(Joint work with M. Brachet (Univ. Lorraine at Metz))

Stabilized Time Schemes for nonlinear parabolic equations

J-P. CHEHAB[1]

[1]LAMFA, UMR 7352, Université de Picardie Jules Verne, Amiens, France
(jean-paul.chehab@u-picardie.fr)

NL2A, CIRM, October 24-28, 2016

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)

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)

Classical antagonism

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

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

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)

Classical antagonism

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

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

- 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

Simplify the implicit system to solve such as reducing the computational cost while keeping good stability properties

- Start from Backward Euler's

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

- Let B be a preconditioner of A, consider the new scheme

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

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

Solution: Residual Smoothing Scheme (RSS) Schemes

Simplify the implicit system to solve such as reducing the computational cost while keeping good stability properties

- Start from Backward Euler's

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

- Let B be a preconditioner of A, consider the new scheme

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

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

This have been considered independently by A. Cohen, Averbuch, and Israeli ('98, unpublished) and by Costa ('98), then Costa, Dettori, Gottlieb and Temam ('01) (but in a 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

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

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

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

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

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

So 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 $u^{(k)}$.

Fully Nonlinear RSS

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

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

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

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

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.

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.

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* $M = Id - \Delta t(Id + \tau \Delta t B)^{-1} A$ *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

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

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*

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

RSS-scheme is first order accurate 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

1: $u^{(0)}$ given
2: **for** (; k; =)0,1, $\cdots$ until convergence
3: **Solve** $(Id + \tau \frac{\Delta t}{2} B)v_1 = -\frac{\Delta t}{2} F(u^{(k)})$,
4: **Set** $u_1 = u^{(n)} + v_1$,
5: **Solve** $(Id + \tau \frac{\Delta t}{2} B)v_2 = -\frac{\Delta t}{2} F(u_1)$,
6: **Set** $u_2 = u_1 + v_2$,
7: **Solve** $(Id + \tau \Delta t B)v_3 = -\Delta t F(u^{(k)})$,
8: **Set** $u_3 = u^{(n)} + v_3$,
9: **Set** $u^{(k+1)} = 2u_2 - u_3$.

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

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

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

and the Strang's Splitting

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

$$\frac{u^{(k+2/3)} - u^{(k+1/3)}}{\Delta t} + \tau_2 B_2(u^{(k+2/3)} - u^{(k+1/3)}) = -A_2 u^{(k+1/3)}, \tag{14}$$

$$\frac{u^{(k+1)} - u^{(k+2/3)}}{\Delta t/2} + \tau_1 B_1(u^{(k+1)} - u^{(k+2/3)}) = -A_1 u^{(k+2/3)}, \tag{15}$$

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

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

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

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

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

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

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.
A natural idea is to use A_2 as preconditioned of A_4 (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 !

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.
A natural idea is to use A_2 as preconditioned of A_4 (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 ! 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

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

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

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

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

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

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 $\tau \geq \frac{\beta^2}{2\alpha} + \frac{\delta^2}{8\alpha\lambda^2_{min}(B)} \geq \frac{\beta^2}{2\alpha}$. 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 preconditioned 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)

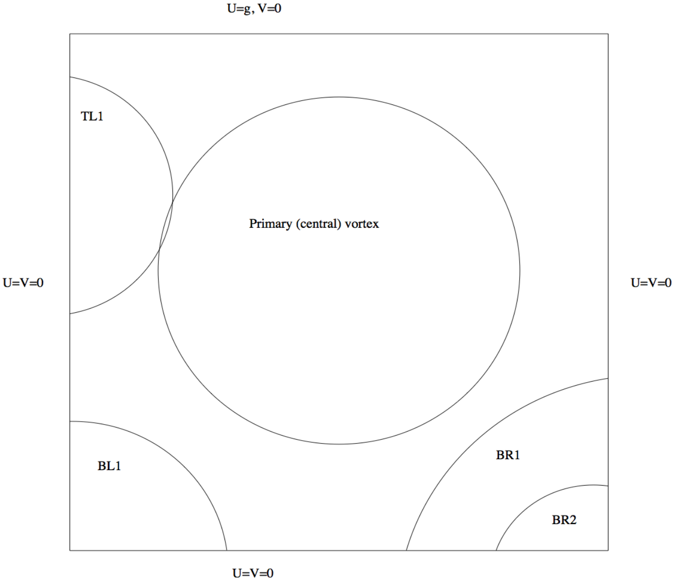
Consider the stream function-vorticity formulation $(\omega - \psi)$ of NSE

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

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

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

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

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** $(;\ k;\ =)0,1,\ \cdots$ 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.

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

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

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

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** $(k; =; 0)$,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

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

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

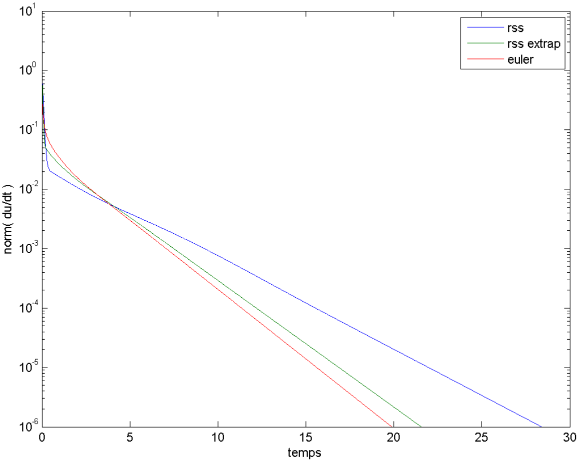


Figure : Convergence to NSE steady state (19) - $\tau = 100$ - $N = 63$ - $Re = 100$ - $\Delta t = 0.01$

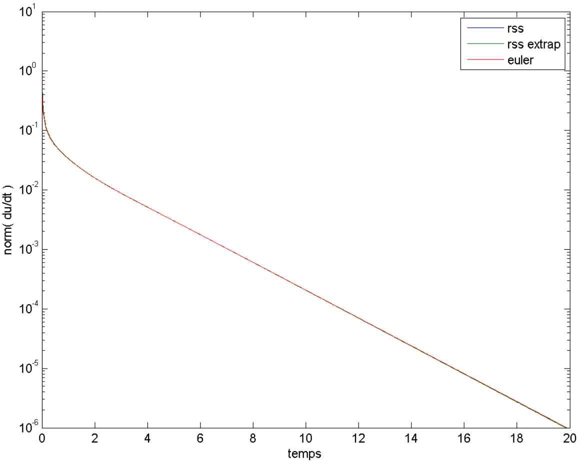


Figure : Convergence to NSE steady state (19) - $\tau = 1$ - $N = 63$ - $Re = 100$ - $\Delta t = 0.01$

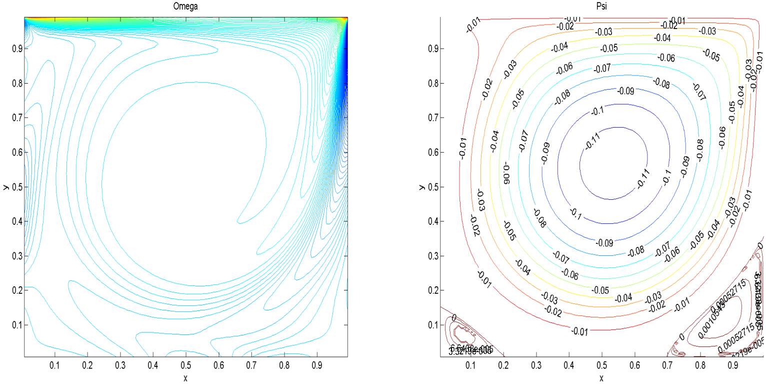


Figure : Solution of NSE (19) - $g \equiv 1$ - $\tau = 1$ - $N = 127$ - $Re = 1000$ - $\Delta t = 0.0005$

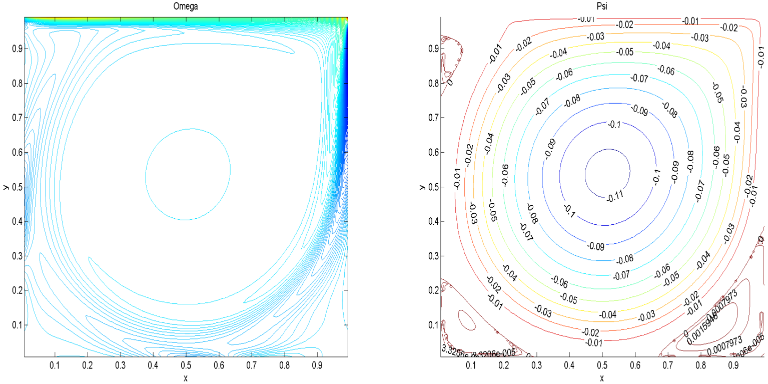
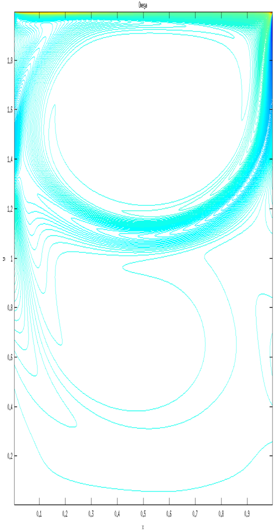
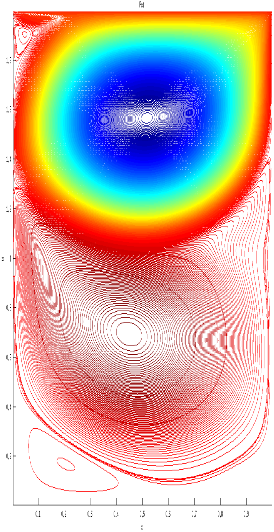


Figure : Solution of NSE (19) - $g \equiv 1$ - $\tau = 1$ - $N = 127$ - $Re = 3200$ - $\Delta t = 0.0005$


Omega
1,8
1,6
1,4
1,2
y 1
0,8
0,6
0,4
0,2
0,1 0,2 0,3 0,4 0,5 0,6 0,7 0,8 0,9
x


Psi
1,8
1,6
1,4
1,2
y 1
0,8
0,6
0,4
0,2
0,1 0,2 0,3 0,4 0,5 0,6 0,7 0,8 0,9
x

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 writes as

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

$$\frac{\partial u}{\partial n} = 0 \tag{24}$$

$$u(0,x) = u_0(x) \tag{25}$$

- 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), $F = \int_{-\infty}^{u} f(v)dv$ 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
- There is a competition between the potential term and the diffusion term: 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 $E(u) = \frac{1}{\epsilon^2} \int_\Omega F(u)dx + \frac{1}{2} \int_\Omega |\nabla u|^2 dx$

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

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

This last equation can be integrated exactly. So the a first RSS-scheme is

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

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 $\lambda >> 1$

$$\underbrace{\frac{\partial u}{\partial t} - \Delta(-\epsilon\Delta u + \frac{1}{\epsilon} f(u))}_{\text{Cahn-Hilliard equation}} \quad \underbrace{+\lambda \chi_{\Omega\setminus D}(x)(u-g)}_{\text{Fidelity term}} = 0, \tag{26, 27}$$

$$\frac{\partial u}{\partial n} = 0 \quad \frac{\partial}{\partial n}\left(\Delta u - \frac{1}{\epsilon^2} f(u)\right) = 0, \tag{28}$$

$$u(0,x) = u_0(x) \tag{29}$$

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

$$\frac{u^{(k+1)} - u^{(k)}}{\Delta t} + A\mu^{(k+1)} + \lambda D(u^{(k+1)} - g) = 0, \tag{30}$$

$$\mu^{(k+1)} = \epsilon A u^{(k+1)} + \frac{1}{\epsilon} f(u^{(k)}) \tag{31}$$

say in the matricidal 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 RSS scheme

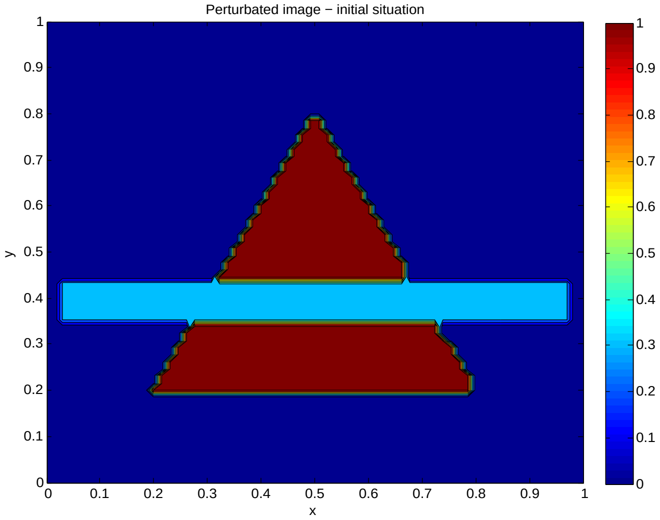
$$\frac{u^{(k+1)}-u^{(k)}}{\Delta t}+\tau B(\mu^{(k+1)}-\mu^{(k)})+A\mu^{(k)}+\lambda D(u^{(k+1)}-u^{(k)})=\lambda_0 D(g-u^{(k)}), \quad (32)$$

$$\mu^{(k+1)}-\mu^{(k)}=\epsilon\tau B(u^{(k+1)}-u^{(k)})+\epsilon A u^{(k)}+\frac{1}{\epsilon}f(u^{(k)})-\mu^{(k)}. \quad (33)$$

say in the matricidal form

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

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)


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

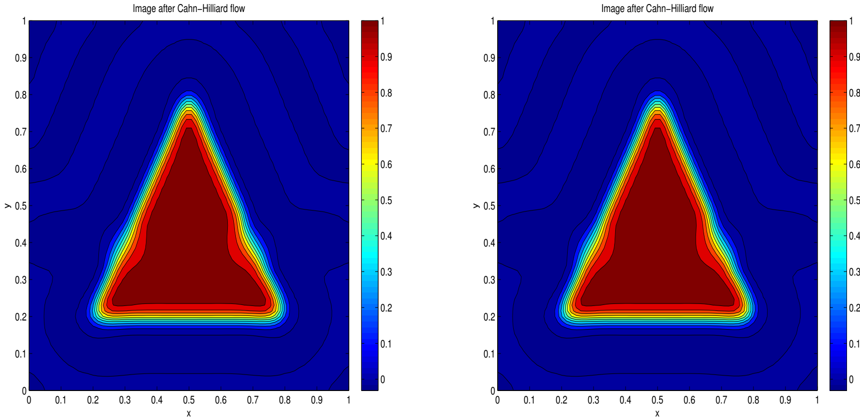


Figure : Inpainting with C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, $N = 64$ - Restored triangle at $T = 0.1$, classical (left) RSS method (right)

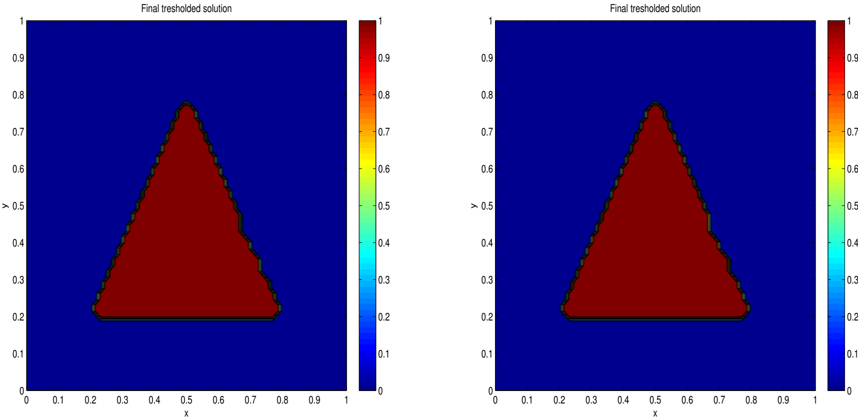


Figure : Inpainting with C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, $N = 64$ - Restored triangle with tresholding at $T = 0.1$, classical (left) RSS method (right)

Method	N	ϵ	Δt	τ	$[0, T]$	quality	CPU factor (iterations)
RSS	$N = 64$	0.05	10^{-3}	1.4	$[0, 0.1]$	EX	12.86
Classic	$N = 64$	0.05	10^{-3}		$[0, 0.1]$	EX	541.37
RSS	$N = 64$	0.05	5.10^{-3}	1.5	$[0, 0.1]$	EX	2.68
Classic	$N = 64$	0.05	5.10^{-3}		$[0, 0.1]$	EX	115.5
RSS	$N = 64$	0.05	10^{-2}	2.8	$[0, 0.1]$	middle	1.42
Classic	$N = 64$	0.5	10^{-2}		$[0, 0.1]$	middle	60.42

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

- 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.

References I

A. Averbuch, A. Cohen, M.Israeli,
A fast and accurate multiscale scheme for parabolic equations,
rapport LAN 1998, unpublished.

S. Bellavia, B. Morini, M. Porcelli,
New Updates of incomplete LU factorizations and applications to large nonlinear systems,
Optimization Methods & software, vol 29 pp 321-340, (2014).

J. Bosch, D. Kay, M. Stoll, and A.J. Wathen, Fast solvers for CahnÐHilliard inpainting, SIAM J. Imag. Sci. 7 (2013), 67Ð97.

J.-P. Chehab, Incremental Unknowns Method and Compact Schemes , M2AN, 32, 1, (1998), 51-83.

References II

M. Brachet and J.-P. Chehab
Stabilized Times Schemes for High Accurate Finite Differences Solutions of Nonlinear Parabolic Equations
Journal of Scientific Computing, 1-37 (), 2016, DOI 10.1007/s10915-016-0223-8

C. Calgaro, J.-P. Chehab, Y. Saad,
Incremental Incomplete LU factorizations with applications to PDES,
Numerical Linear Algebra with Applications, vol 17, 5, p 811–837, 2010.

B. Costa,
Time marching techniques for the nonlinear Galerkin method,
Preprint series of the Institute of Applied Mathematics and Scientific Computing, PhD thesis, Bloomington, Indiana, 1998.

B. Costa. L. Dettori, D. Gottlieb and R. Temam,
Time marching techniques for the nonlinear Galerkin method,
SIAM J. SC. comp., 23, (2001), 1, 46–65.

References III

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.

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

D. J. Eyre,
Unconditionallly Stable One-step Scheme for Gradient Systems,
June 1998, unpublished,
http://www.math.utah.edu/eyre/research/methods/stable.ps.

S. Lele,
Compact Difference Schemes with Spectral Like resolution,
J. Comp. Phys., 103, (1992), 16–42

References IV

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

M. Ribot and M. Schatzman
Stability, convergence and order of the extrapolations of the Residual Smoothing Scheme in energy norm
Confluentes Math. 3 (2011), no. 3, 495–521.