Stabilized Schemes for Phase Fields Models

M. Brachet[*] J.-P. Chehab[†]

July 23, 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 rectriction 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 lake of stability consist in a approximation of the Backward Euler's scheme as follows. Consider the time and space discretization of the heat equation

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

wher A is the stifness 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

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

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

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

[*]Institut Elie Cartan de Lorraine, Université de Lorraine, Site de Metz, Bât. A Ile du Saucy, F-57045 Metz Cedex 1, `matthieu.brachet@math.univ-metz.fr`

[†]Laboratoire Amienois de Mathématiques Fondamentales et Appliquées (LAMFA), UMR 7352, Université de Picardie Jules Verne, 33 rue Saint Leu, 80039 Amiens France , (`Jean-Paul.Chehab@u-picardie.fr`).

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 α and *beta* such that

$$\alpha < Bu, u > \leq < Au, u > \leq \beta < Bu, u >, \ \forall u \in I\!R^n \tag{4}$$

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* $0 < \Delta t < \dfrac{2}{\left(1 - \frac{2\tau}{\beta}\right) \rho(A)}$.

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 table when*

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

Proof. We start from the identity

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

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

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

Using the parallelogram identity on the last term, we find

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

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

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

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 τ_1, τ_2 two positive real numbers. All the matrices are supposed to be symmetric definite positive. We introduce the ADI-RSS schemes

$$\frac{u^{(k+1/2)} - u^{(k)}}{\Delta t} + \tau_1 B_1(u^{(k+1/2)} - u^{(k)}) = -A_1 u^{(k)}, \tag{5}$$
$$\frac{u^{(k+1)} - u^{(k+1/2)}}{\Delta t} + \tau_2 B_2(u^{(k+1)} - u^{(k+1/2)}) = -A_2 u^{(k+1/2)}, \tag{6}$$

and the Strang's Splitting

$$\frac{u^{(k+1/3)} - u^{(k)}}{\Delta t/2} + \tau_1 B_1(u^{(k+1/3)} - u^{(k)}) = -A_1 u^{(k)}, \tag{7}$$
$$\frac{u^{(k+2/3)} - u^{(k+1/3)}}{\Delta t} + \tau_2 B_2(u^{(k+2/3)} - u^{(k+1/3)}) = -A_2 u^{(k+1/3)}, \tag{8}$$
$$\frac{u^{(k+1)} - u^{(k+2/3)}}{\Delta t/2} + \tau_1 B_1(u^{(k+1)} - u^{(k+2/3)}) = -A_1 u^{(k+2/3)}, \tag{9}$$

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

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

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* $0 < \Delta t < Min(\frac{2}{\left(1 - \frac{2\tau_1}{\beta_1}\right)\rho(A_1)}, \frac{2}{\left(1 - \frac{2\tau_2}{\beta_2}\right)\rho(A_2)})$.

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`

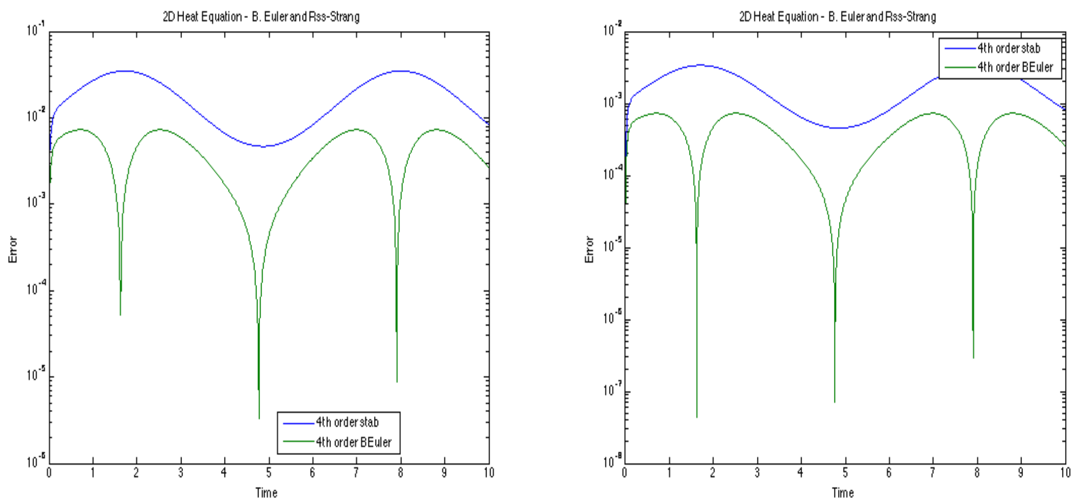

Figure 1: Solution of the heat equation with $\Delta t = 0.01$, (left) and $\Delta t = 0.001$ (right) $n = 31$, $\tau = 1$

The error is clearly in Δt.

2.3.2 3D Heat Equation

The error is clearly in Δt.

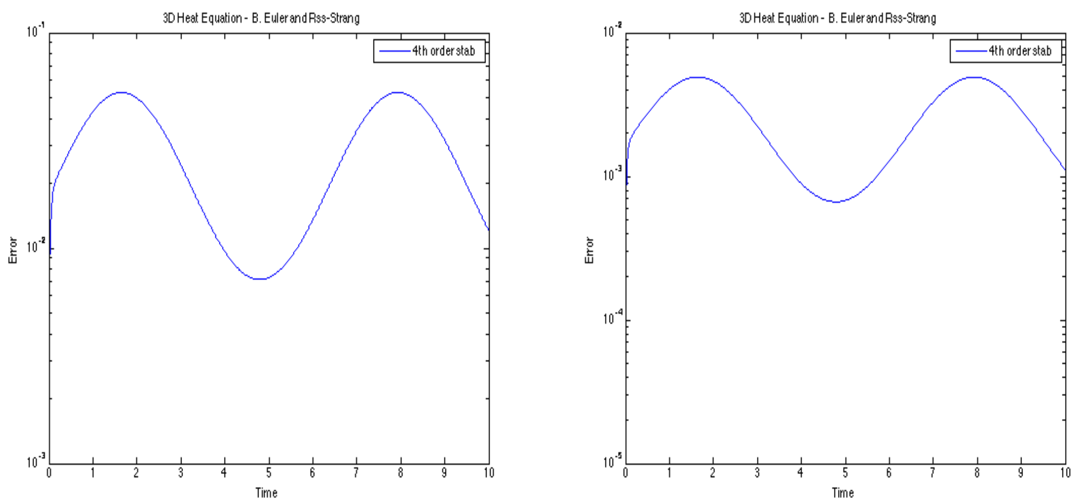

Figure 2: Solution of the 3D heat equation with $\Delta t = 0.01$, (left) and $\Delta t = 0.001$ (right) $n = 31$, $\tau = 1$

3 Allen-Cahn's equation

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

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

where

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

In [1] it was introduced the RSS-scheme

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

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

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

- *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

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

$$\frac{\partial u}{\partial n} = 0, \tag{14}$$

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

$$u(0,x) = u_0(x) \tag{16}$$

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:

$$\frac{\partial u}{\partial t} - \Delta \mu = 0, \tag{17}$$

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

$$\frac{\partial u}{\partial n} = 0, \tag{19}$$

$$\frac{\partial \mu}{\partial n} = 0, \tag{20}$$

$$u(0,x) = u_0(x) \tag{21}$$

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 Ω 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 $\lambda >> 1$

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

$$\underbrace{\text{Cahn-Hilliard equation}} \qquad \underbrace{\text{Fidelity term}} \tag{23}$$

$$\frac{\partial u}{\partial n} = 0 \quad \frac{\partial}{\partial n}\Big(\Delta u - \frac{1}{\epsilon^2} f(u)\Big) = 0, \tag{24}$$
$$u(0,x) = u_0(x) \tag{25}$$

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 $\lambda >> 1$
- The Cahn-Hilliard flow has as effect to connect the fields inside D
- here ϵ 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

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + A\mu^{(k+1)} = 0, \tag{26}$$
$$\mu^{(k+1)} = \epsilon A u^{(k+1)} + \frac{1}{\epsilon} f(u^{(k)}), \tag{27}$$

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

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau B(\mu^{(k+1)} - \mu^{(k)}) + A\mu^{(k)} = 0, \tag{28}$$
$$\mu^{(k+1)} = \epsilon\tau B(u^{(k+1)} - u^{(k)}) + \epsilon A u^{(k)} + \frac{1}{\epsilon} f(u^{(k)}). \tag{29}$$

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

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

and on the other hand

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

Taking the difference of the last two identities, we obtain

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

where

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

The scheme is then stable if $R^{k+1} < R^k$. Hence the stability conditions. ■

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 od Numerical Mathematics, Vol. 88, (1989) Birkhäuser.

[3] C.M. Elliott and A. Stuart The global dynamics of discrete semilinear parabolic equations. SIAM J. Numer. Anal. 30 (1993) 1622–1663.

[4] J. Shen, X. Yang, Numerical Approximations of Allen-Cahn and Cahn-Hilliard Equations. DCDS, Series A, (28), (2010), pp 1669–1691.