Time integration: splitting methods

Marlis Hochbruck, Düsseldorf
Alexander Ostermann, Innsbruck

CPiP 2005, Helsinki
outline

- what are splitting methods?
- linear splitting
  ex: time-dependent Schrödinger equation
- nonlinear splitting
  ex: cubic nonlinear Schrödinger equation
- extensions and references
what is splitting?

consider differential equation

\[ u' = f(u) + g(u), \quad u(0) = u_0 \]

divide et impera: compute (simpler) partial flows

\[ \varphi_t(v_0) := e^{tf}v_0 := v(t) \quad \quad \psi_t(w_0) := e^{tg}w_0 := w(t) \]

and define numerical solution after one step of size \( h \) by

\[ u_1 = \psi_h(\varphi_h(u_0)) = e^{hg}e^{hf}u_0 \approx u(h) \]

splitting is a one-step method
typical problems where splitting may help

time-dependent Schrödinger eq. with smooth potential $V$

\[ i \frac{\partial u}{\partial t} = -\Delta u + V(x, y)u \]

cubic nonlinear Schrödinger eq. (dispersive optical fibres)

\[ i \frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial t^2} + \gamma |u|^2 u \]

nonlinear reaction-diffusion (advection) equations

\[ \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + g(t, u) \]
Lie and Strang splitting for a linear model

consider linear problem

\[ u' = Au + Bu, \quad u(0) = u_0 \]

with true solution \( u(t) = e^{t(A+B)}u_0 \)

Lie splitting

\[ u_{1,L} = e^{hA}e^{hB}u_0 \quad \text{or} \quad u_{1,L} = e^{hB}e^{hA}u_0 \]

symmetric Strang splitting

\[ u_{1,S} = e^{\frac{1}{2}hA}e^{hB}e^{\frac{1}{2}hA}u_0 \quad \text{or} \quad u_{1,S} = e^{\frac{1}{2}hB}e^{hA}e^{\frac{1}{2}hB}u_0 \]

(nearly) same computational work
**local error of splitting**

local error = error after one time step = splitting error

\[
\begin{align*}
u_{1,L} - u(h) &= (e^{hA} e^{hB} - e^{h(A+B)})u_0 \\
&= \left(1 + hA + \frac{h^2}{2} A^2 + \ldots \right) \left(1 + hB + \frac{h^2}{2} B^2 + \ldots \right) \\
&\quad - \left(1 + h(A+B) + \frac{h^2}{2} (A+B)^2 + \ldots \right)u_0 \\
&= \ldots = \frac{h^2}{2} [A, B] u_0 + O(h^3)
\end{align*}
\]

\[
\begin{align*}
u_{1,S} - u(h) &= h^3 \left(\frac{1}{12} [B, [B, A]] - \frac{1}{24} [A, [A, B]]\right)u_0 + O(h^4)
\end{align*}
\]

**commutator** $[A, B] = AB - BA$

**Baker-Campbell-Hausdorff formula**
local error analysis

for unbounded $A$, never expand $e^{tA}$ into a series
alternative: represent solution of

$$u' = Au + g(u), \quad u(0) = v$$

with the variation-of-constants formula instead

$$u(t) = e^{tA}v + \int_0^t e^{(t-s)A}g(u(s))\,ds$$

for the particular case $g(u) = Bu$, we get

$$e^{t(A+B)} = e^{tA} + \int_0^t e^{(t-s)A}Be^{s(A+B)}\,ds$$

reinsert and estimate iterated integral
**local error analysis, cont.**

assumptions on commutators

(a) \[\| [A, B]v \| \leq c_1 \| (-A)^\alpha v \|\]

(b) \[\| [A, [A, B]v] \| \leq c_2 \| (-A)^\beta v \|\]

**Theorem** (Jahnke, Lubich, 2000)

(i) under condition (a) with \(\alpha \geq 0\)

\[
\left\| e^{\frac{1}{2} hA} e^{hB} e^{\frac{1}{2} hA} v - e^{h(A+B)} v \right\| \leq C_1 \cdot h^2 \cdot \| (-A)^\alpha v \|
\]

(ii) under conditions (a) and (b) with \(\beta \geq 1 \geq \alpha\)

\[
\left\| e^{\frac{1}{2} hA} e^{hB} e^{\frac{1}{2} hA} v - e^{h(A+B)} v \right\| \leq C_2 \cdot h^3 \cdot \| (-A)^\beta v \|
\]

\(C_i\) only depends \(c_1, c_i\) and \(\|B\|\).
stability and linear error growth

assume that

\[ \| e^{tA} \| \leq 1, \quad \| e^{tB} \| \leq 1, \quad \| e^{t(A+B)} \| \leq 1 \]

and set \( S = e^{hA} e^{hB} \), \( T = e^{t(A+B)} \). Then

\[ \| S^n \| \leq \| S \|^n \leq (\| e^{tA} \| \cdot \| e^{tB} \|)^n \leq 1 \] (stability)

and

\[ \| S^n - T^n \| = \sum_{j=0}^{n-1} S^j (S - T) T^{n-j-1} \]

\[ \leq \sum_{j=0}^{n-1} \| S^j \| \cdot \| S - T \| \cdot \| T^{n-j-1} \| \leq n \| S - T \| \]

convergence with linear error growth
**application:** time-dependent Schrödinger eq.

we have \( \alpha = \frac{1}{2} \) and \( \beta = 1 \), since

\[
[A, B] \phi(x) = \left[ \frac{d^2}{dx^2}, V(x) \right] \phi(x)
\]

\[
= (V(x)\phi(x))'' - V(x)(\phi(x))''
\]

\[
= V''(x)\phi(x) + 2V'(x)\phi'(x)
\]

this shows that \([A, B]\) is a first-order differential operator

**Theorem** (JL 00) Let \( V \) be \( C^5 \)-smooth. Then

\[
\|U_n - U(t_n)\|_{L^2} \leq \left\{ \begin{array}{ll}
C \cdot h \cdot \|U_0\|_{H^1} \\
C \cdot h^2 \cdot \|U_0\|_{H^2}
\end{array} \right.
\]

uniformly in \( 0 \leq nh \leq T \); the constant \( C \) depends on \( T \), but it is independent of \( n \) and \( h \).
implementation

determine the action of $e^{hA}$ on a spatial vector $v(x)$ in the Fourier space

for example, consider

$$A = i \frac{\partial^2}{\partial x^2} \quad \text{on } (-\pi, \pi)$$

with periodic boundary conditions; thus

$$e^{hA}v = \mathcal{F}^{-1}e^{-ihk^2}\mathcal{F}v$$

efficient numerical implementation:
pseudospectral methods based on FFT

higher dimensions, Dirichlet or Neumann b.c. admissible but restrictions on the domain
numerical experiments

smooth potential $V(x) = 1 - \cos x$ on $(-\pi, \pi)$
nonsmooth potential $V(x) = x + \pi$ on $(-\pi, \pi)$

random initial data in $H^1$ (red) and $H^2$ (blue)

experiments in line with theoretical results
**nonlinear Strang splitting**

consider partial differential equation

\[
\frac{\partial u}{\partial t} = Au + g(u), \quad A = \Delta \text{ or } \pm i\Delta \text{ or } \ldots
\]

partial flows \( \varphi_t(v) = e^{tA}v \) and \( \psi_t(w_0) = w(t) \) for

\[
w' = g(w), \quad w(0) = w_0
\]

**Strang splitting** \( u_{1,S} = (\varphi_{h/2} \circ \psi_h \circ \varphi_{h/2})(u_0) \)

evaluation of \( \varphi \) by Fourier techniques (FFT) or by another exponential integrator

evaluation of \( \psi \) exactly or by a suitable numerical scheme (flow is local)
split-step Fourier method for NLS equation

2D cubic nonlinear Schrödinger equation

\[ i \frac{\partial u}{\partial t} = \Delta u + \gamma |u|^2 u \]

**Theorem** (Bess et al. 2002) For sufficiently small time steps \( h \) we have

\[ \| u_{n,L} - u(t_n) \|_{L^2} \leq C(\| u_0 \|_{H^2}) \cdot h \cdot \| u_0 \|_{H^2} \]
\[ \| u_{n,S} - u(t_n) \|_{L^2} \leq C(\| u_0 \|_{H^4}) \cdot h^2 \cdot \| u_0 \|_{H^4} \]

uniformly in \( 0 \leq nh \leq T \); the constant \( C \) depends on \( T \), but it is independent of \( n \) and \( h \).

optimal order of convergence; constant is not optimal
extensions for the split-step Fourier method

- higher-order splitting methods involve negative time-steps; only for groups
- reaction-diffusion equations

\[ \frac{\partial u}{\partial t} = \Delta u + g(u) \]

ideas of Bess et al. can be adapted

- reactions \( v' = g(v) \) are often very stiff
  use (semi) implicit methods
  stiff operator should be the last in the splitting (Sportisse, 2000)
some references


