Exponential integrators for the Schrödinger equation with time-dependent Hamiltonian

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The Mathematical Problem

The numerical integration of the time-dependent linear matrix differential equation

$$i\frac{d}{dt}u(t) = H(t)\,u(t), \qquad u(0) = u_0 \in \mathbb{C}^d \tag{1}$$

$t \in [0, T]$, $d \gg 1$, and $H(t)$ a Hermitian (usually dense) matrix.

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1. $H(t)$ is a complex Hermitian matrix
2. $H(t)$ is a real symmetric matrix

The Goal

- The numerical integration of the time-dependent Schrödinger Equationt ($\hbar = 1$)

$$i\frac{\partial}{\partial t}\psi(x,t) = -\frac{1}{2\mu}\nabla^2\psi(x,t) + V(x,t)\psi(x,t)$$

$\psi(x,0) = \psi_0(x),\ x \in \mathbb{R}^D,\ t \in [0,T]$. After spatial discretisation one gets the case in which $H(t)$ is real.

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- A quantum two-level system can be written down in the form

$$H(t) = \begin{pmatrix} \omega(t) & C(t) \\ C^*(t) & -\omega(t) \end{pmatrix}$$

  where $\omega(t)$ is a real function and $C(t)$ is, in general, a complex function of t.

Frequently used method

The exponential midpoint method to advance from t_n to $t_{n+1} = t_n + h$

$$u_{n+1} = e^{-ihH(t_n+\frac{h}{2})} u_n$$

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More efficient methods to reach high accuracy?

Methods for the non-autonomous case

I) $H(t)$ **is a complex Hermitian matrix**

i) Time as a new **independent variable**: the (t, t') method

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Peskin, Kosloff and Moiseyev (93-94)

$$i\frac{\partial}{\partial t}\psi(x, t', t) = \mathcal{H}(x, t')\psi(x, t', t),$$

where

$$\mathcal{H}(x, t') = \hat{H}(x, t') - i\frac{\partial}{\partial t'}$$

and then standard methods for the autonomous case can be used with very large time steps.

Main trouble: the linear system to be solved is of a higher dimension, making the algorithms computationally very costly.

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$$i\frac{d}{dt}u = H(t)\,u$$

is equivalent to ($U = (u, u_t) \in \mathbb{C}^{d+1}$)

$$U' = \frac{d}{dt}\left\{ \begin{array}{c} u \\ u_t \end{array} \right\} = \left\{ \begin{array}{c} -iH(u_t)\,u \\ 0 \end{array} \right\} + \left\{ \begin{array}{c} 0 \\ 1 \end{array} \right\} = A(U) + B(U)$$

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$$u_{n+1} = \prod_{j=1}^{m} \mathrm{e}^{-i\,a_j h\, H(t_n + c_j h)}\, u_n,$$

$\{a_j, b_j\}_{j=1}^{m}$ splitting method ($c_j = \sum_{k=1}^{j} b_k$). Efficient methods: 4th-order ($m = 6$); 6th-order ($m = 10$).

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Complex coefficients: $a_j\in\mathbb{C}, b_j\in\mathbb{R}$
4th-order ($m=4$); 6th-order ($m=16$).

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$$\Omega^{[4]} = B_1 + [B_2, B_3], \qquad \text{with} \qquad B_i = h \sum_{j=1}^{K} a_{i,j} A(t_n + c_j \tau)$$

$(\Omega^{[r]} = \Omega + \mathcal{O}(h^{r+1}))$ so that $\Omega^{[4]} u = v_1 + (v_4 - v_5)$ with

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$\Omega^{[6]} u$ involves at least 13 products.

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$c_k \in \mathbb{R}$ are suitable nodes and a_{jk} appropriate coefficients.

$m = 2$: order 4.

$m = 5$: order 6

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$m = 3$: order 5 (with complex coefficients a_{jk}).
$m = 4$: order 6 (with complex coefficients a_{jk}).

$m = 5$: order 6 with one commutator ($[B_{3,1}, B_{3,2}] = \mathcal{O}(h^3)$)

$$u_{n+1} = \mathrm{e}^{B_5}\, \mathrm{e}^{B_4}\, \mathrm{e}^{[B_{3,1},B_{3,2}]}\, \mathrm{e}^{B_2}\, \mathrm{e}^{B_1}\, u_n$$

(real **POSTIVE** coefficients a_{jk}).

The Rosen–Zener model

The Hamiltonian in terms of Pauli matrices is given by

$$H(t) = \frac{1}{2}\omega\sigma_3 + V(t)\sigma_1$$

and in the interaction picture

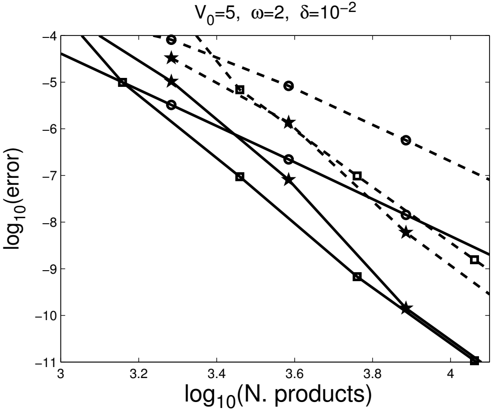
$$H_I(t) = \cos(\omega t)V(t)\,\sigma_1 - \sin(\omega t)V(t)\,\sigma_2 \;\in \mathbb{C}^{2\times 2}$$

A Rosen–Zener model with dissipation of dimension $n = 2k$:

$$H_I(t) = f_1(t)\,\sigma_1 \otimes I_k + f_2(t)\,\sigma_2 \otimes R_k + \delta D_n.$$

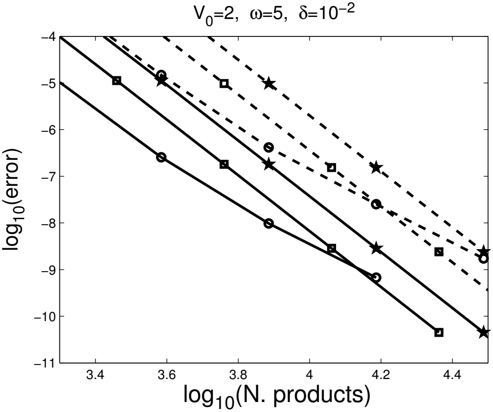
with $D_n = i \times \mathrm{diag}\{-1, -4, \ldots, -n^2\}$, $R_n = \mathrm{tridiag}\{1, 0, 1\}$,
$f_1(t) = \dfrac{V_0\cos(\omega t)}{\cosh(t/T)}$, $\quad f_2(t) = -\dfrac{V_0\sin(\omega t)}{\cosh(t/T)}$, $\quad \delta > 0$,
$T = 1$, $t \in [-5T, 5T]$, $n = 10$.

Example 1:



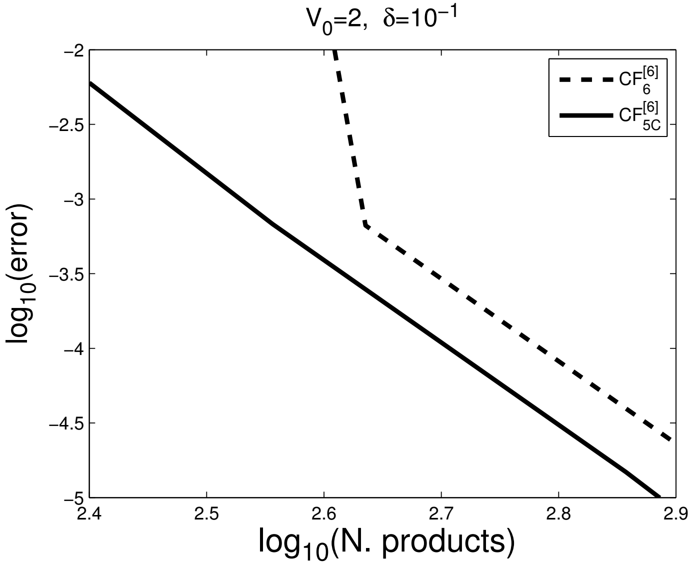
solid lines: 3-exp 5th-order with complex coefs.
dashed lines: 6-exp 6th-order with real coefs.
Taylor of order 4 (circles), 6 (squares) and 8 (stars)

Example 1:



V0=2, ω=5, δ=10−2
−4
−5
−6
−7
−8
−9
−10
−11
3.4
3.6
3.8
4
4.2
4.4
log10(error)
log10(N. products)

Example 1: with dissipation



II:$H(t)$ is a real symmetric matrix

The autonomous case

$$i\,\frac{d}{dt}u = H\,u \quad \Rightarrow \quad u(T) = e^{-i\,T\,H}u(0)$$

where $u \in \mathbb{C}^d$ and $H \in \mathbb{R}^{d\times d}$ is a real and symmetric matrix.

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where $u \in \mathbb{C}^d$ and $H \in \mathbb{R}^{d\times d}$ is a real and symmetric matrix.
Formally, the problem to solve is

$$i\frac{du}{dt} = P^{-1}\begin{pmatrix} E_0 & & & \\ & E_1 & & \\ & & \ddots & \\ & & & E_{d-1} \end{pmatrix} Pu = Hu$$

which is just a set of d harmonic oscillators

Taylor method of order m ($u = q + ip$)

$$\left\{ \begin{array}{c} q_T \\ p_T \end{array} \right\} = \left(\begin{array}{cc} T_1^m & T_2^m \\ -T_2^m & T_1^m \end{array} \right) \left\{ \begin{array}{c} q_0 \\ p_0 \end{array} \right\}$$

$$\frac{T\,\beta}{m} < 0.37$$

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Chebyshev method

$$\left\{ \begin{array}{c} q_C \\ p_C \end{array} \right\} = \left(\begin{array}{cc} C_1^m & C_2^m \\ -C_2^m & C_1^m \end{array} \right) \left\{ \begin{array}{c} q_0 \\ p_0 \end{array} \right\} \qquad \frac{T\,\beta}{m} < 0.90$$

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Symplectic methods

$$\left(\begin{array}{cc} 1 & 0 \\ -b_k y & 1 \end{array} \right) \left(\begin{array}{cc} 1 & a_k y \\ 0 & 1 \end{array} \right) = \left(\begin{array}{cc} 1 & a_k y \\ -b_k y & 1 - a_k b_k y^2 \end{array} \right)$$

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$$K(y) \equiv \prod_{k=1}^{m} \left(\begin{array}{cc} 1 & a_k y \\ -b_k y & 1 - a_k b_k y^2 \end{array} \right) = \left(\begin{array}{cc} K_1^{2m-2} & K_2^{2m-1} \\ K_3^{2m-1} & K_4^{2m} \end{array} \right)$$

$$\left\{ \begin{array}{c} q_S \\ p_S \end{array} \right\} = \left(\begin{array}{cc} K_1^{2m-2} & K_2^{2m-1} \\ K_3^{2m-1} & K_4^{2m} \end{array} \right) \left\{ \begin{array}{c} q_0 \\ p_0 \end{array} \right\} \qquad \frac{T\,\beta}{m} < 2$$

Horner's algorithm for the Taylor method:

$$
\begin{aligned}
&y_0 = u_0 \\
&\textbf{do} \;\; k = 1, m \\
&\quad y_k = u_0 - i \tfrac{T\beta}{m+1-k} \tilde{H} y_{k-1} \\
&\textbf{enddo} \\
&w_T = y_m
\end{aligned}
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Clenshaw algorithm for Chebyshev $(c_k = (-i)^k J_k(T\,\beta))$:

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\begin{aligned}
&d_{m+2} = 0, \qquad d_{m+1} = 0 \\
&\textbf{do} \;\; k = m, 0 \\
&\quad d_k = c_k u_0 + 2\tilde{H}d_{k+1} - d_{k+2} \\
&\textbf{enddo} \\
&w_C \equiv P^C_{m-1}(T\beta\tilde{H})\,u_0 = d_0 - d_2
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\end{array}
$$

Splitting Symplectic methods:

$$
\begin{array}{l}
\textbf{do}\ \ k = 1, m \\
\quad q := q + a_k T\beta\tilde{H}p \\
\quad p := p - b_k T\beta\tilde{H}q \\
\textbf{enddo}
\end{array}
$$

$M_m^{(\theta/m)}$	m	$\beta\tau_{\max}$	y_*/m	$\epsilon(\theta)$	$\mu(\theta)$	$\nu(\theta)$
$M_{10}^{(0.5)}$	10	5	0.63	3.6×10^{-8}	8.7×10^{-11}	9.8×10^{-8}
$M_{10}^{(0.9)}$	10	9	0.94	3.4×10^{-5}	2.9×10^{-5}	1.1×10^{-5}
$M_{20}^{(0.6)}$	20	12	0.79	1.6×10^{-13}	1.4×10^{-13}	5.8×10^{-14}
$M_{20}^{(1)}$	20	20	1.1	4.1×10^{-7}	1.8×10^{-8}	4.8×10^{-7}
$M_{30}^{(0.75)}$	30	22.5	0.84	8.1×10^{-15}	3.3×10^{-16}	1.5×10^{-14}
$M_{30}^{(1)}$	30	30	1.0	4.1×10^{-10}	1.9×10^{-10}	3.1×10^{-10}
$M_{30}^{(1.3)}$	30	39	1.36	2.3×10^{-5}	5.2×10^{-6}	2.2×10^{-5}
$M_{40}^{(1)}$	40	40	1.1	1.8×10^{-12}	4.9×10^{-14}	2.4×10^{-12}
$M_{40}^{(1.2)}$	40	48	1.26	2.1×10^{-8}	2.1×10^{-8}	5.3×10^{-10}
$M_{40}^{(1.4)}$	40	56	1.48	1.48×10^{-5}	4.0×10^{-6}	1.7×10^{-5}
$M_{50}^{(1)}$	50	50	1.07	4.5×10^{-15}	4.5×10^{-15}	2.0×10^{-17}
$M_{50}^{(1.1)}$	50	55	1.13	4.5×10^{-13}	4.2×10^{-13}	4.1×10^{-14}
$M_{50}^{(1.2)}$	50	60	1.26	5.4×10^{-11}	2.7×10^{-11}	3.8×10^{-11}
$M_{50}^{(1.3)a}$	50	65	1.32	1.2×10^{-8}	1.2×10^{-8}	8.3×10^{-10}
$M_{50}^{(1.3)b}$	50	65	1.32	5.9×10^{-7}	9.5×10^{-11}	6.1×10^{-7}
$M_{60}^{(1.1)}$	60	66	1.15	7.2×10^{-15}	7.2×10^{-15}	2.6×10^{-17}
$M_{60}^{(1.2)a}$	60	72	1.3	1.5×10^{-12}	1.1×10^{-12}	8.3×10^{-13}
$M_{60}^{(1.2)b}$	60	72	1.26	4.2×10^{-11}	6.5×10^{-14}	4.6×10^{-11}
$M_{60}^{(1.3)}$	60	78	1.36	1.2×10^{-9}	7.8×10^{-11}	1.2×10^{-9}
$M_{60}^{(1.4)a}$	60	84	1.41	8.4×10^{-8}	2.4×10^{-8}	7.4×10^{-8}
$M_{60}^{(1.4)b}$	60	84	1.46	2.9×10^{-6}	3.7×10^{-9}	2.9×10^{-6}

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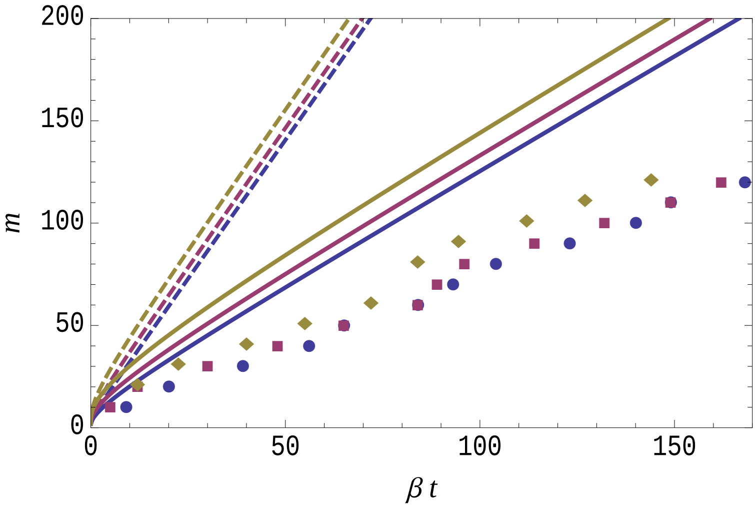


Numerical example 1

(Lubich, Blue book, 2008) To approximate

$$e^{-iH}u_0$$

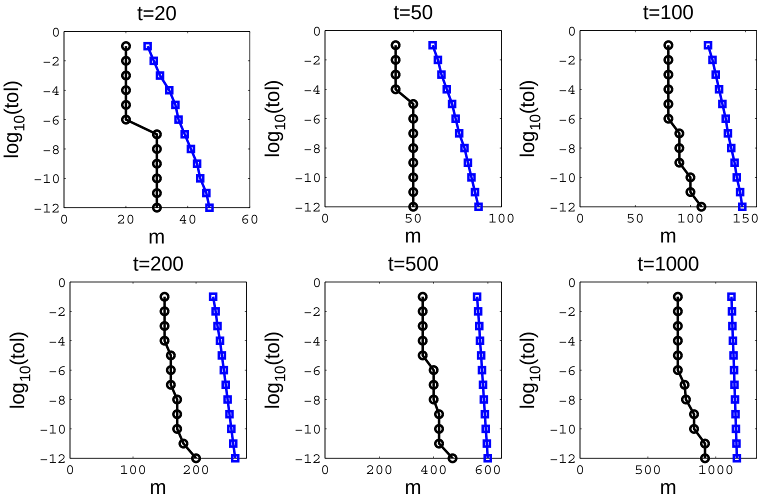
with u_0 a unitary random vector and

$$H = \frac{\lambda}{2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & & \ddots & & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \in \mathbb{R}^{N\times N}, \quad N = 10000$$

$0 \le E_k \le 2\lambda,\ k = 1, 2, \ldots, 10000$
After a shift, $H - \lambda I$, we can take: $T\beta = \lambda = t$
We approximate:

$$e^{-i\,t}e^{-it\hat{H}}u_0, \qquad \hat{H} = (H - t\,I)/t$$

Example:



The Mathematical Problem

$$i\frac{d}{dt}u(t) = H(t)\,u(t), \qquad u(0) = u_0 \in \mathbb{C}^N,$$

It can be written as the $2N$-dimensional real system

$$q' = H(t)p, \qquad p' = -H(t)q.$$

Classical Hamiltonian equations associated to the classical Hamiltonian

$$\mathcal{H}(q,p,t) = \frac{1}{2}p^T H(t)p + \frac{1}{2}q^T H(t)q.$$

Sanz-Serna&Portillo (1996): Time as two dependent variables:

$$\bar{H} = \left(\frac{1}{2}p^T H(p_1)p + p_2\right) + \left(\frac{1}{2}q^T H(q_2)q - q_1\right) = A(P) + B(Q)$$

with $q_1, q_2, p_1, p_2 \in \mathbb{R}$

The Proposed Algorithm

$$q_0 = Re(u_n), \quad p_0 = Im(u_n)$$
$$H_1 = H(t_n + c_1 h), \quad H_2 = H(t_n + c_2 h), \quad H_3 = H(t_n + c_3 h)$$

do $i = 1, m$

$$v = \left(a_{i,1} H_1 + a_{i,2} H_2 + a_{i,3} H_3\right) p_{i-1}$$
$$q_i = q_{i-1} + hv$$
$$v = \left(b_{i,1} H_1 + b_{i,2} H_2 + b_{i,3} H_3\right) q_i$$
$$p_i = p_{i-1} - hv$$

enddo

$$u_{n+1} = q_m + ip_m$$

The system can be written as

$$z' = \begin{pmatrix} 0 & H(t) \\ -H(t) & 0 \end{pmatrix} z = (A(t) + B(t))z$$

where $z = (q, p)^T$ and

$$A(t) = \begin{pmatrix} 0 & H(t) \\ 0 & 0 \end{pmatrix}, \qquad B(t) = \begin{pmatrix} 0 & 0 \\ -H(t) & 0 \end{pmatrix}.$$

The Magnus series expansion allows to write the formal solution in exponential form

$$z(t+h) = e^{\Omega(t,h)} z(t)\,, \qquad \Omega(t,h) = \sum_{k=1}^{\infty} \Omega_k(t,h)$$

Proposed methods

$$z(t+h) \approx \mathrm{e}^{\tilde{A}_{m+1}} \mathrm{e}^{\tilde{B}_m} \mathrm{e}^{\tilde{A}_m} \cdots \mathrm{e}^{\tilde{B}_1} \mathrm{e}^{\tilde{A}_1} z(t)$$

$$\approx \begin{pmatrix} I & \tilde{H}^A_{m+1} \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -\tilde{H}^B_m & I \end{pmatrix} \cdots \begin{pmatrix} I & 0 \\ -\tilde{H}^B_1 & I \end{pmatrix} \begin{pmatrix} I & \tilde{H}^A_1 \\ 0 & I \end{pmatrix} z(t)$$

where

$$\tilde{H}^A_i = h \sum_{j=1}^{k} a_{i,j} H(t + c_j h), \qquad \tilde{H}^B_i = h \sum_{j=1}^{k} b_{i,j} H(t + c_j h),$$

for appropriate coefficients $c_i, a_{i,j}, b_{i,j}$.

SE with Morse Potential and external laser interaction

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2\mu}\frac{\partial^2}{\partial x^2} + V(x) + f(t)x\right)\psi(x,t)$$

with

$$V(x) = D\left(1 - \mathrm{e}^{-\alpha x}\right)^2, \qquad f(t)x = A\cos(\omega t)x$$

$\mu = 1745$, $D = 0.2251$, $\alpha = 1.1741$ *a.u.* (HF molecule in a.u.), $A = 0.011025$ and laser frequency $\omega = 0.01787$.
$x \in [-0.8, 4.32]$, split into $N = 64$ parts and periodic bc.
Initial conditions

$$\phi(x) = \sigma \exp\left(-(\gamma - 1/2)\alpha\, x\right) \exp\left(-\gamma \mathrm{e}^{-\alpha x}\right),$$

$\gamma = 2D/w_0$, $w_0 = \alpha\sqrt{2D/\mu}$ (σ is a normalizing constant).

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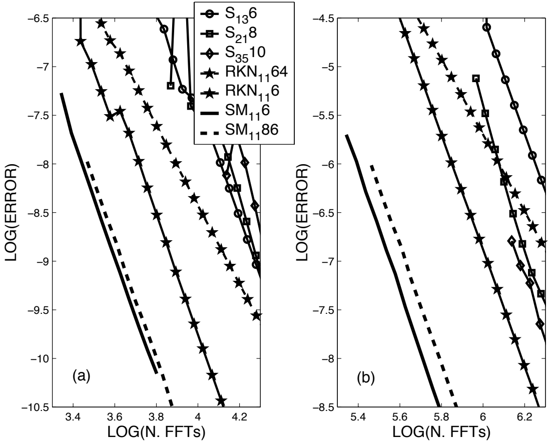
Kormann, Holmgren, and Karlsson, *J. Chem. Phys.* (2008).

Example 1:



S136
S218
S3510
RKN1164
RKN116
SM116
SM1186
LOG(ERROR)
LOG(N. FFTs)
(a)
(b)
−6.5
−7
−7.5
−8
−8.5
−9
−9.5
−10
−10.5
3.4
3.6
3.8
4
4.2
−4.5
−5
−5.5
−6
−6.5
−7
−7.5
−8
−8.5
5.4
5.6
5.8
6
6.2

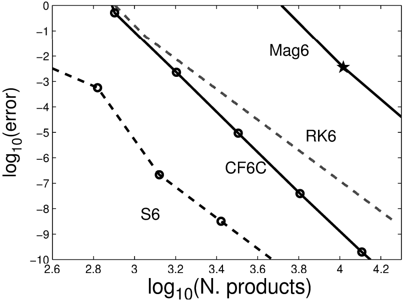
The Rosen–Zener model

$$H(t) = \omega\, \sigma_3 \otimes I_k + f(t)\, \sigma_2 \otimes R_k$$

$R_n = \text{tridiag}\{1, 0, 1\}$,

$$f(t) = \frac{V_0}{\cosh(t/T)}, \quad V_0 = 10, \quad \omega = 10$$

$T = 1,\ t \in [-5T, 5T],\ n = 10.$



0
−1
−2
−3
−4
−5
−6
−7
−8
−9
−10
2.6
2.8
3
3.2
3.4
3.6
3.8
4
4.2
log10(error)
log10(N. products)
Mag6
RK6
CF6C
S6

Diffusion-advection-reaction equation

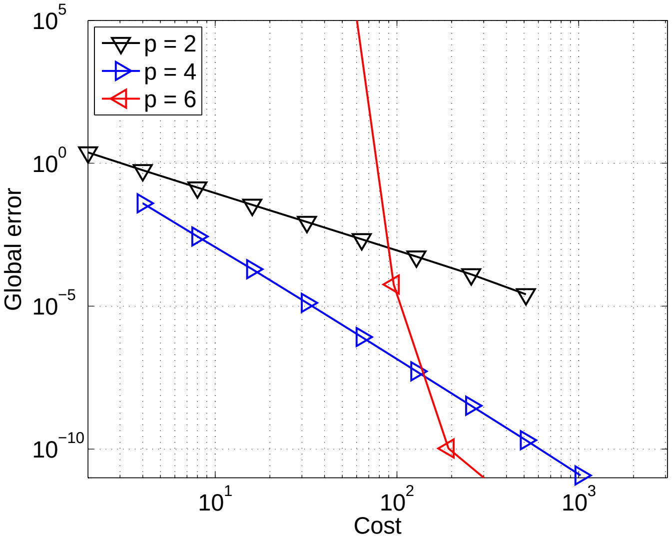
We consider the equation

$$\partial_t u(x,t) = A(x,t)\,u(x,t) = \left(\alpha(x,t)\,\partial_{xx} + \beta(x,t)\,\partial_x + \gamma(x,t)\right) u(x,t)$$

$$\alpha(x,t) = e^{-\cos x}\,(\sin t)^2\,, \qquad \gamma(x,t) = e^{\sin x}\,\left(1 + e^{-t}\right),$$

subject to the initial condition $u(x,0) = \sin(2x)$ and periodic boundary conditions on the spatial interval $\Omega = [0, 2\pi]$.
Number of grid points $M = 100$

Example 2:



Other Applications

For solving the nonlinear perturbed problem

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

with $|\varepsilon| \ll 1$ it can be very useful to have a good integrator for the linear part.

H real and constant

- SB, F. Casas, and A. Murua, J. Comput. Phys. (2015).
- SB, F. Casas and A. Murua, Found. Comp. Math. (2008).
- SB, F. Casas, and A. Murua, SIAM J. Sci. Comput. (2011).

H real and *t*-dependent

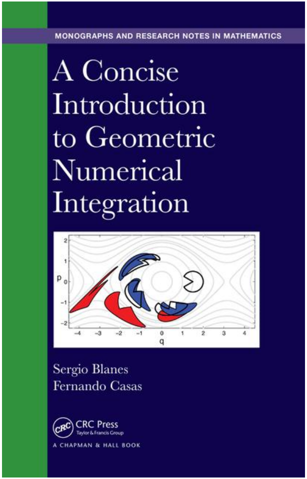
- SB, F. Casas, and A. Murua, Work in progress.
- SB, F. Casas and A. Murua, Int. J. Comp. Math. (2007).
- SB, F. Casas, and A. Murua, RACSAM (2012).

H: *t*-dependent, complex and/or dissipative

- SB, F. Casas, and M. Thalhammer, Work in progress.

Group webpage: http://www.gicas.uji.es

SB and F. Casas, A Concise Introduction to Geometric Numerical Integration, Chapman and Hall/CRC. To appear in April 2016.



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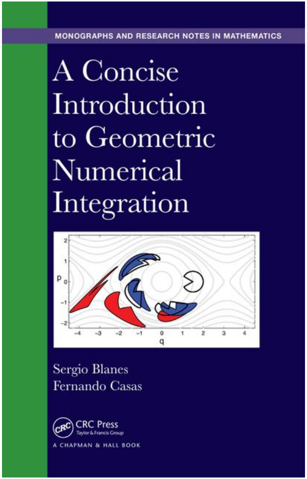

Thank You