Splitting methods for autonomous and non-autonomous perturbed systems

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Goal: The numerical integration of the IVP

$$x' = f(x,t), \qquad x(0) = x_0$$

where $f(x,t)$ is a perturbation of an exactly solvable problem (this also includes some evolutionary PDEs).

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Numerical Integration of Differential Equations

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In the past, researchers were looking for few numerical methods to solve most problems, i.e. to build a black box with a few number of methods implemented.

Soon, it was clear that this was too optimistic due to the huge variety of problems of very different nature, and it was started to look for methods tailored for different classes of problems

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- Multistep methods
- Extrapolation methods
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- Symplectic Integrators
- Lie group methods
- Volume-preserving methods
- Variational integrators
- etc.

The numerical Solution of particular problems

The development of computers allowed to researchers in physics, chemistry, engineering, etc. to study more challenging problems from the computational point of view.

Most of these problems can not be solved by the computer just by using <u>brute force</u> or buying <u>expensive computers</u>. The actual economical situation invites us to develop tailored methods for different classes of problems.

Example of a particular perturbed problem

- The numerical integration of the whole Solar System
- for 60 Myrs
- Backward in time
- to very high accuracy

This problem comes from a research collaboration between geologists and astronomers (talk by A. Farrés).

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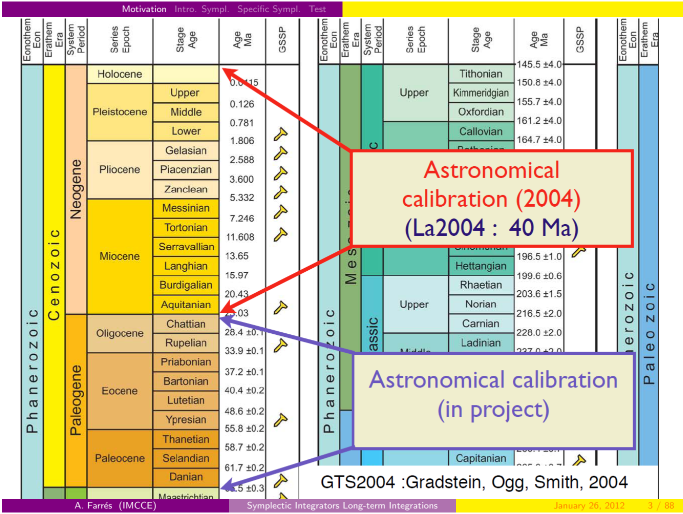
Actual methods (already tailored for this problem) allowed for a faithful integration over 40 Myrs, with good agreement with observations by geologists.

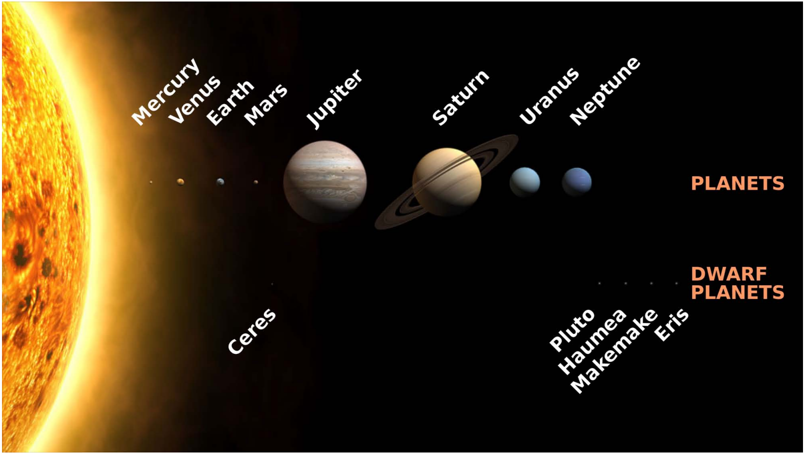
Question: How to develop new methods with better performance than the existing ones for this particular problem?

Example of a particular perturbed problem



Laskar et al., A long-term num. sol. for the insolation quantities of the Earth, Astron. Astroph. (2004) (553 cites at JCR)

Example of a very particular perturbed problem



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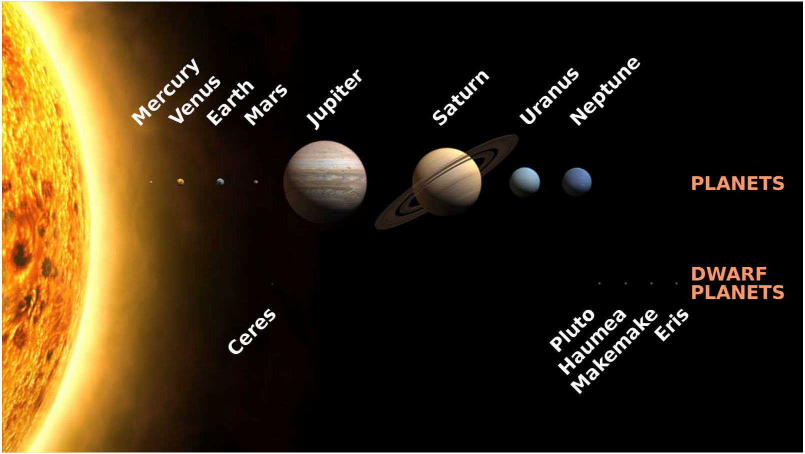

B, Casas, Farrés, Laskar, Makazaga and Murua:
APNUM (2013) and Cel. Mech. & Dyn. Astron. (2013)

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- Numerical Methods valid for most problems
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We present with some detail the steps to follow in order to look for efficient splitting methods to solve perturbed problems.

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4. (Ideally) To collaborate with experts on these fields

Back to the problem: The autonomous case

$$\boxed{x' = f^{[a]}(x) + \varepsilon\, f^{[b]}(x)}$$

where $|\varepsilon| \ll 1$ and each part is exactly solvable

$$x' = f^{[a]}(x) \qquad \longrightarrow \qquad x(h) = \varphi_h^{[a]}(x_0)$$

$$x' = \varepsilon\, f^{[b]}(x) \qquad \longrightarrow \qquad x(h) = \varphi_h^{[b]}(x_0)$$

with h being the time step.

Basic splitting methods

We can use splitting methods

$$\psi^{[1]}: \quad \varphi_h^{[a]} \circ \varphi_h^{[b]}, \qquad \varphi_h^{[b]} \circ \varphi_h^{[a]} \qquad \longrightarrow \quad \mathcal{O}(\varepsilon h^2)$$

$$\psi^{[2]}: \quad \varphi_{h/2}^{[a]} \circ \varphi_h^{[b]} \circ \varphi_{h/2}^{[a]}, \qquad \varphi_{h/2}^{[b]} \circ \varphi_h^{[a]} \circ \varphi_{h/2}^{[b]} \qquad \longrightarrow \quad \mathcal{O}(\varepsilon h^3)$$

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$$\left(\varphi_{h/2}^{[a]} \circ \varphi_h^{[b]} \circ \varphi_{h/2}^{[a]}\right)^N = \varphi_{h/2}^{[a]} \left(\varphi_h^{[b]} \circ \varphi_h^{[a]}\right)^{N-1} \varphi_h^{[b]} \circ \varphi_{h/2}^{[a]}$$

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$$\begin{aligned}
\left(\varphi_{h/2}^{[a]} \circ \varphi_h^{[b]} \circ \varphi_{h/2}^{[a]}\right)^N &= \varphi_{h/2}^{[a]} \left(\varphi_h^{[b]} \circ \varphi_h^{[a]}\right)^{N-1} \varphi_h^{[b]} \circ \varphi_{h/2}^{[a]} \\
&= \varphi_{h/2}^{[a]} \left(\varphi_h^{[b]} \circ \varphi_h^{[a]}\right)^{N} \left(\varphi_{h/2}^{[a]}\right)^{-1}
\end{aligned}$$

Test bench: perturbed harmonic oscillator

Linearly perturbed problem

$$\boxed{H = \frac{1}{2}\left(p^2 + q^2\right) + \frac{\varepsilon}{2} q^2} \qquad (0)$$

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Hamilton equations

$$\frac{d}{dt}\left\{ \begin{array}{c} q \\ p \end{array} \right\} = \left(\begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right) \left\{ \begin{array}{c} q \\ p \end{array} \right\} + \varepsilon \left(\begin{array}{cc} 0 & 0 \\ -1 & 0 \end{array} \right) \left\{ \begin{array}{c} q \\ p \end{array} \right\}$$

i.e. $\quad x' = Ax + \varepsilon Bx, \quad$ whose solution is

$$\left\{ \begin{array}{c} q(t) \\ p(t) \end{array} \right\} = \left(\begin{array}{cc} \cos(\theta_\varepsilon t) & {\chi_\varepsilon}^{-1} \sin(\theta_\varepsilon t) \\ -\chi_\varepsilon \sin(\theta_\varepsilon t) & \cos(\theta_\varepsilon t) \end{array} \right) \left\{ \begin{array}{c} q_0 \\ p_0 \end{array} \right\}$$

with

$$\theta_\varepsilon = \sqrt{1+\varepsilon}, \qquad \chi_\varepsilon = \sqrt{1+\varepsilon}.$$

The perturbed harmonic oscillator

Splitting methods are given by

$$\Psi_h = \prod_{i=1}^{s} \mathrm{e}^{b_i h \varepsilon B} \, \mathrm{e}^{a_i h A} = \prod_{i=1}^{s} \begin{pmatrix} 1 & 0 \\ -b_i h \varepsilon & 1 \end{pmatrix} \begin{pmatrix} \cos(a_i h) & \sin(a_i h) \\ -\sin(a_i h) & \cos(a_i h) \end{pmatrix}$$

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Stability $\Rightarrow \quad |A_h| < 1 \;$ or $\; |A_h| = 1, \; |B_h| + |C_h| = 0$

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$$\Psi_h^N = \begin{pmatrix} \cos(\theta_{\varepsilon,h} N h) & {\chi_{\varepsilon,h}}^{-1} \sin(\theta_{\varepsilon,h} N h) \\ -\chi_{\varepsilon,h} \sin(\theta_{\varepsilon,h} N h) & \cos(\theta_{\varepsilon,h} N h) \end{pmatrix}$$

Back to the basic methods for the perturbed HO

$$\Psi^{[2]}_{BAB} = e^{\frac{h}{2}\varepsilon B}\, e^{hA}\, e^{\frac{h}{2}\varepsilon B}, \qquad \Psi^{[2]}_{ABA} = e^{\frac{h}{2}A}\, e^{h\varepsilon B}\, e^{\frac{h}{2}A}, \qquad \Psi^{[1]}_{BA} = e^{h\varepsilon B}\, e^{hA} \qquad ??$$

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$$\begin{aligned} \Psi_{BAB}^{[2]} &= \begin{pmatrix} 1 & 0 \\ -\frac{h}{2}\varepsilon & 1 \end{pmatrix} \begin{pmatrix} \cos(h) & \sin(h) \\ -\sin(h) & \cos(h) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\frac{h}{2}\varepsilon & 1 \end{pmatrix} \\ &= \begin{pmatrix} \cos(\theta_b h) & \chi_b^{-1}\sin(\theta_b h) \\ -\chi_b \sin(\theta_b h) & \cos(\theta_b h) \end{pmatrix} \end{aligned}$$

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$$\Psi_{ABA}^{[2]} = e^{\frac{h}{2}A}\, e^{h\varepsilon B}\, e^{\frac{h}{2}A} = \begin{pmatrix} \cos(\theta_a h) & \chi_a^{-1}\sin(\theta_a h) \\ -\chi_a \sin(\theta_a h) & \cos(\theta_a h) \end{pmatrix}$$

$$\Psi_{BA}^{[1]} = e^{h\varepsilon B}\, e^{hA} = \begin{pmatrix} \cos(\theta_c h) + \chi_c \sin(\theta_c h) & \chi_d \sin(\theta_c h) \\ -\chi_e \sin(\theta_c h) & \cos(\theta_c h) - \chi_c \sin(\theta_c h) \end{pmatrix}$$

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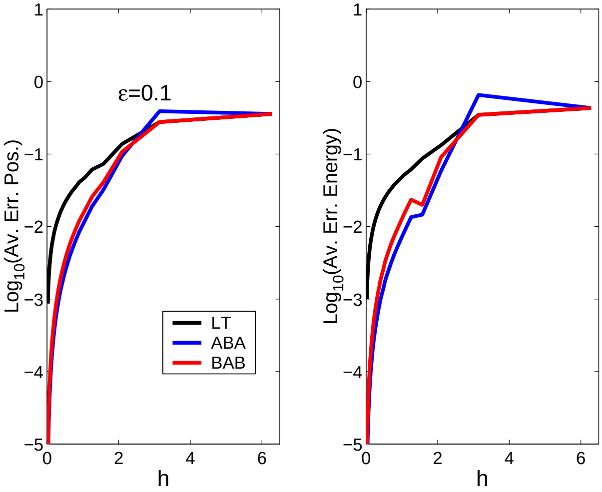
where $\theta_a = \theta_b = \theta_c$!! All methods are conjugate to each other.

Simple numerical example



$$(q_0, p_0) = (1, 1), \;\; t_f = 2\pi$$

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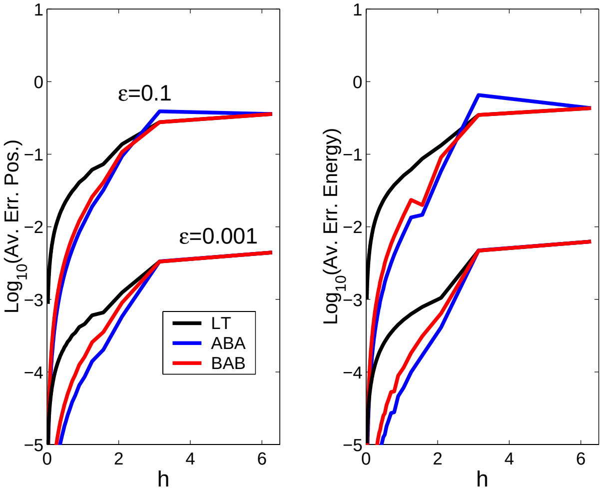

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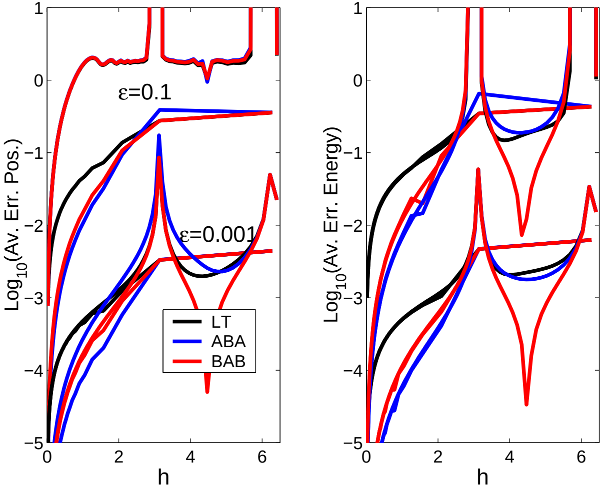
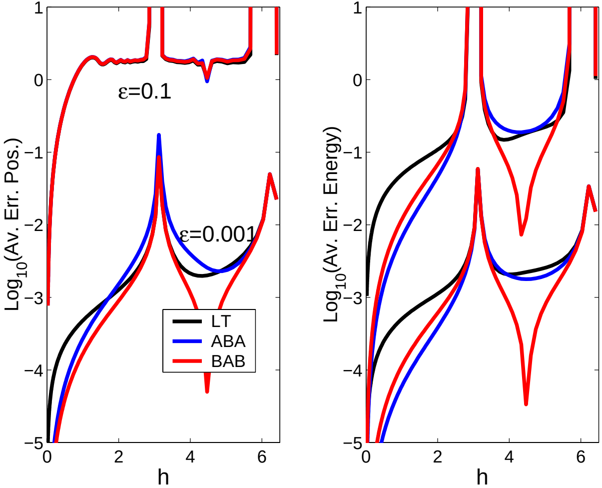


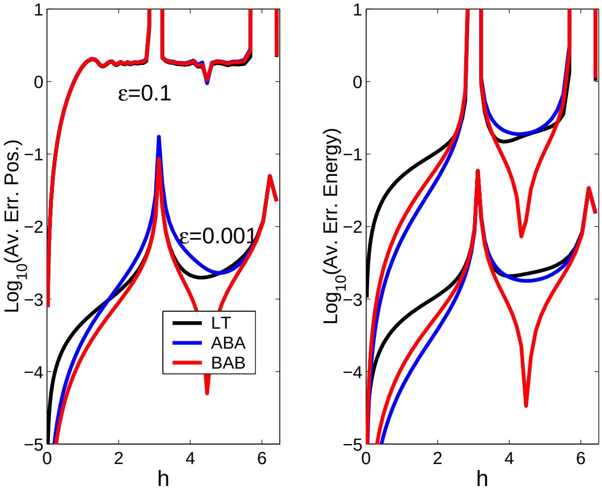
$$(q_0, p_0) = (1, 1), \ t_f = 2000\pi$$

Simple numerical example



Why?

Simple numerical example



Why? **a)** There is a singularity at $h = \pi, \ \forall \varepsilon$;

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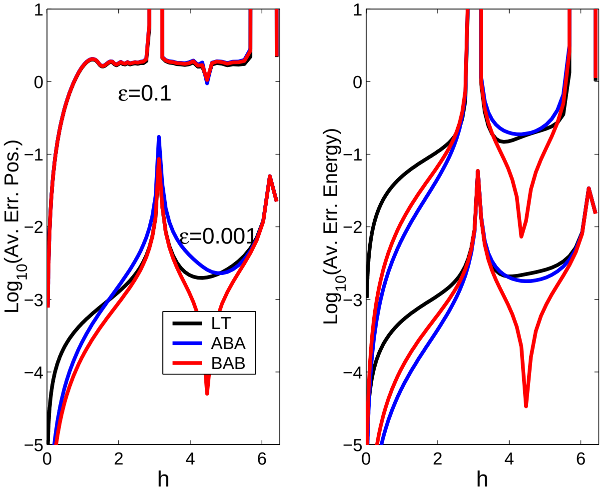

Why? **a)** There is a singularity at $h=\pi, \ \forall\varepsilon$;

b) $\chi_\alpha=\mathcal{O}(\varepsilon), \quad \theta_\alpha=\mathcal{O}(\varepsilon^2)$

Stability limit

If $h = \pi$

$$
\begin{aligned}
\Psi_{BAB}^{[2]} &= \begin{pmatrix} 1 & 0 \\ -\frac{h}{2}\varepsilon & 1 \end{pmatrix} \begin{pmatrix} \cos(h) & \sin(h) \\ -\sin(h) & \cos(h) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\frac{h}{2}\varepsilon & 1 \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \\ -\frac{\pi}{2}\varepsilon & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\frac{\pi}{2}\varepsilon & 1 \end{pmatrix} \\
&= \begin{pmatrix} -1 & 0 \\ \pi\varepsilon & -1 \end{pmatrix}
\end{aligned}
$$

Unstable $\forall\varepsilon$.

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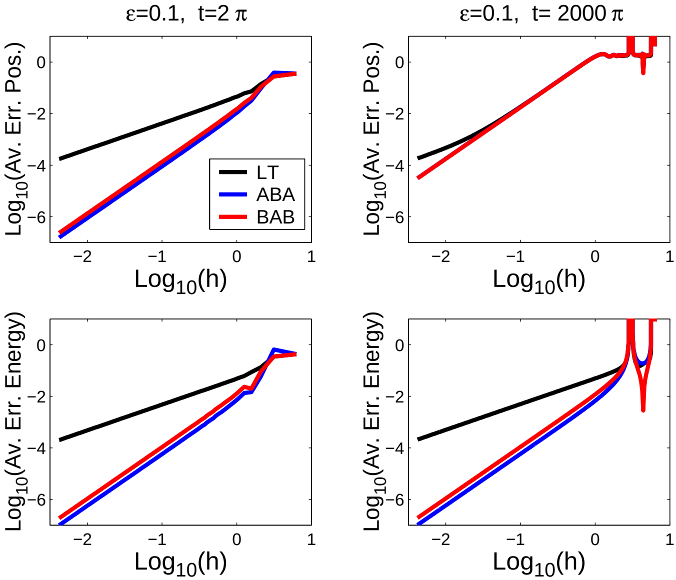

Applications to perturbed systems

- Classical Hamiltonian systems (Solar system)
- Quantum Mechanics
  - Linear and non-linear Schrödinger equation★
  - The eigenvalue problem
- Hybrid Monte Carlo
- Optimal control problems★
- Scaling-Splitting-Squaring to compute $e^{A+\varepsilon B}$
- Parabolic linear and non-linear PDEs★

★ With possible explicit time-dependent dominant part.

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where

$$A = f^{[a]}(x) \cdot \nabla, \qquad B = f^{[b]}(x) \cdot \nabla$$

are Lie operators acting on smooth functions, and the solution can formally be written as

$$\varphi_h(x_0) = \mathrm{e}^{h(A+\varepsilon B)} x_0$$

Back to the problem

$$\Psi(h) = \mathrm{e}^{a_1 hA}\,\mathrm{e}^{b_1 h\varepsilon B} \cdots \mathrm{e}^{a_s hA}\,\mathrm{e}^{b_s h\varepsilon B}$$

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By applying repeatedly the Baker–Campbell–Hausdorff (BCH) formula to a consistent method we can formally write

$$\Psi(h) = \mathrm{e}^{h(A+\varepsilon B+E(h,\varepsilon))}$$

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where

$$\begin{aligned} E \;=\;& h\,\varepsilon\, p_{ab}[A,B] + h^2\,\varepsilon\, p_{aba}[[A,B],A] + h^2\,\varepsilon^2\, p_{abb}[[A,B],B]) \\ & + h^3\,\varepsilon\, p_{abaa}[[[A,B],A],A] + h^3\varepsilon^2 p_{abba}[[[A,B],B],A] \\ & + h^3\varepsilon^3\, p_{abbb}[[[A,B],B],B] + \ldots \end{aligned}$$

Here $[A,B] = AB - BA$ (commutator of Lie operators) and $p_{ab}, p_{abb}, p_{aba}, p_{abbb}, \ldots$ are polynomials in the a_i, b_i.

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$$E = \qquad h^2\, \varepsilon\, p_{aba}[[A,B],A] + h^2\, \varepsilon^2\, p_{abb}[[A,B],B])$$

$$= \mathcal{O}(\varepsilon h^2)$$

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$$\Psi(h) = e^{h(A+\varepsilon B+E(h,\varepsilon))}$$

where

$$E = \qquad h^2 \varepsilon^2 p_{abb}[[A, B], B])$$

$$= \mathcal{O}(\varepsilon h^4 + \varepsilon^2 h^2)$$

Back to the problem

$$\Psi(h) = e^{a_1 hA}\, e^{b_1 h\varepsilon B} \cdots e^{a_s hA}\, e^{b_s h\varepsilon B}$$

By applying repeatedly the Baker–Campbell–Hausdorff (BCH) formula to a consistent method we can formally write

$$\Psi(h) = e^{h(A+\varepsilon B+E(h,\varepsilon))}$$

where

$$E \;=\; h^2\,\varepsilon^2\, p_{abb}[[A,B],B])$$

$$= \mathcal{O}(\varepsilon h^4 + \varepsilon^2 h^2)$$

Method of generalised order (4,2). In general (McLachlan):
$\mathcal{O}(\varepsilon h^{r_1} + \varepsilon^2 h^{r_2} + \cdots + \varepsilon^m h^{r_m}) \;\longrightarrow\; (r_1, r_2, \ldots, r_m) \quad (r_i \geq r_{i+1})$

Generalized order conditions

We make use of the following properties

$$C(h) = \mathrm{e}^{hA} B \mathrm{e}^{-hA} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \frac{1}{3!}[A, [A, [A, B]]] + \ldots$$

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$$\mathrm{e}^{ahA}\, \mathrm{e}^{\varepsilon bhB}\, \mathrm{e}^{-ahA} = \exp\left(\varepsilon b\, h\, \mathrm{e}^{ahA} B \mathrm{e}^{-ahA}\right) = \mathrm{e}^{\varepsilon b\, h\, C(ah)}$$

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$$= \quad \mathrm{e}^{a_1 hA}\, \mathrm{e}^{\varepsilon b_1 hB}\, \mathrm{e}^{-a_1 hA}\, \mathrm{e}^{(a_1 + a_2) hA}\, \mathrm{e}^{\varepsilon b_2 hB}$$

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$$e^{\varepsilon\, b_1 hC(ha_1)}\, e^{\varepsilon\, b_2 hC(h(a_1+a_2))} \simeq e^{h(A+\varepsilon B)}\, e^{-hA}$$

Generalized order conditions

In general

$$\mathrm{e}^{\varepsilon\, b_1 hC(c_1 h)} \cdots \mathrm{e}^{\varepsilon\, b_s hC(c_s h)} \simeq e^{h(A+\varepsilon B)}\, \mathrm{e}^{-hA}$$

$c_k = a_1 + \cdots + a_k.$

Generalized order conditions

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$$\mathrm{e}^{\varepsilon\, b_1 hC(c_1 h)} \cdots \mathrm{e}^{\varepsilon\, b_s hC(c_s h)} \simeq e^{h(A+\varepsilon B)}\, \mathrm{e}^{-hA}$$

$c_k = a_1 + \cdots + a_k$. We expand both sides as power series of ε (Thalhammer, SINUM (2008)). We get generalised order $(r_1, \ldots, r_m)$ if and only if

$$\sum_{1\leq i_1 \leq \cdots \leq i_k \leq s} \frac{b_{i_1} \cdots b_{i_k}}{\sigma_{i_1 \cdots i_k}}\, c_{i_1}^{j_1-1} \cdots c_{i_k}^{j_k-1} = \frac{1}{(j_1 + \cdots + j_k) \cdots (j_1 + j_2) j_1}$$

($\sigma_{i_1 \cdots i_k}$ are given constants) for each $k = 1, \ldots, m$ and each multi-index $(j_1, \ldots, j_k)$ such that $j_1 + \cdots + j_k \leq r_k$.
Lyndon multi-indices allow to find a set of independent order conditions (Murua)

Generalized order conditions

Gen. order	Conditions
$(2n, 2)$	$\sum_{i=1}^{s} b_i\, c_i^{j-1} = \frac{1}{j}, \qquad j = 1, \ldots, n,$ quad. rule
$(2n, 4)$	$\sum_{i=1}^{s} \frac{1}{2} b_i^2 c_i + \sum_{1 \le i < j \le s} b_i b_j c_j = \frac{1}{3}$
$(2n, 6, 4)$	$\sum_{i=1}^{s} \frac{1}{2} b_i^2 c_i^3 + \sum_{1 \le i < j \le s} b_i b_j c_j^3 = \frac{1}{5}$
	$\sum_{i=1}^{s} \frac{1}{2} b_i^2 c_i^3 + \sum_{1 \le i < j \le s} b_i b_j c_i c_j^2 = \frac{1}{10}$

(**B**, Casas, Farrés, Laskar, Makazaga and Murua, APNUM (2013)).

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(**B**, Casas, Farrés, Laskar, Makazaga and Murua, APNUM (2013)).
Valid if $\quad x' = f^{[a]}(x), \quad x' = \varepsilon f^{[b]}(x) \quad$ are exactly solvable

Generalized order conditions

Heliocentric coordinates are very useful for the Solar system, but in these coordinates the Hamiltonian takes de form

$$H = H_K(q,p) + \varepsilon \left(p^2 + V_I(q) \right)$$

or equivalently

$$x' = f^{[a]}(x) + \varepsilon \left(f^{[b,1]}(x) + f^{[b,2]}(x) \right)$$

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The simplest solution

$$\mathrm{e}^{\varepsilon b_i h (B_1 + B_2)} \quad \Rightarrow \quad \mathrm{e}^{\varepsilon b_i h/2 B_1} \, \mathrm{e}^{\varepsilon b_i h B_2} \, \mathrm{e}^{\varepsilon b_i h/2 B_1}$$

and to add the following order condition to the previous Table

$$\boxed{\sum_{i=1}^{s} b_i^3 = 0}$$

Generalized order conditions

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Generalized order conditions for Heliocentric coord.

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List of methods

Methods: $(2n,2)_n, (6,4)_4, (8,4)_5$: (McLachlan, BIT (1995))
New methods optimised for given problems:

- Solar System
  - Jacobi coordinates: $(10,4)_7,\ (8,6,4)_7,\ (10,6,4)_8$
  - Helioc. coord. $(\sum_i b_i^3 = 0)$: $(8,4)_6,\ (8,6,4)_8,\ (10,6,4)_9$
- Parabolic problems
  - Quantum Mech.: Schrödinger eq. in the imaginary time $(6,4)_4,\ (8,4)_5,\ (8,6,4)_7,\ (8,6)_9$ with $a_i, b_i \in \mathbb{C}$
- Scaling-Splitting-Squaring to: $e^{A+\varepsilon B}$ with $a_i \in \mathbb{C},\ b_i \in \mathbb{R}$
- Hybrid Monte Carlo: work in progress
- Other families of methods
  - Methods using derivatives (gradient) of the perturbation.
  - Methods using processor/corrector

Time-dependent problems ??

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Non-autonomous problems:

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$$\nparallel$$

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$$
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Let us first consider

$$x' = Ax + \varepsilon B(t)x$$

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Let us first consider

$$x' = Ax + \varepsilon B(t)x$$

To take the time as a new coordinate and to split as follows

$$\left\{ \begin{array}{l} \dfrac{dx}{dt} = Ax \\ \\ \dfrac{dt_1}{dt} = 1 \end{array} \right. \qquad \text{and} \qquad \left\{ \begin{array}{l} \dfrac{dx}{dt} = \varepsilon B(t_1)x \\ \\ \dfrac{dt_1}{dt} = 0. \end{array} \right.$$

Autonomous system: $\tilde{x}' = \tilde{A}\tilde{x} + \varepsilon \tilde{B}\tilde{x}$

CAUTION: if $a_i \in \mathbb{C}$ then $B(t)$ is evaluated at $t \in \mathbb{C}$.

Time-dependent problems:

Consider now

$$x' = A(t)x + \varepsilon B(t)x$$

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$$x' = A(t)x + \varepsilon B(t)x$$

The simplest trick: to take the time as two new coordinates

$$\left\{ \begin{array}{l} \dfrac{dx}{dt} = A(t_1)x \\[2ex] \dfrac{dt_1}{dt} = 0 \\[2ex] \dfrac{dt_2}{dt} = 1 \end{array} \right. \qquad \text{and} \qquad \left\{ \begin{array}{l} \dfrac{dx}{dt} = \varepsilon B(t_2)x \\[2ex] \dfrac{dt_1}{dt} = 1 \\[2ex] \dfrac{dt_2}{dt} = 0. \end{array} \right.$$

Autonomous system:

$\tilde{x}' = \tilde{A}\tilde{x} + \tilde{B}(\varepsilon)\tilde{x}$ *but* $\tilde{B}(\varepsilon) \neq \mathcal{O}(\varepsilon)$!!!

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Solution: to take the time as only one new coordinate as follows (**B**, Diele, Marangi, Ragni, JCAM (2010))

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$$\tilde{x}' = \tilde{A}\tilde{x} + \varepsilon \tilde{B}\tilde{x}$$

It requires to solve

$$x' = A(t)x$$

to sufficient accuracy. One can use a time-averaging method (e.g. Magnus integrators).

Quantum Mech.: perturbed time-dependent harmonic trap

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

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After spatial discretisation we have

$$iu' = \left(\frac{1}{2}P^2 + \frac{w(t)}{2}X^2\right)u + \varepsilon V(t)u$$

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The dominant part can be solve with one FFT

$$iu' = \left(\frac{1}{2}P^2 + \frac{w(t)}{2}X^2\right)u$$

Bader & **B**, Phys. Rev. E (2011)

Time-dependent reaction-diffusion equation

$$\frac{\partial u}{\partial t} = \alpha(t)^2 \Delta u + \gamma(t) u(1-u)$$

Splitting methods such that: $a_i \in \mathbb{R}^+, \; b_i \in \mathbb{C}^+$.

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Time-dependent reaction-diffusion equation

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Splitting methods such that: $a_i \in \mathbb{R}^+, \ b_i \in \mathbb{C}^+$. To solve exactly with $a_i \in \mathbb{R}^+$

$$\frac{\partial u}{\partial t} = \alpha(t)^2 \Delta u,$$

and, with the time frozen, solve using $b_i \in \mathbb{C}^+$

$$\frac{\partial u}{\partial t} = \tilde{\gamma} u(1-u)$$

One can use methods such that $a_i \in \mathbb{R}^+, \ b_i \in \mathbb{C}^+$. (**B** & Seydaoğlu (2013) Submitted)

Available programs: http://personales.upv.es/ serblaza

$$H = \frac{1}{2}\left(p^2 + q^2\right) + \varepsilon \frac{1}{2} q^2$$

1. $(2s, 2)_n, \ (8, 4)_5, \ (10, 4)_7, \ (8, 6, 4)_7, \ (10, 6, 4)_8$
2. $(a_i, b_i \in \mathbb{C}^+)$: $(6, 4)_4, \ (8, 4)_5, \ (8, 6, 4)_7, \ (8, 6)_9$
3. $(a_i \in \mathbb{R}^+, \ b_i \in \mathbb{C}^+)$: $(4^*, 4)_4, (6, 4)_6$

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$$H = \frac{1}{2}\left(p^2 + w(t)^2 q^2\right) + \varepsilon f(t) q^2$$

5. Methods processors: $(6,4)_2, (7,6,4)_3$, $(7,6,5)_3$

Available programs: http://personales.upv.es/ serblaza

$$H = \frac{1}{2}\left(p^2 + q^2\right) + \varepsilon \frac{1}{2} q^2$$

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5. Methods processors: $(6, 4)_2, (7, 6, 4)_3, \ (7, 6, 5)_3$
6. New methods for Hybrid Monte Carlo (soon) (with Casas and Sanz-Serna)

Numerical Tests:

Solar System with 8 planets in Heliocentric coordinates.

$\mathbf{q}_i, \mathbf{p}_i$: relative positions of each planet with respect to the Sun and conjugate momenta. The Hamiltonian is given by

$$H_{He} = \sum_{i=1}^{8} \left(\frac{m_0 + m_i}{2 m_0 m_i} \|\mathbf{p_i}\|^2 - G \frac{m_0 m_i}{\|\mathbf{q}_i\|} \right) + \sum_{0<i<j\leq n} \left(\frac{\mathbf{p}_i \cdot \mathbf{p}_j}{m_0} - G \frac{m_i m_j}{\Delta_{ij}} \right)$$

where $\Delta_{ij} = \|\mathbf{q}_i - \mathbf{q}_j\|$ for $i, j > 0$.

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2-dimensional pert. Kepler ($e = 0.2, \quad \varepsilon = 10^{-3}$)

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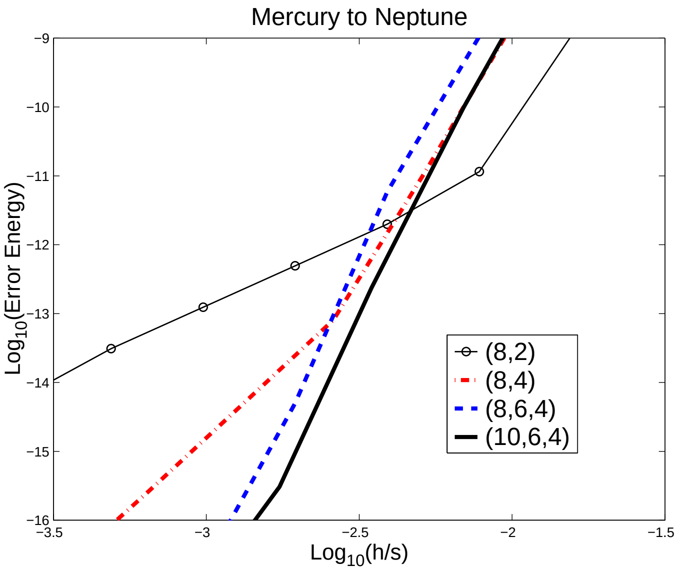
Perturbed oscillator ($(q, p) = (1, 1), \quad \varepsilon = 10^{-3}$)

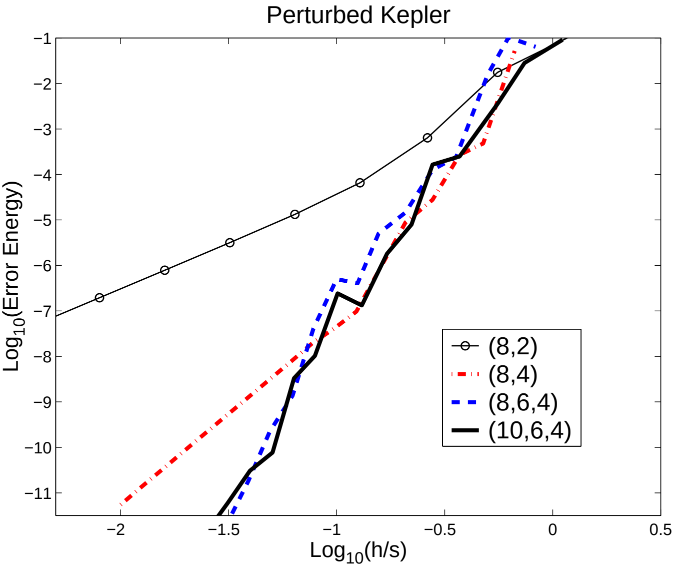
$$H = \frac{1}{2} \left(p^2 + q^2 \right) + \varepsilon \left(\frac{1}{2} p^2 + \frac{1}{4} q^4 \right)$$

Example:



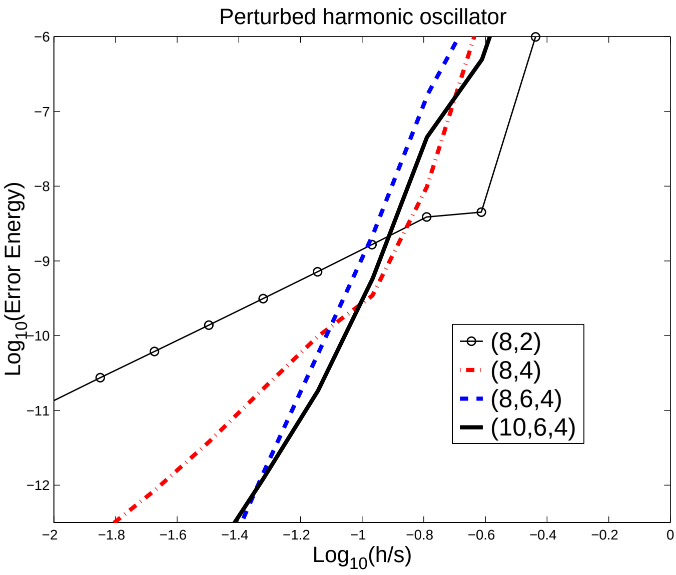
Mercury to Neptune
−9
−10
−11
−12
−13
−14
−15
−16
−3.5
−3
−2.5
−2
−1.5
Log10(Error Energy)
Log10(h/s)
(8,2)
(8,4)
(8,6,4)
(10,6,4)

Example:



Perturbed Kepler
Log10(Error Energy)
Log10(h/s)
−1
−2
−3
−4
−5
−6
−7
−8
−9
−10
−11
−2
−1.5
−1
−0.5
0
0.5
(8,2)
(8,4)
(8,6,4)
(10,6,4)

Example:



Perturbed harmonic oscillator
−6
−7
−8
−9
−10
−11
−12
Log10(Error Energy)
−2
−1.8
−1.6
−1.4
−1.2
−1
−0.8
−0.6
−0.4
−0.2
0
Log10(h/s)
(8,2)
(8,4)
(8,6,4)
(10,6,4)

Conclusions

1. To split a perturbed system into its dominant part and the perturbation is usually convenient even for not necessarily very small perturbations
2. The best splitting method very much depend on the problem to be solves (error in energy or in position, high or low accuracy, short or long time integrations, real or complex coefficients, etc.)
3. We have provided a set of methods tailored for different purposes and implemented in very simple problems to test of their performances as well as their applications on more realistic problems.

Thank you for your attention and
Happy Birthday