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Operator Splitting Methods for Evolution Equations

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Integrable Systems and Scientific Computing

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joint work with Eskil Hansen, Lund University

Introduction

Splitting methods for ODEs

Consider the initial value problem

$$u' = f(u) + g(u), \qquad u(0) \text{ given}$$

Splitting the vector field

$$\begin{aligned} v' &= f(v), \qquad &\Rightarrow \quad v(t) = \varphi_t^{[f]}(v(0)) \\ w' &= g(w), \qquad &\Rightarrow \quad w(t) = \varphi_t^{[g]}(w(0)) \end{aligned}$$

Lie–Trotter splitting (Trotter 1959)

$$u(h) \;\approx\; \varphi_h^{[g]} \circ \varphi_h^{[f]} \,(u(0))$$

Strang–Marchuk splitting (1968)

$$u(h) \;\approx\; \varphi_{h/2}^{[f]} \circ \varphi_h^{[g]} \circ \varphi_{h/2}^{[f]} \,(u(0))$$

Error analysis – the linear case

Initial value problem

$$u' = Au + Bu, \qquad u(t) = \mathrm{e}^{t(A+B)}u(0)$$

Error analysis: bounds for

$$\left\| \mathrm{e}^{tA}\mathrm{e}^{tB} - \mathrm{e}^{t(A+B)} \right\| \le C\, t^{p+1}$$

- Taylor series expansions
- Baker-Campbell–Hausdorff formula (1905/06)

$$\mathrm{e}^{sA}\mathrm{e}^{tB} = \mathrm{e}^{C(s,t)}, \quad C(s,t) \; = \; sA + tB + \frac{st}{2}[A,B] + \ldots$$

expansion in terms of commutators

Hairer, Lubich, Wanner: Geometric Numerical Integration

Error analysis – the nonlinear case

Calculus of Lie derivatives

$$u' = f(u), \qquad D_f = \sum_{j=1}^{n} f_j(u) \frac{\partial}{\partial u_j}$$

gives the representation

$$\varphi_t^{[f]}(u_0) = \exp(tD_f)\mathrm{Id}\,(u_0)$$

Gröbner's permutation lemma (1960)

$$\varphi_t^{[g]} \circ \varphi_t^{[f]} = \exp(tD_f)\exp(tD_g)\mathrm{Id}$$

back to the BCH-formula

Hairer, Lubich, Wanner: Geometric Numerical Integration
Hundsdorfer, Verwer: Numerical Solution of Time-Dependent ADR Eqs.
Sanz-Serna, Calvo: Numerical Hamiltonian Problems

Why using splitting methods?

- geometric numerical integration
  properties of the exact flow are conserved

- partial differential equations
  quest for efficient solvers
  splitting of dimensions
  one large system $\longrightarrow$ many smaller systems (in parallel)
  splitting of physical phenomena (time scales)
  advection, diffusion, reaction
  simpler subsystems

- exact integrators for the single flows are available
  (non)linear Schrödinger eqs., diffusion-reaction eqs.

Splitting methods for PDEs

enormous amount of literature, starting in the 1950's

LOD schemes (locally one dimensional, fractional step methods): Samarskii, Yanenko, Marchuk, ...

ADI schemes (alternating direction implicit):
Douglas, Peaceman, Rachford, ...

in this talk: abstract point of view

evolutionary PDE = ODE in an abstract Banach space

Trotter, Sheng, Schatzman, Descombes, Lubich, Jahnke, Faou, ...

Hundsdorfer, Verwer: Numerical Solution of Time-Dependent Advection-Diffusion-Reaction Equations

Outline

Introduction

Error analysis based on semigroups

High order exponential splitting methods

Error analysis based on semigroups

Linear problem setting

Consider the abstract evolution equation

$$u' = Lu = (A + B)u$$

where L, A and B are of the form

- $E : \mathcal{D}(E) \subseteq H \to H$
- linear and unbounded
- maximal dissipative, i.e.,
  $\mathrm{Re}(Eu, u) \le 0$ and $\mathcal{R}(I - E) = H$

E generates an analytic semigroup of contractions

Linear problem setting, example

Example Elliptic operator on $\Omega \subset \mathbb{R}^d$

$$
\begin{aligned}
Lu &= Au + Bu \\
&= \sum_{i=1}^{s} D_i \left(a_i(x)\ D_i u \right) + \sum_{j=s+1}^{d} D_j \left(a_j(x)\ D_j u \right)
\end{aligned}
$$

- $H = L_2(\Omega)$
- $a_i > 0$ on $\overline{\Omega}$ and boundary conditions
- $a_i > 0$ on Ω and $a_i = 0$ on $\partial\Omega$

Splitting, examples

Four typical examples of splitting methods $S_h u_0 \approx \mathrm{e}^{hL} u_0$

- Lie–Trotter splitting (1959)

  $$S_h = (I - hB)^{-1}(I - hA)^{-1}$$

- Peaceman–Rachford splitting (1955)

  $$S_h = (I - \tfrac{h}{2}B)^{-1}(I + \tfrac{h}{2}A)(I - \tfrac{h}{2}A)^{-1}(I + \tfrac{h}{2}B)$$

- Exponential Lie splitting

  $$S_h = \mathrm{e}^{hB}\mathrm{e}^{hA}$$

- Strang splitting (1968)

  $$S_h = \mathrm{e}^{\frac{1}{2}hA}\mathrm{e}^{hB}\mathrm{e}^{\frac{1}{2}hA}$$

Typical convergence analysis

Telescopic identity

$$(S_h^n - \mathrm{e}^{nhL})u_0 = \sum_{j=0}^{n-1} S_h^{n-j-1}(S_h - \mathrm{e}^{hL})\mathrm{e}^{jhL}u_0$$

Stability $\quad \|S_h^n\| \le C \quad$ for $0 \le nh \le T$

difficult in a general Banach space framework

simple situations:

maximal dissipative operators in Hilbert spaces

relatively bounded operators $\quad \|A^{-\alpha}B\| \le C \quad$ for $0 \le \alpha < 1$

Consistency

Orders require regularity assumptions on initial data / solution

Main goals

Devise and employ an abstract framework which

- allows to prove optimal convergence orders
- allows splitting into unbounded operators
- includes elliptic operators on bounded domains with nonperiodic b.c.

today: concentrate on linear parabolic problems

Many results generalize to
C_0 groups (linear Schrödinger eq. with unbounded potential)
nonlinear parabolic problems

Convergence of the Lie splitting

Consider $\quad u' = Lu, \quad L = A + B$

Theorem

If, under the above assumptions,

i. $\mathcal{D}(L^2) \subseteq \mathcal{D}(AB) \cap \mathcal{D}(A)$

ii. $u_0 \in \mathcal{D}(L^2)$

then the Lie splitting is first order convergent,

$$\|(S_h^n - \mathrm{e}^{nhL})u_0\| \ \le \ Ch \sum_{j=0}^{2} \|L^j u_0\|$$

Note $\quad u_0 \in \mathcal{D}(L^{1+\varepsilon})$ is sufficient if L is sectorial

Hansen, A.O., Numer. Math. (2008)

Proof

Telescopic identity

$$(S_h^n - \mathrm{e}^{nhL})u_0 = \sum_{j=0}^{n-1} S_h^{n-j-1}(S_h - \mathrm{e}^{hL})\mathrm{e}^{jhL}u_0$$

Step I Stability

L, A, B are dissipative

$\Rightarrow \quad \|(I - hA)^{-1}\|, \|(I - hB)^{-1}\|, \|\mathrm{e}^{hL}\| \leq 1$

$\Rightarrow \quad \|S_h^j\|$ and $\|\mathrm{e}^{jhL}\| \leq 1$

Step II Consistency

$S_h - \mathrm{e}^{hL} \;=\; h^2 \; bd.op. \; L^2 \quad \square$

Operator calculus

Let $\lambda_0 := \mathrm{e}^{hL}$, $\quad \ell = hL$

For $j \geq 1$ define the corresponding φ-functions

$$\lambda_j = \frac{1}{h^j} \int_0^h \mathrm{e}^{(h-\tau)L} \frac{\tau^{j-1}}{(j-1)!}\, \mathrm{d}\tau$$

One obtains the recurrence relation

$$\lambda_j = \frac{1}{j!} I + \ell \lambda_{j+1}$$

and, e.g.,

$$\lambda_0 - \lambda_1 = h\big(\lambda_1 - \lambda_2\big)L$$

i.e., one gains one power of h on $\mathcal{D}(L)$.

Operator calculus, cont.

Further introduce

$$a = hA, \quad b = hB$$
$$\alpha = (I - a)^{-1}, \quad \beta = (I - b)^{-1}$$

The corresponding φ_1-function α_1

$$\alpha = I + a\alpha_1 \quad \Rightarrow \quad \alpha_1 = \alpha$$

is particularly simple. Observe that

- $a\alpha = \alpha a$
- $I = \alpha - a\alpha$
- $\beta b\alpha = \beta\alpha b + \beta ba\alpha - \beta\alpha ab \quad \text{on} \ \mathcal{D}(B)$
  because $\beta b = \beta b\alpha - \beta ba\alpha = \beta\alpha b - \beta\alpha ab$

Consistency

$$S_h - \mathrm{e}^{hL} = \beta\alpha - \lambda_0$$

Consistency

$$S_h - \mathrm{e}^{hL} = \beta\alpha - I\lambda_0$$

Consistency

$$
\begin{aligned}
S_h - \mathrm{e}^{hL} &= \beta\alpha - I\lambda_0 \\
&= \beta\alpha - (\beta - b\beta)(\alpha - a\alpha)\lambda_0
\end{aligned}
$$

Consistency

$$
\begin{aligned}
S_h - \mathrm{e}^{hL} &= \beta\alpha - \lambda_0 \\
&= \beta\alpha - (\beta - b\beta)(\alpha - a\alpha)\lambda_0 \\
&= \beta\alpha(I - \lambda_0) + (\beta\alpha a + \beta b\alpha - \beta ba\alpha)\lambda_0
\end{aligned}
$$

Consistency

$$
\begin{aligned}
S_h - \mathrm{e}^{hL} &= \beta\alpha - \lambda_0 \\
&= \beta\alpha - (\beta - b\beta)(\alpha - a\alpha)\lambda_0 \\
&= \beta\alpha(I - \lambda_0) + (\beta\alpha a + \beta b\alpha - \beta b a\alpha)\lambda_0
\end{aligned}
$$

Consistency

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S_h - \mathrm{e}^{hL} &= \beta\alpha - \lambda_0 \\
&= \beta\alpha - (\beta - b\beta)(\alpha - a\alpha)\lambda_0 \\
&= \beta\alpha(I - \lambda_0) + (\beta\alpha a + \beta b\alpha - \beta ba\alpha)\lambda_0 \\
&= -\beta\alpha\ell\lambda_1 + (\beta\alpha a + \beta b\alpha - \beta ba\alpha)\lambda_0
\end{aligned}
$$

Consistency

$$
\begin{aligned}
S_h - \mathrm{e}^{hL} &= \beta\alpha - \lambda_0 \\
&= \beta\alpha - (\beta - b\beta)(\alpha - a\alpha)\lambda_0 \\
&= \beta\alpha(I - \lambda_0) + (\beta\alpha a + \beta b\alpha - \beta ba\alpha)\lambda_0 \\
&= -\beta\alpha\ell\lambda_1 + (\beta\alpha a + {\color{red}\beta b\alpha} - \beta ba\alpha)\lambda_0
\end{aligned}
$$

Consistency

$$
\begin{aligned}
S_h - \mathrm{e}^{hL} &= \beta\alpha - \lambda_0 \\
&= \beta\alpha - (\beta - b\beta)(\alpha - a\alpha)\lambda_0 \\
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&= -\beta\alpha\ell\lambda_1 + (\beta\alpha a + \beta b\alpha - \beta ba\alpha)\lambda_0 \\
&= -\beta\alpha\ell\lambda_1 + \big(\beta\alpha a + \beta\alpha b + \beta ba\alpha - \beta\alpha ab - \beta ba\alpha\big)\lambda_0
\end{aligned}
$$

Consistency

$$\begin{aligned} S_h - \mathrm{e}^{hL} &= \beta\alpha - \lambda_0 \\ &= \beta\alpha - (\beta - b\beta)(\alpha - a\alpha)\lambda_0 \\ &= \beta\alpha(I - \lambda_0) + (\beta\alpha a + \beta b\alpha - \beta ba\alpha)\lambda_0 \\ &= -\beta\alpha\ell\lambda_1 + (\beta\alpha a + \beta b\alpha - \beta ba\alpha)\lambda_0 \\ &= -\beta\alpha\ell\lambda_1 + \big(\beta\alpha a + \beta\alpha b + \beta ba\alpha - \beta\alpha ab - \beta ba\alpha\big)\lambda_0 \\ &= \beta\alpha\ell(\lambda_0 - \lambda_1) - \beta\alpha ab\lambda_0 \end{aligned}$$

Consistency

$$
\begin{aligned}
S_h - \mathrm{e}^{hL} &= \beta\alpha - \lambda_0 \\
&= \beta\alpha - (\beta - b\beta)(\alpha - a\alpha)\lambda_0 \\
&= \beta\alpha(I - \lambda_0) + (\beta\alpha a + \beta b\alpha - \beta ba\alpha)\lambda_0 \\
&= -\beta\alpha\ell\lambda_1 + (\beta\alpha a + \beta b\alpha - \beta ba\alpha)\lambda_0 \\
&= -\beta\alpha\ell\lambda_1 + \big(\beta\alpha a + \beta\alpha b + \beta ba\alpha - \beta\alpha ab - \beta ba\alpha\big)\lambda_0 \\
&= \beta\alpha\ell(\lambda_0 - \lambda_1) - \beta\alpha ab\lambda_0 \\
&= \beta\alpha\ell^2(\lambda_1 - \lambda_2) - \beta\alpha ab\lambda_0
\end{aligned}
$$

Consistency

$$
\begin{aligned}
S_h - \mathrm{e}^{hL} &= \beta\alpha - \lambda_0 \\
&= \beta\alpha - (\beta - b\beta)(\alpha - a\alpha)\lambda_0 \\
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&= -\beta\alpha\ell\lambda_1 + \big(\beta\alpha a + \beta\alpha b + \beta ba\alpha - \beta\alpha ab - \beta ba\alpha\big)\lambda_0 \\
&= \beta\alpha\ell(\lambda_0 - \lambda_1) - \beta\alpha ab\lambda_0 \\
&= \beta\alpha\ell^2(\lambda_1 - \lambda_2) - \beta\alpha ab\lambda_0 \\
&= h^2 S_h\big((\lambda_1 - \lambda_2)L^2 - AB\mathrm{e}^{hL}\big)
\end{aligned}
$$

Consistency

$$
\begin{aligned}
S_h - \mathrm{e}^{hL} &= \beta\alpha - \lambda_0 \\
&= \beta\alpha - (\beta - b\beta)(\alpha - a\alpha)\lambda_0 \\
&= \beta\alpha(I - \lambda_0) + (\beta\alpha a + \beta b\alpha - \beta ba\alpha)\lambda_0 \\
&= -\beta\alpha\ell\lambda_1 + (\beta\alpha a + \beta b\alpha - \beta ba\alpha)\lambda_0 \\
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&= \beta\alpha\ell(\lambda_0 - \lambda_1) - \beta\alpha ab\lambda_0 \\
&= \beta\alpha\ell^2(\lambda_1 - \lambda_2) - \beta\alpha ab\lambda_0 \\
&= h^2 S_h\big((\lambda_1 - \lambda_2)L^2 - AB I \mathrm{e}^{hL}\big)
\end{aligned}
$$

Consistency

$$
\begin{aligned}
S_h - \mathrm{e}^{hL} &= \beta\alpha - \lambda_0 \\
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&= -\beta\alpha\ell\lambda_1 + \big(\beta\alpha a + \beta\alpha b + \beta ba\alpha - \beta\alpha ab - \beta ba\alpha\big)\lambda_0 \\
&= \beta\alpha\ell(\lambda_0 - \lambda_1) - \beta\alpha ab\lambda_0 \\
&= \beta\alpha\ell^2(\lambda_1 - \lambda_2) - \beta\alpha ab\lambda_0 \\
&= h^2 S_h\big((\lambda_1 - \lambda_2)L^2 - AB\,I\,\mathrm{e}^{hL}\big) \\
&= h^2 S_h\big((\lambda_1 - \lambda_2)L^2 - AB(I - L)^{-2}\mathrm{e}^{hL}(I - L)^2\big) \qquad \square
\end{aligned}
$$

Further results

- First order convergence for exponential Lie splitting. Rules for commutation involve (higher) φ-functions.
- Second order convergence for Peaceman–Rachford and Strang splitting.
- Many more methods can be analyzed. E.g., a second order splitting method for the Heston model in finance, involving cross derivatives.
- Extension to nonautonomous problems.
- Non-stiff order conditions are sufficient for exponential splitting in the stiff case (under appropriate regularity assumptions). Hansen, A.O., Math. Comp. (2009)

High order splitting methods for analytic semigroups exist

Exponential splitting

Consider the abstract evolution equation

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

and its approximate solution via an exponential splitting method

$$u_n \; = \; S_h^n u_0 \; \approx \; \mathrm{e}^{nhL} u_0 \; = \; u(nh).$$

A single time step of length h is given by the operator

$$S_h \; = \; \prod_{j=1}^{s} \mathrm{e}^{\gamma_j hA} \mathrm{e}^{\delta_j hB} \; = \; \mathrm{e}^{\gamma_s hA} \mathrm{e}^{\delta_s hB} \cdots \mathrm{e}^{\gamma_1 hA} \mathrm{e}^{\delta_1 hB}.$$

An order barrier for analytic semigroups?

Common belief: Splitting methods for analytic semigroups are of second order at most.

- Splitting schemes with real coefficients necessarily have at least one negative coefficient whenever $p \geq 3$.
- One can not make use of such schemes as the semigroups are not well defined for negative times t.

However, there are plenty of schemes of order $p \geq 3$ with complex coefficients with positive real parts.

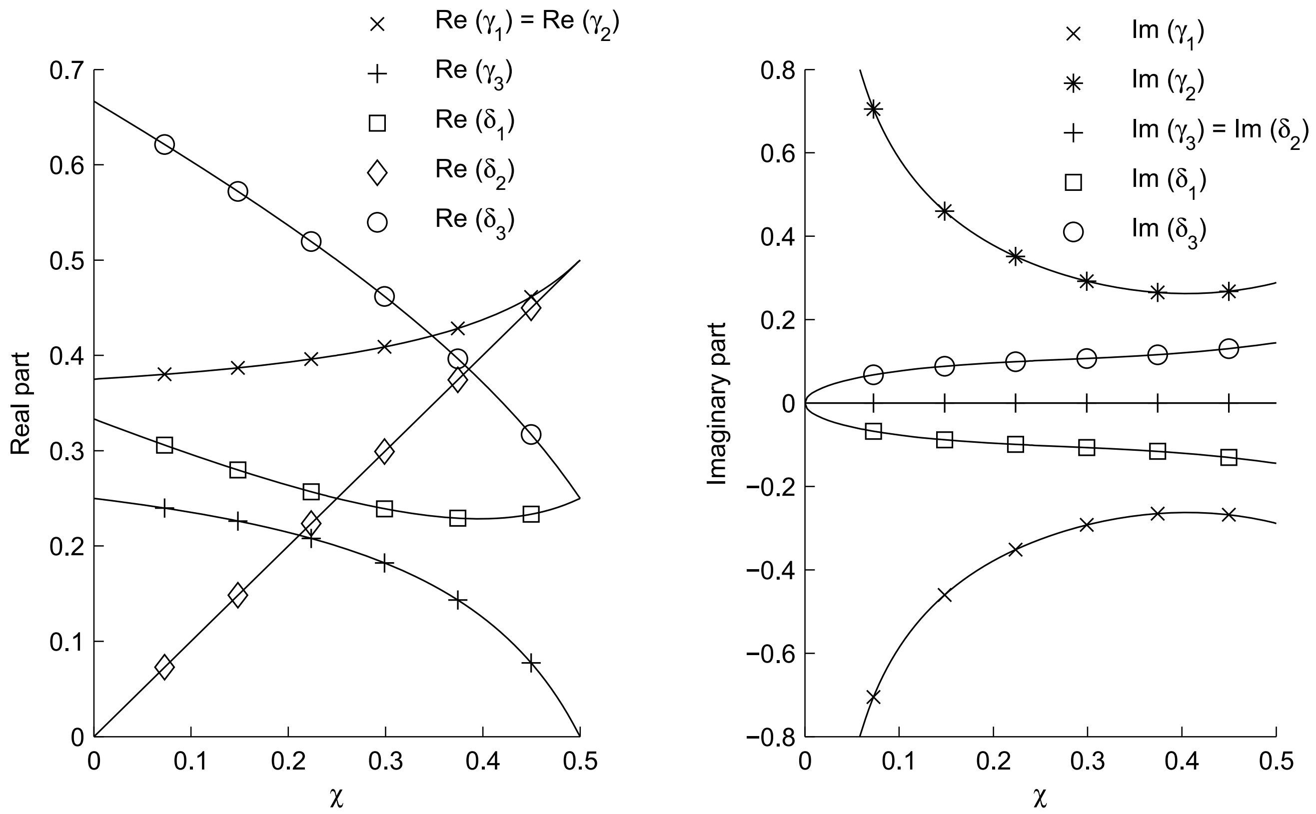
$\longrightarrow$ analytic semigroups

Sheng (1989), Blanes, Casas (2005)

Hansen, A.O. (2008), Castella, Chartier, Descombes, Vilmart (2008)

A family of third order methods with three stages

Five order conditions in six unknowns; take, e.g. $\delta_2 = \chi$ as a free parameter. System can be solved analytically.



A particular case

A particular case is obtained for $\chi = \frac{1}{2}$, resulting in

$$\Psi_h(\tfrac{1}{2}) = \mathrm{e}^{\left(\frac{1}{4}-\mathrm{i}\,\frac{\sqrt{3}}{12}\right)hB}\,\mathrm{e}^{\left(\frac{1}{2}-\mathrm{i}\,\frac{\sqrt{3}}{6}\right)hA}\,\mathrm{e}^{\frac{1}{2}hB}\,\mathrm{e}^{\left(\frac{1}{2}+\mathrm{i}\,\frac{\sqrt{3}}{6}\right)hA}\,\mathrm{e}^{\left(\frac{1}{4}+\mathrm{i}\,\frac{\sqrt{3}}{12}\right)hB}$$

It only requires, in average, the evaluation of four semigroup actions instead of the normal six.

Suzuki (1990)
"It should be noted the scheme [involving negative time steps] cannot be applied to a diffusion operator ..."

Bandrauk (1990), Chambers (2003), Prosen, Pižorn (2008)
Hamiltonian problems, Schrödinger equation

Hansen, A.O. (2008)

Composition methods

The following lemma is the key for constructing high order splitting methods.

Lemma

Let S_h be a one step method of classical order q. If

$$\sigma_1 + \ldots + \sigma_m = 1 \qquad \textit{and} \qquad \sigma_1^{q+1} + \ldots + \sigma_m^{q+1} = 0,$$

then the composition method $S_{\sigma_m h} \ldots S_{\sigma_1 h}$ is at least of classical order $q+1$.

If the composition is symmetric, i.e., if $\sigma_{m-\ell+1} = \sigma_\ell$ for all ℓ, then the order of the resulting scheme is even.

Suzuki (1990), Yoshida (1990), McLachlan (1995)

Two term compositions

We have $\sigma_1 = \sigma$ and $\sigma_2 = 1 - \sigma$. Solve

$$\sigma^{q+1} + (1-\sigma)^{q+1} = 0 \qquad \text{or} \qquad \left(\frac{\sigma}{1-\sigma}\right)^{q+1} = -1.$$

By taking logarithms

$$\log \frac{\sigma}{1-\sigma} = \frac{1+2\ell}{q+1}\pi \mathrm{i}$$

we easily derive that all solutions are given by

$$\sigma = \frac{1}{2} + \mathrm{i}\, \frac{\sin\left(\dfrac{2\ell+1}{q+1}\pi\right)}{2 + 2\cos\left(\dfrac{2\ell+1}{q+1}\pi\right)} \quad \text{for} \quad \begin{cases} -\frac{q}{2} \le \ell \le \frac{q}{2} - 1 & \text{if } q \text{ even}, \\ -\frac{q+1}{2} \le \ell \le \frac{q-1}{2} & \text{if } q \text{ odd}. \end{cases}$$

Coefficients with the smallest arguments (angles) for $\ell = 0$.

Two term compositions, cont.

Consider the two term compositions

$$\Phi_h(k,2) = \Phi_{\sigma_{k,2}h}(k-1,2)\,\Phi_{\sigma_{k,1}h}(k-1,2), \qquad k \geq 1,$$

where $\Phi_h(0,2) = \mathrm{e}^{\frac{1}{2}hB}\mathrm{e}^{hA}\mathrm{e}^{\frac{1}{2}hB}$ is the Strang splitting.

Theorem

Let $1 \leq k \leq 4$. Then the exponential splitting schemes $\Phi_h(k,2)$ with above coefficients are of order $p = k+2$. □

The optimal coefficients have the arguments:

S_h	$\Phi_h(0,2)$	$\Phi_h(1,2)$	$\Phi_h(2,2)$	$\Phi_h(3,2)$	$\Phi_h(4,2)$
φ	0°	30°	52.50°	70.50°	85.50°
p	2	3	4	5	6

Symmetric four term compositions

Starting again from the Strang splitting $\Phi_h(0,4)$ we consider

$$\Phi_h(k,4) = \Phi_{\sigma_{k,1}h}(k-1,4)\,\Phi_{\sigma_{k,2}h}(k-1,4)\,\Phi_{\sigma_{k,2}h}(k-1,4)\,\Phi_{\sigma_{k,1}h}(k-1,4), \qquad k \geq 1,$$

with coefficients $\sigma_{k,1}$ and $\sigma_{k,2}$.
By eliminating $\sigma_{k,2}$ we obtain the order condition $(q = 2k)$

$$\sigma^{q+1} + \left(\frac{1}{2} - \sigma\right)^{q+1} = 0 \qquad \text{or} \qquad \left(\frac{2\sigma}{1-2\sigma}\right)^{q+1} = -1.$$

The solutions with minimal arguments are then

$$\sigma_{k,1} = \frac{1}{4} + \mathrm{i}\,\frac{\sin\left(\frac{\pi}{2k+1}\right)}{4 + 4\cos\left(\frac{\pi}{2k+1}\right)}, \qquad \sigma_{k,2} = \overline{\sigma}_{k,1}, \qquad \varphi = \frac{\pi}{2(2k+1)}$$

Symmetric four term compositions, cont.

Consider the compositions $\Phi_h(0,4) = \mathrm{e}^{\frac{1}{2}hB}\mathrm{e}^{hA}\mathrm{e}^{\frac{1}{2}hB}$ and

$$\Phi_h(k,4) = \Phi_{\sigma_{k,1}h}(k-1,4)\,\Phi_{\sigma_{k,2}h}(k-1,4)$$
$$\Phi_{\sigma_{k,2}h}(k-1,4)\,\Phi_{\sigma_{k,1}h}(k-1,4), \qquad k \geq 1.$$

Theorem

Let $1 \leq k \leq 6$. Then the exponential splitting schemes $\Phi_h(k,4)$ are of order $p = 2k+2$. □

The optimal coefficients have the arguments:

S_h	$\Phi_h(1,4)$	$\Phi_h(2,4)$	$\Phi_h(3,4)$	$\Phi_h(4,4)$	$\Phi_h(5,4)$	$\Phi_h(6,4)$
φ	30°	48°	60.86°	70.86°	79.04°	85.96°
p	4	6	8	10	12	14

Convergence – analytic framework

Consider

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

where the operators L, A and B have the following properties:

- They are linear and (possibly) unbounded with domain in a Banach space X;
- They generate analytic semigroups for parameters in the sector
$$\Sigma_\varphi = \{z \in \mathbb{C} : |\arg z| < \varphi\}, \qquad \varphi \in (0, \pi/2];$$
- A and B satisfy the stability bounds
$$\|e^{zA}\| \le e^{\omega|z|} \quad \text{and} \quad \|e^{zB}\| \le e^{\omega|z|}$$
for some $\omega \ge 0$ and all $z \in \Sigma_\varphi$.

Convergence for analytic semigroups

Theorem

Under the above (and certain regularity) assumptions, consider an exponential splitting method S_h of classical order p, with all its coefficients γ_j and δ_j in the sector $\Sigma_\varphi \subset \mathbb{C}$. Then

$$\left\| \left(S_h^n - \mathrm{e}^{nhL} \right) u_0 \right\| \leq Ch^p, \qquad 0 \leq nh \leq T,$$

where the constant C can be chosen uniformly on bounded time intervals and, in particular, independent of n and h.

Proof. Under our assumptions, the classical order conditions imply convergence. □

Hansen, A.O., Math. Comp. (2009)

Numerical examples

Dimension splitting of the elliptic operator $L = A + B$, where

$$Au = \sum_{i=1}^{s} D_i \left(a_i D_i u\right) \quad \text{and} \quad Bu = \sum_{j=s+1}^{d} D_j \left(a_j D_j u\right).$$

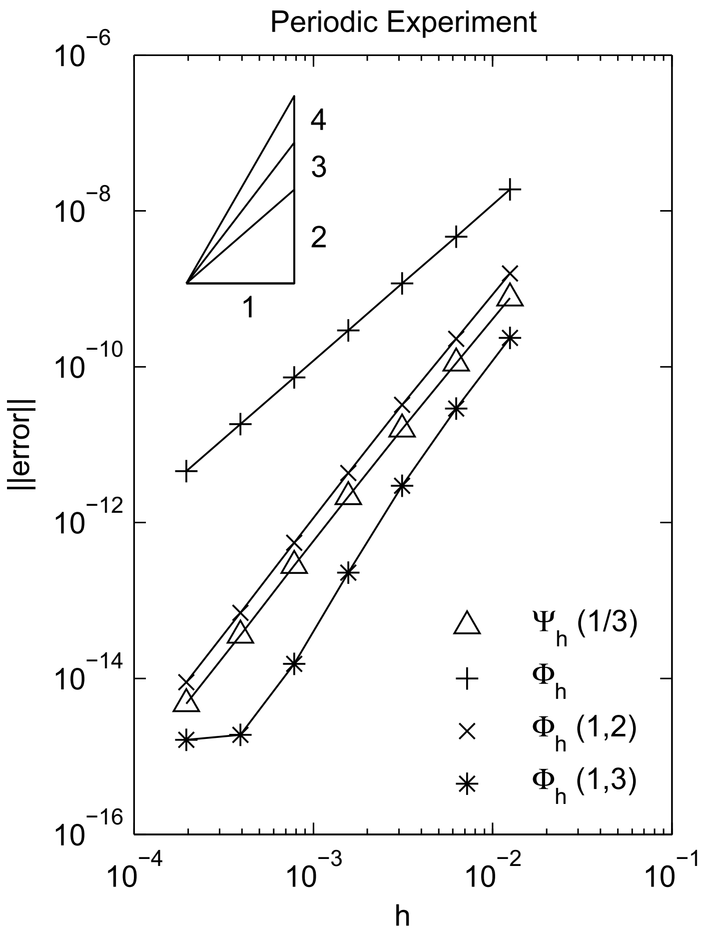
In the examples below: $s = 1$, $d = 2$.

Discretization in space with standard finite differences

$$(A_{\Delta x} U)_{i,j} = \frac{a_{i+1/2,j}(U_{i+1,j} - U_{i,j}) - a_{i-1/2,j}(U_{i,j} - U_{i-1,j})}{(\Delta x)^2}$$

Periodic boundary conditions

$$u' = D_1(aD_1 u) + D_2(aD_2 u), \qquad \Omega = \mathbb{T}^2, \qquad (x_1, x_2) \in [0,1)^2$$

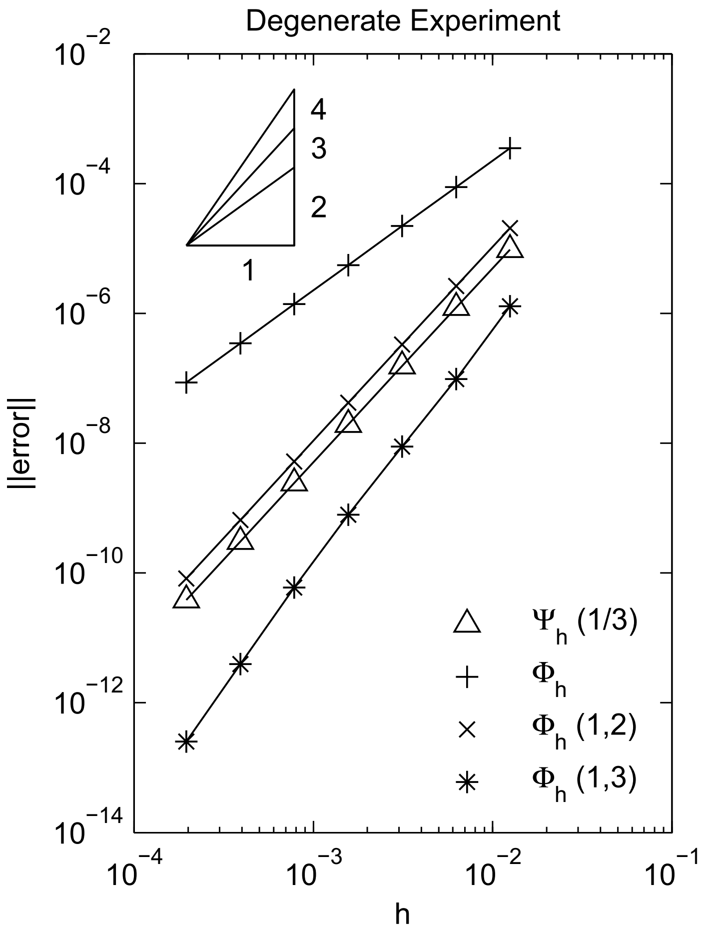


$$a(x_1, x_2) = \sin(2\pi x_1)\sin(2\pi x_2) + 2$$
$$u_0(x_1, x_2) = \sin(2\pi x_1)\sin(2\pi x_2)$$

T/h	Ψ_h	Φ_h	$\Phi_h(1,2)$	$\Phi_h(1,3)$
16	2.77	2.02	2.78	3.02
32	2.82	2.00	2.82	3.29
64	2.87	2.00	2.91	3.70
128	2.94	2.00	2.97	3.90
256	2.97	2.00	2.99	3.03
512	2.93	2.00	2.95	0.21

Degenerate case

$$u' = D_1(aD_1u) + D_2(aD_2u), \qquad \Omega = (0,1)^2$$

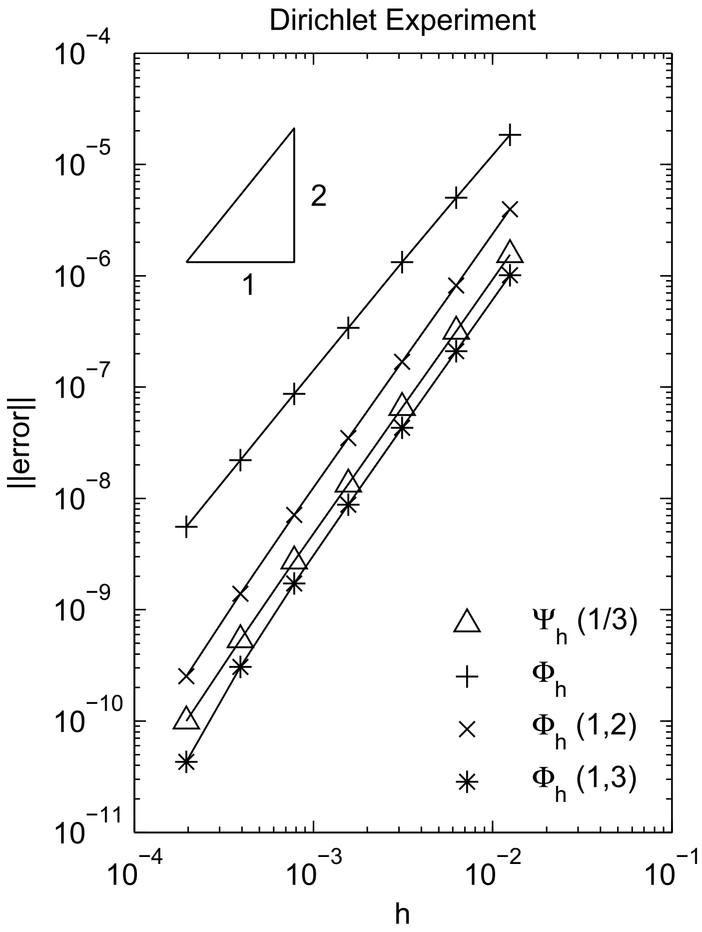


$$a(x_1,x_2) = 16x_1(1-x_1)x_2(1-x_2)$$
$$u_0(x_1,x_2) = \sin(3\pi x_1)\cos(3\pi x_2)$$

T/h	Ψ_h	Φ_h	$\Phi_h(1,2)$	$\Phi_h(1,3)$
16	2.96	1.99	2.96	3.72
32	2.99	2.00	2.99	3.46
64	2.99	2.00	2.99	3.48
128	2.99	2.00	3.00	3.73
256	3.00	2.00	3.00	3.90
512	3.00	2.00	3.00	3.97

Dirichlet boundary conditions

$$u' = D_1(aD_1 u) + D_2(aD_2 u), \qquad \Omega = (0,1)^2$$



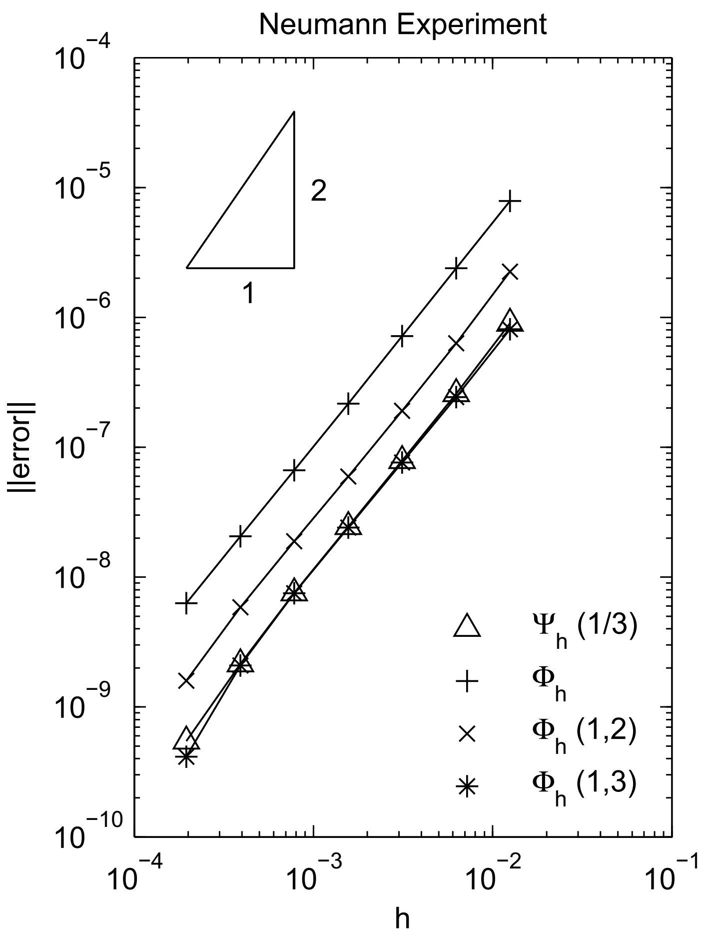
$$a(x_1, x_2) = 16x_1(1-x_1)x_2(1-x_2) + 1$$

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

T/h	Ψ_h	Φ_h	$\Phi_h(1,2)$	$\Phi_h(1,3)$
16	2.28	1.88	2.27	2.27
32	2.28	1.93	2.27	2.28
64	2.28	1.95	2.28	2.30
128	2.30	1.97	2.30	2.35
256	2.34	1.98	2.34	2.49
512	2.43	1.99	2.47	2.83

Neumann boundary conditions

$$u' = D_1(aD_1u) + D_2(aD_2u), \qquad \Omega = (0,1)^2$$

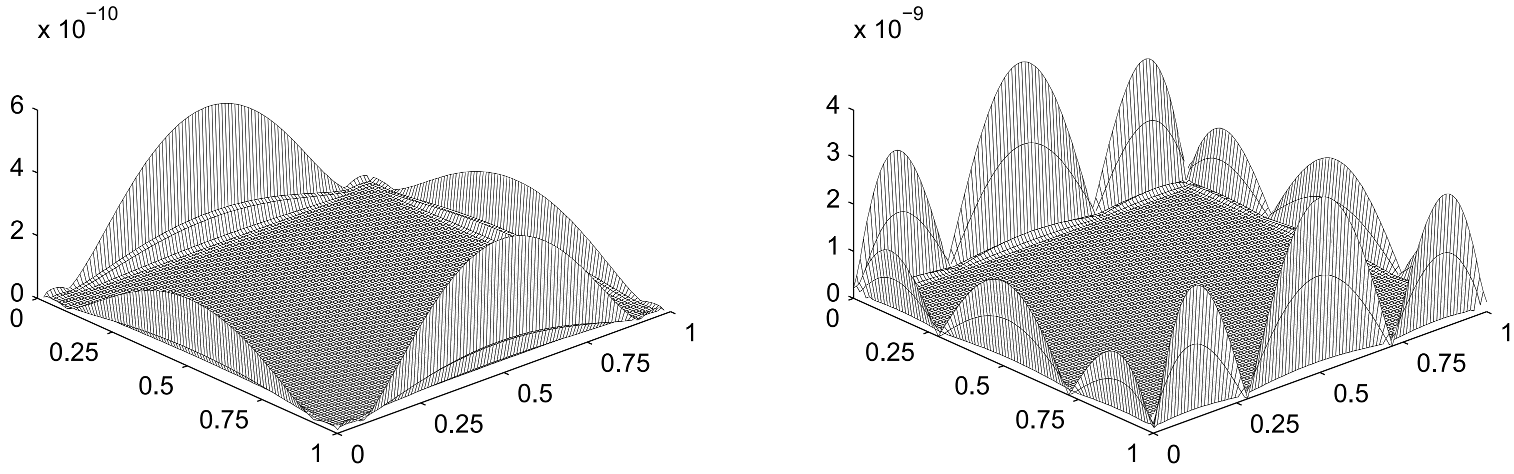


$$a(x_1,x_2) = 16x_1(1-x_1)x_2(1-x_2)+1$$

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

T/h	Ψ_h	Φ_h	$\Phi_h(1,2)$	$\Phi_h(1,3)$
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

Error localization



Errors at time $T = 0.1$ for $\Phi_h(1,3)$, with $h = T/512$, when applied to the Dirichlet (left) and Neumann (right) problems.

The full order of convergence is obtained in subdomains bounded away from the boundary.

Lubich, A. O. (1995)

Conclusions and outlook

Framework for analyzing convergence of splitting methods.

- Semigroup theory.
- Optimal orders under appropriate regularity assumptions.
- High-order splitting for parabolic problems.
- Composition methods up to order 14.
- Order reduction for Dirichlet and Neumann b.c.
  Full order of convergence away from boundaries.

Some references

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