Splitting methods for explicitly time-dependent systems

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Workshop in honor to the 60th birthday of Siu A. Chin
"High-order actions and their applications in many-body, few-body, classical problems"

Barcelona, March 24-26, 2009

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Introduction

We analyze splitting methods for separable and explicitly time-dependent systems

$$\frac{d}{dt}\mathrm{x} = \mathrm{f}_A(\mathrm{x}, t) + \mathrm{f}_B(\mathrm{x}, t)$$

where we assume that

$$\frac{d}{dt}\mathrm{x} = \mathrm{f}_A(\mathrm{x}) \qquad \frac{d}{dt}\mathrm{x} = \mathrm{f}_B(\mathrm{x})$$

are easy to solve and we can use highly efficient splitting methods which take into account the particular structure of the vector fields

Introduction

For the general problem

$$\frac{d}{dt}\mathrm{x} = \mathrm{f}(\mathrm{x}, t)$$

most books simply recommend to take the time as a new coordinate

$$\frac{d}{dt}\mathrm{x} = \mathrm{f}(\mathrm{x}, x_t)$$
$$\frac{d}{dt}x_t = 1$$

or equivalently

$$\frac{d}{dt}\mathrm{y} = \mathbf{F}(\mathrm{y})$$

with $\mathrm{y} = (\mathrm{x}, x_t)^T$, and then to use the methods for the autonomous problems. However, in many cases, the structure of the vector field $\mathbf{F}(\mathrm{y})$ differs from the structure of $\mathrm{f}(\mathrm{x})$ and this forces to use less efficient numerical methods.

Example: the linear problem

$$\frac{d}{dt}\mathrm{x} = A(t)\mathrm{x}$$

$$\begin{aligned} \tfrac{d}{dt}\mathrm{x} &= A(x_t)\mathrm{x} \\ \tfrac{d}{dt}x_t &= 1 \end{aligned}$$

but there exist other methods which consider the time differently and lead into more efficient methods for an important number of problems.

In the separable case, the previous procedure generalizes introducing two new coordinates for the time

$$\begin{aligned} \tfrac{d}{dt}\mathrm{x} &= \mathrm{f}_A(\mathrm{x}, x_1) + \mathrm{f}_B(\mathrm{x}, x_2) \\ \tfrac{d}{dt}x_1 &= 1 \\ \tfrac{d}{dt}x_2 &= 1 \end{aligned}$$

with the splitting

$$\left\{ \begin{aligned} \tfrac{d}{dt}\mathrm{x} &= \mathrm{f}_A(\mathrm{x}, x_1) \\ \tfrac{d}{dt}x_1 &= 0 \\ \tfrac{d}{dt}x_2 &= 1 \end{aligned} \right. \qquad \left\{ \begin{aligned} \tfrac{d}{dt}\mathrm{x} &= \mathrm{f}_B(\mathrm{x}, x_2) \\ \tfrac{d}{dt}x_1 &= 1 \\ \tfrac{d}{dt}x_2 &= 0 \end{aligned} \right.$$

In the Hamiltonian formalism, for the time-dependent Hamiltonian

$$H(\mathbf{q},\mathbf{p},t) = T(\mathbf{p},t) + V(\mathbf{q},t)$$

this is equivalent to introduce two new coordinates and associated momenta in the following way

$$H = \Big(T(\mathbf{p},q_1) + p_2\Big) + \Big(V(\mathbf{q},q_2) + p_1\Big)$$

Then, one has to solve a general separable system

$$\frac{d}{dt}\mathbf{y} = \mathbf{F}_A(\mathbf{y}) + \mathbf{F}_B(\mathbf{y})$$

with $\quad \mathbf{y} = (\mathbf{x}, x_1, x_2)^T$

We will show different techniques which consider the time as a special parameter and lead into more efficient algorithms.

Splitting Methods

Consider the linear time dependent SE

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

It is separable in its kinetic and potential parts. The solution of the discretised equation is given by

$$i\frac{d}{dt}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t) \quad \Rightarrow \quad \mathbf{c}(t) = e^{-it\mathbf{H}}\mathbf{c}(0)$$

where $\mathbf{c} = (c_1, \ldots, c_N)^T \in \mathbb{C}^N$ and $\mathbf{H} = \mathbf{T} + \mathbf{V} \in \mathbb{R}^{N\times N}$ Hermitian matrix.
Fourier methods are frequently used

$$\begin{array}{ll} (\mathbf{V}\mathbf{c})_i = V(x_i)c_i & N \text{ products} \\ \mathbf{T}\mathbf{c} = \mathcal{F}^{-1}\mathbf{D}_T\,\mathcal{F}\mathbf{c} & \mathcal{O}(N\log N) \text{ operations} \end{array}$$

$\mathcal{F}$ is the fast Fourier transform (FFT)

Consider the Strang-splitting or leap-frog second order method

$$U_2(\tau) \equiv e^{\tau/2\mathbf{V}}\, e^{\tau\mathbf{T}}\, e^{\tau/2\mathbf{V}}$$

Notice that

$$\left(e^{\tau\mathbf{V}}\mathbf{c}\right)_i = e^{\tau V(x_i)} c_i$$

the exponentials are computed only once and are stored at the beginning.

Similarly, for the kinetic part we have

$$e^{\tau\mathbf{T}}\mathbf{c} = \mathcal{F}^{-1} e^{\tau\mathbf{D}_T} \mathcal{F}\mathbf{c}$$

$$[\mathbf{V},[\mathbf{V},[\mathbf{V},\mathbf{T}]]] = \mathbf{0}$$

Consider $\mathbf{c} = \mathbf{q} + i\mathbf{p}$ then $$i\frac{d}{dt}(\mathbf{q} + i\mathbf{p}) = \mathbf{H}(\mathbf{q} + i\mathbf{p})$$

Hamiltonian system: $\mathcal{H} = \frac{1}{2}\mathbf{p}^T\mathbf{H}\mathbf{p} + \frac{1}{2}\mathbf{q}^T\mathbf{H}\mathbf{q}$

$$\frac{d}{dt}\left\{ \begin{array}{c} \mathbf{q} \\ \mathbf{p} \end{array} \right\} = \left(\begin{array}{cc} 0 & \mathbf{H} \\ -\mathbf{H} & 0 \end{array} \right) \left\{ \begin{array}{c} \mathbf{q} \\ \mathbf{p} \end{array} \right\}$$

with formal solution

$$\mathbf{O}(t) = \left(\begin{array}{cc} \cos(t\mathbf{H}) & \sin(t\mathbf{H}) \\ -\sin(t\mathbf{H}) & \cos(t\mathbf{H}) \end{array} \right)$$

It is an orthogonal and symplectic operator.

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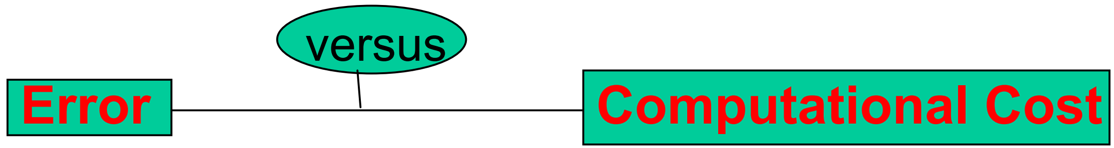
Taking z=(q,p), then z'=(A+B)z

Notice that $[\mathrm{A}, [\mathrm{A}, [\mathrm{A}, \mathrm{B}]]] = [\mathrm{B}, [\mathrm{B}, [\mathrm{B}, \mathrm{A}]]] = 0$

Efficiency of a Method



It is possible to improve the efficiency if:

- $\|B\| \ll \|A\|$

- $[B,[B,[B,A]]] = 0$

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- $[B,[B,A]]$ easy to compute (mod. pot.)

- Using the Processing Technique

$$\mathbf{U}_n = \mathbf{U}_P \mathbf{U}_K \mathbf{U}_P^{-1} \quad \Longrightarrow \quad \mathbf{U}_n^p = \mathbf{U}_P \mathbf{U}_K^p \mathbf{U}_P^{-1}$$

Higher Orders

The well known fourth-order composition scheme

$$\mathrm{U}_4(h) = \mathrm{U}_2(\alpha_1 h)\mathrm{U}_2(\alpha_0 h)\mathrm{U}_2(\alpha_1 h)$$

with

$$\alpha_1 = \frac{1}{2 - 2^{1/3}}, \quad \alpha_0 = 1 - 2\alpha_1$$

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Or in general

$$\mathbf{U}_{2n+2}(h) = \mathbf{U}_{2n}^p(\alpha_1 h)\mathbf{U}_{2n}(\alpha_0 h)\mathbf{U}_{2n}^p(\alpha_1 h)$$

with

$$\alpha_1 = \frac{1}{2p - (2p)^{1/(2n+1)}}, \quad \alpha_0 = 1 - 2\alpha_1$$

-Creutz-Gocksh(89)
-Suzuki(90)
-Yoshida(90)

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Excellent trick!!

In practice, **they show low performance!!**

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Order	4	6	8	10
	3- For-Ru(89)	**7**-Yoshida(90)	**15**-Yoshida(90)	**31**-Suz-Um(93)
	Yos(90),etc.	**9**-McL(95)	Suz-Um(93)	**31-33**-Ka-Li(97)
	5-Suz(90)	Kahan-Li(97)	**15-17**-McL(95)	**33**-Tsitouras(00)
	McL(95)	**11-13**-Sof-Spa(05)	Kahan-Li(97)	**31-35**-Wanner(02)
			19-21-Sof-Spa(05)	**31-35**-Sof-Spa(05)
			24SS-Ca-SS(93)	

Processed				
	P**3-17**-McL(02)	P**5-15**	P**9-19**	P**15-25**
		B-Casas-Murua(06)		

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$$\begin{aligned} \mathbf{U}_n(h) &= e^{hb_k\mathbf{B}}\, e^{ha_k\mathbf{A}} \;\ldots\; e^{hb_1\mathbf{B}}\, e^{ha_1\mathbf{A}} \\ &= \Phi_1^*(d_k h)\Phi_1(c_k h) \;\cdots\; \Phi_1^*(d_1 h)\Phi_1(c_1 h) \end{aligned}$$

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$$\mathbf{U}_n(h) = e^{hb_k\mathbf{H}_0}\, e^{\epsilon ha_k\mathbf{H}_1} \;\ldots\; e^{hb_1\mathbf{H}_0}\, e^{\epsilon ha_1\mathbf{H}_1} \qquad \|\epsilon\mathbf{H}_1\| \ll \|\mathbf{H}_0\|$$

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$$\mathbf{U}_n = \mathbf{U}_P \mathbf{U}_K \mathbf{U}_P^{-1} \quad \Longrightarrow \quad \mathbf{U}_n^p = \mathbf{U}_P \mathbf{U}_K^p \mathbf{U}_P^{-1}$$

Let us consider again the linear time dependent SE

$$i\frac{d}{dt}\mathbf{c}(t) = \mathbf{H}\mathbf{c}(t) \quad \Rightarrow \quad \mathbf{c}(t) = e^{-it\mathbf{H}}\mathbf{c}(0)$$

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Order	4	6	8	10	12
	4,6	**6**	**8**	**10**	**12**
			Gray-Manolopoulos(96)		
11-29		**11**	**11**	**17**	B-Casas-Murua(08)

Processed				
	P**3,4**	P**3,4**	P**4-5**	McL-Gray(97)

P**2-40** **orders: 2-20** B-Casas-Murua(06)

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We have built splitting methods for the harmonic oscillator!!!

$$\frac{d}{dt}\left\{ \begin{array}{c} q \\ p \end{array} \right\} = \Bigg[\underbrace{\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}}_{A} + \underbrace{\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}}_{B} \Bigg] \left\{ \begin{array}{c} q \\ p \end{array} \right\}$$

Exact solution (ortogonal and symplectic)

$$O(t) = \begin{pmatrix} \cos(t) & \sin(t) \\ -\sin(t) & \cos(t) \end{pmatrix}$$

We consider the composition

$$M(h) = \prod_{i=1}^{m} e^{ha_i A}\, e^{hb_i B}$$

Notice that

$$e^{hA}\, e^{hB} = \begin{pmatrix} 1 & h \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -h & 1 \end{pmatrix} = \begin{pmatrix} 1 - h^2 & h \\ -h & 1 \end{pmatrix}$$

Schrödinger equation with a Morse potential

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

with

$$V(x) = D(1 - e^{-\alpha x})^2$$

$$\mu = 1745,\ D = 0.2251,\ \alpha = 1.1741$$

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Initial conditions

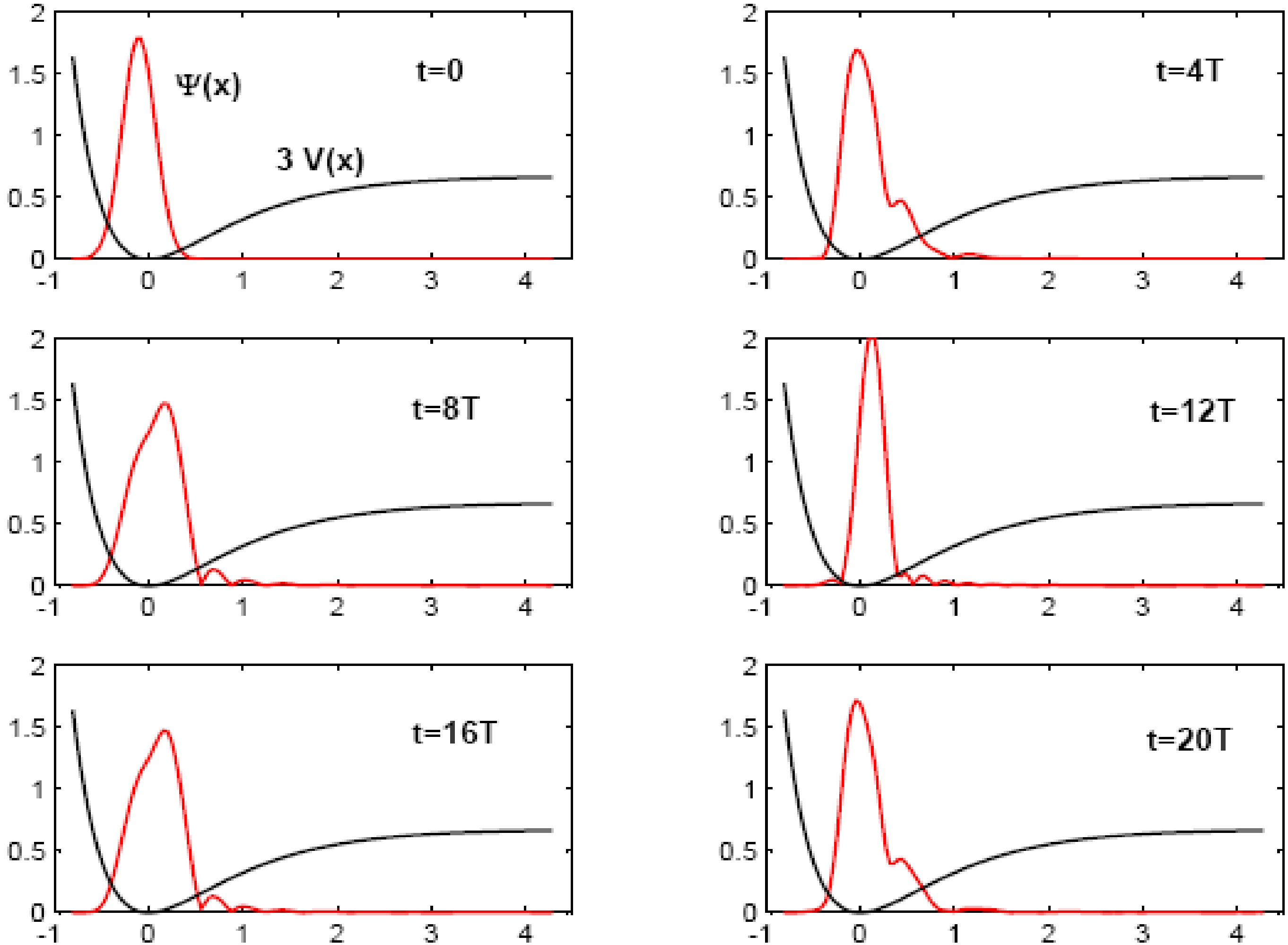
$$\psi(x,t) = \rho \exp\Big(-\beta(x-\bar{x})^2\Big)$$

$$\beta = \sqrt{D\mu\alpha^2/2},\ \bar{x} = -0.1 \quad (\rho \text{ norm. const.})$$

$$t \in [0, 20\,T] \quad \text{with} \quad T = 2\pi/\Big(\alpha\sqrt{2D/\mu}\Big)$$

$$x \in [-0.8, 4.32], \text{ split into } N = 128 \text{ parts}$$

Gaussian wave fuction in a Morse potential



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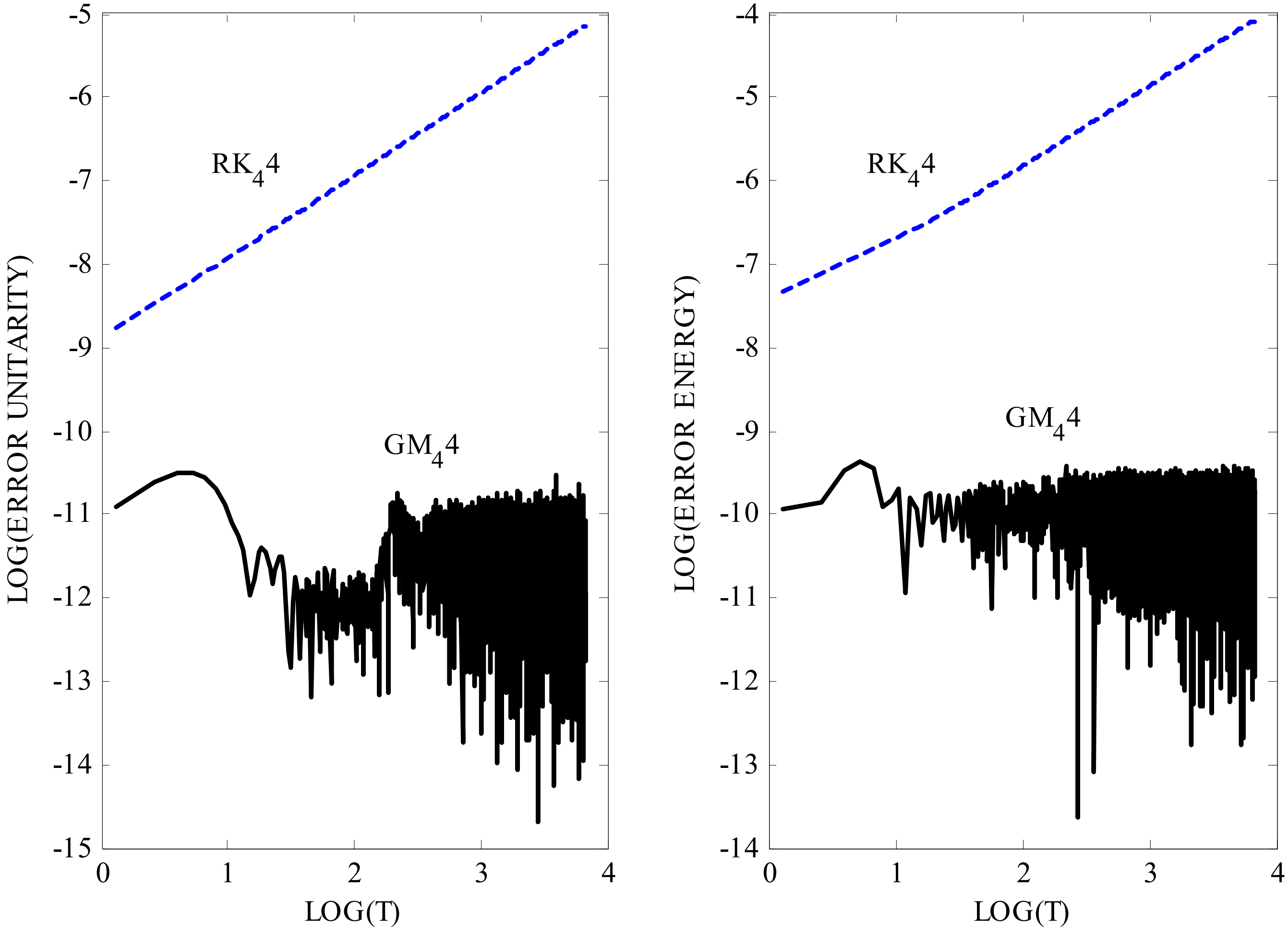

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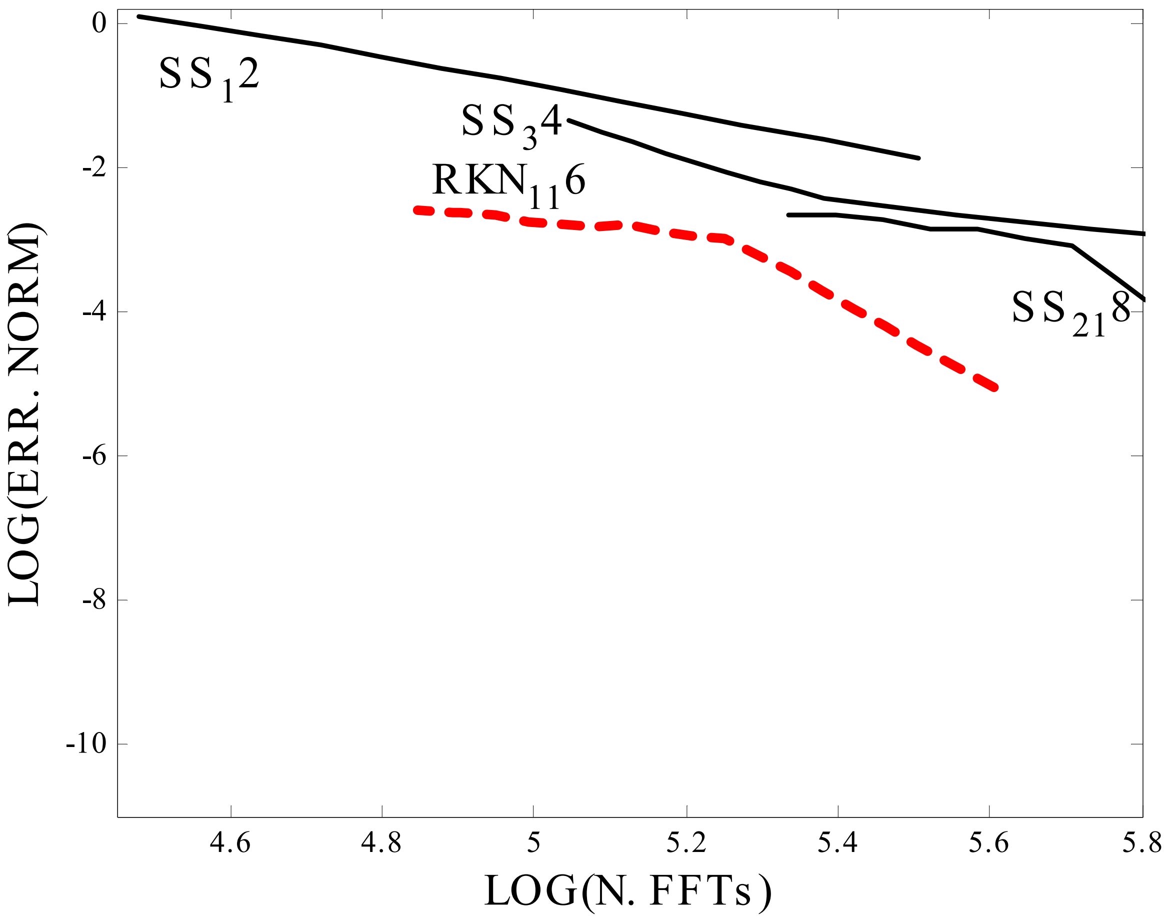

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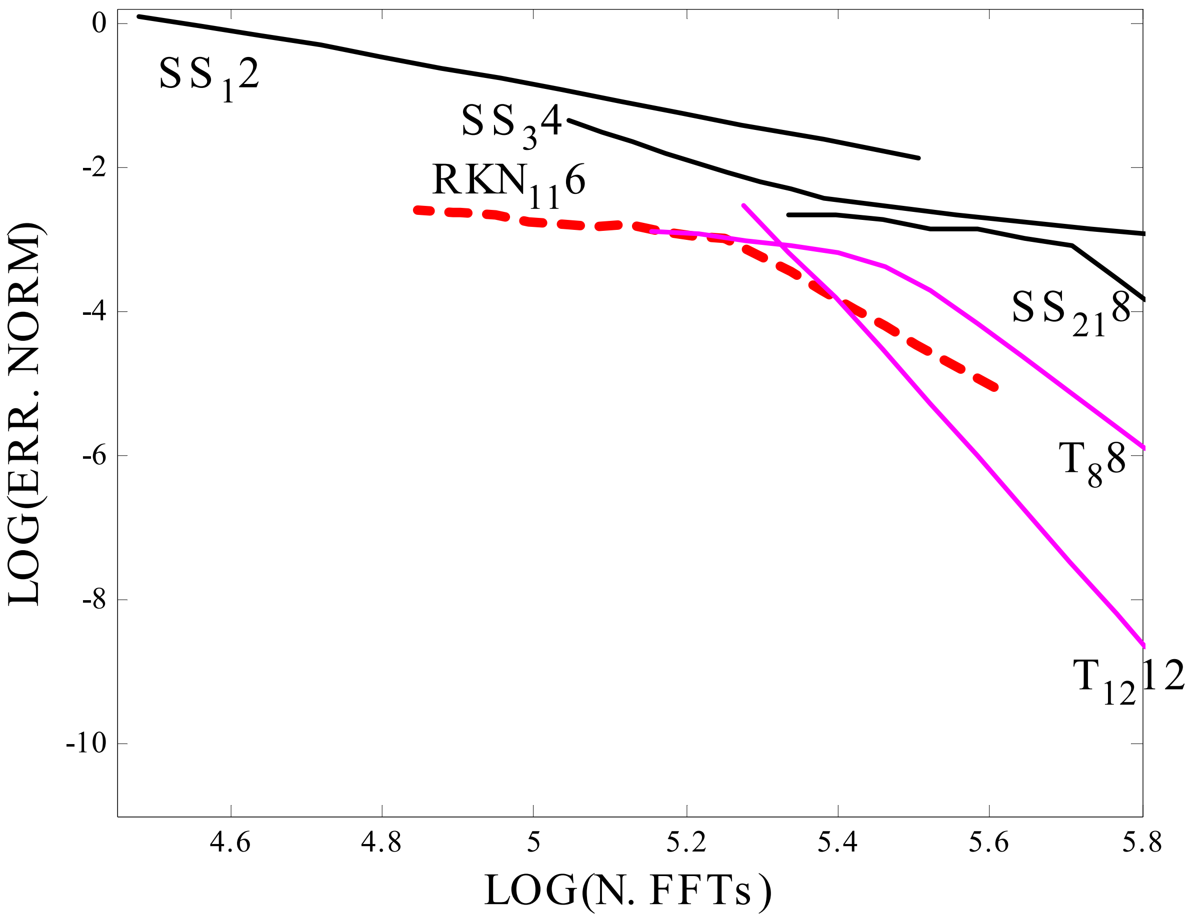

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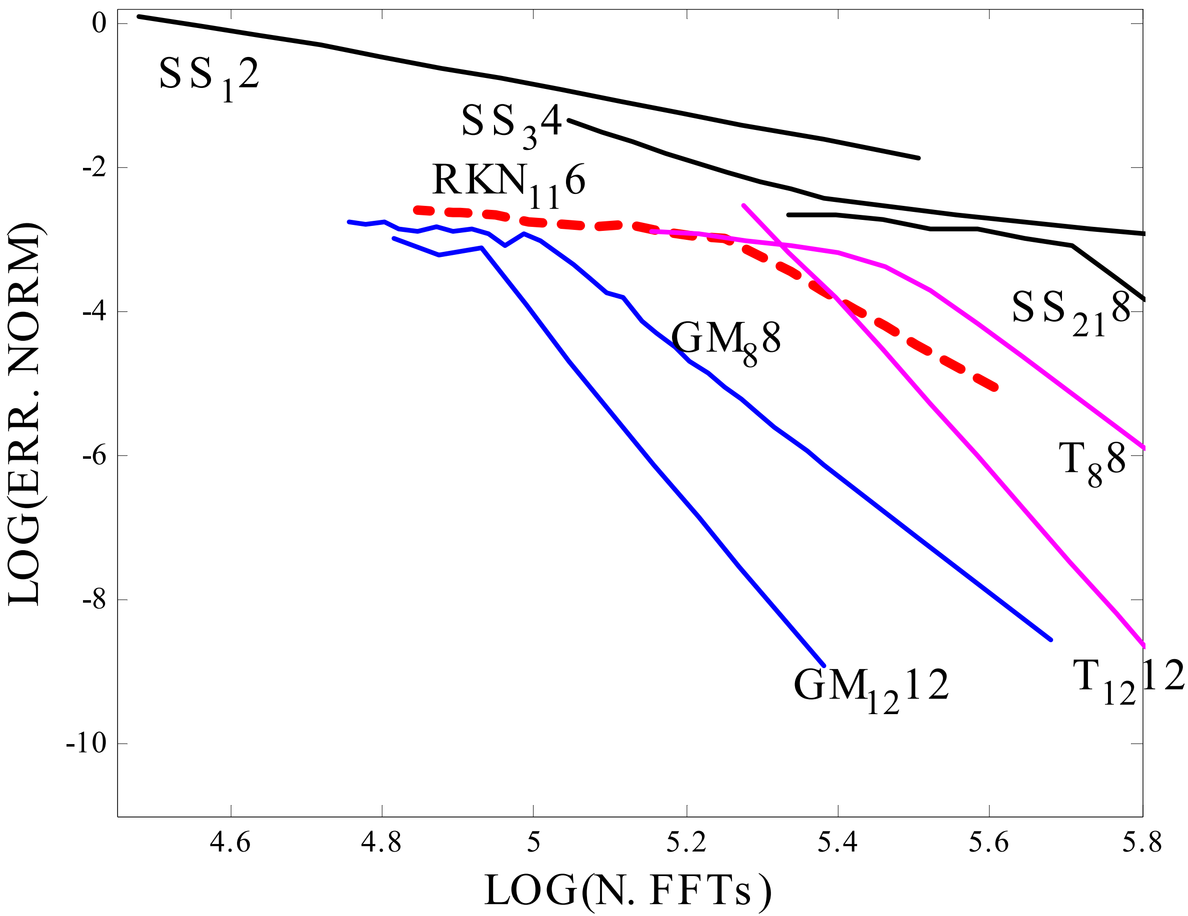

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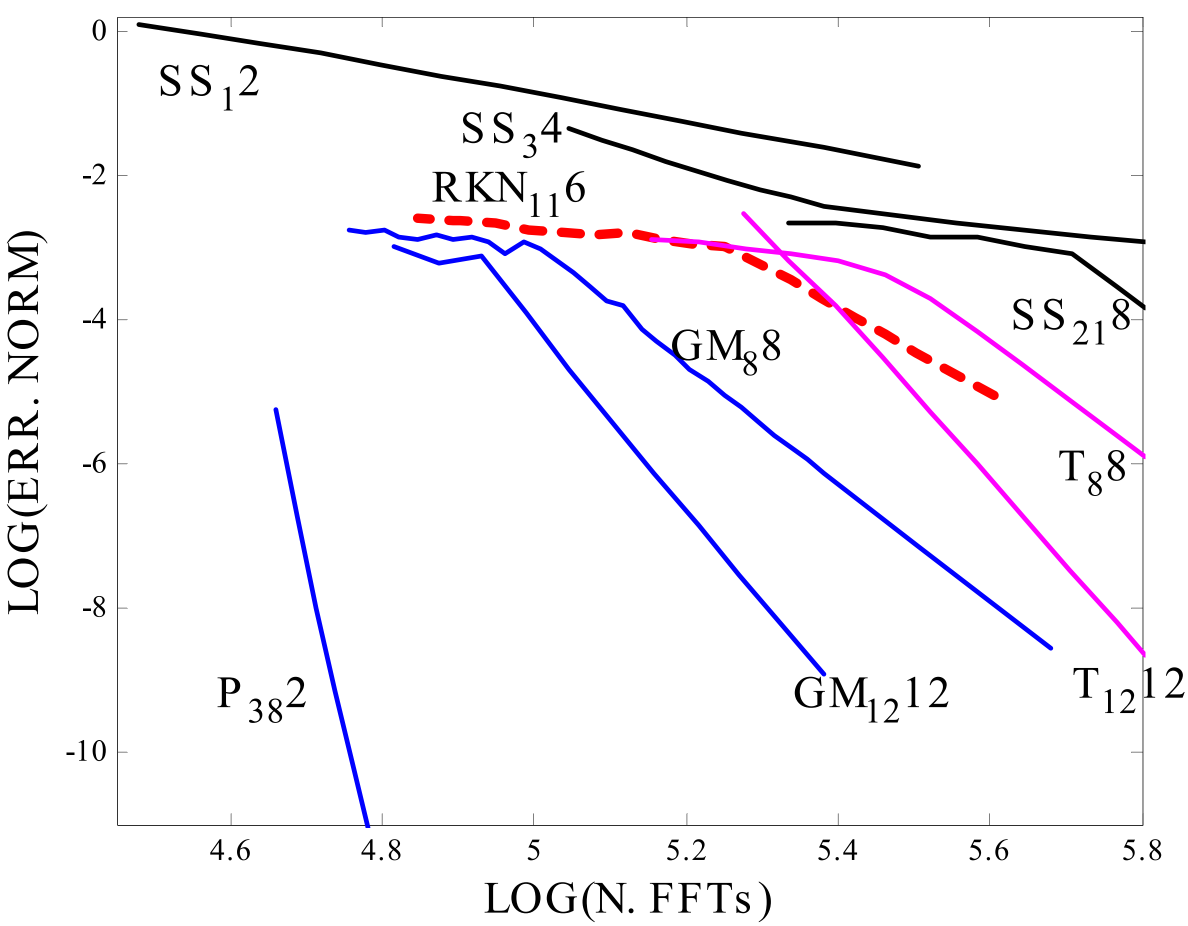

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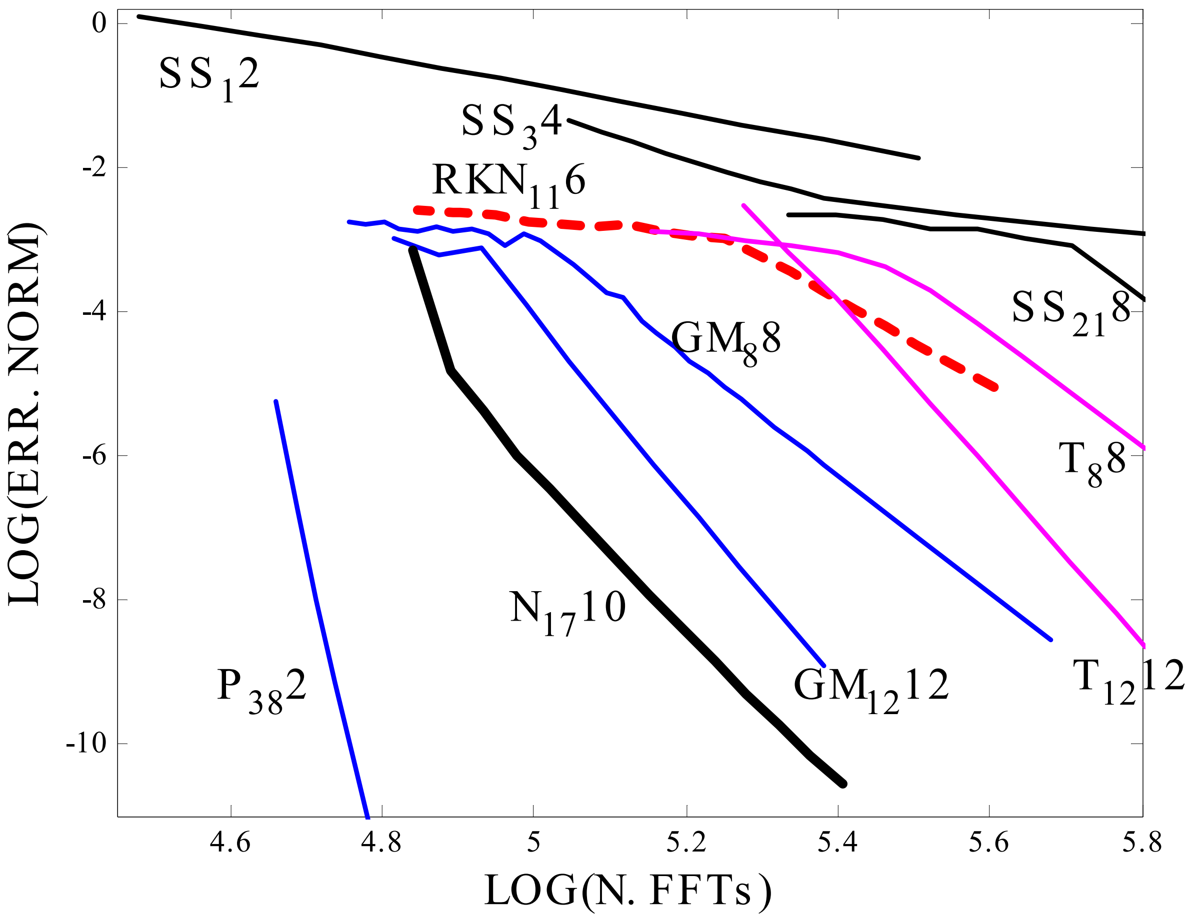


Applications to other Problems

To numerically solve the linear time dependent system

$$x' = M(t)y, \qquad y' = -N(t)x$$

and the solution can not be written in a closed form

The simplest solution is to convert the system into autonomous

$$\begin{aligned} x' &= M(y_t)y & \qquad y' &= -N(x_t)x \\ x_t' &= 1 & \qquad y_t' &= 1 \end{aligned}$$

where $x_t, y_t \in \mathbb{R}$ The system is no longer linear and the most efficient methods can not be used

We consider **appropriate time averages** to approximate the solution up to a given order in the time step. This allows us to use the previous techniques developed for splitting methods

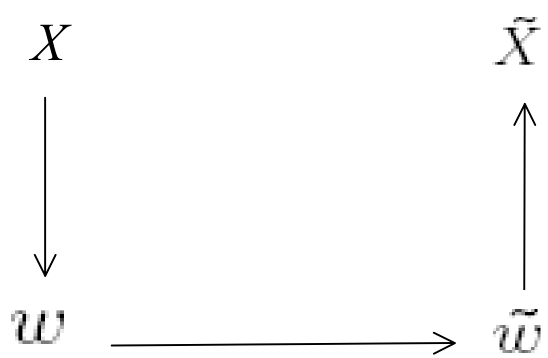
Lie Group Methods

Many differential equations can be written in the following matrix form

$$\frac{dX}{dt} = A(t, X)X$$

If $X(0) \in G$, and $A : \mathbb{R} \times G \longrightarrow g$ then the solution remains in the group.

Consider $\Phi : g \to G$, then write the solution as $X = \Phi(w)$ and look for the DE for w. To preserve the Lie algebra structure is easier than the Lie group. We get an approximation $\tilde{w}$ in the Lie algebra and then $\tilde{X} = \Phi(\tilde{w}) \in G$



Linear non-autonomous systems

$$\frac{dX}{dt} = A(t)X, \qquad X(0) = I$$

with $A(t) \in \mathbb{R}^{d\times d}$

If $A(t)$ is		then X is
skew-hermitic	$\longrightarrow$	unitary
skew-symmetric	$\longrightarrow$	orthogonal
$\mathrm{Tr}(A) = 0$	$\longrightarrow$	$\det X = 1$
$A = JS$	$\longrightarrow$	symplectic
	$\vdots$	

$X(t) \in$ Lie group G if $A(t) \in$ Lie algebra g

$$
\begin{aligned}
X(h) &= e^{\Omega(h)} X_0 && \text{Magnus} \\
&= e^{F_1(h)} e^{F_2(h)} \ldots X_0 && \text{Fer} \\
&= e^{S_1(h)} e^{S_2(h)} \ldots e^{S_2(h)} e^{S_1(h)} X_0 && \text{Sym. Fer} \\
&= \left(I - \frac{1}{2} C(h)\right)^{-1} \left(I + \frac{1}{2} C(h)\right) X_0 && \text{Cayley} \\
&\simeq e^{c_1 h A(d_1 h)} \ldots e^{c_m h A(d_m h)} X_0 && \text{Splitting}
\end{aligned}
$$

This theory allows us to build relatively simple methods at different orders:

A **second order method** is given by:

$$X_{n+1} = \exp\left(\frac{h}{2}A_{1/2}\right)X_n$$

with $A_{1/2} = A(t_n + \frac{h}{2})$

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A **fourth order method** is given by:

$$X_{n+1} = \exp\left(\frac{h}{2}(A_1 + A_2) - h^2\frac{\sqrt{3}}{12}[A_1, A_2]\right)X_n$$

with $A_i = A(t_n + c_i h)$ and $c_{1,2} = \frac{1}{2} \mp \frac{\sqrt{3}}{6}$

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Methods using different quadratures and higher order methods with a moderate number of commutators also exist.

Applications to other Problems

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We consider **appropriate time averages** to approximate the solution up to a given order in the time step. This allows us to use the previous techniques developed for splitting methods

Let us consider $z = (x, y)^T$ then

$$z' = \Big(A(t) + B(t)\Big) z$$

with

$$A(t) = \begin{pmatrix} 0 & M(t) \\ 0 & 0 \end{pmatrix}, \quad B(t) = \begin{pmatrix} 0 & 0 \\ -N(t) & 0 \end{pmatrix}$$

We approximate the solution by the composition

$$K(t,h) = e^{A_m(t,h)} e^{B_m(t,h)} \cdots e^{A_1(t,h)} e^{B_1(t,h)}$$
$$= \begin{pmatrix} I & M_m \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -N_m & I \end{pmatrix} \cdots \begin{pmatrix} I & M_1 \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -N_1 & I \end{pmatrix}$$

with the averages

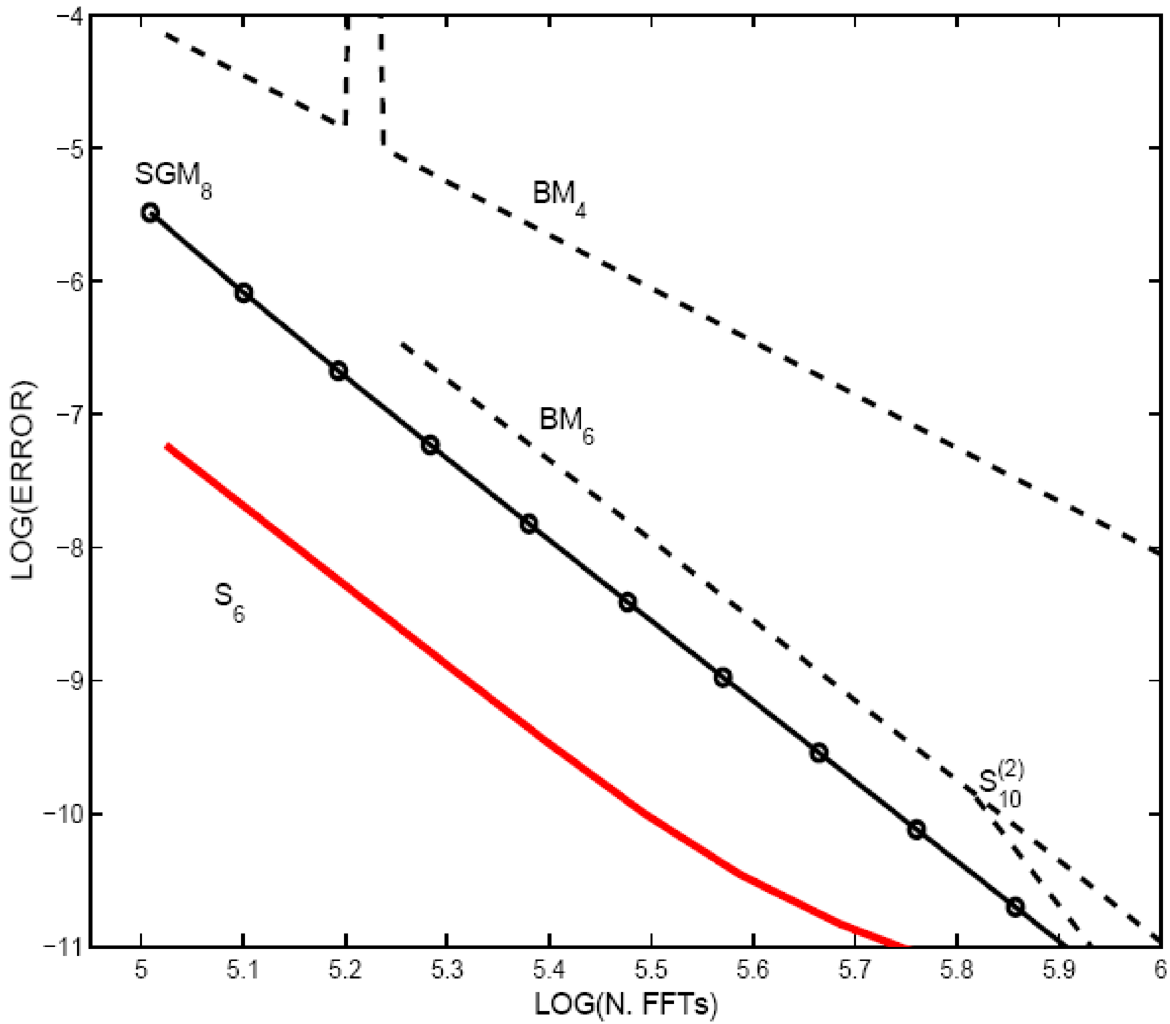
$$M_i = h \sum_{j=1}^{k} \rho_{ij} M(t + c_j h), \quad N_i = h \sum_{j=1}^{k} \sigma_{ij} N(t + c_j h)$$

Gaussian wave fuction in a Morse potential

with laser field $V_I(x,t) = A\cos(\omega t)x$

$A = 0{,}011025$

$w = 0{,}01787$



Second Example: Let us consider the classical Hamiltonian

$$H(\mathbf{q},\mathbf{p},t) = H_0(\mathbf{q},\mathbf{p},t) + H_1(\mathbf{q},t)$$

such that $H_0(\mathbf{q},\mathbf{p},t)$ is solvable if the time is frozen and the kinetic part is quadratic in momentum, and $H_1(\mathbf{q},t)$ is a small perturbation.

This is the case, e.g. if we take

$$V(\mathbf{q},t) = V_0(\mathbf{q},t) + V_1(\mathbf{q},t)$$

where V_0 is the linear part and V_1 is the non-linear part so we split

$$H(\mathbf{q},\mathbf{p},t) = \Big(T(\mathbf{p}) + V_0(\mathbf{q},t)\Big) + V_1(\mathbf{q},t)$$

If the time is frozen

$$H(\mathbf{q},\mathbf{p},t) = \Big(T(\mathbf{p}) + V_0(\mathbf{q})\Big) + V_1(\mathbf{q})$$

we can use very efficient splitting methods:

Nyström + [V,[V,T]] + near-integrable + processing

The standard procedure to consider the time as a new parameter do not allow to use many of these advantages, and then one has to use less efficient methods

A procedure which allows to use all these tools is to treat the time as follows

$$H(\mathbf{q},\mathbf{p},t) = \Big(T(\mathbf{p}) + V_0(\mathbf{q},q_t) + p_t\Big) + V_1(\mathbf{q},q_t)$$

This splitting requires to solve accurately the linear systems

$$H(\mathbf{q},\mathbf{p},t) = T(\mathbf{p}) + V_0(\mathbf{q},q_t) + p_t$$

which is equivalent to

$$H(\mathbf{q},\mathbf{p},t) = T(\mathbf{p}) + V_0(\mathbf{q},t)$$

And

$$H(\mathbf{q},\mathbf{p},t) = V_1(\mathbf{q},q_t)$$

but, with the time frozen

Numerical Example: Let us consider the Hamiltonian

$$H(q,p,t) = \left(\frac{1}{2}p^2 + \frac{1}{2}f(t)q^2\right) + \varepsilon \sum_{j=1}^{k} \cos(q - \omega_j t)$$

It describes the motion of a charged particle in a time-dependent magnetic field perturbed by k electrostatic plane waves, each with the same wavenumber and amplitude, but with different temporal frequencies ω_j

To solve accurately the linear system (e.g. with a Magnus integrator)

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

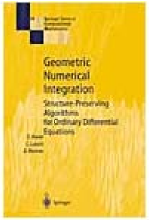
and the frozen Hamiltonian, which depends only on coordinates

$$H(q,p,t) = \varepsilon \sum_{j=1}^{k} \cos(q - \omega_j q_t)$$

Conclusions

- Splitting methods are powerful tools for numerically solving the separable systems
- If the system is explicitly time-dependent, splitting methods can also be used
- To consider the time as a new coordinate in the standard way can not be the most appropriate procedure
- If the time is treated properly, we can take profit of the advantage of splitting methods taylored for problems with particular structure

Basic References



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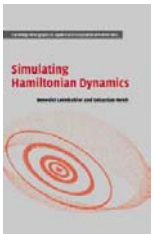

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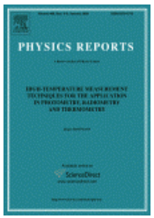

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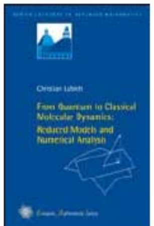

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Splitting methods for explicitly time-dependent systems

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Workshop in honor to the 60th birthday of Siu A. Chin
"High-order actions and their applications in many-body, few-body, classical problems"

Barcelona, March 24-26, 2009

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