Composition and splitting methods with complex times for (complex) parabolic equations

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Outline

1. **Context**
   - Parabolic partial differential equations
   - Splitting and composition methods
2. **Methods obtained by iterative compositions**
   - Double,triple and quadruble jump methods
   - Limitations
3. **Numerical experiments**
   - Linear reaction-diffusion equation
   - Fischer's equation
   - Complex Ginzburg-Landau equation
4. **Future work**

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   - Parabolic partial differential equations
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One-dimensional problems

The most simple reaction-diffusion equation involves the concentration u of a single substance in one spatial dimension

$$\partial_t u = D\partial_x^2 u + F(u),$$

and is also referred to as the Kolmogorov-Petrovsky-Piscounov equation. Specific forms appear in the litterature:

- the choice $F(u) = 0$ yields the heat equation;
- the choice $F(u) = u(1-u)$ yields Fisher's equation and is used to describe the spreading of biological populations;
- the choice $F(u) = u(1-u^2)$ describes Rayleigh-Benard convection;
- the choice $F(u) = u(1-u)(u-\alpha)$ with $0 < \alpha < 1$ arises in combustion theory and is referred to as Zeldovich'equation.

More general problems

More dimensions

Several component systems allow for a much larger range of possible phenomena. They can be represented as

$$\begin{pmatrix} \partial_t u_1 \\ \vdots \\ \partial_t u_d \end{pmatrix} = \begin{pmatrix} D_1 & & \\ & \ddots & \\ & & D_d \end{pmatrix} \begin{pmatrix} \Delta u_1 \\ \vdots \\ \Delta u_n \end{pmatrix} + \begin{pmatrix} F_1(u_1, \dots, u_d) \\ \vdots \\ F_d(u_1, \dots, u_d) \end{pmatrix}$$

Diffusion operator with a complex number $\delta \in \mathbb{C}$

For instance, the complex Ginzburg-Landau equation with a polynomial non-linearity has the form

$$\frac{\partial u}{\partial t} = \alpha \Delta u - \sum_{j=0}^{K} \beta_j |u|^{2j} u, \quad K \in \mathbb{N}, \quad (\beta_1, \dots, \beta_K) \in \mathbb{C}_+^K.$$

Two classes of methods for two different situations

In this work, we consider **composition** and **splitting** methods with **complex coefficients** of the form

$$e^{b_1 hB} e^{a_1 hA} e^{b_2 hB} e^{a_2 hA} \dots e^{b_s hB} e^{a_s hA}$$

for the following two situations:

- Reaction-diffusion equations with **real** diffusion coefficient. The important feature of $A = D\Delta$ here is that is has a **real** spectrum: hence, any method involving complex steps with positive real part is suitable.
- Complex Ginzburg-Landau equation. The values of the $\tilde{a}_i := \arg(\beta) + \arg(a_i)$ determine the stability. It is thus of importance to minimize the value of $\max_{i=1,\dots,s} |\arg(a_i)|$. Methods such that all a_i's are positive reals are ideal with that respect.

Outline

Order conditions for composition

One way to raise the order is to consider **composition** methods of the form

$$\Psi_h := \Phi_{\gamma_s h} \circ \ldots \circ \Phi_{\gamma_1 h}.$$

Theorem

Let Φ_h be a method of (classical) order p. If

$$\gamma_1 + \ldots + \gamma_s = 1 \text{ and } \gamma_1^{p+1} + \ldots + \gamma_s^{p+1} = 0$$

then $\Psi_h := \Phi_{\gamma_s h} \circ \ldots \circ \Phi_{\gamma_1 h}$ has at least order $p + 1$.

Double jump methods ([HO])

Composition methods $\Phi_h^{[p]}$ of order p can be constructed by induction:

$$\Phi_h^{[2]} = \Phi_h, \qquad \Phi_h^{[p+1]} = \Phi_{\gamma_{p,1}h}^{[p]} \circ \Phi_{\gamma_{p,2}h}^{[p]} \quad \text{for } p \geq 2.$$

The method $\Phi_h^{[p]}$ requires $s = 2^{p-1}$ compositions of Φ_h with **combined** coefficients γ_1, ..., γ_s which are of the form

$$\prod_{k=2}^{p-1} \gamma_{k,i_k}, \quad i_k \in \{1, 2\}.$$

Theorem

For $p = 3, 4, 5, 6$, the coefficients $\gamma_j, j = 1, \ldots, 2^{p-1}$, have arguments less than $\pi/2$.

Triple jump methods $s=3$ ([HO] and [CCDG])

Symmetric composition methods $\Phi_h^{[p]}$ of even order p can be constructed by induction:

$$\Phi_h^{[2]} = \Phi_h, \qquad \Phi_h^{[p+2]} = \Phi_{\gamma_{p,1}h}^{[p]} \circ \Phi_{\gamma_{p,2}h}^{[p]} \circ \Phi_{\gamma_{p,1}h}^{[p]} \quad \text{for } p \geq 2.$$

The method $\Phi_h^{[p]}$ requires $s = 3^{p/2-1}$ compositions of Φ_h with **combined** coefficients γ_1, ..., γ_s.

Theorem

By appropriately choosing the solutions of the order condition $2\gamma_{p,1}^{p+1} + (1-\gamma_{p,1})^{p+1} = 0$, the coefficients $\gamma_j, j = 1, \ldots, 3^{p/2-1}$, have arguments less than $\pi/2$ for $p = 2, 4, 6, 8, 10, 12, 14$.

Quadruple jump methods $s = 4$ ([HO] and [CCDG])

Symmetric composition methods $\Phi_h^{[p]}$ of order p (p even) can be constructed by induction:

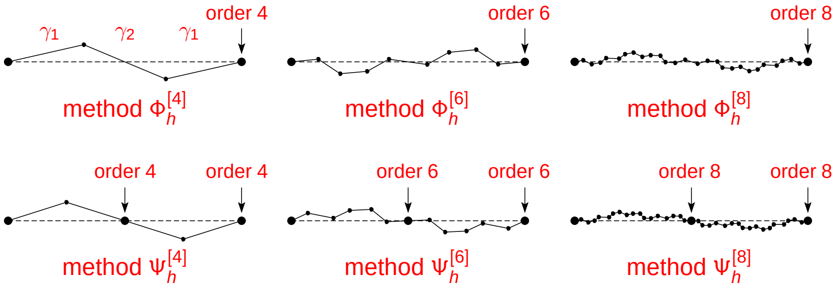
$$\Psi_h^{[0]} = \Phi_h, \quad \Psi_h^{[p+2]} = \Psi_{\gamma_4 h}^{[p]} \circ \Psi_{\gamma_3 h}^{[p]} \circ \Psi_{\gamma_2 h}^{[p]} \circ \Psi_{\gamma_1 h}^{[p]}, \; p \geq 2$$

of order $p + 2$. The method $\Psi_h^{[p]}$ requires $s = 4^{p/2-1}$ compositions of Φ_h with **combined** coefficients γ_1, ..., γ_s.

Theorem

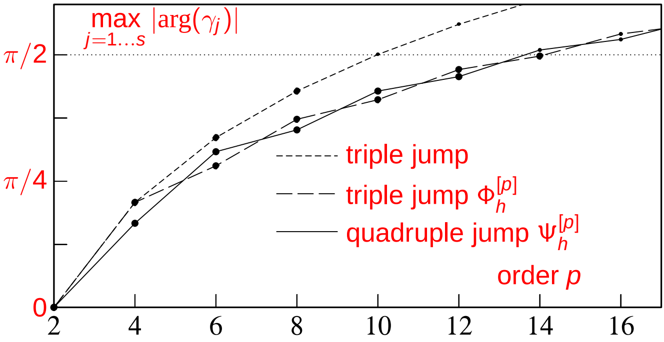
For $p = 2, 4, 6, 8, 10, 12, 14$, the coefficients γ_i for $i = 1, \ldots, 4^{p/2-1}$, have arguments less than $\pi/2$.

Triple and Quadruple jump methods ([HO] and [CCDG])



Diagrams of coefficients for compositions methods

Triple and Quadruple jump methods ([HO] and [CCDG])



Values of $\max_{j=1\dots s} |\arg \gamma_j|$ for various compositions methods

An order barrier for symmetric methods constructed by composition

Theorem

Consider a **symmetric** *p-th order method with $p > 14$ constructed through the iterative* **symmetric** *composition*

$$\Psi_h^{[p+2]} = \Psi_{\gamma_{p,s_p} h}^{[p]} \circ \Psi_{\gamma_{p,s_p-1} h}^{[p]} \circ \cdots \circ \Psi_{\gamma_{p,2} h}^{[p]} \circ \Psi_{\gamma_{p,1} h}^{[p]}, \quad p \geq 2$$

starting from a **symmetric method of order** 2. *Then one of the coefficients*

$$\prod_{k=1}^{r} \gamma_{2k,i_{2k}}, \quad i_{2k} \in \{1, \ldots, s_{2k}\}, \qquad r \in \{1, \ldots, \frac{p}{2}\}$$

has a strictly negative real part.

Methods obtained by solving directly the full order conditions

It is hoped (and partly proved) that

1. methods of order higher than 14 can be achieved
2. more efficient methods can be constructed (with smaller error constants)
3. splitting methods where the a_i's are positive and of high-order can be obtained

We now present numerical results for the methods obtained up to now.

Outline

Linear reaction-diffusion equation with periodic potential

Our first test-problem is the scalar equation in one-dimension

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

where:

- $V(x,t) = 2 + \sin(2\pi x)$ is a *linear* potential.
- $u(x,t)$ is the unknown periodic function on the x-interval $[0,1]$.

Discretization in space

After discretization in space ($\Delta x = 1/(N+1)$ and $x_i = i\Delta x$ for $i = 1, \dots, N$), we arrive at the differential equation

$$\dot{U} = AU + BU, \tag{1}$$

where the Laplacian Δ has been approximated by the matrix A of size $N \times N$ given by

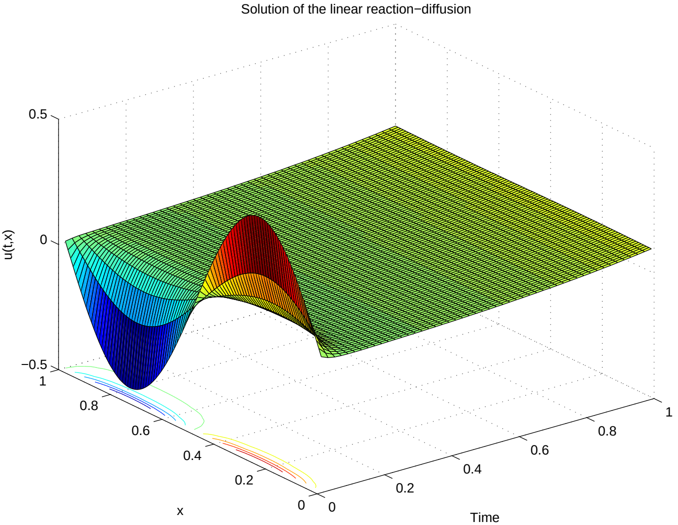
$$A = (\Delta x)^2 \begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ 1 & & & 1 & -2 \end{pmatrix},$$

and where $B = \mathrm{Diag}(V(x_1), \dots, V(x_N))$.

Discretization in time

Since the eigenvalues of A are large and negative, and those of B small, both $e^{h\alpha A}$ and $e^{h\beta B}$ are well-defined, provided $\Re(\alpha) \geq 0$.

Exact solution



The semi-linear reaction-diffusion equation of Fischer

Our second test-problem is the scalar equation

$$\frac{\partial u(x,t)}{\partial t} = \Delta u(x,t) + F(u(x,t)) \tag{2}$$

where:

- $F(u)$ is now a **non-linear** reaction term: $F(u) = u(1-u)$.
- $u(x,t)$ is the unknown **periodic** function on the x-interval $[0,1]$.

Discretization in space

After discretization in space as in the linear case, we arrive at the ordinary differential equation

$$\dot{U} = AU + F(U),$$

where

$$A = (\Delta x)^2 \begin{pmatrix} -2 & 1 & & & 1 \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ 1 & & & 1 & -2 \end{pmatrix},$$

and $F(U)$ is now defined by

$$F(U) = \big(u_1(1-u_1), \ldots, u_N(1-u_N)\big).$$

Discretization in time

The ODE is split into, on the one hand, a linear equation, and on the other hand, the non-linear ordinary differential equation

$$\frac{du_i}{dt} = u_i(1 - u_i),$$

with initial condition

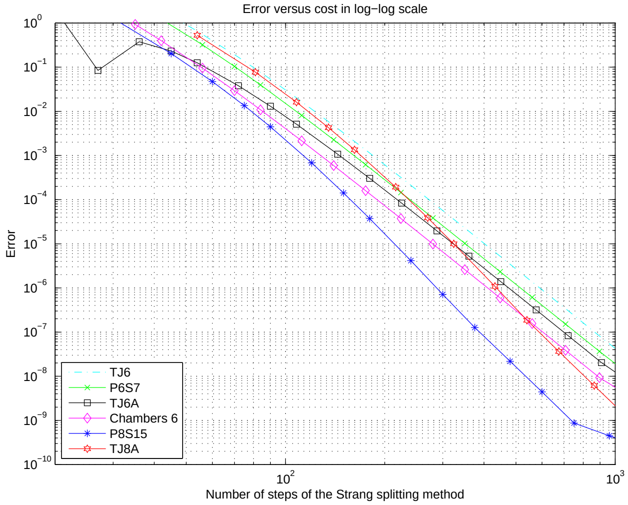
$$U(0) = (u_1(0), \ldots, u_N(0)).$$

This is a holomorphic differential equation which can be solved analytically for each component as

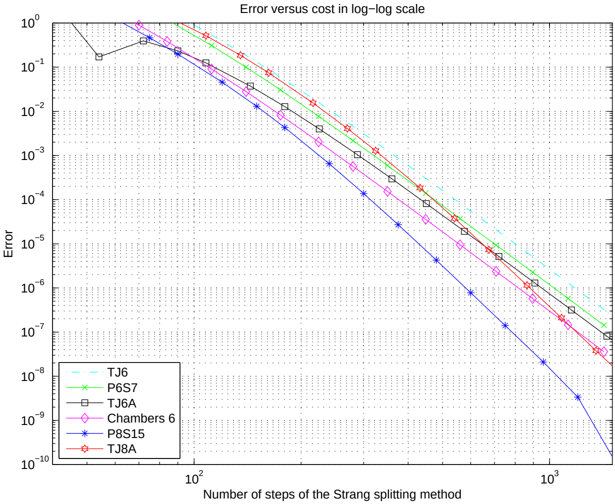
$$u_i(t) = u_i(0) + u_i(0)(1 - u_i(0))\frac{(e^t - 1)}{1 + u_i(0)(e^t - 1)},$$

Clearly, $u_i(t)$ is well defined for small complex time t.

Results for the linear equation



Results for Fischer's equation



The semi-linear Complex Ginzburg-Landau equation

Our third test problem is the complex Ginzburg-Landau equation on the domain $(x,t) \in [-100,100] \times [0,100]$

$$\frac{\partial u(x,t)}{\partial t} = \alpha \Delta u(x,t) + \varepsilon u(x,t) - \beta |u(x,t)|^2 u(x,t)$$

with:

- $(x,t) \in [-100,100] \times [0,100]$
- $\alpha = 1 + ic_1$, $\beta = 1 - ic_3$ and $c_1 = 1$, $c_3 = -2$ and $\varepsilon = 1$.
- $u_0(x) = \frac{0.8}{\cosh(x-10)^2} + \frac{0.8}{\cosh(x+10)^2}$.

Exact solution (amplitude)

For the values of the parameters considered here, plane wave solutions establish themselves quickly after a transient phase.

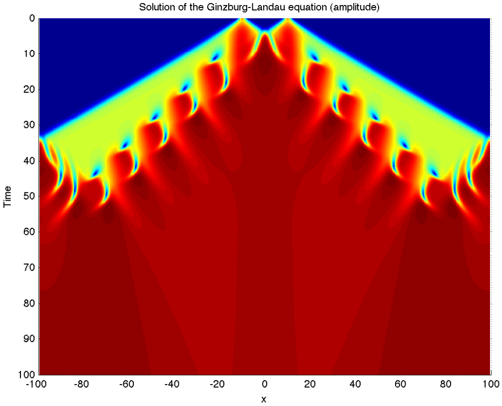


Figure: Colormaps of the amplitude $|u(x,t)|$.

Exact solution (real or imaginary parts)

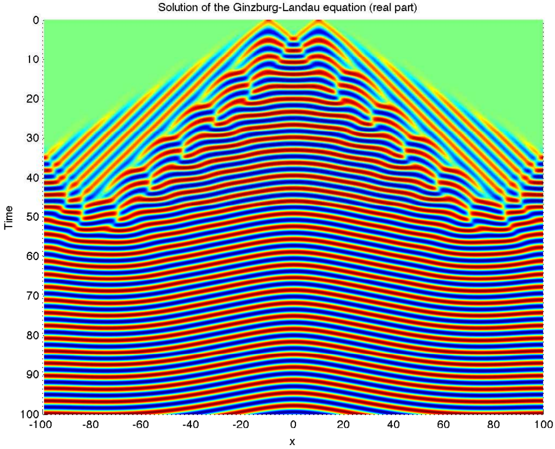


Figure: Colormaps of the real part $\Re(u(x,t))$.

Discretization in space

After discretization in space:

- $x_i = i\Delta x$ for $i = 1, \ldots, N$ with $\Delta x = 1/(N+1)$;
- $U = (u_1, \ldots, u_N) \in \mathbb{C}^N$, where $u_i(t) \approx u(x_i, t)$;

one obtains the ODE:

$$\dot{U} = \alpha AU + \varepsilon U - \beta F(U),$$

where A stands as before for the Laplacian and where

$$F(U) = \left(|u_1|^2 u_1, \ldots, |u_N|^2 u_N\right).$$

Discretization in time (I)

The ODE is split into, on the one hand, a linear equation

$$\dot{U} = \alpha A U + \varepsilon U,$$

and on the other hand, the non-linear equation

$$\dot{U} = -\beta F(U).$$

1. Solution $U(t) = e^{\varepsilon t} e^{t \alpha A} U_0$ (first part) can be extended to $t \in \mathbb{C}$.
2. Each component of the second system evolves according to
$$\dot{u}_i = -\beta |u_i|^2 u_i$$
so that, for $t \in \mathbb{R}$ small enough
$$u_i(t) = e^{-\frac{\beta}{2}\log(1+2|u_i(0)|^2 t)} u_i(0).$$

Discretization in time (II)

Alert

Since $u \mapsto |u|^2 u$ is **not** a holomorphic function, the “natural” extension of $u_i(t)$ to $\mathbb{C}$ is not valid!

We rewrite the system for $V(t) = \Re(U(t))$ and $W(t) = \Im(U(t))$:

$$\begin{cases} \dot{V} &= AV - c_1 AW + \varepsilon V - G(V + c_3 W) \\ \dot{W} &= c_1 AV + AW + \varepsilon W - G(-c_3 V + W) \end{cases}$$

where G is the diagonal matrix with $G_{i,i} = v_i^2 + w_i^2$.

At the cost of double dimension

we can now solve the equation for complex time $t \in \mathbb{C}$ with $\Re(t) \geq 0$.

Discretization in time (III)

After a linear change of variables $(V, W) \mapsto (\tilde{V}, \tilde{W})$ the solution of the **non-linear part** reads

$$\begin{cases} \tilde{v}_i(t) &= \tilde{v}_i(0) e^{-\frac{\beta}{2}\log(1+2t\tilde{M}_i(0))} \\ \tilde{w}_i(t) &= \tilde{w}_i(0) e^{-\frac{\bar{\beta}}{2}\log(1+2t\tilde{M}_i(0))} \end{cases}, \qquad \tilde{M}_i(0) := 4i\tilde{v}_i(0)\tilde{w}_i(0).$$

Definition of log

The logarithm refers to the principal value of $\log(z)$ for complex numbers: if $z = (a+ib) = re^{i\theta}$ with $-\pi < \theta \leq \pi$, then

$$\begin{aligned} \log z &:= \ln r + i\theta = \ln|z| + i \arg z \\ &= \ln(|a+ib|) + 2i \arctan\left(\frac{b}{a+\sqrt{a^2+b^2}}\right). \end{aligned}$$

$\log(z)$ is **not defined** for $z \in \mathbb{R}^-$.

Discretization in time (IV)

One step $U_0 \mapsto U_1$ of a splitting method $(a_1, b_1, \dots, a_s, b_s)$:

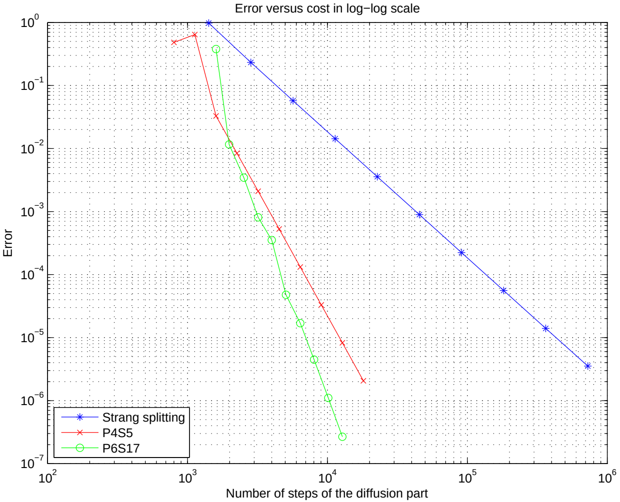
1. Initialize $V_0 = \Re(U_0)$ and $W_0 = \Im(U_0)$
2. Compute $(V_0, W_0) \mapsto (\tilde{V}_0, \tilde{W}_0)$
3. Set $k = s$
4. Compute $\tilde{V}_{1/2} := \tilde{V}(b_k h)$ and $\tilde{W}_{1/2} := \tilde{W}(b_k h)$
5. Compute $\tilde{V}_1 = e^{\varepsilon a_k h} \exp(h a_k \alpha A) \tilde{V}_{1/2}$ and $\tilde{W}_1 = e^{\varepsilon a_k h} \exp(h a_k \bar{\alpha} A) \tilde{W}_{1/2}$
6. Decrement k by 1
7. If $k \geq 1$, set $\tilde{V}_0 = \tilde{V}_1$, $\tilde{W}_0 = \tilde{W}_1$ and go to step 4.
8. Compute $(\tilde{V}_1, \tilde{W}_1) \mapsto (V_1, W_1)$

Methods considered

We test here three different methods of orders 2, 4 and 6:

1. Strang's splitting
$$e^{h/2B}e^{hA}e^{h/2B}$$
2. P4S5 , a fourth-order method of [CCDV]:
$$e^{b_1hB}e^{ahA}e^{b_2hB}e^{ahA}e^{b_3hB}e^{ahA}e^{b_2hB}e^{ahA}e^{b_1hB}$$
where the b_i's are complex with positive real parts, and $a = 1/4$.
3. P6S17 , a sixth-order method of [BCCM]:
$$e^{b_1hV}e^{ahA}\dots e^{b_8hV}e^{ahA}e^{b_9hV}e^{ahA}e^{b_8hV}\dots e^{ahA}e^{b_1hV}$$
where the b_i's are complex with positive real parts, and $a = 1/16$.

Results for the Complex Ginzburg-Landau equation



Outline

Ongoing and future work

- further study of optimal composition methods
- further study of methods involving complex coefficients for only one operator
- methods for other classes of problems

THANK YOU FOR YOUR ATTENTION