Stabilized Schemes for Phase Fields Models

M. Brachet* J.-P. Chehab†

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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

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

where 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 [4]

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 (10) and (13) 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 (1) is unconditionally stable*
- *If* $\tau < \frac{\beta}{2}$, *then (1) 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 (1) 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. ■ The RSS-Gear's scheme can beg implemented as follows:

Algorithm 1 : RSS-Gear

1: **for** $k = 0, 1, \cdots$ until convergence **do**
2: **Solve** $(3.Id + \tau 2\Delta t B)\delta = -2\Delta t(u^{(k)} - u^{(k-1)} + Au^{(k)})$
3: **Set** $u^{(k+1)} = u^{(k)} + \delta$
4: **end for**

Of course, more general RSS version of time scheme can be obtained by approaching directly the implicit part of the iteration matrix for instance for the Crank-Nicolson scheme:

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \frac{1}{2}(Au^{(k+1)} + Au^{(k)}) = 0, \tag{5}$$
$$\tag{6}$$

This scheme can be rewritten as

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \frac{1}{2}(Au^{(k+1)} - Au^{(k)}) = -Au^{(k)}, \tag{7}$$
$$\tag{8}$$

and implemented following the two steps:

- Solve $(Id + \frac{\Delta t}{2}A)\delta = -\Delta t A u^{(k)}$
- Set $u^{(k+1)} = u^{(k)} + \delta$

The RSS scheme consists in replacing the implicit part by a simplified one using a preconditioning matrix B of A, namely

- Solve $(Id + \tau\frac{\Delta t}{2}B)\delta = -\Delta t A u^{(k)}$
- Set $u^{(k+1)} = u^{(k)} + \delta$

The implementation of the RSS-CN scheme reads as

Algorithm 2 : RSS Crank-Nicolson

1: **for** $k = 0, 1, \cdots$ until convergence **do**
2: **Solve** $(Id + \frac{\tau\Delta t}{2}B)\delta = -\Delta t A u^{(k)}$
3: **Set** $u^{(k+1)} = u^{(k)} + \delta$
4: **end for**

This scheme is consistent with the classical CN one since, for $\tau = 1$ and $B = A$ the original method is recovered. We can easily derive the following stability result for this scheme PROVE STABILITY RESULT FOR RSS CN

Proposition 2.3 *Assume that A and B are two SPD matrices. Under hypothesis (4), we have the following stability conditions:*

- *If $\tau \geq \beta$, the schemes (10) and (13) are unconditionally stable (i.e. stable $\forall\ \Delta t > 0$)*
- *If $\tau < \beta$, then the scheme is stable for $0 < \Delta t < \dfrac{2}{\left(1 - \frac{\tau}{\beta}\right)\rho(A)}$.*

Proof. It suffices to replace τ by $\frac{\tau}{2}$ in Proposition (2.1). ■

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

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

$$\frac{u^{(k+1)} - u^{(k+1/2)}}{\Delta t} + \tau_2 B_2(u^{(k+1)} - u^{(k+1/2)}) = -A_2 u^{(k+1/2)}, \tag{10}$$

and the Strang's Splitting

$$\frac{u^{(k+1/3)} - u^{(k)}}{\Delta t/2} + \tau_1 B_1(u^{(k+1/3)} - u^{(k)}) = -A_1 u^{(k)}, \tag{11}$$

$$\frac{u^{(k+2/3)} - u^{(k+1/3)}}{\Delta t} + \tau_2 B_2(u^{(k+2/3)} - u^{(k+1/3)}) = -A_2 u^{(k+1/3)}, \tag{12}$$

$$\frac{u^{(k+1)} - u^{(k+2/3)}}{\Delta t/2} + \tau_1 B_1(u^{(k+1)} - u^{(k+2/3)}) = -A_1 u^{(k+2/3)}, \tag{13}$$

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

$$\frac{u^{(k+i/m)} - u^{(k+(i-1)/m)}}{\Delta t} + \tau_i B_i(u^{(k+i/m)} - u^{(k+(i-1)/m)}) = -A_i u^{(k+(i-1)/m)}, \tag{14}$$

We recall that

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

Proposition 2.4 *Under hypothesis (4), we have the following stability conditions:*

- *If* $\tau_i \geq \frac{\beta_i}{2}, i = 1, 2$ *the scheme (10)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* $0 < \Delta t < Min\left(\frac{2}{\left(1 - \frac{2\tau_1}{\beta_1}\right)\rho(A_1)}, \frac{2}{\left(1 - \frac{2\tau_2}{\beta_2}\right)\rho(A_2)}\right)$.

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

2.3 Numerical illustrations

Before presenting the stabilized schemes for phase fields models, we give hereafter some numerical illustration son linear problems when discretized in space by finite differences compact schemes, focusing on Neumann boundary conditions. We propose as in [4] to use a (lower) second order discretization matrix for preconditioning the underlining matrices. We first consider the Ellptic Neumann problem then the Heat equation.

2.3.1 Finite difference Preconditioning for compact schemes and the Neumann problem

WE BRIEFFLY RECALL SOME RESULTS OF BRACHET-CHEHAB AND POINT OUT THE HOMOGENEOUS NEUMANN BC. AN ILLUSTRATION IS THE SOLUTION OF THE NEUMANN PROBLEM (2D, 3D)

We give hereafter numerical results on the solution of 2D and 3D Neumann problems

$$\alpha u - \Delta u = f \quad \text{in } \Omega =]0,1[^{2,3}, \tag{15}$$

$$\frac{\partial u}{\partial n} = 0 \qquad \text{on } \partial\Omega \tag{16}$$

when discretized by fourth order compact schemes. The preconditioning matrix the usual five point scheme finite difference schemes. A random r.h.s `b=1-2*rand(N,1)` is chosen so in order to have the presence of a late number of frequencies. The initial data is $u = 0$, the tolerance parameter 10^{-10}, we took $\alpha = \beta = 1$ but the results are very close for other values of these parameters. The result we report is the maximum number of external iterations to convergence, on 5 independent numerical resolutions, the number of discretization point per direction n is reported as (n). The stiffnes matrices are of respective sizes $n^2 \times n^2$ (2D problem) and $n^3 \times n^3$ (3D problem). The preconditioning systems are solved using the cosine fft.,

Of course, due the implicity of the scheme, the fourth order discretization matrix A of $-\Delta$ is nonsymmetric while the preconditioning matrix B is. However, in practice the RSS method is still efficient. This is due to the small size of the skewsymmetric part of A, see [4].

Problem	# it. (n)	# it. (n))	# it. (n)	# it. (n)	#it. (n)	#it. (n)
Poisson 2D	16 (n=15)	15 (n=31)	14 (n=63)	13 (n=127)	12 (n=255)	(n=511)
Poisson 3D	30 (n=15)	30 (n=31)	(n=63)			

Table 1: Solutions of 2D and 3D Neumann problem with GMRES and second order preconditioner

2.3.2 Heat Equation

For the 2D and the 3D heat equation, we here compare different RSS schemes presented above (ADI, Gear's, CN and Euler's) in order to illustrate the stability results and to point out the owl of the stabilization parameter τ.

USE THE MATLAB CODES IN THE DIRECTORY ADI_MATLAB. see program `chaleur_2D_splitting.m`

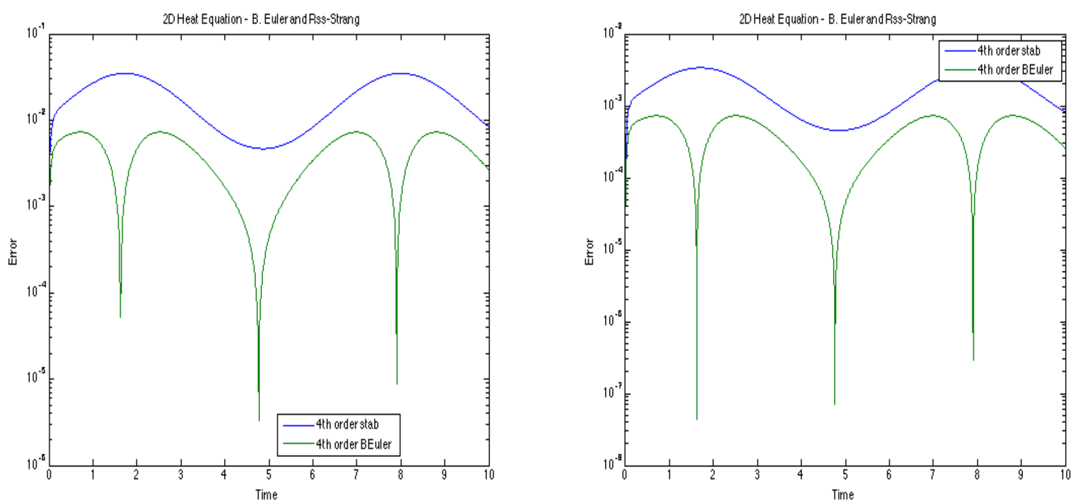

Figure 1: Solution of the heat equation with $\Delta t = 0.01$, (left) and $\Delta t = 0.001$ (right) $n = 31$, $\tau = 1$

The error is clearly in Δt.

We now consider the 3D Heat equation, with Homogeneous Neumann BC.
The error is clearly in Δt.

- Solution of the Neumann Problem with Preconditioned GMRES `solve Neum 3D CS.m`
- Neumann Problem `test dct neumann.m`

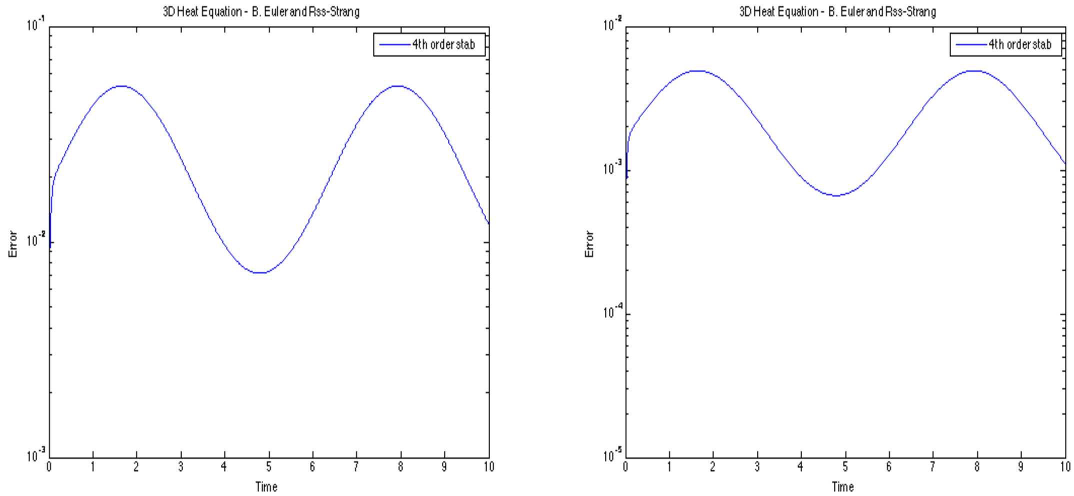

Figure 2: Solution of the 3D heat equation with $\Delta t = 0.01$, (left) and $\Delta t = 0.001$ (right) $n = 31$, $\tau = 1$

- Heat equation `test chaleur.m`
-

3 Allen-Cahn's equation

3.1 The Models

3.1.1 Phase transition equation

The Allen-Cahn equation

$$\frac{\partial u}{\partial t} + M(-\Delta u + \frac{1}{\epsilon^2} f(u)) = 0 \tag{17}$$

$$\frac{\partial u}{\partial n} = 0 \tag{18}$$

$$u(0, x) = u_0(x), \tag{19}$$

describes the process of phase separation in iron alloys [Allen-Cahn, 1972, 1973], including order-disorder transitions: M is the mobilty (taken to be 1 for simplicity), $F = \int_{-\infty}^{u} f(v)dv$ is the free energy, u is the (non-conserved) order parameter, ϵ is the interface length. The homogenous Neumann boundary condition implies that there is not a loss of mass outside the domain Ω. It is important to note that here is a competition between the potential term and the diffusion term: regularization in phase transition.

3.1.2 Inpainting

$$\frac{\partial u}{\partial t} = \nabla . \left(\frac{\nabla u}{|\nabla u|} \right) + \lambda_0 \chi_{x \in \Omega \setminus \Omega_0} (f(x) - c) = 0, \quad x \in \Omega, t > 0 \tag{20}$$

$$\frac{\partial u}{\partial n} = 0, \qquad \partial \Omega, t > 0 \tag{21}$$

see [12]

3.1.3 Image segmentation

$$\epsilon \frac{\partial u}{\partial t} = \epsilon \nabla . \left(g(|\nabla G_\sigma * U_0|) \nabla u \right) + g(|\nabla G_\sigma * U_0|) \left(\frac{1}{\epsilon} f_0(u) + \epsilon F |\nabla u| \right), \quad \Omega \tag{22}$$

$$\frac{\partial u}{\partial n} = 0, \quad \partial \Omega \tag{23}$$

Her $\epsilon > 0$, $f_0(u) = \frac{1}{2} au(1-u)(u-1/2)$ with $a >> 0$ is derived from the double well potential ; finally F is bounded continuous function of x, g is $\mathcal{C}^\infty$ and positive and $U_0 \in L^\infty$. We impose furthermore the conditions

$$0 \leq \gamma_1 \leq g(x) \leq \gamma 2$$

We refer the reader to [1, 11]

3.2 Energy diminuishing schemes

We here first recall somme schemes and their stability conditions, see also [4]. First of all, we consider a semi-implicit RSS-Scheme applied to the pattern evolution A-C equation:

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau B(u^{(k+1)} - u^{(k)}) + \frac{1}{\epsilon^2} f(u^{(k)}) = -Au^{(k)}. \tag{24}$$

We set $E(u) = \frac{1}{2} < Au, u > +\frac{1}{\epsilon^2} < F(u), \mathbf{1} >$, where F is a primitive of f that we choose such that $F(0) = 0$; $\mathbf{1}$ is the vector whose components are all equal to 1. We say that the scheme is energy decreasing if

$$E(u^{(k+1)}) < E(u^{(k)}).$$

We have the stability result, [4]:

Theorem 3.1 *Assume that f is $\mathcal{C}^1$ and $| f' |_\infty \leq L$. We have the following stability conditions*

- *If $\tau \geq \frac{\beta}{2}$ then*
  - *if $\left(\frac{\tau}{\beta} - \frac{1}{2}\right)\lambda_{min} - \frac{L}{2\epsilon^2} \geq 0$ then the scheme is unconditionally stable,*
  - *if $\left(\frac{\tau}{\beta} - \frac{1}{2}\right)\lambda_{min} - \frac{L}{2\epsilon^2} < 0$ then the scheme is stable for*

$$0 < \Delta t < \frac{1}{\frac{L}{2\epsilon^2} - \left(\frac{\tau}{\beta} - \frac{1}{2}\right)\lambda_{min}},$$

- *If $\tau < \frac{\beta}{2}$ then the scheme is stable for*

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

Of course, it gives a hard time step reduction. A way to overcome this drawback is to consider directly AC equation as a gradient system with a natural diminishing energy property. A first inconditionnally stable scheme is ([7, 8])

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + Au^{(k+1)} + \frac{1}{\epsilon^2} DF(u^{(k)}, u^{(k+1)}) = 0, \tag{25}$$

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 [4] it was introduced the RSS-scheme

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau B(u^{(k+1)} - u^{(k)}) + DF(u^{(k+1)}, u^{(k)}) = -Au^{(k)} \tag{26}$$

which enjoys of the following stability condition, see [4] for the proof.

Proposition 3.2 *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*

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

Another way to obtain a unconditionally stable scheme is to use the so-called convex splitting, [9, 6] We follow [9] and make the assumptions

$$\begin{array}{ll} F(u) \geq 0, & \forall u \in I\!R^n, \\ F(u) \to +\infty & \text{ as } \|u\| \to +\infty, \\ < J(\nabla F)(u)u, u >\geq \lambda & \forall u \in I\!R^n. \end{array} \tag{27}$$

We now make the following additional hypothesis ($\mathcal{C}$)

i. We assume that F can be splitted as follows

$$F(u) = F_c(u) - F_e(u),$$

where $F_* \in \mathcal{C}^2(I\!R^n, I\!R)$, $* = c$ or $* = e$.

ii. F_* is strictly convex in $I\!R^n$, $* = c$ or $* = e$.

iii. $< [\nabla F_e(u)]u, u >\geq -\lambda$, $\forall u \in I\!R^n$.

We can now state the stability result:

Theorem 3.3 *Consider the RSS-convex splitting scheme*

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau B(u^{(k+1)} - u^{(k)}) + \nabla F_c(u^{(k+1)}) = -Au^{(k)} + \nabla F_e(u^{(k)}), \tag{28}$$

Then

- *If $(\tau\beta - \frac{1}{2}\rho(A) + \left(\hat{\lambda} - |\lambda|\right) > 0$ then the scheme is unconditionally stable*
- *Else it is stable under condition*

$$0 < \Delta t < \frac{1}{(\frac{1}{2} - \tau\beta)\rho(A) + |\lambda| - \hat{\lambda}}.$$

3.3 Splitting schemes

We follow [11] who proposed for the Double Well potential case the scheme ($F(u) = \frac{1}{4}(1-u^2)^2$) the splitting scheme

$$\frac{u^* - u^{(k)}}{\Delta t} + \frac{1}{2}(Au^* + Au^{(k)}) = 0, \tag{29}$$

$$\frac{u^{(k+1)} - u^*}{\Delta t} = \frac{u^{(k+1)} - (u^{(k+1)})^3}{\epsilon^2} \tag{30}$$

The last equation ca be simplified since it correspond to a one-step approximation by backward Euler's to the differential equation

$$\frac{du}{dt} = \frac{u - u^3}{\epsilon^3} \tag{31}$$

whose the solution is

$$u(t) = \frac{u(0)}{\sqrt{e^{-2\frac{t}{\epsilon^2}} + u(0)^2(1 - e^{-2\frac{t}{\epsilon^2}})}}$$

Hence the simplified scheme

$$\frac{u^* - u^{(k)}}{\Delta t} + \frac{1}{2}(Au^* + Au^{(k)}) = 0, \tag{32}$$

$$u^{(k+1)} = \frac{u^*}{\sqrt{e^{-2\frac{\delta t}{\epsilon^2}} + (u^*)^2(1 - e^{-2\frac{\delta t}{\epsilon^2}})}} \tag{33}$$

is rather considerers and have nice stability properties, see [11].

To implement RRS-like version of this splitting scheme it then suffices to replace the first step by a RSS-CN scheme as proposed in section 2. We then obtain the RSS-splitting scheme

Algorithm 3 : RSS splitting dor Allen Cahn

for $k = 0, 1, \cdots$ **do**
  Solve $(Id + \frac{\tau \Delta t}{2}\epsilon B)\delta = -\Delta t A u^{(k)}$
  Set $u^{(*)} = u^{(k)} + \delta$
  Set $u^{(k+1)} = \dfrac{u^*}{\sqrt{e^{-2\frac{\delta t}{\epsilon^2}} + (u^*)^2(1 - e^{-2\frac{\delta t}{\epsilon^2}})}}$
end for

SEE Program `RSSsplittingAC3DCS.m`.

It must be noted that replacing the Crank Nicolson scheme by Backward Euler schemes gives not a stable scheme.
ADD HERE A STABILITY RESULT FOR THIS SCHEME

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

$$\frac{\partial u}{\partial t} - \Delta(-\Delta u + \frac{1}{\epsilon^2} f(u)) = 0, \tag{34}$$

$$\frac{\partial u}{\partial n} = 0, \tag{35}$$

$$\frac{\partial}{\partial n}\left(\Delta u - \frac{1}{\epsilon^2} f(u)\right) = 0, \tag{36}$$

$$u(0,x) = u_0(x) \tag{37}$$

This equation enjoys of the following 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 classical way to study and to simulate CH is to decouple the equation as follows:

$$\frac{\partial u}{\partial t} - \Delta\mu = 0, \qquad \text{in } \Omega, t > 0 \tag{38}$$

$$\mu = -\Delta u + \frac{1}{\epsilon^2} f(u), \qquad \text{in } \Omega, tt > 0 \tag{39}$$

$$\frac{\partial u}{\partial n} = 0, \frac{\partial \mu}{\partial n} = 0, \qquad \text{on } \partial\Omega, t > 0 \tag{40}$$

$$u(0,x) = u_0(x) \qquad \text{in } \Omega \tag{41}$$

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 $\lambda >> 1$

$$\frac{\partial u}{\partial t} - \Delta(-\epsilon\Delta u + \frac{1}{\epsilon} f(u)) \quad + \lambda\chi_{\Omega\setminus D}(x)(u-g) = 0, \tag{42}$$

$$\underbrace{\text{Cahn-Hilliard equation}} \qquad \underbrace{\text{Fidelity term}} \tag{43}$$

$$\frac{\partial u}{\partial n} = 0 \quad \frac{\partial}{\partial n}\left(\Delta u - \frac{1}{\epsilon^2} f(u)\right) = 0, \tag{44}$$

$$u(0,x) = u_0(x) \tag{45}$$

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

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + A\mu^{(k+1)} = 0, \tag{46}$$

$$\mu^{(k+1)} = \epsilon A u^{(k+1)} + \frac{1}{\epsilon} f(u^{(k)}), \tag{47}$$

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

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

see [13] We derive the RSS-Scheme from the backward Euler's (46)-(47) by replacing $Az^{(k+1)}$ by $\tau B(z^{(k+1)} - z^{(k)}) + Az^{(k)}$ for $z = u$ or $z = \mu$. We obtain

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau B(\mu^{(k+1)} - \mu^{(k)}) + A\mu^{(k)} = 0, \tag{48}$$

$$\mu^{(k+1)} = \epsilon\tau B(u^{(k+1)} - u^{(k)}) + \epsilon A u^{(k)} + \frac{1}{\epsilon} f(u^{(k)}). \tag{49}$$

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 (48)-(51) is unconditionally stable.*

Proof. We take the scalar product of (48) with $u^{(k+1)} - u^{(k)}$ and of (51) with $\mu^{(k+1)}$. After the use of the parallelogram identity and usual simplifications, we obtain, on the one hand

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

and on the other hand

$$\begin{array}{rl}
< u^{(k+1)} - u^{(k)}, \mu^{(k+1)} > & = \tau < B(u^{(k+1)} - u^{(k)}), u^{(k+1)} - u^{(k)} > \\
& + \frac{1}{2} \big(< Au^{(k+1)}, u^{(k+1)} > - < Au^{(k)}, u^{(k)} > - < A(u^{(k+1)} - u^{(k)}), u^{(k+1)} - u^{(k)} > \big)
\end{array}$$

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. ■ We now describe the practical solution. We can write

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

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

$$\begin{cases} X_1 + \tau\Delta t B X_2 = F1, \\ -\tau\epsilon B X_1 + X_2 = F_2. \end{cases}$$

Hence

$$(Id + \tau^2\Delta t\epsilon B^2)X_2 = F_2 + \epsilon\tau B F1$$

Then,

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

We can resume the solution as

Algorithm 4 : RSS Cahn-Hilliard

```
for k = 0, 1, ··· until convergence do
    Set F_1 = −Δt A μ^(k) and F_2 = −μ^(k) + ϵ A u^(k) + (1/ϵ) f(u^(k))
    Solve (Id + τ^2 Δt ϵ B^2) δμ = F_2 + τ ϵ B F_1
    Set μ^(k+1) = μ^(k) + δμ
    Set u^(k+1) = u^(k) − τ Δt B δμ
end for
```

When considering the inpainting model, the RSS scheme can be written as

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau B(\mu^{(k+1)} - \mu^{(k)}) + A\mu^{(k)} + \lambda_0 D(u^{(k+1)} - g) = 0, \quad (50)$$

$$\mu^{(k+1)} = \epsilon\tau B(u^{(k+1)} - u^{(k)}) + \epsilon A u^{(k)} + \frac{1}{\epsilon} f(u^{(k)}). \quad (51)$$

say in the matricidal form

$$\begin{pmatrix} Id + \delta t\lambda_0 D & \tau\Delta t B \\ -\epsilon\tau B & Id \end{pmatrix} \begin{pmatrix} u^{(k+1)} - u^{(k)} \\ \mu^{(k+1)} - \mu^{(k)} \end{pmatrix} = \begin{pmatrix} \Delta t(\lambda_0 D(g - u^{(k)}) - Au^{(k)}) \\ \epsilon Au^{(k)} + \frac{1}{\epsilon} fF(u^{(k)}) - \mu^{(k)} \end{pmatrix}$$

The implementation of the scheme reads as

Algorithm 5 : RSS Cahn-Hilliard for implainting

1: **for** $k = 0, 1, \cdots$ until convergence **do**
2: **Set** $F_1 = \Delta t(\lambda_0 D(g - u^{(k)}) - Au^{(k)})$
3: **Set** $F_2 = -\mu^{(k)} + \epsilon Au^{(k)} + \frac{1}{\epsilon} f(u^{(k)})$
4: **Solve** $(Id + \lambda_0 D + \tau^2\Delta t\epsilon B^2)\delta = F_1 - \tau\Delta t B F_2$
5: **Set** $\delta\mu = F_2 + \epsilon\tau B\delta$
6: **Set** $u^{(k+1)} = u^{(k)} + \delta$
7: **Set** $\mu^{(k+1)} = \mu^{(k)} + \delta\mu$
8: **end for**

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

- ALLEN CAHN + SPLITTING + CN-RSS ON THE LINEAR PART `RSS splitting AC3D CS.m` (WITH FFT)
- ALLEN CAHN 3D + EULER-RSS WITH SPLITTING IN EVERY DIRECTION `AC 3D RSS.m` (WITHOUT FFT)

- ALLEN CAHN 2D + FFT Allen Cahn fft.m (WITHOUT CS)

APPLICATIONS : PATTERNS, IMAGE RESTAURATION (???) see `http://fr.mathworks.com/discove` see [11] p 1604.

5.2.1 Patterns dynamics

5.2.2 Image segmentation

5.3 Cahn-Hilliard equation

USE THE (NON RSS BUT STABILIZED AS IN BERTOZZI PAPER) CODEs IN THE DIRECTORY CH_INPAINTING

- PATTERNS COMPUTATION: IMPLICIT EXPLIT SCHEME WITH FFT 3DCahn Hilliard fft.m (NON RSS)
- INPAINTING 2D test CH2D RSS solver1.m (without fft), see [5], p22

APPLICATIONS: 2D (3D) PATTERNS,
2D, 3D INPAINTING (SEE WHATEN et al)

5.3.1 Patterns dynamics

Method	N	ϵ	Δt	τ	$[0,T]$	$\|error\|_\infty$	CPU
RSS	$N=64$	0.5	10^{-3}	5	$[0,1]$	0.0194	7.358853
RSS	$N=64$	0.5	10^{-3}	2	$[0,1]$	0.0084	7.196025
Classic	$N=64$	0.5	10^{-3}		$[0,1]$	0.0047	1661.661410
RSS	$N=64$	0.5	10^{-2}	2.2	$[0,1]$	0.0773	0.795797
Classic	$N=64$	0.5	10^{-2}		$[0,1]$	0.0486	157.812224

Table 2: 2D Allen-Cahn equation: simulation of patterns - RSS-semi-implicit scheme vs classic semi-implicit scheme, exact solution is $u(x,y,t) = \cos(\pi x)\cos(\pi y)\exp(sin(3\pi t))$, $\Omega = [0,1]^2$ pgm Allen Cahn fft RSS.m

Method	N	ϵ	Δt	τ	$[0,T]$	$\|error\|_\infty$	CPU
RSS	$N=32$	0.5	10^{-3}	5	$[0,1]$	5.960^{-2}	94.874912
RSS	$N=32$	0.5	10^{-3}	2	$[0,1]$	$3.03\ 10^{-2}$	94.874912
Classic	$N=32$	0.5	10^{-3}		$[0,1]$	$2.1\ 10^{-2}$	210.545565
RSS	$N=32$	0.5	10^{-2}	2	$[0,1]$	0.3123	9.495254
RSS	$N=32$	0.5	10^{-2}	1.9	$[0,1]$	0.3066	9.819845
Classic	$N=32$	0.5	10^{-2}		$[0,1]$	0.2586	21.360027

Table 3: 3D Allen-Cahn equation: simulation of patterns - RSS-Lie splitting scheme vs classic Lie -splitting scheme, exact solution is $u(x,y,z,t) = \cos(\pi x)\cos(\pi y)\cos(\pi z)\exp(sin(3\pi t))$, $\Omega = [0,1]^3$ pgm Allen Cahn fft.m

5.3.2 Inpainting

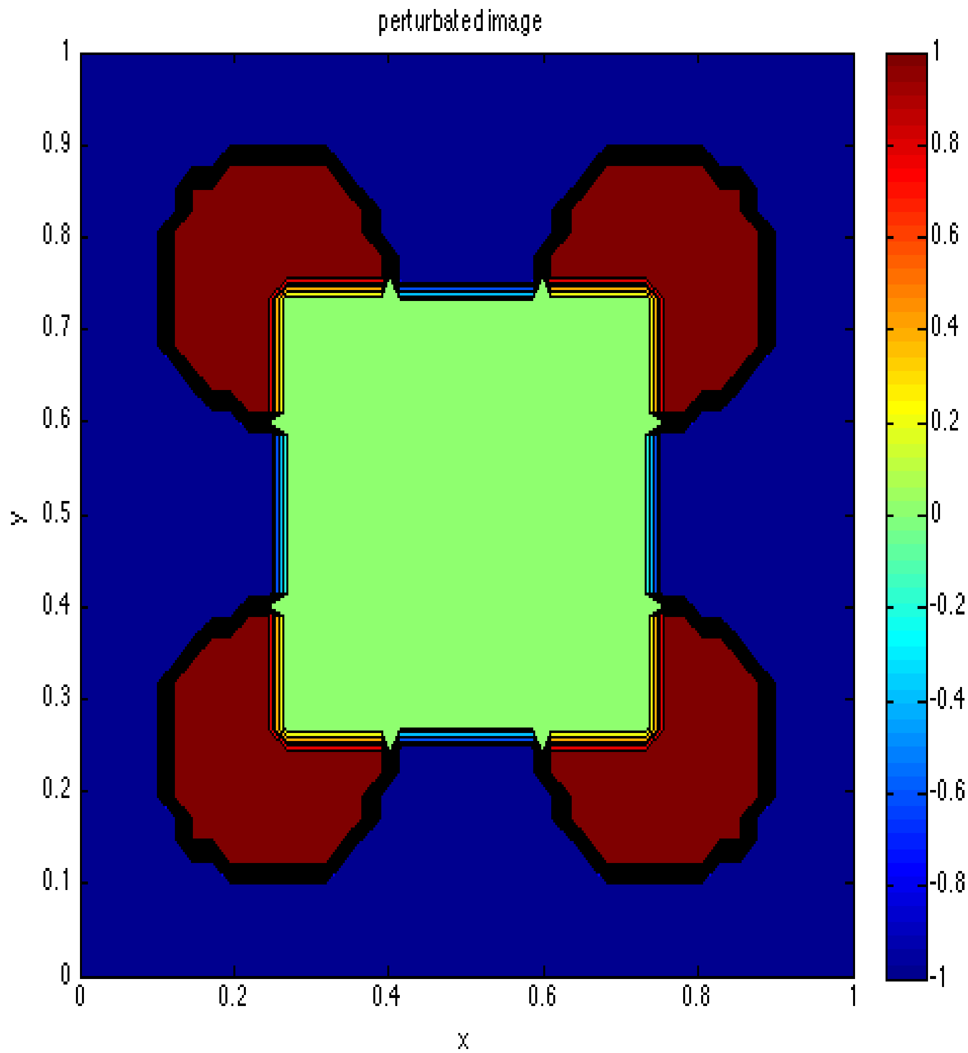

Figure 3: Inpainting with C-H. $\Delta t = 0.01$, $\epsilon = 0.5$, $\tau = 2.2$, N=64$-Initialinpaintedimage$

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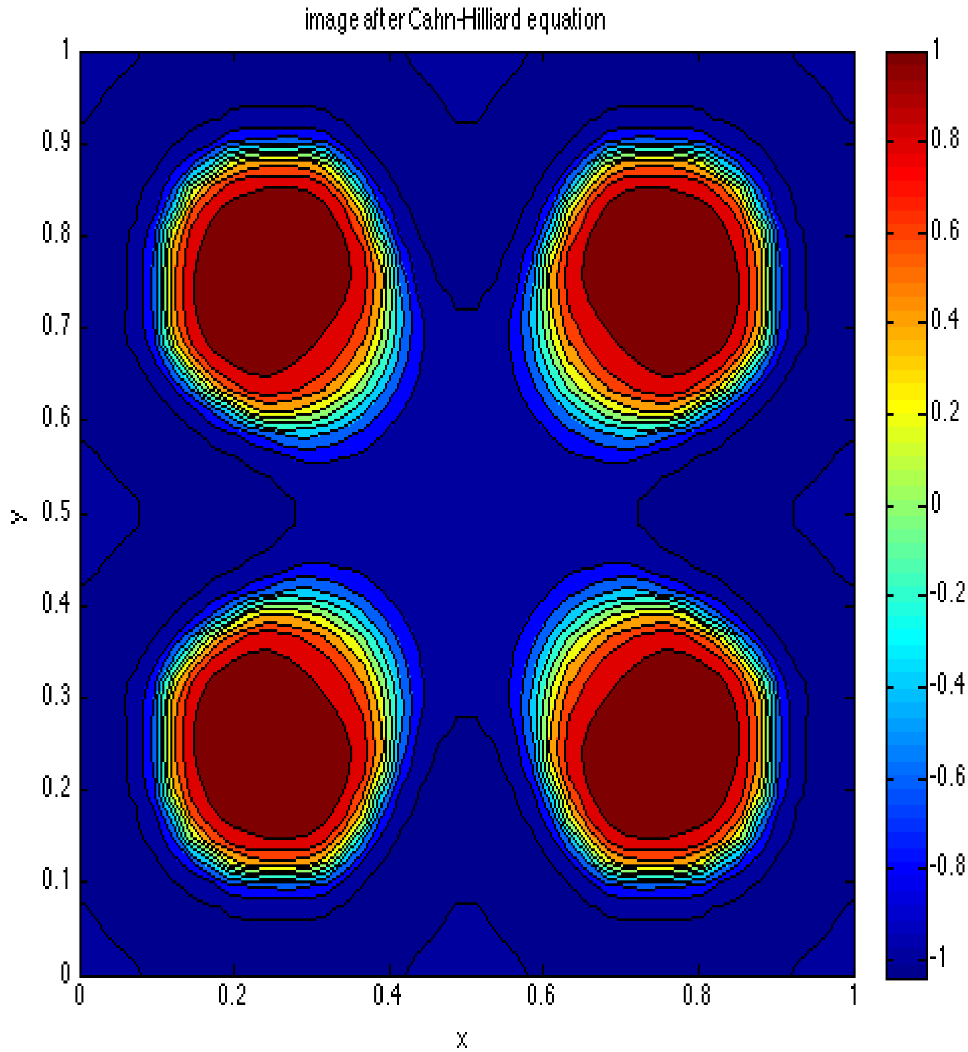

Figure 4: Inpainting with C-H. $\Delta t = 0.01$, $\epsilon = 0.5$, $\tau = 2.2$, N=64$-finalimagecpu = 2540.61$

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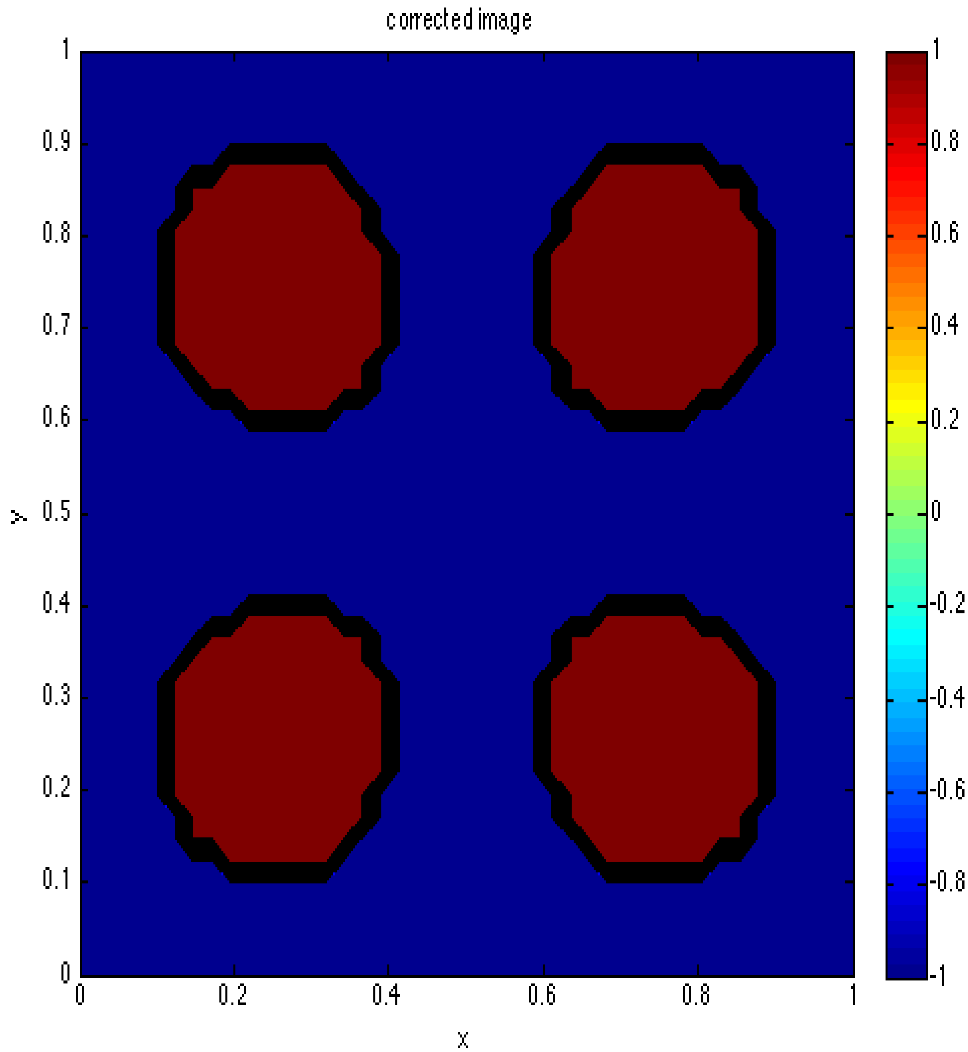

Figure 5: Inpainting with C-H. $\Delta t = 0.01$, $\epsilon = 0.5$, $\tau = 2.2$, N=64$-finaltresholdedimagecpu =$ 2540.61

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