Splitting methods (with processing) for near-integrable problems

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Based on a work with

- Sergio Blanes
- Ariadna Farrés
- Jacques Laskar
- Ander Murua
- Joseba Makazaga

I. INTRODUCTION

Some history

- In Oberwolfach GNI workshop (2011), J. Laskar proposed to construct more accurate and efficient integrators for the integration of the Solar System
- The goal: to achieve round off error (in extended arithmetic) with the minimum computational cost
- Very accurate methods, to be used for long integration time intervals
- The methods should be symplectic and well adapted to the near-integrable structure of the Hamiltonian problem
- Result (until now):
  - S. Blanes, F.C., A. Farrés, J. Laskar, J. Makazaga and A. Murua. New families of symplectic splitting methods for numerical integration in dynamical astronomy. *Appl. Numer. Math.* **68** (2013), 58-72
  - A. Farrés, J. Laskar, S. Blanes, F. Casas, J. Makazaga and A. Murua. High precision symplectic integrators for the Solar System. *Celest. Mech. Dyn. Astr.* **116** (2013), 141-174

Purpose of the talk

1. To review the work done and the constructed methods
2. To propose 'new' strategies to get improved? integrators: use of *processing*

We first review the simplified model of the Solar System for which the new methods have been designed:

The non-relativistic gravitational N-body problem

Non-relativistic gravitational N-body problem

- Motion of $n+1$ particles (the Sun, with mass m_0, and n planets with masses m_i, $i = 1, \ldots, n$) only affected by their mutual gravitational interaction
- Hamiltonian system with

$$H = \frac{1}{2} \sum_{i=0}^{n} \frac{\|\mathbf{p}_i\|^2}{m_i} - G \sum_{0 \le i < j \le n} \frac{m_i m_j}{\|\mathbf{q}_i - \mathbf{q}_j\|} \qquad (1)$$

- $\mathbf{q}_i$ and $\mathbf{p}_i = m_i \dot{\mathbf{q}}_i$: position and momenta of the $n+1$ bodies in a barycentric reference frame.
- Planets evolve around the central mass following almost Keplerian orbits
- By an appropriate change of coordinates one can rewrite (1) as

$$H = K + V_I, \qquad \text{where} \qquad |V_I| \ll |K|.$$

- Jacobi and Heliocentric coordinates

- Jacobi coord.: $H_J(Q_J, P_J) = K_J(Q_J, P_J) + V_I^{[J]}(Q_J)$
- Heliocentric coord.:
  $H_H(Q_H, P_H) = K_H(Q_H, P_H) + V_I^{[H]}(Q_H, P_H)$
- K_J, K_H: sum of independent unperturbed Kepler problems
- $V_I^{[J]}$, $V_I^{[H]}$: perturbations depending on the interactions of the planets
- $|V_I^{[J]}| \ll |K_J|$, $|V_I^{[H]}| \ll |K_H|$, but an important difference:

$$V_I^{[J]}(Q_J), \qquad \text{and} \qquad V_I^{[H]}(Q_H, P_H)$$

so that $V_I^{[H]}(Q_H, P_H)$ can be written as

$$V_I^{[H]}(Q_H, P_H) = V_{I_1}^{[H]}(Q_H) + V_{I_2}^{[H]}(P_H)$$

- Particular example of a *near-integrable Hamiltonian system*:

$$H(q,p;\varepsilon) = H^{[a]}(q,p) + \varepsilon H^{[b]}(q,p), \qquad (2)$$

  where $\varepsilon \ll 1$ and $H^{[a]}$ is exactly integrable.
- In Jacobi coordinates, $H^{[b]}(q)$
- In heliocentric coordinates, $H^{[b]}(q,p) = H_1^{[b]}(q) + H_2^{[b]}(p)$
- It makes sense to take into account this special structure when designing integration methods to approximate its dynamics.
- Splitting methods as compositions of the flows corresponding to $H^{[a]}$ and $H^{[b]}$ or $H^{[a]}$, $H_1^{[b]}$, $H_2^{[b]}$
- A particular goal: to achieve the same accuracy in both types of coordinates

II. SPLITTING METHODS FOR NEAR-INTEGRABLE SYSTEMS

General framework

- Generic differential equation of the form

$$x' = f^{[a]}(x) + \varepsilon f^{[b]}(x), \qquad x(0) = x_0 \in \mathbb{R}^D, \tag{3}$$

where $|\varepsilon| \ll 1$ and each part

$$x' = f^{[a]}(x), \qquad x' = \varepsilon f^{[b]}(x) \tag{4}$$

is exactly solvable (or can be numerically solved up to round off accuracy) with solutions

$$x(\tau) = \varphi_\tau^{[a]}(x_0), \qquad x(\tau) = \varphi_\tau^{[b]}(x_0)$$

respectively, at $t = \tau$, the time step.

- If $\varphi_\tau(x_0)$ is the *exact solution* then $\psi_\tau = \varphi_\tau^{[b]} \circ \varphi_\tau^{[a]}$ provides a first-order approximation,

$$\psi_\tau(x_0) = \varphi_\tau(x_0) + \mathcal{O}(\tau^2)$$

General framework

- Higher order approximations can be obtained by

$$\psi_\tau = \varphi^{[a]}_{a_{s+1}\tau} \circ \varphi^{[b]}_{b_s\tau} \circ \varphi^{[a]}_{a_s\tau} \circ \cdots \circ \varphi^{[b]}_{b_1\tau} \circ \varphi^{[a]}_{a_1\tau} \tag{5}$$

  for appropriately chosen coefficients a_i, b_i.
- The splitting method ψ_τ is of order r if for all $x \in \mathbb{R}^D$,

$$\psi_\tau(x) = \varphi_\tau(x) + \mathcal{O}(\tau^{r+1}) \quad \text{as} \quad \tau \to 0. \tag{6}$$

- Consistency condition:

$$\sum_{i=1}^{s+1} a_i = 1, \qquad \sum_{i=1}^{s} b_i = 1. \tag{7}$$

- Symmetric / left-right palindromic compositions: $a_{s+2-i} = a_i$, $b_{s+1-i} = b_i$. Then, if (7) holds, *order 2*

Lie operators

- In term of the *Lie operators* A and B associated with $f^{[a]}$ and $f^{[b]}$,

$$A\,g(x) = \left.\frac{d}{d\tau}\right|_{\tau=0} g(\varphi_\tau^{[a]}(x)), \qquad B\,g(x) = \left.\frac{d}{d\tau}\right|_{\tau=0} g(\varphi_\tau^{[b]}(x)),$$

  one has

$$g(\varphi_\tau(x)) = \mathrm{e}^{\tau(A+\varepsilon B)} g(x),$$

- Then, for all functions g,

$$g(\varphi_\tau^{[a]}(x)) = \mathrm{e}^{\tau\,A}\,g(x), \qquad g(\varphi_\tau^{[b]}(x)) = \mathrm{e}^{\tau\,\varepsilon\,B}\,g(x). \quad (8)$$

- Analogously, for the integrator

$$\psi_\tau = \varphi^{[a]}_{a_{s+1}\tau} \circ \varphi^{[b]}_{b_s\tau} \circ \varphi^{[a]}_{a_s\tau} \circ \cdots \circ \varphi^{[b]}_{b_1\tau} \circ \varphi^{[a]}_{a_1\tau}$$

one has

$$g(\psi_\tau(x)) = \Psi(\tau)\, g(x),$$

where $\Psi(\tau)$ is

$$\Psi(\tau) = \mathrm{e}^{a_1\tau A}\, \mathrm{e}^{b_1\tau\varepsilon B} \cdots \mathrm{e}^{a_s\tau A}\, \mathrm{e}^{b_s\tau\varepsilon B}\, \mathrm{e}^{a_{s+1}\tau A}. \qquad (9)$$

Generalized order

- Two parameters: τ and ε
- We are interested in how the local error $\psi_\tau(x) - \varphi_\tau(x)$ decreases as $\varepsilon \to 0$
- Any consistent symmetric method the local error satisfies $\psi_\tau(x) = \varphi_\tau(x) + \mathcal{O}(\varepsilon\,\tau^3)$ or $\Psi(\tau) - \mathrm{e}^{\tau(A+\varepsilon\,B)} = \mathcal{O}(\varepsilon\,\tau^3)$
- If $\psi_\tau(x) = \varphi_\tau(x) + \mathcal{O}(\varepsilon\,\tau^5 + \varepsilon^2\,\tau^3)$ then the method is of (generalized) order $(4, 2)$ (R.I. McLachlan)
- In general, a splitting method is of generalized order $(r_1, r_2, \ldots, r_m)$ if

$$\psi_\tau(x) = \varphi_\tau(x) + \mathcal{O}(\varepsilon\tau^{r_1+1} + \varepsilon^2\tau^{r_2+1} + \cdots + \varepsilon^m\tau^{r_m+1}).$$

$r_1 \geq r_2 \geq \cdots \geq r_m$

In particular,

- $(8,2)$: $\psi_\tau(x) - \varphi_\tau(x) = \mathcal{O}(\varepsilon\tau^9 + \varepsilon^2\tau^3 + \cdots)$
- $(8,4)$: $\psi_\tau(x) - \varphi_\tau(x) = \mathcal{O}(\varepsilon\tau^9 + \varepsilon^2\tau^5 + \varepsilon^3\tau^5 + \cdots)$
- $(8,6,4)$: $\psi_\tau(x) - \varphi_\tau(x) = \mathcal{O}(\varepsilon\tau^9 + \varepsilon^2\tau^7 + \varepsilon^3\tau^5 + \cdots)$
- $(10,6,4)$: $\psi_\tau(x) - \varphi_\tau(x) = \mathcal{O}(\varepsilon\tau^{11} + \varepsilon^2\tau^7 + \varepsilon^3\tau^5 + \cdots)$

Independent generalized order conditions obtained in

- S. Blanes, F.C., A. Farrés, J. Laskar, J. Makazaga and A. Murua. New families of symplectic splitting methods for numerical integration in dynamical astronomy. *Appl. Numer. Math.* **68** (2013), 58-72

by considering a particular subset of multi-indices called *Lyndon multi-indices*

Generalized order	Lyndon multi-indices
$(8,2)$	$(3),(5),(7)$
$(8,4)$	(3), (5), (7), $(1,2)$
$(8,6,4)$	(3), (5), (7), $(1,2)$, $(1,4)$, $(2,3)$
$(10,6,4)$	(3), (5), (7), (9), $(1,2)$, $(1,4)$, $(2,3)$

Multi-index	Condition
$(j),\ \ j \geq 1$	$\displaystyle\sum_{i=1}^{s} b_i\, c_i^{j-1} = \frac{1}{j}$
$(1,2)$	$\displaystyle\sum_{i=1}^{s} \frac{1}{2} b_i^2 c_i + \sum_{1\leq i<j\leq s} b_i b_j c_j = \frac{1}{3}$
$(1,4)$	$\displaystyle\sum_{i=1}^{s} \frac{1}{2} b_i^2 c_i^3 + \sum_{1\leq i<j\leq s} b_i b_j c_j^3 = \frac{1}{5}$
$(2,3)$	$\displaystyle\sum_{i=1}^{s} \frac{1}{2} b_i^2 c_i^3 + \sum_{1\leq i<j\leq s} b_i b_j c_i c_j^2 = \frac{1}{10}$

$c_i = \sum_{j=1}^{i} a_j,\ i = 1,2,\ldots,s,\ c_{s+1} = 1$

New numerical schemes (Jacobi coordinates)

- $(10, 4)$: 7 stages

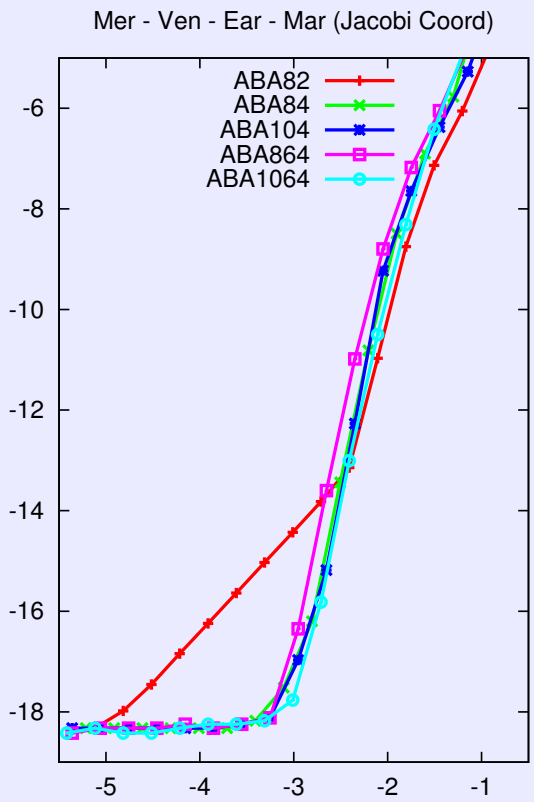
$$a_1\, b_1\, a_2\, b_2\, a_3\, b_3\, a_4\, b_4\, a_4\, b_3\, a_3\, b_2\, a_2\, b_1\, a_1$$

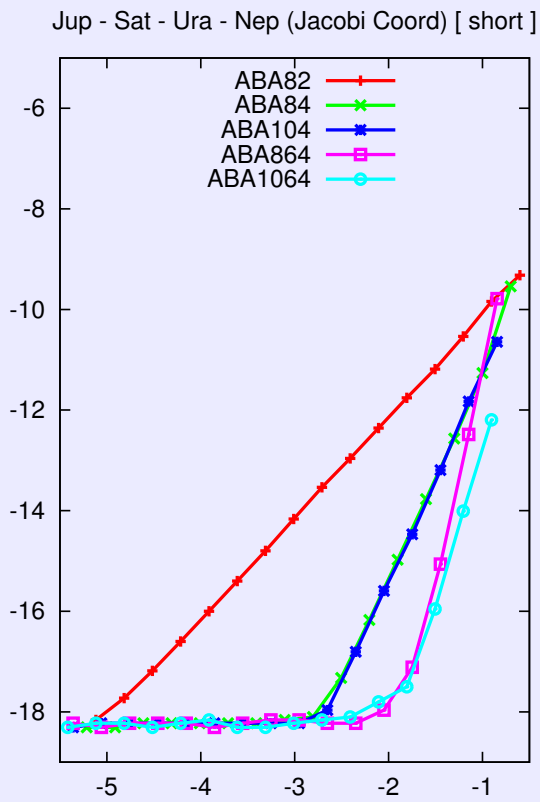
- $(8, 6, 4)$: 7 stages
- $(10, 6, 4)$: 8 stages

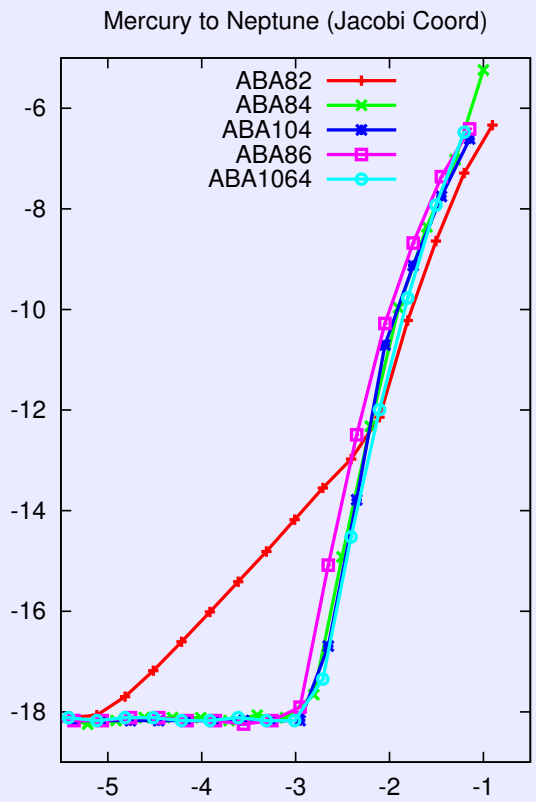
$$a_1\, b_1\, a_2\, b_2\, a_3\, b_3\, a_4\, b_4\, a_5\, b_4\, a_4\, b_3\, a_3\, b_2\, a_2\, b_1\, a_1\,.$$

- This requires solving the order conditions, applying optimization procedures, homotopy continuation methods, etc.

Illustration: Solar System in Jacobi coordinates







Heliocentric coordinates

- Now the system is of the form

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

- 'Idea': consider a composition

$$\widetilde{\psi}_\tau = \varphi^{[a]}_{a_1\tau} \circ \widetilde{\varphi}^{[b]}_{b_1\tau} \circ \varphi^{[a]}_{a_2\tau} \circ \cdots \circ \widetilde{\varphi}^{[b]}_{b_1\tau} \circ \varphi^{[a]}_{a_1\tau}$$

  where $\widetilde{\varphi}^{[b]}_\tau$ is an approximation of $\varphi^{[b]}_\tau$ obtained by some numerical integrator applied to $\varepsilon(f^{[b]}(x) + f^{[c]}(x))$,

- In particular,

$$\widetilde{\varphi}^{[b]}_{b_i\tau} = \varphi^{[b]}_{b_i\tau/2} \circ \varphi^{[c]}_{b_i\tau} \circ \varphi^{[b]}_{b_i\tau/2}$$

- But in this way, the resulting method is only of order 2!.

- Series of differential operators associated with $\widetilde{\psi}_\tau$

$$\widetilde{\Psi}(\tau) = \mathrm{e}^{a_1\tau A}\,\widetilde{\Phi}^{[b]}_{b_1\tau}\cdots\mathrm{e}^{a_2\tau A}\,\widetilde{\Phi}^{[b]}_{b_1\tau}\,\mathrm{e}^{a_1\tau A}$$

with

$$\widetilde{\Phi}^{[b]}_{b_j\tau} = \mathrm{e}^{b_j\tau B+(b_j\tau\varepsilon)^3 D_3+(b_j\tau\varepsilon)^5 D_5+\cdots}$$

- By applying the BCH formula, the new term

$$\left(\sum_{j=1}^{s} b_j^3\right)\varepsilon^3\tau^3 D_3$$

appears in the expression of the (vector field of the) modified Hamiltonian

- We impose, in addition to the previous generalized order conditions,

$$\sum_{j=1}^{s} b_j^3 = 0$$

and the resulting method can be made of order $\mathcal{O}(\tau^5\varepsilon^5)$

Result:

- Symmetric schemes with 1 additional stage
- Order (8,4) with 6 stages, minimum number (13 maps, 25 exponentials)

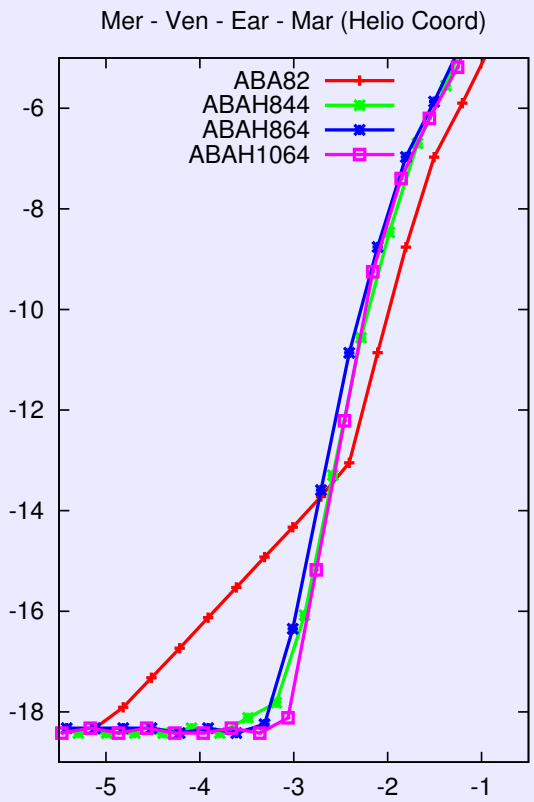
$$\begin{aligned}\psi_\tau \;=\; & \varphi^{[a]}_{a_1\tau} \circ \widetilde{\varphi}^{[b]}_{b_1\tau} \circ \varphi^{[a]}_{a_2\tau} \circ \widetilde{\varphi}^{[b]}_{b_2\tau} \circ \varphi^{[a]}_{a_3\tau} \circ \widetilde{\varphi}^{[b]}_{b_3\tau} \circ \varphi^{[a]}_{a_4\tau} \circ \widetilde{\varphi}^{[b]}_{b_3\tau} \\ & \circ \varphi^{[a]}_{a_3\tau} \circ \widetilde{\varphi}^{[b]}_{b_2\tau} \circ \varphi^{[a]}_{a_2\tau} \circ \widetilde{\varphi}^{[b]}_{b_1\tau} \circ \varphi^{[a]}_{a_1\tau}.\end{aligned}$$

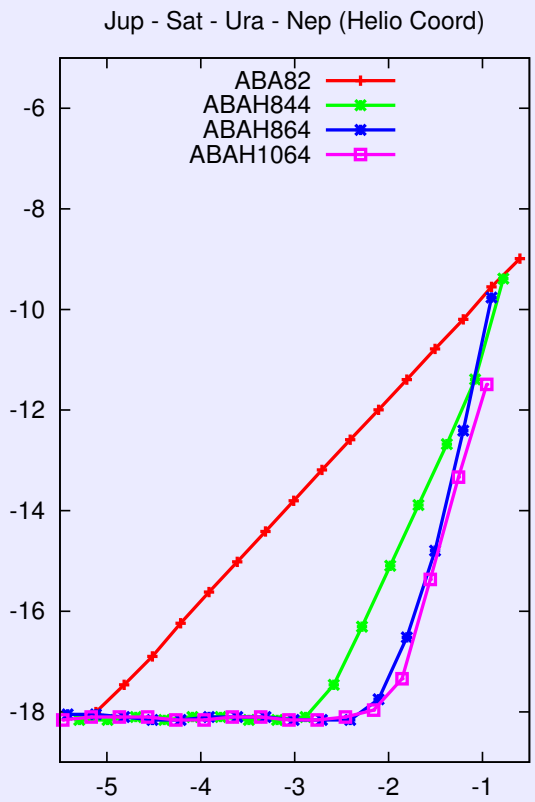
- Order (8,6,4), 8 stages
- Order (10,6,4), 9 stages (9 order conditions)
- In comparison a method (10,6,4) of the form

$$\psi_\tau = \varphi^{[a]}_{a_{s+1}\tau} \circ \varphi^{[c]}_{c_s\tau} \circ \varphi^{[b]}_{b_s\tau} \circ \varphi^{[a]}_{a_s\tau} \circ \cdots \circ \varphi^{[c]}_{c_1\tau} \circ \varphi^{[b]}_{b_1\tau} \circ \varphi^{[a]}_{a_1\tau}$$

requires 23 order conditions

Illustration: Solar System in Heliocentric coordinates





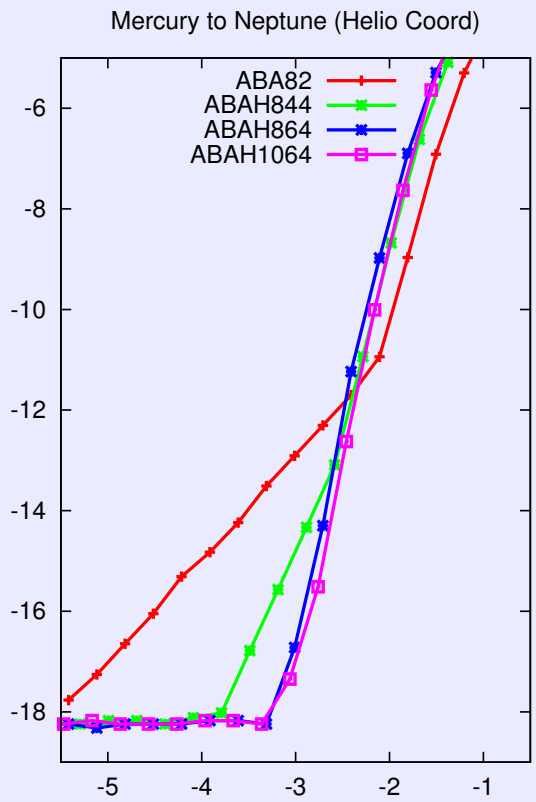
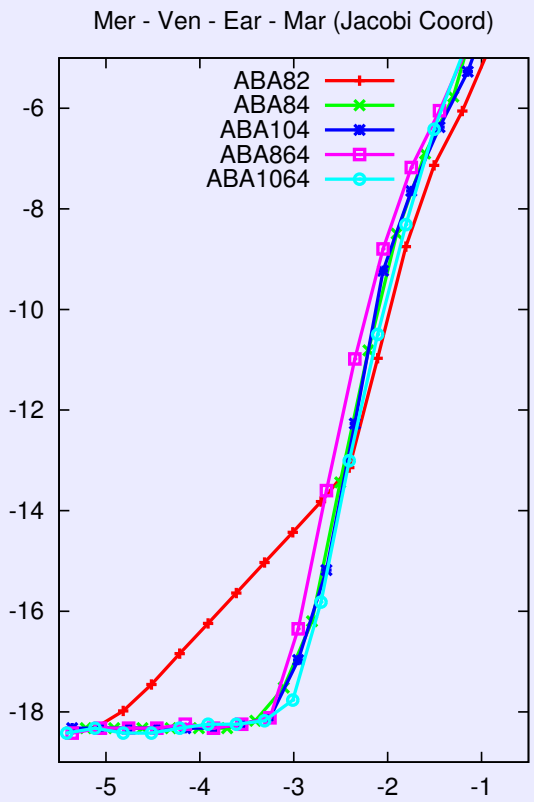
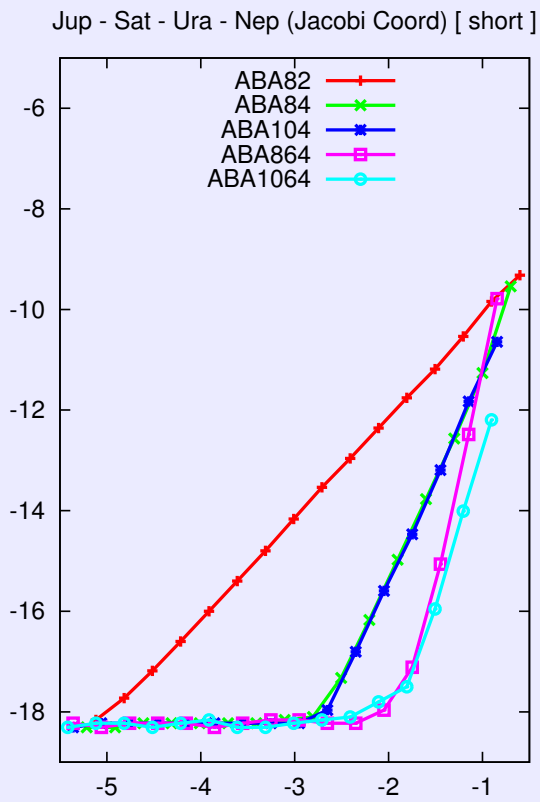
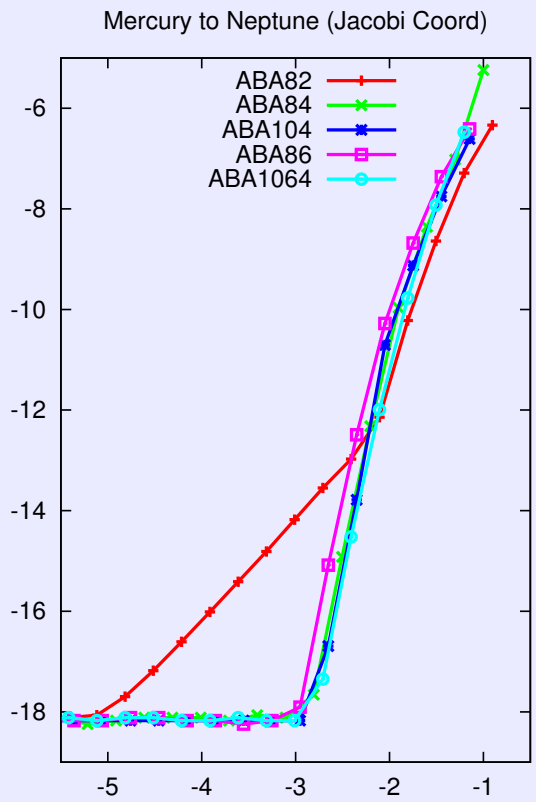


Illustration: Solar System in Jacobi coordinates







New directions

- Is it possible to construct even more efficient schemes?
- One possibility: the use of processing
- Methods with a reduced number of stages
- Appropriate for long term integrations
- Well suited (we believe) for near-integrable problems

III. PROCESSOR AND STARTER

Processing

- Methods of the form

$$\hat{\psi}_\tau = \pi_\tau^{-1} \circ \psi_\tau \circ \pi_\tau$$

- We *enhance*, *correct* or *process* the numerical scheme ψ_τ (the kernel) with a (near-identity) map π_τ (the processor or corrector) so that the resulting method $\hat{\psi}_\tau$ is 'better' than ψ_τ.
- After n steps,

$$\hat{\psi}_\tau^n = \pi_\tau^{-1} \circ \psi_\tau^n \circ \pi_\tau$$

- Introduced by J. Butcher in 1969 in the context of Runge–Kutta methods
- Processing + splitting: McLachlan, Wisdom, Sanz-Serna, Blanes, Ros, Murua,...

Effective order

- ψ_τ is of *effective order* r if a processor π_τ exists for which $\hat{\psi}_\tau$ is of order r,

$$\hat{\psi}_\tau = \pi_\tau^{-1} \circ \psi_\tau \circ \pi_\tau = \varphi_\tau + \mathcal{O}(\tau^{r+1})$$

- Many order conditions can be satisfied by π_τ, and thus ψ_τ must verify a much reduced set of conditions (less stages!!)
- Splitting + processing for near-integrable problems
- ... In particular for the integration of the Solar System (very long time integrations with a few intermediate outputs)

Analysis

$$\hat{\psi}_\tau = \pi_\tau^{-1} \circ \psi_\tau \circ \pi_\tau$$

- Analysis as in the usual case: with operators
- For the kernel $\psi_\tau \quad \Rightarrow \quad \Psi(\tau) = \exp(K)$
- For the processor $\pi_\tau \quad \Rightarrow \quad \Pi(\tau) = \exp(P)$
- Then

$$\hat{\Psi}(\tau) = \mathrm{e}^{\hat{F}} = \Pi(\tau)\Psi(\tau)\Pi^{-1}(\tau) = \mathrm{e}^{P}\mathrm{e}^{K}\mathrm{e}^{-P}$$

and thus

$$\hat{F} = \mathrm{e}^{P} K \mathrm{e}^{-P} = \mathrm{e}^{\mathrm{ad}_P} K$$

- Both the kernel and the processor are built as compositions:

$$\begin{aligned} \mathrm{e}^{K} &= \mathrm{e}^{a_1\tau A}\,\mathrm{e}^{b_1\tau\varepsilon B}\cdots\mathrm{e}^{a_s\tau A}\,\mathrm{e}^{b_s\tau\varepsilon B}\,\mathrm{e}^{a_{s+1}\tau A} \\ \mathrm{e}^{P} &= \mathrm{e}^{c_1\tau A}\,\mathrm{e}^{d_1\tau\varepsilon B}\cdots\mathrm{e}^{c_q\tau A}\,\mathrm{e}^{d_q\tau\varepsilon B}\,\mathrm{e}^{c_{q+1}\tau A} \end{aligned}$$

- Symmetric kernel. Then

$$\sum_{j=1}^{s+1} a_j = \sum_{j=1}^{s} b_j = 1, \qquad \sum_{j=1}^{q+1} c_j = \sum_{j=1}^{q} d_j = 0$$

Procedure

1. Solve the effective order conditions for the kernel (more stages than strictly necessary for optimization, etc.): very good kernels
2. Given a particular kernel, solve the conditions for the processor

Remark: It is important to evaluate π_τ as accurately as possible, whereas π_τ^{-1} can be safely approximate (the error does not propagate). (just the opposite of G. Vilmart's problem for SDE)

- Several processed splitting methods exist involving less stages for near-integrable problems
- For simple examples they show an excellent behavior
- In the integration of the Solar System, however, they present some drawbacks (*instabilities*, etc.)
- Instabilities can be traced to the fact that

$$\sum_{j=1}^{q+1} c_j = \sum_{j=1}^{q} d_j = 0$$

  for the processor, which can produce *large* coefficients
- Is there any procedure to avoid that?

Starter

- The use of a starter (J. Butcher, 1969)
- Consider 3 steps of a processed method (in terms of series of differential operators):

$$\begin{aligned} \mathrm{e}^{P}\mathrm{e}^{3K}\mathrm{e}^{-P} &= \left(\mathrm{e}^{P}\mathrm{e}^{K}\right)\mathrm{e}^{K}\left(\mathrm{e}^{K}\mathrm{e}^{-P}\right) \\ &\equiv \mathrm{e}^{T}\mathrm{e}^{K}\mathrm{e}^{V} \end{aligned}$$

- T and V are power series expansions in terms of A, B and their nested Lie brackets $[A,B]$, $[A,[A,B]]$, $[B,[A,B]]$, etc
- Coefficients of T and V can be obtained from those of P and K
- Order conditions to be satisfied by P translate into conditions for T and V

- Since K is symmetric and of effective order r, then it is true that
$$V(\tau) = -T(-\tau) + \mathcal{O}(\tau^{r+1}),$$
so that
$$(\mathrm{e}^{T})^{*} \equiv \mathrm{e}^{-T(-\tau)} = \mathrm{e}^{V(\tau)} + \mathcal{O}(\tau^{r+1}),$$
and
$$\mathrm{e}^{T}\mathrm{e}^{K}(\mathrm{e}^{T})^{*} = \mathrm{e}^{3\hat{F}} + \mathcal{O}(\tau^{r+1})$$
- We consider the composition $\mathrm{e}^{T}\mathrm{e}^{K}(\mathrm{e}^{T})^{*}$ as our approximation
- ... but in this case to the exact solution after time 3τ

- We construct the starter e^{T} as the composition

$$\mathrm{e}^{T} = \mathrm{e}^{\alpha_1 \tau A}\, \mathrm{e}^{\beta_1 \tau \varepsilon B} \cdots \mathrm{e}^{\alpha_q \tau A}\, \mathrm{e}^{\beta_q \tau \varepsilon B}$$

  so that

$$(\mathrm{e}^{T})^{*} = \mathrm{e}^{\beta_q \tau \varepsilon B}\, \mathrm{e}^{\alpha_q \tau A} \cdots \mathrm{e}^{\beta_1 \tau \varepsilon B}\, \mathrm{e}^{\alpha_1 \tau A}$$

- Advantages:
  - The whole method is *symmetric*
  - Now $\sum_{j=1}^{q} \alpha_j = \sum_{j=1}^{q} \beta_j = 1$ and the coefficients are more reduced in size
- Our aim: to construct methods $(8,4)$, $(8,6,4)$, $(10,6,4)$ with processing involving less stages to be used in the integration of the Solar System (Jacobi and Heliocentric)

Jacobi

- $(s, 4)$: kernel with 2 stages involving only complex solutions $\Rightarrow$ minimum number of stages: 3
- But with 3 stages, already methods $(s, 6, 4)$
- $(8, 6, 4)$.
  - Kernel with 3 stages: $a_1 b_1 a_2 b_2 a_2 b_1 a_1$. 2 solutions
  - Starter with (at least) 5 stages
  - Add more stages in the kernel for optimization (4 or 5)
- Same strategy for Heliocentric coordinates: add one additional stage in the kernel

Work in progress