Sympletic Methods for Long-Term Integration of the Solar System

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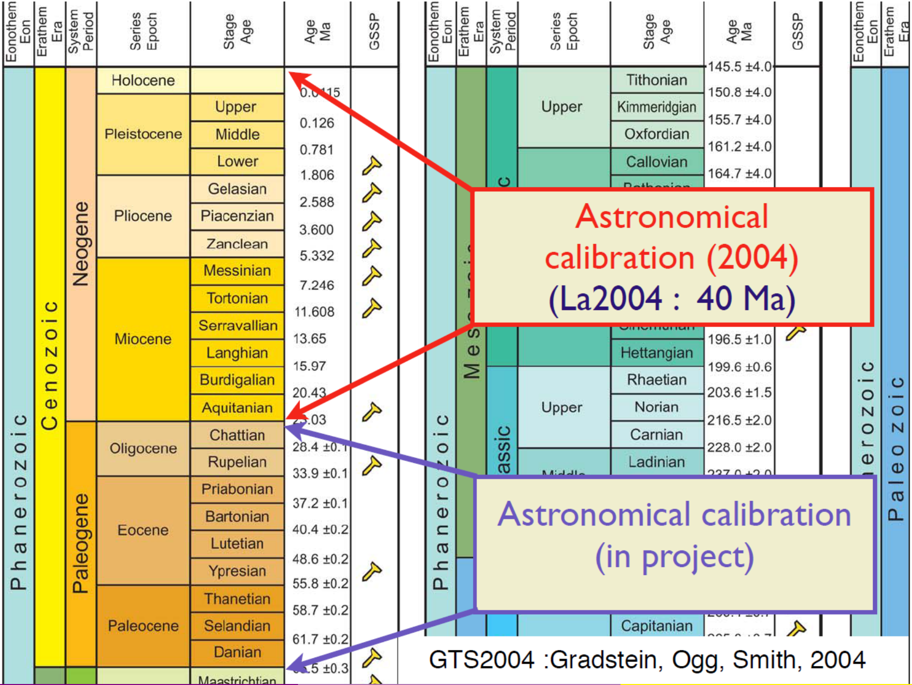
Overview of the Talk

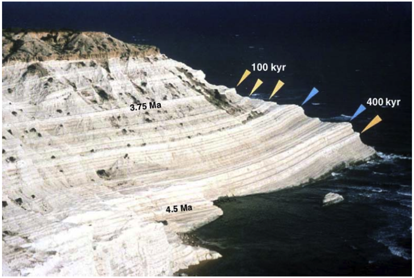
1. *Why do we want long-term integrations of the Solar System ?*
2. *The N-Body Problem (Toy model for the Planetary motion)*
3. *Symplectic Splitting Methods for Hamiltonian Systems*

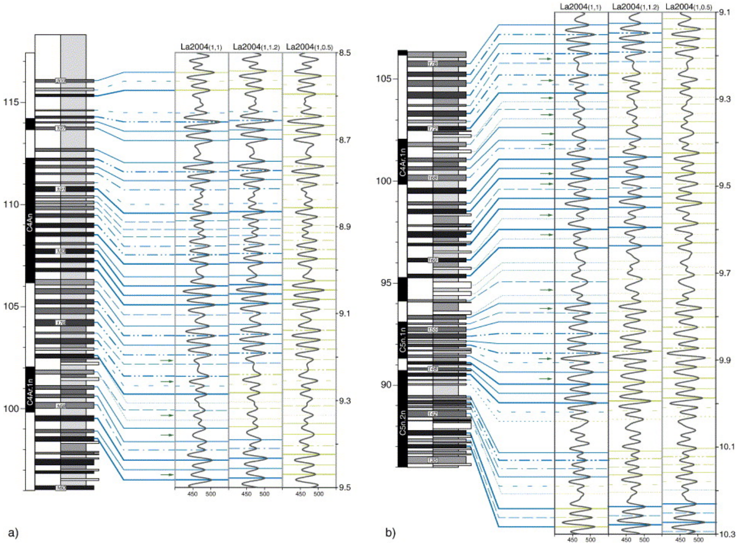
GTS_{next}-EU
towards the next generation Geological Time Scale for the last 100 million years

PEOPLE
MARIE CURIE ACTIONS


Eonothem Eon
Erathem Era
System Period
Series Epoch
Stage Age
Age Ma
GSSP
Phanerozoic
Cenozoic
Neogene
Paleogene
Holocene
Pleistocene
Pliocene
Miocene
Oligocene
Eocene
Paleocene
Upper
Middle
Lower
Gelasian
Piacenzian
Zanclean
Messinian
Tortonian
Serravallian
Langhian
Burdigalian
Aquitanian
Chattian
Rupelian
Priabonian
Bartonian
Lutetian
Ypresian
Thanetian
Selandian
Danian
Maastrichtian
0.126
0.781
1.806
2.588
3.600
5.332
7.246
11.608
13.65
15.97
20.43
28.4 ±0.1
33.9 ±0.1
37.2 ±0.1
40.4 ±0.2
48.6 ±0.2
55.8 ±0.2
58.7 ±0.2
61.7 ±0.2
Mesozoic
Paleozoic
Upper
Tithonian
Kimmeridgian
Oxfordian
Callovian
Hettangian
Rhaetian
Norian
Carnian
Ladinian
Capitanian
145.5 ±4.0
150.8 ±4.0
155.7 ±4.0
161.2 ±4.0
164.7 ±4.0
196.5 ±1.0
199.6 ±0.6
203.6 ±1.5
216.5 ±2.0
228.0 ±2.0
Astronomical calibration (2004)
(La2004 : 40 Ma)
Astronomical calibration
(in project)
GTS2004 :Gradstein, Ogg, Smith, 2004


Solasaga


100 kyr
400 kyr
3.75 Ma
4.5 Ma


a)
b)
La2004(1,1)
La2004(1,1.2)
La2004(1,0.5)
C4An
C4Ar.1n
C5n.1n
C5n.2n
115
110
105
100
95
90
8.5
8.7
8.9
9.1
9.3
9.5
9.7
9.9
10.1
10.3
450
500

La2010: A new orbital solution for the long term motion of the Earth.

J. Laskar[1], A. Fienga[1,2], M. Gastineau[1], and H. Manche[1]

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March 8, 2011

Abstract. We present here a new solution for the astronomical computation of the orbital motion of the Earth spanning from 0 to −250 Myr. The main improvement with respect to the previous numerical solution La2004 (Laskar et al. 2004) is an improved adjustment of the parameters and initial conditions through a fit over 1 Myr to a special version of the high accurate numerical ephemeris INPOP08 (Fienga et al. 2009). The precession equations have also been entirely revised and are no longer averaged over the orbital motion of the Earth and Moon. This new orbital solution is now valid over more than 50 Myr in the past or in the future with proper phases of the eccentricity variations. Due to chaotic behavior, the precision of the solution decreases rapidly beyond this time span, and we discuss the behavior of various solutions beyond 50 Myr. For paleoclimate calibrations, we provide several different solutions that are all compatible with the most precise planetary ephemeris. We have thus reached the time where geological data are now required to discriminate among planetary orbital solutions beyond 50 Myr.

1. Introduction

Due to gravitational planetary perturbations, the elliptical

& Holman 1991), confirming the chaotic behavior found by Laskar (1989, 1990). Following the improvement of com-

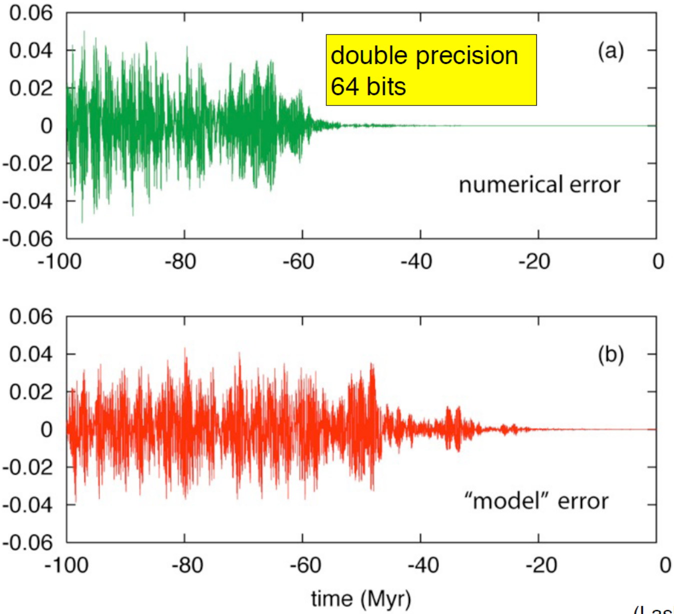
Planetary Solution

- La2004 : numerical, simplified,
  tuned to DE406 (6000 yr)

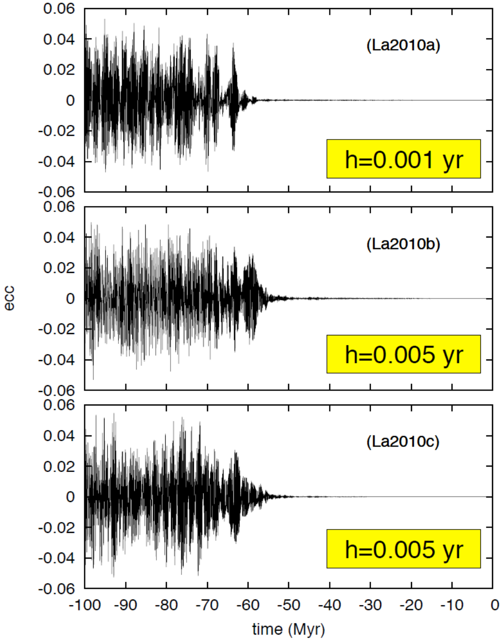
- INPOP : numerical, "complete",
  adjusted to 45000 observations.
  1 Myr : 6 months of CPU.

- La2010 : numerical, less simplified,
  tuned to INPOP (1 Myr).
  250Myr : 18 months of CPU.

eccentricity of the Earth (La2004)



(Laskar et al, 2004)



Numerical Precision

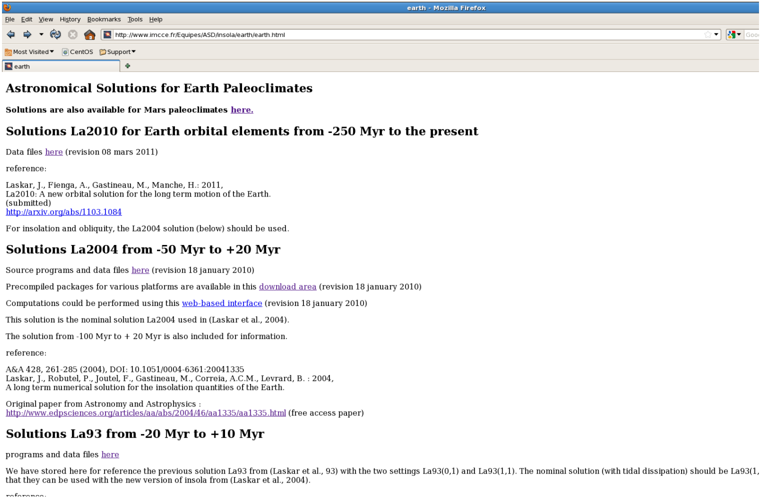
La2010a
is fine for 60 Myr

But
18 months of CPU
for 250 Myr !

(Laskar et al, 2010)

For further information

http://www.imcce.fr/Equipes/ASD/insola/earth/earth.html



Astronomical Solutions for Earth Paleoclimates

Solutions are also available for Mars paleoclimates here.

Solutions La2010 for Earth orbital elements from -250 Myr to the present

Data files here (revision 08 mars 2011)

reference:

Laskar, J., Fienga, A., Gastineau, M., Manche, H.: 2011,
La2010: A new orbital solution for the long term motion of the Earth.
(submitted)
http://arxiv.org/abs/1103.1084

For insolation and obliquity, the La2004 solution (below) should be used.

Solutions La2004 from -50 Myr to +20 Myr

Source programs and data files here (revision 18 january 2010)

Precompiled packages for various platforms are available in this download area (revision 18 january 2010)

Computations could be performed using this web-based interface (revision 18 january 2010)

This solution is the nominal solution La2004 used in (Laskar et al., 2004).

The solution from -100 Myr to + 20 Myr is also included for information.

reference:

A&A 428, 261-285 (2004), DOI: 10.1051/0004-6361:20041335
Laskar, J., Robutel, P., Joutel, F., Gastineau, M., Correia, A.C.M., Levrard, B. : 2004,
A long term numerical solution for the insolation quantities of the Earth.

Original paper from Astronomy and Astrophysics :
http://www.edpsciences.org/articles/aa/abs/2004/46/aa1335/aa1335.html (free access paper)

Solutions La93 from -20 Myr to +10 Myr

programs and data files here

We have stored here for reference the previous solution La93 from (Laskar et al., 93) with the two settings La93(0,1) and La93(1,1). The nominal solution (with tidal dissipation) should be La93(1,
that they can be used with the new version of insola from (Laskar et al., 2004).

The Challenge

1. The NUMERICAL PRECISION of the solution. We want to be sure that the precision is not a limiting factor.
2. The SPEED of the algorithm. As La2010a took nearly 18 months to complete.

The N - Body Problem

The N-Body Problem

We consider that we have $n+1$ particles (n planets + the Sun) interacting between each other due to their mutual gravitational attraction.

We consider:

- $\mathbf{u_0}, \mathbf{u_1}, \ldots, \mathbf{u_n}$ and $\dot{\mathbf{u}}_\mathbf{0}, \dot{\mathbf{u}}_\mathbf{1}, \ldots, \dot{\mathbf{u}}_\mathbf{n}$ the position and velocities of the $n+1$ bodies with respect to the centre of mass.
- $\tilde{\mathbf{u}}_\mathbf{i} = m_i \dot{\mathbf{u}}_\mathbf{i}$ the conjugated momenta.

The equations of motion are Hamiltonian:

$$H = \frac{1}{2}\sum_{i=0}^{n} \frac{||\tilde{\mathbf{u}}_\mathbf{i}||^2}{m_i} - G \sum_{0\le i<j\le n} \frac{m_i m_j}{||\mathbf{u_i} - \mathbf{u_j}||}. \tag{1}$$

Notice that the Hamiltonian is naturally split as $H = T(p) + U(q)$.

The N-Body Problem (Planetary Case)

In an appropriate set of coordinates:

$$H = H_A(p, q) + \varepsilon H_B(q)$$

$$H = H_A(a) + \varepsilon H_B(a, \lambda, e, \omega, i, \Omega)$$

Where H_A corresponds to the **Keplerian motion** and H_B to the **Planetary interactions**.

Change of variables:

$$(p, q) \longrightarrow (a, \lambda, e, \omega, i, \Omega)$$

(Wisdom & Holman, 1991
Kinoshita, Yoshida, Nakai, 1991)

Jacobi Coordinates

We consider the position of each planet (P_i) w.r.t. the centre of mass of the previous planets ($P_0, \ldots, P_{i-1}$).

$$\left.\begin{array}{rcl} \mathbf{v_0} & = & (m_0\mathbf{u_0} + \cdots + m_n\mathbf{u_n})/\eta_n \\ \mathbf{v_i} & = & \mathbf{u_i} - (\sum_{j=0}^{i-1} m_j\mathbf{u_j})/\eta_{i-1} \end{array}\right\}, \qquad \left.\begin{array}{rcl} \tilde{\mathbf{v}}_0 & = & \tilde{\mathbf{u}}_0 + \cdots + \tilde{\mathbf{u}}_n \\ \tilde{\mathbf{v}}_i & = & (\eta_{i-1}\tilde{\mathbf{u}}_i - m_i(\sum_{j=0}^{i-1} \mathbf{u_j}))/\eta_i \end{array}\right\}.$$

where $\eta_i = \sum_{j=0}^{i} m_j$.

In this set of coordinates the Hamiltonian is naturally split into two part: $H_J = H_{Kep} + H_{pert}$:

$$H_J = \sum_{i=1}^{n} \left(\frac{1}{2}\frac{\eta_i}{\eta_{i-1}}\frac{||\tilde{\mathbf{v}}_i||^2}{m_i} - G\frac{m_i\eta_{i-1}}{\mathbf{v_i}} \right) + G\left[\sum_{i=2}^{n} m_i \left(\frac{\eta_{i-1}}{||\mathbf{v_i}||} - \frac{m_0}{||\mathbf{r_i}||} \right) - \sum_{0<i<j\leq n} \frac{m_i m_j}{\Delta_{ij}} \right],$$

where $\Delta_{i,j} = ||\mathbf{u_i} - \mathbf{u_j}||$.

Heliocentric Coordinates

We consider relative position of each planet (P_i) with respect to the Sun (P_0).

$$\left.\begin{array}{rcl} \mathbf{r_0} & = & \mathbf{u_0} \\ \mathbf{r_i} & = & \mathbf{u_i} - \mathbf{u_0} \end{array}\right\}, \qquad \left.\begin{array}{rcl} \tilde{\mathbf{r}}_\mathbf{0} & = & \tilde{\mathbf{u}}_\mathbf{0} + \cdots + \tilde{\mathbf{u}}_\mathbf{n} \\ \tilde{\mathbf{r}}_\mathbf{i} & = & \tilde{\mathbf{u}}_\mathbf{i} \end{array}\right\},$$

In this set of coordinates the Hamiltonian is naturally split into two part: $H_H = H_{Kep} + H_{pert}$:

$$H_H = \sum_{i=1}^{n} \left(\frac{1}{2} ||\tilde{\mathbf{r}}_\mathbf{i}||^2 \left[\frac{m_0 + m_i}{m_0 m_i} \right] - G \frac{m_0 m_i}{\mathbf{r_i}} \right) + \sum_{0<i<j\leq n} \left(\frac{\tilde{\mathbf{r}}_\mathbf{i} \cdot \tilde{\mathbf{r}}_\mathbf{j}}{m_0} - G \frac{m_i m_j}{\Delta_{ij}} \right),$$

where $\Delta_{i,j} = ||\mathbf{r_i} - \mathbf{r_j}||$.

Jacobi Vs Heliocentric coordinates

In both cases we have $H = H_{Kep} + H_{pert}$. But:

- $H_H = H_A(p, q) + \varepsilon(H_B(q) + H_C(p))$,
- $H_J = H_A(p, q) + \varepsilon H_B(q)$,

where H_A, H_B and H_C are integrable on their own.

Remarks:

- the size of the perturbation in Jacobi coordinates is smaller that the size of the perturbation in Heliocentric coordinates, giving a better approximation of the real dynamics.
- the expressions in Heliocentric coordinates are easier to handle, and do not require a specific order on the planets.

Jacobi Vs Heliocentric (size of perturbation)

np,case	Heliocentric Pert.	Jacobi Pert.
2, MV	5.264837243090217E-011	2.507597928893501E-011
2, JS	2.336559877558003E-006	8.255625324341979E-007
4, MM	9.165205211655520E-010	6.334248585000000E-010
4, JN	2.718444355584028E-006	8.716288751176844E-007
8, MN	2.804289442433957E-006	8.715850310304487E-007
8, VP	2.802584202262463E-006	8.715856645507914E-007
9, All	2.804292431703275E-006	8.715852470196316E-007

Table: Size of the perturbation in Heliocentric Vs Jacobi coordinates for different type of planetary configurations.

Jacobi Vs Heliocentric coordinates

i, j	Heliocentric Pert.	Jacobi Pert.
1,2	5.26483724309021731E-011	2.50759792889350194E-011
2,3	7.59739225393103695E-010	5.95009062984183148E-010
3,4	3.48299827426021253E-011	5.52675544625019969E-011
4,5	6.43324771287086414E-009	3.25222776727405301E-010
5,6	2.33655987755800395E-006	8.25562532434197998E-007
6,7	5.62192585020240051E-008	1.31346460445138887E-008
7,8	5.38356857904020469E-009	2.86142920053947548E-009
8,9	4.52500558799539687E-013	2.40469325009519492E-013

Table: Size of the perturbation in Heliocentric Vs Jacobi coordinates for the consecutive pair of planets. Here, 1 = Mercury, 2 = Venus, 3 = Earth-Moon Barycentre, 4 = Mars, 5 = Jupiter, 6 = Saturn, 7 = Uranus, 8 = Neptune, 9 = Pluto.

Symplectic Splitting Methods for Hamiltonian Systems

Splitting Methods for Hamiltonian Systems

Let $H(q,p)$ be a Hamiltonian, where (q,p) are a set of canonical coordinates.

$$\frac{dz}{dt} = \{H, z\} = L_H z, \tag{2}$$

where $z = (q,p)$ and $\{\ ,\ \}$ is the Poisson Bracket ($\{F, G\} = F_q G_p - F_p G_q$).

The formal solution of Eq. (2) at time $t = \tau$ that starts at time $t = \tau_0$ is given by,

$$z(\tau) = \exp(\tau L_H) z(\tau_0). \tag{3}$$

- The main idea is to build approximations for $\exp(\tau L_H)$ that preserve the symplectic character.
- We focus on the special case $H = H_A + \varepsilon H_B$, where H_A and H_B are integrable on its own. This is the case of the N-body planetary system, where the system can be expressed as a Keplerian motion plus a small perturbation due to their mutual interaction.

Splitting Methods for Hamiltonian Systems

The formal solution of Eq. (2) at time $t = \tau$ that starts at time $t = \tau_0$ is given by,

$$z(\tau) = \exp(\tau L_H) z(\tau_0) = \exp[\tau(A + \varepsilon B)] z(\tau_0). \tag{4}$$

where $A \equiv L_{H_A}, B \equiv L_{H_B}$.

We recall that H_A and H_B are integrable, hence we can compute $\exp(\tau A)$ and $\exp(\tau B)$ explicitly.

We will construct symplectic integrators, $S_n(\tau)$, that approximate $\exp[\tau(A + \varepsilon B)]$ by an appropriate composition of $\exp(\tau A)$ and $\exp(\tau \varepsilon B)$:

$$\mathcal{S}_n(\tau) = \prod_{i=1}^{n} \exp(a_i \tau A) \exp(b_i \tau \varepsilon B)$$

Splitting Methods for Hamiltonian Systems

Using the Baker-Campbell-Hausdorff (BHC) formula for the product of two exponential of non-commuting operators X and Y:

$$\exp X \exp Y = \exp Z,$$

with

$$Z = X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}([X,[X,Y]] - [Y,[Y,X]]) + \frac{1}{24}[X,[Y,[Y,X]]] + \dots,$$

and $[X,Y] := XY - YX$.

This ensures us that is we have an nth order integrating scheme:

$$\prod_{i=1}^{k} \exp(a_i \tau A) \exp(b_i \tau B) = \exp(\tau D_{\tilde{H}}).$$

Then $\tilde{H} = H + \tau^n H_n + o(\tau^n)$ and the error in energy is of order τ^n.

Two simple examples

- $S_1(\tau) = \exp(\tau A)\exp(\tau B)$,

$$K = A + B + \frac{\tau}{2}[A, B] + \frac{\tau^2}{12}\left([A, [A, B]] + [B, [B, A]]\right) + \dots$$

- $S_2(\tau) = \exp(\tau/2A)\exp(\tau B)\exp(\tau/2A)$,

$$K = A + B + \frac{\tau^2}{6}\left([A, [A, B]] + [B, [B, A]]\right) + \dots$$

Many Authors like Ruth(1983), Neri (1987) and Yoshida(1990) among others have found appropriate set coefficientscients a_i, b_i in order to have a High Order symplectic integrator (4th, 6th, 8th, ...).

Splitting Methods for Hamiltonian Systems

Let us call $\mathcal{S}_n(\tau) = \exp(\tau K)$. Where,

$$\mathcal{S}_n(\tau) = \prod_{i=1}^{n} \exp(a_i \tau A) \exp(b_i \tau \varepsilon B) = \exp(\tau K), \tag{5}$$

The BCH theorem ensures us that $K \in L(\{A, B\})$, the Lie algebra generated by A and B, and it can be expanded as a double asymptotic series in τ and ε:

$$\begin{aligned} \tau K \;&=\; \tau p_{1,0} A \;+\; \varepsilon \tau p_{1,1} B \;+\; \varepsilon \tau^2 p_{2,1}[A, B] \\ &+ \varepsilon \tau^3 p_{3,1}[A,[A,B]] \;+\; \varepsilon^2 \tau^3 p_{3,2}[B,[B,A]] \\ &+ \varepsilon \tau^4 p_{4,1}[A,[A,[A,B]]] \;+\; \varepsilon^2 \tau^4 p_{4,2}[A,[B,[B,A]]] \;+\; \varepsilon^3 \tau^4 p_{4,3}[B,[B,[B,A]] + \ldots, \end{aligned}$$

where $p_{i,j}$ are polynomials in a_i and b_i.

Splitting Methods for Hamiltonian Systems

We will say that a method $\mathcal{S}_n(\tau)$ has order p if $K = A + \varepsilon B + o(\tau^p)$.

- Hence, the coefficients a_i, b_i must satisfy:

$$p_{1,0} \; = \; 1, \qquad p_{1,1} \; = \; 1, \qquad p_{i,j} \; = \; 0, \text{ for } i = 2, \ldots, p.$$

Remark:

- It is easy to check that,

$$\begin{aligned} p_{0,1} &= a_1 + a_2 + \cdots + a_n = 1, \\ p_{1,1} &= b_1 + b_2 + \cdots + b_n = 1. \end{aligned}$$

- If $S_n(\tau) = S_n(-\tau)$ then all the terms of order τ^{2k+1} are cancelled out.

Splitting Methods for Hamiltonian Systems

$$\mathcal{S}_n(\tau) = \prod_{i=1}^{n} \exp(a_i \tau A) \exp(b_i \varepsilon \tau B) = \exp(\tau K),$$

In general $\varepsilon \ll \tau$ (or at least $\varepsilon \approx \tau$), so we are more interested in killing the error terms with small powers of ε. We will find the coefficient a_i, b_i such that:

$$|\tau K - \tau(A + \varepsilon B)| = \mathcal{O}(\varepsilon \tau^{s_1+1} + \varepsilon^2 \tau^{s_2+1} + \varepsilon^3 \tau^{s_3+1} + \cdots + \varepsilon^m \tau^{s_m+1}). \qquad (6)$$

Definition

We will say that the method $\mathcal{S}_n(\tau)$ has n stages if it requires n evaluations of $\exp(\tau A)$ and $\exp(\tau B)$ per step-size.

Definition

We will say that the method $\mathcal{S}_n(\tau)$ has order $(s_1, s_2, s_3, \dots)$ if it satisfies Eq. (6).

$\mathcal{SABA}_n$ or McLachlan (2n,2) methods

McLachlan, 1995; Laskar & Robutel, 2001, considered symmetric schemes that only killed the terms of order $\tau^k\varepsilon$ for $k = 1, ..., 2n$.

$$\mathcal{S}_m(\tau) = \exp(a_1\tau A)\exp(b_1\tau B)\ldots\exp(b_1\tau B)\exp(a_1\tau A).$$

The main advantages are that:

- We only need n stages to have a method of order $(2n, 2)$.
- We can guarantee that for all n the coefficients a_i, b_i will always be positive.

- McLachlan, 1995: "*Composition methods in the presence of small parameters*", BIT 35(2), pp. 258-268.

- Laskar & Robutel, 2001: "*High order symplectic integrators for perturbed Hamiltonian systems*", Celestial Mechanics and Dynamical Astronomy 80(1), 39-62.

$\mathcal{SABA}_n$ or McLachlan (2n,2) methods

McLachlan, 1995; Laskar & Robutel, 2001

id	order	stages	a_i	b_i
SABA1 or ABA22	$(2,2)$	1	$a_1 = 1/2$	$b_1 = 1$
SABA2 or ABA42	$(4,2)$	2	$a_1 = 1/2 - \sqrt{3}/6$ $a_2 = \sqrt{3/3}$	$b_1 = 1/2$
SABA3 or ABA62	$(6,2)$	3	$a_1 = 1/2 - \sqrt{15}/10$ $a_2 = \sqrt{15}/10$	$b_1 = 5/18$ $b_2 = 4/9$
SABA4 or ABA82	$(8,2)$	4	$a_1 = 1/2 - \sqrt{525 + 70\sqrt{30}}/70$ $a_2 = \left(\sqrt{525 + 70\sqrt{30}} - \sqrt{525 - 70\sqrt{30}}\right)/70$ $a_3 = \sqrt{525 - 70\sqrt{30}}/35$	$b_1 = 1/4 - \sqrt{30}/72$ $b_2 = 1/4 + \sqrt{30}/72$
SBAB1 or BAB22	$(2,2)$	1	$a_1 = 1$	$b_1 = 1/2$
SBAB2 or BAB42	$(4,2)$	2	$a_1 = 1/2$	$b_1 = 1/6$ $b_2 = 2/3$
SBAB3 or BAB62	$(6,2)$	3	$a_1 = 1/2 - \sqrt{5}/10$ $a_2 = \sqrt{5}/5$	$b_1 = 1/12$ $b_2 = 5/12$
SBAB4 or BAB82	$(8,2)$	4	$a_1 = 1/2 - \sqrt{3/7}/2$ $a_2 = \sqrt{3/7}/2$	$b_1 = 1/20$ $b_2 = 49/180$ $b_3 = 16/45$

Table: Table of coefficients for the ABA, BAB methods of order $(2s,2)$ for $s = 1,\ldots,4$.

$\mathcal{SABA}_n$ or McLachlan (2n,2) methods

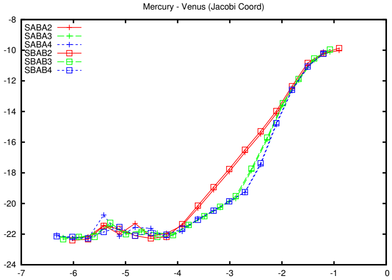


Figure: Comparison of the performance of the $SABA_n$ and $SBAB_n$ schemes for the couples Mercury - Venus (left) and the Jupiter-Saturn (right) (**Jacobi Coordinates**) In log scale maximum error energy Vs. cost (τ/n).

$\mathcal{SABA}_n$ or McLachlan (2n,2) methods

- As we have seen in the figures above, the main limiting factor of these methods are the terms of order $\tau\varepsilon^2$, which become relevant when τ is small.

- We recall that in the methods described above we have:

$$K \;=\; (A \;+\; \varepsilon B) \;+\; \varepsilon\tau^{2n}p_{2n,1}[A,[A,[A,B]]] \;+\; \varepsilon^2\tau^2 p_{3,2}[B,[B,A]] + \ldots,$$

- There are in the literature several options to kill the terms of order $\tau^2\varepsilon^2\{\{A,B\},B\}$.

Symplectic Integrator (killing the terms of higher order)

Let $S_0(\tau)$ be any of the given symmetric symplectic schemes previously described:

$$\mathcal{S}_0(\tau) = \exp(a_1\tau A)\exp(b_1\tau B)\dots\exp(b_1\tau B)\exp(a_1\tau A) = \exp(\tau K),$$

where $K = (A + \varepsilon B) + \varepsilon\tau^{2n}p_{2n,1}[A,[A,[A,B]]] + \varepsilon^2\tau^2 p_{3,2}[B,[B,A]] + \dots.$

In order to kill the terms of order $\varepsilon^2\tau^2$ we can:

1. Add a corrector term: $\exp(-\tau^3\varepsilon^2 c/2L_C)S_0(\tau)\exp(-\tau^3\varepsilon^2 c/2L_C)$.
2. Composition method: $S_0^m(\tau)S_0(c\tau)S_0^m(\tau)$, where $c = -(2m)^{-1/3}$.
3. Add extra stages: $S(\tau) = \prod_{i=1}^{m}\exp(a_i\tau A)\exp(b_i\tau B)$, with $m > n$.

Hence, the reminder will be $\tau^{2n}\varepsilon + \tau^4\varepsilon^2$, having methods of order $(2n, 4)$.

The corrector term L_C

This option was proposed by *Laskar & Robutel, 2001*.

$$K = (A + \varepsilon B) + \varepsilon^2\tau^2 p_{3,2}[B,[B,A]] + \varepsilon\tau^{2n} p_{2n,1}[A,[A,[A,B]]] + \dots,$$

Notice that if A is quadratic in p and B depends only of q then $[B,[B,A]]$ is integrable.

We will consider $SC_n(\tau) = \exp(-\tau^3\varepsilon^2 b/2L_C)S_n(\tau)\exp(-\tau^3\varepsilon^2 b/2L_C)$, with $C = \{\{A,B\},B\}$.

order	c_{ABA_n}	c_{BAB_n}
1	$1/12$	$1/24$
2	$(2-\sqrt{3})/24$	$1/72$
3	$(54-13\sqrt{15})/648$	$(13-5\sqrt{5})/288$
4	0.003396775048208601331532157783492144	$(3861-791\sqrt{21})/64800$

REMARK: This procedure only works in Jacobi coordinates.

Composition method

The idea behind this option was first discussed by *Yoshida (1990)*. generalise

- He showed that if $S(\tau)$ is a symplectic methods of order $2k$, then it is possible to find a new method of order $2k+2$ by taking

$$S(\tau)S(c\tau)S(\tau),$$

where c must satisfy, $c^{2k+1}+2=0$.

- We can generalise these as:

$$S^m(\tau)S(c\tau)S^m(\tau),$$

where now, $c=-(2m)^{1/(2k+1)}$.

- With this simple composition methods we can transform any of the $(2s,2)$ methods described above to $(2s,4)$ method.

REMARK: This procedure works for both set of coordinates.

Adding an extra stage (McLachlan (2s,4))

McLachlan discussed the possibility of adding an extra stage to methods of order $(2s, 2)$ in order to get rid of the $\varepsilon^2\tau^2$ terms:

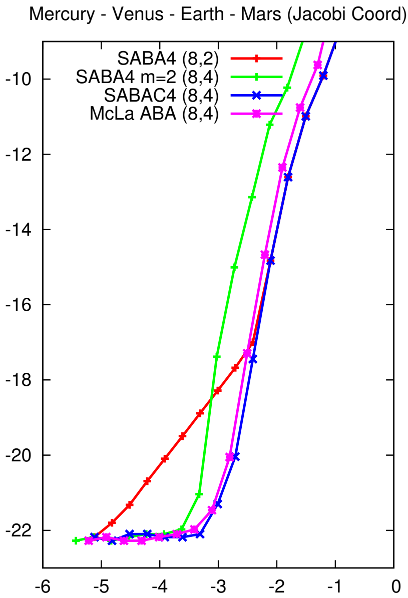
$$S(\tau) = \prod_{i=1}^{n+1} \exp(a_i \tau A) \exp(b_i \tau B)$$

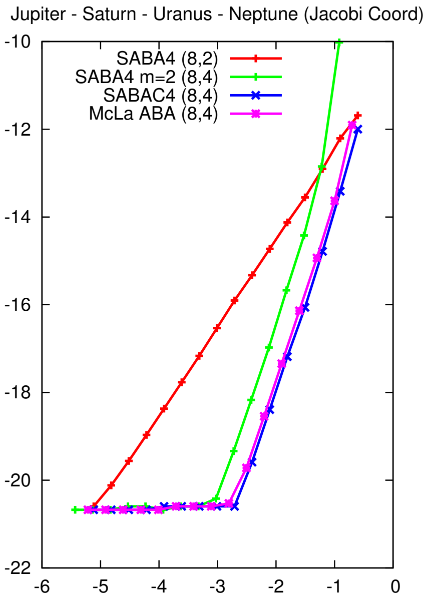
.

id	order	stages	a_i	b_i
ABA64	$(6,4)$	4	$---$	$---$
BAB64	$(6,4)$	4	$a_1 = -0.0437514219173$ $a_2 = 0.5437514219173$	$b_1 = 0.53163862458135$ $b_2 = -0.3086019704406$ $b_3 = 0.55392669171851$
ABA84	$(8,4)$	5	$a_1 = 0.07534696026989$ $a_2 = 0.51791685468825$ $a_3 = -0.0932638149581$	$b_1 = 0.19022593937367$ $b_2 = 0.84652407044352$ $b_3 = -1.0735000196344$
BAB84	$(8,4)$	5	$a_1 = -0.00758691311877$ $a_2 = 0.31721827797316$ $a_3 = 0.38073727029120$	$b_1 = 0.81186273854451$ $b_2 = -0.6774803995321$ $b_3 = 0.36561766098765$

Notice that we no longer have positive values for the coefficients a_i, b_i.

Jacobi Coordinates (first results)





A couple of REMARKS !!

Remark 1: Splitting Methods in Heliocentric Coordinates

We recall that in Heliocentric coordinates:

$$H(p,q) = H_A(p,q) + \varepsilon(H_B(q) + H_C(p)).$$

- We can use the same integrating schemes introduced above:

$$S(\tau) = \prod_{i=1}^{n} \exp(a_i \tau A) \exp(b_i \tau (B + C)),$$

- We can use the approximation:

$$\exp(\tau(B + C)) = \exp(\tau/2C) \exp(\tau B) \exp(\tau/2C).$$

Example (Leap-Frog method):

$$S_1(\tau) = \exp(\tau/2A) \exp(\tau/2C) \exp(\tau B) \exp(\tau/2C) \exp(\tau/2A).$$

REMARK: this introduces an extra error term in the approximation of order $\varepsilon^3\tau^3$.

Remark 2: Compensated Summation

When we solve numerically an ODE, we essentially have a recursive evaluation of the form:

$$y_{n+1} = y_n + \delta_n, \tag{7}$$

where y_n is the approximated solution and δ_n is the increment to be done.

- Usually $|\delta_n| \ll |y_n|$.
- The evaluation of Eq. (7) can cause larger rounding errors that the computation of δ_n.

To reduce this round-off error we can use the so called the *"compensated summation"* algorithm introduced by *Kahan 1965*.

- Kahan W., 1965: "*Pracniques: further remarks on reducing truncation errors*" Communications of the ACM 8(1) pp.40.

- also see: `http://en.wikipedia.org/wiki/Kahan_summation_algorithm`.

Remark 2: Compensated Summation

Definition (Compensated Summation Algorithm)

Let y_0 and $\{\delta_n\}_{n\geq 0}$ be given and assume that we want to compute the terms $y_{n+1} = y_n + \delta_n$.

We start with $e = 0$ and compute $y_1, y_2, \dots$ as follows:

$$
\begin{aligned}
&\textit{for}\ \ n = 0, 1, 2, \dots\ \ \textit{do} \\
&\qquad a = y_n \\
&\qquad e = e + \delta_n \\
&\qquad y_{n+1} = a + e \\
&\qquad e = e + (a - y_{n+1}) \\
&\textit{enddo}
\end{aligned}
$$

Notice that with this algorithm is to accumulate the rounding errors in e and feed them back into the summation when possible.

Remark 2: Compensated Summation

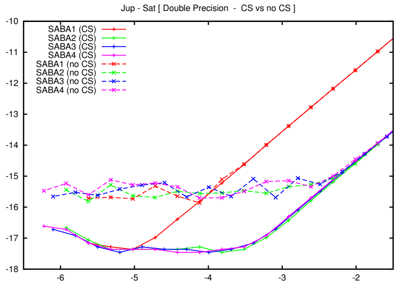
The CODE would look something like this:

```
subroutine pas_B(Xplan,XPplan,tau)
implicit none
integer i
real(TREAL),intent(in) ::  tau
real(TREAL),dimension(3,nplan),intent(inout)::  Xplan,XPplan
real(TREAL), dimension(3)::  AUX

call Accelera(Xplan)
do i=1,nplan
   AUX = XPplan(:,i)
   err(4:6,i,1) = err(4:6,i,1) - tau*(cG*Acc(:,i))
   XPplan(:,i) = AUX + err(4:6,i,1)
   err(4:6,i,1) = err(4:6,i,1) + (AUX - XPplan(:,i))
end do
end subroutine pas_B
```

Remark 2: Compensated Summation

Results: Compensated Summation Vs No Compensated Summation



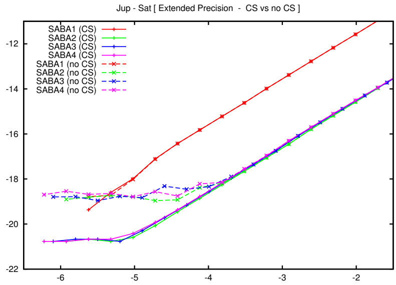
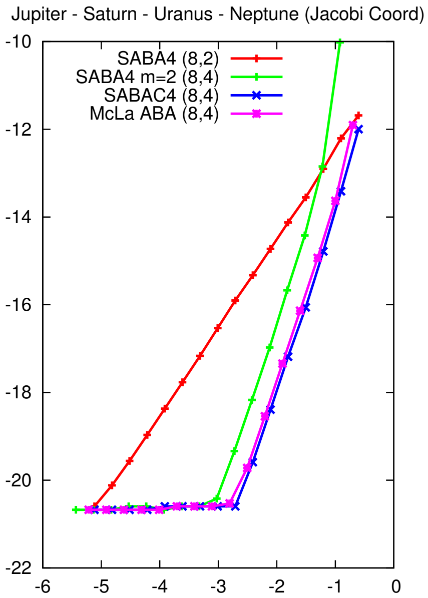
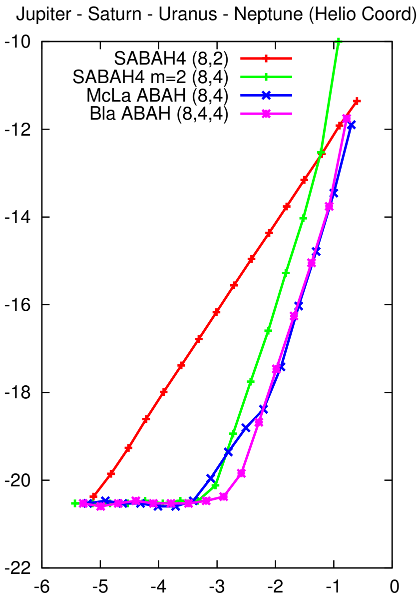


Figure: Maximum variation of the energy versus cost of the $\mathcal{SABA}_n$ schemes on the Sun - Jupiter - Saturn three body problem, with and without the compensated summation. Results using **double precision** arithmetics (left) and **extended precision** arithmetics (right).

End of REMARKS !!

Jacobi vs Heliocentric (first results)





More Splitting Methods (work with S. Blanes et.al)

Our goal is to find new splitting symplectic schemes that will improve the results already discussed.

- Improve the performance of McLachlan in Heliocentric Coordinates.
- Build new schemes for Jacobi Coordinates.
- Build new schemes for Heliocentric Coordinates.

Compare the performance of all of these schemes trying to find the optimal one for our purpose.

Heliocentric Coordinates (Improving McLachlan)

As we have already discussed, in Heliocentric coordinates, we use $\exp(\tau/2C)\exp(\tau B)\exp(\tau/2C)$ to integrate the perturbation part.

- This introduces in our approximation error terms of order $\varepsilon^3\tau^2$ that can become important for small step-sizes. For instance, the McLachlan methods of order $(8,4)$ becomes a method of order $(8,4,2)$
- In order to improve the performance of these scheme, we can add an extra stage to get rid of these term.

$$\prod_{i=1}^{m+1} \exp(a_i\tau A)\exp(b_i\varepsilon\tau B)$$

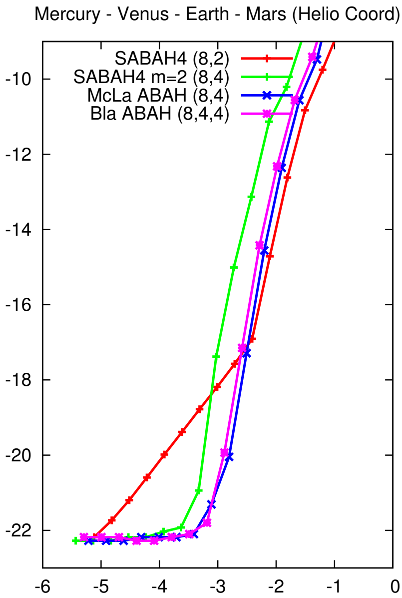
- We must add the extra condition:

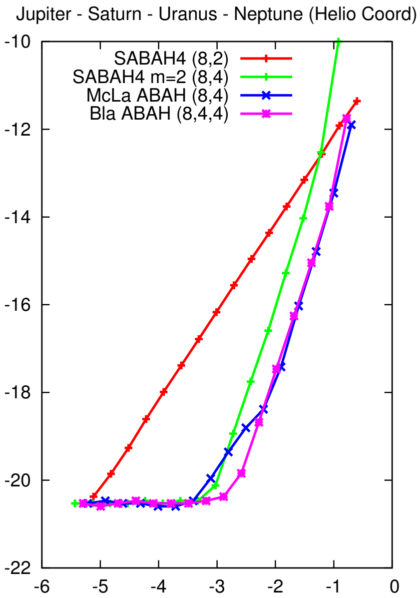
$$b_1^3 + b_2^3 + \cdots + b_m^3 = 0$$

Heliocentric Coordinates (Improving McLachlan)

id	order	n	a_i	b_i
ABAH84	$(8,4)$	5	$a_1 = 0.07534696026989288842$ $a_2 = 0.51791685468825678230$ $a_3 = -0.09326381495814967072$	$b_1 = 0.19022593937367661925$ $b_2 = 0.84652407044352625706$ $b_3 = -1.07350001963440575260$
BAB84	$(8,4)$	5	$a_1 = -0.00758691311877$ $a_2 = 0.31721827797316$ $a_3 = 0.38073727029120$	$b_1 = 0.81186273854451$ $b_2 = -0.6774803995321$ $b_3 = 0.36561766098765$
ABAH844	$(8,4,4)$	6	$a_1 = 0.27414026894340187 62$ $a_2 = -0.10756843844016423 06$ $a_3 = -0.04801850259060169 26$ $a_4 = 0.76289334417472809 43$	$b_1 = 0.64088579516251271 78$ $b_2 = -0.85857544895678285 67$ $b_3 = 0.71768965379427013 89$
BABH844	$(8,4,4)$	6	$a1 = -0.16395870306792437 05$ $a2 = 0.77958251810828947 12$ $a3 = -0.11562381504036510 07$	$b1 = 0.13084241046155891 09$ $b2 = -0.01086448146405448 25$ $b3 = 1.02817800959539007 77$ $b4 = -1.29631187718578901 23$

Heliocentric Coordinates (Improving McLachlan)





New Schemes

In this philosophy, we can always add extra stages in order to kill the desired terms in the error approximation.

$$S_m(\tau) = \prod_{i=1}^{m} \exp(a_i \tau A) \exp(b_i \varepsilon \tau B)$$

We need:

- First to decide which are the most relevant terms that might be limiting our splitting scheme.
- Find the minimal set of coefficients that fulfil our requirements (not trivial).

Possible drawbacks:

- Sometimes many stages are required having no actual gain in the performance of the scheme.
- We will no longer have positive coefficients. This can sometimes produce big rounding error propagation for long term-integration.

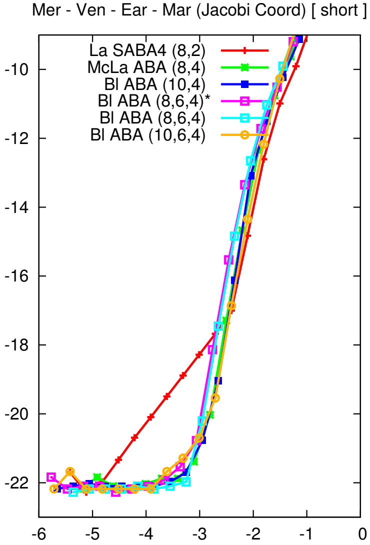
New Schemes for Jacobi Coordinates

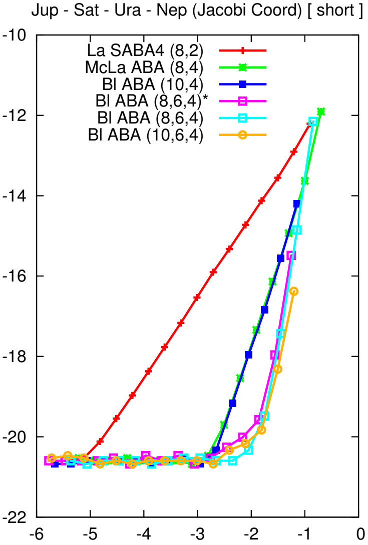
id	order	n	a_i	b_i
ABA82	$(8,2)$	4	$a_1 = 0.06943184420297371$ $a_2 = 0.26057763400459815$ $a_3 = 0.33998104358485626$	$b_1 = 0.17392742256872692$ $b_2 = 0.32607257743127307$
ABA84	$(8,4)$	5	$a_1 = 0.07534696026989288$ $a_2 = 0.51791685468825678$ $a_3 = -0.09326381495814967$	$b_1 = 0.19022593937367661$ $b_2 = 0.84652407044352625$ $b_3 = -1.07350001963440575$
ABA104	$(10,4)$	7	$a_1 = 0.04706710064597250$ $a_2 = 0.18475693541708810$ $a_3 = 0.28270600567983620$ $a_4 = -0.01453004174289681$	$b_1 = 0.11888191736819701$ $b_2 = 0.24105046055150156$ $b_3 = -0.27328666670532380$ $b_4 = 0.82670857757125044$
ABA864	$(8,6,4)$	7	$a_1 = 0.07113342649822311 7$ $a_2 = 0.24115342795664009 8$ $a_3 = 0.52141176177281478 9$ $a_4 = -0.33369861622767800$	$b_1 = 0.18308368747219722 1$ $b_2 = 0.31078285989857486 9$ $b_3 = -0.02656461851195880$ $b_4 = 0.06539614228237341 8$
ABA864* eo$(10,8,6)$	$(8,6,4)$	9	$a_1 = 0.04537121303269675$ $a_2 = 0.26635548892881057$ $a_3 = 0.47099647540428644$ $a_4 = -0.04269356620573340$ $a_5 = 0.5 - (a_1 + a_2 + a_3 + a_4)$	$b_1 = 0.11069709214141803$ $b_2 = 0.45662174680086315$ $b_3 = 0.44701929136469362$ $b_4 = -0.57503410931598372$ $b_5 = 1 - 2(b_1 + b_2 + b_3 + b_4)$
ABA1064	$(10,6,4)$	8	$a_1 = 0.03809449742241219$ $a_2 = 0.14529871611691374$ $a_3 = 0.20762769572554125$ $a_4 = 0.43590970365152615$ $a_5 = -0.65386122583278670$	$b_1 = 0.09585888083707521$ $b_2 = 0.20444615314299878$ $b_3 = 0.21707034797899110$ $b_4 = -0.01737538195906509$

New Schemes for Heliocentric Coordinates

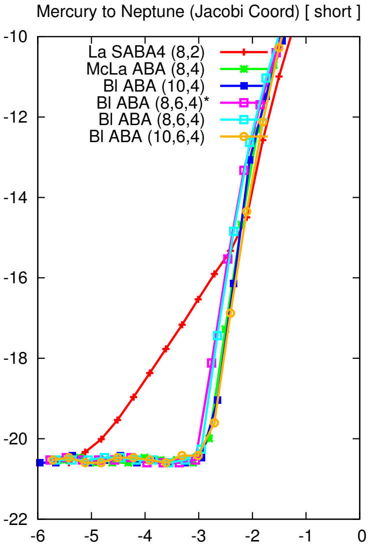
id	order	n	a_i	b_i
ABAH82	$(8, 2)$	4	$a_1 = 0.0694318442029737123$ $a_2 = 0.2605776340045981552$ $a_3 = 0.3399810435848562648$	$b_1 = 0.1739274225687269286$ $b_2 = 0.3260725774312730713$
ABAH84	$(8, 4)$	5	$a_1 = 0.07534696026989288842$ $a_2 = 0.51791685468825678230$ $a_3 = -0.09326381495814967072$	$b_1 = 0.19022593937367661925$ $b_2 = 0.84652407044352625706$ $b_3 = -1.07350001963440575260$
ABAH844	$(8, 4, 4)$	6	$a_1 = 0.2741402689434018762$ $a_2 = -0.1075684384401642306$ $a_3 = -0.04801850259060169267$ $a_4 = 0.7628933441747280943$	$b_1 = 0.6408857951625127178$ $b_2 = -0.8585754489567828567$ $b_3 = 0.7176896537942701389$
ABAH864	$(8, 6, 4)$	8	$a_1 = 0.06810235651658372084$ $a_2 = 0.2511360387221033233$ $a_3 = -0.07507264957216562516$ $a_4 = -0.009544719701745007811$ $a_5 = 0.5307579480704477134$	$b_1 = 0.16844325936189545343$ $b_2 = 0.4243177173742677224$ $b_3 = -0.5858109694681756812$ $b_4 = 0.4930499927320125053$
ABAH1064	$(10, 6, 4)$	9	$a_1 = 0.04731908697653382270$ $a_2 = 0.2651105235748785159$ $a_3 = -0.009976522883811240843$ $a_4 = -0.05992919973494155126$ $a_5 = 0.2574761120673404534$	$b_1 = 0.11968846245853220353$ $b_2 = 0.37529558553793742504$ $b_3 = -0.46845934183259937836$ $b_4 = 0.33513973427558970103$ $b_5 = 0.27667111912108009750$

Results for Jacobi (I)

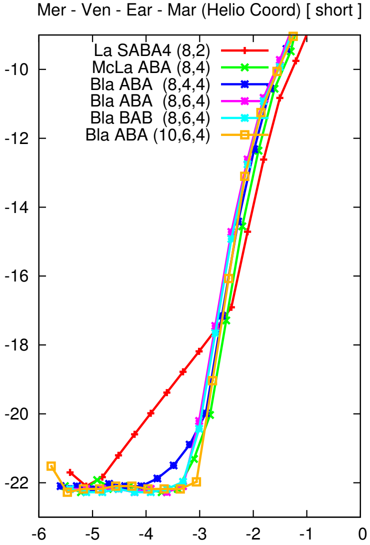


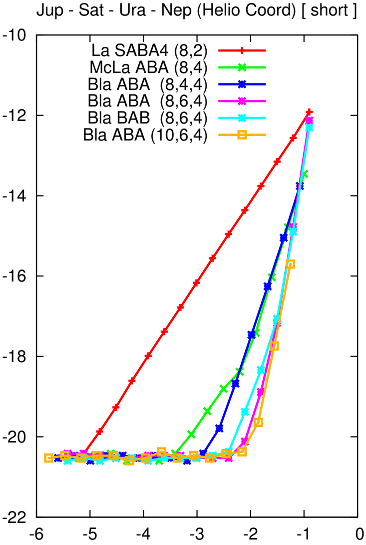


Results for Jacobi (II)

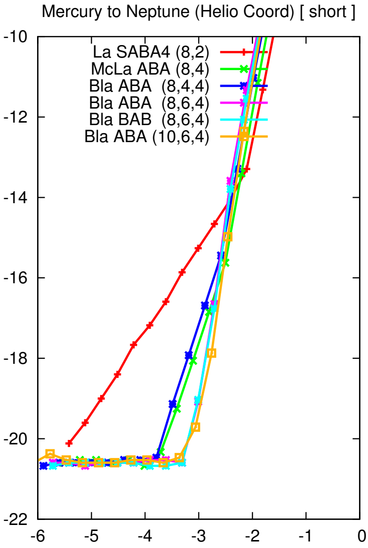


Results for Heliocentric (I)

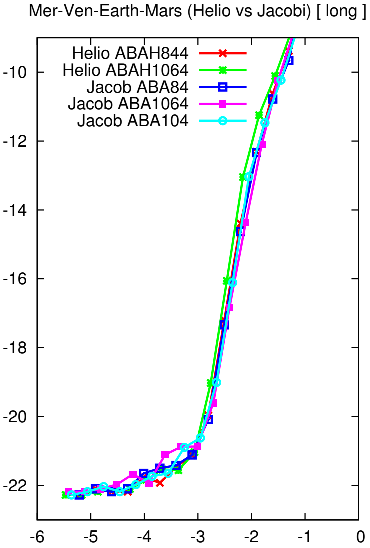


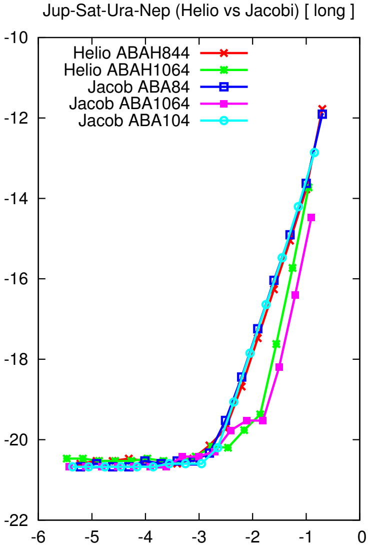


Results for Heliocentric (II)

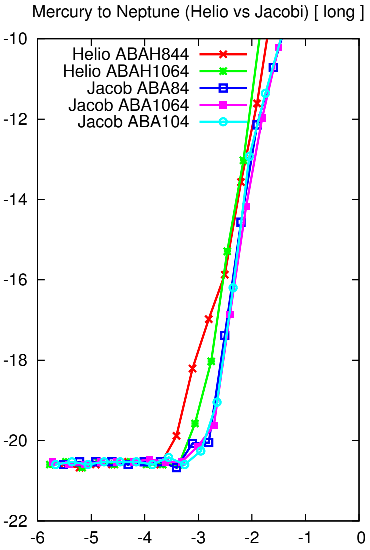


Results Jacobi Vs Heliocentric (I)





Results Jacobi Vs Heliocentric (II)



Final Comments

- Jacobi coordinates offer better results than Heliocentric coordinates.
- The use of a "corrector" is needed in order to improve the efficiency of the splitting methods.
- Adding extra stages in order to improve the error approximation (i.e. methods of order $(8, 4, 4)$, $(8, 6, 4)$, ...) in many cases improves the results.
- The high angular momenta of Mercury is the main limiting factor on the optimal step-size.

Thank You for Your Attention