Splitting methods with real-complex coefficients for separable non-autonomous semi-linear reaction-diffusion equation of Fisher

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XXIII CEDYA

Castellón, September 9, 2013

The Problem

Non-autonomous separable PDE

$$\frac{du}{dt} = \hat{A}(t,u) + \hat{B}(t,u), \qquad u(0) = u_0$$

$\Rightarrow$ $u(x,t) \in \mathbb{R}^D$.

$\Rightarrow$ (Possibly unbounded) Operators $\hat{A}$, $\hat{B}$ and $\hat{A}+\hat{B}$ generate C^0 semi-groups for positive t over a finite or infinite Banach space.

Inhomogeneous Non-Autonomous Heat Equation

$$\frac{\partial u}{\partial t} = \alpha(t)\Delta u + V(x,t)u, \quad \text{or} \quad \frac{\partial u}{\partial t} = \nabla(a(x,t)\nabla u) + V(x,t)u$$

Reaction-diffusion equations

$$\frac{\partial u}{\partial t} = D(t)\Delta u + \hat{B}(t,u), \quad t \geq 0, x \in \mathbb{R}^d \quad \text{or} \quad x \in \mathbb{T}^d$$

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For simplicity,

(Apparently) Linear form

$$\frac{du}{dt} = A(t)u + B(t)u,$$

$\Rightarrow$ A, B are the Lie operators associated to $\hat{A}$, $\hat{B}$, i.e.

$$A(t) \equiv \hat{A}(t,u)\frac{\partial}{\partial u}, \qquad B(t) \equiv \hat{B}(t,u)\frac{\partial}{\partial u}$$

which act on functions of u.

Simplest Methods For Autonomous Problems

⇒ Autonomous problem

$$\frac{du}{dt} = Au + Bu,$$

⇒ Subproblems

$$\frac{du}{dt} = Au \qquad \text{and} \qquad \frac{du}{dt} = Bu$$

⇒ Denote by e^{hA}, e^{hB} the exact h-flows for each problem respectively.

⇒ *Lie-Trotter splitting*

$$e^{hA}\, e^{hB} \qquad \text{or} \qquad e^{hB}\, e^{hA},$$

- $S(h) = e^{h(A+B)} + \mathcal{O}(h^2)$.

⇒ *Strang splitting*

$$S(h) = e^{h/2\,A}\, e^{hB}\, e^{h/2\,A} \qquad \text{or} \qquad S(h) = e^{h/2\,B}\, e^{hA}\, e^{h/2\,B}$$

- $S(h) = e^{h(A+B)} + \mathcal{O}(h^3)$.

⇒ High-order approximations

$$\Psi(h) = e^{hb_{s+1}B}\, e^{ha_sA} \cdots e^{hb_2B}\, e^{ha_1A}\, e^{hb_1B},$$

at any order exist.

$\Rightarrow$ Negative coefficients for *order* > 2.

- A and B generate C^0 semi-groups.
- Flows e^{tA} and/or e^{tB} may not be well-defined for negative times, for instance, for the Laplacian operator

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$\Rightarrow$ Goal evaluation $A(t), B(t)$ at real times.

Splitting method having one set of coefficients real and positive valued

$$a_i \in \mathbb{R}^+, \qquad b_i \in \mathbb{C}^+, \qquad (\text{or} \quad a_i \in \mathbb{C}^+, \qquad b_i \in \mathbb{R}^+).$$

- In order to numerically solve the system.

$\Rightarrow$ Take time as a new coordinate and split the system as (Blanes et al., JCAM, 2010)

$$\begin{cases} \frac{du}{dt}(t) = A(t_1)u \\ \frac{dt_1}{dt}(t) = 1 \end{cases} \quad \text{and} \quad \begin{cases} \frac{du}{dt}(t) = B(t_1)u \\ \frac{dt_1}{dt}(t) = 0. \end{cases}$$

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Splitting methods for non-autonomous perturbed systems

Suppose that

$$\|B(t)\| \ll \|A(t)\|, \ \forall t.$$

$\Rightarrow$ $B = \varepsilon B_\varepsilon$ with $|\varepsilon| \ll 1$

$\Rightarrow$ A and B are qualitatively different for perturbed problems

$\Rightarrow$ s-stage symmetric BAB compositions

$$\Psi(h) = \mathrm{e}^{hb_{s+1}\varepsilon B}\, \mathrm{e}^{ha_s A} \cdots \mathrm{e}^{hb_2 \varepsilon B}\, \mathrm{e}^{ha_1 A}\, \mathrm{e}^{hb_1 \varepsilon B},$$

with $a_{s+1-i} = a_i, \ b_{s+2-1} = b_i, \ i = 1, 2, \ldots,$

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$$\Psi(h) = \mathrm{e}^{ha_{s+1}A}\, \mathrm{e}^{hb_s\varepsilon B} \, \cdots \, \mathrm{e}^{ha_2 A}\, \mathrm{e}^{hb_1\varepsilon B}\, \mathrm{e}^{ha_1 A},$$

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Order conditions

⇒ For consistent methods ($\sum_i a_i = \sum_i b_i = 1$)

$$\Psi(h) = \mathrm{e}^{h(A+\varepsilon B)+E(h,\varepsilon)}$$

$$\begin{aligned} E(h,\varepsilon) &= h^3\ (\varepsilon\, p_{aba}[[A,B],A] + \varepsilon^2\, p_{abb}[[A,B],B]) \\ &\quad + h^5\ (\varepsilon\, p_{abaaa}[[[[A,B],A],A],A] + \mathcal{O}(\varepsilon^2)) + \mathcal{O}(\varepsilon h^7). \end{aligned}$$

⇒ Following (Blanes et al., APNUM, 2013), for the ABA composition

$$\begin{aligned} p_{aba} &= \frac{1}{2}\sum_{i=1}^{s} b_i c_i (1-c_i) - \frac{1}{12}, \\ p_{abb} &= \sum_{i=1}^{s} \frac{1}{2} b_i^2 c_i + \sum_{1\le i<j\le s} b_i b_j c_j - \frac{1}{3}, \\ p_{abaaa} &= \sum_{i=1}^{s} b_i\, c_i^4 - \frac{1}{5}. \end{aligned}$$

- $c_i = \sum_{j=0}^{i} a_j$,
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- $c_i = \sum_{j=0}^{i} a_j$,
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$\Rightarrow$ Fourth-order methods require to satisfy

$$p_{aba} = 0, \qquad p_{abb} = 0$$

- Fails a_i, b_i real and positive
- Goal $a_i \in \mathbb{R}^+$ and $b_i \in \mathbb{C}^+$.
- Fix $a_i \in (0,1)$ and leave the b_i to solve the order conditions.

$\Rightarrow$ It is not usually possible to concatenate the last map in one step with the first one in the following step in case of *ABA* composition.

$\Rightarrow$ In practice a *ABA* composition with the same number of exponentials as a *BAB* composition can be computationally more costly up to one additional stage.

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New Fourth-order methods

$\Rightarrow$ Fourth-order methods with a 4-stage composition

$$(b_1\ a_1\ b_2\ a_2\ b_3\ a_2\ b_2\ a_1\ b_1)$$

consistency conditions

$$a_1 + a_2 = \frac{1}{2}, \qquad 2(b_1 + b_2) + b_3 = 1.$$

- Fix $a_i \in (0, 1/2)$.
- Choice $a_1 = \frac{1}{4}$ obtained in (Castella et al., BIT, 2009).

$\Rightarrow$ Take a_1 as a free parameter to minimise the dominant error term[1]

$$\min_{a_1 \in (0,1/2)} |Re(p_{abaaa})| = \min_{a_1 \in (0,1/2)} \left| \sum_{i=1}^{4} Re(b_i)\, c_i^4 - \frac{1}{5} \right|.$$

[1] $u_{n+1} = Re(\Psi(h) u_n)$.

⇒ A 6-stage composition

$$(b_1\ a_1\ b_2\ a_2\ b_3\ a_3\ b_4\ a_3\ b_3\ a_2\ b_2\ a_1\ b_1)$$

⇒ The coefficients b_i are used to satisfy the conditions

$$p_{aba} = 0, \qquad p_{abb} = 0, \qquad p_{abaaa} = 0.$$

⇒ We just take $a_1 = a_2 = a_3 = \frac{1}{6}$.

⇒ Methods which derived in this work can be seen our paper (Blanes et al., Submitted).

Splitting methods

$\Rightarrow$ Standard Strang decomposition for non-autonomous system

$$S(h) = e^{h/2\, B_1}\, e^{hA_0}\, e^{h/2\, B_0} \qquad (1)$$

$\Rightarrow A_i = A(t_n + ih),\; B_i = B(t_n + ih).$

Split the system

$$\begin{cases} \frac{du}{dt}(t) = A(t_1)u \\ \frac{dt_1}{dt}(t) = 0 \\ \frac{dt_2}{dt}(t) = 1 \end{cases} \quad \text{and} \quad \begin{cases} \frac{du}{dt}(t) = B(t_2)u \\ \frac{dt_1}{dt}(t) = 1 \\ \frac{dt_2}{dt}(t) = 0. \end{cases}$$

$\Rightarrow$ Fourth order extrapolation method

$$\Phi^{[4]}(h) = \frac{4}{3} e^{\frac{h}{4}\, B_1}\, e^{\frac{h}{2} A_{1/2}}\, e^{\frac{h}{2}\, B_{1/2}}\, e^{\frac{h}{2} A_0}\, e^{\frac{h}{4}\, B_0} - \frac{1}{3} e^{\frac{h}{2}\, B_1}\, e^{hA_0}\, e^{\frac{h}{2}\, B_0}. \qquad (2)$$

⇒ Following schemes are then considered:

⇒ with real coefficients

- **Strang**: The second-order symmetric Strang splitting method (1);
- **(6,2)**: The symmetric splitting method of effective order (6,2) given in (McLachlan, BIT, 1995);
- **(EXT4)**: The fourth-order extrapolation method (2);

⇒ with complex coefficients and $a_i \in \mathbb{R}^+$

- **(RC4)**: The 4-stage fourth-order method from (Castella et al., BIT, 2009);
- **(O4)**: The 4-stage fourth-order method built in (Blanes et al. , MATCMP, 2013), whose coefficients are available at `http://www.gicas.uji.es/Research/splitting-complex.html` and referred as "Order 4 (optimized)";
- **(SM4)**: The new optimized 4-stage fourth-order method given in (Blanes et al., Submitted) ;
- **(SM(6,4))**: The new 6-stage fourth-order method are given in (Blanes et al., Submitted);

The semi-linear reaction-diffusion equation of Fisher

$$\frac{\partial u}{\partial t} = \alpha(t)^2 \Delta u + F(u,t), \qquad u(x,0) = u_0(x),$$

⇒ Periodic boundary conditions in the space domain $[0,1]$.

⇒ Fisher's potential

$$F(u) = \gamma(t) u(1-u), \qquad \gamma(t) = \frac{2 - e^{-\beta t}}{100}$$

⇒ $\alpha(t) = \frac{1}{4} + \mu \cos(wt)$.

⇒ Discretization in space,

$$\frac{dU}{dt} = \alpha(t)^2 AU + F(U,t),$$

⇒ $U = (U_1, \ldots, U_N) = (u_1, \ldots, u_N) \in \mathbb{R}^N$.

⇒ A is $N \times N$ circulant matrix.

⇒ $F(U,t) = \gamma(t)\big(U_1(1-U_1), \ldots, U_N(1-U_N)\big)$.

Splitting technique

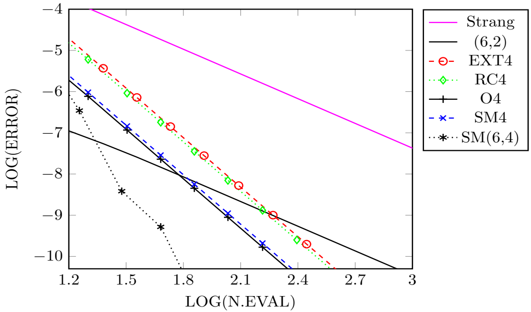
$$\begin{cases} \frac{dU}{dt}(t) = \alpha(t_1)^2 A \Delta U \\ \frac{dt_1}{dt}(t) = 1 \end{cases} \quad \text{and} \quad \begin{cases} \frac{dU}{dt}(t) = \gamma_1 U(1-U) \\ \frac{dt_1}{dt}(t) = 0. \end{cases}$$

$\Rightarrow$ $\gamma_1 = \gamma(t_1)$

Analytic solution of scalar equations

$$u(x,h) = u_0(x) + u_0(x)(1-u_0(x)) \frac{(\mathrm{e}^{\gamma_1 h} - 1)}{1 + u_0(x)(\mathrm{e}^{\gamma_1 h} - 1)}$$

$\Rightarrow$ $u(x,h)$ is well-defined for small complex time h.



⇒ $u_0(x) = \sin(2\pi x)$.

⇒ $\beta = 1, \mu = 1/8, w = 4, N = 100$ at final time $t = 1$.

⇒ Compute the error (in the 2-norm) at the final time $t = 1$ by applying the same composition methods as in the linear case.

⇒ N.EVAL is number of evaluations of the flow A.

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Thank you for your attention