Castellón, September 2010

Splitting methods with complex times for parabolic equations

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This is joint work with

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Plan of the talk

Paper published in BIT 49 (2009).
Similar results are derived independently by
E. Hensen & A. Ostermann (BIT 49, 2009).

1. Context
   - Reaction-diffusion problems
   - Splitting and composition methods
2. Splitting methods with complex coefficients
   - Construction of new high-order methods
   - Convergence for the linear case with exponential maps
3. Numerical experiments
   - Reaction-diffusion with Fisher's non-linear potential.
   - Exponential maps and Peaceman-Rachford approx.
4. Future work

Part 1

Context

- Reaction-diffusion problems
- Splitting and composition methods

Reaction-diffusion problems

The most simple reaction-diffusion equation involves the concentration $u(x,t)$ of a single substance in one spatial dimension

$$\partial_t u(x,t) = D\partial_x^2 u(x,t) + F(u(x,t)) \qquad D > 0$$

and is also known as the Kolmogorov-Petrovsky-Piscounov eq.

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and is also known as the Kolmogorov-Petrovsky-Piscounov eq. Specific forms appear in the literature:

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

Lie-Trotter and Strang Splitting

Let us illustrate the methods on the linear case

$$\frac{\partial u}{\partial t} = \Delta u + V u, \quad V \text{ linear.}$$

Lie-Trotter (order 1)
Splitting methods basically rely on the identity

$$e^{h(\Delta + V)} = e^{h\Delta}\, e^{hV} + \mathcal{O}\left(h^2\right).$$

Strang splitting
The symmetric version

$$e^{h/2\,V} e^{h\Delta} e^{h/2\,V}$$

yields an approximation of order 2.

High-order general compositions

One can consider general splitting methods of the form

$$e^{b_1 hV} e^{a_1 h\Delta} e^{b_2 hV} e^{a_2 h\Delta} \dots e^{b_s hV} e^{a_s h\Delta}.$$

Baker-Campbell-Hausdorff formula yields order conditions in terms of the coefficients a_j, b_j (these are not straightforward to solve for high orders).

$$e^{hA} e^{hB} = e^{h(A+B) + \frac{h^2}{2}[A,B] + \dots}$$

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Also, raising the order can be achieved by considering composition methods of the form

$$\Psi_h := \Phi_{\gamma_s h} \circ \dots \circ \Phi_{\gamma_1 h},$$

where Φ_h is a given basic method, e.g.

- $\Phi_h = e^{h/2V} e^{h\Delta} e^{h/2V}$

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- $\Phi_h = e^{h/2V} e^{h\Delta} e^{h/2V}$
- $\Phi_h = \underbrace{\left(\mathrm{Id} - \frac{h}{2}V\right)^{-1}}_{\text{implicit Euler}} \underbrace{\left[\left(\mathrm{Id} - \frac{h}{2}A\right)^{-1} \left(\mathrm{Id} + \frac{h}{2}A\right)\right]}_{\text{implicit midpoint}} \underbrace{\left(\mathrm{Id} + \frac{h}{2}V\right)}_{\text{explicit Euler}}.$

(Peaceman-Rachford formula, 55’)

A disappointing result: order barrier 2

The heat equation is not reversible. Thus, only splitting methods using $e^{ha_j\Delta}$ with coefficients $a_j > 0$ can be used.

Consider a splitting method of order p for $e^{h(A+B)}$ of the form

$$e^{ha_sA}e^{hb_sB}\dots e^{ha_1A}e^{hb_1B}$$

Theorem (Sheng 89', Suzuki 91', Sussman & Wisdom 92')
For $p > 2$ there exists j such that $a_j < 0$ or $b_j < 0$.

Theorem (Goldman & Kaper 96')
For $p > 2$ there exist j, k such that $a_j < 0$ and $b_k < 0$.

An elegant geometric proof obtained by Blanes & Casas 05'.

Possible remedies to the order barrier

- Extrapolation method

$$\frac{4}{3}\Phi_{h/2} \circ \Phi_{h/2} - \frac{1}{3}\Phi_h.$$

  Formal order 4, but unstable with the Peaceman-Rachford approximation.

- An extrapolation method is considered in Schatzman '01 and taken from Dia '96,

$$\frac{45}{64}\Phi_{h/3} \circ \Phi_{h/3} \circ \Phi_{h/3} + \frac{1}{2}\Phi_{h/2} \circ \Phi_{h/2} - \frac{13}{64}\Phi_h.$$

  Although the formal order of this method is 4, the true order of convergence is not clearly understood.

Possible remedies to the order barrier

- Allow for the use of complex coefficients such that $\Re(a_i) > 0$.

  The idea of using complex coefficients in numerical methods is not new:

  - Rosenbrock 63'
  - Suzuki 90' (composition methods)
  - Gegechkori, Rogava & Tsiklauri 02', 04' (orders 3 & 4, convex combinations)
  - Chambers 03' (Celestial mechanics)
  - Bandrauk, Dehghanian & Lu. 06' (orders 3 & 4)

  (see also the recent survey by Blanes, Casas & Murua, 10').

Part 2

Splitting methods with complex coefficients

- Construction of new high-order methods
- Convergence for the linear case with exponential maps

Jump methods

Theorem Let Φ_h be a method of 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 $p + 1$.

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

Proof. The idea is to show that if the basic method has order p,

$$\Phi_h(y) = \varphi_h(y) + C(y)h^{p+1} + \mathcal{O}(h^{p+2}),$$

where φ_h denotes the exact flow, then

$$\Psi_h(y) = \varphi_h(y) + C(y)(\gamma_1^{p+1} + \ldots + \gamma_s^{p+1})h^{p+1} + \mathcal{O}(h^{p+2}).$$

$\square$

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

Triple jump method.
If $s = 3$ and $\gamma_1 = \gamma_3$ (symmetry) there is a unique real solution

$$\gamma_1 = \gamma_3 = \frac{1}{2 - 2^{1/(p+1)}}, \qquad \gamma_2 = -\frac{2^{1/(p+1)}}{2 - 2^{1/(p+1)}}.$$

and for Φ_h symmetric of order p, Ψ_h is of order $p+2$.

This procedure can be repeated iteratively up to any order
(Creutz & Gocksch 89', Forest 89', Suzuki 90', Yoshida 90)

Double jump method of Suzuki 90' $s = 2$

$$\gamma_1 + \gamma_2 = 1, \quad \gamma_1^{p+1} + \gamma_2^{p+1} = 0.$$

Solving the equations for $s = 2$, no real but complex solutions:

$$\gamma_1^{(p)} = \overline{\gamma_2^{(p)}} = \left(1 + e^{\frac{i\pi}{p+1}}\right)^{-1}.$$

Suzuki constructed methods of high-order by induction:

$$\Phi_h^{(1)} = \Phi_h, \qquad \Phi_h^{(p+1)} = \Phi_{\gamma_2^{(p)} h}^{(p)} \circ \Phi_{\gamma_1^{(p)} h}^{(p)}, \quad \text{for } p \geq 1.$$

The above construction with complex coefficients is explicitly given by Suzuki (Phys. Lett. A 90' and J. Math. Phys. 91') as an introduction for his popular composition methods involving only real coefficients.
In fact, it yields coefficients with positive real parts up to order 6.

New triple jump methods $s = 3$

$$\gamma_1 + \gamma_2 + \gamma_3 = 1, \quad \gamma_1^{p+1} + \gamma_2^{p+1} + \gamma_3^{p+1} = 0.$$

Solving the equations for even p.

There are $p+1$ solutions in $\mathbb{C}$: for $k = 0, \ldots p$,

$$\gamma_{1,k}^{(p)} = \gamma_{3,k}^{(p)} = \frac{1}{2 - 2^{1/(p+1)} e^{2ik\pi/(p+1)}}, \quad \gamma_{2,k}^{(p)} = -\frac{2^{1/(p+1)} e^{2ik\pi/(p+1)}}{2 - 2^{1/(p+1)} e^{2ik\pi/(p+1)}}.$$

Optimal solutions

The two conjugate solutions $(\gamma_1^{(p)}, \gamma_2^{(p)}, \gamma_3^{(p)})$ and $(\overline{\gamma}_1^{(p)}, \overline{\gamma}_2^{(p)}, \overline{\gamma}_3^{(p)})$ which minimize $\max_j |\arg(\gamma_{j,k}^{(p)})|$ are obtained for $k = \pm p/2$:

$$\gamma_1^{(p)} = \gamma_3^{(p)} = \frac{e^{i\pi/(p+1)}}{2e^{i\pi/(p+1)} + 2^{1/(p+1)}}, \quad \gamma_2^{(p)} = \frac{2^{1/(p+1)}}{2e^{i\pi/(p+1)} + 2^{1/(p+1)}}.$$

Notice that these solutions also minimize $|\gamma_1| + |\gamma_2| + |\gamma_3|$.

New triple jump methods $s = 3$

Similarly, symmetric composition methods $\Phi_h^{(p)}$ of order p (p even) can be constructed by induction:

$$\Phi_h^{(2)} = \Phi_h, \qquad \Phi_h^{(p+2)} = \Phi^{(p)}_{\gamma_3^{(p)} h} \circ \Phi^{(p)}_{\gamma_2^{(p)} h} \circ \Phi^{(p)}_{\gamma_1^{(p)} h} \quad \text{for } p \geq 2.$$

Theorem
The method $\Phi_h^{(p)}$ requires $s = 3^{p/2-1}$ compositions of Φ_h with combined coefficients $\gamma_1, \dots, \gamma_s$.
For $p = 2, 4, 6, 8$, the coefficients $\gamma_j, j = 1, \dots, 3^{p/2-1}$, have positive real parts.

New triple jump methods $s = 3$

An improvement to reduce the quantity $\max_{i=1\ldots s} |\arg(\gamma_i)|$ is to replace coefficients $(\gamma_1^{(p)}, \gamma_2^{(p)}, \gamma_3^{(p)})$ by $(\overline{\gamma}_1^{(p)}, \overline{\gamma}_2^{(p)}, \overline{\gamma}_3^{(p)})$ alternatively, e.g.

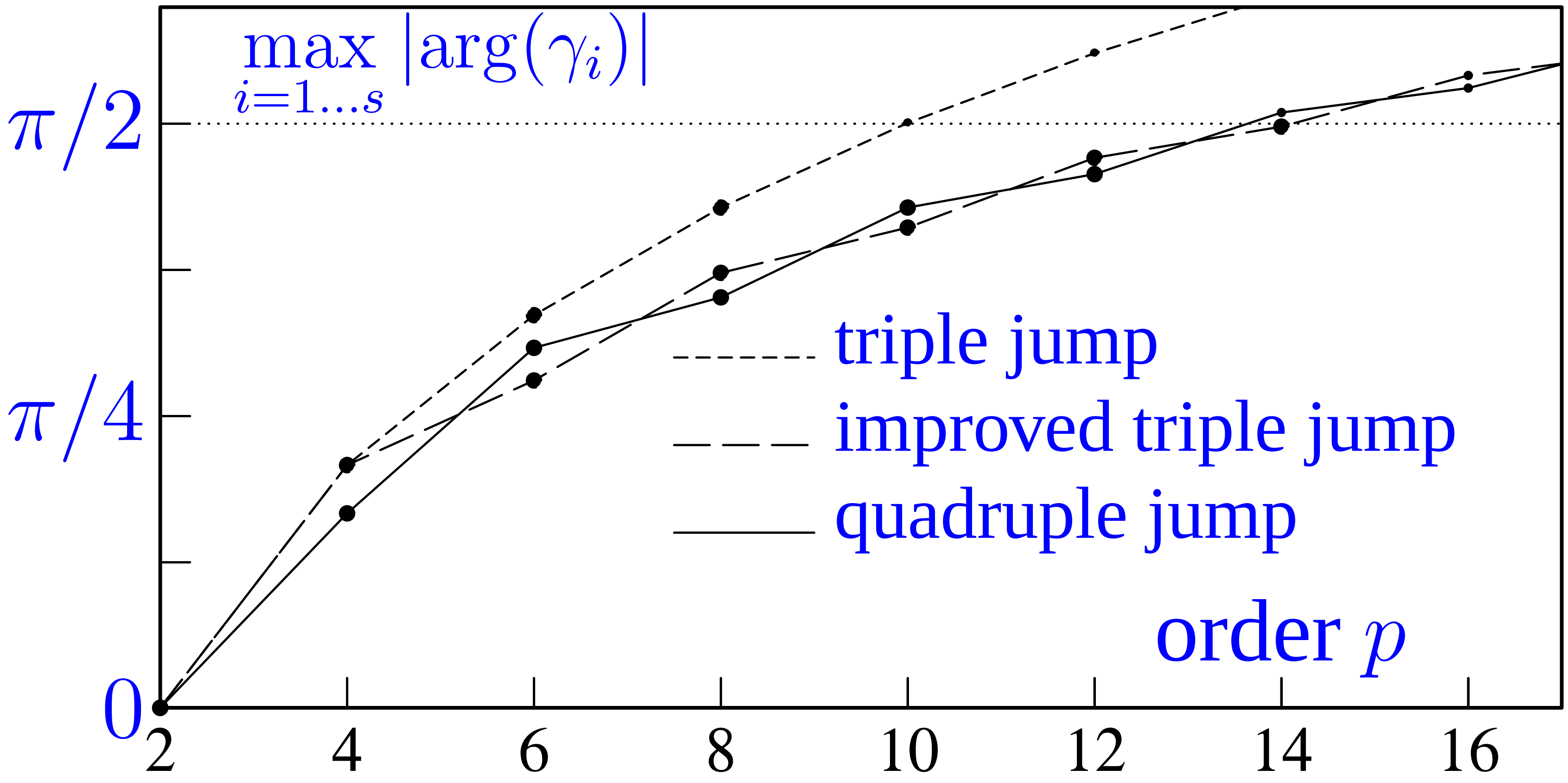
$$\Phi_h^{(p+2)} = \Phi^{(p)}_{\gamma_3^{(p)} h} \circ \Phi^{(p)}_{\gamma_2^{(p)} h} \circ \Phi^{(p)}_{\gamma_1^{(p)} h} \qquad \text{if } p/2 \text{ odd},$$

$$\Phi_h^{(p+2)} = \Phi^{(p)}_{\overline{\gamma}_3^{(p)} h} \circ \Phi^{(p)}_{\overline{\gamma}_2^{(p)} h} \circ \Phi^{(p)}_{\overline{\gamma}_1^{(p)} h} \qquad \text{else}.$$

Theorem

The method $\Phi_h^{(p)}$ requires $s = 3^{p/2-1}$ compositions of Φ_h with combined coefficients $\gamma_1, \ldots, \gamma_s$.
For $p = 2, 4, 6, 8, 10, 12, 14$, the coefficients γ_j for $j = 1, \ldots, 3^{p/2-1}$, have positive real parts.

Triple and Quadruple jump methods:angles



Values of $\max_{j=1\ldots s} |\arg \gamma_j|$
versus order of composition methods.

New quadruple jump methods $s = 4$

Take $\Phi_h^{(p)}$, symmetric method of order p, and consider

$$\Psi_h^{(p+2)} = \Phi^{(p)}_{\gamma_4^{(p)} h} \circ \Phi^{(p)}_{\gamma_3^{(p)} h} \circ \Phi^{(p)}_{\gamma_2^{(p)} h} \circ \Phi^{(p)}_{\gamma_1^{(p)} h}$$

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Solving the equations for even p.
The two complex conjugate solutions with minimal sum of moduli and minimal $\max_{j=1\ldots4} |\arg(\gamma_{j,k}^{(p)})|$) are obtained for

$$\gamma_1^{(p)} = \overline{\gamma}_2^{(p)} = \overline{\gamma}_3^{(p)} = \gamma_4^{(p)} = \frac{1}{4} + i\frac{\sin(\pi/(p+1))}{4 + 4\cos(\pi/(p+1))}.$$

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Theorem

The method $\Psi_h^{(p)}$ requires $s = 4 \cdot 3^{p/2-2}$ compositions of Φ_h with combined coefficients γ_1, ..., γ_s.

For $p = 4, 6, 8, 10, 12$, the coefficients γ_i for $i = 1, \ldots, 4^{p/2-1}$, have positive real parts.

An accurate approximation at midstep

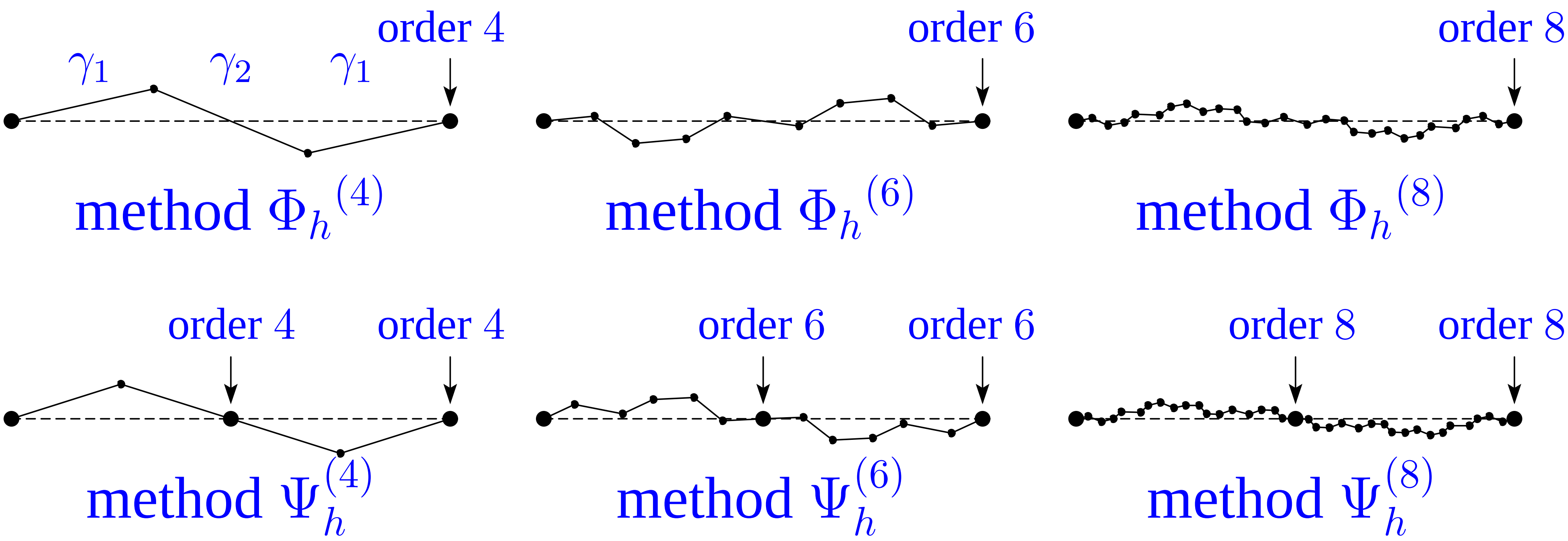
An interesting feature is that we obtain an accurate approximation of the solution at midstep (notice $\gamma_1 + \gamma_2 = 1/2$).

Indeed, consider the method of order $p+2$:

$$\begin{aligned} y_{n+1/2} &= (\Phi^{(p)}_{\gamma_2 h} \circ \Phi^{(p)}_{\gamma_1 h})(y_n), \\ y_{n+1} &= (\Phi^{(p)}_{\gamma_1 h} \circ \Phi^{(p)}_{\gamma_2 h})(y_{n+1/2}). \end{aligned}$$

As a matter of fact, $(2\gamma_1, 2\gamma_2)$ and $(2\gamma_2, 2\gamma_1)$ are solutions of the order $p+1$ equations with $s=2$, so that $y_{n+1/2}$ yields an approximation of the solution at time $t = t_n + h/2$ with local error $\mathcal{O}(h^{p+2})$.

Triple and Quadruple jump methods:diagrams



Diagrams of coefficients for compositions methods

Example: $\Psi_h^{(4)} = \Phi_{\gamma_1 h}^{(2)} \circ \Phi_{\overline{\gamma} h}^{(2)} \circ \Phi_{\overline{\gamma} h}^{(2)} \circ \Phi_{\gamma h}^{(2)}, \qquad \gamma = \frac{1}{4} + i\frac{\sqrt{3}}{12}.$

Convergence in the linear case for exponential maps

Theorem

Under some reasonable assumptions on the linear operators A, B and L = $A + B$, an exponential splitting method

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

with coefficients in an appropriate sector of the right-side complex plane and of formal order p remains of order p for the linear equation $u_t = Au + Bu$.

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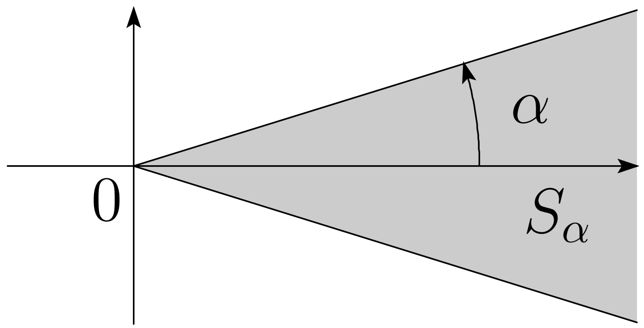
with coefficients in an appropriate sector of the right-side complex plane and of formal order p remains of order p for the linear equation $u_t = Au + Bu$.
Proof
The proof is a direct consequence of a previous result of Hansen & Ostermann (2008) for splittings of the form

$$L = A_1 + A_2 + A_3 + \dots + A_s$$

where the A_j's generate continous semigroups on H (Hilbert space), and satisfy certain smoothness assumptions.

In our setting: mα-dissipative operators

$$A : D(A) \subset H \to H$$



$$\forall u \in D(A), -(Au, u) \in S_\alpha,$$

$\forall z \notin S_\alpha, zId + A$ isomorphism :$D(A) \to H.$

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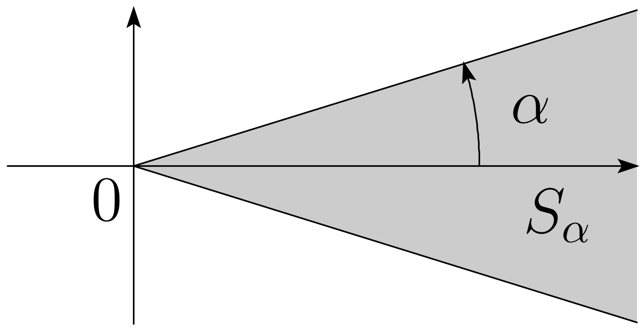


$$\forall u \in D(A), -(Au, u) \in S_\alpha,$$
$$\forall z \notin S_\alpha, zId + A \text{ isomorphism } : D(A) \to H.$$

- A mα-dissipative operator A with $0 \le \alpha \le \pi/2$ generates a continuous semi-group on H and is a contraction operator:

$$\forall t \ge 0, \|e^{tA} u\|_H \le \|u\|_H.$$

- Here: $a_i \Delta$ is mα-dissipative in $L^2(\mathbb{R}^d)$ with $\alpha = |\arg(a_i)|$.

Part 3

Numerical experiments

- Reaction-diffusion with Fisher's non-linear potential.
- Exponential maps and Peaceman-Rachford approx.

Reaction-diffusion with Fisher's non-linear potential

We consider the scalar equation in one-dimension on $\mathbb{T} \sim (0, 1)$

$$u_t = \Delta u + u(1 - u).$$

After discretization in space, we arrive at the ODE

$$\dot{U} = AU + \left(u^1(1 - u^1), \ldots, u^N(1 - u^N)\right)^T \in \mathbb{R}^N$$

The scalar differential equation

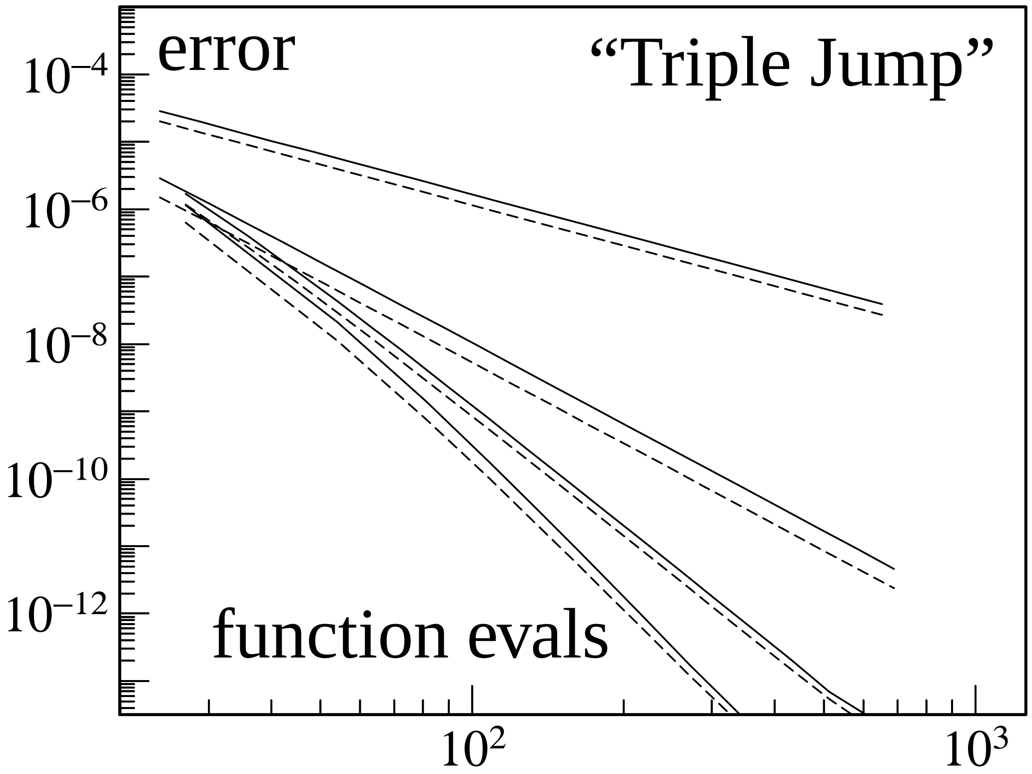
$$\frac{du}{dz} = u(1 - u), \qquad u(0) = u_0$$

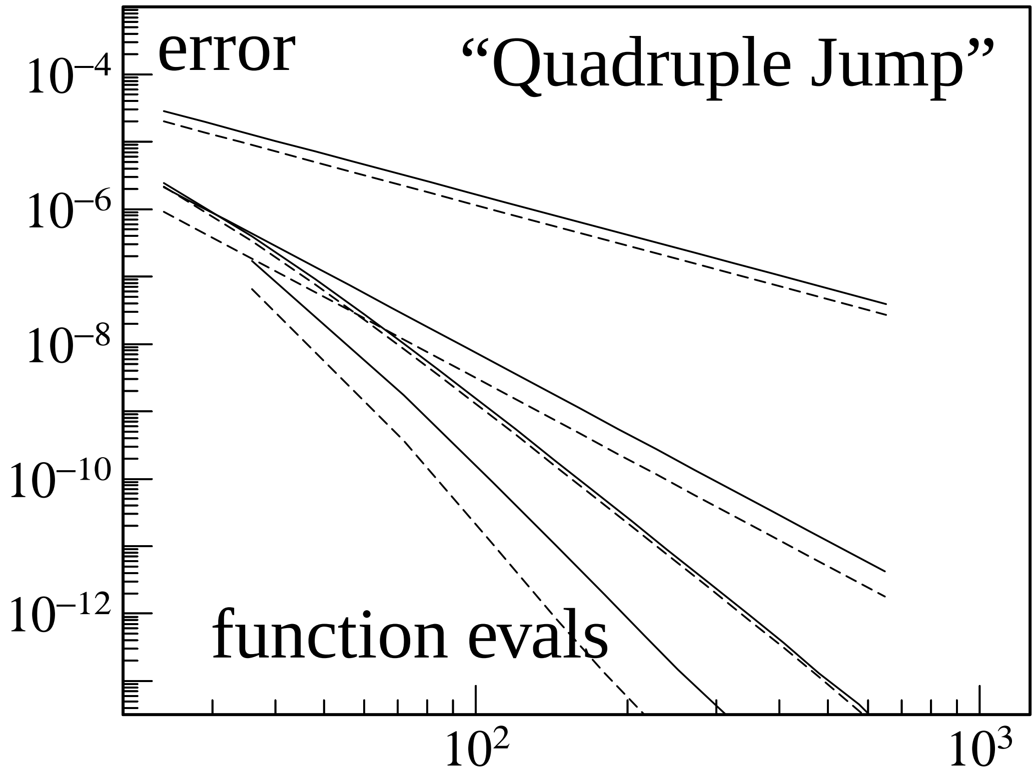
can be solved analytically as

$$u(z) = u_0 + u_0(1 - u_0)\frac{(e^z - 1)}{1 + u_0(e^z - 1)},$$

which is well defined for small complex time z.

Triple and Quadruple jump methods

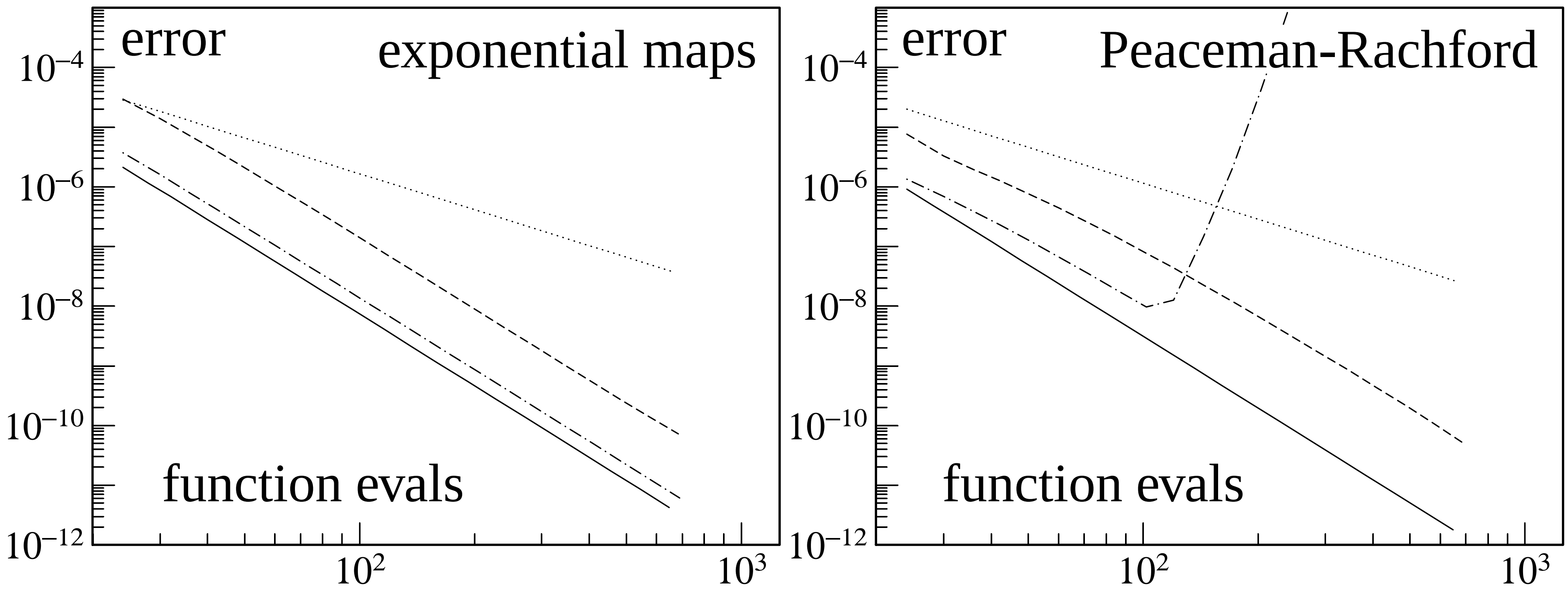




Composition methods of orders 2,4,6,8.

Solid lines: exponentials. Dashes lines: Peaceman Rachford.

Triple and Quadruple jump methods



Solid lines: Quadruple jump method of order 4.
Dashes lines and dashes-dotted lines: Extrapolation methods.
Dotted lines: Strang splitting.

Perspectives

- systematic study of optimal composition methods
- convergence analysis for non-linear problems
- methods involving complex coefficients for only one operator: e.g. the order 4 method

$$e^{b_1 hV} e^{a_1 hA} e^{b_2 hV} e^{a_2 hA} e^{b_3 hV} e^{a_2 hA} e^{b_2 hV} e^{a_1 hA} e^{b_1 hV}$$

where $b_1 = 1/10 - i/30$, $b_2 = 4/15 + 2i/15$,
$b_3 = 4/15 - i/5$ are complex, and
$a_1 = a_2 = a_3 = a_4 = 1/4$ are reals.
May be useful e.g. for the Schrödinger equation with a non-linear potential.