Superconvergence of the Strang splitting when using the Crank-Nicolson scheme for parabolic PDEs with oblique boundary conditions

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Joint work with

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Introduction: the Strang splitting method

For parabolic semilinear problems of the form

$$\begin{aligned} \partial_t u(x,t) &= Du(x,t) + f(x,u(x,t)) \ \text{ in } \Omega \times (0,T], \\ Bu(x,t) &= b(x) \ \text{ on } \partial\Omega \times (0,T], \\ u(x,0) &= u_0(x) \ \text{ in } \Omega, \end{aligned}$$

we consider time discretizations with splitting methods:

$$\phi_t^f : \qquad \partial_t u(x,t) = f(x,u(x,t)) \quad \text{in } \Omega \times (0,T],$$

$$\phi_t^D : \qquad \begin{aligned} \partial_t u(x,t) &= Du(x,t) \quad \text{in } \Omega \times (0,T], \\ Bu(x,t) &= b(x) \text{ on } \partial\Omega \times (0,T]. \end{aligned}$$

For approximating $u(t_n,x) \simeq u_n(x)$, $t_n = n\tau$, the Strang splitting method writes

$$u_{n+1} = \phi^f_{\frac{\tau}{2}} \circ \phi^D_{\tau} \circ \phi^f_{\frac{\tau}{2}}(u_n),$$

Or alternatively, another version writes:

$$u_{n+1} = \phi^D_{\frac{\tau}{2}} \circ \phi^f_{\tau} \circ \phi^D_{\frac{\tau}{2}}(u_n).$$

Introduction: the Crank-Nicolson

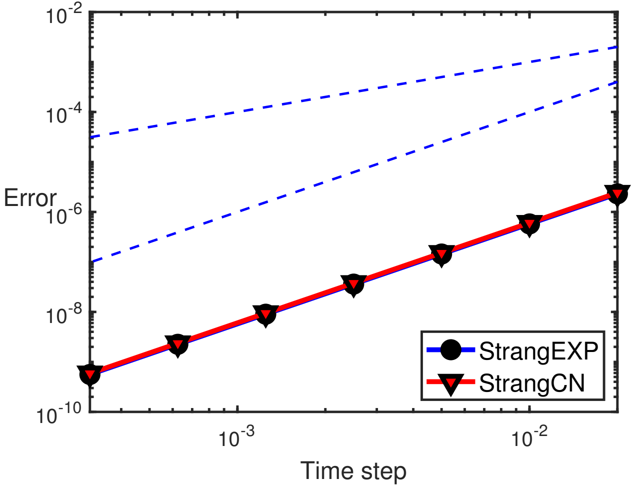
It is typical to approximate the exact flow of the diffusion part,

$$u(t) = \phi_t^D(u_0) : \qquad \begin{array}{rcl} \partial_t u &=& Du \quad \text{in } \Omega \times (0,T], \\ Bu &=& b \quad \text{on } \partial\Omega \times (0,T], \end{array}$$

either with a Krylov method, or with a Runge-Kutta type method, such as the Crank-Nicolson method (formally of order two),

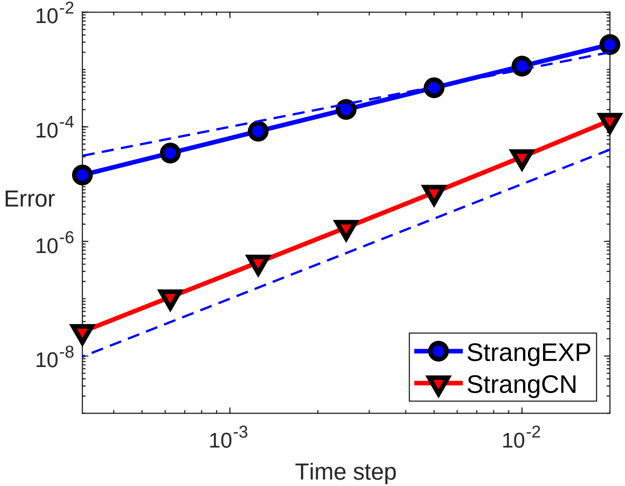
$$u_1 = \phi_\tau^{D,CN}(u_0) : \qquad \begin{array}{rcl} \frac{u_1(x)-u_0(x)}{\tau} &=& D\frac{u_1(x)+u_0(x)}{2} \quad \text{in } \Omega, \\ B\frac{u_0(x)+u_1(x)}{2} &=& b(x) \quad \text{on } \partial\Omega. \end{array}$$

A numerical example on $\Omega = (0,1)$



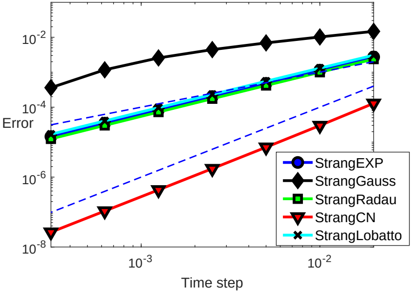
$$\partial_t u = \partial_{xx} u + e^{-x} \text{ on } \Omega, \quad \partial_x u + u = 1 \text{ on } \partial\Omega, \quad u(x,0) = 1.$$

A numerical example: order reduction!

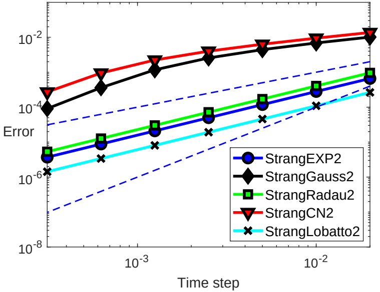


$$\partial_t u = \partial_{xx} u + 1 \text{ on } \Omega, \quad u = 1 \text{ on } \partial\Omega, \quad u(x,0) = 1.$$

With other approximations of the diffusion part?



$$u_{n+1} = \phi^{f}_{\frac{\tau}{2}} \circ \phi^{D}_{\tau} \circ \phi^{f}_{\frac{\tau}{2}}(u_n)$$



$$u_{n+1} = \phi^{D}_{\frac{\tau}{2}} \circ \phi^{f}_{\tau} \circ \phi^{D}_{\frac{\tau}{2}}(u_n)$$

$$\partial_t u = \partial_{xx} u + 1 \text{ on } \Omega, \quad u = 1 \text{ on } \partial\Omega, \quad u(x,0) = 1.$$

What happened?

An observation from [W. Hundsdorfer and J. Verwer. 1994]: the reason of the order reduction is that $w = \phi^f_\tau(u_n)$ does not preserve the boundary conditions, i.e. $Bu_n = b \not\Longrightarrow Bw = b$ for $Bf(u) \neq 0$.

Possible remedies to order reduction in splitting methods:

- [L. Einkemmer and A. Ostermann, 2016] Modify the splitting as:

$$u_{n+1} = \phi^{D+q_n}_{\frac{\tau}{2}} \circ \phi^{f-q_n}_{\tau} \circ \phi^{D+q_n}_{\frac{\tau}{2}}(u_n),$$

  where q_n is chosen such that $Bq_n = Bf(u_n) + \mathcal{O}(\tau)$ on $\partial\Omega$.

- [G. Bertoli and V., 2020] Consider a five step splitting method as

$$u_{n+1} = \phi^{f}_{\frac{\tau}{2}} \circ \phi^{-q_n}_{\frac{\tau}{2}} \circ \phi^{D+q_n}_{\tau} \circ \phi^{-q_n}_{\frac{\tau}{2}} \circ \phi^{f}_{\frac{\tau}{2}}(u_n)$$

  where q_n is computed only using the source flow output $\phi^f_{\frac{\tau}{2}}(u_n)$ such that $w = \phi^{-q_n}_{\frac{\tau}{2}} \circ \phi^f_{\frac{\tau}{2}}(u_n)$ satisfies the boundary conditions $Bw = b$ up to $\mathcal{O}(\tau^2)$.

Note: In this talk, we shall not use the above "repair" techniques.

Contents

G. Bertoli, C. Besse, and V., Superconvergence of the Strang splitting when using the Crank-Nicolson scheme for parabolic PDEs with oblique boundary conditions, Submitted (2020), Hal:hal-02992821v1, arXiv:2011.05178.

Superconvergence of splitting with Crank-Nicolson

For the diffusion-reaction problem, consider the splitting method

$$u_{n+1} = \phi^f_{\frac{\tau}{2}} \circ \phi^{D,CN}_\tau \circ \phi^f_{\frac{\tau}{2}}(u_n),$$

where the diffusion part is approximated by the Crank-Nicolson scheme.

Theorem (order two of convergence for $f = f(x)$)

Let $u_0 \in W^{2,p}(\Omega)$ with $Bu_0 = b$ on $\partial\Omega$ and $f = f(x) \in L^p(\Omega)$. Then the global error $e_n = u_n - u(t_n)$ satisfies

$$\|e_n\|_{L^p(\Omega)} \leq \frac{C\tau^2}{t_n}, \qquad e_n = \left(r(\tau A)^n - e^{n\tau A}\right) A^{-1}(Du_0 + f),$$

where A is the restriction of the operator D to the set of functions satisfying the homogeneous boundary condition $Bu(x) = 0$ on $\partial\Omega$, and $r(z) = \frac{1+\frac{z}{2}}{1-\frac{z}{2}}$ is the stability function of the CN scheme.

Preservation of stationary states

Corollary

For $f = f(x)$, the splitting method with Crank-Nicolson preserves stationary states.

Proof.

For a stationary solution $(\partial_t u(x,t) = 0)$, $Du_0 + f = 0$ yields

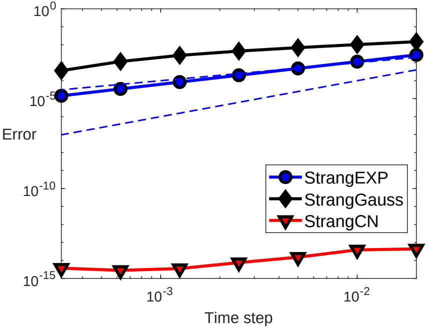
$$e_n = \left(r(\tau A)^n - e^{n\tau A}\right) A^{-1}(Du_0 + f) = 0$$

and $u_n = u_0$ for all n. □

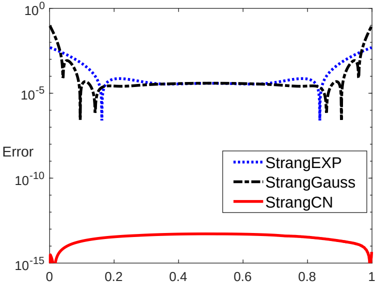
Remark 1. This result does not persist for $\phi_{\frac{\tau}{2}}^{D,CN} \circ \phi_{\tau}^{f} \circ \phi_{\frac{\tau}{2}}^{D,CN}$.

Remark 2. This result does not persist for nonlinear sources terms $f = f(x,u)$. See algebraic characerization of B-series in [McLachlan, K. Modin, H. Munthe-Kaas, O. Verdier, 2016].

Numerical experiments: errors for stationary states



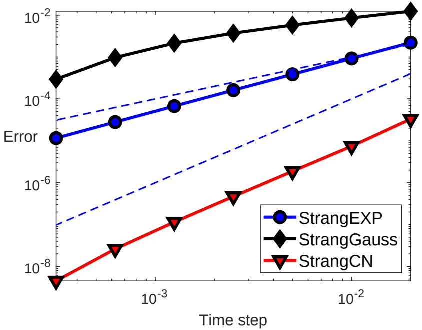
Error $u_n - u(t_n)$



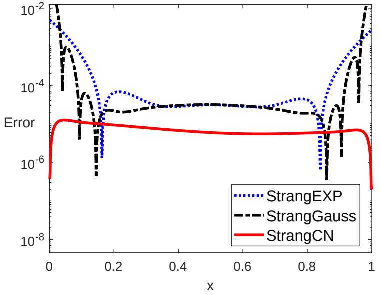
error profile $|u_n(x) - u(t_n, x)|$ for timestep $\tau = 10^{-2}$

$$\partial_t u = \partial_{xx} u - 1 \text{ on } \Omega = (0,1), \quad u = u_0 \text{ on } \partial\Omega, \quad u(x,0) = x^2/2.$$

Stationary states for $f = f(u)$



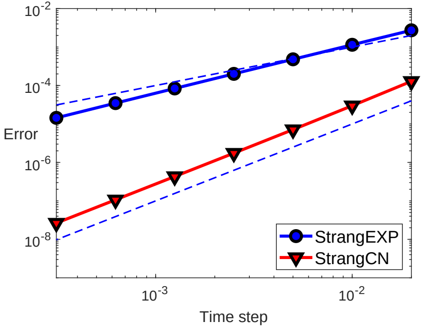
Error $u_n - u(t_n)$



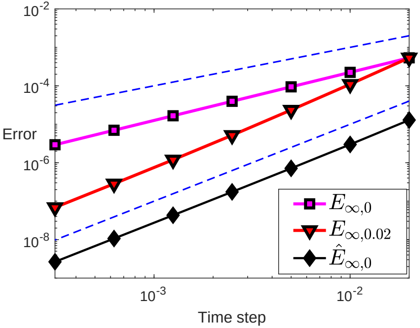
error profile $|u_n(x) - u(t_n, x)|$ for $\tau = 10^{-2}$.

$$\partial_t u = \partial_{xx} u + u \text{ on } \Omega, \quad u = u_0 \text{ on } \partial\Omega, \quad u(x,0) = u_0(x) = \cos(x).$$

Optimality of the error bound $\|u_n - u(t_n)\|_{L^p(\Omega)} \leq C\tau^2/t_n$



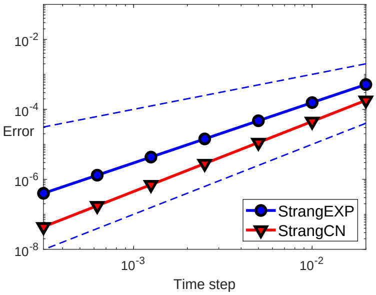
$L^2(\Omega)$ error at final time T



$L^\infty(0, T, L^2(\Omega))$ error
$L^\infty(0.02, T, L^2(\Omega))$ error
$L^\infty(0, T, L^2(\Omega))$ error for $tu(t)$

$$\partial_t u = \partial_{xx} u + 1 \text{ on } \Omega = (0,1), \quad u = 1 \text{ on } \partial\Omega, \quad u(x,0) = 1.$$

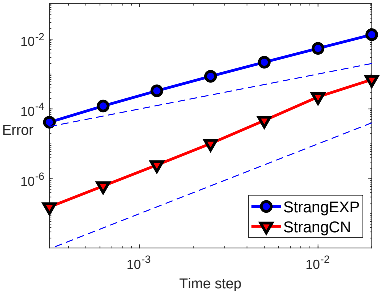
Numerical experiments on $\Omega = (0,1)^2$: nonlinear case



$$f(u) = u$$

Robin boundary conditions

$$u + \partial_n u = u_0 \text{ on } \partial\Omega$$



$$f(u) = u^2$$

Dirichlet + Neumann boundary conditions

$$\partial_t u = \Delta u + f(u) \text{ on } \Omega, \quad u(x,0) = u_0(x).$$

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Analytical framework

$D = \sum_{i,j=1}^{d} \frac{\partial}{\partial x_i}\left(a_{ij}(x)\frac{\partial}{\partial x_j}\right) + \sum_{i=1}^{d} b_i(x)\frac{\partial}{\partial x_i},$

$Bu(x) = \sum_{i=1}^{d} \beta_i(x)\frac{\partial u(x)}{\partial x_i} + \alpha(x)u(x).$

A lifting procedure to deal with $Bu = b$ on $\partial\Omega$. We define the operator $(A, \mathcal{D}(A))$ as the restriction of D to the domain $\mathcal{D}(A) = \{u \in W^{2,p}(\Omega); Bu = 0 \text{ on } \partial\Omega\}$, i.e. $Au = Du$ for $u \in \mathcal{D}(A)$.

The operator A is a closed densely defined linear operator satisfying:

- The resolvent set $\rho(A) = \{\lambda \in \mathbb{C}\ ;\ \lambda I - A \text{ is an isomorphism}\}$, contains, for a fixed $\theta \in (0, \frac{\pi}{2})$, the closure of the set $\Sigma_\theta = \{z \in \mathbb{C}\ ;\ z \neq 0,\ |\arg(z)| < \pi - \theta\}$, i.e. $\rho(A) \supset \overline{\Sigma}_\theta$.
- For all $\lambda \in \Sigma_\theta$, the resolvent $R(\lambda, A) = (\lambda I - A)^{-1}$, satisfies the following bound for the operator norm, where $M \geq 1$,

$$\|R(\lambda, A)\| \leq \frac{M}{|\lambda|}.$$

Main ingredient 1: Homogeneous case

Theorem (see [A. Hansbo, 1999] in a general Banach space case)

For $u_0 \in \mathcal{D}(A)$,

$$\|(r(\tau A)^n - e^{\tau n A})u_0\|_{L^p(\Omega)} \leq \frac{C\tau^2}{t_n}\|Au_0\|_{L^p(\Omega)},$$

where C is a constant independent of u_0, τ, n and $t_n = n\tau$.

Main ingredient 2: Local error representation

Consider the splitting method

$$u_{n+1} = \phi^f_{\frac{\tau}{2}} \circ \phi^{D,CN}_\tau \circ \phi^f_{\frac{\tau}{2}}(u_n) = \mathcal{S}_\tau(u_n).$$

Proposition

The local error $\delta_{n+1} = \mathcal{S}_\tau(u(t_n)) - u(t_{n+1})$ of the splitting with CN satisfies

$$\delta_{n+1} = (r(\tau A) - e^{\tau A})A^{-1}e^{t_n A}(Du_0 + f).$$

Remark: this local estimate is specific to the splitting method with the Crank-Nicolson scheme.

Global error

Proof.

The global error $e_n = u_n - u(t_n)$ satisfies

$$e_{n+1} = \mathcal{S}_\tau(u_n) - \mathcal{S}_\tau u(t_n) + \mathcal{S}_\tau u(t_n) - u(t_{n+1}) = \mathcal{S}_\tau(u_n) - \mathcal{S}_\tau u(t_n) + \delta_{n+1}.$$

Hence

$$e_{n+1} = r(\tau A)e_n + \delta_{n+1}$$

$$\begin{aligned} e_n &= \sum_{k=0}^{n-1} r(\tau A)^{n-k-1}\delta_{k+1} \\ &= \Big(\big(r(\tau A) - e^{\tau A}\big)\sum_{k=0}^{n-1} r(\tau A)^{n-k-1} e^{k\tau A}\Big) A^{-1}(Du_0 + f) \\ &= \big(r(\tau A)^n - e^{n\tau A}\big) A^{-1}(Du_0 + f). \end{aligned}$$

□

Return to the local error representation

We take $z \in W^{2,p}(\Omega)$ with $Bz = b$ on $\partial\Omega$ and define $\tilde{u} = u - z$, which satisfies the following differential problem with homogeneous boundary conditions,

$$
\begin{aligned}
\partial_t \tilde{u}(x,t) &= D\tilde{u}(x,t) + f(x, \tilde{u}(x,t) + z(x)) + Dz(x) \quad \text{in } \Omega \times (0,T], \\
B\tilde{u}(x,t) &= 0 \quad \text{on } \partial\Omega \times (0,T], \\
\tilde{u}(x,0) &= u_0(x) - z(x) \quad \text{in } \Omega.
\end{aligned}
$$

By the Duhamel formula,

$$\tilde{u}(t) = e^{tA}(u_0 - z) + \int_0^t e^{(t-s)A}(f(\tilde{u}(s) + z) + Dz)ds.$$

Using $\tilde{u}(t_n) \in \mathcal{D}(A)$, we deduce

$$u(t_n + \tau) = z + e^{\tau A}(u(t_n) - z) + \int_0^\tau e^{(\tau - s)A}(f(u(t_n + s)) + Dz)ds.$$

Return to the local error representation

We have the following representation of δ_{n+1}:

$$\delta_{n+1} = (r(\tau A) - e^{\tau A})(u(t_n) - z) + (r(\tau A) - e^{\tau A})A^{-1}Dz \\ + \frac{\tau}{2}(r(\tau A) + I)f - A^{-1}(e^{\tau A} - I)f.$$

Using $r(y) - e^y = \frac{y}{2}(r(y) + 1) - (e^y - 1)$,

$$\delta_{n+1} = (r(\tau A) - e^{\tau A})(u(t_n) - z + A^{-1}Dz + A^{-1}f).$$

Using $\tilde{u} = u - z$, recall $\partial_t \tilde{u}(t) = A\tilde{u}(t) + f + Dz$. Hence,

$$\delta_{n+1} = (r(\tau A) - e^{\tau A})A^{-1}\partial_t \tilde{u}(t_n).$$

Using the variation of constant formula, we obtain,

$$\begin{aligned}\partial_t \tilde{u}(t_n) &= Ae^{t_n A}\tilde{u}_0 + A\int_0^{t_n} e^{(t_n - s)A}(f + Dz)ds + f + Dz \\ &= Ae^{t_n A}\tilde{u}_0 + (e^{t_n A} - I)(f + Dz) + f + Dz \\ &= e^{t_n A}(A\tilde{u}_0 + f + Dz) = e^{t_n A}(Du_0 + f).\end{aligned}$$

Summary

- Surprisingly, the Crank-Nicolson scheme performs better that the exact solution in the Strang splitting, avoiding order reduction phenomena and preserving stationary states for $f = f(x)$.
- This seems specific to the Crank-Nicolson scheme among classical implicit Runge-Kutta methods.
- Remark: we noted numerically that the order two convergence of the Strang splitting method with Crank-Nicolson presented in this paper does not persist for dispersive problems, e.g.

$$i\partial_t u = \partial_{xx} u + 1 \text{ on } \Omega, \quad u = 1 \text{ on } \partial\Omega, \quad u(x,0) = 1.$$

Current works:

- Nonlinear $f(u)$?
- Case of absorbing boundary conditions?

G. Bertoli, C. Besse, and V., Superconvergence of the Strang splitting when using the Crank-Nicolson scheme for parabolic PDEs with oblique boundary conditions, Submitted (2020), Hal:hal-02992821v1, arXiv:2011.05178.