iSyMBA: A Symplectic Massive Bodies Integrator with Planets Interpolation

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ABSTRACT
A planetary instability occurring at time < 100 My after formation of the giant planets in our solar system can be responsible for some characteristics of the inner solar system. However, the actual influence of the instability on the terrestrial planet formation is not well understood. The simulations of terrestrial planet formation are very CPU-expensive, and this limits the exploration of different instability scenarios. To include the effects of the giant planets instability in the simulations of terrestrial planets formation in a feasible way, we approach the problem in two steps. First, we model and record an evolution of the giant planets that replicates the present outer solar system in the end. Then, we use that orbital record, properly interpolated, as the input for a second step to simulate its effects on the terrestrial planet formation. For this second step, we developed iSyMBA, a symplectic massive bodies algorithm, where “i” stands for interpolation. iSyMBA is a very useful code to accurately evaluate the effects of planetary instabilities on minor body reservoirs, while accounting for close encounters among massive objects. We provide a detailed description of how iSyMBA was developed and implemented to study terrestrial planet formation. Adapting iSyMBA for other problems that demand interpolation from previous simulations can be done following the method described here.

Key words: methods: numerical – software: development – software: simulations – planets and satellites: formation

1 INTRODUCTION
Current theories of the early evolution of the solar system invoke a temporary instability of the giant planets, that would have happened sometime after the dissipation of the gas in the protoplanetary nebula (see Nesvorný 2018, for a review). This instability led to mutual scattering of the giant planets while they were radially migrating due to the interaction with an outer massive disk of remnant planetesimals. The instability is required to explain many dynamical features that are currently observed in the different populations of solar system bodies. These include the angular momentum deficit of the giant planets (e.g. Nesvorný & Morbidelli 2012; Deienno et al. 2017), the inclinations of asteroids in the main belt (e.g. Roig & Nesvorný 2015; Deienno et al. 2018), the existence of Jupiter trojans (e.g. Nesvorný et al. 2013), the orbital architecture of the Kuiper belt (e.g. Nesvorný 2015; Gomes et al. 2018), the excited orbit of Mercury (e.g. Roig et al. 2016), the dynamical characteristics of the satellites of the jovian planets (e.g. Deienno et al. 2014; Nesvorný et al. 2014b,a), among others.

The first instability models (Tsiganis et al. 2005) assumed that the instability may have happened around 600 My after the dissipation of the gas in the protoplanetary nebula, helping to trigger the Lunar Late Heavy Bombardment (LHB; Gomes et al. 2005; Bottke et al. 2012). Recent models, however, propose that the instability may have happened as early as ~ 10 My after the dissipation of the gas (Nesvorný 2018). This means that the instability might have played a relevant role in the accretion of the terrestrial planets (e.g. Clement et al. 2018, 2019; Nesvorný et al. 2021).

Using fully self consistent models to study the effects of the instability in the early evolution of the solar system may be an unfeasible task. In general, such models need to consider at least three ingredients: the giant planets, the disk of massive planetesimals that drives the migration of the giant planets, and the population of bodies affected by the instability. We refer to the latter as the target population, and it may be represented either by test particles or by mutually interacting massive bodies. This requires to explore a large number of model parameters and over a wide range of values, implying the need for hundreds or thousands of computationally expensive numerical simulations that, in most cases, lead to meaningless results.

An alternative to overcome these limitations is to use simplified, yet realistic, models where the amount of free parameters is smaller, and the user have more control over the range of possible evolutions of the system. This involves, for example, to drop off the disk of planetesimals and consider a prescribed evolution of the giant planets. This prescribed evolution might be as simple as an ad hoc evolution, mimicked by using artificial forces, or as complex as a realistic evolution obtained from other previous simulations (e.g. Nesvorný et al. 2017; Deienno et al. 2018).

Here, we develop a numerical integration method that exploits the latter approach. In this method, the evolution of the giant planets is stored in a file at regular intervals, and their positions and velocities for a given time are obtained by interpolation. Our aim is to construct a symplectic N body integrator for the target population, that has the giant planets interpolation scheme embedded in it.
Symplectic integrators are a particular class of numerical integrators, specifically designed to solve Hamiltonian problems (Yoshida 1993). Their main property is the conservation of a quantity $\tilde{H}$, referred to as the surrogate Hamiltonian, that is very close to the original Hamiltonian $H$ of the problem. Our choice for a symplectic algorithm has two motivations: (i) these algorithms have proven to be fast and reliable, allowing for long term simulations of planetary $N$-body systems with less computational cost than traditional integration algorithms (e.g. Wisdom & Holman 1991), and (ii) we intend to use the set of subroutines and packages of the well-tested and publicly available symplectic integrators Swift (Levison & Duncan 1993) and SyMBA (Duncan et al. 1998), with the necessary modifications, as the basis for our algorithm.

When the target population consists of massless particles, the construction of a symplectic integrator with embedded interpolation is relatively straightforward (e.g. Beaugé et al. 2002; Roig & Nesvorný 2015). On the other hand, when the target populations consist of massive bodies that interact with each other and may develop close encounters, including the giant planets interpolation in a symplectic way requires some specific considerations that turn the development of the algorithm more difficult. One particular problem is related to the fact that the system of giant planets has a centre-of-mass that differs from that of the target population. This requires a specific splitting of the Hamiltonian that is not accounted for in full $N$-body symplectic integrators.

Here, we focus on the case when the target population is in the inner solar system, and we describe the construction of the algorithm. For its recent applications, we refer the reader to Nesvorný et al. (2021) and DeSouza et al. (2021). The paper is organised as follows. In Sect. 2, we revise the basic concepts, provide the detailed description of the new algorithm, and perform some validation tests. In Sect. 3, we briefly discuss the possible parallelization strategies for the new code. The last section is devoted to the conclusions.

2 SYMPLECTIC INTEGRATION WITH INTERPOLATION

2.1 SyMBA

Before proceeding with the description of SyMBA, we will briefly review the basics of SyMBA (see Duncan et al. 1998, for more details). SyMBA stands for Symplectic Massive Bodies Algorithm, and it is a second order symplectic integrator for the planetary $N$ body problem, that allows for close encounters between massive bodies.

Let us assume a set of $N$ bodies of masses $m_i$ orbiting around the Sun (or any central star) of mass $M \gg m_i$, and introduce the Poincaré canonical coordinates $r_i, p_i$ such that $r_i$ are heliocentric positions and $p_i = m_i v_i$ are barycentric momenta (barycentric velocities). Throughout this work, primed variables are referred to the centre-of-mass of the system, and not primed variables are referred to the Sun. The Hamiltonian of the system is then composed of three parts:

$$H(r, p') = H_{\text{Kep}} + H_{\text{Int}} + H_{\text{Sun}}$$ (1)

where

$$H_{\text{Kep}}(r, p') = \sum_{i=1}^{N} \left( \frac{|p_i|^2}{2m_i} - \frac{G M m_i}{|r_i|} \right)$$ (2)

represents the two body motion of the bodies around the Sun,

$$H_{\text{Int}}(r) = -\sum_{i=1}^{N-1} \sum_{k=i+1}^{N} \frac{G m_i m_k}{|r_i - r_k|}$$ (3)

is the gravitational interaction potential between the bodies, and

$$H_{\text{Sun}}(p') = \frac{1}{2M} \sum_{i=1}^{N} |p_i'|^2$$ (4)

is the barycentric kinetic energy of the Sun.

Whenever $H_{\text{Int}}, H_{\text{Sun}} \ll H_{\text{Kep}}$, a second order symplectic integration over a time step $\tau$ is obtained through the following sequence of steps:

Step 1. Evolve the system only through $H_{\text{Sun}}$, over $\tau/2$; this applies a linear drift (LD) to the positions $r$.

Step 2. Evolve the system only through $H_{\text{Int}}$, over $\tau/2$; this applies an impulse or kick (K) to the momenta $p'$.

Step 3. Evolve the system only through $H_{\text{Kep}}$, over $\tau$; this applies a drift (D) to each body along a Keplerian orbit.

Step 4. Evolve the system only through $H_{\text{Int}}$, over $\tau/2$; this applies again a kick (K) to the momenta $p'$.

Step 5. Evolve the system only through $H_{\text{Sun}}$, over $\tau/2$; this applies again a linear drift (LD) to the positions $r$.

The integration over a time step $\tau$ is then schematised by a sequence LD - K - D - K - LD. The detailed flowchart of the algorithm is shown in Fig. 1.

However, when a close encounter between two bodies arises, the condition $H_{\text{Int}} \ll H_{\text{Kep}}$ is no longer satisfied and the above sequence is no longer valid. In a traditional numerical integrator, the increase of the $H_{\text{Int}}$ term during the close encounter is usually compensated by a decrease of the time step $\tau$, such as to keep the impulse $-\tau \partial H_{\text{Int}}/\partial r$ limited. However, in a symplectic integrator the time step must be kept fixed over the whole integration. This is a well known limitation of symplectic algorithms, since the surrogate Hamiltonian $\tilde{H}$, that is preserved by the algorithm, is such that $\tilde{H} \approx H + O(\tau^n)$, being $n$ the order of the integrator. Thus, any change in the time step would break the conservation of $\tilde{H}$.

The solution proposed by Duncan et al. (1998) and Chambers (1999) to circumvent this limitation consists into split the term $H_{\text{Int}}$ into pieces, weighted by a function that depends on the distance between the different pairs of bodies. Consider, for example, a two-terms splitting, $H_{\text{Int}} = H_{\text{Int}}^{(1)} + H_{\text{Int}}^{(2)}$, where:

$$H_{\text{Int}}^{(1)} = -\sum_{i=1}^{N-1} \sum_{k=i+1}^{N} \frac{G m_i m_k}{r_{ik}} (1 - w_{1,ik})$$

$$H_{\text{Int}}^{(2)} = -\sum_{i=1}^{N-1} \sum_{k=i+1}^{N} \frac{G m_i m_k}{r_{ik}} w_{1,ik}$$ (5)

Here, $r_{ik} = |r_i - r_k|$, and $w_{1,ik}$ is a sigmoid-like weight function:

$$w_{1,ik} = \begin{cases} 1 & r_{ik} \geq R_{l,ik} \\ \phi \left( \frac{r_{ik} - R_{l+1,ik}}{R_{l,1+ik} - R_{l+1,ik}} \right) & R_{l+1,ik} \leq r_{ik} < R_{l,ik} \\ 0 & r_{ik} < R_{l,1+ik} \end{cases}$$ (6)

where $\phi$ is a suitable odd degree polynomial, and $R_{l,1}, R_{l+1,1}$ are defined in terms of the mutual Hill radii. Then, the sequence of steps over a time step $\tau$ becomes:

Step 1. Evolve the system only through $H_{\text{Sun}}$, over $\tau/2$

Step 2. Evolve the system only through $H_{\text{Int}}^{(1)}$, over $\tau/2$

Step 3. Repeat from 1 to $q$ ($q > 1$, integer)

Step 3.1. Evolve the system only through $H_{\text{Int}}^{(1)}$, over $\tau/2q$

Step 3.2. Evolve the system only through $H_{\text{Kep}}$, over $\tau/q$

Step 3.3. Evolve the system only through $H_{\text{Int}}^{(0)}$, over $\tau/2q$
Step 4. Evolve the system only through $H_{\text{int}}^{(1)}$ over $\tau/2$

Step 5. Evolve the system only through $H_{\text{Sun}}$, over $\tau/2$

When $r_{ik} \geq R_{i,ik}$ (no close encounters), $H_{\text{int}}^{(0)} = 0$ and step 3 reduces to a single evolution of $H_{\text{Kepl}}$ over $\tau$. On the other hand, when $r_{ik} < R_{i+1,ik}$ (close encounter), $H_{\text{int}}^{(1)} = 0$, and step 3 effectively performs the symplectic integration using a smaller step time $\tau/q$.

The above sequence can be represented as:

$$\text{LD} - K^{(1)} = \left( K^{(0)} - D - K^{(0)} \right) q - K^{(1)} - \text{LD}$$

This strategy can be recursively extended to an arbitrary sequence of weight functions for radii $R_{1,ik} > R_{2,ik} > \ldots > R_{n,ik} > R_{n+1,ik}$, associating smaller and smaller time steps to each weight function. In SyMBA, $R_{n+1,ik}$ is usually set to be of the order of the planetary radii, and $R_{1,ik}$ is of the order of a few Hill radii.

2.2 iSyMBA

In order to apply the above concepts to develop iSyMBA, we consider three different categories of bodies:

(i) Giant planets: represented by $J$ bodies of masses $\mu_j$, $j = 1, \ldots, J$. The positions $\rho_j$ and velocities $v_j$ of these bodies are directly read from a file, where they are stored at regular time intervals, and are interpolated down to the desired time step.\(^1\) The giant planets perturb the other two bodies categories in the simulation, but they do not suffer any perturbation, neither among them, nor from other bodies.

(ii) Terrestrial protoplanets: represented by $T$ bodies of masses $m_i \geq m_{\text{tiny}}, i = 1, \ldots, T$. The positions $\rho_i$ and velocities $v_i$ of these bodies are advanced through a second order symplectic integrator. They feel their mutual gravitational perturbations, as well as those from the giant planets and from the terrestrial planetesimals. Terrestrial protoplanets may also feel relativistic perturbations, if required.

(iii) Terrestrial planetesimals: represented by $N - T$ bodies of masses $m_i < m_{\text{tiny}}, i = T+1, \ldots, N$. The positions $\rho_i$ and velocities $v_i$ of these bodies are also advanced through a second order symplectic integrator. They do not feel their mutual gravitational perturbations, but they are perturbed by both the giant planets and the terrestrial protoplanets. They also perturb the terrestrial protoplanets.

As in the original SyMBA code, $m_{\text{tiny}}$ is a constant mass threshold, that we set, for example, to 2 $M_\text{Moon}$ in Nesvorný et al. (2021). We refer to the set of terrestrial protoplanets and planetesimals simply as the terrestrial bodies.

In the following, we describe in detail the different parts of the code. The flowchart of the algorithm is presented in Fig. 2.

2.2.1 Giant planets interpolation

The positions and velocities of the giant planets are obtained from a previous, and independent, simulation of the migration of these planets by interaction with a transneptunian disk of planetesimals (e.g. Nesvorný & Morbidelli 2012; Deienno et al. 2018). The output of this simulation, i.e. heliocentric positions and velocities (or heliocentric orbital elements) of the giant planets, as well as their masses and the Sun mass, are stored in a file at 1-yr intervals. The masses are not necessarily constant during such evolution, since the planets and the Sun may accrete planetesimals while migrating and grow in mass.

Let $\rho_{ib}, v_{ib}, \mu_b$ be the position, velocity, and mass of a given giant planet at time $t_b$, and $\rho_e, v_e, \mu_e$ the corresponding values at a posterior time $t_e$. Let also $M_b$ and $M_e$ the corresponding masses of the Sun. Assume that we want to interpolate this trajectory over a time step $\tau = (t_e - t_b)/n$. The interpolation method consists of the following steps.

Step 1. Advance $\rho_{ib}, v_{ib}$ from $t_b$ to $t_e$ along a Keplerian orbit, considering the central mass $M_b + \mu_b$, to obtain the sequence of values $\rho_{ib}^{(i)}, v_{ib}^{(i)}$, for times $t_i = t_b + i \tau, i = 0, \ldots, n$.

Step 2. Recede $\rho_e, v_e$ from $t_e$ to $t_b$ along a Keplerian orbit, considering the central mass $M_e + \mu_e$, to obtain the sequence of values $\rho_e^{(i)}, v_e^{(i)}$, for times $t_j = t_e - j \tau, j = 0, \ldots, n$.

Step 3. Compute the interpolated values at time $t_b \leq t_k \leq t_e$ through a weighted average:

\[
\rho_k = (1 - w_k)\rho_{ib}^{(k)} + w_k\rho_e^{(n-k)}
\]
\[
v_k = (1 - w_k)v_{ib}^{(k)} + w_kv_e^{(n-k)}
\]
\[
\mu_k = (1 - w_k)\mu_b + w_k\mu_e
\]
\[
M_k = (1 - w_k)M_b + w_kM_e
\]

where $w_k = k/n, k = 0, \ldots, n$.

We recall that these interpolated coordinates are heliocentric. A similar interpolation strategy was already implemented in the Swift_RNVS3 integrator to deal with encounters of test particles.
to massive bodies (Levison & Duncan 1993), and the corresponding subroutine has been adapted with the necessary modifications to account for mass changes.

The interpolation of a giant planet that disappears from the system, either by escaping or by merging to another giant, can be performed only until the last registry of that planet stored in the file. In such case, since the orbits are stored at 1-yr intervals, we lose only a few months of evolution of the giant that disappears. This is not expected to have any significant influence on the evolution of the target population over million years. Moreover, in the case of a merging between two giant planets, one giant disappears but another has its mass increased. This latter giant will be properly interpolated since the interpolation scheme takes into account any variation of the planet’s mass.

It is worth noting that the symplectic algorithm described in the next sections is independent of the particular interpolation scheme. Other interpolation routines, different that the one presented here, can be applied with the same result.

### 2.2.2 Terrestrial bodies integration

The key contribution to the development of the algorithm consists in the second order symplectic integrator to advance the orbits of the terrestrial bodies over a time step \( \tau \). This is constituted by a specific sequence of Lie series, applied to a non autonomous Hamiltonian of the form:

\[
H(\mathbf{r}, \mathbf{p'}, t) = H_{\text{Kep}} + H_{\text{Pert}} + H_{\text{Jov}} + H_{\text{Sun}}
\]

where, again, \( \mathbf{r}, \mathbf{p'} \) are the Poincaré canonical coordinates. The Hamiltonian is time dependent though the heliocentric positions \( \mathbf{r} \), and the barycentric momenta (velocities) \( \dot{\mathbf{p'}} = \mu_j \mathbf{v'} \) of the giant planets, which are computed from the interpolated heliocentric values (Sect. 2.2.1). It is worth noting that the barycentric momenta \( \mathbf{p'}, \mathbf{\dot{p}}' \) are referred to the centre-of-mass of the whole system, i.e. considering the terrestrial bodies and the giant planets altogether.

The different terms of the Hamiltonian are:

\[
H_{\text{Kep}}(\mathbf{r}, \mathbf{p'}) = \sum_{i=1}^{N} \frac{\left| \mathbf{p'}_i \right|^2}{2m_i} + \frac{G M m_i}{|\mathbf{r}_i|}
\]

that represents the two body motion of the terrestrial bodies around the Sun, of mass \( M \).

\[
H_{\text{Pert}}(\mathbf{r}) = -\sum_{i=1}^{N-1} \sum_{k=N+1}^{N} \frac{G m_i m_k}{|\mathbf{r}_i - \mathbf{r}_k|}
\]

which is the mutual gravitational perturbation among the terrestrial bodies,

\[
H_{\text{Jov}}(\mathbf{r}, t) = -\sum_{i=1}^{N} \sum_{j=1}^{J} G m_i \mu_j \frac{\mathbf{r}_i - \mathbf{r}_j(t)}{|\mathbf{r}_i - \mathbf{r}_j(t)|}
\]

that gives the direct gravitational perturbation of the giant planets on the terrestrial bodies, and

\[
H_{\text{Sun}}(\mathbf{p'}, t) = \frac{1}{2M} \sum_{i=1}^{N} \left| \mathbf{p'}_i + \sum_{j=1}^{J} \mathbf{v'}_j(t) \right|^2
\]

that represents the linear momentum of the Sun around the centre-of-mass of the whole system.

The detailed sequence of operations for a single step time integration, from \( t \) to \( t + \tau \), is as follows:

Step 1. Start with the heliocentric positions and velocities \( \mathbf{r}, \mathbf{v} \) of all the terrestrial bodies, obtained from the previous time step, as well as the heliocentric positions and velocities \( \mathbf{p}, \mathbf{v} \) interpolated for the giant planets, at time \( t \).

Step 2. Calculate the heliocentric acceleration \( \mathbf{a}_i \) on the terrestrial protoplanets due to relativistic corrections (Quinn et al. 1991):

\[
\mathbf{a}_{i,j} = \frac{G M}{c^2 |\mathbf{r}_i|^3} \left( 4 \mathbf{r}_i \cdot \mathbf{v}_i \mathbf{v}_i - \mathbf{v}_i \cdot \mathbf{v}_i \mathbf{r}_j + 4M \frac{\mathbf{F}_i}{|\mathbf{r}_i|} \right), \quad i = 1, \ldots, T
\]

Step 3. Apply a kick, over \( \tau/2 \), in the barycentric velocities \( \mathbf{v'} \) of the terrestrial protoplanets due to the relativistic acceleration correction:

\[
\mathbf{v}_i \leftarrow \mathbf{v}_i + \frac{\tau}{2} \mathbf{a}_{i,j}, \quad i = 1, \ldots, T
\]

Step 4. Convert the heliocentric positions \( \mathbf{r} \) of the terrestrial bodies due to the giant planets contribution to the Sun momentum:

\[
\mathbf{r}_i \leftarrow \mathbf{r}_i + \frac{\tau}{2M} \sum_{j=1}^{J} \mu_j \mathbf{v}'_j, \quad i = 1, \ldots, N
\]

Step 5. Compute the heliocentric accelerations \( \mathbf{a}_{i,j} \) on the terrestrial bodies due to the giant planets:

\[
\mathbf{a}_{i,j} = -\sum_{j=1}^{J} \frac{G \mu_j \mathbf{r}_i - \mathbf{r}_j(t)}{|\mathbf{r}_i - \mathbf{r}_j(t)|^3}, \quad i = 1, \ldots, N
\]

Step 6. Apply a kick, over \( \tau/2 \), in the heliocentric velocities \( \mathbf{v} \) of the terrestrial bodies due to these accelerations:

\[
\mathbf{v}_i \leftarrow \mathbf{v}_i + \frac{\tau}{2} \mathbf{a}_{i,j}, \quad i = 1, \ldots, N
\]

Step 7. Perform a linear drift, over \( \tau/2 \), of the heliocentric positions \( \mathbf{r} \) of the terrestrial bodies due to the giant planets contribution to the Sun momentum:

\[
\mathbf{r}_i \leftarrow \mathbf{r}_i + \frac{\tau}{2M} \sum_{k=1}^{N} m_k \mathbf{v}'_k, \quad i = 1, \ldots, N
\]

Step 8. Perform a linear drift, over \( \tau/2 \), of the heliocentric positions \( \mathbf{r} \) of the terrestrial bodies due to their own contribution to the Sun momentum:

\[
\mathbf{r}_i \leftarrow \mathbf{r}_i + \frac{\tau}{2M} \sum_{k=1}^{N} m_k \mathbf{v}'_k, \quad i = 1, \ldots, N
\]

Step 9. Compute the heliocentric mutual accelerations \( \mathbf{a}_{i,j} \) of the terrestrial protoplanets and planetesimals:

\[
\mathbf{a}_{i,j} = -\sum_{k=1}^{N} \frac{G m_k \mathbf{r}_i - \mathbf{r}_k}{|\mathbf{r}_i - \mathbf{r}_k|^3}, \quad i = 1, \ldots, T
\]

\[
\mathbf{a}_{i,j} = -\sum_{k=1}^{T} \frac{G m_k \mathbf{r}_i - \mathbf{r}_k}{|\mathbf{r}_k - \mathbf{r}_i|^3}, \quad k = T + 1, \ldots, N
\]

Step 10. Apply a kick, over \( \tau/2 \), in the barycentric velocities \( \mathbf{v}' \) of the terrestrial bodies due to these accelerations:

\[
\mathbf{v}_i \leftarrow \mathbf{v}_i + \frac{\tau}{2} \mathbf{a}_{i,j}, \quad i = 1, \ldots, N
\]
Step 1. Drift the heliocentric positions \( \mathbf{r} \) and barycentric velocities \( \mathbf{v} \) of the terrestrial protoplanets and planetesimals along the Keplerian orbits generated by the Hamiltonian \( H_{\text{Kep}} \) (Eq. 9), over a full time step \( \tau \).

Step 2. Recompute the heliocentric mutual accelerations \( \mathbf{a}_T \) of the terrestrial bodies (Eq. 20).

Step 3. Apply a kick, over \( \tau/2 \), in the barycentric velocities \( \mathbf{v}' \) due to \( \mathbf{a}_R \).

Step 4. Convert: \( \mathbf{v}, \mathbf{v} \) to \( \mathbf{v}', \mathbf{u}' \) for all bodies.

Step 5. Compute Accelerations: \( \mathbf{a}_T \) on \( \mathbf{PP} \) and \( \mathbf{PL} \) due to \( \mathbf{GP} \).

Step 6. Apply a kick, over \( \tau/2 \), in \( \mathbf{v}' \) due to \( \mathbf{a}_T \).

Step 7. Apply a Linear Drift over \( \tau/2 \) in \( \mathbf{r} \) due to \( \mathbf{GP} \) own momentum on the Sun.

Step 8. Convert: \( \mathbf{v} \) to \( \mathbf{v}' \) for \( \mathbf{GP} \) at \( t+\tau \).

Step 9. Apply a Linear Drift over \( \tau/2 \) in \( \mathbf{r} \) due to \( \mathbf{GP} \) momentum on the Sun.

Step 10. Apply a kick over \( \tau/2 \) in \( \mathbf{v}' \) due to \( \mathbf{a}_T \).

Step 11. Drift \( \mathbf{r} \) and \( \mathbf{v}' \) along keplerian orbits via \( H_{\text{Kep}} \) over \( \tau \).

Step 12. Recompute the heliocentric velocities \( \mathbf{v}' \) of the terrestrial bodies due to their own contribution to the Sun momentum (Eq. 19).

Step 13. Apply a kick, over \( \tau/2 \), in the barycentric velocities \( \mathbf{v}' \) due to the giant planets (Eq. 14).

Step 14. Perform a linear drift, over \( \tau/2 \), of the heliocentric positions \( \mathbf{r} \) of the terrestrial bodies due to the giant planets contribution to the Sun momentum (Eq. 18).

Step 15. Convert the heliocentric velocities \( \mathbf{v} \) of the giant planets at \( t+\tau \) to barycentric \( \mathbf{v}' \), with respect to the centre-of-mass of the whole system:

\[
\mathbf{v}' = - \sum_{i=1}^{N} m_i \mathbf{v}'_i + \sum_{j=1}^{J} \mu_j \mathbf{v}'_j \\
M + \sum_{j=1}^{J} \mu_j \\
\mathbf{v}'_j = \mathbf{v}_j + \mathbf{V}', \quad j = 1, \ldots, J
\]  

(22)

Step 16. Perform a linear drift, over \( \tau/2 \), of the heliocentric positions \( \mathbf{r} \) of the terrestrial bodies due to the giant planets (Eq. 16).

Step 17. Recompute the heliocentric accelerations \( \mathbf{a}_T \) on the terrestrial bodies due to the giant planets (Eq. 17).

Step 18. Apply a kick, over \( \tau/2 \), in the barycentric velocities \( \mathbf{v}' \) of the terrestrial bodies due to these accelerations (Eq. 17).

Step 19. Convert back the barycentric velocities \( \mathbf{v}' \) of the terrestrial bodies to heliocentric \( \mathbf{v} \):

\[
\mathbf{v}' = - \sum_{i=1}^{N} m_i \mathbf{v}'_i + \sum_{j=1}^{J} \mu_j \mathbf{v}'_j \\
M \\
\mathbf{v}_i = \mathbf{v}'_i - \mathbf{V}', \quad i = 1, \ldots, N
\]  

(23)

Step 20. Recalculate the heliocentric acceleration \( \mathbf{a}_R \) on the terrestrial protoplanets due to relativistic corrections (Eq. 13).

Step 21. Apply a kick, over \( \tau/2 \), in the heliocentric velocities \( \mathbf{v} \) of the terrestrial protoplanets due to the relativistic acceleration correction (Eq. 14).

Step 22. Return to step 2.

At variance with the standard SyMBA code, that uses a LD - K - D - K - LD sequence, iSyMBA uses a KJ - LDJ - LD sequence, where the sub-indices J, T refer to jovian and terrestrial, respectively, with an additional outer K sequence for relativistic corrections, if required. This specific sequence has three advantages over other possible sequences:

(i) The giant planets perturbations (Eq. 16) do not need to be recomputed at the beginning of each time step; they can be recovered from the final values of the previous time step.

(ii) If relativistic corrections are not accounted for, there is no need to recompute the barycentric velocities at the beginning of each time step (Eq. 15); they can be recovered from the final values of the previous time step.

(iii) The innermost LDJ - KTJ - DKT - KLT sequence (steps 8 to 14), that treats the interactions among the terrestrial bodies solely, could be executed by the standard SyMBA algorithm.

2.2.3 Treatment of close encounters among terrestrial bodies

Close encounters among terrestrial protoplanets, or between terrestrial protoplanets and planetesimals, are manipulated by iSyMBA using the same strategy of SyMBA, i.e. by splitting the
potential term (Eq. 10) as:

\[ H_{\text{pert}}(r) = H^{(0)}_{\text{pert}} + \sum_{i=1}^{n} H^{(s)}_{\text{pert}} \]

\[ H^{(0)}_{\text{pert}} = \sum_{i=1}^{T-1} \sum_{k=1}^{N} \sum_{l=1}^{K} \frac{G m_i m_k}{r_{ik}} \left[ 1 - w_{l,ik} \right] \]

\[ H^{(s)}_{\text{pert}} = \sum_{i=1}^{T-1} \sum_{k=1}^{N} \sum_{l=1}^{K} \frac{G m_i m_k}{r_{ik}} w_s \left[ 1 - w_{l,ik} \right] \]

where the \( w_{l,ik} \) are given by Eq. (6). The propagation of the orbits of any two bodies involved in an encounter during the innermost LD through the nested application of a \( K - D - T \) sequence (steps 8 to 14), is carried out recursively through the nested application of a \( K - D - T \) sequence to the Hamiltonian \( \left\{ \left( H_{\text{Kep}} + H^{(0)}_{\text{pert}} + H^{(1)}_{\text{pert}} \right) + \ldots + H^{(n)}_{\text{pert}} \right\} \), using smaller and smaller time steps \( \tau = \tau / 3^l, l = 1, \ldots, n \).

For this stage, we use the original \( \text{iSyMBA} \) subroutines, with little modifications. Bodies are always merged whenever they reach the last stage of the recursion and get closer than \( R_{\alpha+1,ik} \).

2.2.4 Treatment of close encounters between terrestrial bodies and giant planets

Close encounters with giant planets are not properly manipulated by \( \text{iSyMBA} \). The application of a splitting strategy to the term \( \tilde{H}_{\text{Jov}} \) (Eq. 11) would demand additional interpolations of the giant planets orbits, down to smaller and smaller time steps. This would also require significant changes to the standard \( \text{iSyMBA} \) recursive subroutines, which turns to be a quite complex task. Therefore, we leave this implementation to a future work.

Currently, the way \( \text{iSyMBA} \) deals with such close encounters is to keep tracking the distances between the protoplanets/planetesimals and the giant planets, and discard the former when they get closer to a giant planet than the sum of their individual Hill radii. This solution proved to be adequate for our purposes, since the disk of terrestrial bodies is interior to Jupiter’s orbit. Thus, we may expect that close encounters of planetesimals with the giant planets will be rare, and they eventually will affect only the outer edge of the disk. In particular, using the results of Nesvorný et al. (2021), we verified that, when the disk extends up to 4 au with a radial surface density profile \( \Sigma(r) = r^{-1} \), less than 30% of the planetesimals experienced close encounters with Jupiter during the simulations.

2.2.5 Treatment of small perihelion passages

The \( \text{iSyMBA} \) code does not properly treat the \( \tilde{H}_{\text{Sun}} \) term increase (Eq. 12) when a terrestrial body experiences a small perihelion passage or get too close to the Sun. This limitation also exists in the standard \( \text{SyMBA} \) code. In such cases, the code relies only in the setup of a sufficiently small time step to resolve the perihelion passage without loosing too much precision. In Nesvorný et al. (2021), we setup a time step \( \tau = 3-7 \) days, which proved to be good enough in that application. Bodies are discarded whenever they reach heliocentric or perihelion distances smaller than a given threshold, set by the user.

2.2.6 Symplecticity and energy conservation

The symplecticity of \( \text{iSyMBA} \) is guaranteed by the conservation of the corresponding surrogate Hamiltonian:

\[ \mathcal{H} = H_{\text{Kep}} + H_{\text{pert}} + H_{\text{Sun}} + H_{\text{pert,i}} + \frac{1}{2} H_{\text{pert,j}} + \sum_{i=0}^{n} \frac{\tau^2}{12} \left[ H_{\text{Kep}} + H_{\text{pert,i}} + H_{\text{Kep}} + \frac{1}{2} H_{\text{pert,j}} \right] \]

where \([,]\) represents the Lagrange brackets. In practice, the total energy can be computed as the sum of the barycentric kinetic and potential energies, taking into account all the three categories of bodies in the system:

\[ E = \frac{1}{2} M \dot{V}^2 + \sum_{i=1}^{N} \frac{G m_i V_i^2}{r_i} + \sum_{j=1}^{J} \frac{1}{2} \sum_{k=1}^{J} \frac{G m_j \mu_k}{|r_{ij} - r_{kj}|} \]

\[ - \sum_{i=1}^{N} \frac{G m_i}{F_i} - \sum_{i=1}^{T-1} \sum_{k=1}^{N} \sum_{l=1}^{K} \frac{G m_i m_k}{r_{ik}} \left[ 1 - w_{l,ik} \right] \]

\[ - \sum_{j=1}^{J} \sum_{k=1}^{J} \frac{G m_j \mu_k}{|r_{ij} - r_{kj}|} \]

It is worth recalling that in \( \text{iSyMBA} \), the model Hamiltonian is non autonomous. Therefore, the energy is not expected to be constant, but it should display periodic oscillations with bounded amplitude.

2.3 Validation tests

The \( \text{iSyMBA} \) algorithm has been validated as follows. We consider a system consisting of \( J \) giant planets and \( T \) terrestrial planets, and perform a simulation over 1 My using the standard \( \text{SyMBA} \), i.e. allowing for all the planets to be mutually perturbed. The output (orbital elements) of this simulation for the giant planets is stored in a file every 1 year, while the output for the terrestrial planets is stored in a separate file every 1000 years. Then, we repeat the simulation using \( \text{iSyMBA} \), with the same initial conditions for the terrestrial planets, and interpolating the giant planets’ orbits from the ones previously stored. The output of this simulation is recorded every 1000 years, and it is directly compared to the previous output from \( \text{SyMBA} \). In all the simulations, we check that the total energy of the system, computed from Eq. (28), is well behaved.

We apply the above validation test to two different systems. The first one is the present solar system, with 4 terrestrial and 4 giant planets. Initial conditions are taken from the JPL Ephemerides. Relativistic perturbations are not taken into account, and there are no close encounters between the planets. We call this the 4G4T model.

The second system is a fictitious system composed of 5 giant planets and 20 terrestrial bodies. The giant planets are Jupiter, Saturn, and 3 ice giants, initially in a mutual resonant and compact orbital configuration (see DeSouza et al. 2021, for example). The 20 terrestrial bodies are represented by planetary embryos with a total mass of \( 5 M_\oplus \). These bodies are uniformly distributed in a very narrow annulus, between 0.95 and 1.05 au, with eccentricities < 0.01 and inclinations < 0.001. The idea of this setup is to force close encounters between the terrestrial bodies, in order to test the behaviour of \( \text{iSyMBA} \) under such conditions. Relativistic
Table 1. Maximum differences in the orbital elements of the terrestrial planets, over 1 My, for the validation test using the 4G4T model (see text).

|        | \( \delta a/a \) | \( \delta e/e \) | \( \delta I/I \) | \( \delta \varpi (\degree) \) |
|--------|------------------|------------------|------------------|------------------|
| Mercury | 1.5 \times 10^{-6} | 9 \times 10^{-5} | 4 \times 10^{-5} | 6 \times 10^{-3} |
| Venus  | 2.5 \times 10^{-5} | 6 \times 10^{-3} | 2 \times 10^{-3} | 2 \times 10^{-1} |
| Earth  | 4 \times 10^{-5}  | 1.5 \times 10^{-2} | 6 \times 10^{-3} | 5 \times 10^{-1} |
| Mars   | 3 \times 10^{-5}  | 1.5 \times 10^{-3} | 2 \times 10^{-4} | 4 \times 10^{-2} |

perturbations are not taken into account either. We call this the 5G20T model.

Figure 3 shows a result from the 4G4T model. The panels display the evolution of the orbital elements of Mercury from the iSyMBA simulation (in magenta), and the SyMBA simulation (in black, but not visible due to overlapping). The differences between the two codes are shown in green. The behaviour is similar for the other terrestrial planets. Table 1 summarises the maximum relative differences found in this validation test. The total energy of the system behaves as expected, and the differences between the two codes in no larger than 10^{-5} over the whole time span.

In the 5G20T model, reproducing the exact evolution of the system with iSyMBA is not feasible, because the system is chaotic, and the small differences caused by the many collisions/mergers produce quantitatively different results. We verify, however, that the total energy of the system is well behaved, as shown in Fig. 5, with a bounded amplitude for iSyMBA that is only twice than in the 4G4T model without collisions. Although the number of collisions recorded in SyMBA and iSyMBA is not the same, the latter is able to reproduce quite well the first few collisions in the simulation. An example of this is shown in Fig. 6. We note that the merger happens at slightly different times in each case. Such small differences quickly propagate, and in a few tens of years each code starts to produce its own set of collisions, not matching each other anymore.

The above validation tests allow us to conclude that iSyMBA shows the desired behaviour in terms of simulation results.

3 PARALLELISATION STRATEGY

Aiming to improve the performance of iSyMBA, we have implemented multi-threading parallelisation using OpenMP. The following discussion does not intend to be comprehensive, and it is only applicable to the specific test models described below. Our aim is to provide some clues about the possible best strategies to parallelise the code, that eventually can be also taken into account to parallelise iSyMBA itself.

There is no unique strategy to parallelise a code, and sometimes the best approach is obtained by first redesigning the original serial code. Here, however, the idea is to adopt a parallelisation strategy that keeps the original serial structure of the iSyMBA subroutines with minimum or no changes.

The following discussion is based on two different test models: one considering 100 terrestrial proto-planets and 1 000 planetesimals (e.g. Nesvorný et al. 2021), which we refer to as m100n1000 model, and another considering 10 proto-planets and 10 000 planetesimals, which we called m10n10000 model. In both cases the number of giant planets is 5. In all the tests, we use the same total time span and the same time step. We also keep the amount of I/O operations to the minimum required. We define the normalised execution time as the ratio \( T_{\text{par}}/T_{\text{ser}} \), where \( T_{\text{ser}} \) is the total execution time of the serial code, without any parallelisation, and \( T_{\text{par}} \) is the execution time of the parallelised code. All the tests have been performed in Intel Core i7 processors, using GNU Fortran.

There are basically two types of structures that can be parallelised in iSyMBA using OpenMP:

(i) the operations that require double loops over the terrestrial bodies, like the mutual acceleration calculations (Eqs. 13, 16 and 20), the check for close encounters, and the energy computation (Eq. 28), and

(ii) the calculations that require single loops over the bodies, including the Keplerian drifts, the linear drifts, the kicks, the coordinate changes, the loops to deal with interpolation of the giant planets, etc.

We will discuss each structure separately.

3.1 Single loops

Parallelisation of the single loops within the code has to be carefully evaluated, because it may provide little or no improvement of the execution speed. For example, in the LD - K - D - K - LD integration scheme, the Keplerian drifts are, in theory, the second most CPU-expensive step, after the accelerations calculation. However, in our simulations, the Keplerian drifts take between 5% to 20% of the total run time in a serial run. Therefore, their parallelisation might not contribute significantly to improve performance.

We have verified that, in the m100n1000 simulations, parallelisation of the single loops makes the code only \( \sim 1.2 \) times faster, but in the m10n10000 simulations, it becomes \( \sim 2.3 \) times faster.

We have also verified that parallelisation of any loop within the recursive integration of close encounters (see Sect. 2.2.3) must be avoided, since it may slow down execution speed by a factor of 2. This concern, in particular, the subroutines symba7_step_recur and symba7_kick. We note, however, that there is no actual need to parallelise any part of the recursion, because it only affects the pair of bodies involved in an encounter, and these are not too frequent per time step.

After several experiments, we conclude that multi-threading parallelisation has to focus on the double loops, as explained below, and on the single loops that performs the most complex calculations, like the Keplerian drifts, the loops to deal with the interpolation of the giant planets, the relativistic corrections, the oblateness potential, and the discard subroutines.

3.2 Double loops

The strategy applied for parallelisation of the double loops influences the execution speed. A double loop to compute the accelerations between proto-planets and planetesimals typically reads:

\[
\text{do } i \text{ from } 1 \text{ to } m \\
\quad \text{do } j \text{ from } i+1 \text{ to } n \\
\quad \quad a(j) = a(j) + \text{accel}_{ij} \\
\quad \quad a(i) = a(i) + \text{accel}_{ij} \\
\text{end do} \\
\text{end do}
\]

where \( m \) is the number of self gravitating proto-planets, \( n \) is the number of planetesimals, and \( a() \) is an array of dimension \( n \). In this case, one possible strategy is to parallelise the outer loop over \( i \), and the other possibility is to parallelise the inner loop over \( j \).

Figure 7 shows the normalised execution time for the different models and strategies, as a function of the number of threads.
Figure 3. Comparison between the output from SyMBA (black) and iSyMBA (over-plotted in magenta) for the orbital elements of planet Mercury, over 1 My of evolution, in the 4G4T model (see text for the simulation details): \( a \), semi-major axis, \( e \) eccentricity, \( I \) inclination, and \( \sigma \) longitude of perihelion. The smaller panels show the relative differences (in green), except for \( \sigma \) that shows the absolute difference.

The solid lines correspond to the case in which the outer loops are parallelised, while the dashed lines correspond to the case in which the inner loops are parallelised. We note that, when using few threads, there is no significant difference between one strategy or the other, although parallelisation of the outer loops performs a bit better. On the other hand, when using many threads, each strategy has advantages over the other depending on the values of \( m \) and \( n \).

For the simulations of the m100n1000 model, parallelisation of the outer loops provides \( \sim 1.5 \) times faster execution times with respect to the parallelisation of the inner loops. On the other hand, for the simulations of the m10n10000 model, it is the parallelisation of the inner loops that provides \( \sim 1.3 \) times faster execution times than parallelising the outer loops.\(^2\)

This behaviour may be related to the fact that initialisation and execution of a parallel loop involve several tasks, besides the calculations within the loop, that may produce some latency in the

\(^2\) These tests have been performed using 8 threads.
Figure 4. Comparison between the total energy of the system from SyMBA (black) and from iSyMBA (magenta), in the 4G4T model (see text). Since the iSyMBA Hamiltonian is nonautonomous, the energy displays oscillations with amplitude $< 10^{-5}$, with respect to the SyMBA energy.

Figure 5. Comparison between the total energy of the system from SyMBA (black) and from iSyMBA (magenta), in the 5G20T model (see text). Again, the iSyMBA energy displays oscillations with amplitude $< 2 \times 10^{-5}$, with respect to the SyMBA energy.

Execution. When parallelising an inner loop, the parallel threads have to be initialised/allocated for every iteration of the outer loop, and this may cause a lot of latency. If the outer loop is small, as in $m = 10$, the latency does not have a big impact. However, if the outer loop is bigger, as in $m = 100$, the impact of latency may become significant.

Parallelisation of the outer loops has a couple of additional peculiarities that should be taken into account. The first one refers to the fact that the number of iterations over $j$, in the inner loop, is smaller for larger $i$. This means that the amount of work to be done by each iteration over $i$ is different. One possibility is choosing between a cyclic or a block scheduling. A cyclic schedule distributes the loop iterations in a round-robin fashion among the available threads, and should provide better performance in our case. The other possibility is choosing between static or dynamic scheduling. We have verified that using a combination of static and cyclic scheduling provides $\sim 1.1$ times faster execution times than either a dynamic or block scheduling.

The second peculiarity in parallelising the outer loops refers to the occurrence of data racing conditions over the accelerations array $a_i$. A racing condition arises when two or more processes running in different threads try to modify or update the same variable at the same time. Fortunately, Fortran OpenMP has the capability of performing array reduction, which allows to properly update $a_i$, avoiding data race.

Although multi-threading parallelisation, in our case, may improve execution speed by a factor of 3 to 6, the improvement is not linear with the number of threads and, as shown in Fig. 7, it tends to stabilise for $\geq 10$ threads.

Figure 6. Detail of an encounter/merger between two terrestrial bodies in the 5G20T model. The SyMBA simulation is shown in black, and iSyMBA in magenta. Full and dashed lines identify each of the bodies, respectively.

Figure 7. The performance of iSyMBA for different multi-threading parallelisation strategies. The solid lines correspond to the parallelisation of the outer loop in double loops, while the dashed lines correspond to the parallelisation of the inner loop. The colours identify the test models with different numbers of proto-planets ($m$) and planetesimals ($n$). The execution time has been normalised with respect to the serial execution time (see text for details). The green dotted line represents a linear trend, for reference purposes.
4 CONCLUSIONS

In this work, we described how to implement the necessary modifications to embed an orbit interpolation scheme into the symplectic planetary $N$-body integrator SyMBA. Our algorithm, named iSyMBA, allows to study the effects of a prescribed evolution of a set of planets on a target population of massive bodies, that interact with each other through close encounters.

iSyMBA is a very useful code to accurately evaluate the effects of planetary instabilities on the accretion processes in the terrestrial planets region. These include the growth of protoplanetary embryos (Nesvorný et al. 2021), the Moon-forming impact (DeSouza et al. 2021), and the origin of Mercury.

Although iSyMBA has been primarily developed and implemented to study terrestrial planet formation, the method presented here could be easily modified to study the evolution of other populations, that requires orbit interpolation from previously developed simulations, while accounting for close encounters among massive objects.

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DATA AVAILABILITY

iSyMBA is freely available under request to the corresponding author.

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