Parareal Algorithms for the Cahn-Hilliard Equation

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1 Introduction

In this work we are interested in designing time parallel algorithm for the Cahn-Hilliard (CH) equation. The CH equation

$$\begin{aligned} \frac{\partial u}{\partial t} &= \Delta f(u) - \varepsilon^2 \Delta^2 u \quad \text{for } (x,t) \in \Omega(\subset \mathbb{R}) \times (0,T], \\ \frac{\partial u}{\partial n} &= \frac{\partial(\Delta u)}{\partial n} = 0 \quad \text{for } (x,t) \in \partial\Omega \times (0,T], \\ u(x,0) &= u_0(x) \quad \text{for } x \in \Omega, \end{aligned} \tag{1}$$

is a prototype to display the evolution of a binary melted alloy below the critical temperature; see [2, 3]. The nonlinear function $f(u)$ satisfies $f(u) = F'(u)$, where $F(u) = 0.25(u^2-1)^2$ is the homogeneous free energy. As the solution u of (1) takes values in $[-1,1]$, the function $f(u)$ becomes Lipschitz with Lipschitz constant 2. The solution of (1) involves two different dynamics, one being the phase separation which is rapid in time and phase regions are separated by the interface of width $\varepsilon(0 < \varepsilon \ll 1)$. Another is phase coarsening which is slower in time, during this stage the solution lean towards an equilibrium state which reduces the internal energy. The energy associated with the CH equation is

$$\mathscr{E}(u) := \int_\Omega \left(F(u) + \frac{\varepsilon^2}{2} |\nabla u|^2 \right) dx,$$

known as the Ginzburg-Landau free energy functional. The energy functional $\mathscr{E}(u)$ and total mass $\int_\Omega u$ satisfy the following

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$$\frac{d}{dt}\mathscr{E}(u) \leq 0, \qquad \frac{d}{dt}\int_{\Omega} u = 0.$$

And the energy minimization and mass conservation property of (1) is expected to be preserved by numerical method. To deal with that, Eyre proposed an unconditionally gradient stable scheme in [4, 5]. The idea is to split the homogeneous free energy $F(u)$ into the sum of a convex and a concave term, and then treat the convex term implicitly and the concave term explicitly to obtain a nonlinear approximation for the CH equation (1) in 1D as:

$$u_j^{n+1} - u_j^n = \Delta t A(u_j^{n+1})^3 - \Delta t A u_j^n - \varepsilon^2 \Delta t A^2 u_j^{n+1}, \tag{2}$$

where Δt is the time step and A is the discrete Laplacian and the scheme is $O(\Delta t + \Delta x^2)$ accurate [4, 5]. To get a linear approximation of (1) the term $(u_j^{n+1})^3$ in (2) is rewritten as $(u_j^n)^2 u_j^{n+1}$ to get the following

$$u_j^{n+1} - u_j^n = \Delta t A(u_j^n)^2 u_j^{n+1} - \Delta t A u_j^n - \varepsilon^2 \Delta t A^2 u_j^{n+1}, \tag{3}$$

which is also an unconditionally gradient stable scheme and has the same accuracy as the nonlinear scheme (2), see [4]. This is known as linearly stabilized splitting scheme (LSS). We also use the following semi-implicit Euler (SIE) approximation of (1)

$$u_j^{n+1} - u_j^n = \Delta t A(u_j^n)^3 - \Delta t A u_j^n - \varepsilon^2 \Delta t A^2 u_j^{n+1}, \tag{4}$$

though it is not a physically relevant approximation as the scheme is not gradient stable [5]. The solution of (1) involves long time dynamics, namely phase coarsening stage, thus the CH equation (1) needs to be simulated over long time window to get the solution. Therefore it is of great importance to develop efficient time parallel method for (1) to speed-up the computation. To achieve this we construct the Parareal methods [9] for (1). The Parareal method has been successfully applied to: fluid-structure interaction in [6], Navier-Stokes equation in [7], molecular-dynamics in [1]. The main objective of this work is to adapt the Parareal algorithm for the CH equation (1) and study the convergence behaviour.

We introduce the Parareal algorithm in one spatial dimension for the CH equation in Section 2. In Section 3 we discuss stability and convergence property of the Parareal method. To illustrate our theoretical findings, the accuracy and robustness of the proposed algorithms, we present the numerical results in Section 4.

2 Parareal method

To solve the following system of ODEs

$$\frac{du}{dt} = f(u), \quad u(0) = u_0, \quad t \in (0, T], \tag{5}$$

Lions et al. proposed the Parareal algorithm in [9], where $f\colon \mathbb{R}^+ \times \mathbb{R}^d \to \mathbb{R}^d$ is Lipschitz. The method constitutes of the following strategy: first a non-overlapping

decomposition of time domain $(0,T]$ into N smaller subintervals of uniform size, i.e., $(0,T] = \cup_{n=1}^{N}[T_{n-1},T_n]$ with $T_n - T_{n-1} = \Delta T = T/N$, secondly one divides each time slice $[T_{n-1},T_n]$ into J smaller time slices with $\Delta t = \Delta T/J$, then a fine propagator F which is expensive but accurate, and a coarse propagator G which is cheap but may be inaccurate are assigned to compute the solution in fine grid and coarse grid, respectively. Then the Parareal algorithm for (5) starts with an initial approximation U_n^0 at T_n's, obtained by the coarse operator G and solve for $k = 0,1,\ldots$

$$\begin{aligned} U_0^{k+1} &= u_0, \\ U_{n+1}^{k+1} &= G(T_{n+1},T_n,U_n^{k+1}) + F(T_{n+1},T_n,U_n^k) - G(T_{n+1},T_n,U_n^k), \end{aligned} \tag{6}$$

where $S(T_{n+1},T_n,U_n^k)$ provides solution at T_{n+1} by taking the initial solution U_n at T_n for the k-th iteration for $S = F$ or G. The Parareal solution U_{n+1}^{k+1} converges towards the fine resolution in finite step. To get a practical parallel algorithm we should have $k \ll N$.

Now to employ discrete Parareal method for the CH equation (1) we discretize (1) as shown earlier and denote U_n^k as $u(jh,T_n), j = 1,2,\ldots,N_x$ in (6) for k-th iteration, where h is spatial mesh size and N_x is number of nodes in spatial domain. We fix the fine propagator F to be the LSS scheme (3) in (6). For the coarse operator G in (6) we consider the following three choices:

(i) The coarse propagator G is given by the LSS scheme in (3).

(ii) The coarse propagator G is given by the SIE scheme in (4).

(iii) The coarse propagator G is given by the implicit scheme of the heat equation

$$u_t = 2\Delta u, \tag{7}$$

which is a linearization of (1) with respect a constant solution and then truncate the fourth order derivative term as ε is small.

The third choice of coarse operator is interesting as the equation (7) does not represent the underlying physics of the equation (1). Here we study the convergence behaviour of the Parareal algorithm corresponding to the coarse operators (ii) and (iii). The coarse operator corresponding to (ii) and (iii) can be written as

$$G_{\mathrm{SI}}(U) = \left(I + \varepsilon^2 \Delta T A^2\right)^{-1} \left(U + \Delta T A f(U)\right), \quad U \in \mathbb{R}^{N_x}, \tag{8a}$$

$$G_{\mathrm{IH}}(U) = \left(I - 2\Delta T A\right)^{-1} U, \quad U \in \mathbb{R}^{N_x} \tag{8b}$$

respectively, and $A = \frac{1}{h^2}[1 \ -2 \ \ 1] \in \mathbb{R}^{N_x \times N_x}$ with $A(1,2) = 2 = A(N_x,N_x-1)$ is the discrete Laplacian with homogeneous Neumann boundary conditions.

3 Stability and convergence result

In this section, we discuss the stability and convergence issues related to the coarse operators in (8). We start with a few auxiliary results.

Lemma 1 (Growth of coarse operators)

The coarse operators in (8) *satisfy the growth condition*

$$\| G_{SI}(U) \| \leq \| U \|, \quad \forall U \in \mathbb{R}^{N_x} \tag{9a}$$

$$\| G_{IH}(U) \| \leq \| U \|, \quad \forall U \in \mathbb{R}^{N_x}. \tag{9b}$$

Proof The eigenvalues of A are $\lambda_p = \frac{2}{h^2}\left\{\cos\left(\frac{(p-1)\pi}{N_x-1}\right)-1\right\}, p = 1,\cdots,N_x$. Clearly, λ_p's are distinct and satisfy $\lambda_p \leq 0, \forall p$. By taking norm on (8a) and using Lipschitz condition on f we get $\| G_{\mathrm{SI}}(U) \| \leq \max_{\lambda_p}\left|\frac{1+2\Delta T\lambda_p}{1+\varepsilon^2\Delta T\lambda_p^2}\right| \| U \|$. Now the function $g(x) = \frac{1-2\Delta Tx}{1+\varepsilon^2\Delta Tx^2} \leq 1$, $\forall x \geq 0$. Hence, we have (9a). Now $\| (I-2\Delta TA)^{-1} \| = \frac{1}{\min_{\lambda_p}\{1-2\Delta T\lambda_p\}} = 1$. Then by taking norm on (8b) we have (9b). □

Lemma 2 (Lipschitz property of G)

The coarse operators in (8) *satisfy the Lipschitz condition*

$$\| G_{SI}(T_{n+1},T_n,U) - G_{SI}(T_{n+1},T_n,V) \| \leq \| U-V \|, \quad \forall U,V \in \mathbb{R}^{N_x} \tag{10a}$$

$$\| G_{IH}(T_{n+1},T_n,U) - G_{IH}(T_{n+1},T_n,V) \| \leq \| U-V \|, \quad \forall U,V \in \mathbb{R}^{N_x}. \tag{10b}$$

Proof The results are straight forward. □

Lemma 3 (Local truncation error (LTE) differences)

Let $F(T_{n+1},T_n,U)$ be the fine operator in (3)*. For any coarse operators among $G_{SI}(T_{n+1},T_n,U), G_{IH}(T_{n+1},T_n,U)$ in* (8)*, the following LTE differences hold*

$$F(T_{n+1},T_n,U) - G_{SI}(T_{n+1},T_n,U) = c_2(U)\Delta T^2 + c_3(U)\Delta T^3 + \cdots, \tag{11a}$$

$$F(T_{n+1},T_n,U) - G_{IH}(T_{n+1},T_n,U) = c_1'(U)\Delta T + c_2'(U)\Delta T^2 + \cdots, \tag{11b}$$

where $c_j(U)$, $c_{j'}'(U)$ are continuously differentiable function for $j = 2,3,\ldots$, $j' = 1,2,\ldots$

Proof Let $S(T_{n+1},T_n,U)$ be the exact solution of (1). Since F and G_{SI} have LTE of $O(\Delta T^2)$, we have

$$\begin{aligned} &F(T_{n+1},T_n,U) - G_{\mathrm{SI}}(T_{n+1},T_n,U) \\ &\quad = F(T_{n+1},T_n,U) - S(T_{n+1},T_n,U) + S(T_{n+1},T_n,U) - G_{\mathrm{SI}}(T_{n+1},T_n,U) \\ &\quad = \widetilde{c_2}(U)\Delta T^2 + \widetilde{c_3}(U)\Delta T^3 + \cdots + \widehat{c_2}(U)\Delta T^2 + \widehat{c_3}(U)\Delta T^3 + \cdots \\ &\quad = c_2(U)\Delta T^2 + c_3(U)\Delta T^3 + \cdots. \end{aligned}$$

Similarly one can obtain LTE differences for G_{IH}. □

Theorem 1 (Stability) *Let $G_{SI}(T_{n+1},T_n,U_n)$ be the coarse operator in* (8a)*, then the corresponding Parareal method is stable, i.e., for each n and k, there exist a constant C such that*

$$\| U_{n+1}^{k+1} \| \leq \| u_0 \| + C\Delta T^2 (n+1) \left(\max_{0\leq j\leq n} \| U_j^k \| \right).$$

Proof Taking norm in the correction step (6) we have

$$\begin{aligned} \| U_{n+1}^{k+1} \| &\leq \| G_{\mathrm{SI}}(T_{n+1},T_n,U_n^{k+1}) \| + \| F(T_{n+1},T_n,U_n^k) - G_{\mathrm{SI}}(T_{n+1},T_n,U_n^k) \| \\ &\leq \| U_n^{k+1} \| + C\Delta T^2 \| U_n^k \|, \end{aligned} \tag{12}$$

where in the 2nd inequality we use (9a) and (11a). Taking the sum over n on the recurrence relation (12) we have

$$\| U_{n+1}^{k+1} \| - \| U_0^{k+1} \| \leq C\Delta T^2 \sum_{j=0}^{n} \| U_j^k \| \leq C\Delta T^2 (n+1) \left(\max_{0\leq j\leq n} \| U_j^k \| \right).$$

Now using $U_0^{k+1} = u_0$ we get the stated result. □

Theorem 2 (Stability) *Let $G_{IH}(T_{n+1},T_n,U_n)$ be the coarse operator in* (8b)*, then the corresponding Parareal method is stable, i.e., for each n and k, there exist a constant C such that*

$$\| U_{n+1}^{k+1} \| \leq \| u_0 \| + C\Delta T (n+1) \left(\max_{0\leq j\leq n} \| U_j^k \| \right).$$

Proof Proof can be obtained by following Theorem 1. □

Theorem 3 (Convergence) *Let $F(T_{n+1},T_n,U_n)$ be the fine operator in* (3) *and $G_{SI}(T_{n+1},T_n,U_n)$ be the coarse operator in* (8a)*. The propagator F and G_{SI} satisfy LTE differences* (11a) *and G_{SI} satisfies Lipschitz condition* (10a)*, then the corresponding Parareal method satisfies the following error estimation*

$$\| U(T_n) - U_n^k \| \leq \frac{C_3'}{C_1'} \frac{(C_1'\Delta T^2)^{k+1}}{(k+1)!} \prod_{j=0}^{k} (n-j),$$

where the constants C_1', C_3' are related to LTE.

Theorem 4 (Convergence) *Let $F(T_{n+1},T_n,U_n)$ be the fine operator in* (3) *and $G_{IH}(T_{n+1},T_n,U_n)$ be the coarse operator in* (8b)*. The propagator F and G_{IH} satisfy LTE differences* (11b) *and G_{IH} satisfies Lipschitz condition* (10b)*, then the corresponding Parareal method satisfies the following error estimation*

$$\| U(T_n) - U_n^k \| \leq \frac{C_3''}{C_1''} \frac{(C_1''\Delta T)^{k+1}}{(k+1)!} \prod_{j=0}^{k} (n-j),$$

where the constants C_1'', C_3'' are related to LTE.

The proof of Theorems 3 & 4 is followed by the argument of the proof of Theorem 1 in [8].

4 Numerical illustration

We now show numerical experiments of Parareal method for (1) corresponding to three different coarse operators. We consider the random initial condition for (1). The Parareal error is measured in $L^\infty(0,T;L^2)$, and we fix the spatial domain $\Omega = (0,2)$.

4.1 $F =$ LSS, $G =$ LSS

We first run the numerical experiments of Parareal method corresponding to fine and coarse operator as LSS scheme (3). We plot the error curves for short as well as long time window on the left panel in Figure 1 with $\varepsilon^2 = 0.01$, $J = 40$ and $h = 1/64$. The method converges in four iterations to the fine solution of temporal accuracy $O(10^{-4})$ for different T. For $T = 1$ we can see that the Parareal method 20 times faster than the serial method on single processor. To see the dependency of the parameter ε, we plot the error curve on the right in Figure 1 for different ε by fixing $T = 1$, $N = 80$, $J = 40$. We observe that the method behaves similar irrespective of any choice of ε. On the left of the Figure 2 we plot error curves for more refined solution for $T = 1$, $N = 80$, $J = 40$, $\varepsilon^2 = 0.01$. We observe that the convergence is independent of mesh parameters.

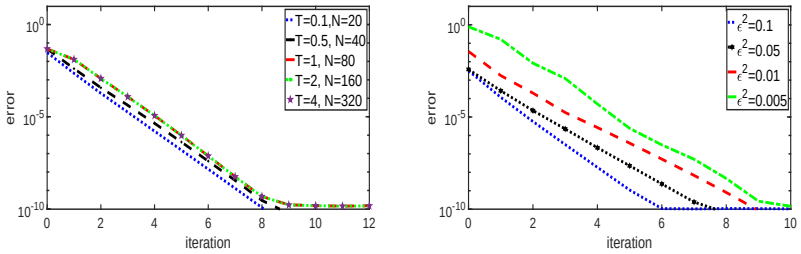

Fig. 1 On the left: different T and N; On the right: different choice of ε.

4.2 $F =$ LSS, $G =$ SIE

Now we run experiments of Parareal method corresponding to fine operator as LSS scheme (3) and coarse operator as SIE scheme (4). We plot the error curves on the right panel in Figure 2 for short as well as long time window with the parameters $\varepsilon^2 = 0.01$, $h = 1/64$, $J = 40$. Ignoring the cost of computing the coarse operator, it is visible that a reasonable speed up is possible; for example to get the solution at

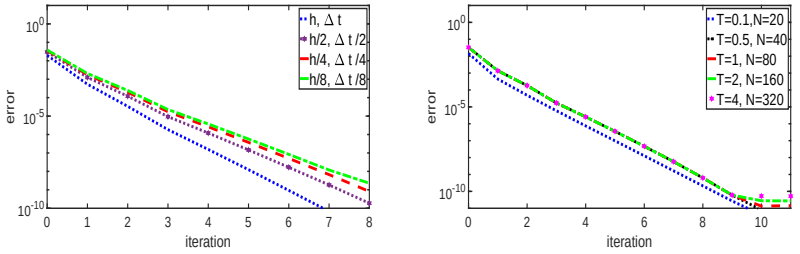

Fig. 2 On the left: different $h, \Delta t$ for LSS; On the right: different T, N for SIE.

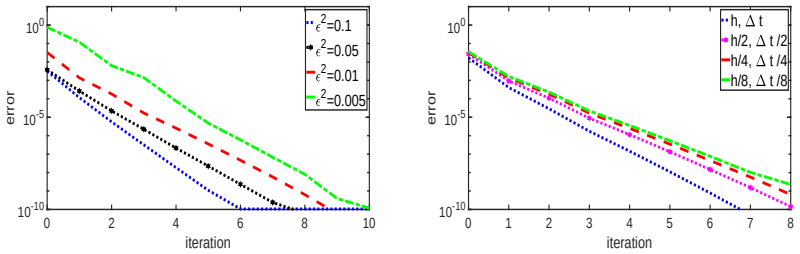

Fig. 3 On the left: different ε; On the right: different $h, \Delta t$.

$T = 4$ with an accuracy of $O(10^{-4})$ the method needs four iterations and this implies that the solution can be obtained 80 times faster than serial method on a single processor. We plot the error curves on the left in Figure 3 for different ε by taking $T = 1, N = 80, J = 40$ and we see that the convergence is independent of the choice of ε. On the right of the Figure 3 we plot error curves for more refined solution for $T = 1$, $N = 80$, $J = 40$, $\varepsilon^2 = 0.01$. We see that the convergence is independent of mesh parameters.

4.3 $F =$ LSS, $G =$ IH

We finally take the fine operator as LSS scheme (3) and coarse operator as implicit scheme of (7).We plot the error curves on the left in Figure 4 for short as well as long time window with the parameters $\varepsilon^2 = 0.01$, $h = 1/64$, $J = 40$ and small ΔT. We observe the convergence but it is not immediate. Even if we take reasonably large ΔT we obtain convergence but with very less speed up, see on the right of Figure 4. Even though the heat equation (7) as coarse operator provide solution we need further investigation to obtain the speed up.

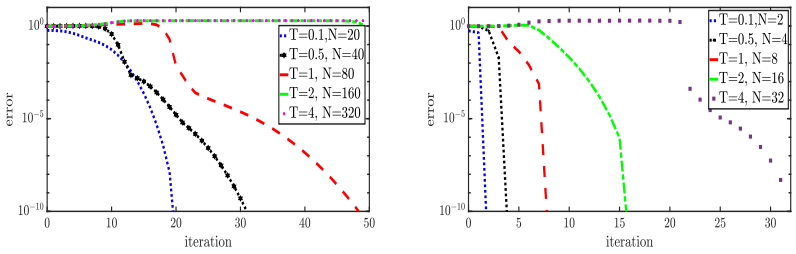

Fig. 4 On the left: small ΔT; On the right: large ΔT.

5 Conclusions

We formulated and studied the Parareal methods for the CH equation in 1D. We gave stability and convergence estimates of the Parareal method for different choices of coarse operator. Lastly we presented numerical experiments for all the proposed algorithms.

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