Time integration: splitting methods

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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

$$v' = f(v), \quad v(0) = v_0 \qquad\qquad w' = g(w), \quad w(0) = w_0$$

$$\varphi_t(v_0) := \mathrm{e}^{tf} v_0 := v(t) \qquad\qquad \psi_t(w_0) := \mathrm{e}^{tg} w_0 := w(t)$$

and define numerical solution after one step of size h by

$$u_1 = \psi_h\bigl(\varphi_h(u_0)\bigr) = \mathrm{e}^{hg}\mathrm{e}^{hf} u_0 \;\approx\; u(h)$$

splitting is a one-step method

typical problems where splitting may help

time-dependent Schrödinger eq. with smooth potential V

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

cubic nonlinear Schrödinger eq. (dispersive optical fibres)

$$\mathrm{i}\,\frac{\partial u}{\partial x} = \frac{\partial^2 u}{\partial t^2} + \gamma|u|^2 u$$

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 $u(t) = \mathrm{e}^{t(A+B)}u_0$

Lie splitting

$$u_{1,L} = \mathrm{e}^{hA}\mathrm{e}^{hB}u_0 \qquad \text{or} \qquad u_{1,L} = \mathrm{e}^{hB}\mathrm{e}^{hA}u_0$$

symmetric Strang splitting

$$u_{1,S} = \mathrm{e}^{\frac{1}{2}hA}\mathrm{e}^{hB}\mathrm{e}^{\frac{1}{2}hA}u_0 \qquad \text{or} \qquad u_{1,S} = \mathrm{e}^{\frac{1}{2}hB}\mathrm{e}^{hA}\mathrm{e}^{\frac{1}{2}hB}u_0$$

(nearly) same computational work

local error of splitting

local error = error after one time step = splitting error

$$u_{1,L} - u(h) = \left(\mathrm{e}^{hA}\mathrm{e}^{hB} - \mathrm{e}^{h(A+B)}\right)u_0$$
$$= \Big(1 + hA + \tfrac{h^2}{2}A^2 + \ldots\Big)\Big(1 + hB + \tfrac{h^2}{2}B^2 + \ldots\Big)$$
$$- \Big(1 + h(A+B) + \tfrac{h^2}{2}(A+B)^2 + \ldots\Big)u_0$$
$$= \ldots = \frac{h^2}{2}\big[A,B\big]u_0 + \mathcal{O}(h^3)$$

$$u_{1,S} - u(h) = h^3\Big(\tfrac{1}{12}\big[B,[B,A]\big] - \tfrac{1}{24}\big[A,[A,B]\big]\Big)u_0 + \mathcal{O}(h^4)$$

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

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

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

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

reinsert and estimate iterated integral

local error analysis, cont.

assumptions on commutators

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

(b) $\big\|\big[A,[A,B]v\big]\big\| \le c_2 \|(-A)^\beta v\|$

Theorem (Jahnke, Lubich, 2000)

(i) under condition (a) with $\alpha \ge 0$

$$\Big\|\mathrm{e}^{\frac{1}{2}hA}\mathrm{e}^{hB}\mathrm{e}^{\frac{1}{2}hA}v - \mathrm{e}^{h(A+B)}v\Big\| \le C_1 \cdot h^2 \cdot \|(-A)^\alpha v\|$$

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

$$\Big\|\mathrm{e}^{\frac{1}{2}hA}\mathrm{e}^{hB}\mathrm{e}^{\frac{1}{2}hA}v - \mathrm{e}^{h(A+B)}v\Big\| \le C_2 \cdot h^3 \cdot \|(-A)^\beta v\|$$

C_i only depends $c_1,\ c_i$ and $\|B\|$.

stability and linear error growth

assume that

$$\|e^{tA}\| \le 1, \qquad \|e^{tB}\| \le 1, \qquad \|e^{t(A+B)}\| \le 1$$

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

$$\|S^n\| \le \|S\|^n \le \big(\|e^{tA}\| \cdot \|e^{tB}\|\big)^n \le 1 \qquad \text{(stability)}$$

and

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

$$\le \sum_{j=0}^{n-1} \|S^j\| \cdot \|S-T\| \cdot \|T^{n-j-1}\| \le n\,\|S-T\|$$

convergence with linear error growth

application: time-dependent Schrödinger eq.

we have $\alpha = 1/2$ and $\beta = 1$, since

$$[A, B]\,\phi(x) = \left[\frac{\mathrm{d}^2}{\mathrm{d}\,x^2}, V(x)\right]\phi(x) = \big(V(x)\phi(x)\big)'' - V(x)\big(\phi(x)\big)'' = V''(x)\phi(x) + 2V'(x)\phi'(x)$$

this shows that $[A, B]$ is a first-order differential operator

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

$$\|U_n - U(t_n)\|_{L^2} \leq \begin{cases} C \cdot h \cdot \|U_0\|_{H^1} \\ C \cdot h^2 \cdot \|U_0\|_{H^2} \end{cases}$$

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

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

with periodic boundary conditions; thus

$$\mathrm{e}^{hA} v = \mathcal{F}^{-1} \mathrm{e}^{-\mathrm{i}hk^2} \mathcal{F} v$$

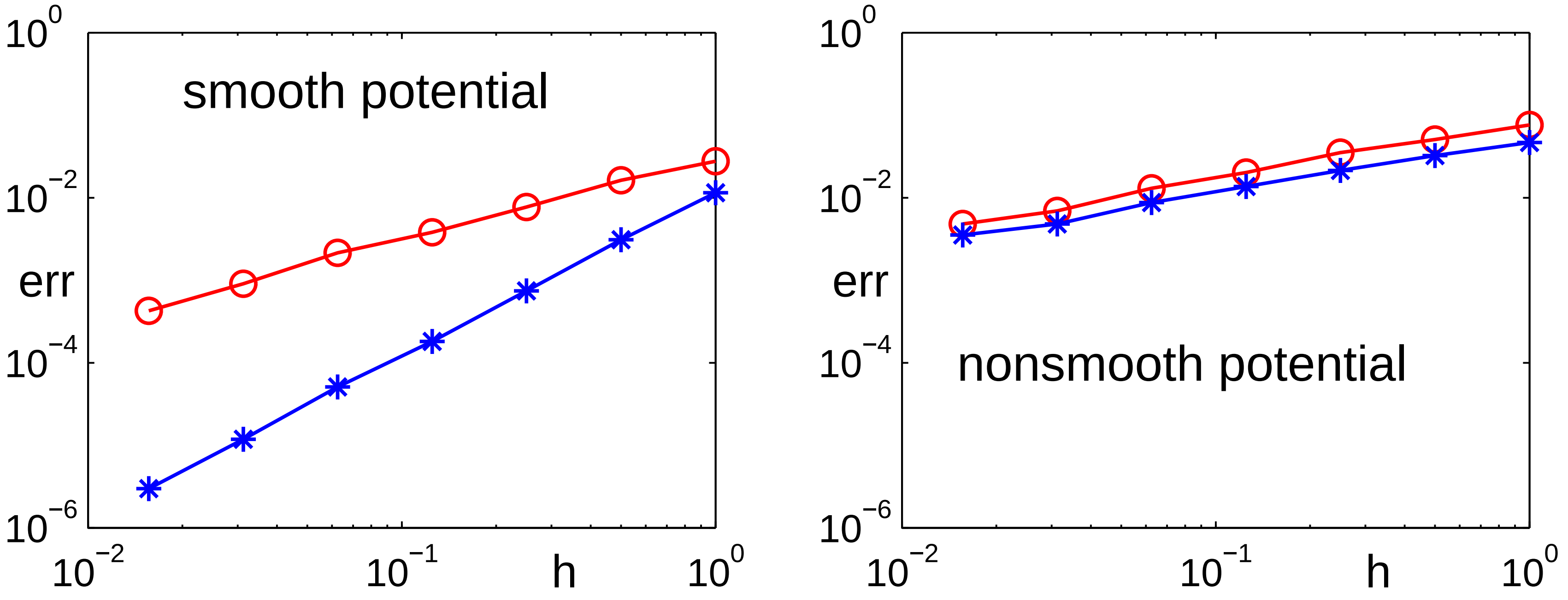
efficient numerical implementation:
pseudospectral methods based on FFT

higher dimensions, Dirichlet or Neumann b.c. admissable
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

$$\frac{\partial u}{\partial t} = Au + g(u), \qquad A = \Delta \ \text{ or } \ \pm \mathrm{i}\Delta \ \text{ or } \ \ldots$$

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

$$w' = g(w), \quad w(0) = w_0$$

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

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

evaluation of ψ exactly or by a suitable numerical scheme (flow is local)

split-step Fourier method for NLS equation

2D cubic nonlinear Schrödinger equation

$$\mathrm{i}\,\frac{\partial u}{\partial t} = \Delta u + \gamma |u|^2 u$$

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

$$\|u_{n,L} - u(t_n)\|_{L^2} \le C\big(\|u_0\|_{H^2}\big) \cdot h \cdot \|u_0\|_{H^2}$$

$$\|u_{n,S} - u(t_n)\|_{L^2} \le C\big(\|u_0\|_{H^4}\big) \cdot h^2 \cdot \|u_0\|_{H^4}$$

uniformly in $0 \le nh \le T$; 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

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