Splitting methods for multiscale problems

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Joint work with
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Multiscale numerical methods for
differential equations, Rennes 2015

Splitting methods for initial value problems

Consider the initial value problem

$$u' = A(u) + B(u), \qquad u(0) = u_0$$

Splitting the vector field

$$\begin{aligned} v' = A(v) \qquad &\to \qquad v(t) = \varphi_t^{[A]}(v_0) \\ w' = B(w) \qquad &\to \qquad w(t) = \varphi_t^{[B]}(w_0) \end{aligned}$$

Lie–Trotter splitting (Trotter 1959)

$$u(\tau) \;\approx\; \varphi_\tau^{[B]} \circ \varphi_\tau^{[A]}\,(u_0)$$

Strang–Marchuk splitting (1968)

$$u(\tau) \;\approx\; \varphi_{\tau/2}^{[A]} \circ \varphi_\tau^{[B]} \circ \varphi_{\tau/2}^{[A]}\,(u_0)$$

Nonlinear Schrödinger equations

Cubic nonlinear Schrödinger equation

$$\mathrm{i}\,\partial_t u = (-\Delta + |u|^2)u$$

In the previous notation

$$Au = \mathrm{i}\,\Delta u, \qquad B(u) = -\mathrm{i}\,|u|^2 u$$

The flow of B can be computed exactly. Note that

$$\mathrm{i}\,w_t \overline{w} = |w|^4$$

implies $w_t \overline{w} \in \mathrm{i}\,\mathbb{R}$ and thus

$$(|w|^2)_t = 0, \qquad w(t) = \mathrm{e}^{-\mathrm{i}\,|w_0|^2 t} w_0$$

High-order methods by composition.

Error analysis for PDEs – the linear case

Initial value problem

$$u' = Au + Bu, \qquad \text{e.g.,}\quad A = \mathrm{i}\Delta, \quad B = \mathrm{i}\,V(x)$$

Error analysis: expand exact solution

$$\begin{aligned} u(\tau) &= \mathrm{e}^{\tau A}u_0 + \int_0^\tau \mathrm{e}^{(\tau-s)A}Bu(s)\,\mathrm{d}s \\ &= \mathrm{e}^{\tau A}u_0 + \int_0^\tau \mathrm{e}^{(\tau-s)A}B\mathrm{e}^{sA}u_0\,\mathrm{d}s + \mathcal{O}(\tau^2) \end{aligned}$$

and numerical solution

$$\begin{aligned} u_1 &= \mathrm{e}^{\tau A}\mathrm{e}^{\tau B}u_0 \\ &= \mathrm{e}^{\tau A}\Big(1 + \tau B + \mathcal{O}(\tau^2)\Big)u_0 \\ &= \mathrm{e}^{\tau A}u_0 + \tau\mathrm{e}^{\tau A}Bu_0 + \mathcal{O}(\tau^2) \end{aligned}$$

Error analysis for PDEs – cont.

Take the difference of the exact

$$u(\tau) = \mathrm{e}^{\tau A} u_0 + \int_0^\tau \mathrm{e}^{(\tau - s)A} B \mathrm{e}^{sA} u_0 \, \mathrm{d}s + \mathcal{O}(\tau^2)$$

and the numerical solution

$$u_1 = \mathrm{e}^{\tau A} u_0 + \tau \mathrm{e}^{\tau A} B u_0 + \mathcal{O}(\tau^2)$$

and use the quadrature rule

$$\int_0^\tau f(s) \, \mathrm{d}s = \tau f(0) + \int_0^\tau \int_0^s f'(\sigma) \, \mathrm{d}\sigma \, \mathrm{d}s,$$

where

$$f(s) = \mathrm{e}^{(\tau - s)A} B \mathrm{e}^{sA} u_0, \qquad f'(\sigma) = \mathrm{e}^{(\tau - \sigma)A} [B, A] \mathrm{e}^{\sigma A} u_0$$

Order of consistency requires smoothness.
(T. Jahnke, C. Lubich, *BIT*, 2000)

Error analysis for PDEs – the nonlinear case

Lemma [Gröbner–Alekseev formula]. Consider

$$u'(t) = A(u(t)) + B(u(t)), \quad u(0) = u_0$$
$$w'(t) = A(w(t)) \quad \text{with solution } E_A(t, w_0)$$

Then

$$u(t) = E_A(t, u_0) + \int_0^t \partial_2 E_A\left(t - s, u(s)\right) B\left(u(s)\right) \mathrm{d}s$$

Proof. Fundamental theorem of calculus.

- 'Back to the linear case.'
- Temporal and spatial smoothness of the exact solution required.
- Stability, however, can be tricky.

Outline

Burgers type nonlinearities

Many interesting equations in physics are of the form

$$u_t = P(\partial_x)u + uu_x,$$

where P is a polynomial of $\deg P \geq 2$ and with $\operatorname{Re} P(\mathrm{i}\xi) \leq 0$:

$$u_t = u_{xx} + uu_x \qquad \text{viscous Burgers equation}$$

$$u_t = u_{xxx} + uu_x \qquad \text{Korteweg–de Vries equation}$$

$$u_t = u_{xxxxx} - u_{xxx} + uu_x \qquad \text{Kawahara equation}$$

Splitting: linear part $Au = P(\partial_x)u$
Burgers nonlinearity $B(u) = uu_x$

Abstract convergence analysis for Strang splitting:
smooth initial data, exact flows, periodic b.c.
(H. Holden, C. Lubich, N. Risebro, *Math. Comp.*, 2013)

Kadomtsev–Petviashvili equation

KP models the evolution of nonlinear, long waves of small amplitude with slow dependence on the transverse coordinate.
(B. Kadomtsev and V. Petviashvili, *Sov. Phys. Dokl.*, 1970)

Cross swell [haule croisée, Kreuzsee] at Île de Ré (wikipedia, Michel Griffon).

Kadomtsev–Petviashvili equation

KP is a model for nonlinear wave propagation

$$\left(\partial_t u + 6uu_x + \varepsilon^2 u_{xxx}\right)_x + \lambda u_{yy} = 0$$

Description of long wavelength waves, where

$\lambda = 1$	(weak surface tension)	KP I model
$\lambda = -1$	(strong surface tension)	KP II model

In evolution form

$$\partial_t u + 6uu_x + \varepsilon^2 u_{xxx} + \lambda \partial_x^{-1} u_{yy} = 0$$

Soliton solutions; appearance of small scale oscillations.

Numerical comparisons (exponential integrators).
(C. Klein and K. Roidot, *SIAM J. Sci. Comput.*, 2011)

KP equation, splitting

We split the KP equation into

$$v_t = Av = -\varepsilon^2 v_{xxx} - \lambda \partial_x^{-1} v_{yy}$$
$$w_t = B(w) = -6ww_x$$

and use Strang splitting on a regular spatial grid.

For the linear part, we use FFT (with regularized Fourier multiplier).

For the nonlinear advection part, we use the method of characteristics

$$w(\tau, x, y) = w_1(x, y) = w_0(x - \tau w_1(x, y), y)$$

This equation is solved by a few fixed-point iterations; requires interpolation of $w_0(\cdot, y)$.

Can be done in parallel (y is a parameter).

KP equation, exponential integrator

Alternative discretization by an exponential integrator (relying on the above splitting)

$$u_{n+1} = \mathrm{e}^{\tau A} u_n + \tau \varphi_1(\tau A) B(u_n) + \tau \varphi_2(\tau A) \left(B(U) - B(u_n) \right),$$

where

$$U = \mathrm{e}^{\tau A} u_n + \tau \varphi_1(\tau A) B(u_n)$$

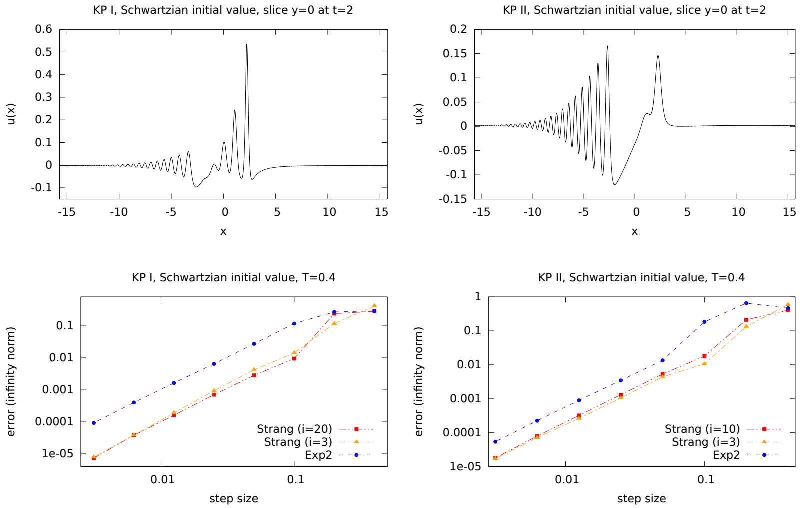
The φ_i functions are given by the recurrence relation

$$z\varphi_{k+1}(z) = \varphi_k(z) - \varphi_k(0), \qquad \varphi_0(z) = \mathrm{e}^z$$

Exponential integrators treat the advection explicitly and require a CFL condition.

(M. Hochbruck, A.O., *Acta Numerica*, 2010)

Initial value $u_0(x,y) = -\frac{1}{2}\partial_x \operatorname{sech}^2\left(\sqrt{x^2+y^2}\right)$

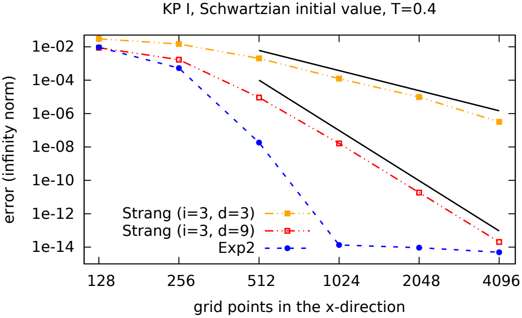


$$\Omega = [-5\pi, 5\pi]^2, \quad \varepsilon = 0.1, \quad 2^{11} \times 2^9 \text{ grid points for } (x,y)$$

Loss of exponential convergence

The ninth degree polynomial interpolation is approximately three times as costly as the cubic interpolation.

Nevertheless, Strang splitting is still twice as fast compared to the exponential integrator of order 2.

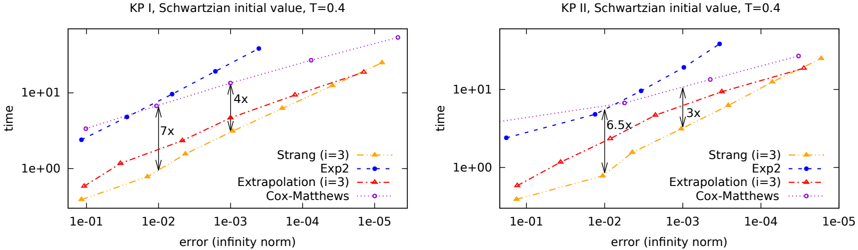


$\Omega = [-5\pi, 5\pi]^2, \quad \varepsilon = 0.1, \quad 2^9$ grid points for y, $\quad \tau = 0.01$

Performance

Compare performance of splitting methods (order 2 and 4) with two exponential integrators.

(S. Cox and P. Matthews, *J. Comput. Phys.*, 2002)



$\Omega = [-5\pi, 5\pi]^2, \quad \varepsilon = 0.1, \quad 2^{11} \times 2^9$ grid points

For $d = 9$ the fourth-order methods behave almost identically.

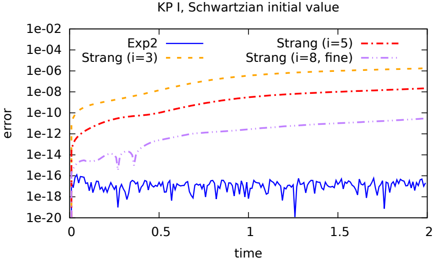
Conservation of mass: $|m(t) - m(0)|$

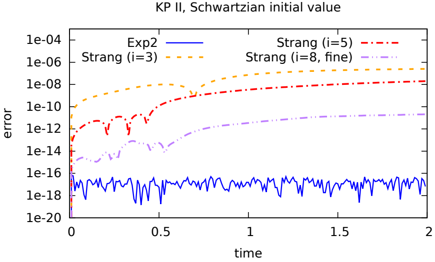
Total mass

$$m(t) = \int_\Omega u(t,x,y)\,\mathrm{d}(x,y)$$

is conserved by exponential integrators.

(L. Einkemmer, A.O., *J. Comput. Phys.*, 2015)



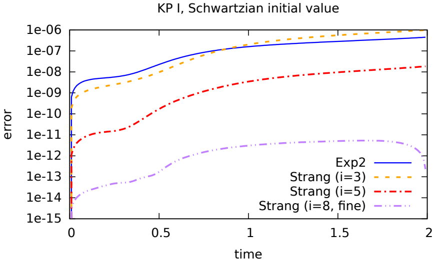


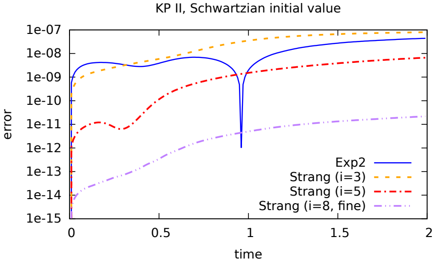
$\Omega = [-5\pi, 5\pi]^2$, $\quad \varepsilon = 0.1$, $\quad 2^{11} \times 2^9$ grid points, $\quad \tau = 0.01$

fine grid: $2^{13} \times 2^9$

Conservation of momentum

KP has quadratic invariant $$\int_\Omega u(t,x,y)^2 \,\mathrm{d}(x,y)$$





$\Omega = [-5\pi, 5\pi]^2$, $\quad \varepsilon = 0.1$, $\quad 2^{11} \times 2^9$ grid points, $\quad \tau = 0.01$

fine grid: $2^{13} \times 2^9$

Outline

Burgers type nonlinearities

Reaction-diffusion equations

Positivity preservation

Conclusions

Reaction-diffusion equation

Reaction-diffusion initial-boundary value problem

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

where

- $u(t) = u(t,x)$ for $0 < t \le T$ 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 $f(0) = 0$);
- $b \colon [0, T] \times \partial\Omega \to \mathbb{R}$ is allowed to depend on time.

Reaction-diffusion splitting

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

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	1.999
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

First analysis

Reduction to homogeneous Dirichlet boundary conditions: let

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

and consider $U = u - z$ which satisfies

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

Written as an abstract parabolic problem

$$\begin{aligned} U_t &= AU + k(t) + g(t, U) \\ U(0) &= u_0 - z_0, \end{aligned}$$

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

Lie splitting

Splitting the problem

$$U_t = AU + k(t) + g(t, U), \quad U_n = u(t_n) - z(t_n)$$

gives

$$v(t_n + \tau) = \mathrm{e}^{\tau A} U_n + \int_0^\tau \mathrm{e}^{(\tau - s)A} k(t_n + s)\,\mathrm{d}s$$

and

$$w(t_n + \tau) = U_n + \tau g(t_n, U_n) + \int_0^\tau (\tau - s) w''(t_n + s)\,\mathrm{d}s,$$

hence (blue after red)

$$\mathcal{L}_\tau U_n = \mathrm{e}^{\tau A} U_n + \tau \mathrm{e}^{\tau A} g(t_n, U_n) + \int_0^\tau \mathrm{e}^{(\tau - s)A} k(t_n + s)\,\mathrm{d}s + \int_0^\tau \mathrm{e}^{\tau A} (\tau - s) w''(t_n + s)\,\mathrm{d}s$$

Local error of Lie splitting

Expansion of the exact solution

$$U(t_n+\tau) = \mathrm{e}^{\tau A} U_n + \int_0^\tau \mathrm{e}^{(\tau-s)A} k(t_n+s)\,\mathrm{d}s + \int_0^\tau \mathrm{e}^{(\tau-s)A} g(t_n+s, U(t_n+s))\,\mathrm{d}s.$$

Combining these results we get for the local error

$$\mathcal{L}_\tau U_n - U(t_n+\tau) = \int_0^\tau \mathrm{e}^{\tau A}(\tau-s) w''(t_n+s)\,\mathrm{d}s - \int_0^\tau \int_0^s \ell_n'(\xi)\,\mathrm{d}\xi\mathrm{d}s,$$

where

$$\ell_n(s) = \mathrm{e}^{(\tau-s)A} g(t_n+s, U(t_n+s))$$

and thus

$$\ell_n'(s) = -\mathrm{e}^{(\tau-s)A} A g(t_n+s, U(t_n+s)) + \mathrm{e}^{(\tau-s)A} \partial_s g(t_n+s, U(t_n+s))$$

Abstract convergence, classical Lie splitting

Theorem. (L. Einkemmer, A.O., *SIAM J. Sci. Comput.*, 2015)
The classical 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

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

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.

Essential modification step

Satisfy a compatibility condition for the nonlinearity.
(E. Hansen, F. Kramer, A.O., *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:

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

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

Abstract convergence, Strang splitting

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

Proof. The leading error term is now $A^2 g(t, U(t))$.

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

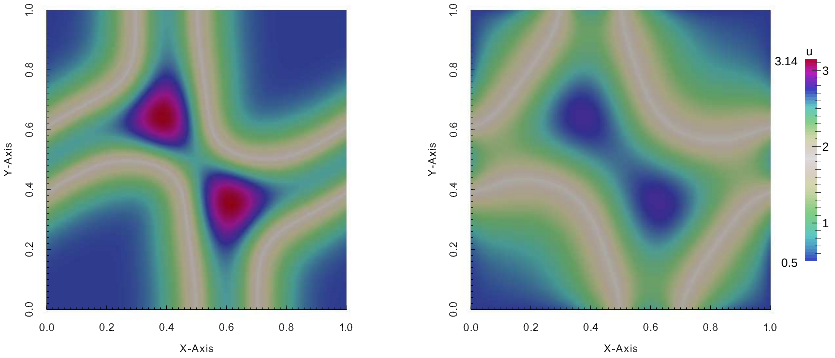
Remark. Spatially smooth functions lie in $\mathcal{D}((-\Delta)^{1/4-\varepsilon})$; therefore one observes order 1.25 in L^2 for uncorrected splitting (order $1 + \frac{1}{2p}$ in L^p).

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	2.002
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



	Strang		Strang (modified)	
step size	ℓ^∞ error	order	ℓ^∞ error	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

Strang preserves positivity

Theorem. For the numerical solution of $u' = Au + f(u)$, consider the Strang splitting. If the semigroups e^{tA} and $\varphi_t^{[f]}$ are positive, then the Strang splitting is positive as well.

Proof. Composition of positive operators is positive.

Example. Chafee–Infante equation

$$u_t - u_{xx} = u - u^3.$$

The semigroups e^{tA} and $\varphi_t^{[f]}$ are positive. Moreover, the set

$$Y = \{v \in X \,;\, v(\Omega) \subseteq [0,1]\}$$

is invariant under f, e^{tA}, $\varphi_t^{[f]}$ and the exact flow.

Positivity of full discretization

Let $\Omega \subset \mathbb{R}^2$ be polygonal and consider

$$u_t - \Delta u = 0, \quad u|_{\partial\Omega} = 0$$

together with its FE discretization (linear, lumped mass)

$$D_h u_h'(t) + S_h u_h(t) = 0$$

Theorem. (V. Thomeé, L. Wahlbin, *Math. Comp.*, 2008)
Let $A_h = -D_h^{-1} S_h$. The solution matrix $\mathrm{e}^{\tau A_h}$ is positive for all τ if and only if the triangulation $\mathcal{T}_h$ is Delaunay.

Combined with Strang splitting this gives a second-order positive scheme.

Conclusions

- Splitting methods for evolutionary PDEs;
- Attenuate the CFL condition;
- Methods are computationally attractive;
- Non-periodic boundary conditions require care;
- Good geometric properties.

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