Geometric integrators with complex coefficients

Sergio Blanes

Instituto de Matemática Multidisciplinar
Universitat Politècnica de València

FoCM'11, Budapest, July 4-14, 2011

Joint work, at different parts, with:

P. Bader, F. Casas, P. Chartier, J. Makazaga, and A. Murua

The numerical integration of non-reversible systems using high order splitting methods with complex coefficients (having positive real part) has been recently considered

Example: The linear heat equation with potential

$$\frac{\partial}{\partial t}\mathbf{u} = \triangle \mathbf{u} + V(x)\mathbf{u}$$

Introduction

The numerical integration of non-reversible systems using high order splitting methods with complex coefficients (having positive real part) has been recently considered

Example: The linear heat equation with potential

$$\frac{\partial}{\partial t}\mathbf{u} = \triangle \mathbf{u} + V(x)\mathbf{u}$$

New families of numerical methods have appeared which deserve further analysis.

The numerical integration of non-reversible systems using high order splitting methods with complex coefficients (having positive real part) has been recently considered

Example: The linear heat equation with potential

$$\frac{\partial}{\partial t}\mathbf{u} = \triangle \mathbf{u} + V(x)\mathbf{u}$$

New families of numerical methods have appeared which deserve further analysis.

Some questions:

- $\exists$ methods at any order with coefficients having positive real parts?
- Are the new methods efficient?
- Are useful for long time integrations? Backward error analysis?

Introduction

- From the computational point of view:
  – The numerical methods can be more involved and computationally more expensive.

Introduction

- From the computational point of view:
  – The numerical methods can be more involved and computationally more expensive.
- From the theoretical point of view:
  – Singularities in the complex domain can appear
  – Bounded solutions in the real space are unbounded in the complex domain, and this can affect to the stability of the methods
  – The evolution of the solution on the extended manifold in the complex domain needs to be studied

Example: The Volterra-Lotka problem

Let us consider the Volterra–Lotka problem

$$\dot{u} = u(v - 2), \qquad \dot{v} = v(1 - u)$$

First integral: $I(u, v) = \ln(uv^2) - (u + v)$.

Example: The Volterra-Lotka problem

Let us consider the Volterra–Lotka problem

$$\dot{u} = u(v-2), \qquad \dot{v} = v(1-u)$$

First integral: $I(u,v) = \ln(uv^2) - (u+v)$.
It can be considered as a Hamiltonian system with

$$H = (2p - e^p) + (q - e^q)$$

with $q = \ln u,\ p = \ln v$
Split: $f_A = (u(v-2), 0), \quad f_B = (0, v(1-u))$

A simple 4*th*-order method

Given a symmetric 2nd order $\mathcal{S}^{[2]}$ one gets a 4th order integrator $\mathcal{S}^{[4]} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ as

$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]},$$

$$2\alpha + \beta = 1, \qquad 2\alpha^3 + \beta^3 = 0$$

A simple 4*th*-order method

Given a symmetric 2nd order $\mathcal{S}^{[2]}$ one gets a 4th order integrator $\mathcal{S}^{[4]} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ as

$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]},$$

$$2\alpha + \beta = 1, \qquad 2\alpha^3 + \beta^3 = 0$$

$$\alpha = \frac{1}{2 - 2^{1/3}} \simeq 1.35 > 1, \qquad \beta = 1 - 2\alpha \simeq -1.7 < 0$$

A simple 4*th*-order method

Given a symmetric 2nd order $\mathcal{S}^{[2]}$ one gets a 4th order integrator $\mathcal{S}^{[4]} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ as

$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]},$$

$$2\alpha + \beta = 1, \qquad 2\alpha^3 + \beta^3 = 0$$

$$\alpha = \frac{1}{2 - 2^{1/3}} \simeq 1.35 > 1, \qquad \beta = 1 - 2\alpha \simeq -1.7 < 0$$

$$\alpha \simeq 0.324 \pm i0.135, \qquad \beta \simeq 0.351 \mp i0.269$$

A simple 4*th*-order method

Given a symmetric 2nd order $\mathcal{S}^{[2]}$ one gets a 4th order integrator $\mathcal{S}^{[4]} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ as

$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]},$$

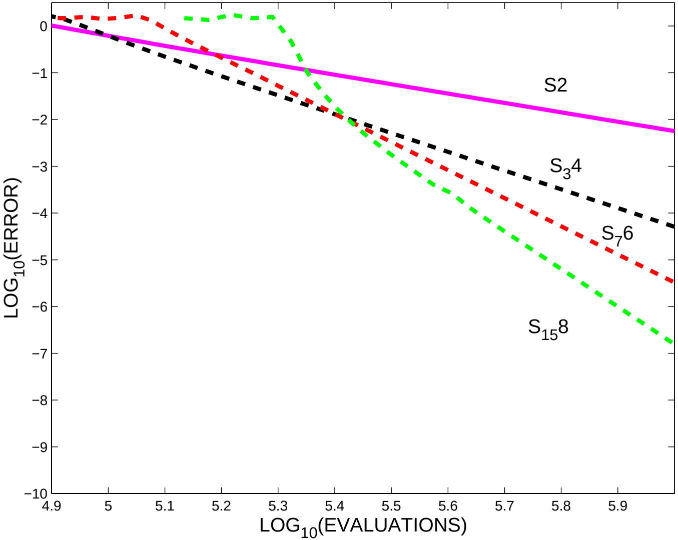
$$2\alpha + \beta = 1, \qquad 2\alpha^3 + \beta^3 = 0$$

$$\alpha = \frac{1}{2 - 2^{1/3}} \simeq 1.35 > 1, \qquad \beta = 1 - 2\alpha \simeq -1.7 < 0$$

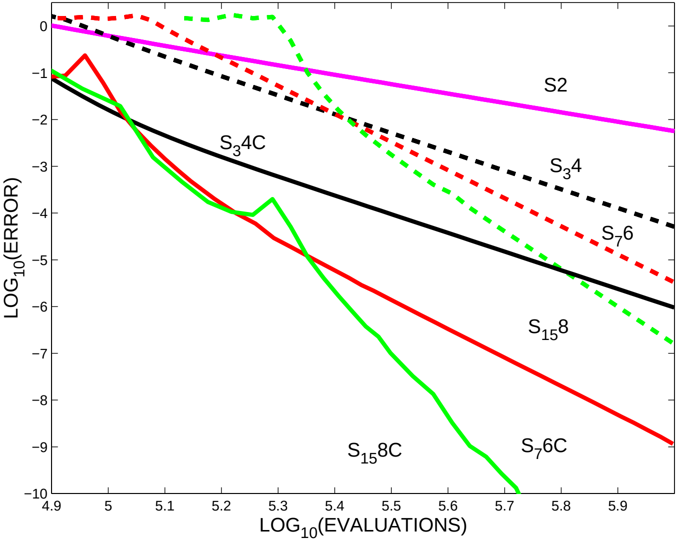
$$\alpha \simeq 0.324 \pm i0.135, \qquad \beta \simeq 0.351 \mp i0.269$$

Initial conditions $(u_0, v_0) = (4, 2), \quad t \in [0, 1000]$

Example: The Volterra-Lotka problem



Example:



0
−1
−2
−3
−4
−5
−6
−7
−8
−9
−10
4.9
5
5.1
5.2
5.3
5.4
5.5
5.6
5.7
5.8
5.9
LOG10(ERROR)
LOG10(EVALUATIONS)
S2
S34C
S34
S76
S158
S158C
S76C

4*th*−order Methods by Composition

$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha_k h}^{[2]} \circ \cdots \circ \mathcal{S}_{\alpha_1 h}^{[2]}$$

$4th-$order Methods by Composition

$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha_k h}^{[2]} \circ \cdots \circ \mathcal{S}_{\alpha_1 h}^{[2]}$$

Order conditions

$$\sum_{i=1}^{k} \alpha_i = 1, \qquad \sum_{i=1}^{k} \alpha_i^3 = 0$$

$4th-$order Methods by Composition

$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha_k h}^{[2]} \circ \cdots \circ \mathcal{S}_{\alpha_1 h}^{[2]}$$

Order conditions

$$\sum_{i=1}^{k} \alpha_i = 1, \qquad \sum_{i=1}^{k} \alpha_i^3 = 0$$

If $\alpha_i \in \mathbb{R}$ then

$$\exists\, j \;/\; \alpha_j < 0$$

$4th-$order Methods by Composition

$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha_k h}^{[2]} \circ \cdots \circ \mathcal{S}_{\alpha_1 h}^{[2]}$$

Order conditions

$$\sum_{i=1}^{k} \alpha_i = 1, \qquad \sum_{i=1}^{k} \alpha_i^3 = 0$$

If $\alpha_i \in \mathbb{R}$ then

$$\exists\, j \;/\; \alpha_j < 0$$

If $\alpha_i \in \mathbb{C}$ then

$$\max_{i=1,\ldots,k} \mathrm{Arg}(\alpha_i) - \min_{i=1,\ldots,k} \mathrm{Arg}(\alpha_i) \geq \frac{\pi}{3}.$$

Given a **symmetric** method of order $2p$, $\mathcal{S}^{[2p]}(h)$, we can define a recursion by **symmetric** compositions

$$\mathcal{S}^{[2p+2]}(h) = \prod_{i=1}^{m_p} \mathcal{S}^{[2p]}(\alpha_{p,i} h)$$

Given a **symmetric** method of order $2p$, $\mathcal{S}^{[2p]}(h)$, we can define a recursion by **symmetric** compositions

$$\mathcal{S}^{[2p+2]}(h) = \prod_{i=1}^{m_p} \mathcal{S}^{[2p]}(\alpha_{p,i} h)$$

$$\sum_{i=1}^{m_p} \alpha_{p,i} = 1 \qquad \text{and} \qquad \sum_{i=1}^{m_p} \alpha_{p,i}^{2p+1} = 0.$$

Given a **symmetric** method of order $2p, \mathcal{S}^{[2p]}(h)$, we can define a recursion by **symmetric** compositions

$$\mathcal{S}^{[2p+2]}(h) = \prod_{i=1}^{m_p} \mathcal{S}^{[2p]}(\alpha_{p,i} h)$$

$$\sum_{i=1}^{m_p} \alpha_{p,i} = 1 \qquad \text{and} \qquad \sum_{i=1}^{m_p} \alpha_{p,i}^{2p+1} = 0.$$

Starting from $\mathcal{S}^{[2]}(h)$, we have

$$\mathcal{S}^{[2(p+1)]}(h) = \prod_{i_p=1}^{m_p} \left(\prod_{i_{p-1}=1}^{m_{p-1}} \left(\cdots \left(\prod_{i_1=1}^{m_1} \mathcal{S}^{[2]}(\alpha_{p,i_p} \alpha_{p-1,i_{p-1}} \cdots \alpha_{1,i_1} h) \right) \cdots \right) \right.$$

Given a **symmetric** method of order $2p, \mathcal{S}^{[2p]}(h)$, we can define a recursion by **symmetric** compositions

$$\mathcal{S}^{[2p+2]}(h) = \prod_{i=1}^{m_p} \mathcal{S}^{[2p]}(\alpha_{p,i} h)$$

$$\sum_{i=1}^{m_p} \alpha_{p,i} = 1 \qquad \text{and} \qquad \sum_{i=1}^{m_p} \alpha_{p,i}^{2p+1} = 0.$$

Starting from $\mathcal{S}^{[2]}(h)$, we have

$$\mathcal{S}^{[2(p+1)]}(h) = \prod_{i_p=1}^{m_p} \left(\prod_{i_{p-1}=1}^{m_{p-1}} \left(\cdots \left(\prod_{i_1=1}^{m_1} \mathcal{S}^{[2]}(\alpha_{p,i_p} \alpha_{p-1,i_{p-1}} \cdots \alpha_{1,i_1} h) \right) \cdots \right) \right)$$

Castella, Chartier, Descombes, & Vilmart, BIT 49 (2009), 487-508, and Hansen & Ostermann, BIT 49 (2009), 527-542, obtained methods up to order 14 with coefs. having positive real part.

$$\mathcal{S}_h^{[2]} \to \mathcal{S}_h^{[4]} \to \mathcal{S}_h^{[6]} \to \mathcal{S}_h^{[8]} \to \ldots \mathcal{S}_h^{[14]} \to \mathcal{S}_h^{[16]}$$

Lemma

For $k \geq 2$ and $r \geq 2$, consider $(z_1, \ldots, z_k) \in (\mathbb{C}_+)^k$ such that $\sum_{i=1}^k z_i^r = 0$. Then we have

$$\max_{i=1,\ldots,k} \operatorname{Arg}(z_i) - \min_{i=1,\ldots,k} \operatorname{Arg}(z_i) \geq \frac{\pi}{r}.$$

Lemma

For $k \geq 2$ and $r \geq 2$, consider $(z_1, \ldots, z_k) \in (\mathbb{C}_+)^k$ such that $\sum_{i=1}^k z_i^r = 0$. Then we have

$$\max_{i=1,\ldots,k} \mathrm{Arg}(z_i) - \min_{i=1,\ldots,k} \mathrm{Arg}(z_i) \geq \frac{\pi}{r}.$$

Proof.

If

$$\max_{i=1,\ldots,k} \mathrm{Arg}(z_i) - \min_{i=1,\ldots,k} \mathrm{Arg}(z_i) < \frac{\pi}{r}.$$

then

$$\max_{i=1,\ldots,k} \mathrm{Arg}(z_i^r) - \min_{i=1,\ldots,k} \mathrm{Arg}(z_i^r) < \pi.$$

and obviously $\sum_{i=1}^k z_i^r \neq 0$. □

Theorem

Starting from a second-order symmetric method $\mathcal{S}^{[2]}(h)$*, all methods* $\mathcal{S}^{[2p]}(h)$ *of order* $2p = 16, 18, \ldots$ *from the previous recursion have at least one coefficient with negative real part.*

Proof.

We assume that all methods $\mathcal{S}^{[2q]}(h)$, $q = 1, \ldots, p$ have all their coefficients in $\mathbb{C}_+$. Using Lemma 1 we have

$$\forall q = 1, \ldots, p, \quad \max_{i=1,\ldots,m_q} \mathrm{Arg}(\alpha_{q,i}) - \min_{i=1,\ldots,m_q} \mathrm{Arg}(\alpha_{q,i}) \geq \frac{\pi}{2q+1},$$

so that

$$\max_{i_1,\ldots,i_p} \mathrm{Arg}\left(\prod_{j=1}^{p} \alpha_{j,i_j}\right) - \min_{i_1,\ldots,i_p} \mathrm{Arg}\left(\prod_{j=1}^{p} \alpha_{j,i_j}\right) \geq \frac{\pi}{3} + \cdots + \frac{\pi}{2p+1}.$$

Since $\frac{1}{3} + \frac{1}{5} + \cdots + \frac{1}{15} > 1$, then $2p = 14$ is an upper bound. □

Composition Methods with Complex Coefficients

Proof.

We assume that all methods $\mathcal{S}^{[2q]}(h)$, $q = 1, \ldots, p$ have all their coefficients in $\mathbb{C}_+$. Using Lemma 1 we have

$$\forall q = 1, \ldots, p, \quad \max_{i=1,\ldots,m_q} \mathrm{Arg}(\alpha_{q,i}) - \min_{i=1,\ldots,m_q} \mathrm{Arg}(\alpha_{q,i}) \geq \frac{\pi}{2q+1},$$

so that

$$\max_{i_1,\ldots,i_p} \mathrm{Arg}\left(\prod_{j=1}^{p} \alpha_{j,i_j}\right) - \min_{i_1,\ldots,i_p} \mathrm{Arg}\left(\prod_{j=1}^{p} \alpha_{j,i_j}\right) \geq \frac{\pi}{3} + \cdots + \frac{\pi}{2p+1}.$$

Since $\frac{1}{3} + \frac{1}{5} + \cdots + \frac{1}{15} > 1$, then $2p = 14$ is an upper bound. □

This is a sharp bound since methods of order 14 have been obtained

Composition Methods with Complex Coefficients

From the computational point of view, it is more efficient to build methods directly by the composition

$$\mathcal{S}^{[2p]}(h) = \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_s h)$$

We have built methods of order 6 and 8:

$$\begin{aligned} \mathcal{S}^{[6]}(h) &= \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_7 h) \\ \mathcal{S}^{[8]}(h) &= \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_{15} h) \end{aligned}$$

Composition Methods with Complex Coefficients

From the computational point of view, it is more efficient to build methods directly by the composition

$$\mathcal{S}^{[2p]}(h) = \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_s h)$$

We have built methods of order 6 and 8:

$$\begin{aligned} \mathcal{S}^{[6]}(h) &= \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_7 h) \\ \mathcal{S}^{[8]}(h) &= \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_{15} h) \end{aligned}$$

We have also built methods of order 16 with coefficients having their real part positive. The procedure followed is:

$$\mathcal{S}_h^{[2]} \to \mathcal{S}_h^{[8]} \to \mathcal{S}_h^{[16]}$$

Composition Methods with Complex Coefficients

From the computational point of view, it is more efficient to build methods directly by the composition

$$\mathcal{S}^{[2p]}(h) = \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_s h)$$

We have built methods of order 6 and 8:

$$\begin{aligned} \mathcal{S}^{[6]}(h) &= \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_7 h) \\ \mathcal{S}^{[8]}(h) &= \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_{15} h) \end{aligned}$$

We have also built methods of order 16 with coefficients having their real part positive. The procedure followed is:

$$\mathcal{S}_h^{[2]} \to \mathcal{S}_h^{[8]} \to \mathcal{S}_h^{[16]}$$

$\exists$ methods at all orders?

Composition Methods with Complex Coefficients

From the computational point of view, it is more efficient to build methods directly by the composition

$$\mathcal{S}^{[2p]}(h) = \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_s h)$$

We have built methods of order 6 and 8:

$$\begin{aligned} \mathcal{S}^{[6]}(h) &= \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_7 h) \\ \mathcal{S}^{[8]}(h) &= \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_{15} h) \end{aligned}$$

We have also built methods of order 16 with coefficients having their real part positive. The procedure followed is:

$$\mathcal{S}_h^{[2]} \to \mathcal{S}_h^{[8]} \to \mathcal{S}_h^{[16]}$$

$\exists$ methods at all orders? We are still ignorant

Composition Methods with Complex Coefficients

From the computational point of view, it is more efficient to build methods directly by the composition

$$\mathcal{S}^{[2p]}(h) = \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_s h)$$

We have built methods of order 6 and 8:

$$\begin{aligned}
\mathcal{S}^{[6]}(h) &= \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_7 h) \\
\mathcal{S}^{[8]}(h) &= \mathcal{S}^{[2]}(\gamma_1 h) \cdots \mathcal{S}^{[2]}(\gamma_{15} h)
\end{aligned}$$

We have also built methods of order 16 with coefficients having their real part positive. The procedure followed is:

$$\mathcal{S}_h^{[2]} \to \mathcal{S}_h^{[8]} \to \mathcal{S}_h^{[16]}$$

$\exists$ methods at all orders? We are still ignorant, but at a higher level of ignorance!

Example: The Volterra-Lotka problem

$$\dot{u} = u(v-2), \qquad \dot{v} = v(1-u)$$

$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]},$$

$$\alpha \simeq 0.324 + i0.135, \qquad \beta \simeq 0.351 - i0.269$$

Initial conditions $(u_0, v_0) = (4, 2)$, time step: $h = \frac{1}{8}$
Measure the relative error: $|I - I_0|/|I_0|$ with
$I(u, v) = \ln(uv^2) - (u + v)$.

Example: The Volterra-Lotka problem

$$\dot{u} = u(v-2), \qquad \dot{v} = v(1-u)$$

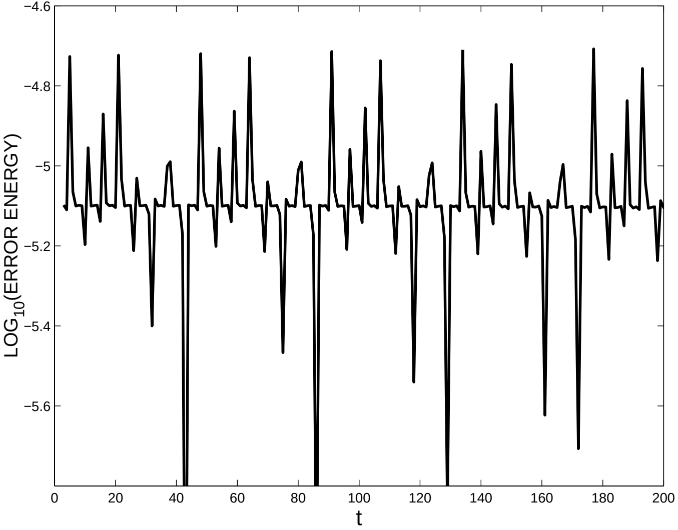
$$\mathcal{S}_h^{[4]} = \mathcal{S}_{\alpha h}^{[2]} \circ \mathcal{S}_{\beta h}^{[2]} \circ \mathcal{S}_{\alpha h}^{[2]},$$

$$\alpha \simeq 0.324 + i0.135, \qquad \beta \simeq 0.351 - i0.269$$

Initial conditions $(u_0, v_0) = (4, 2)$, time step: $h = \frac{1}{8}$
Measure the relative error: $|I - I_0|/|I_0|$ with
$I(u,v) = \ln(uv^2) - (u+v)$.

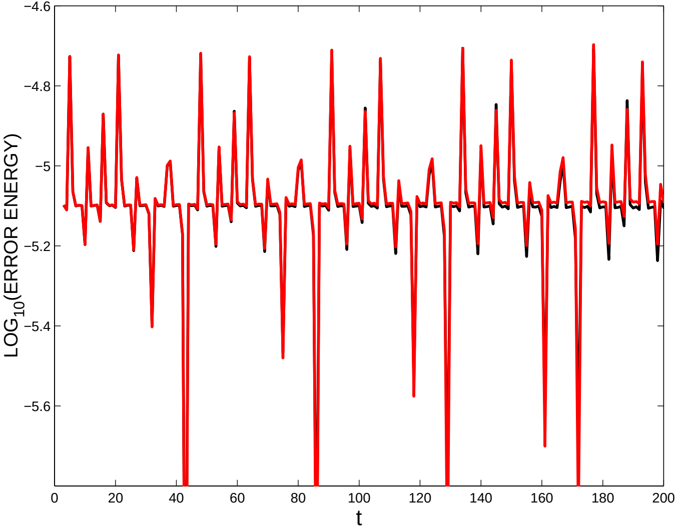
- I) Projection at the end of the integration
- II) Projection at each step

Example:



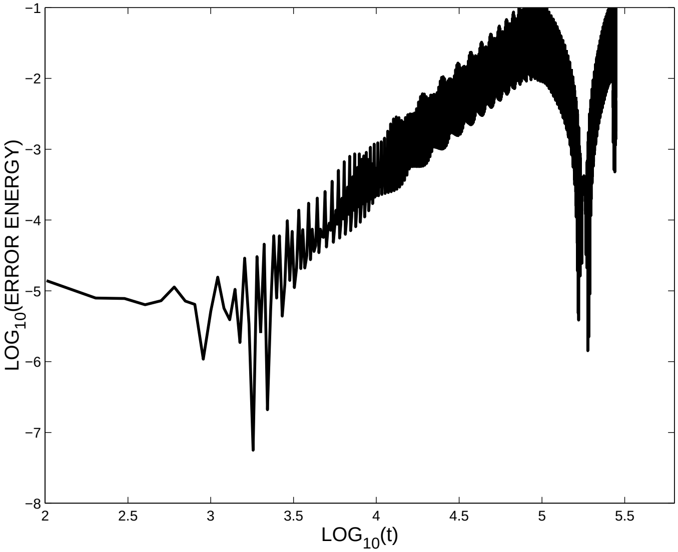
−4.6
−4.8
−5
−5.2
−5.4
−5.6
LOG10(ERROR ENERGY)
0
20
40
60
80
100
120
140
160
180
200
t

Example:

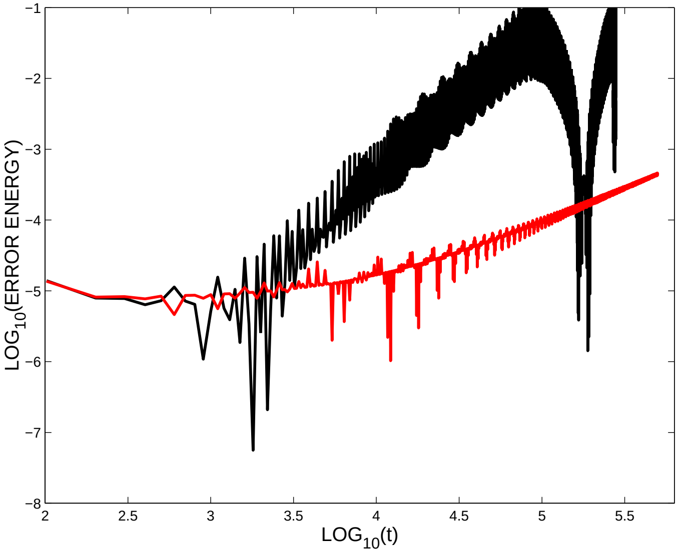


−4.6
−4.8
−5
−5.2
−5.4
−5.6
0
20
40
60
80
100
120
140
160
180
200
t
LOG10(ERROR ENERGY)

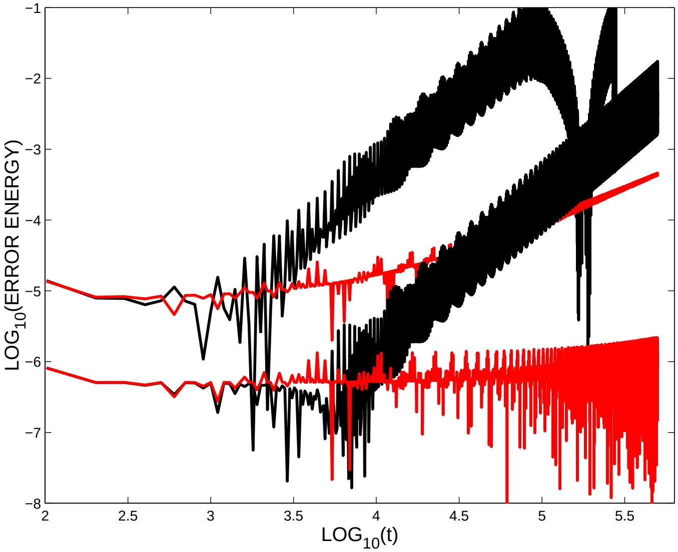
Example:



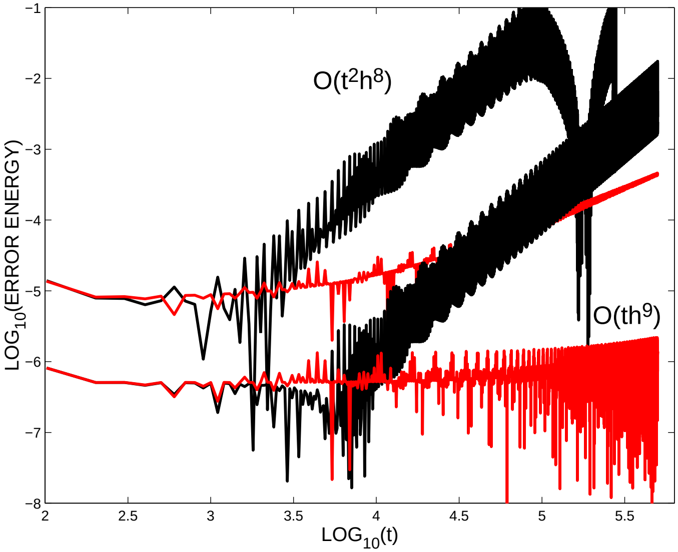
Example:



Example:



Example:



O(t²h⁸)
O(th⁹)
LOG₁₀(ERROR ENERGY)
LOG₁₀(t)
−1
−2
−3
−4
−5
−6
−7
−8
2
2.5
3
3.5
4
4.5
5
5.5

Projection into the real space. Informal proof

Let $\Phi(h) = e^{hF}$ denote the exact solution and $S_r(h)$ a with complex coefficients method of order $r = \min\{q, p\}$ such that

$$S_r(h) = \exp\left(hF + h^{q+1}F_R + ih^{p+1}F_I\right)$$

Projection into the real space. Informal proof

Let $\Phi(h) = e^{hF}$ denote the exact solution and $S_r(h)$ a with complex coefficients method of order $r = \min\{q, p\}$ such that

$$
\begin{aligned}
S_r(h) &= \exp\left(hF + h^{q+1}F_R + ih^{p+1}F_I\right) \\
&= \exp\left(ih^{p+1}\hat{F}_I\right)\exp\left(hF + h^{q+1}\hat{F}_R\right)
\end{aligned}
$$

Projection into the real space. Informal proof

Let $\Phi(h) = e^{hF}$ denote the exact solution and $S_r(h)$ a with complex coefficients method of order $r = \min\{q, p\}$ such that

$$\begin{aligned}
S_r(h) &= \exp\left(hF + h^{q+1}F_R + ih^{p+1}F_I\right) \\
&= \exp\left(ih^{p+1}\hat{F}_I\right)\exp\left(hF + h^{q+1}\hat{F}_R\right) \\
&= \left(I + ih^{p+1}\hat{F}_I - h^{2p+2}\hat{F}_I^2 + \dots\right)\exp\left(hF + h^{q+1}\hat{F}_R\right)
\end{aligned}$$

Projection into the real space. Informal proof

Let $\Phi(h) = e^{hF}$ denote the exact solution and $S_r(h)$ a with complex coefficients method of order $r = \min\{q, p\}$ such that

$$\begin{aligned} S_r(h) &= \exp\left(hF + h^{q+1}F_R + ih^{p+1}F_I\right) \\ &= \exp\left(ih^{p+1}\hat{F}_I\right)\exp\left(hF + h^{q+1}\hat{F}_R\right) \\ &= \left(I + ih^{p+1}\hat{F}_I - h^{2p+2}\hat{F}_I^2 + \dots\right)\exp\left(hF + h^{q+1}\hat{F}_R\right) \end{aligned}$$

F_R, F_I are elements of the Lie algebra associated to the components of F, but $\hat{F}_I^2$ is not in the Lie algebra.

Projection into the real space. Informal proof

Let $\Phi(h) = e^{hF}$ denote the exact solution and $S_r(h)$ a with complex coefficients method of order $r = \min\{q, p\}$ such that

$$
\begin{aligned}
S_r(h) &= \exp\left(hF + h^{q+1}F_R + ih^{p+1}F_I\right) \\
&= \exp\left(ih^{p+1}\hat{F}_I\right)\exp\left(hF + h^{q+1}\hat{F}_R\right) \\
&= \left(I + ih^{p+1}\hat{F}_I - h^{2p+2}\hat{F}_I^2 + \ldots\right)\exp\left(hF + h^{q+1}\hat{F}_R\right)
\end{aligned}
$$

F_R, F_I are elements of the Lie algebra associated to the components of F, but $\hat{F}_I^2$ is not in the Lie algebra.
To project at the end corresponds to ($t = Nh$)

$$
Re\left(S_p^N(h)\right) = \left(I - t^2h^{2p}\check{F}_I^2 + \ldots\right)\exp\left(t(F + h^q\check{F}_R)\right)
$$

Projection into the real space. Informal proof

Let $\Phi(h) = e^{hF}$ denote the exact solution and $S_r(h)$ a with complex coefficients method of order $r = \min\{q, p\}$ such that

$$\begin{aligned} S_r(h) &= \exp\left(hF + h^{q+1}F_R + ih^{p+1}F_I\right) \\ &= \exp\left(ih^{p+1}\hat{F}_I\right)\exp\left(hF + h^{q+1}\hat{F}_R\right) \\ &= \left(I + ih^{p+1}\hat{F}_I - h^{2p+2}\hat{F}_I^2 + \dots\right)\exp\left(hF + h^{q+1}\hat{F}_R\right) \end{aligned}$$

F_R, F_I are elements of the Lie algebra associated to the components of F, but $\hat{F}_I^2$ is not in the Lie algebra.
To project at the end corresponds to ($t = Nh$)

$$Re\left(S_p^N(h)\right) = \left(I - t^2h^{2p}\check{F}_I^2 + \dots\right)\exp\left(t(F + h^q\check{F}_R)\right)$$

while to project at each step corresponds to

$$Re\left(S_p(h)\right)^N = \left(I - th^{2p+1}\check{F}_I^2 + \dots\right)\exp\left(t(F + h^q\check{F}_R)\right)$$

Some other problems of interest

(a) The linear Schrödinger equation ($\hbar = 1$):

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left(-\frac{1}{2m}\nabla^2 + V(x)\right)\Psi(x,t)$$

$$\mathbf{u}(h) = e^{ih(\Delta+\mathbf{V})}\mathbf{u}_0$$

Methods with $a_i \in \mathbb{R}^+,\ b_i \in \mathbb{C}$.

Some other problems of interest

(a) The linear Schrödinger equation ($\hbar = 1$):

$$i\frac{\partial}{\partial t}\Psi(x,t) = \left(-\frac{1}{2m}\nabla^2 + V(x)\right)\Psi(x,t)$$

$$\mathbf{u}(h) = e^{ih(\Delta+\mathbf{V})}\mathbf{u}_0$$

Methods with $a_i \in \mathbb{R}^+, \ b_i \in \mathbb{C}$.

(b) The LSE integrated in the pure imaginary time

$$\frac{\partial}{\partial \tau}\Psi(x,\tau) = \left(\frac{1}{2m}\nabla^2 - V(x)\right)\Psi(x,\tau)$$

Methods with $a_i, \ b_i \in \mathbb{C}_+$.

In addition $[V,[V,[V,\nabla^2]]] = 0$

References

- R.I. McLachlan and R. Quispel, Splitting methods, *Acta Numerica* **11** (2002), pp. 341-434.
- SB, F. Casas, and A. Murua, Splitting and composition methods in the numerical integration of differential equations. Bol. Soc. Esp. Math. Apl., 45 (2008), 87–143.
- F. Castella, P. Chartier, S. Descombes, and G. Vilmart, Splitting methods with complex times for parabolic equations, BIT 49 (2009), 487–508.
- E. Hansen and A. Ostermann, High order splitting mehtods for analytic semigroup exist, BIT 49 (2009), 527–542.
- SB, F. Casas, and A. Murua, Splitting methods with complex coefficients. Bol. Soc. Esp. Math. Apl., 50 (2010), 47–61.
- SB, F. Casas, P. Chartier, and A. Murua, Splitting methods with complex coefficients for some classes of evolution equations. Submitted.

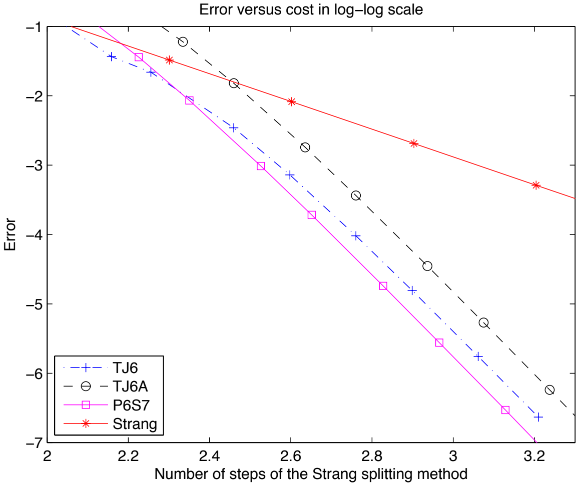
Numerical Examples: A linear parabolic equation

Let us consider the scalar equation in one-dimension

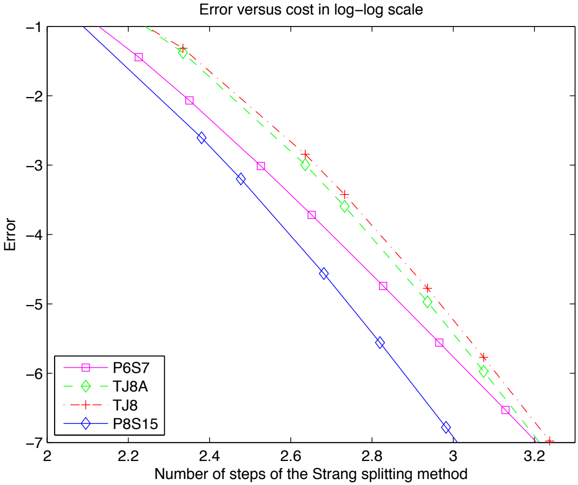
$$\frac{\partial u}{\partial t} = \Delta u + (2 + \sin(2\pi x))\, u$$

$u(x, 0) = \sin(2\pi x)$
$x \in [0, 1]$ with $N = 100$
periodic boundary conditions.

Example:


Error versus cost in log−log scale
Error
Number of steps of the Strang splitting method
−1
−2
−3
−4
−5
−6
−7
2
2.2
2.4
2.6
2.8
3
3.2
TJ6
TJ6A
P6S7
Strang

Example:



Error versus cost in log–log scale
−1
−2
−3
−4
−5
−6
−7
Error
2
2.2
2.4
2.6
2.8
3
3.2
Number of steps of the Strang splitting method
P6S7
TJ8A
TJ8
P8S15