Splitting schemes for Schrödinger equations

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Outline

1. Standard numerical analysis of operator splitting
   - Operator splitting
   - Error estimate / Lie formalism / Finite dimension
   - Error estimate / Lie formalism / Infinite dimension
2. Non standard numerical analysis of operator splitting
   - Critical parameters come into play
   - An exact local error representation
3. An example
   - Gross–Pitaevskii equation
4. Conclusions

Outline

Basis of operator splitting

System to be solved (t : time interval)

$$U(t) = T^t U_0 \qquad \begin{cases} \partial_t U - i\Delta U = i f(U) \\ U(0) = U_0 \end{cases}$$

Two elementary "blocks".

$$V(t) = X^t V_0 \qquad \begin{cases} \partial_t V - i\Delta V = 0 \\ V(0) = V_0 \end{cases}$$

$$W(t) = Y^t W_0 \qquad \begin{cases} \partial_t W = i f(W) \\ W(0) = W_0 \end{cases}$$

"Explicit" solutions - L^2 norm is conserved

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Basis of operator splitting

First order methods :

Lie Formulae.

$$L_1^t U_0 = X^t Y^t U_0 \qquad L_1^t U_0 - T^t U_0 = O(t^2),$$

$$L_2^t U_0 = Y^t X^t U_0 \qquad L_2^t U_0 - T^t U_0 = O(t^2),$$

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Basis of operator splitting

Second order methods :

Strang Formulae.

$$S_1^t\, U_0 = Y^{t/2}\, X^t\, Y^{t/2}\, U_0 \qquad S_1^t\, U_0 - T^t\, U_0 = O(t^3),$$

$$S_2^t\, U_0 = X^{t/2}\, Y^t\, X^{t/2}\, U_0 \qquad S_2^t\, U_0 - T^t\, U_0 = O(t^3),$$

Higher order

$$Z^t\, U_0 = X^{a_1 t}\, Y^{b_1 t}\, X^{a_2 t}\, Y^{b_2 t} \dots X^{a_s t}\, Y^{b_s t}\, U_0,$$

with (real or complex) method coefficients $(a_j, b_j)_{j=1}^{s}$.

Basis of operator splitting

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Higher order

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with (real or complex) method coefficients $(a_j, b_j)_{j=1}^{s}$.

Basis of operator splitting

$$
\begin{aligned}
Z^t U_0 &= X^{a_1 t}\, Y^{b_1 t} X^{a_2 t}\, Y^{b_2 t} \dots X^{a_s t}\, Y^{b_s t}\, U_0, \\
&= T^t U_0 + O(t^{p+1}).
\end{aligned}
$$

A fourth-order method involving four compositions by Yoshida, i.e., $p = s = 4$, possesses the real coefficients

$$
a_1 = 0\,, \quad a_2 = a_4 = \gamma_1 = \frac{1}{2-\sqrt[3]{2}}\,, \quad a_3 = \gamma_2 = -\frac{\sqrt[3]{2}}{2-\sqrt[3]{2}}\,,
$$
$$
b_1 = b_4 = \tfrac{1}{2}\,\gamma_1\,, \quad b_2 = b_3 = \tfrac{1}{2}\,(\gamma_1 + \gamma_2)\,.
$$

Basis of operator splitting

The coefficients of a favourable fourth-order splitting method proposed by S. Blanes and P.C. Moan, J. Comput. Appl. Math. (2002), and a related third-order splitting method (Embedded formula) constructed by M. Thalhammer are displayed in next table :

j	a_j
1	0
2,7	0.245298957184271
3,6	0.604872665711080
4,5	$\frac{1}{2} - (a_2 + a_3)$

j	b_j
1,7	0.0829844064174052
2,6	0.396309801498368
3,5	-0.0390563049223486
4	$1 - 2(b_1 + b_2 + b_3)$

j	$\hat{a}_j$
1	a_1
2	a_2
3	a_3
4	a_4
5	0.3752162693236828
6	1.4878666594737946
7	-1.3630829287974774

j	$\hat{b}_j$
1	b_1
2	b_2
3	b_3
4	b_4
5	0.4463374354420499
6	-0.0060995324486253
7	0

Adaptive Splitting Time Step

With two time integration solvers :

$$Sp_1^{\Delta t} U_0 - T^{\Delta t} U_0 = \mathcal{O}(\Delta t^p) \quad \Longrightarrow \quad \text{Splitting formula}$$

$$\widetilde{Sp}_1^{\Delta t} U_0 - T^{\Delta t} U_0 = \mathcal{O}(\Delta t^{p-1}) \quad \Longrightarrow \quad \text{Embedded spl. formula}$$

and considering

$$\left\| Sp_1^{\Delta t} U_0 - \widetilde{Sp}_1^{\Delta t} U_0 \right\| \approx \mathcal{O}(\Delta t^{p-1}) < Tol$$

yields

$$\Delta t_{new} = \Delta t \sqrt[p-1]{\frac{Tol}{\left\| Sp_1^{\Delta t} U_0 - \widetilde{Sp}_1^{\Delta t} U_0 \right\|}}$$

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Outline

Error estimate

Error estimate -> Lie formalism. For an ODE $\dot{y} = f_1(y)$, we denote by φ_1^t the exact solution, we introduce the differential operator (Lie derivative)

$$D_1 = \sum_j f_{1,j} \frac{\partial}{\partial y_j}.$$

For a smooth function from $\mathbb{R}^n$ to $\mathbb{R}^n$, we have

$$\frac{d}{dt} F\left(\varphi_1^t(y_0)\right) = F'\left(\varphi_1^t(y_0)\right) f_1\left(\varphi_1^t(y_0)\right) = (D_1 F)\left(\varphi_1^t(y_0)\right)$$

Error estimate

By iterations, the Taylor's expansion of $F\left(\varphi_1^t(y_0)\right)$ in $t=0$ gives (formally)

$$F\left(\varphi_1^t(y_0)\right)=\sum_{k\geq 0}\frac{t^k}{k!}\left(D_1^k F\right)(y_0)=e^{tD_1}F(y_0).$$

With $F=$Id, we obtain

$$\varphi_1^t(y_0)=e^{tD_1}\mathrm{Id}(y_0).$$

Error estimate

Moreover, if we introduce a second flow φ_2^t, we have :

$$\left(\varphi_2^t \varphi_1^t\right)(y_0) = e^{tD_1} e^{tD_2} \mathrm{Id}(y_0).$$

Error estimate

Then if we denote by φ_3^t the exact solution of $\dot{y} = (f_1 + f_2)(y)$, we have the following relation :

$$\varphi_3^t(y_0) - \left(\varphi_2^t \varphi_1^t\right)(y_0) = e^{t(D_1+D_2)}\mathrm{Id}(y_0) - e^{tD_1}e^{tD_2}\mathrm{Id}(y_0),$$

we then work with linear operators ! For example, for two linear operators A et B, we have

$$e^{t(A+B)} - e^{tA}e^{tB} = \frac{t^2}{2}[A,B] + O(t^3),$$

this yields,

$$\varphi_3^t(y_0) - \left(\varphi_2^t \varphi_1^t\right)(y_0) = \frac{t^2}{2}[D_1,D_2]\mathrm{Id}(y_0) + O(t^3),$$

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and $[D_1, D_2]$ is now a Lie bracket...

$$[D_1, D_2] = \sum_i \left(\sum_j \left(\frac{\partial f_{1,i}}{\partial y_j} f_{2,j} - \frac{\partial f_{2,i}}{\partial y_j} f_{1,j} \right) \right) \frac{\partial}{\partial y_i}$$

We are not limited to the finite dimension...

$$\left(D_1 = \sum_j f_{1,j} \frac{\partial}{\partial y_j} \right)$$

Error estimate

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Outline

Error estimate

We consider an initial value problem of the form

$$\begin{cases} u'(t) = F\big(u(t)\big)\,, \quad 0 \leq t \leq T\,, \\ u(0) \text{ given}\,, \end{cases}$$

where the structure of the unbounded nonlinear operator $F : D(F) \subset X \to X$ suggests a decomposition into two parts

$$F(v) = A(v) + B(v)\,, \qquad v \in D(A) \cap D(B)\,,$$

with unbounded nonlinear operators $A : D(A) \subset X \to X$ and $B : D(B) \subset X \to X$, such that $D(F) = D(A) \cap D(B) \neq \emptyset$.

Error estimate

The exact solution of the evolutionary problem is (formally) given by

$$u(t) = \mathscr{E}_F\big(t, u(0)\big)\,, \qquad 0 \leq t \leq T\,,$$

with evolution operator $\mathscr{E}_F$ depending on the actual time and the initial value. We employ the formal notation

$$u(t) = e^{tD_F} u(0)\,, \qquad 0 \leq t \leq T\,,$$

which is suggestive of the (less involved) linear case. Here, the evolution operator e^{tD_F} and the Lie-derivative D_F associated with F are given by

$$e^{tD_F} G\, v = G\big(\mathscr{E}_F(t, v)\big)\,, \quad 0 \leq t \leq T\,, \qquad D_F G\, v = G'(v)\, F(v)\,,$$

for any unbounded nonlinear operator $G : D(G) \subset X \to X$ with Fréchet derivative G'.

Error estimate

Whenever G is the identity operator, we write

$$e^{tD_F} v = \mathscr{E}_F(t, v), \quad 0 \le t \le T, \qquad D_F v = F(v),$$

for short.
We note the relation

$$D_F = \frac{d}{dt}\Big|_{t=0} e^{tD_F}$$

This is in accordance with the identity $L = \frac{d}{dt}|_{t=0}\, e^{tL}$, valid for instance for any bounded linear operator $L : X \to X$ with the exponential function defined by the power series.

Error estimate

Recalling that for example, for two linear operators A et B, we have

$$e^{t(A+B)} - e^{tA}e^{tB} = \frac{t^2}{2}[A,B] + O(t^3),$$

We apply this formula in the nonlinear framework with Δ and f.

Error estimate

$$
\begin{aligned}
([D_f, D_\Delta]\mathrm{Id})\,u_0 &= (D_f(D_\Delta \mathrm{Id}) - D_\Delta(D_f \mathrm{Id}))\,u_0,\\
&= (D_\Delta \mathrm{Id})'(u_0) f(u_0) - (D_f \mathrm{Id})'(u_0)\frac{\partial^2 u_0}{\partial x^2},\\
&= \frac{\partial^2}{\partial x^2}(f(u_0)) - f'(u_0)\frac{\partial^2 u_0}{\partial x^2}
\end{aligned}
$$

and

$$
\frac{\partial^2 f(u_0)}{\partial x^2} - f'(u_0)\frac{\partial^2 u_0}{\partial x^2} = f''(u_0)\left(\frac{\partial u_0}{\partial x}\right)^2.
$$

Application to Lie et Strang formulae yields

$$T^t u_0 - Y^t X^t u_0 = -\frac{t^2}{2} f''(u_0)(\partial_x u_0)^2 + O(t^3),$$

$$T^t u_0 - Y^{t/2} X^t Y^{t/2} u_0 =$$

$$-i\frac{t^3}{24}\left(2f^{(4)}(u_0)(\partial_x u_0)^4 + 8f^{(3)}(u_0)(\partial_x u_0)^2(\partial_{xx} u_0)\right)$$

$$-i\frac{t^3}{6} f''(u_0)(\partial_{xx} u_0)^2$$

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\end{aligned}$$

Outline

We consider the following time-dependent nonlinear Schrödinger equation for $\psi : \mathbb{R}^d \times [0,T] \to \mathbb{C} : (x,t) \mapsto \psi(x,t)$

$$\begin{cases} i\,\varepsilon\,\partial_t \psi(x,t) = -\frac{1}{2}\,\varepsilon^2 \Delta\,\psi(x,t) + U(x)\,\psi(x,t) + \vartheta\,\left|\psi(x,t)\right|^2 \psi(x,t), \\ \psi(x,0) \text{ given}, \qquad x \in \mathbb{R}^d, \quad 0 \le t \le T, \end{cases}$$

with (small) parameter $\varepsilon > 0$, real-valued external potential $U : \mathbb{R}^d \to \mathbb{R}$, and coupling constant $\vartheta \in \mathbb{R}$, imposing asymptotic boundary conditions on the unbounded domain.

The above problem is related to the time-dependent Gross–Pitaevskii equation which arises in the description of the macroscopic wave function of a Bose–Einstein condensate.

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Could we give a sense to the previous estimates ?

For small parameter values $0 < \varepsilon \ll 1$, the above mentioned approach is *not* appropriate to provide optimal local and global error bounds with respect to ε; thus, different techniques are needed for a better theoretical understanding of the error behaviour of splitting methods for nonlinear evolutionary problems...

First idea : Taylor expansions...

C. Besse, B. Bidégaray et S. Descombes, Order estimates in time of splitting methods for the nonlinear Schrödinger equation, SIAM J. Numer. Anal., Vol. 40, No. 1, (2002), pp 26-40.

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Outline

Error estimate

Theorem (Local error representation)

For our nonlinear evolutionary problem the defect operator

$$\mathscr{L}(t,v) = e^{tD_A}\, e^{tD_B}\, v - e^{D_{A+B}}\, v$$

of the Lie splitting method $\mathscr{S}(t,v) = e^{tD_A}\, e^{tD_B}\, v$ *possesses the integral representation*

$$\mathscr{L}(t,v) = \int_0^t \int_0^{\tau_1} e^{\tau_1 D_A}\, e^{\tau_2 D_B}\, [D_A, D_B]\, e^{(\tau_1-\tau_2)D_B}\, e^{(t-\tau_1)D_F}\, v\, d\tau_2\, d\tau_1$$

$$= \int_0^t \int_0^{\tau_1} \partial_2 \mathscr{E}_F\big(t-\tau_1, \mathscr{S}(\tau_1, v)\big)\, \partial_2 \mathscr{E}_B\big(\tau_1-\tau_2, \mathscr{E}_A(\tau_1, v)\big) \times [B,A]\Big(\mathscr{E}_B\big(\tau_2, \mathscr{E}_A(\tau_1, v)\big)\Big)\, d\tau_2\, d\tau_1 .$$

Error estimate

In regard to the primal initial value problem

$$\begin{cases} \frac{d}{dt}\,\mathscr{E}_F(t,v) = F\big(\mathscr{E}_F(t,v)\big)\,, \quad 0 \leq t \leq T\,, \\ \mathscr{E}_F(0,v) = v\,, \end{cases}$$

we determine the following time derivative

$$\begin{aligned} \tfrac{d}{dt}\,\mathscr{S}(t,v) &= B\Big(\mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big)\Big) + \partial_2\mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big)\,A\big(\mathscr{E}_A(t,v)\big) \\ &= F\big(\mathscr{S}(t,v)\big) + \partial_2\mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big)\,A\big(\mathscr{E}_A(t,v)\big) - A\big(\mathscr{S}(t,v)\big) \end{aligned}$$

Error estimate

Consequently, we obtain the initial value problem

$$\begin{cases} \frac{d}{dt}\mathscr{S}(t,v) = F\big(\mathscr{S}(t,v)\big) + R(t,v)\,, & 0 \leq t \leq T\,, \\ \mathscr{S}(0,v) = v\,, \end{cases}$$

which involves the time-dependent remainder

$$R(t,v) = \partial_2 \mathscr{E}_B\big(t, \mathscr{E}_A(t,v)\big)\, A\big(\mathscr{E}_A(t,v)\big) - A\big(\mathscr{S}(t,v)\big)\,, \qquad 0 \leq t \leq T$$

and we apply now the nonlinear variation-of-constants formula...

Error estimate

Theorem (Gröbner–Alekseev formula)

The analytical solutions of the following initial value problems

$$v'(t) = H\big(t, v(t)\big) = G\big(v(t)\big) + R\big(t, v(t)\big)\,, \quad 0 \le t \le T\,, v(0) = v_0,$$

$$v'(t) = G\big(v(t)\big)\,, \quad 0 \le t \le T\,, v(0) = v_0$$

are related through the nonlinear variation-of-constants formula

$$\mathscr{E}_H(t, v_0) = \mathscr{E}_G(t, v_0) + \int_0^t \partial_2 \mathscr{E}_G\big(t-\tau, \mathscr{E}_H(\tau, v_0)\big)\, R\big(\tau, \mathscr{E}_H(\tau, v_0)\big)\, d\tau,$$

and this yields the formula.

Outline

We illustrate the local error behaviour when applied to the one-dimensional Gross–Pitaevskii equation under an initial condition in classical Wentzel–Kramers–Brillouin form :

$$\begin{cases} \mathrm{i}\,\partial_t \psi(x,t) = \Big(-\tfrac{1}{2}\,\varepsilon\,\partial_{xx} + \tfrac{1}{\varepsilon}\,U(x) + \tfrac{1}{\varepsilon}\,\vartheta\,\big|\psi(x,t)\big|^2\Big)\,\psi(x,t)\,, \\ \psi(x,0) = \rho_0(x)\,\mathrm{e}^{\mathrm{i}\,\sigma_0(x)/\varepsilon}\,, \qquad x \in \Omega\,, \quad 0 \le t \le T\,, \end{cases}$$

for a function $\psi : \Omega \times [0,T] \to \mathbb{C} : (x,t) \mapsto \psi(x,t)$, where $\Omega \subset \mathbb{R}$ denotes a (suitably chosen) bounded interval.
We assume the external real potential $U : \Omega \to \mathbb{R}$ and the functions $\rho_0, \sigma_0 : \Omega \to \mathbb{R}$ defining the initial condition to be sufficiently often differentiable with bounded derivatives.
Finally

$$U(x) = \tfrac{1}{2}\,\omega^2 x^2\,, \qquad x \in \Omega\,,$$

for a positive weight $\omega > 0$.

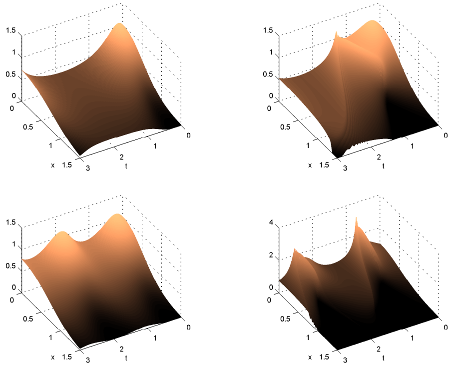

Figure: Time evolution with $\vartheta = 1$. Solution values $|\psi(x,t)|^2$, $(x,t) \in [0,1.5] \times [0,3]$, for $(\varepsilon,\omega) = (1,1)$ (top left), $(\varepsilon,\omega) = (10^{-2},1)$ (top right), $(\varepsilon,\omega) = (1,2)$ (bottom left), and $(\varepsilon,\omega) = (10^{-2},2)$ (bottom right).

The nonlinear Schrödinger equation may be cast into the form of an abstract initial value problem with linear operator $A : D(A) \subset X \to X$ and nonlinear operator $B : D(B) \subset X \to X$ defined by

$$A = \varepsilon \hat{A}, \quad \hat{A} = \frac{1}{2} i \partial_{xx}, \qquad B = \frac{1}{\varepsilon} \hat{B}, \quad \hat{B}(v) = -i \left(U + \vartheta |v|^2 \right) v.$$

$$U = 0\,, \quad \sigma_0 = 0\,:$$

Numerical results indicate that, in the present example,

- For $\Delta t/\varepsilon$ in a certain range the local error of the Lie splitting method is dominated by $C_1\,\Delta t^3/\varepsilon$,
- For $\Delta t/\varepsilon$ exceeding a certain value the local error becomes unsatisfactorily large,
- For $\Delta t = \varepsilon$, $\left\|\mathscr{L}(\varepsilon, u_0)\right\|_{L^2} \leq C\,\varepsilon^2$.

$$\left\|\mathscr{L}(\Delta t, u_0)\right\|_{L^2} \leq \left(C_0 + C_1\frac{\Delta t}{\varepsilon} + C_2\frac{\Delta t^2}{\varepsilon^2} + C_3\frac{\Delta t^3}{\varepsilon^3}\right)\Delta t^2.$$

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General case ($U \neq 0$)...

$$\sigma_0 = 0: \qquad \left\| \mathscr{L}(\Delta t, u_0) \right\|_{L^2} \leq P\left(\frac{\Delta t}{\varepsilon}\right) \Delta t^2, \quad P(\xi) = \sum_{j=0}^{3} C_j \, \xi^j,$$

$$\partial_x \sigma_0 \neq 0: \qquad \left\| \mathscr{L}(\Delta t, u_0) \right\|_{L^2} \leq Q\left(\frac{\Delta t}{\varepsilon}\right) \Delta t, \quad Q(\xi) = \sum_{j=0}^{\infty} C_j \, \xi^j,$$

- Splitting methods for Schrödinger equations
- Numerical analysis in several cases even in the presence of critical parameters
- A first step in the explanation of "good" and "bad" behaviours in numerical simulation.