Stabilized Time Schemes for High Accurate Finite Differences Solutions of Nonlinear Parabolic Equations

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Outline

Motivation

Consider the dynamical system (obtained after discretization in space)

$$\begin{aligned} \frac{du}{dt} + Au = f, \\ u(0) = u_0, \end{aligned} \tag{1}$$

A : stiffness matrix (SPD)

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- Explicit time schemes (such as Forward Euler''s) produce fast iterations but suffer from hard time step restriction

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$$0 < \Delta t < \frac{2}{\rho(A)}$$

- Implicit time schemes (such as Backward Euler's) are stable but need to solve a linear system at each step, sometimes with a full matrix.

Solution: Residual Smoothing Scheme (RSS) Schemes

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$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \quad \underbrace{\tau B(u^{(k+1)} - u^{(k)})}_{\text{Stabilization term}} \quad + Au^{(k)} = f, \tag{2}$$

Here $\tau > 0$ can be tuned to enhance the stability

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Considered independently by A. Cohen-Averbuch-Israeli ('98, unpublished) and by Costa ('98), then Costa-Dettori-Gottlieb-Temam ('01) (Fourier point of view) ; Studied by Ribot ('03) then Ribot-Schatzman('11); C-Costa ('02,'03, '04) applied the method with hierarchical pre conditioners in Finite Differences

Natural questions and outline

- Give a general approach for nonlinear parabolic equations
- Give conditions on B and τ to guarantee enhanced stability conditions (as compared to Forward and Backward Euler's)
- Accuracy of the schemes
- Situations in which the approach is interesting (two different levels of discretization)
- Applications: simulations of nonlinear parabolic PDE

$$\frac{du}{dt} + F(u) = 0, t > 0, \tag{3}$$

$$u(0) = u_0, \tag{4}$$

here $F : \mathbb{R}^N \to \mathbb{R}^N$ is a regular map
The backward Euler's scheme reads

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

Now writing

$$F(u^{(k+1)}) \simeq F(u^{(k)}) + F'(u^{(k)})(u^{(k+1)} - u^{(k)}),$$

where $F'(u^{(k)})$ denotes the differential of F at $u^{(k)}$, we get

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + F'(u^{(k)})(u^{(k+1)} - u^{(k)}) + F(u^{(k)}) = 0,$$

Finally

$$u^{(k+1)} = u^{(k)} - \Delta t(Id + \Delta t F'(u^{(k)}))^{-1} F(u^{(k)}).$$

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$\Longrightarrow$ with $\Phi(v) = v - u^{(k)} + \Delta t F(v)$: $u^{(k+1)}$ is the first iterate of Newton-Raphson applied to $\Phi(v)$ when starting from $u^{(k)}$

Fully Nonlinear RSS

Now, if we replace $F'(u^{(k)})$ by a preconditioner τB_k, we find

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \quad \tau \underbrace{B_k(u^{(k+1)} - u^{(k)})}_{\text{Global stabilization}} \quad + F(u^{(k)}) = 0, \tag{5}$$

and $u^{(k+1)}$ is thus the first iteration of a quasi Newton Method applied to $\Phi(v)$ when starting from the initial guess $u^{(k)}$.

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and $u^{(k+1)}$ is thus the first iteration of a quasi Newton Method applied to $\Phi(v)$ when starting from the initial guess $u^{(k)}$.
The efficiency of this stabilized scheme is closely related to the cost of the computation of the pre-conditioner of the jacobian matrix which changes at each iteration: use technique of updating factorizations (Calgaro-C-Saad, Bellavia et al)

Semi Nonlinear RSS

if $F(u)$ can be expressed as $F(u) = Au + f(u)$, we define the scheme

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \quad \tau \underbrace{B(u^{(k+1)} - u^{(k)})}_{\text{Stabilization of the linear part}} \quad + F(u^{(k)}) = 0, \tag{6}$$

where B is a pre-conditioner of A.

Assume A and B are SPD.

$$(\mathcal{H}) \qquad \alpha < Bu, u > \leq < Au, u > \leq \beta < Bu, u >, \ \forall u \in \mathbb{R}^N.$$

α and β can depend on the dimension N. If not the matrix B is said to be an inconditionnal pre-conditioner of A.

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Theorem

Under hypothesis $\mathcal{H}$, we have the following stability conditions:

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

Theorem

We consider the two sequences

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

and

$$\frac{v^{(k+1)} - v^{(k)}}{\Delta t} + Av^{(k+1)} = f,$$

with $u^{(0)} = v^{(0)}$. *We let* $M = Id - \Delta t(Id + \tau\Delta tB)^{-1}A$ *and we assume that* $\| M \| < 1$, *then, there exists* $\gamma \in [0, 1[$ *such that*

$$\| u^{(k)} - v^{(k)} \| \leq \Delta t^2 \| \tau B - A \| \frac{1}{1-\gamma} \| f - Av^{(0)} \|, \forall k \geq 0.$$

As a consequence RSS is first order accurate in time

Consider the reaction-diffusion equation (of Allen-Cahn's type):

$$\frac{\partial u}{\partial t} - \Delta u + \frac{1}{\epsilon^2} f(u) = 0, \quad x \in \Omega, t > 0, \tag{7}$$

$$\frac{\partial u}{\partial n} = 0 \qquad \partial\Omega, t > 0, \tag{8}$$

$$u(x, 0) = u_0(x) \qquad x \in \Omega, \tag{9}$$

where $\epsilon > 0$ is a given parameter. The (semi nonlinear) RSS scheme applied to the discretized scheme writes as

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau B(u^{(k+1)} - u^{(k)}) = -Au^{(k)} - \frac{1}{\epsilon^2} f(u^{(k)}). \tag{10}$$

We set $E(u) = \frac{1}{2} < Au, u > + \frac{1}{\epsilon^2} < F(u), \mathbf{1} >$, where F is a primitive of f.
The scheme is energy decreasing if

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

If $F \geq 0$ (this will be the case in the applications) then $E \geq 0$ so the stability is obtained.

Theorem

Assume that f is $\mathcal{C}^1$ and $\mid f' \mid_\infty \leq L$. We have the following stability conditions (energy diminishing conditions)

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

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

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

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

RSS-scheme is only first order accurate and a classical way to improve the accuracy is to use Richardson extrapolation, as follows (see A. Cohen *et al*):

$$\frac{du}{dt} = F(u),$$

by the forward Euler scheme defines the iterations

$$u^{k+1} = u^k + \Delta t F(u^k) = G_{\Delta t}(u^k).$$

The smoothed sequence is defined by

$$\begin{aligned} v_1 &= G_{\Delta t}(u^k), \\ v_{2,0} &= G_{\Delta t/2}(u^k), \\ v_{2,1} &= G_{\Delta t/2}(v_{2,0}), \\ u^{k+1} &= 2v_{2,1} - v_1. \end{aligned}$$

It is second order accurate in time.

Below the Extrapolated RSS scheme

Algorithm 1 : Extrapolated RSS Scheme

$u^{(0)}$ given
for **do**$k = 0, 1, \cdots$ until convergence
  Solve $(Id + \tau \frac{\Delta t}{2} B) v_1 = -\frac{\Delta t}{2} F(u^{(k)})$,
  Set $u_1 = u^{(n)} + v_1$,
  Solve $(Id + \tau \frac{\Delta t}{2} B) v_2 = -\frac{\Delta t}{2} F(u_1)$,
  Set $u_2 = u_1 + v_2$,
  Solve $(Id + \tau \Delta t B) v_3 = -\Delta t F(u^{(k)})$,
  Set $u_3 = u^{(n)} + v_3$,
  Set $u^{(k+1)} = 2u_2 - u_3$.
end for

Ribot and Schatzman ('11) have studied the general Richardson extrapolation in the infinite dimensional case (A and B are operators).

Gear's Scheme $\frac{3u^{(k+1)}-4u^{(k)}+u^{(k-1)}}{2\Delta t}+Au^{(k+1)}=0$

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

- If $\tau \geq \frac{\beta}{2}$, then the scheme is unconditionally stable
- If $\tau < \frac{\beta}{2}$, then the scheme is table when $0<\Delta t<\dfrac{2}{\rho(A)(1-\frac{2\tau}{\beta})}$

Crank Nicolson's Scheme $\frac{u^{(k+1)}-u^{(k)}}{\Delta t}+\frac{1}{2}(Au^{(k+1)}+Au^{(k)})=0$

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

- If $\tau \geq \beta$, the scheme is unconditionally stable
- If $\tau < \beta$, then the scheme is stable for $0<\Delta t<\dfrac{2}{\left(1-\frac{\tau}{\beta}\right)\rho(A)}$.

Lie (or Strang) Splitting

$$\frac{u^{(k+1/2)}-u^{(k)}}{\Delta t}+\tau_1 B_1(u^{(k+1/2)}-u^{(k)})=-A_1u^{(k)}, \quad (11)$$

$$\frac{u^{(k+1)}-u^{(k+1/2)}}{\Delta t}+\tau_2 B_2(u^{(k+1)}-u^{(k+1/2)})=-A_2u^{(k+1/2)}, \quad (12)$$

and the Strang's Splitting

$$\frac{u^{(k+1/3)}-u^{(k)}}{\Delta t/2}+\tau_1 B_1(u^{(k+1/3)}-u^{(k)})=-A_1u^{(k)}, \quad (13)$$

$$\frac{u^{(k+2/3)}-u^{(k+1/3)}}{\Delta t}+\tau_2 B_2(u^{(k+2/3)}-u^{(k+1/3)})=-A_2u^{(k+1/3)}, \quad (14)$$

$$\frac{u^{(k+1)}-u^{(k+2/3)}}{\Delta t/2}+\tau_1 B_1(u^{(k+1)}-u^{(k+2/3)})=-A_1u^{(k+2/3)}, \quad (15)$$

We have the same type of stability conditions as for RSS Euler's scheme.

Compact Scheme (Lele's approach, '92)

- A way to obtain a high level of accuracy with a finite difference scheme (spectral-like resolution)
- Approaching a linear operator (differentiation, interpolation) by a rational (instead of polynomial-like) finite differences scheme
- Let $U = (U_1, \cdots, U_n)^T$ denotes a vector whose the components are the approximations of a regular function u at (regularly spaced) grid points $x_i = ih$, $i = 1, \cdots, n$. We compute approximations of $V_i = \mathcal{L}(u)(x_i)$ as solution of a system

$$P.V = QU,$$

so the approximation matrix is formally $B = P^{-1}Q$.

- Fourth order scheme for the first derivative

$$P = tridiag(\frac{1}{4}, 1, \frac{1}{4}), Q = \frac{1}{2h}\begin{pmatrix} a_1 & a_2 & a_3 & a_4 & \\ -\frac{3}{2} & 0 & \frac{3}{2} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{3}{2} & 0 & \frac{3}{2} \\ & -a_4 & -a_3 & -a_2 & -a_1 \end{pmatrix},$$

with $a_1 = -2$, $a_2 = 3$, $a_3 = -\frac{2}{3}$ and $a_4 = \frac{1}{8}$.

- Fourth order scheme for the second derivative

$$P = tridiag(\frac{1}{10}, 1, \frac{1}{10}), Q = \frac{1}{h^2}\begin{pmatrix} a_1 & a_2 & a_3 & a_4 & a_5 & & \\ -\frac{6}{5} & \frac{12}{5} & -\frac{6}{5} & & & & \\ & -\frac{6}{5} & \frac{12}{5} & -\frac{6}{5} & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -\frac{6}{5} & \frac{12}{5} & -\frac{6}{5} & \\ & & & & -\frac{6}{5} & \frac{12}{5} & -\frac{6}{5} \\ & & a_{N-4} & a_{N-3} & a_{N-2} & a_{N-1} & a_N \end{pmatrix}$$

here the constant a_1, a_2, a_3, ... are given by

$$a_1 = -\frac{67}{60}, a_2 = -\frac{7}{12}, a_3 = \frac{13}{10}, a_4 = -\frac{61}{120}, a_5 = \frac{1}{12}.$$

Passage to higher dimension by tensorial product: if A_{xx}^N denotes the discretization matrix on $[0,1]$ associated to Dirichlet Boundary conditions, using N internal discretization points, then

$$Id \otimes A_{xx}^N$$

We denote by A_2 the laplacian matrix associated to the usual Second order FD scheme (3 pts in 1D, 5 pts in 2D, 7 points in 3D) and by A_4 the one associated to 4th order CS

$$\text{2D laplacian matrix : } Id \otimes A_{xx}^N + A_{yy}^N \otimes Id$$

Application to the solution of Poisson Problem (H.D.BC)

Let A_2 (resp. A_4) be the second order (resp. the fourth order) discretization matrix of $-\Delta$ on a regular grid composed of N internal points per direction.
A natural idea is to use A_2 (B) as a preconditioner of A_4 (A) (C '98)

- Multiplication of A_4 by a vector needs to solve additional linear systems
- A_2 is sparse: (cheap) sparse factorization techniques can be used to precondition A_2 then A_4 and then solve efficiently the linear system in A_4; notice that fast solvers as Sine-FFT can be used also

Pb	# it. (n)	# it. (n)	# it. (n)	# it. (n)	#it. (n)	#it. (n)
2D	12 (n=15)	11 (n=31)	10 (n=63)	10 (n=127)	9 (n=255)	8 (n=511)
3D	12 (n=15)	11 (n=31)	11 (n=63)			

Table : Solutions of 2D and 3D Poisson problem with GMRES, 4th order CS discretization and second order preconditioner

Remark : A_4 is not symmetric, so the previous stability results do not apply !

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Remark : A_4 is not symmetric, so the previous stability results do not apply !
In fact, it works while the symmetry defect $\delta = \|A - A^T\|$ is small and this is the case here, see next theorem

Application to the Heat equation

The RSS scheme writes as

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau A_2(u^{(k+1)} - u^{(k)}) + A_4 u^{(k)} = f. \qquad (16)$$

The numerical treatment of non homogeneous (possibly time depending) Dirichlet boundary conditions can be realized with the RSS approach.
Let $A_m(u, n)$, $m = 2, 4$, be the m*th* order finite difference discretization of $-\Delta$ of u with Dirichlet conditions at time $n\Delta t$, note that this operator is affine.
The stabilized scheme writes formally as

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau(A_2(u^{(k+1)}, k+1) - A_2(u^{(k)}, k)) + A_4(u^{(k)}, k) = f, \qquad (17)$$

Making the approximation $A_2(u^{(k+1)}, k+1) \simeq A_2(u^{(k+1)}, k)$, we obtain

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau A_2(u^{(k+1)} - u^{(k)}) + A_4(u^{(k)}, k) = f. \qquad (18)$$

Theorem

Let $A \in \mathcal{M}_n(\mathbb{R}^N)$. We assume that A is positive definite and B a symmetric definite positive preconditioning matrix of A satisfy hypothesis $\mathcal{H}$. We set $\delta = \| A - A^T \|$ and $\Phi(\xi) = (\beta^2 - 2\alpha\tau)\xi + \frac{1}{4\xi}\delta^2$. Assume that $\frac{\beta^2}{2\alpha} - \frac{\delta^2}{8\alpha\lambda_{min}(B)^2} \geq 0$. Then the RSS scheme has the following stability conditions

i. *if $\tau \geq \frac{\beta^2}{2\alpha} + \frac{\delta^2}{8\alpha\lambda_{min}^2(B)} \geq \frac{\beta^2}{2\alpha}$. then the scheme is unconditionally stable.*

ii. *If $\tau \leq \frac{\beta^2}{2\alpha} - \frac{\delta^2}{8\alpha\lambda_{max}(B)^2}$ then the scheme is stable under condition*

$$0 < \Delta t < \frac{2\alpha}{\Phi(\lambda_{max}(B))}$$

iii. *If $\frac{\beta^2}{2\alpha} - \frac{\delta^2}{8\alpha\lambda_{max}(B)^2} \leq \tau < \frac{\beta^2}{2\alpha} + \frac{\delta^2}{8\alpha\lambda_{min}(B)^2}$ then the scheme is stable under condition*

$$0 < \Delta t < \frac{2\alpha}{\Phi(\lambda_{min}(B))}$$

Avdantages

- Use fast solvers:
  - For Poisson problems with Dirichlet BC:

$$A_4 u = f$$

    use sin- FFT or Multigrid as preconditioner for solving preconditioning systems $A_2 z = r$
  - For the Heat equation

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau A_2(u^{(k+1)} - u^{(k)}) + A_4(u^{(k)}, k) = f.$$

    use sin-FFT
- More generally, use the sparse linear algebra preconditioning techniques for the fast solution of the implicit part

RSS for solving 2D incompressible Navier-Stokes equations (NSE)

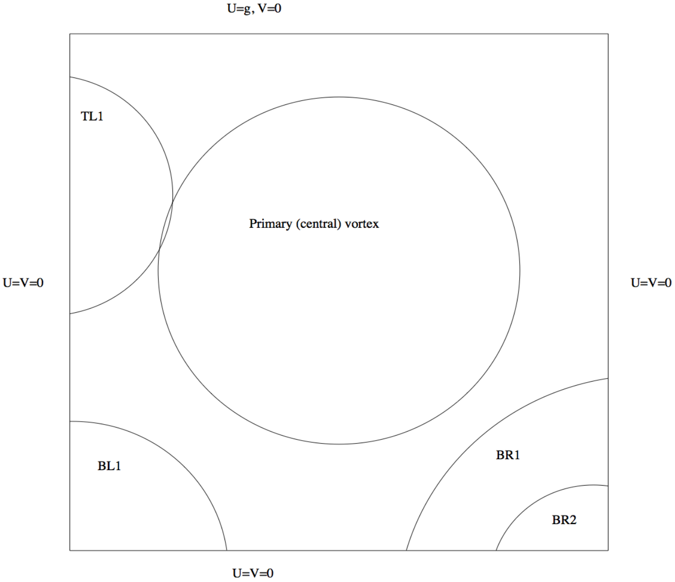
Consider the stream function-vorticity formulation $(\omega - \psi)$ of NSE

$$\frac{\partial \omega}{\partial t} - \frac{1}{Re}\Delta\omega + \frac{\partial \psi}{\partial y}\frac{\partial \omega}{\partial x} - \frac{\partial \psi}{\partial x}\frac{\partial \omega}{\partial y} = 0, \quad \text{in } \Omega, \tag{19}$$

$$\Delta\psi = \omega, \quad \text{in } \Omega. \tag{20}$$

$$\omega(x, y, 0) = \omega_0(x, y), \tag{21}$$

that we supplement with proper boundary conditions. We denote by $\Gamma_i \;\; i = 1, .., 4$ the sides of the unit square Ω as follows: Γ_1 is the lower horizontal side, Γ_3 is the upper horizontal side, Γ_2 is the left vertical side, and Γ_4 is the right vertical side.


U=g, V=0
TL1
Primary (central) vortex
U=V=0
U=V=0
BL1
BR1
BR2
U=V=0

Basic NSE semi implicit Scheme

The Equations are discretized in space with Fourth order CS.

Algorithm 2 Navier-Stokes

1: (ω^0, ψ^0) given as solution of the Stokes problem
2: **for** **do** $k = 0, 1, \cdots$ until convergence
3: **Update** the boundary terms in $\omega^{(k+1)}$ of $\psi^{(k)}$ using fourth order extrapolation
4: **Compute** $\omega^{(k+1)}$ by solving.

$$\frac{\omega^{(k+1)} - \omega^{(k)}}{\Delta t} + \frac{1}{Re} A_4 \omega^{(\star)} + D_4^y \psi^{(k)} .* D_4^x \omega^{(k)} - D_4^x \psi^{(k)} .* D_4^y \omega^{(k)} = 0$$

5: **Compute** ψ^{n+1}as solution of the Poisson equation

$$A_4 \psi^{(k+1)} = \omega^{(k+1)}$$

6: **end for**

Here $\star = k$ or $\star = k + 1$

Algorithm 3 RSS-Navier-Stokes

1: (ω^0, ψ^0) given as solution of the Stokes problem
2: **for** k **do**=0,1, ... until convergence
3: **Update** the boundary terms in $\omega^{(k+1)}$ of $\psi^{(k)}$ using fourth order extrapolation
4: **Compute** $\omega^{(k+1)}$ by solving.

$$\begin{array}{c} \dfrac{\omega^{(k+1)} - \omega^{(k)}}{\Delta t} + \tau \dfrac{1}{Re} A_2(\omega^{(k+1)} - \omega^{(k)}) \\ + D_4^y \psi^{(k)} .* D_4^x \omega^{(k)} - D_4^x \psi^{(k)} .* D_4^y \omega^{(k)} \end{array} = -\frac{1}{Re} A_4 \omega^{(k)}$$

5: **Compute** ψ^{n+1}as solution of the Poisson equation

$$A_4 \psi^{(k+1)} = \omega^{(k+1)}$$

6: **end for**

Numerical results

Implementation

Systems in ω solved using sin-FFT, those in ψ using sin-FFT preconditioning

Benchmark

We distinguish two different driven flows, according to the choice of the boundary conditions on the velocity. More precisely we have

- $g(x) = 1$: Cavity A (lid driven cavity)
- $g(x) = (1-(1-2x)^2)^2$: Cavity B (regularized lid driven cavity)

These are the considered geometries

- Lid Driven cavity on a square domain All the results have been compared with those of Ghia & Ghia (JCP '82), Bruneau & Jouron ('90) Goyon ('96), Ben Artzi-Croisille-Fishelov (2005)
- Lid Driven cavity on a rectangular model (or double cavity) All the results have been compared with those of Bruneau & Jouron ('90) Goyon ('96)

A double check has been run, varying the spatial discretization

The effect of the stabilization

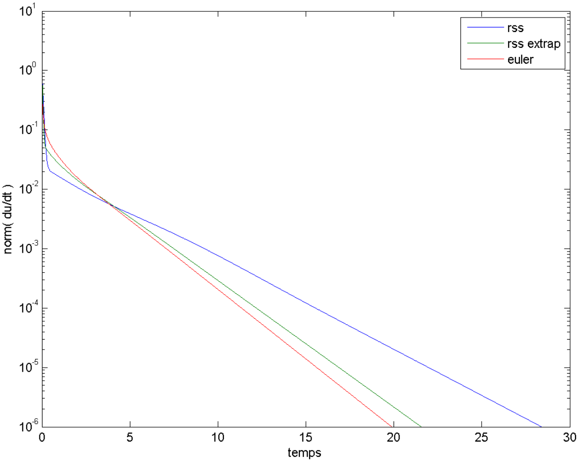


Figure : Convergence to NSE steady state (19) - $\tau = 100$ - $N = 63$ - $Re = 100$ - $\Delta t = 0.01$

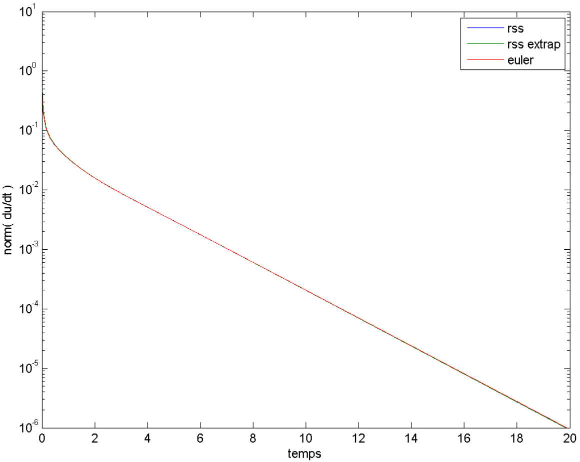


Figure : Convergence to NSE steady state (19) - $\tau = 1$ - $N = 63$ - $Re = 100$ - $\Delta t = 0.01$

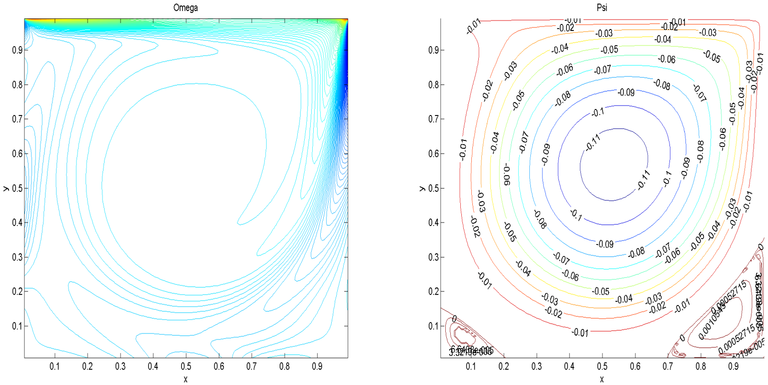


Figure : Solution of NSE (19) - $g \equiv 1$ - $\tau = 1$ - $N = 127$ - $Re = 1000$ - $\Delta t = 0.0005$

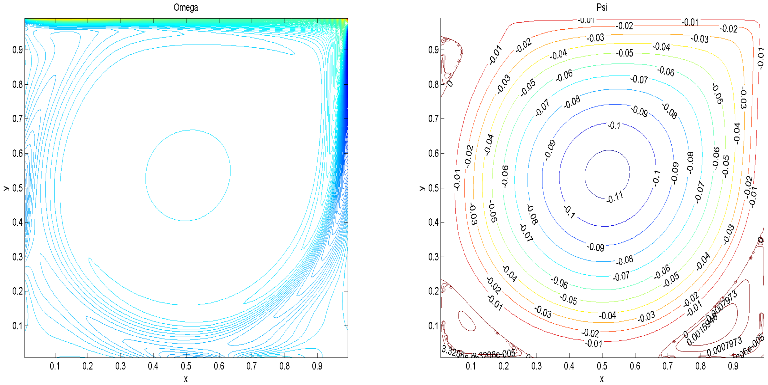
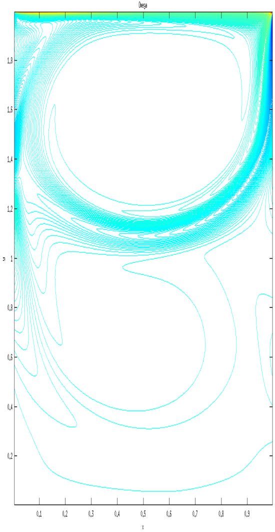
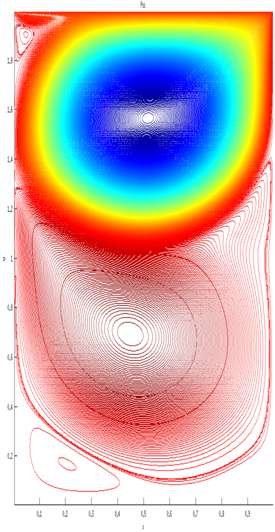


Figure : Solution of NSE (19) - $g \equiv 1$ - $\tau = 1$ - $N = 127$ - $Re = 3200$ - $\Delta t = 0.0005$





Nonlinear RSS Scheme

The (semi linear) RRS-scheme becomes less interesting as *Re* increases. Idea use Nonlinear RSS version.

$$\left(\frac{1}{\Delta t} Id + \tau\left(\frac{1}{Re}A_2 + diag(D_y\psi^{(k)})D_x - diag(D_x\psi^{(k)})D_y\right)\right)\delta^{(k)} = -F(\psi^{(k)}, \omega^{(k)}) \quad (22$$

with $\delta^{(k)} = \omega^{(k+1)} - \omega^{(k)}$, where A_2 is the second order laplacian matrix, $diag(D_y\psi^{(k)})$ (resp. $diag(D_x\psi^{(k)})$) is the diagonal matrix with the discrete (second order accurate) approximation of $\dfrac{\partial\psi^{(k)}}{\partial x}$ (resp. $\dfrac{\partial\psi^{(k)}}{\partial y}$) at grid points as entries; D_x (resp. D_y) denote the (second order accurate) first derivative matrix in x (resp. in y) on the cartesian grid.
$-F(\psi^{(k)}, \omega^{(k)})$ is the high order compact scheme discretisation of $-\dfrac{1}{Re}\Delta\omega + \dfrac{\partial\phi}{\partial y}\dfrac{\partial\omega}{\partial x} - \dfrac{\partial\phi}{\partial x}\dfrac{\partial\omega}{\partial y}$.

Method τ Extrap.	RSS Δt no	RSS Δt_{max} no	RSS T_c no	RSS Δt yes	RSS Δt_{max} yes	RSS T_c yes	NLRSS Δt yes	NLRSS Δt_{max} yes	NLRSS T_c yes
$\tau = 1$	0.005	0.005	56.21	0.005	0.01	56.81			
	0.01		***	0.01		56.79	0.01	0.02	56.86
	0.02		***	0.02	***		0.02		56.96
$\tau = 30$	0.05	0.04	NC	0.05	0.08	47.95	0.05	0.7	65.05
	0.1		***	0.1		***	0.1		62.5
	0.7		***	0.7		***	0.7		321.3

Table : RSS (left) RSS with Extrapolation (center) and extrapolated NLRSS (right) $Re = 1000$, $n = 127$, $\epsilon = 10^{-5}$

Allen-Cahn Equation for the Phase separation

$$\frac{\partial u}{\partial t} + M(-\Delta u + \frac{1}{\epsilon^2} f(u)) = 0 \quad (23)$$

$$\frac{\partial u}{\partial n} = 0 \quad (24)$$

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

- It 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), $F = \displaystyle\int_{-\infty}^{u} f(v)dv$ is the free energy, u is the (non-conserved) **order parameter**, ϵ is the **interface length**.
- Homogenous Neumann boundary condition implies that there is not a loss of mass outside the domain Ω
- Potential and diffusion compete: regularization in phase transition
- Maximum principle: if $|u_0(x)| \leq \beta$ then $|u(x,t)| \leq \beta$, where β is the magnitude of largest zero of f.

It is a gradient flow $E(u) = \frac{1}{\epsilon^2} \int_\Omega F(u)dx + \frac{1}{2} \int_\Omega |\nabla u|^2 dx$

some potentials

- Double Well potential $F(u) = \frac{1}{4}(1-u^2)^2$ or Ginzburg-Landau double Well potential
- Truncated double-well potential

$$\tilde{F}(u) = \begin{cases} \dfrac{3M^2-1}{2}u^2 + 2M^3u + \dfrac{1}{4}(3M^4+1) & \text{if } u > M \\ \dfrac{1}{4}(1-u^2)^2 & \text{if } u \in [-M, M] \\ \dfrac{3M^2-1}{2}u^2 + 2M^3u + \dfrac{1}{4}(3M^4+1) & \text{if } u < -M \end{cases}$$

- Logarithmic free energy

$$F(u) = \frac{\theta}{2}\,(1+u)\ln 1 + u + (1-u)\ln 1 - u - \frac{\theta_c}{2}u^2$$

An inconditionnally stable scheme is ([Elliott1989, ElliottStuart1993])

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + Au^{(k+1)} + \frac{1}{\epsilon^2} DF(u^{(k)}, u^{(k+1)}) = 0, \tag{26}$$

where

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

Theorem

Consider the RSS-scheme

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau B(u^{(k+1)} - u^{(k)}) + \frac{1}{\epsilon^2} DF(u^{(k+1)}, u^{(k)}) = -Au^{(k)} \tag{27}$$

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*

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

When $F(u) = \frac{1}{4}(1-u^2)^2$ is considered, one can split the AC equation as

$$\frac{\partial u}{\partial t} - \Delta u = 0,$$
$$\frac{\partial u}{\partial t} + \frac{1}{\epsilon^2} F'(u) = 0,$$

This last equation can be integrated exactly (Li-Jeong-Choi-Lee-Kim '15). So the a first RSS-scheme is

$$\frac{u^{(*)} - u^{(k)}}{\Delta t} + \tau B(u^{(*)} - u^{(k)}) = -Au^{(k)},$$
$$\mathrm{u}^{(k+1)} = \frac{u^*}{\sqrt{e^{-2\frac{\Delta t}{\epsilon^2}} + (u^*)^2(1 - e^{-2\frac{\Delta t}{\epsilon^2}})}}$$

The first (RRS) step can be splitted in ADI sub steps.

Method	N	ϵ	Δt	τ	$[0, T]$	$\|error\|_\infty$	CPU factor
RSS	$N = 64$	0.5	10^{-3}	5	$[0, 1]$	0.0194	1
RSS	$N = 64$	0.5	10^{-3}	2	$[0, 1]$	0.0084	1
Classic	$N = 64$	0.5	10^{-3}		$[0, 1]$	0.0047	226
RSS	$N = 64$	0.5	10^{-2}	2.2	$[0, 1]$	0.0773	1
Classic	$N = 64$	0.5	10^{-2}		$[0, 1]$	0.0486	226

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

Method	N	ϵ	Δt	τ	$[0, T]$	$\|\|error\|\|_\infty$	CPU factor
RSS	$N = 32$	0.5	10^{-3}	5	$[0, 1]$	5.960^{-2}	1
RSS	$N = 32$	0.5	10^{-3}	2	$[0, 1]$	$3.03\ 10^{-2}$	1
Classic	$N = 32$	0.5	10^{-3}		$[0, 1]$	$2.1\ 10^{-2}$	2.22
RSS	$N = 32$	0.5	10^{-2}	2	$[0, 1]$	0.3123	1
RSS	$N = 32$	0.5	10^{-2}	1.9	$[0, 1]$	0.3066	1
Classic	$N = 32$	0.5	10^{-2}		$[0, 1]$	0.2586	2.22

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

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 $\lambda >> 1$

$$\underbrace{\frac{\partial u}{\partial t} - \Delta(-\epsilon \Delta u + \frac{1}{\epsilon} f(u))}_{\text{Cahn-Hilliard equation}} \quad \underbrace{+\lambda \chi_{\Omega \setminus D}(x)(u-g)}_{\text{Fidelity term}} = 0, \tag{28, 29}$$

$$\frac{\partial u}{\partial n} = 0 \quad \frac{\partial}{\partial n}\left(\Delta u - \frac{1}{\epsilon^2} f(u)\right) = 0, \tag{30}$$

$$u(0,x) = u_0(x) \tag{31}$$

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.

The Reference scheme

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + A\mu^{(k+1)} + \lambda D(u^{(k+1)} - g) = 0, \tag{32}$$

$$\mu^{(k+1)} = \epsilon A u^{(k+1)} + \frac{1}{\epsilon} f(u^{(k)}) \tag{33}$$

say in the matricial form

$$\begin{pmatrix} Id + \Delta t \lambda D & \Delta t A \\ -\epsilon A & Id \end{pmatrix} \begin{pmatrix} u^{(k+1)} \\ \mu^{(k+1)} \end{pmatrix} = \begin{pmatrix} u^{(k)} + \Delta t \lambda D g \\ \frac{1}{\epsilon} f(u^{(k)}) \end{pmatrix}$$

The linear system can be solved by using a (incomplete) LU block decomposition; technique of approximation of Schur's complement can be applied for the optimization (Bosh-Kay-Stoll-Wathen '13)

The Reference scheme

Algorithm 5 : RSS Cahn-Hilliard for implainting (formal LU)

1: **for** $k = 0, 1, \cdots$ until a stopping criterion is satisfied, **do**
2: **Set** $F_1 = u^{(k)} + \Delta t \lambda_0 Dg$
3: **Set** $F_2 = \frac{1}{\epsilon} f(u^{(k)})$
4: **Solve** $(Id + \lambda_0 D + \Delta t \epsilon A^2) u^{(k+1)} = F_1 - \tau \Delta t A F_2$
5: **Set** $\mu^{(k+1)} = F_2 + \epsilon A u^{(k+1)}$
6: **end for**

The RSS scheme

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + \tau B(\mu^{(k+1)} - \mu^{(k)}) + A\mu^{(k)} + \lambda D(u^{(k+1)} - u^{(k)}) = \lambda_0 D(g - u^{(k)}), \quad (34)$$

$$\mu^{(k+1)} - \mu^{(k)} = \epsilon\tau B(u^{(k+1)} - u^{(k)}) + \epsilon A u^{(k)} + \frac{1}{\epsilon} f(u^{(k)}) - \mu^{(k)}. \quad (35)$$

say in the matricial form

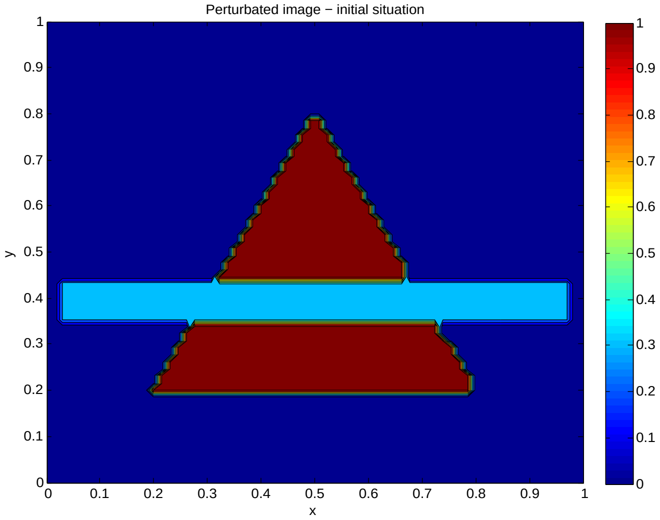
$$\begin{pmatrix} Id + \Delta t\lambda D & \tau\Delta t B \\ -\epsilon\tau B & Id \end{pmatrix} \begin{pmatrix} u^{(k+1)} - u^{(k)} \\ \mu^{(k+1)} - \mu^{(k)} \end{pmatrix} = \begin{pmatrix} \Delta t(\lambda D(g - u^{(k)}) - A u^{(k)}) \\ \epsilon A u^{(k)} + \frac{1}{\epsilon} f(u^{(k)}) - \mu^{(k)}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

The linear system can be solved by using a (incomplete) LU block decomposition; technique of approximation of Schur's complement can be applied for the optimization (Bosh-Kay-Stoll-Wathen '13)

The RSS scheme

Algorithm 7 : RSS Cahn-Hilliard for implainting (formal LU)

1: **for** $k = 0, 1, \cdots$ until a stopping criterion is satisfied, **do**
2: **Set** $F_1 = \Delta t(\lambda_0 D(g - u^{(k)}) - Au^{(k)})$
3: **Set** $F_2 = -\mu^{(k)} + \epsilon A u^{(k)} + \frac{1}{\epsilon} f(u^{(k)})$
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**


Perturbated image − initial situation
y
x
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

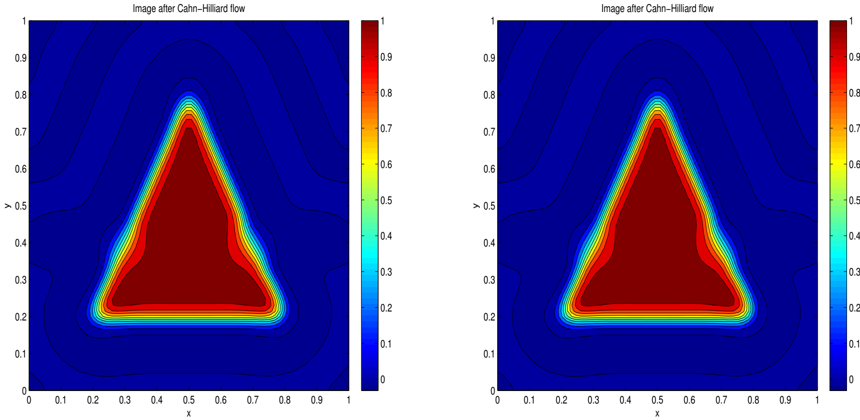


Figure : Inpainting with C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, $N = 64$ - Restored triangle at $T = 0.1$, classical (left) RSS method (right)

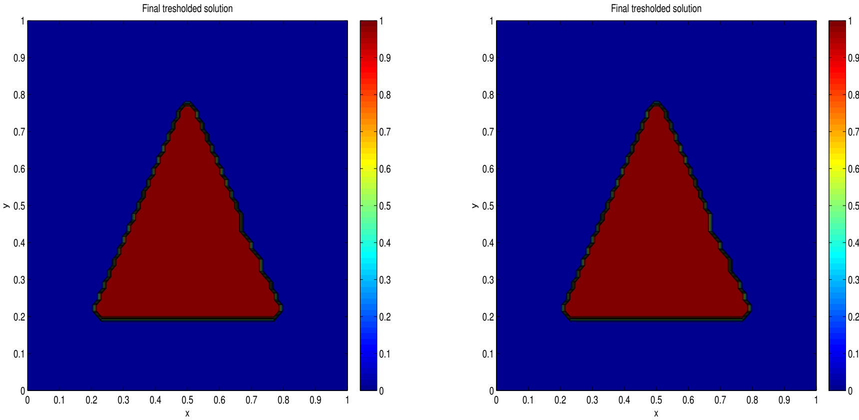


Figure : Inpainting with C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, $N = 64$ - Restored triangle with thresholding at $T = 0.1$, classical (left) RSS method (right) ayt

Method	N	ϵ	Δt	τ	$[0,T]$	quality	CPU factor (iterations)
RSS	$N=64$	0.05	10^{-3}	1.4	$[0,0.1]$	EX	1
Classic	$N=64$	0.05	10^{-3}		$[0,0.1]$	EX	>10
RSS	$N=64$	0.05	5.10^{-3}	1.5	$[0,0.1]$	EX	1
Classic	$N=64$	0.05	5.10^{-3}		$[0,0.1]$	EX	>10
RSS	$N=64$	0.05	10^{-2}	2.8	$[0,0.1]$	middle	1
Classic	$N=64$	0.5	10^{-2}		$[0,0.1]$	middle	>10

Table : 2D Cahn-Hilliard Inpainting equation, the triangle example: , $\Omega=[0,1]^2$, $\lambda=90000$

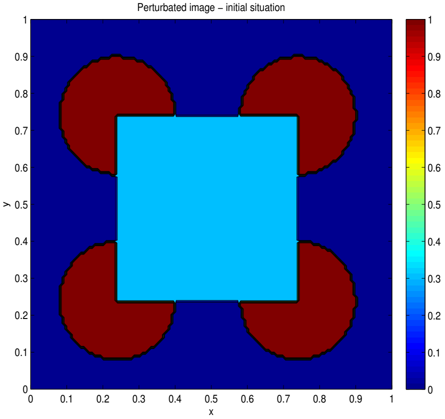


Figure : Inpainting with C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, $N = 128$ - Initial inpainted image

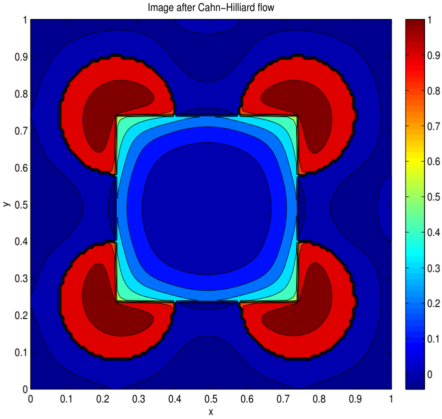


Figure : Inpainting with C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, $N = 128$ - image at $t = 0.005$

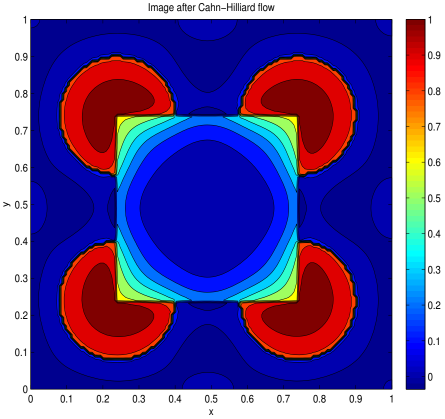


Figure : Inpainting with C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, $N = 128$ - image at $t = 0.008$

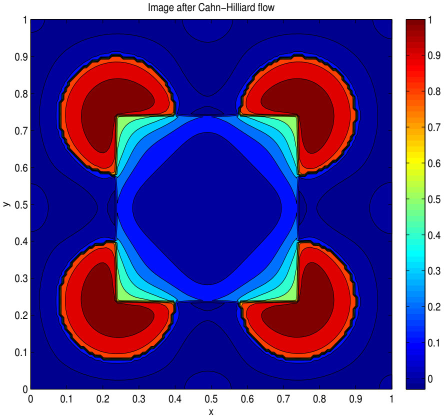


Figure : Inpainting with C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, $N = 128$ - image at $t = 0.01$

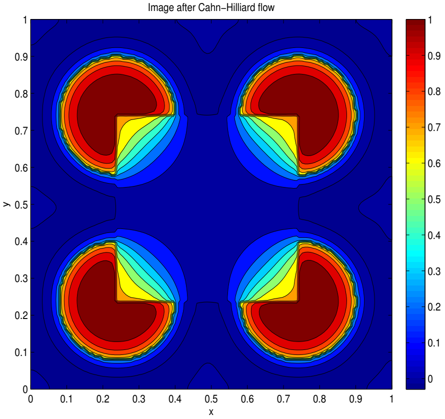


Figure : Inpainting with C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, $N = 128$ - image at $t = 0.02$

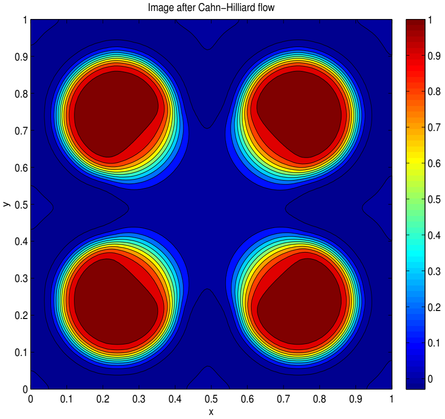


Figure : Inpainting with C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, $N = 128$ - image at $t = 0.1$

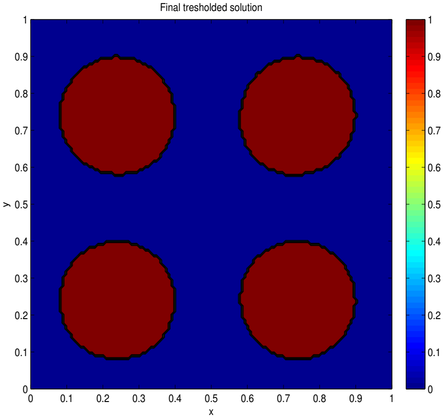


Figure : Inpainting with C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, $N = 128$ - thresholded image at $t = 0.1$

The 3-D Case (New)

movie `inpainting_bar.avi`

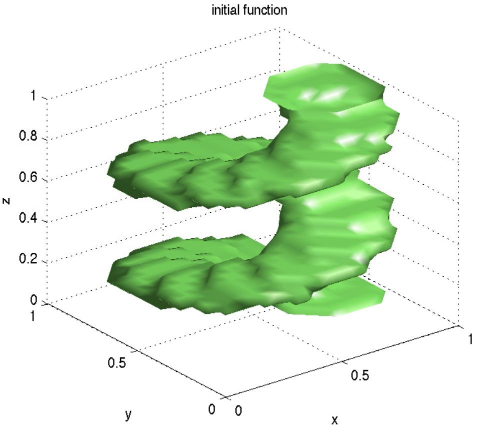


Figure : Inpainting 3D with C-H. $\Delta t = 1.e-7$, $\lambda = 100000$, $\epsilon = 0.05$, $N = 20$ -

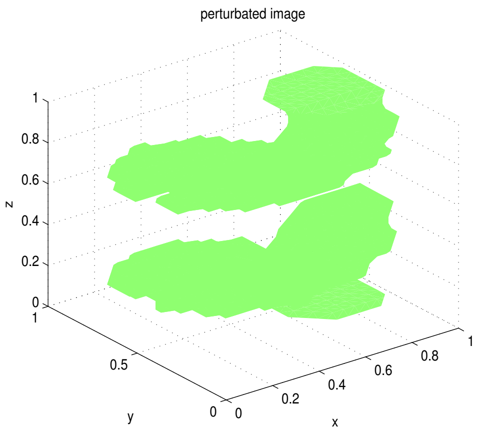


Figure : Inpainting 3D with C-H. $\Delta t = 1.e-7$, $\lambda = 100000$, $\epsilon = 0.05$, $N = 20$

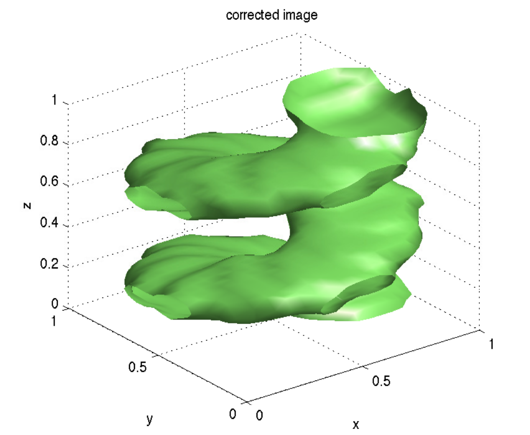


Figure : Inpainting 3D with C-H. $\Delta t = 1.e-7$, $\lambda = 100000$, $\epsilon = 0.05$, $N = 20$

movie `inpainting_spiral.avi`

- RSS approach for parabolic equations present a compromise for preserving the stability of (semi)-implicit time schemes while simplifying the solution a each time step.
- Versatility: possibility to apply the technique to a large number of times schemes

- RSS approach for parabolic equations present a compromise for preserving the stability of (semi)-implicit time schemes while simplifying the solution a each time step.
- Versatility: possibility to apply the technique to a large number of times schemes
- Main issue: saving computational time for a comparable precision
- Adaptive versions by varying τ at each iterations
- Limitation to
  - parabolic equations: RSS does not apply interestingly, e.g., to Airy equation then not to KdV.
  - finite differences when dealing with different discretization level (or accuracy): change point of view for FEM (work in progress w . C A. K.)


Salamat
Спасибо
谢谢
Eskerrik asko
Дзякуй
Thank You
Merci
Kiitos
Asante
Grazie
dziękuję
ありがとう
köszönöm
Tak

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