Splitting methods with boundary corrections

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Joint work with
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Strang's paper, SIAM J. Numer. Anal., 1968

$$u_t = Au_x + Bu_y, \qquad u(0) = u_0.$$

$$S_k^{(5)} f = \mathrm{e}^{\frac{k}{2}A\partial_x}\mathrm{e}^{kB\partial_y}\mathrm{e}^{\frac{k}{2}A\partial_x} f$$

or rather second-order approximations to the exponentials

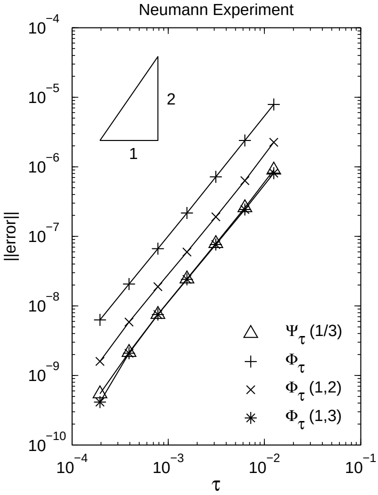
The first question is whether this alternation of one-dimensional operators retains second order accuracy. This can be decided only by a computation:

$$S_k^{(5)} f \approx \left(I + \frac{k}{2}A\partial_x + \frac{k^2}{8}A^2\partial_x^2\right)\left(I + kB\partial_y + \frac{k^2}{2}B^2\partial_y^2\right) \cdot \left(I + \frac{k}{2}A\partial_x + \frac{k^2}{8}A^2\partial_x^2\right) f$$

$$\approx f + k(Af_x + Bf_y) + \frac{k^2}{2}(A^2 f_{xx} + (AB + BA)f_{xy} + B^2 f_{yy}),$$

Neumann boundary conditions

$$\partial_t u = \partial_1(a\partial_1 u) + \partial_2(a\partial_2 u), \qquad \Omega = (0,1)^2$$

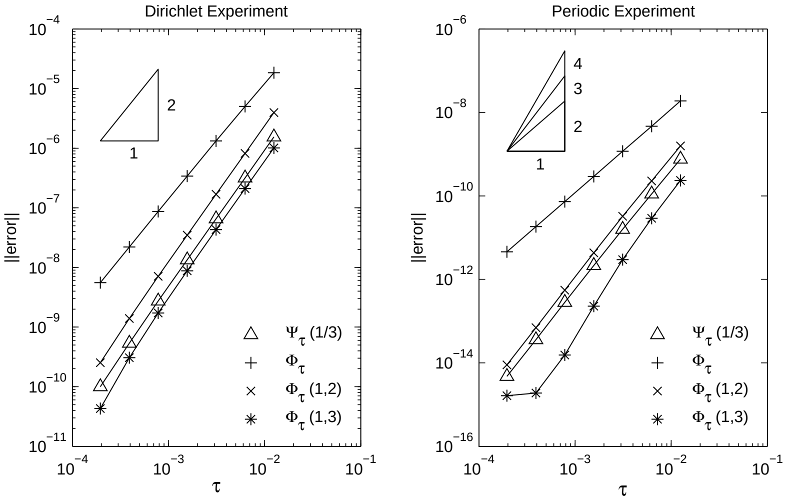


$$a(x_1,x_2) = 16x_1(1-x_1)x_2(1-x_2)+1$$

$$u_0(x_1,x_2) = c\,\exp\left(-\frac{1}{x_1(1-x_1)} - \frac{1}{x_2(1-x_2)}\right)$$

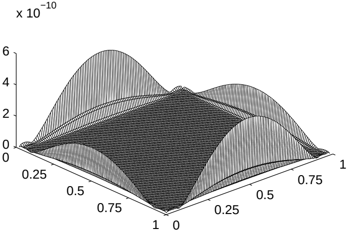
T/τ	Ψ_τ	Φ_τ	$\Phi_\tau(1,2)$	$\Phi_\tau(1,3)$
16	1.80	1.71	1.83	1.73
32	1.72	1.74	1.73	1.68
64	1.68	1.73	1.68	1.66
128	1.70	1.70	1.66	1.69
256	1.81	1.69	1.69	1.84
512	1.98	1.71	1.88	2.34

Dirichlet and periodic boundary conditions

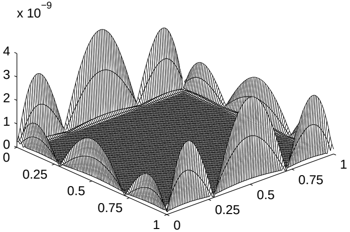


E. Hansen, A.O., High order splitting methods for analytic semigroups exist. *BIT Numer. Math.* 49, 527–542 (2009)

Error is concentrated on the boundary



Dirichlet problem



Neumann problem

Pointwise errors at time $T = 0.1$ for the splitting $\Phi_h(1,3)$, step size $\tau = T/512$.

Large errors are located along a thin strip around the boundary.

Outline

Diffusion-reaction splitting

Oblique boundary conditions

References

Diffusion-reaction equations: Dirichlet problem

Diffusion-reaction initial-boundary value problem

$$
\begin{aligned}
u_t &= Du + f(u) \\
u|_{\partial\Omega} &= b \\
u(0) &= u_0
\end{aligned}
$$

where

- $u = u(t, x)$ for $0 < t \leq T$ and $x \in \Omega \subset \mathbb{R}^d$;
- D is an elliptic differential operator (e.g., the Laplacian);
- $f : \mathbb{R} \to \mathbb{R}$ is the reaction term (usually $f(0) = 0$);
- b: $[0, T] \times \partial\Omega \to \mathbb{R}$ is allowed to depend on time.

Diffusion-reaction splitting

The system $$u_t = Du + f(u), \quad u|_{\partial\Omega} = b$$

is split up into $$v_t = Dv, \quad v|_{\partial\Omega} = b$$
$$w_t = f(w)$$

Numerical example in $\Omega = (0,1)$ with $u_0(x) = 1 + \sin^2 \pi x$, $f(u) = u^2$, 500 grid points, $b_0 = b_1 = 1$. Error at $t = 0.1$

	Strang		Strang (modified)	
step size	ℓ^2 error	order	ℓ^2 error	order
2.000e-02	1.524e-03	–	1.320e-05	–
1.000e-02	6.337e-04	1.2659	3.303e-06	1.9990
5.000e-03	2.628e-04	1.2697	8.264e-07	1.9987
2.500e-03	1.085e-04	1.2766	2.066e-07	1.9998
1.250e-03	4.444e-05	1.2875	5.152e-08	2.0039

Error analysis for Lie splitting

Reduction to homogeneous Dirichlet boundary conditions: let

$$Dz = 0, \quad z|_{\partial\Omega} = b$$

and consider $U = u - z$ which satisfies

$$\begin{aligned} U_t &= DU + f(U+z) - z_t, \quad U|_{\partial\Omega} = 0, \\ U(0) &= u_0 - z_0. \end{aligned}$$

Write PDE as an abstract parabolic problem

$$U_t = AU + k(t) + g(t, U), \quad U(0) = u_0 - z_0,$$

where $\mathcal{D}(A) = H^2(\Omega) \cap H_0^1(\Omega)$, e.g., and split.

The leading term in the local error is then

$$\tau^2 \cdot A\, g(t_k, U(t_k)).$$

Abstract convergence, classic Lie splitting

Theorem. (L. Einkemmer, AO, *SIAM J. Sci. Comput.*, 2015)
The classic Lie splitting is convergent of order $\tau\,|\log\tau|$, i.e.

$$\|u_n - u(t_n)\| \le C\tau(1 + |\log\tau|), \qquad 0 \le n\tau \le T,$$

where C depends on T but is independent of τ and n.

Proof. We employ the parabolic smoothing property

$$\|\mathrm{e}^{tA}(-tA)^{\alpha}\| \le C, \qquad \alpha \ge 0$$

to bound

$$\tau^2 \sum_{k=0}^{n-1} \mathrm{e}^{(n-k-1)\tau A} A g(t_k, U(t_k))$$

which is the leading error term.

Numerical results for Lie splitting

Numerical example in $\Omega = (0,1)$ with $u_0(x) = 1 + \sin^2 \pi x$, $f(u) = u^2$, 500 grid points, $b_0 = b_1 = 1$. Error at $t = 0.1$

	Lie		Lie (modified)	
step size	ℓ^∞ error	order	ℓ^∞ error	order
2.000e-02	2.872e-01	–	2.144e-01	–
1.000e-02	3.546e-03	6.3396	2.166e-03	6.6297
5.000e-03	1.957e-03	0.8575	1.090e-03	0.9910
2.500e-03	1.051e-03	0.8974	5.465e-04	0.9955
1.250e-03	5.526e-04	0.9269	2.737e-04	0.9977
6.250e-04	2.864e-04	0.9483	1.369e-04	0.9988
3.125e-04	1.468e-04	0.9636	6.849e-05	0.9994

Essential modification step

The critical error term is: $\mathrm{e}^{(n-k-1)\tau A} A g(t_k, U(t_k))$

Satisfy a compatibility condition for the nonlinearity.
(E. Hansen, F. Kramer, AO, *Appl. Numer. Math.*, 2012)

Split the nonlinearity $f(U+z)$ into a term $g(t,U)$ such that $g(t,0)=0$ and a second term that does not depend on U.

Obvious choice:

$$v_t = Dv + f(z) - z_t, \quad v|_{\partial\Omega} = 0$$
$$w_t = f(w+z) - f(z)$$

Modified nonlinearity $g(t,U) = f(U + z(t)) - f(z(t))$
satisfies $g(t,0) = 0$ as required.

Abstract convergence, Strang splitting

Theorem. (L. Einkemmer, AO, *SIAM J. Sci. Comput.*, 2015)
The classic Strang splitting is first-order convergent.
The modified Strang splitting is second-order convergent.

Proof. The leading error term is $\mathrm{e}^{(n-k-1)\tau A} A^2 g(t_k, U(t_k))$.

- One power of A is bounded by parabolic smoothing;
- Another power of A is bounded by the modification.

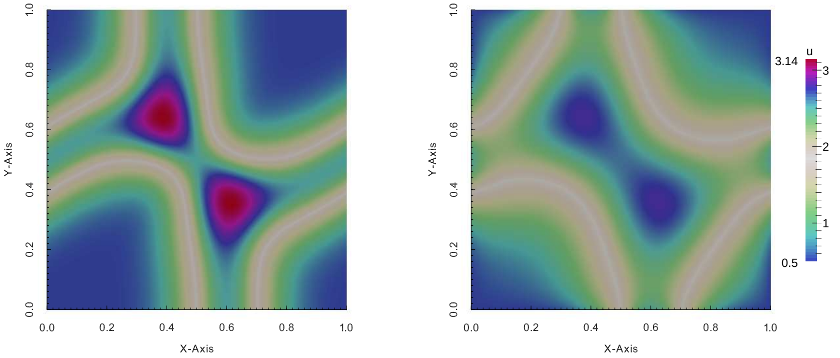
Remark. Spatially smooth functions lie in $\mathcal{D}((-\Delta)^{1/4-\varepsilon})$; therefore one observes order 1.25 in L^2 for uncorrected splitting (order $1 + \frac{1}{2p}$ in L^p).

1D example, time dependent boundary conditions

1D example, $\Omega = (0, 1)$, and $f(u) = u^2$,
initial value $u_0(x) = 1 + \sin^2 \pi x$, 500 grid points,
boundary values $b_0(t) = b_1(t) = 1 + \sin 5t$.

	Strang		Strang (modified)	
step size	ℓ^∞ error	order	ℓ^∞ error	order
2.000e-02	2.060e-02	–	4.399e-04	–
1.000e-02	9.913e-03	1.0554	1.099e-04	2.0005
5.000e-03	4.724e-03	1.0694	2.748e-05	2.0002
2.500e-03	2.212e-03	1.0947	6.867e-06	2.0005
1.250e-03	1.008e-03	1.1341	1.714e-06	2.0020
6.250e-04	4.407e-04	1.1932	4.263e-07	2.0079
3.125e-04	1.813e-04	1.2817	1.043e-07	2.0316

2D example, time invariant boundary conditions



step size	Strang ℓ^∞ error	Strang order	Strang (modified) ℓ^∞ error	Strang (modified) order
0.1	8.449277e-01	–	1.835188e-02	–
0.05	6.570760e-01	0.362768	4.962590e-03	1.88676
0.025	4.063934e-01	0.693183	1.263375e-03	1.97381
0.0125	1.670386e-01	1.2827	3.326822e-04	1.92507

Outline

Diffusion-reaction splitting

Oblique boundary conditions

References

Model problem with oblique b.c.

Diffusion-reaction problem on domain $\Omega \subset \mathbb{R}^d$

$$
\begin{aligned}
u_t &= Du + f(u) \\
Bu|_{\partial\Omega} &= b \\
u(0) &= u_0
\end{aligned}
$$

where

- $D = \sum_{i,j=1}^d d_{ij}(x)\partial_{ij} + \sum_{i=1}^d d_i(x)\partial_i + d_0(x)I$ is an elliptic operator with positive definite $(d_{ij}(x))$;
- $B = \sum_{i=1}^d \beta_i(x)\partial_i + \alpha(x)I$ is a first-order operator;
- B satisfies the uniform non tangentiality condition

$$
\inf_{x\in\partial\Omega} \left| \sum_{i=1}^d \beta_i(x) n_i(x) \right| > 0.
$$

Neumann problem: $\alpha = 0$, $\beta_i(x) = \sum_{j=1}^d d_{ij}(x) n_j(x)$ for all i.

Condition on the correction

Choose as correction a smooth function q that satisfies the boundary conditions of $f(u)$

$$Bq_n(0)|_{\partial\Omega} = Bf(u(t_n))|_{\partial\Omega} + \mathcal{O}(\tau).$$

Since

$$\begin{aligned} Bf(u)|_{\partial\Omega} &= \alpha f(u)|_{\partial\Omega} + f'(u)\textstyle\sum_{i=1}^{d} \beta_i(x)\partial_i u|_{\partial\Omega} \\ &= \alpha f(u)|_{\partial\Omega} + f'(u)(b - \alpha u)|_{\partial\Omega} \end{aligned}$$

and our numerical methods converge at least with order one, we can simply take

$$Bq_n|_{\partial\Omega} = \alpha f(u_n)|_{\partial\Omega} + f'(u_n)\big(b_n - \alpha u_n\big)|_{\partial\Omega}.$$

Dirichlet case: $\alpha = 1$, $\beta_1 = \ldots = \beta_s = 0$ and $q|_{\partial\Omega} = f(b)$.
(previously called $f(z)$)

Modified splitting

With the correction q_n satisfying

$$Bq_n|_{\partial\Omega} = \alpha f(u_n)|_{\partial\Omega} + f'(u_n)\big(b_n - \alpha u_n\big)|_{\partial\Omega}.$$

at hand, we consider the boundary-corrected splitting

$$\begin{aligned} \partial_t v_n &= Dv_n + q_n, \quad Bv_n|_{\partial\Omega} = b_n \\ \partial_t w_n &= f(w_n) - q_n, \end{aligned}$$

and solve it on the time interval $[t_n, t_{n+1}]$ by the standard Lie or Strang approach.

Modified Strang splitting

For a given initial value u_n, first solve

$$\partial_t v_n = Dv_n + q_n, \quad Bv_n|_{\partial\Omega} = b_n$$

with initial value $v_n(0) = u_n$ to obtain $v_n(\frac{\tau}{2})$.

Next, integrate $\partial_t w_n = f(w_n) - q_n$ with initial value $w_n(0) = v_n(\frac{\tau}{2})$ to obtain $w_n(\tau)$.

Finally, integrate once more

$$\partial_t \tilde{v}_n = D\tilde{v}_n + q_n, \quad B\tilde{v}_n|_{\partial\Omega} = b_n$$

but this time with initial value $\tilde{v}_n(0) = w_n(\tau)$, and set

$$u_{n+1} = \mathcal{S}_\tau u_n = \tilde{v}_n(\tfrac{\tau}{2}).$$

Convergence results

Theorem. (L. Einkemmer, AO, arXiv:1601.02288, 2016)
The modified Strang splitting scheme is second-order convergent. More precisely, the global error satisfies

$$\|u_n - u(t_n)\| \le C\tau^2(1 + |\log\tau|), \qquad 0 \le n\tau \le T,$$

where C depends on T but is independent of τ and n.

Orders of convergence for classic Strang splitting in various norms:

boundary type	L^1	L^2	L^∞
$\beta_1 = \ldots = \beta_d = 0$	1.50	1.25	1.00
$\exists j$ with $\beta_j \neq 0$	2.00	1.75	1.50

Inhomogeneous Neumann boundary conditions

We take $f(u) = u^2$, $\Omega = (0,1)$ with $b_0 = 0$ and $b_1 = 1$, 500 points.
Admissible correction $q_n(s,x) = x^2 u_n(1)$.

	Strang		Strang	
step size	ℓ^∞ error	order	ℓ^2 error	order
3.125e-02	1.806e-01	–	8.733e-02	–
1.562e-02	2.211e-04	9.67	2.130e-05	12.00
7.812e-03	7.684e-05	1.52	6.364e-06	1.74
3.906e-03	2.638e-05	1.54	1.895e-06	1.75
1.953e-03	8.897e-06	1.57	5.612e-07	1.76

	Strang (modified)		Strang (modified)	
step size	ℓ^∞ error	order	ℓ^2 error	order
3.125e-02	8.752e-02	–	5.471e-02	–
1.562e-02	1.495e-05	12.51	3.931e-06	13.76
7.812e-03	3.868e-06	1.95	9.773e-07	2.01
3.906e-03	1.002e-06	1.95	2.428e-07	2.01
1.953e-03	2.603e-07	1.94	6.023e-08	2.01

Mixed Dirichlet/Neumann boundary conditions

Dirichlet b.c. (with $b_0 = 1$) and Neumann b.c. (with $b_1 = 1$).
Correction is given by $q_n(s, x) = 1 + 2xu_n(1)$.

	Strang		Strang	
step size	ℓ^∞ error	order	ℓ^2 error	order
1.250e-02	5.718e-03	–	5.815e-04	–
6.250e-03	2.736e-03	1.06	2.379e-04	1.29
3.125e-03	1.288e-03	1.09	9.652e-05	1.30
1.563e-03	5.904e-04	1.13	3.855e-05	1.32
7.813e-04	2.596e-04	1.19	1.499e-05	1.36

	Strang (modified)		Strang (modified)	
step size	ℓ^∞ error	order	ℓ^2 error	order
1.250e-02	8.222e-05	–	2.567e-05	–
6.250e-03	2.087e-05	1.98	6.426e-06	2.00
3.125e-03	5.292e-06	1.98	1.609e-06	2.00
1.563e-03	1.341e-06	1.98	4.031e-07	2.00
7.813e-04	3.395e-07	1.98	1.009e-07	2.00

Various possible corrections

Problem with Dirichlet b.c. ($b_0 = 1, b_1 = 2$) and 500 grid points. The error is given at $t = 0.1$ with a step size $\tau = 1.25 \cdot 10^{-3}$.

method	correction	ℓ^∞ error
Lie	none	2.31e-03
Lie (mod.)	harmonic: $q = 1 + x$	1.20e-03
Lie (mod.)	$q = 1 + x + \sin \pi x$	2.43e-03
Lie (mod.)	$q = 1 + x + \sin 10\pi x$	3.21e-03

method	correction	ℓ^∞ error
Strang	none	1.84e-03
Strang (mod.)	harmonic: $q = 1 + x$	1.20e-06
Strang (mod.)	$q = 1 + x + \sin \pi x$	1.27e-06
Strang (mod.)	$q = 1 + x + \sin 10\pi x$	7.02e-05

References

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