

# Stabilized Schemes for Phase Fields Models

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July 28, 2016

## Abstract

## 1 Introduction

## 2 The RSS-schemes for parabolic problems

The forward Euler's scheme is known to be stable only for small time steps; this restriction can be hard when considering heat-equation, the basic linear part of reaction-diffusion equations on which we focus here. This is due to the necessity of not allowing the expansion of high mode components which leads to the divergence of the scheme. A way to overcome the lack of stability consist in a approximation of the Backward Euler's scheme as follows. Consider the time and space discretization of the heat equation

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + Au^{(k+1)} = 0, \quad (1)$$

wher  $A$  is the stiffness matrix,  $\Delta t > 0$ , the time step; here  $u^{(k)}$  is the approximation of the solution at time  $t = k\Delta t$  in the spatial approximation space. To simplify the linear system that must be solved at each step, we replace  $Au^{(k+1)}$  by  $\tau B(u^{(k+1)} - u^{(k)}) + Au^{(k)}$ , where  $\tau \geq 0$  and where  $B$  is a preconditioner of  $A$ . This leads to the so-called RSS scheme

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau B(u^{(k+1)} - u^{(k)}) + Au^{(k)} = 0. \quad (2)$$

Chosing a "good" and appropriate preconditioner for enhancing the stability of the scheme (2) as respect to the forward Euler scheme is not *a priori* an easy task. Rewriting (2) as

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau Bu^{(k+1)} + (A - \tau B)u^{(k)} = 0. \quad (3)$$

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## 2.1 RSS-Schemes and stabilization

Let  $A$  and  $B$  be two  $n \times n$  symmetric positive definite matrices. We assume that there exist two strictly positive constant  $\alpha$  and  $\beta$  such that

$$\alpha < Bu, u > \leq Au, u > \leq \beta < Bu, u >, \quad \forall u \in \mathbb{R}^n \quad (4)$$

We first recall the following basic result [1]

**Proposition 2.1** *Assume that  $A$  and  $B$  are two SPD matrices. Under hypothesis (4), we have the following stability conditions:*

- If  $\tau \geq \frac{\beta}{2}$ , the schemes (6) and (9) are unconditionally stable (i.e. stable  $\forall \Delta t > 0$ )
- If  $\tau < \frac{\beta}{2}$ , then the scheme is stable for  $0 < \Delta t < \frac{2}{\left(1 - \frac{2\tau}{\beta}\right) \rho(A)}$ .

Of course we can consider second order schemes such as Gear's and apply the RSS stabilization. We can prove similar stability results:

**Proposition 2.2** *Consider the RSS-scheme derived from Gear's method*

$$\frac{1}{2\Delta t}(3u^{(k+1)} - 4u^{(k)} + u^{(k-1)}) + \tau B(u^{(k+1)} - u^{(k)}) + Au^k = 0$$

We have the following stability conditions

- If  $\tau \geq \frac{\beta}{2}$ , then (5) is unconditionally stable
- If  $\tau < \frac{\beta}{2}$ , then (5) is stable when

$$0 < \Delta t < \frac{2}{\rho(A)(1 - \frac{2\tau}{\beta})}$$

**Proof.** We start from the identity

$$\begin{aligned} < 3u^{(k+1)} - 4u^{(k)} + u^{(k-1)}, u^{(k+1)} - u^{(k)} > &= 2\|u^{(k+1)} - u^{(k)}\|^2 + \frac{1}{2}(\|u^{(k+1)} - u^{(k)}\|^2 \\ &\quad - \|u^{(k)} - u^{(k-1)}\|^2 + \|u^{(k+1)} - 2u^{(k)} + u^{(k-1)}\|^2) \end{aligned}$$

We now take the scalar product of each term of (5) with  $u^{(k+1)} - u^{(k)}$  and obtain

$$\begin{aligned} &2\|u^{(k+1)} - u^{(k)}\|^2 + \frac{1}{2}(\|u^{(k+1)} - u^{(k)}\|^2 - \|u^{(k)} - u^{(k-1)}\|^2 + \|u^{(k+1)} - 2u^{(k)} + u^{(k-1)}\|^2) \\ &+ 2\Delta t (\tau < B(u^{(k+1)} - u^{(k)}), u^{(k+1)} - u^{(k)} > + < Au^{(k)}, u^{(k+1)} - u^{(k)} >) = 0 \end{aligned}$$

Using the parallelogram identity on the last term, we find

$$\begin{aligned} &2\|u^{(k+1)} - u^{(k)}\|^2 + \frac{1}{2}(\|u^{(k+1)} - u^{(k)}\|^2 - \|u^{(k)} - u^{(k-1)}\|^2 + \|u^{(k+1)} - 2u^{(k)} + u^{(k-1)}\|^2) \\ &+ 2\Delta t (\tau < B(u^{(k+1)} - u^{(k)}), u^{(k+1)} - u^{(k)} > \\ &+ \frac{1}{2}(< Au^{(k+1)}, u^{(k+1)} > - < Au^{(k)}, u^{(k)} > - < A(u^{(k+1)} - u^{(k)}), u^{(k+1)} - u^{(k)} >) = 0 \end{aligned}$$

Now, we let  $E^{k+1} = \frac{1}{2} \langle Au^{(k+1)}, u^{(k+1)} \rangle + \frac{1}{2} \|u^{(k+1)} - u^{(k)}\|^2$  and we obtain,

$$2\|u^{(k+1)} - u^{(k)}\|^2 + \frac{1}{2}\|u^{(k+1)} - 2u^{(k)} + u^{(k-1)}\|^2 + 2\Delta t(E^{k+1} - E^k) + 2\Delta t(\tau \langle B(u^{(k+1)} - u^{(k)}), u^{(k+1)} - u^{(k)} \rangle - \frac{1}{2} \langle A(u^{(k+1)} - u^{(k)}), u^{(k+1)} - u^{(k)} \rangle)$$

The stability is obtained when  $E^{k+1} < E^k$ , hence the conditions. ■

## 2.2 A ADI-RSS Scheme

Consider the linear differential system

$$\frac{dU}{dt} + AU = 0$$

with  $A = A_1 + A_2$ . Let  $B_1$  and  $B_2$  be preconditioners of  $A_1$  and  $A_2$  respectively and  $\tau_1, \tau_2$  two positive real numbers. All the matrices are supposed to be symmetric definite positive. We introduce the ADI-RSS schemes

$$\frac{u^{(k+1/2)} - u^{(k)}}{\Delta t} + \tau_1 B_1(u^{(k+1/2)} - u^{(k)}) = -A_1 u^{(k)}, \quad (5)$$

$$\frac{u^{(k+1)} - u^{(k+1/2)}}{\Delta t} + \tau_2 B_2(u^{(k+1)} - u^{(k+1/2)}) = -A_2 u^{(k+1/2)}, \quad (6)$$

and the Strang's Splitting

$$\frac{u^{(k+1/3)} - u^{(k)}}{\Delta t/2} + \tau_1 B_1(u^{(k+1/3)} - u^{(k)}) = -A_1 u^{(k)}, \quad (7)$$

$$\frac{u^{(k+2/3)} - u^{(k+1/3)}}{\Delta t} + \tau_2 B_2(u^{(k+2/3)} - u^{(k+1/3)}) = -A_2 u^{(k+1/3)}, \quad (8)$$

$$\frac{u^{(k+1)} - u^{(k+2/3)}}{\Delta t/2} + \tau_1 B_1(u^{(k+1)} - u^{(k+2/3)}) = -A_1 u^{(k+2/3)}, \quad (9)$$

Of course these approach can be applied in more general situations, eg considering  $A = \sum_{i=1}^m A_i$

and  $B = \sum_{i=1}^m B_i$  and the splitting

$$\frac{u^{(k+i/m)} - u^{(k+(i-1)/m)}}{\Delta t} + \tau_i B_i(u^{(k+i/m)} - u^{(k+(i-1)/m)}) = -A_i u^{(k+(i-1)/m)}, \quad (10)$$

We recall that

As a direct consequence of proposition 2.1, we can prove the following result

**Proposition 2.3** *Under hypothesis (4), we have the followig stability conditions:*

- If  $\tau_i \geq \frac{\beta_i}{2}, i = 1, 2$  the scheme (6) is unconditionally stable (i.e. stable  $\forall \Delta t > 0$ )

- If  $\tau_i < \frac{\beta_i}{2}$ ,  $i = 1, 2$ , then the scheme is stable for  $0 < \Delta t < \text{Min}(\frac{2}{(1 - \frac{2\tau_1}{\beta_1})\rho(A_1)}, \frac{2}{(1 - \frac{2\tau_2}{\beta_2})\rho(A_2)})$ .

**Proof.** It suffices to apply proposition 2.1 to each system. ■

## 2.3 Numerical results

USE THE MATLAB CODES IN THE DIRECTORY ADI\_MATLAB.

### 2.3.1 2D Heat Equation

see program `chaleur_2D_splitting.m`

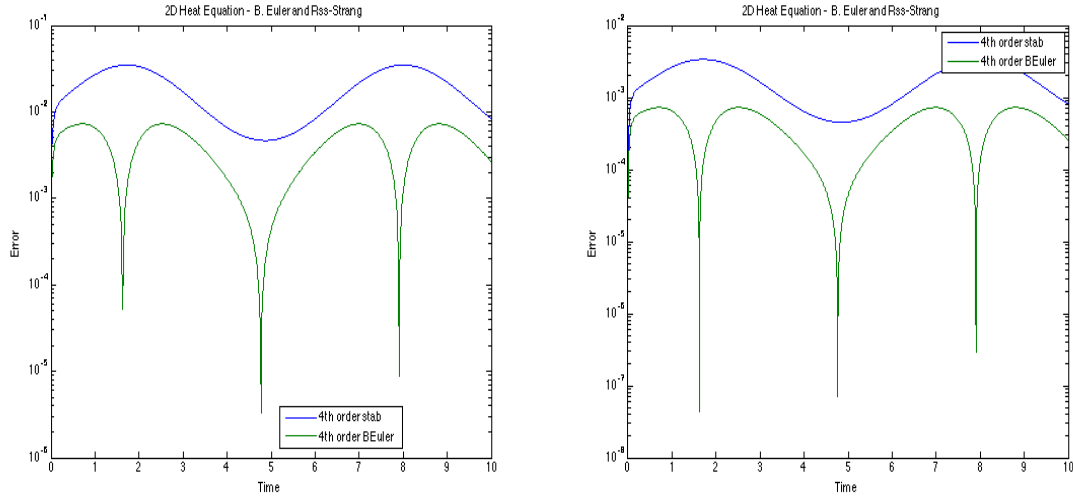


Figure 1: Solution of the heat equation with  $\Delta t = 0.01$ , (left) and  $\Delta t = 0.001$  (right)  $n = 31$ ,  $\tau = 1$

The error is clearly in  $\Delta t$ .

### 2.3.2 3D Heat Equation

The error is clearly in  $\Delta t$ .

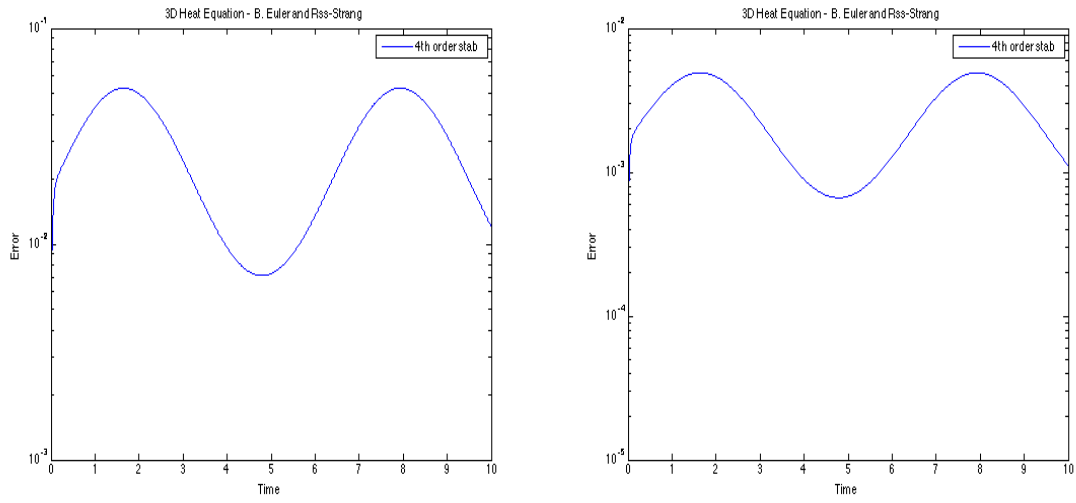


Figure 2: Solution of the 3D heat equation with  $\Delta t = 0.01$ , (left) and  $\Delta t = 0.001$  (right)  $n = 31$ ,  $\tau = 1$

### 3 Allen-Cahn's equation

A first inconditionnally stable scheme is ([2, 3])

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + Au^{(k+1)} + \frac{1}{\epsilon^2} DF(u^{(k)}, u^{(k+1)}) = 0, \quad (11)$$

where

$$DF(u, v) = \begin{cases} \frac{F(u) - F(v)}{u - v} & \text{if } u \neq v, \\ f(u) & \text{if } u = v. \end{cases}$$

In [1] it was introduced the RSS-scheme

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau B(u^{(k+1)} - u^{(k)}) + DF(u^{(k+1)}, u^{(k)}) = -Au^{(k)} \quad (12)$$

which enjoys of the following stability condition, see [1] for the proof.

**Proposition 3.1** *Under hypothesis  $\mathcal{H}$*

- *if  $\tau \geq \frac{\beta}{2}$ , the RSS scheme is unconditionally stable,*
- *if  $\tau < \frac{\beta}{2}$ , the RSS scheme is stable under condition*

$$0 < \Delta t < \frac{\beta}{\rho(A)(\frac{\beta}{2} - \tau)}.$$

## 4 Cahn-Hilliard's equation

### 4.1 The models

#### 4.1.1 Cahn Hilliard and Patterns

The CH equation describes the process of phase separation, by which the two components of a binary fluid spontaneously separate and form domains pure in each component. It writes as

$$\frac{\partial u}{\partial t} - \Delta(-\Delta u + \frac{1}{\epsilon^2}f(u)) = 0, \quad (13)$$

$$\frac{\partial u}{\partial n} = 0, \quad (14)$$

$$\frac{\partial}{\partial n} \left( \Delta u - \frac{1}{\epsilon^2}f(u) \right) = 0, \quad (15)$$

$$u(0, x) = u_0(x) \quad (16)$$

We have the properties

- Conservation of the mass:  $\bar{u} = \int_{\Omega} u(x, t) dx = \int_{\Omega} u_0(x) dx$
- Decay of the energy in time

$$\frac{\partial E(u)}{\partial t} = - \int_{\Omega} |\nabla(-\Delta u + \frac{1}{\epsilon^2}f(u))|^2 dx \leq 0$$

A nice way to study and to simulate CH is to decouple the equation as follows:

$$\frac{\partial u}{\partial t} - \Delta \mu = 0, \quad (17)$$

$$\mu = -\Delta u + \frac{1}{\epsilon^2}f(u), \quad (18)$$

$$\frac{\partial u}{\partial n} = 0, \quad (19)$$

$$\frac{\partial \mu}{\partial n} = 0, \quad (20)$$

$$u(0, x) = u_0(x) \quad (21)$$

#### 4.1.2 The inpainting problem

Cahn hilliard equations allow here to in paint a tagged picture. Let  $g$  be the original image and  $D \subset \Omega$  the region of  $\Omega$  in which the image is deterred. The idea is to add a penalty term that forces the image to remain unchanged in  $\Omega \setminus D$  and to reconnect the fields of  $g$  inside  $D$ . Let  $\lambda \gg 1$

$$\frac{\partial u}{\partial t} - \Delta(-\epsilon \Delta u + \frac{1}{\epsilon}f(u)) + \lambda \chi_{\Omega \setminus D}(x)(u - g) = 0, \quad (22)$$

$$\underbrace{\frac{\partial u}{\partial t} - \Delta(-\epsilon \Delta u + \frac{1}{\epsilon}f(u))}_{\text{Cahn-Hilliard equation}} \quad \underbrace{+ \lambda \chi_{\Omega \setminus D}(x)(u - g)}_{\text{Fidelity term}} = 0 \quad (23)$$

$$\frac{\partial u}{\partial n} = 0 \quad \frac{\partial}{\partial n} \left( \Delta u - \frac{1}{\epsilon^2} f(u) \right) = 0, \quad (24)$$

$$u(0, x) = u_0(x) \quad (25)$$

Here  $\chi_{\Omega \setminus D}(x) = \begin{cases} 1 & \text{if } x \in \Omega \setminus D, \\ 0 & \text{else} \end{cases}$

- The presence of the penalization term  $\lambda \chi_{\Omega \setminus D}(x)(u - g)$  forces the solution to be close to  $g$  in  $\Omega \setminus D$  when  $\lambda \gg 1$
- The Cahn-Hilliard flow has as effect to connect the fields inside  $D$
- here  $\epsilon$  will play the role of the "contrast". A post-processing is possible using a thresholding procedure.

## 4.2 The RSS-Scheme

The semi-implicit scheme

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + A\mu^{(k+1)} = 0, \quad (26)$$

$$\mu^{(k+1)} = \epsilon A u^{(k+1)} + \frac{1}{\epsilon} f(u^{(k)}), \quad (27)$$

suffers from a hard time step restriction, its energy stability is guaranteed for

$$0 < \Delta < \epsilon^2$$

see [4] We derive the RSS-Scheme from the backward Euler's (26)-(27) by replacing  $Az^{(k+1)}$  by  $\tau B(z^{(k+1)} - z^{(k)}) + Az^{(k)}$  for  $z = u$  or  $z = \mu$ . We obtain

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau B(\mu^{(k+1)} - \mu^{(k)}) + A\mu^{(k)} = 0, \quad (28)$$

$$\mu^{(k+1)} = \epsilon \tau B(u^{(k+1)} - u^{(k)}) + \epsilon A u^{(k)} + \frac{1}{\epsilon} f(u^{(k)}). \quad (29)$$

We remark that this scheme preserves the steady state. We now address a stability analysis. We first consider the linear case ( $f \equiv 0$ ).

**Theorem 4.1** *Assume that  $f \equiv 0$ . If  $\tau > \beta$ , then the scheme (28)-(29) is unconditionally stable.*

**Proof.** We take the scalar product of (28) with  $u^{(k+1)} - u^{(k)}$  and of (29) with  $\mu^{(k+1)}$ . After the use of the parallelogram identity and usual simplifications, we obtain, on the one hand

$$\begin{aligned} & \langle u^{(k+1)} - u^{(k)}, \mu^{(k+1)} \rangle + \frac{\Delta t \tau}{2} (\langle B\mu^{(k+1)}, \mu^{(k+1)} \rangle - \langle B\mu^{(k)}, \mu^{(k)} \rangle) \\ & \langle B(\mu^{(k+1)} - \mu^{(k)}), \mu^{(k+1)} - \mu^{(k)} \rangle \\ & + \frac{\Delta t}{2} (\langle A\mu^{(k+1)}, \mu^{(k+1)} \rangle - \langle A\mu^{(k)}, \mu^{(k)} \rangle) \\ & - \langle A(\mu^{(k+1)} - \mu^{(k)}), \mu^{(k+1)} - \mu^{(k)} \rangle = 0, \end{aligned}$$



and on the other hand

$$\begin{aligned} \langle u^{(k+1)} - u^{(k)}, \mu^{(k+1)} \rangle &= \tau \langle B(u^{(k+1)} - u^{(k)}), u^{(k+1)} - u^{(k)} \rangle \\ &\quad + \frac{1}{2} (\langle Au^{(k+1)}, u^{(k+1)} \rangle - \langle Au^{(k)}, u^{(k)} \rangle - \langle A(u^{(k+1)} - u^{(k)}), u^{(k+1)} - u^{(k)} \rangle) \end{aligned}$$

Taking the difference of the last two identities, we obtain

$$\begin{aligned} &\{\tau \langle B(u^{(k+1)} - u^{(k)}), u^{(k+1)} - u^{(k)} \rangle - \frac{1}{2} \langle B(u^{(k+1)} - u^{(k)}), u^{(k+1)} - u^{(k)} \rangle\} \\ &+ \Delta t \left\{ \frac{\tau}{2} \langle B(\mu^{(k+1)} - \mu^{(k)}), \mu^{(k+1)} - \mu^{(k)} \rangle - \frac{1}{2} \langle B(\mu^{(k+1)} - \mu^{(k)}), \mu^{(k+1)} - \mu^{(k)} \rangle \right\} \\ &+ R^{k+1} - R^k = 0, \end{aligned}$$

where

$$R^{k+1} = \frac{1}{2} \langle Au^{(k+1)}, u^{(k+1)} \rangle + \Delta t \langle B\mu^{(k+1)}, \mu^{(k+1)} \rangle + \frac{\Delta t}{2} \langle A\mu^{(k+1)}, \mu^{(k+1)} \rangle.$$

The scheme is then stable if  $R^{k+1} < R^k$ . Hence the stability conditions. ■ We now describe the practical solution. We can write

$$\begin{pmatrix} Id & \tau\Delta t B \\ -\epsilon\tau B & Id \end{pmatrix} \begin{pmatrix} u^{(k+1)} - u^{(k)} \\ \mu^{(k+1)} \end{pmatrix} = \begin{pmatrix} -\Delta t Au^{(k)} \\ \epsilon Au^{(k)} + F(u^{(k)}) \end{pmatrix}$$

The matrix of the system can be factorized as Block LU

$$M = \begin{pmatrix} Id & \tau\Delta t B \\ -\epsilon\tau B & Id \end{pmatrix} = \begin{pmatrix} Id & 0 \\ -\epsilon\tau B & Id \end{pmatrix} \begin{pmatrix} Id & \tau\Delta t B \\ 0 & S \end{pmatrix}$$

where  $S = Id + \tau^2 \Delta t \epsilon B^2$  is the Schur complement. We have to solve the coupled linear system

$$\begin{cases} X_1 + \tau\Delta t B X_2 = F_1, \\ -\tau\epsilon B X_1 + X_2 = F_2. \end{cases}$$

Hence

$$(Id + \tau^2 \Delta t \epsilon B^2) X_2 = F_2 + \epsilon\tau B F_1$$

Then,

$$X_1 = F_1 - \tau\Delta t B X_2$$

We can resume the solution as

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**Algorithm 1** : RSS Cahn-Hilliard

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- 1: **for**  $k = 0, 1, \dots$  until convergence **do**
  - 2:     **Set**  $F_1 = -tA\mu^{(k)}$  and  $F_2 = -\mu^{(k)} + \epsilon Au^{(k)} + \frac{1}{\epsilon} f(u^{(k)})$
  - 3:     **Solve**  $(Id + \tau^2 \Delta t \epsilon B^2) \delta\mu = F_2 + \tau\epsilon B F_1$
  - 4:     **Set**  $\mu^{(k+1)} = \mu^{(k)} + \delta\mu$
  - 5:     **Set**  $u^{(k+1)} = u^{(k)} - \tau\Delta t B \delta\mu$
  - 6: **end for**
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## 5 Numerical Results

### 5.1 Implementation

The applications we are interested with are Allen-Cahn and Cahn-Hilliard equations to which homogeneous Neumann boundary conditions are associated. We proceed as in [?] and we first discretize in space the equation with high order finite difference compact schemes; the matrix  $A$  corresponds then to the laplacien with Homogenous Neumann BC (HNBC). Matrix  $B$  is the (sparse) second order laplacian matrix with HNBC. For a fast solution of linear systems in the RSS, we will use the cosine-fft to solve the Neumann problems with matrix  $Id + \tau \Delta t B$ . `test_Neumann_2D.m` is a (non RSS) solver that uses cos-fft for 2D neumann problem on the square

### 5.2 Allen-Cahn equation

`Allen_Cahn_fft.m` runs (a non RSS) Allen-Cahn with semi-implicit scheme and cos-fft, see directory AC\_CH: this seems correct

Also `Allen_Cahn_fft_3D.m` runs ( a non RSS) Allen-Cahn with semi-implicit scheme and cos-fft, see directory AC\_CH: To check

### 5.3 Cahn-Hilliard equation

USE THE (NON RSS BUT STABILIZED AS IN BERTOZZI PAPER) CODEs IN THE DIRECTORY CH\_INPAINTING

## References

- [1] Matthieu Brachet, Jean-Paul Chehab, Stabilized Times Schemes for High Accurate Finite Differences Solutions of Nonlinear Parabolic Equations, J Sci Comput (2016), DOI 10.1007/s10915-016-0223-8
- [2] C.M. Elliott, The Chan-Hilliard Model for the Kinetics of Phase Separation, *in* Mathematical Models for Phase Change Problems, International Series of Numerical Mathematics, Vol. 88, (1989) Birkhäuser.
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- [4] J. Shen, X. Yang, Numerical Approximations of Allen-Cahn and Cahn-Hilliard Equations. DCDS, Series A, (28), (2010), pp 1669–1691.