delta x^2} + \frac{2}{\Delta y^2} + \frac{2}{\Delta z^2})\mu_{ijk}^{n+\frac{1}{2}} = \frac{c_{ijk}^{n}}{\Delta t} \\ + \frac{\mu_{i+1,jk}^{n+\frac{1}{2}} + \mu_{i-1,jk}^{n+\frac{1}{2}}}{\Delta x^2} + \frac{\mu_{i,j+1,k}^{n+\frac{1}{2}} + \mu_{i,j-1,k}^{n+\frac{1}{2}}}{\Delta y^2} + \frac{\mu_{ij,k+1}^{n+\frac{1}{2}} + \mu_{ij,k-1}^{n+\frac{1}{2}}}{\Delta z^2}. \end{gathered}$$

After applying the standard discrete Laplacian operator to (6.3.19), we get

$$\begin{aligned} & -(\epsilon_1^2 + \epsilon_3^2)(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2})c_{ijk}^{n+1} \\ & -\epsilon_3^2(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2})d_{ijk}^{n+1} + \mu_{ijk}^{n+\frac{1}{2}} \\ = \; & \frac{1}{2}\frac{\partial F}{\partial c}(c_{ijk}^{n}, d_{ijk}^{n}) - \frac{\epsilon_1^2 + \epsilon_3^2}{2}\Delta_d c_{ijk}^{n} - \frac{\epsilon_3^2}{2}\Delta_d d_{ijk}^{n} + \frac{1}{2}\frac{\partial F}{\partial c}(c_{ijk}^{n+1}, d_{ijk}^{n+1}) \\ & -\frac{\epsilon_1^2 + \epsilon_3^2}{2\Delta x^2}(c_{i+1,jk}^{n+1} + c_{i-1,jk}^{n+1}) - \frac{\epsilon_1^2 + \epsilon_3^2}{2\Delta y^2}(c_{i,j+1,k}^{n+1} + c_{i,j-1,k}^{n+1}) \\ & -\frac{\epsilon_1^2 + \epsilon_3^2}{2\Delta z^2}(c_{ij,k+1}^{n+1} + c_{ij,k-1}^{n+1}) - \frac{\epsilon_3^2}{2\Delta x^2}(d_{i+1,jk}^{n+1} + d_{i-1,jk}^{n+1}) \\ & -\frac{\epsilon_3^2}{2\Delta y^2}(d_{i,j+1,k}^{n+1} + d_{i,j-1,k}^{n+1}) - \frac{\epsilon_3^2}{2\Delta z^2}(d_{ij,k+1}^{n+1} + d_{ij,k-1}^{n+1}). \end{aligned}$$

After linearize $\frac{\partial F}{\partial c}(c_{ijk}^{n+1}, d_{ijk}^{n+1})$ about $(c_{ijk}^{m}, d_{ijk}^{m})$, then we have

$$\begin{aligned} \frac{\partial F}{\partial c}(c_{ijk}^{n+1}, d_{ijk}^{n+1}) = \frac{\partial F}{\partial c}(c_{ijk}^{m}, d_{ijk}^{m}) + \frac{\partial^2 F}{\partial c^2}(c_{ijk}^{m}, d_{ijk}^{m})(c_{ijk}^{n+1} - c_{ijk}^{m}) \\ + \frac{\partial^2 F}{\partial c \partial d}(c_{ijk}^{m}, d_{ijk}^{m})(d_{ijk}^{n+1} - d_{ijk}^{m}). \end{aligned}$$

$$-[(\epsilon_1^2+\epsilon_3^2)(\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta z^2})+\frac{1}{2}\frac{\partial^2 F}{\partial c^2}(c_{ijk}^m,d_{ijk}^m)]c_{ijk}^{n+1}$$

$$-[\epsilon_3^2(\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta z^2})+\frac{1}{2}\frac{\partial^2 F}{\partial c\partial d}(c_{ijk}^m,d_{ijk}^m)]d_{ijk}^{n+1}+\mu_{ijk}^{n+\frac{1}{2}}$$

$$\begin{aligned}
&=\frac{1}{2}\frac{\partial F}{\partial c}(c_{ijk}^n,d_{ijk}^n)-\frac{\epsilon_1^2+\epsilon_3^2}{2}\Delta_d c_{ijk}^n-\frac{\epsilon_3^2}{2}\Delta_d d_{ijk}^n\\
&+\frac{1}{2}\frac{\partial F}{\partial c}(c_{ijk}^m,d_{ijk}^m)-\frac{1}{2}\frac{\partial^2 F}{\partial c^2}(c_{ijk}^m,d_{ijk}^m)c_{ijk}^m-\frac{1}{2}\frac{\partial^2 F}{\partial c\partial d}(c_{ijk}^m,d_{ijk}^m)d_{ijk}^m\\
&-\frac{\epsilon_1^2+\epsilon_3^2}{2\Delta x^2}(c_{i+1,jk}^{n+1}+c_{i-1,jk}^{n+1})-\frac{\epsilon_1^2+\epsilon_3^2}{2\Delta y^2}(c_{i,j+1,k}^{n+1}+c_{i,j-1,k}^{n+1})\\
&-\frac{\epsilon_1^2+\epsilon_3^2}{2\Delta z^2}(c_{ij,k+1}^{n+1}+c_{ij,k-1}^{n+1})-\frac{\epsilon_3^2}{2\Delta x^2}(d_{i+1,jk}^{n+1}+d_{i-1,jk}^{n+1})\\
&-\frac{\epsilon_3^2}{2\Delta y^2}(d_{i,j+1,k}^{n+1}+d_{i,j-1,k}^{n+1})-\frac{\epsilon_3^2}{2\Delta z^2}(d_{ij,k+1}^{n+1}+d_{ij,k-1}^{n+1}).
\end{aligned}$$

For the second equation, we have

$$\frac{d_{ijk}^{n+1}-d_{ijk}^n}{\Delta t} = \Delta_d \nu_{ijk}^{n+\frac{1}{2}} \tag{6.3.19}$$

$$\begin{aligned}
\nu_{ijk}^{n+\frac{1}{2}} &= \frac{1}{2}[\frac{\partial F}{\partial d}(c_{ijk}^{n+1},d_{ijk}^{n+1})+\frac{\partial F}{\partial d}(c_{ijk}^n,d_{ijk}^n)]\\
&-\frac{\epsilon_3^2}{2}\Delta_d(c_{ijk}^{n+1}+c_{ijk}^n)-\frac{\epsilon_2^2+\epsilon_3^2}{2}\Delta_d(d_{ijk}^{n+1}+d_{ijk}^n).
\end{aligned} \tag{6.3.20}$$

Applying the standard Laplacian operator to the equation (6.3.19), we get

$$\frac{d_{ijk}^{n+1}}{\Delta t}-(\frac{\nu_{i+1,jk}^{n+\frac{1}{2}}-2\nu_{ijk}^{n+\frac{1}{2}}+\nu_{i-1,jk}^{n+\frac{1}{2}}}{\Delta x^2}+\frac{\nu_{i,j+1,k}^{n+\frac{1}{2}}-2\nu_{ijk}^{n+\frac{1}{2}}+\nu_{i,j-1,k}^{n+\frac{1}{2}}}{\Delta y^2}$$

$$+\frac{\nu_{ij,k+1}^{n+\frac{1}{2}}-2\nu_{ijk}^{n+\frac{1}{2}}+\nu_{ij,k-1}^{n+\frac{1}{2}}}{\Delta z^2})=\frac{d_{ijk}^n}{\Delta t}$$

$$\frac{d_{ijk}^{n+1}}{\Delta t}+(\frac{2}{\Delta x^2}+\frac{2}{\Delta y^2}+\frac{2}{\Delta z^2})\nu_{ijk}^{n+\frac{1}{2}}=\frac{d_{ijk}^n}{\Delta t}$$

$$+\frac{\nu_{i+1,jk}^{n+\frac{1}{2}}+\nu_{i-1,jk}^{n+\frac{1}{2}}}{\Delta x^2}+\frac{\nu_{i,j+1,k}^{n+\frac{1}{2}}+\nu_{i,j-1,k}^{n+\frac{1}{2}}}{\Delta y^2}+\frac{\nu_{ij,k+1}^{n+\frac{1}{2}}+\nu_{ij,k-1}^{n+\frac{1}{2}}}{\Delta z^2}$$

$$
\begin{aligned}
&-\epsilon_3^2(\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta z^2})c_{ijk}^{n+1}-(\epsilon_2^2+\epsilon_3^2)(\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta z^2})d_{ijk}^{n+1}\\
&+\nu_{ijk}^{n+\frac{1}{2}}=\frac{1}{2}\frac{\partial F}{\partial d}(c_{ijk}^n,d_{ijk}^n)-\frac{\epsilon_3^2}{2}\Delta_d c_{ijk}^n-\frac{\epsilon_2^2+\epsilon_3^2}{2}\Delta_d d_{ijk}^n\\
&+\frac{1}{2}\frac{\partial F}{\partial d}(c_{ijk}^{n+1},d_{ijk}^{n+1})-\frac{\epsilon_3^2}{2\Delta x^2}(c_{i+1,jk}^{n+1}+c_{i-1,jk}^{n+1})\\
&-\frac{\epsilon_3^2}{2\Delta y^2}(c_{i,j+1,k}^{n+1}+c_{i,j-1,k}^{n+1})-\frac{\epsilon_3^2}{2\Delta z^2}(c_{ij,k+1}^{n+1}+c_{ij,k-1}^{n+1})\\
&-\frac{\epsilon_2^2+\epsilon_3^2}{2\Delta x^2}(d_{i+1,jk}^{n+1}+d_{i-1,jk}^{n+1})-\frac{\epsilon_2^2+\epsilon_3^2}{2\Delta y^2}(d_{i,j+1,k}^{n+1}+d_{i,j-1,k}^{n+1})\\
&-\frac{\epsilon_2^2+\epsilon_3^2}{2\Delta z^2}(d_{ij,k+1}^{n+1}+d_{ij,k-1}^{n+1})
\end{aligned}
$$

Finally, linearize $\frac{\partial F}{\partial d}(c_{ijk}^{n+1},d_{ijk}^{n+1})$ about (c_{ijk}^m,d_{ijk}^m) to get

$$
\begin{aligned}
\frac{\partial F}{\partial d}(c_{ijk}^{n+1},d_{ijk}^{n+1})=\frac{\partial F}{\partial d}(c_{ijk}^m,d_{ijk}^m)&+\frac{\partial^2 F}{\partial c\partial d}(c_{ijk}^m,d_{ijk}^m)(c_{ijk}^{n+1}-c_{ijk}^m)\\
&+\frac{\partial^2 F}{\partial d^2}(c_{ijk}^m,d_{ijk}^m)(d_{ijk}^{n+1}-d_{ijk}^m).
\end{aligned}
$$

$$
\begin{aligned}
&-[\epsilon_3^2(\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta z^2})+\frac{1}{2}\frac{\partial^2 F}{\partial c\partial d}(c_{ijk}^m,d_{ijk}^m)]c_{ijk}^{n+1}\\
&-[(\epsilon_2^2+\epsilon_3^2)(\frac{1}{\Delta x^2}+\frac{1}{\Delta y^2}+\frac{1}{\Delta z^2})+\frac{1}{2}\frac{\partial^2 F}{\partial d^2}(c_{ijk}^m,d_{ijk}^m)]d_{ijk}^{n+1}+\nu_{ijk}^{n+\frac{1}{2}}
\end{aligned}
$$

$$
\begin{aligned}
&=\frac{1}{2}\frac{\partial F}{\partial d}(c_{ijk}^n,d_{ijk}^n)-\frac{\epsilon_3^2}{2}\Delta_d c_{ijk}^n-\frac{\epsilon_2^2+\epsilon_3^2}{2}\Delta_d d_{ijk}^n\\
&+\frac{1}{2}\frac{\partial F}{\partial d}(c_{ijk}^m,d_{ijk}^m)-\frac{1}{2}\frac{\partial^2 F}{\partial c\partial d}(c_{ijk}^m,d_{ijk}^m)c_{ijk}^m-\frac{1}{2}\frac{\partial^2 F}{\partial d^2}(c_{ijk}^m,d_{ijk}^m)d_{ijk}^m\\
&-\frac{\epsilon_3^2}{2\Delta x^2}(c_{i+1,jk}^{n+1}+c_{i-1,jk}^{n+1})-\frac{\epsilon_3^2}{2\Delta y^2}(c_{i,j+1,k}^{n+1}+c_{i,j-1,k}^{n+1})-\frac{\epsilon_3^2}{2\Delta z^2}(c_{ij,k+1}^{n+1}+c_{ij,k-1}^{n+1})\\
&-\frac{\epsilon_2^2+\epsilon_3^2}{2\Delta x^2}(d_{i+1,jk}^{n+1}+d_{i-1,jk}^{n+1})-\frac{\epsilon_2^2+\epsilon_3^2}{2\Delta y^2}(d_{i,j+1,k}^{n+1}+d_{i,j-1,k}^{n+1})\\
&-\frac{\epsilon_2^2+\epsilon_3^2}{2\Delta z^2}(d_{ij,k+1}^{n+1}+d_{ij,k-1}^{n+1}).
\end{aligned}
$$

Let us rewrite equations (6.3.17)-(6.3.20) as follows.

$$
\mathbf{NSO}(c^{n+1},\mu^{n+\frac{1}{2}},d^{n+1},\nu^{n+\frac{1}{2}})=(g_1^n,g_2^n,g_3^n,g_4^n),
$$

where the nonlinear system operator (**NSO**) is defined as

$$\begin{aligned}\mathbf{NSO}(c^{n+1},\mu^{n+\frac{1}{2}},d^{n+1},\nu^{n+\frac{1}{2}}) &= (\frac{c_{ij}^{n+1}}{\Delta t}-\Delta\mu_{ij}^{n+\frac{1}{2}},\\ &\quad \mu_{ij}^{n+\frac{1}{2}}-\frac{1}{2}f_1(c_{ij}^{n+1},d_{ij}^{n+1})+\frac{\epsilon_1^2+\epsilon_3^2}{2}\Delta_d c_{ij}^{n+1}+\frac{\epsilon_3^2}{2}\Delta_d d_{ij}^{n+1},\\ &\quad \frac{d_{ij}^{n+1}}{\Delta t}-\Delta_d\nu_{ij}^{n+\frac{1}{2}},\\ &\quad \nu_{ij}^{n+\frac{1}{2}}-\frac{1}{2}f_2(c_{ij}^{n+1},d_{ij}^{n+1})+\frac{\epsilon_2^2+\epsilon_3^2}{2}\Delta_d d_{ij}^{n+1}+\frac{\epsilon_3^2}{2}\Delta_d c_{ij}^{n+1})\end{aligned}$$

and the source term is

$$\begin{aligned}(g_1^n,g_2^n,g_3^n,g_4^n) &= (\frac{c_{ij}^n}{\Delta t},\ \frac{1}{2}f_1(c_{ij}^n,d_{ij}^n)-\frac{\epsilon_1^2+\epsilon_3^2}{2}\Delta_d c_{ij}^n-\frac{\epsilon_3^2}{2}\Delta_d d_{ij}^n,\\ &\quad \frac{d_{ij}^n}{\Delta t},\ \frac{1}{2}f_2(c_{ij}^n,d_{ij}^n)-\frac{\epsilon_2^2+\epsilon_3^2}{2}\Delta_d d_{ij}^n-\frac{\epsilon_3^2}{2}\Delta_d c_{ij}^n).\end{aligned}$$

In the following description of one **FAS** cycle, we assume a sequence of grids Ω_k (Ω_{k-1} is coarser than Ω_k by factor 2). Given the number η of pre- and post- smoothing relaxation sweeps, an iteration step for the nonlinear multigrid method using the V-cycle is formally written as follows:

FAS multigrid cycle

Let $\{c_k^{m+1},\mu_k^{m+\frac{1}{2}},d_k^{m+1},\nu_k^{m+\frac{1}{2}}\}$

$$=FAScycle(k,c_k^m,\mu_k^{m-\frac{1}{2}},d_k^m,\nu_k^{m-\frac{1}{2}},\mathbf{NSO}_k,{g_1}_k^n,{g_2}_k^n,{g_3}_k^n,{g_4}_k^n,\eta).$$

That is, $\{c_k^m,\mu_k^{m-\frac{1}{2}},d_k^m,\nu_k^{m-\frac{1}{2}}\}$ and $\{c_k^{m+1},\mu_k^{m+\frac{1}{2}},d_k^{m+1},\nu_k^{m+\frac{1}{2}}\}$ are the approximations of $\{c_k^{n+1}(x_i,y_j),\ \mu_k^{n+\frac{1}{2}}(x_i,y_j),\ d_k^{n+1}(x_i,y_j),\ \nu_k^{n+\frac{1}{2}}(x_i,y_j)\}$ before and after an FAScycle.

Now, define the FAScycle.

(1) Presmoothing

Compute $\{\bar{c}_k^m,\ \bar{\mu}_k^{m-\frac{1}{2}},\ \bar{d}_k^m,\ \bar{\nu}_k^{m-\frac{1}{2}}\}$ by applying η smoothing steps to $\{c_k^m,\ \mu_k^{m-\frac{1}{2}},d_k^m,\ \nu_k^{m-\frac{1}{2}}\}$

$$\begin{aligned}&\{\bar{c}_k^m,\ \bar{\mu}_k^{m-\frac{1}{2}},\ \bar{d}_k^m,\ \bar{\nu}_k^{m-\frac{1}{2}}\}\\ &=SMOOTH^\eta(c_k^m,\mu_k^{m-\frac{1}{2}},d_k^m,\nu_k^{m-\frac{1}{2}},\mathbf{NSO}_k,{g_1}_k^n,{g_2}_k^n,{g_3}_k^n,{g_4}_k^n),\end{aligned}$$

which means performing η smoothing steps with initial approximation $c_k^m,\mu_k^{m-\frac{1}{2}},d_k^m,\nu_k^{m-\frac{1}{2}},{g_1}_k^n,{g_2}_k^n,{g_3}_k^n,{g_4}_k^n$, and $SMOOTH$ relaxation operator to get the approximation $\{\bar{c}_k^m,\ \bar{\mu}_k^{m-\frac{1}{2}},\ \bar{d}_k^m,\ \bar{\nu}_k^{m-\frac{1}{2}}\}$.

One $SMOOTH$ relaxation operator step consists of solving the system (6.3.21)-(6.3.23) given below by 4×4 matrix inversion for each ijk:

$$\frac{\bar{c}^m_{ijk}}{\Delta t} + \frac{6}{h^2}\bar{\mu}^{m-\frac{1}{2}}_{ijk} = {g_1}^n_{ijk} + \frac{\mu^{m-\frac{1}{2}}_{i+1,jk} + \bar{\mu}^{m-\frac{1}{2}}_{i-1,jk} + \mu^{m-\frac{1}{2}}_{i,j+1,k} + \bar{\mu}^{m-\frac{1}{2}}_{i,j-1,k} + \mu^{m-\frac{1}{2}}_{ij,k+1} + \bar{\mu}^{m-\frac{1}{2}}_{ij,k-1}}{h^2}. \quad (6.3.21)$$

$$\begin{aligned}
-[\frac{6\epsilon^2}{h^2} &+ \frac{1}{2}\frac{\partial^2 F}{\partial c^2}(c^m_{ijk}, d^m_{ijk})]\bar{c}^m_{ijk} - [\frac{3\epsilon^2}{h^2} + \frac{1}{2}\frac{\partial^2 F}{\partial c \partial d}(c^m_{ijk}, d^m_{ijk})]\bar{d}^m_{ijk} + \bar{\mu}^{m-\frac{1}{2}}_{ijk} \\
&= {g_2}^n_{ijk} + \frac{1}{2}\frac{\partial F}{\partial c}(c^m_{ijk}, d^m_{ijk}) - \frac{1}{2}\frac{\partial^2 F}{\partial c^2}(c^m_{ijk}, d^m_{ijk})c^m_{ijk} - \frac{1}{2}\frac{\partial^2 F}{\partial c \partial d}(c^m_{ijk}, d^m_{ijk})d^m_{ijk} \\
&\quad -\frac{\epsilon^2}{h^2}(c^m_{i+1,jk} + \bar{c}^m_{i-1,jk} + c^m_{i,j+1,k} + \bar{c}^m_{i,j-1,k} + c^m_{ij,k+1} + \bar{c}^m_{ij,k-1}) \\
&\quad -\frac{\epsilon^2}{2h^2}(d^m_{i+1,jk} + \bar{d}^m_{i-1,jk} + d^m_{i,j+1,k} + \bar{d}^m_{i,j-1,k} + d^m_{ij,k+1} + \bar{d}^m_{ij,k-1}).
\end{aligned}$$

$$\frac{\bar{d}^m_{ijk}}{\Delta t} + \frac{6}{h^2}\bar{\nu}^{m-\frac{1}{2}}_{ijk} = {g_3}^n_{ijk} + \frac{\nu^{m-\frac{1}{2}}_{i+1,jk} + \bar{\nu}^{m-\frac{1}{2}}_{i-1,jk} + \nu^{m-\frac{1}{2}}_{i,j+1,k} + \bar{\nu}^{m-\frac{1}{2}}_{i,j-1,k}}{h^2} + \frac{\nu^{m-\frac{1}{2}}_{ij,k+1} + \bar{\nu}^{m-\frac{1}{2}}_{ij,k-1}}{h^2}. \quad (6.3.22)$$

$$\begin{aligned}
-[\frac{3\epsilon^2}{h^2} &+ \frac{1}{2}\frac{\partial^2 F}{\partial c \partial d}(c^m_{ijk}, d^m_{ijk})]\bar{c}^m_{ijk} - [\frac{6\epsilon^2}{h^2} + \frac{1}{2}\frac{\partial^2 F}{\partial d^2}(c^m_{ijk}, d^m_{ijk})]\bar{d}^m_{ijk} + \bar{\nu}^{m-\frac{1}{2}}_{ijk} \\
&= {g_4}^n_{ijk} + \frac{1}{2}\frac{\partial F}{\partial d}(c^m_{ijk}, d^m_{ijk}) - \frac{1}{2}\frac{\partial^2 F}{\partial c \partial d}(c^m_{ijk}, d^m_{ijk})c^m_{ijk} - \frac{1}{2}\frac{\partial^2 F}{\partial d^2}(c^m_{ijk}, d^m_{ijk})d^m_{ijk} \\
&\quad -\frac{\epsilon^2}{2h^2}(c^m_{i+1,jk} + \bar{c}^m_{i-1,jk} + c^m_{i,j+1,k} + \bar{c}^m_{i,j-1,k} + c^m_{ij,k+1} + \bar{c}^m_{ij,k-1}) \\
&\quad -\frac{\epsilon^2}{h^2}(d^m_{i+1,jk} + \bar{d}^m_{i-1,jk} + d^m_{i,j+1,k} + \bar{d}^m_{i,j-1,k} + d^m_{ij,k+1} + \bar{d}^m_{ij,k-1}).
\end{aligned}$$

(2) Compute the defect

$$\begin{aligned}
&(\overline{\mathrm{def}_1}^m_k, \overline{\mathrm{def}_2}^m_k, \overline{\mathrm{def}_3}^m_k, \overline{\mathrm{def}_4}^m_k) \\
&= ({g_1}^n_k, {g_2}^n_k, {g_3}^n_k, {g_4}^n_k) - \mathbf{NSO}_k(\bar{c}^m_k, \bar{\mu}^{m-\frac{1}{2}}_k, \bar{d}^m_k, \bar{\nu}^{m-\frac{1}{2}}_k).
\end{aligned}$$

(3) Restrict the defect and $\{\bar{c}^m_k,\ \bar{\mu}^{m-\frac{1}{2}}_k,\ \bar{d}^m_k,\ \bar{\nu}^{m-\frac{1}{2}}_k\}$

$$(\overline{\mathrm{def}_1}^m_{k-1}, \overline{\mathrm{def}_2}^m_{k-1}, \overline{\mathrm{def}_3}^m_{k-1}, \overline{\mathrm{def}_4}^m_{k-1}) = I^{k-1}_k(\overline{\mathrm{def}_1}^m_k, \overline{\mathrm{def}_2}^m_k, \overline{\mathrm{def}_3}^m_k, \overline{\mathrm{def}_4}^m_k)$$

$$(\bar{c}^m_{k-1}, \bar{\mu}^{m-\frac{1}{2}}_{k-1}, \bar{d}^m_{k-1}, \bar{\nu}^{m-\frac{1}{2}}_{k-1}) = I^{k-1}_k(\bar{c}^m_k, \bar{\mu}^{m-\frac{1}{2}}_k, \bar{d}^m_k, \bar{\nu}^{m-\frac{1}{2}}_k).$$

The restriction operator I_k^{k-1} maps k-level functions to $(k-1)$-level functions.

$$\begin{aligned} d_{k-1}(x_i,y_j,z_k) &= I_k^{k-1} d_k(x_i,y_j,z_k) \\ &= \frac{1}{8}[d_k(x_i-\frac{h}{2},y_j-\frac{h}{2},z_k-\frac{h}{2})+d_k(x_i-\frac{h}{2},y_j+\frac{h}{2},z_k-\frac{h}{2}) \\ &\quad +d_k(x_i+\frac{h}{2},y_j-\frac{h}{2},z_k-\frac{h}{2})+d_k(x_i+\frac{h}{2},y_j+\frac{h}{2},z_k-\frac{h}{2}) \\ &\quad +d_k(x_i-\frac{h}{2},y_j-\frac{h}{2},z_k+\frac{h}{2})+d_k(x_i-\frac{h}{2},y_j+\frac{h}{2},z_k+\frac{h}{2}) \\ &\quad +d_k(x_i+\frac{h}{2},y_j-\frac{h}{2},z_k+\frac{h}{2})+d_k(x_i+\frac{h}{2},y_j+\frac{h}{2},z_k+\frac{h}{2})]. \end{aligned}$$

That is, coarse grid values are obtained by averaging the eight nearby fine grid values.

(4) Compute the right-hand side

$$\begin{aligned} ({g_1}_{k-1}^n,{g_2}_{k-1}^n,{g_3}_{k-1}^n,{g_4}_{k-1}^n) &= (\overline{\text{def}}{}_{1\,k-1}^{\;m},\overline{\text{def}}{}_{2\,k-1}^{\;m},\overline{\text{def}}{}_{3\,k-1}^{\;m},\overline{\text{def}}{}_{4\,k-1}^{\;m}) \\ &\quad +\mathbf{NSO}_{k-1}(\bar{c}_{k-1}^m,\bar{\mu}_{k-1}^{m-\frac{1}{2}},\bar{d}_{k-1}^m,\bar{\nu}_{k-1}^{m-\frac{1}{2}}). \end{aligned}$$

(5) Compute an approximate solution $\{\hat{c}_{k-1}^m,\ \hat{\mu}_{k-1}^{m-\frac{1}{2}},\ \hat{d}_{k-1}^m,\ \hat{\nu}_{k-1}^{m-\frac{1}{2}}\}$ **of the coarse grid equation on** Ω_{k-1}**, i.e.**

$$\mathbf{NSO}_{k-1}(c_{k-1}^m,\mu_{k-1}^{m-\frac{1}{2}},d_{k-1}^m,\nu_{k-1}^{m-\frac{1}{2}}) = ({g_1}_{k-1}^n,{g_2}_{k-1}^n,{g_3}_{k-1}^n,{g_4}_{k-1}^n). \tag{6.3.23}$$

If $k=1$, we explicitly invert a 4×4 matrix to obtain the solution. If $k>1$, we solve (6.3.23) by performing a **FAS** k-grid cycle using $\{\bar{c}_{k-1}^m,\ \bar{\mu}_{k-1}^{m-\frac{1}{2}},\bar{d}_{k-1}^m,\ \bar{\nu}_{k-1}^{m-\frac{1}{2}}\}$ as an initial approximation:

$$\begin{aligned} \{\hat{c}_{k-1}^m,\hat{\mu}_{k-1}^{m-\frac{1}{2}},\hat{d}_{k-1}^m,\hat{\nu}_{k-1}^{m-\frac{1}{2}}\} &= \text{FAScycle}(k-1,\bar{c}_{k-1}^m,\bar{\mu}_{k-1}^{m-\frac{1}{2}},\bar{d}_{k-1}^m,\bar{\nu}_{k-1}^{m-\frac{1}{2}}, \\ &\qquad \mathbf{NSO}_{k-1},{g_1}_{k-1}^n,{g_2}_{k-1}^n,{g_3}_{k-1}^n,{g_4}_{k-1}^n\eta). \end{aligned}$$

(6) Compute the coarse grid correction (CGC):

$$\begin{aligned} \hat{v_1}_{k-1}^m &= \hat{c}_{k-1}^m-\bar{c}_{k-1}^m. \\ \hat{v_2}_{k-1}^{m-\frac{1}{2}} &= \hat{\mu}_{k-1}^{m-\frac{1}{2}}-\bar{\mu}_{k-1}^{m-\frac{1}{2}}. \\ \hat{v_3}_{k-1}^m &= \hat{d}_{k-1}^m-\bar{d}_{k-1}^m. \\ \hat{v_4}_{k-1}^{m-\frac{1}{2}} &= \hat{\nu}_{k-1}^{m-\frac{1}{2}}-\bar{\nu}_{k-1}^{m-\frac{1}{2}}. \end{aligned}$$

(7) Interpolate the correction

$$\begin{aligned} \hat{v_1}_k^m &= I_{k-1}^k\hat{v_1}_{k-1}^m. \\ \hat{v_2}_k^{m-\frac{1}{2}} &= I_{k-1}^k\hat{v_2}_{k-1}^{m-\frac{1}{2}}. \\ \hat{v_3}_k^m &= I_{k-1}^k\hat{v_3}_{k-1}^m. \\ \hat{v_4}_k^{m-\frac{1}{2}} &= I_{k-1}^k\hat{v_4}_{k-1}^{m-\frac{1}{2}}. \end{aligned}$$

The interpolation operator I_{k-1}^k maps (k-1)-level functions to k-level functions. Here, the coarse values are simply transferred to the four nearby fine grid points, i.e. $v_k(x_i, y_j, z_k) = I_{k-1}^k v_{k-1}(x_i, y_j, z_k) = v_{k-1}(x_i + \frac{h}{2}, y_j + \frac{h}{2}, z_k + \frac{h}{2})$ for $i,\ j$ and k odd-numbered integers. The values at the other node points are given by

$$\begin{aligned} v_k(x_i + h, y_j, z_k) &= v_k(x_i, y_j + h, z_k) = v_k(x_i + h, y_j + h, z_k) \\ &= v_k(x_i, y_j, z_k + h) = v_k(x_i + h, y_j, z_k + h) = v_k(x_i, y_j + h, z_k + h) \\ &= v_k(x_i + h, y_j + h, z_k + h) = v_{k-1}(x_i + \frac{h}{2}, y_j + \frac{h}{2}, z_k + \frac{h}{2}), \end{aligned}$$

where $i,\ j$ and k are odd.

(8) Compute the corrected approximation on Ω_k

$$\begin{aligned} c_k^{m,\text{ after } CGC} &= \bar{c}_k^m + \hat{v_1}_k^m. \\ \mu_k^{m-\frac{1}{2},\text{ after } CGC} &= \bar{\mu}_k^{m-\frac{1}{2}} + \hat{v_2}_k^{m-\frac{1}{2}}. \\ d_k^{m,\text{ after } CGC} &= \bar{d}_k^m + \hat{v_3}_k^m. \\ \nu_k^{m-\frac{1}{2},\text{ after } CGC} &= \bar{\nu}_k^{m-\frac{1}{2}} + \hat{v_4}_k^{m-\frac{1}{2}}. \end{aligned}$$

(9) Postsmoothing

Compute $\{c_k^{m+1}, \mu_k^{m+\frac{1}{2}}, d_k^{m+1}, \nu_k^{m+\frac{1}{2}}\}$ by applying ν smoothing steps to $c_k^{m,\text{ after } CGC}$, $\mu_k^{m-\frac{1}{2},\text{ after } CGC}$, $d_k^{m,\text{ after } CGC}$, $\nu_k^{m-\frac{1}{2},\text{ after } CGC}$

$$\begin{aligned} &\{c_k^{m+1}, \mu_k^{m+\frac{1}{2}}, d_k^{m+1}, \nu_k^{m+\frac{1}{2}}\} \\ &= SMOOTH^{\eta}(c_k^{m,\text{ after } CGC}, \mu_k^{m-\frac{1}{2},\text{ after } CGC}, d_k^{m,\text{ after } CGC}, \\ &\qquad \nu_k^{m-\frac{1}{2},\text{ after } CGC}, \mathbf{NSO}_k, {g_1}_k^n, {g_2}_k^n, {g_3}_k^n, {g_4}_k^n). \end{aligned}$$

This completes the description of a nonlinear FAScycle.

6.4 Numerical experiments

We consider a ternary system in a one dimension domain, $\Omega = [0, 1]$. The free energy F is given by

$$F(c_1, c_2) = \frac{1}{4}[c_1^2 c_2^2 + c_2^2(1 - c_1 - c_2)^2 + (1 - c_1 - c_2)^2 c_1^2],$$

To fix ideas, let $M_1 = M_2 = 1$ and $\epsilon_1 = \epsilon_2 = \epsilon_3 = \epsilon$ for simplicity.

Then, the partial differential equations (6.1.1) and (6.1.2) become

$$\frac{\partial c_1(x,t)}{\partial t} = \Delta_d \mu_1(x,t), \qquad \frac{\partial c_2(x,t)}{\partial t} = \Delta_d \mu_2(x,t), \tag{6.4.24}$$

$$\mu_1(x,t) = \frac{\partial F}{\partial c_1}(c_1,c_2) - 2\epsilon^2 \Delta_d c_1(x,t) - \epsilon^2 \Delta_d c_2(x,t), \tag{6.4.25}$$

$$\mu_2(x,t) = \frac{\partial F}{\partial c_2}(c_1,c_2) - \epsilon^2 \Delta_d c_1(x,t) - 2\epsilon^2 \Delta_d c_2(x,t), \tag{6.4.26}$$

where $(x,t) \in [0,1] \times [0,T]$.

4.A Convergence test

To obtain an estimate of the rate of convergence, we perform a number of simulations for a sample initial problem on a set of increasingly finer grids. The initial data is

$$c_1(x) = c_2(x) = 1/4 + 0.01\cos(3\pi x) + 0.04\cos(5\pi x) \tag{6.4.27}$$

on a domain, $\Omega = [0,1]$. The numerical solutions are computed on the uniform grids, $\Delta x = \frac{1}{2^n}$ for $n = 5, 6, 7, 8, 9,$ and 10. For each case, the calculations are run to time t = 0.2, the uniform time steps, $\Delta t = 0.1\Delta x$ and $\epsilon = 0.005$, are used to establish the convergence rates.

In our formulation of the method for ternary (**C-H**) system, since a cell centered grid is used, we define the error to be the discrete L_2-norm of the difference between that grid and the average of the next finer grid cells covering it:

$$e_{h/\frac{h}{2}\,i} \stackrel{def}{=} c_{h\,i} - \left(c_{\frac{h}{2}\,2i} + c_{\frac{h}{2}\,2i-1}\right)/2.$$

The rate of convergence is defined as the ratio of successive errors: $\log_2(||e_{h/\frac{h}{2}}||/||e_{\frac{h}{2}/\frac{h}{4}}||)$.

Table 6.1: Convergence Results — Concentration c_1.

Case	32-64	rate	64-128	rate	128-512	rate	512-1024
L_2	9.69e-3	2.54	1.66e-3	2.11	3.86e-4	2.03	9.43e-5

The errors and rates of convergence are given in table 6.1. The results suggest that the scheme is indeed second order accurate. In Fig. 6.1, the time evolution of the energy $\mathcal{E}(\mathbf{c})$ with same initial data (6.4.27) is shown. As expected from theorem 6.1, the energy is non-increasing and tends to a constant value. This is in fact a local equilibrium for Neumann boundary conditions.

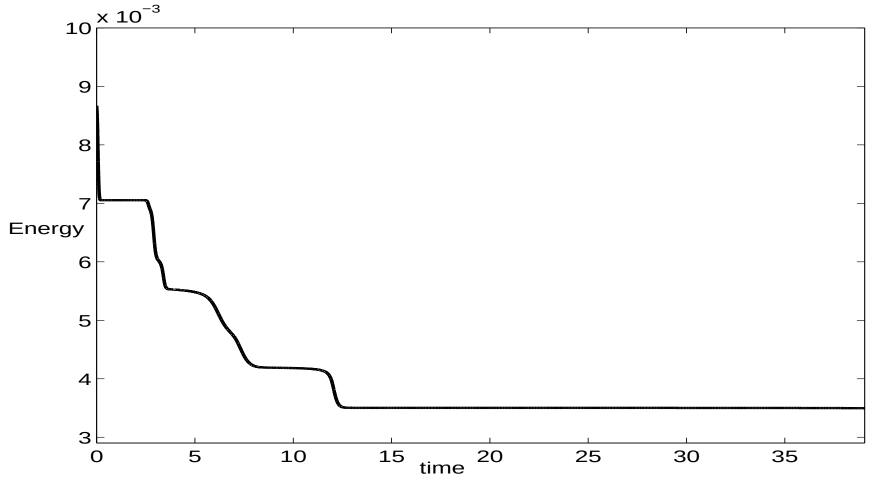

Figure 6.1: Energy decrease

4.B Linear stability analysis

Let the mean concentration take the form $\mathbf{m} = (m_1, m_2, m_3)$ where $m_i > 0\,\forall i$ and $m_3 = 1 - m_1 - m_2$. We seek a solution of the form

$$c_1(x,t) = m_1 + \sum_{n=1}^{\infty} \alpha_n(t)\cos(n\pi x)$$

$$c_2(x,t) = m_2 + \sum_{n=1}^{\infty} \beta_n(t)\cos(n\pi x)$$

$$c_3(x,t) = m_3 + \sum_{n=1}^{\infty} \gamma_n(t)\cos(n\pi x)$$

where $\mid \alpha_n(t) \mid, \mid \beta_n(t) \mid$, and $\mid \gamma_n(t) \mid \ll 1$; note that $\alpha_n(t) + \beta_n(t) + \gamma_n(t) = 0$. Linearizing $\frac{\partial F(c_1,c_2)}{\partial u_i}$ about $(m_1,\ m_2)$, then we have

$$\begin{aligned}
\frac{\partial F(c_1,c_2)}{\partial c_1} &= \frac{\partial F(m_1,m_2)}{\partial c_1} + \frac{\partial^2 F(m_1,m_2)}{\partial c_1^2}(c_1 - m_1) \\
&\quad + \frac{\partial^2 F(m_1,m_2)}{\partial c_1 c_2}(c_2 - m_2), \\
\frac{\partial F(c_1,c_2)}{\partial c_2} &= \frac{\partial F(m_1,m_2)}{\partial c_2} + \frac{\partial^2 F(m_1,m_2)}{\partial c_1 c_2}(c_1 - m_1) \\
&\quad + \frac{\partial^2 F(m_1,m_2)}{\partial c_2^2}(c_2 - m_2)
\end{aligned}$$

and substituting into (6.4.25), (6.4.26), up to first order, also let $m_1 = m_2 = m$ for simplicity, then we have

$$\begin{aligned}\frac{\partial c_1}{\partial t} &= \frac{\partial^2 F(m,m)}{\partial c_1^2}\Delta_d c_1 + \frac{\partial^2 F(m,m)}{\partial c_1 c_2}\Delta_d c_2 - 2\epsilon^2\Delta_d^2 c_1 - \epsilon^2\Delta_d^2 c_2,\\ \frac{\partial c_2}{\partial t} &= \frac{\partial^2 F(m,m)}{\partial c_1 c_2}\Delta_d c_1 + \frac{\partial^2 F(m,m)}{\partial c_2^2}\Delta_d c_2 - 2\epsilon^2\Delta_d^2 c_2 - \epsilon^2\Delta_d^2 c_1.\end{aligned}$$

$$\begin{aligned}\frac{\partial c_1}{\partial t} &= (7.5m^2 - 4m + 0.5)\Delta_d c_1 + (6m^2 - 2m)\Delta_d c_2 \qquad (6.4.28)\\ &\quad -2\epsilon^2\Delta_d^2 c_1 - \epsilon^2\Delta_d^2 c_2,\\ \frac{\partial c_2}{\partial t} &= (6m^2 - 2m)\Delta_d c_1 + (7.5m^2 - 4m + 0.5)\Delta_d c_2 \qquad (6.4.29)\\ &\quad -2\epsilon^2\Delta_d^2 c_2 - \epsilon^2\Delta_d^2 c_1.\end{aligned}$$

After substitution $c_1 = m + \alpha(t)\cos(n\pi x),\;\; c_2 = m + \beta(t)\cos(n\pi x)$ in (6.4.28), (6.4.29), respectively. We get

$$\begin{pmatrix}\alpha_n(t)\\ \beta_n(t)\end{pmatrix}' = \mathbf{A}\begin{pmatrix}\alpha_n(t)\\ \beta_n(t)\end{pmatrix} = \begin{pmatrix} a & b\\ b & a\end{pmatrix}\begin{pmatrix}\alpha_n(t)\\ \beta_n(t)\end{pmatrix}$$

where

$$\begin{aligned} a &= -(n\pi)^2(7.5m^2 - 4m + 0.5) - 2\epsilon^2(n\pi)^4,\\ b &= -(n\pi)^2(6m^2 - 2m) - \epsilon^2(n\pi)^4.\end{aligned}$$

The solution to the system of ODEs is given by

$$\begin{pmatrix}\alpha_n(t)\\ \beta_n(t)\end{pmatrix} = e^{At}\begin{pmatrix}\alpha_n(0)\\ \beta_n(0)\end{pmatrix}.$$

And eigenvalues of A are

$$\begin{aligned}\lambda_1 &= -(n\pi)^2[13.5m^2 - 6m + 0.5 + 3\epsilon^2(n\pi)^2],\\ \lambda_2 &= -(n\pi)^2[1.5m^2 - 2m + 0.5 + \epsilon^2(n\pi)^2].\end{aligned}$$

In Fig. 6.2, the theoretical growth rate λ_1 is compared to that obtained from the nonlinear scheme. The numerical growth rate is defined by

$$\tilde{\lambda_1}_k = \log\left(\frac{\max_i |{c_1}_i^n - 0.25|}{\max_i |{c_1}_i^0 - 0.25|}\right)/t_n.$$

Here, we used $(m_1, m_2, m_3) = (0.25, 0.25, 0.5)$, initial data $c_1(x) = c_2(x) = 0.25 + 0.01\cos(k\pi x)$ and $\epsilon = 0.01$, $\Delta t = 10^{-4}$, $h = 1/128$ and $t_n = 0.02$. The graph shows that the linear analysis (solid line) and numerical solution (circle) are in good agreement.

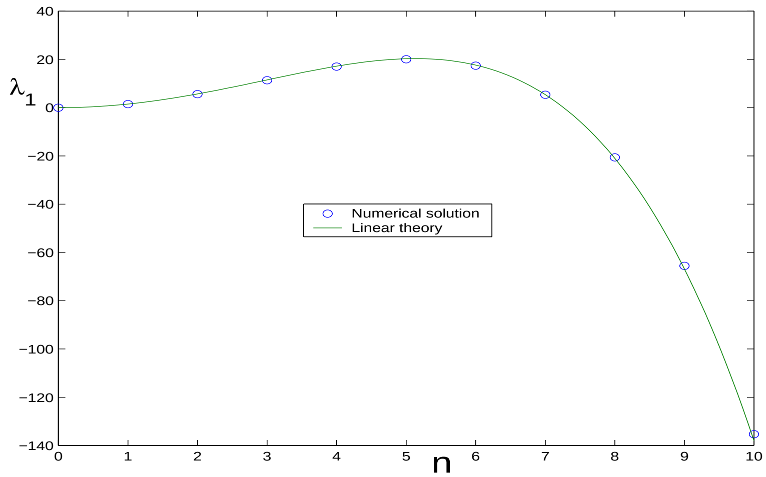

Figure 6.2: growth rate for the different wave number n

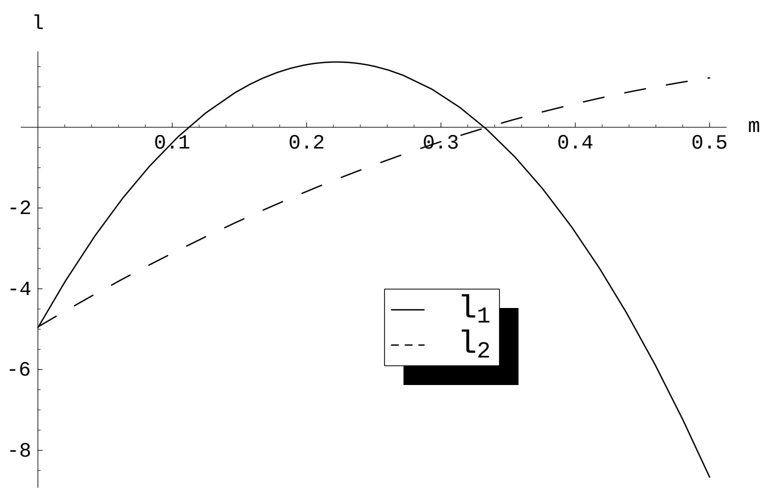

Figure 6.3: Eigenvalues with $c_1 = c_2 = m,\ n = 1,$ and $\epsilon = 0.005$.

Fig. 6.3 shows the eigenvalues, $\lambda_1 = -(n\pi)^2[13.5m^2 - 6m + 0.5 + 3\epsilon^2(n\pi)^2],\ \lambda_2 = -(n\pi)^2[1.5m^2 - 2m + 0.5 + \epsilon^2(n\pi)^2]$, when $m_1 = m_2 = m$ and $\epsilon = 0.005, n = 1$.

We chose $\Delta x = 1/128,\ \Delta t = 0.001,$ and $\epsilon = 0.005$. The initial conditions were random perturbations of the uniform state $\mathbf{m}$. We stop the numerical computations when the error between $(m+1)^{th}-$ and $m^{th}-$ iterations become less than 10^{-7}. That is

$$\|\mathbf{c}^{m+1} - \mathbf{c}^{m}\| \leq 10^{-7}.$$

The pictures are arranged in a matrix format with time increasing to the right in rows then down columns. The final numerical solution plotted in Fig. 6.4 is a stationary numerical solution, that is, the stopping criterion for the iterative procedure is satisfied in a single step from one time level to the next, for example, $\|\mathbf{c}^{n+1} - \mathbf{c}^{n}\| \leq 10^{-7}$.

We performed three experiments with initial data taking $m_1 = 0.22,\ 0.4,$ and 0.05. In the first experiment with $m_1 = 0.22$, where $\lambda_1 > 0$ and $\lambda_2 < 0$. Initially the third phase c_3 dominates. Moreover, for some time the evolution is in the direction of $c_1 = c_2$ with a two-phase structure (see Fig. 6.4 t = 0.16). However, at a time shortly after t = 1.40, we see growth in the phases c_1 and c_2. At a time t = 10.5, we see three phases are separated and there is always a phase that resides in the interfacial region.

In the second experiment with $m_1 = 0.4$, where $\lambda_1 < 0$ and $\lambda_2 > 0$. The evolution, after the quench, shows two phases with either c_1 or c_3 dominating (see Fig. 6.5, t = 0.16, 0.78; decomposition proceeds like a binary alloy). And at t = 11.6, three three phases are separated.

In the third experiment with $m_1 = 0.05$, where $\lambda_1 < 0$ and $\lambda_2 < 0$. Initial perturbation is not enough to initiate domain growth, instead the small perturbation is damped and the evolution is to homogeneous mixture state (see Fig. 6.6, t = 5.31).

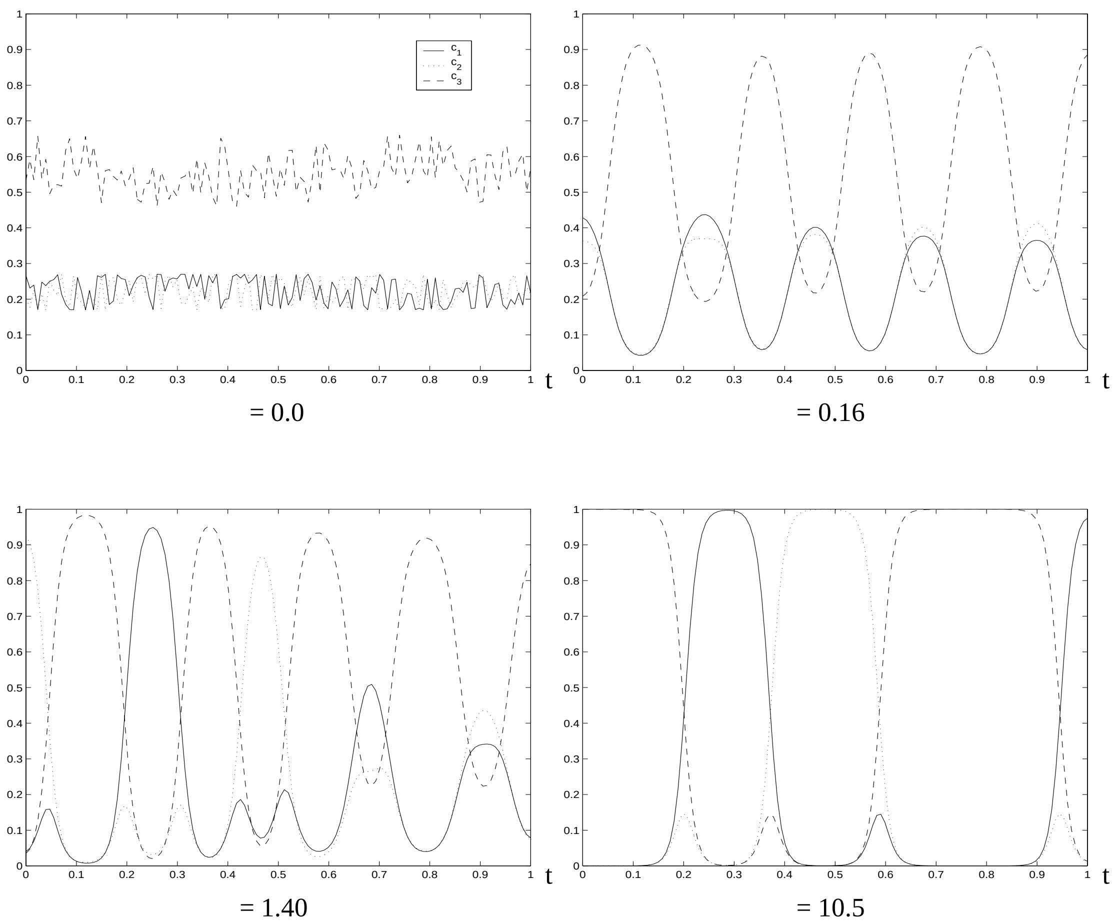

Figure 6.4: $(m_1, m_2, m_3) = (0.22, 0.22, 0.56)$.

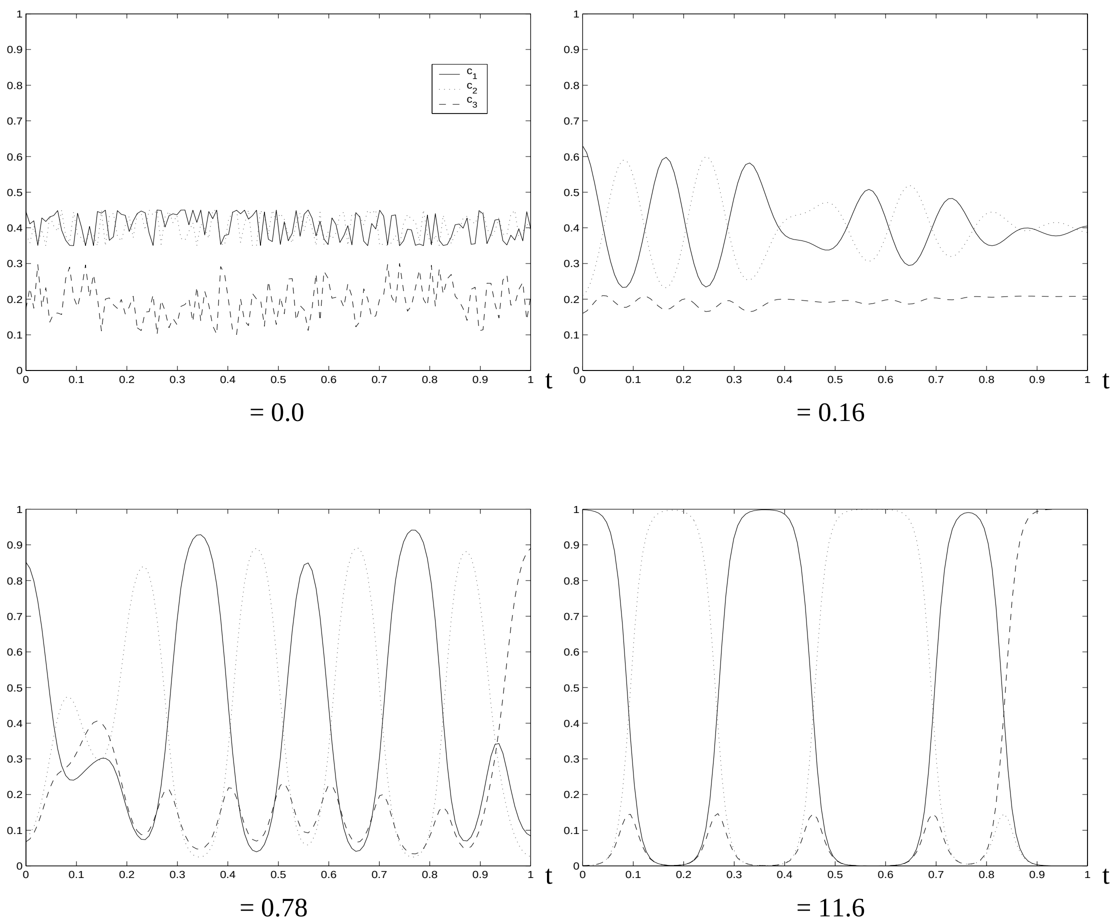

Figure 6.5: $(m_1, m_2, m_3) = (0.4, 0.4, 0.2)$.

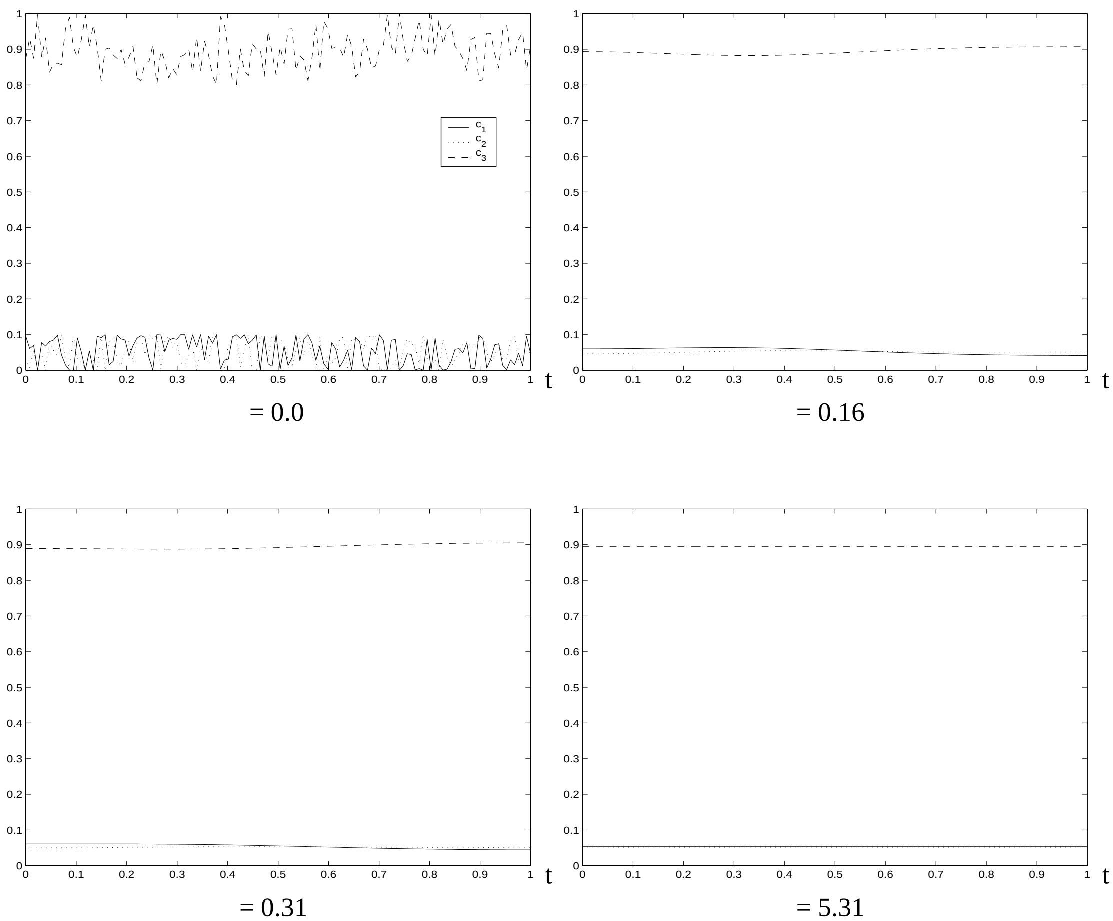

Figure 6.6: $(m_1, m_2, m_3) = (0.05, 0.05, 0.9)$.