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Long-time averaging for integrable Hamiltonian dynamics

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Summary Given a Hamiltonian dynamics, we address the question of computing the space-average (referred as the *ensemble* average in the field of molecular simulation) of an observable through the limit of its time-average. For a completely integrable system, it is known that ergodicity can be characterized by a diophantine condition on its frequencies and that the two averages then coincide. In this paper, we show that we can improve the rate of convergence upon using a filter function in the time-averages. We then show that this convergence persists when a numerical symplectic scheme is applied to the system, up to the order of the integrator.

Key words integrable Hamitonian systems – averaging – filtering – Riemann sums – symplectic solvers – invariant tori

1 Introduction

Consider a Hamiltonian dynamics in $\mathbb{R}^d \times \mathbb{R}^d$

$$\begin{cases} \dot{p}(t) = -\nabla_q H(p(t), q(t)),\ p(0) = p_0, \\ \dot{q}(t) = \quad \nabla_p H(p(t), q(t)),\ q(0) = q_0. \end{cases} \tag{1}$$

Let $M(p_0, q_0)$ be the manifold $\{(p,q) \in \mathbb{R}^{2d} \,|\, H(p,q) = H(p_0,q_0)\}$. The solution of (1) is a dynamical system on $M(p_0, q_0)$ with the invariant measure

$$d\rho(p,q) = \frac{d\sigma(p,q)}{\|\nabla H(p,q)\|_2},$$

where $d\sigma(p,q)$ is the measure induced on $M(p_0,q_0)$ by the Euclidean measure of $\mathbb{R}^{2d}$, and $\|\cdot\|_2$ the Euclidean norm in $\mathbb{R}^{2d}$.

It is a common problem to estimate the *space* average of an observable A over the manifold $M(p_0,q_0)$

$$\frac{\int_{M(p_0,q_0)} A(p,q)d\rho(q,p)}{\int_{M(p_0,q_0)} d\rho(q,p)}, \tag{2}$$

through the limit of the *time* average

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T A(p(t),q(t))dt, \tag{3}$$

where $(p(t),q(t))$ is the solution of (1). Our wish is here to give a sound ground to (and in some cases improve [4]) the numerical simulations of (3) commonly used in the field of molecular dynamics.

The conditions under which the two quantities (2) and (3) coincide are not known in general and it is out of the scope of this paper to investigate them. In contrast, in the case of an *integrable* system, a well-known result of Arnold [2] states that, under a *non-resonant* condition on the frequency vector associated with the initial condition, the space average of a continuous function on the manifold

$$S(p_0,q_0) = \{(p,q) \in \mathbb{R}^d \times \mathbb{R}^d \ ; \\ I_1(p,q) = I_1(p_0,q_0), \ldots, I_d(p,q) = I_d(p_0,q_0)\}, \tag{4}$$

where $I_1,\ldots,I_d$ are the d invariants of the problem (1), coincide with the long-time average of this function. Moreover, if the frequencies satisfy a *diophantine* condition, the convergence is of order T^{-1}. Integrable and near-integrable systems under some diophantine condition will thus constitute a natural framework for the present work.

In the following, we consider a completely integrable Hamiltonian system (1) in the sense of the Arnold-Liouville theorem [2,5]: There exist d invariants $I_1 = H, I_2,\ldots,I_d$ in involution (i.e. their Poisson Bracket $\{I_i,I_j\} = 0$) such that their gradient are everywhere independent, and the trajectories of the system remain bounded. Under these conditions, there exist action-angles variables (a,θ) in a neighborhood U of $S(p_0,q_0)$. We have $(p,q) = \psi(a,\theta)$, where ψ is a symplectic transformation

$$\psi : D \times \mathbb{T}^d \ni (a,\theta) \mapsto (p,q) \in U,$$

with $\mathbb{T}^d = (\mathbb{R}/2\pi\mathbb{Z})^d$ the standard d-dimensional flat torus, and D a neighborhood in $\mathbb{R}^d$ of the point a_0 such that $(a_0, \theta_0) = \psi^{-1}(p_0, q_0)$. By definition of action-angle variables, the Hamiltonian $H(p,q)$ of (1) writes $H(p,q) = K(a)$ in the coordinates (a, θ), and thus the dynamics reads

$$\begin{cases} \dot{a}(t) = 0, \\ \dot{\theta}(t) = \omega(a(t)), \end{cases} \tag{5}$$

where $\omega = \partial K/\partial a$ is the frequency vector associated with the problem. The solution of this system for initial data (a_0, θ_0) simply writes $a(t) = a_0$ and $\theta(t) = \omega(a_0)t + \theta_0$.

For fixed $(a_0, \theta_0) = \psi(p_0, q_0)$, the image of $S(p_0, q_0)$ by ψ^{-1} is the torus $\{a_0\} \times \mathbb{T}^d$. On this torus, the measure $d\theta$ is invariant by the flow of (5). Considering the pull-back of this measure by the transformation ψ, we thus get a measure $d\mu(p,q)$ on $S(p_0, q_0)$ which is invariant by the flow of (1). For any function $A(p,q)$ defined on $S(p_0, q_0)$ we define the *space* average:

$$\langle A \rangle := \frac{\int_{S(p_0,q_0)} A(p,q) d\mu(p,q)}{\int_{S(p_0,q_0)} d\mu(p,q)} = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} A \circ \psi(a_0, \theta) d\theta \tag{6}$$

For a fixed time T, the *time* average is defined as

$$\langle A \rangle(T) := \frac{1}{T} \int_0^T A(p(t), q(t)) dt. \tag{7}$$

In a first step, we will investigate the extent to which the convergence of the time average (7) toward the space average (6) can be accelerated through the use of weighted integrals of the form

$$\langle A \rangle_\varphi(T) := \frac{\int_0^T \varphi\left(\frac{t}{T}\right) A(p(t), q(t)) dt}{\int_0^T \varphi\left(\frac{t}{T}\right) dt}, \tag{8}$$

where φ is a smooth function with compact support in $[0,1]$ (later on, we will refer to φ as the *filter* function). In a second step, we will consider the time-discretization of (8), i.e. the discretization of both the integral through Riemann sums and the trajectory with symplectic integrators. In particular, we will derive estimates of the convergence with respect to T and the size h of the time-grid, which are in perfect agreement with the numerical experiments conducted in [4].

2 The complete analysis of the d-dimensional harmonic oscillator

In this section, we illustrate the main ideas of the paper in the rather simple situation of the d-dimensional harmonic oscillator, where most of the analysis can be conducted in an explicit way. Hereafter, $H(p,q)$ is thus the Hamiltonian function from $\mathbb{R}^d \times \mathbb{R}^d$ to $\mathbb{R}$ defined as

$$H(p,q) = \frac{1}{2}\sum_{k=1}^{d}(\omega_k^2 q_k^2 + p_k^2), \tag{9}$$

and the corresponding dynamics is governed by the equations

$$\begin{cases} \dot{p}_k = -\omega_k^2 q_k \\ \dot{q}_k = \quad\;\; p_k \end{cases}, \; k = 1,\dots,d.$$

The exact trajectory lies on the d-dimensional manifold $S(p_0,q_0)$ defined by (4) where the $I_k(p,q) = \frac{1}{2}\left(\omega_k^2 q_k^2 + p_k^2\right)$ are the conserved energies of the d oscillators. Hence, denoting $r_k^0 = \sqrt{2I_k(p_0,q_0)}$, $k = 1,\dots,d$ and $z = (\omega_1 q_1 + ip_1,\dots,\omega_d q_d + ip_d)$ the aggregated vector of rescaled positions and momenta, the exact solution is of the form

$$z(t) = \left(r_1^0 e^{i(\omega_1 t+\phi_1)},\dots,r_d^0 e^{i(\omega_d t+\phi_d)}\right), \tag{10}$$

where $\phi = (\phi_1,\dots,\phi_d)$ depends on the initial conditions (p_0,q_0). As a consequence, the space average (6) we wish to approximate may be written here as:

$$\langle A\rangle = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d}(A\circ\Theta)(r^0,\theta)d\theta,$$

where $\Theta(r^0,\theta) = (\frac{r_1^0}{\omega_1}\cos(\theta_1), r_1^0\sin(\theta_1),\dots,\frac{r_d^0}{\omega_d}\cos(\theta_d), r_d^0\sin(\theta_d))$. As for the *time*-average (7), it reads:

$$\langle A\rangle(T) = \frac{1}{T}\int_0^T (A\circ\Theta)(r^0,\omega t+\phi)dt.$$

In order to estimate the rate of convergence of (7) toward (6), we expand $A\circ\Theta$ in Fourier series (the conditions under which this expansion is valid will be detailed in the following sections):

$$(A\circ\Theta)(r^0,\theta) = \sum_{\alpha\in\mathbb{Z}^d}\widehat{A\circ\Theta}(r^0,\alpha)e^{i\alpha\cdot\theta},$$

where $\alpha \cdot \theta = \alpha_1 \theta_1 + \ldots + \alpha_d \theta_d$ and with:

$$\widehat{A \circ \Theta}(r^0, \alpha) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} (A \circ \Theta)(r^0, \theta) e^{-i\alpha \cdot \theta} d\theta.$$

In particular, $\widehat{A \circ \Theta}(r^0, 0) = \langle A \rangle$. Hence, we have:

$$|\langle A \rangle - \langle A \rangle(T)| \leq \frac{1}{T} \sum_{\alpha \in \mathbb{Z}^d,\, \alpha \neq 0} \frac{2|\widehat{A \circ \Theta}(r^0, \alpha)|}{|\alpha \cdot \omega|}. \tag{11}$$

This infinite sum can then be bounded if we assume, on one hand, that the vector of frequencies $\omega = (\omega_1, \ldots, \omega_d)$ satisfies *Siegel's diophantine condition*

$$\exists\, \gamma, \nu > 0, \quad \forall\, \alpha \in \mathbb{Z}^d, \quad |\alpha \cdot \omega| > \gamma |\alpha|^{-\nu}, \tag{12}$$

and on the other hand, that the Fourier coefficients decay sufficiently rapidly. This relatively poor rate of convergence ($1/T$) may now be considerably improved by considering *iterated* averages of the form:

$$\langle A \rangle_k(T) := \frac{1}{T^k} \int_0^T \ldots \int_0^T (A \circ \Theta)(r^0, (t_1 + \ldots + t_k)\, \omega + \phi) dt_1 \ldots dt_k. \tag{13}$$

Using Fourier expansions as in (11), we indeed obtain in a very similar way the following error estimate for (13):

$$|\langle A \rangle - \langle A \rangle_k(T)| \leq \frac{1}{T^k} \sum_{\alpha \in \mathbb{Z}^d,\, \alpha \neq 0} \frac{2|\widehat{A \circ \Theta}(r^0, \alpha)|}{|\alpha \cdot \omega|^k}, \tag{14}$$

and under slightly more stringent bounds on the $|\widehat{A \circ \Theta}(r^0, \alpha)|$, (14) leads to a rate of convergence of $1/T^k$. Inspired by these computations, and noticing that (13) is a special case of (8) (more precisely $\langle A \rangle_k(T/k) = \langle A \rangle_\varphi(T)$ with $\varphi \equiv \chi^{*k}_{[0,1/k]}$, the k^{th}-convolution of the characteristic function of $[0, 1/k]$), we will consider in the sequel more general *filter*-functions and demonstrate that the rate of convergence can be further improved.

Now, a natural question that arises is whether the techniques exposed above are amenable to numerical computations, when both the trajectory $z(t)$ and the integrals (7) or (13) are approximated using numerical schemes. In the case of the harmonic oscillator, it turns out that the numerical trajectory $z^h(t_n)$ (i.e. the approximation at time $t_n = nh$ of $z(t_n)$), as soon as the underlying scheme is a symplectic (or symmetric) Runge-Kutta method [3], may be interpreted as the exact solution of a harmonic oscillator with *modified* frequencies $\omega_k^h = \omega_k \Theta(h\omega_k)$. In particular, the numerical trajectory lies on the same manifold $S(q_0, p_0)$ as the exact one. For the velocity-Verlet scheme, the numerical trajectory would lie on an invariant torus $\mathcal{O}(h^2)$-close to $S(q_0, p_0)$. This situation is more typical of what happens for general integrable Hamiltonian systems. In our situation, we have:

$$z^h(t_n) = \left(r_1^0 e^{i(\omega_1 \Theta(h\omega_1)t_n + \phi_1)}, \ldots, r_d^0 e^{i(\omega_d \Theta(h\omega_d)t_n + \phi_d)} \right),$$

where Θ is a smooth function defined by

$$\Theta(y) = \frac{1}{y} \arctan \left(\frac{R(iy) - R(-iy)}{i(R(iy) + R(-iy))} \right),$$

$R(z)$ being the *stability function* of the method (in fact, Θ is real-analytic as soon as R has no pole on the imaginary axis and satisfies $\Theta(y) = 1 + \mathcal{O}(y^r)$ where r denotes the order of convergence of the Runge-Kutta method). As a consequence, the Riemann sum associated with (13) (note that (15) with $k = 1$ corresponds to (7)) reads, for $T = nh$, $n \in \mathbb{N}$,

$$\langle A \rangle_k^{\mathrm{Rie}}(T) := \frac{1}{n^k} \sum_{j_1=0}^{n-1} \ldots \sum_{j_k=0}^{n-1} (A \circ \Theta)(r^0, (j_1 + \ldots + j_k) h \, \omega \, \Theta(\omega h) + \phi), \tag{15}$$

where $\omega\Theta(\omega h) = (\omega_1 \Theta(\omega_1 h), \ldots, \omega_d \Theta(\omega_d h))$, so that using once again Fourier expansions, we get straightforwardly:

$$|\langle A \rangle - \langle A \rangle_k^{\mathrm{Rie}}(T)| \leq \frac{1}{n^k} \sum_{\alpha \in \mathbb{Z}^d, \, \alpha \neq 0} |\widehat{A \circ \Theta}(r^0, \alpha)| \left| \frac{e^{inh\alpha \cdot (\omega\Theta(\omega h))} - 1}{e^{ih\alpha \cdot (\omega\Theta(\omega h))} - 1} \right|^k. \tag{16}$$

Bounding the above infinite sum now requires to bound the term $|e^{inx} - 1| / |e^{ix} - 1|$ for x of the form $x = h\alpha \cdot (\omega\Theta(\omega h))$. To this aim, we use the following two inequalities

$$\exists \, C_0, x_0 > 0, \ \forall n \in \mathbb{N}, \ \forall |x| \leq x_0, \ \left| \frac{e^{inx} - 1}{e^{ix} - 1} \right| \leq C_0 \frac{1}{|x|}, \tag{17}$$

$$\forall n \in \mathbb{N}, \ \forall x \in \mathbb{R}, \ \left| \frac{e^{inx} - 1}{e^{ix} - 1} \right| \leq n, \tag{18}$$

according to whether $|x|$ is small (17) or not (18). The bound we are looking for is now based on the following lemma:

Lemma 1 *Assume that the vector of frequencies* ω *satisfies the diophantine condition* (12) *and the Runge-Kutta method is of order* r. *Then, there exist strictly positive constants* c *and* h_0 *such that*

$$\forall\, h \le h_0 \quad \forall\, \alpha \in \mathbb{Z}^d, \quad |\alpha \cdot (\omega\, \Theta(\omega h))| \le \frac{\gamma}{2}\, |\alpha|^{-\nu} \Longrightarrow |\alpha| \ge c\, h^{-\frac{r}{\nu+1}}.$$

Proof. Assume that there exists $\alpha \in \mathbb{Z}^d$ such that

$$|\alpha \cdot (\omega\, \Theta(\omega h))| \le \frac{\gamma}{2}\, |\alpha|^{-\nu}.$$

Then, from $\Theta(h\omega_k) = 1 + \mathcal{O}(|h\,\omega_k|^r)$, we obtain for h sufficiently small:

$$\begin{aligned} \frac{\gamma}{2}\, |\alpha|^{-\nu} &\ge |\omega \cdot \alpha| - C|\alpha|\, |h\,\omega|^r, \\ &\ge \gamma|\alpha|^{-\nu} - C|\alpha|\, |h\,\omega|^r, \end{aligned}$$

where C is the strictly positive constant contained in the term $\mathcal{O}$ (note that if $\Theta \equiv 1$, although the constant C is zero, there is no α violating condition (12) and the lemma remains valid). Hence,

$$|\alpha| \ge \left(\frac{\gamma}{2C|\omega|^r}\, h^{-r} \right)^{\frac{1}{\nu+1}}.$$

∎

But for $|\alpha| \le ch^{-r/(\nu+1)}$ we have $|h\alpha \cdot \omega\Theta(\omega h)| \le \tilde{c}h^{1-r/(\nu+1)}$ for a constant $\tilde{c}$ independent of h. Hence if $\nu > r-1$, then for small enough h we have $|h\alpha \cdot \omega\Theta(\omega h)| \le x_0$ defined in (17). Now we can split the sum in (16) into

$$\sum_{1 \le |\alpha| \le ch^{-\frac{r}{\nu+1}}} |\widehat{A \circ \Theta}(r^0, \alpha)|\, \frac{C_0^k}{n^k h^k |\alpha \cdot (\omega\, \Theta(\omega h))|^k} + \sum_{|\alpha| \ge ch^{-\frac{r}{\nu+1}}} |\widehat{A \circ \Theta}(r^0, \alpha)|. \qquad (19)$$

Using the estimate of Lemma 1 for the first term and assuming that the Fourier coefficients decay sufficiently rapidly, it then follows that

$$|\langle A \rangle - \langle A \rangle_k^{\mathrm{Rie}}(T)| = \mathcal{O}\left(\frac{1}{T^k} + h^r \right). \qquad (20)$$

This seems to be the best possible estimate attainable, since the term in $1/T^k$ is the intrinsic error component of the *iterated*-average, whereas the term h^r inevitably comes into play when using a numerical scheme of order r. It is worth noticing that there is **no secular component** in the numerical error h^r owing to the **symplecticity of the time-integrator**.

Our aim in next sections is now to prove estimates that generalize (20) in the following two directions:

1. for *filtered*-averages with general filter functions;
2. for integrable Hamiltonian system with bounded trajectories.

3 Approximation of the average: The continuous case

The function φ considered in Formula (8) is somewhat arbitrary. The most commonly used function in practice is $\varphi \equiv 1$, which corresponds to the usual *time*-average as defined in (7), for which convergence when T tends to infinity is rather slow (with rate $1/T$). For the harmonic oscillator, we have seen that the use of *iterated*-averages (which can be seen as a special case of *filtered*-averages) allows for a significant acceleration of the convergence. Theorem 1 below shows that with increasingly smooth functions φ satisfying appropriate zero boundary conditions, it is possible to improve the rate of convergence to $1/T^k$ for any integer $k > 1$, not only for the harmonic oscillator, but for a general integrable Hamiltonian system. It is then natural to investigate what happens in the limit when k tends to infinity. To this aim, we shall consider, as an example of infinitely differentiable functions φ with compact support $[0,1]$ that satisfy $\varphi^{(k)}(0) = \varphi^{(k)}(1) = 0$ for any $k \in \mathbb{N}$, the function ξ defined below:

$$\begin{aligned} \xi : [0,1] &\longrightarrow [0,+\infty[\\ x &\longmapsto \exp\left(-\frac{1}{x(1-x)}\right). \end{aligned} \tag{21}$$

In the sequel, we shall assume that the estimates

$$\|\xi^{(k)}\|_{\mathrm{L}^1} := \int_0^1 |\xi^{(k)}(x)|dx \leq \mu\beta^k k^{\delta k}, \tag{22}$$

$$\|\xi^{(k)}\|_{\mathrm{L}^\infty} := \sup_{x\in[0,1]} |\xi^{(k)}(x)| \leq \mu\beta^k k^{\delta k}, \tag{23}$$

hold for some strictly positive constants μ, β and δ. The existence of such constants will be shown in Lemma 3.

Theorem 1 *Consider the completely integrable system* (1)*, and assume that the diophantine condition* (12) *is satisfied for* $\omega(a_0)$ *defined in* (5) *by the initial condition* (q_0, p_0)*, with* $(q_0, p_0) = \psi(a_0, \theta_0)$*. Consider a function* $A \in C^0(\mathbb{R}^d, \mathbb{R}^d)$ *(the observable). Recall that to this function we associate the* space*-average* $\langle A\rangle$*, the* time*-average* $\langle A\rangle(T)$ *and the* filtered *time-average* $\langle A\rangle_\varphi(T)$ *respectively defined in* (6)*,* (7) *and* (8)*, where* $\varphi \in C^0(0,1)$ *is a* filter *function (assumed to be positive). Then we have the following convergence estimates:*

1. *If A is real analytic on $\mathbb{R}^d \times \mathbb{R}^d$, then there exists a constant c depending on A, d, ν and γ such that*

$$|\langle A\rangle(T) - \langle A\rangle| \leq \frac{c}{T}.$$

2. *If φ is $C^{k+1}(0,1)$ with $\varphi^{(j)}(0) = \varphi^{(j)}(1) = 0$ for all $j = 0, \ldots, k-1$, and if A is real analytic on $\mathbb{R}^d \times \mathbb{R}^d$, then there exist positive constants c_0 and R depending on A, φ, d, ν and γ, such that (here $\nu \in \mathbb{N}$, though a similar formula holds for general ν using the Γ function)*

$$|\langle A\rangle_\varphi(T) - \langle A\rangle| \leq \frac{c_0 R^{k+1}(\nu(k+1)+1)!}{T^{k+1}} \times \frac{(|\varphi^{(k)}(0)| + |\varphi^{(k)}(1)| + \|\varphi^{(k+1)}\|_{\mathrm{L}^1})}{\|\varphi\|_{\mathrm{L}^1}}.$$

3. *If ξ defined in (21) is taken as the filter function and if A is real analytic on $\mathbb{R}^d \times \mathbb{R}^d$, then there exist strictly positive constants c_1, κ and ρ depending on A, d, ν and γ, such that*

$$|\langle A\rangle_\xi(T) - \langle A\rangle| \leq c_1 e^{-\kappa T^{1/\rho}}.$$

Proof. Statement 1. is proved in Arnold [2]. It may also be obtained as a special case of 2. with $\varphi \equiv 1$. Now, if A is real-analytic on $\mathbb{R}^d \times \mathbb{R}^d$, then so is $A \circ \psi$ on the d-dimensional torus $\mathbb{T}^d$ and we can expand it as a Fourier series

$$(A \circ \psi)(a_0, \alpha) = \sum_{\alpha \in \mathbb{Z}^d} \widehat{A \circ \psi}(a_0, \alpha) e^{i\alpha \cdot \theta},$$

with exponentially decaying coefficients:

$$\forall \alpha \in \mathbb{Z}^d, \ |\widehat{A \circ \psi}(a_0, \alpha)| \leq C e^{-\frac{|\alpha|}{C}},$$

where C is a strictly positive real constant. The integral over $\mathbb{T}^d$ of the first coefficient of the series ($\alpha = 0$) is straightforwardly identified as the space-average

$$\widehat{A \circ \psi}(a_0, 0) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} (A \circ \psi)(a_0, \theta) d\theta.$$

Writing $\int_0^T \varphi\left(\frac{t}{T}\right) dt = T\|\varphi\|_{\mathrm{L}^1} := \chi^{-1}$, the error can be computed as follows:

$$\langle A\rangle_\varphi(T) - \langle A\rangle = \chi \sum_{\alpha \in \mathbb{Z}^d,\, \alpha \neq 0} \widehat{A \circ \psi}(a_0, \alpha) \int_0^T \varphi\Big(\frac{t}{T}\Big) e^{i\alpha \cdot (\theta_0 + t\omega(a_0))} dt \quad (24)$$

$$= \chi \sum_{\alpha \in \mathbb{Z}^d,\, \alpha \neq 0} \widehat{A \circ \psi}(a_0, \alpha) e^{i(\alpha \cdot \theta_0)} \int_0^T \varphi\Big(\frac{t}{T}\Big) e^{it(\alpha \cdot \omega(a_0))} dt.$$

Now, the running term of the series can be integrated by parts

$$\int_0^T \varphi\Big(\frac{t}{T}\Big) e^{it(\alpha\cdot\omega(a_0))}dt = \left[\frac{\varphi\big(\frac{t}{T}\big)e^{it(\alpha\cdot\omega(a_0))}}{i(\alpha\cdot\omega(a_0))}\right]_0^T - \frac{1}{Ti(\alpha\cdot\omega(a_0))}\int_0^T \varphi'\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}dt.$$

Integrating repeatedly by parts, this last term writes

$$\frac{e^{iT(\alpha\cdot\omega(a_0))}\varphi(1)-\varphi(0)}{i(\alpha\cdot\omega(a_0))} - \frac{1}{Ti(\alpha\cdot\omega(a_0))}\int_0^T \varphi'\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}dt$$
$$= \ldots = \frac{(-1)^k}{(Ti(\alpha\cdot\omega(a_0)))^k}\int_0^T \varphi^{(k)}\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}dt,$$

and eventually,

$$\int_0^T \varphi\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}dt = \frac{(-1)^k}{(Ti(\alpha\cdot\omega(a_0)))^{k+1}}T\left[\varphi^{(k)}\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}\right]_0^T - \frac{(-1)^k}{(Ti(\alpha\cdot\omega(a_0)))^{k+1}}\int_0^T \varphi^{(k+1)}\Big(\frac{t}{T}\Big)e^{it(\alpha\cdot\omega(a_0))}dt.$$

Inserting this expression in equation (24) and taking the moduli of both sides, we finally get the bound

$$|\langle A\rangle_\varphi(T)-\langle A\rangle| \le \frac{(|\varphi^{(k)}(0)|+|\varphi^{(k)}(1)|+\|\varphi^{(k+1)}\|_{\mathrm{L}^1})}{T^{k+1}\|\varphi\|_{\mathrm{L}^1}} \times \sum_{\alpha\in\mathbb{Z}^d,\ \alpha\neq 0}\frac{|\widehat{A\circ\psi}(a_0,\alpha)|}{|\alpha\cdot\omega(a_0)|^{k+1}}$$

It remains to justify the convergence of the series considered above (and to bound its limit). This is a consequence of the diophantine condition $|\alpha\cdot\omega(a_0)| \le \frac{\gamma}{|\alpha|^\nu}$, which gives here

$$\sum_{\alpha\in\mathbb{Z}^d,\ \alpha\neq 0}\frac{|\widehat{A\circ\psi}(a_0,\alpha)|}{|\alpha\cdot\omega(a_0)|^{k+1}} \le \sum_{\alpha\in\mathbb{Z}^d,\ \alpha\neq 0} Ce^{-\frac{|\alpha|}{C}}\left(\frac{|\alpha|}{\gamma^{1/\nu}}\right)^{\nu(k+1)},$$
$$\le C\eta^{\nu(k+1)}\sum_{\alpha\in\mathbb{Z}^d,\ \alpha\neq 0} e^{-\frac{|\alpha|}{C}}\left(\frac{|\alpha|}{\eta\gamma^{1/\nu}}\right)^{\nu(k+1)}.$$

We now take $\eta = \frac{2C}{\gamma^{1/\nu}}$ so that $1/(\gamma^{1/\nu}\eta) = 1/(2C)$ and we obtain:

$$\sum_{\alpha\in\mathbb{Z}^d,\ \alpha\neq 0} \frac{|\widehat{A\circ\psi}(a_0,\alpha)|}{|\alpha\cdot\omega(a_0))|^{k+1}} \leq C\eta^{\nu(k+1)}(\nu(k+1)+1)! \sum_{\alpha\in\mathbb{Z}^d} e^{-\frac{|\alpha|}{2C}},$$
$$\leq \frac{C(2C)^{\nu(k+1)}(8C)^d}{\gamma^{k+1}}(\nu(k+1)+1)!,$$

where we have used $x^n \leq e^x(n+1)!$. Statement 3. is a consequence of Statement 2. with a suitably chosen k: since $\xi^{(k)}(0) = \xi^{(k)}(1) = 0$ for any $k \in \mathbb{N}$, we have indeed that for all $k \geq 0$:

$$|\langle A\rangle_\xi(T) - \langle A\rangle| \leq c_1 \left(\frac{r_1}{T}\right)^{k+1} (k+1)^{\delta(k+1)}(\nu(k+1)+1)!,$$

with $c_1 = c_0\mu$ and $r_1 = R\beta$, μ and β being the constants of (22). Now let $\tilde{\nu}$ be the nearest integer to ν toward infinity. This gives:

$$|\langle A\rangle_\xi(T) - \langle A\rangle| \leq c_1 \left(\frac{r_1\tilde{\nu}^{\tilde{\nu}}}{T}\right)^{k+1} (k+1)^{(\delta+\tilde{\nu})(k+1)},$$
$$\leq c_1 e^{f(k+1)},$$

where $f(\ell) = \ell[\log(r_1\tilde{\nu}^{\tilde{\nu}}/T) + (\delta+\tilde{\nu})\log(\ell)]$. The minimum of f for positive ℓ is attained for $\ell = \frac{1}{e}\left(\frac{T}{r_1\tilde{\nu}^{\tilde{\nu}}}\right)^{1/(\tilde{\nu}+\delta)}$ and is worth

$$f_{min} = -\frac{(\delta+\tilde{\nu})}{e}\left(\frac{T}{r_1\tilde{\nu}^{\tilde{\nu}}}\right)^{\frac{1}{(\delta+\tilde{\nu})}}.$$

■

Remark 1 In the proof of Theorem 1, one gets $c_0 = C(8C)^d$, $R = (2C)^\nu/\gamma$, $c_1 = \mu c_0$, $\kappa = -(\delta+\tilde{\nu})e^{-1}\tilde{\nu}^{-\frac{\tilde{\nu}}{\tilde{\nu}+\delta}}$ and $\rho = (\delta+\tilde{\nu})$, where $\tilde{\nu} = \nu+1$. The values of these constants rely heavily on the sharpness of estimates (22) and it is likely that they might be improved. Nevertheless, the convergence behavior would be essentially the same for large dimensions: even if ξ was analytic, one would get $\rho = 1+\tilde{\nu}$. More noticeably, since almost all frequencies $\omega(a_0)$ satisfy the diophantine condition for some γ as soon as $\nu > d-1$, we may think of $\tilde{\nu}$ as being d and thus δ as being approximately $1+d$. The rate of convergence thus directly depends on the dimension of the phase-space.

4 Semi-discrete averages

We now wish to investigate whether the estimates of Theorem 1 persist when one replaces the integrals by Riemann sums. It turns out, quite remarkably, that its proof can be almost readily adapted, if one assumes the additional *non-resonance* condition [5], i.e. if, given a step-size h, there exist positive constants γ^* and ν^* such that for all $\alpha \in \mathbb{Z}^d$, the following estimate holds:

$$\left| \frac{1 - e^{i\alpha \cdot h\omega(a_0)}}{h} \right| \geq \gamma^* |\alpha|^{-\nu^*}. \tag{25}$$

Though this condition might appear very restrictive at first glance, the probability of picking an $h \in [0, h_0]$ violating (25) goes to zero with h_0, whenever the diophantine condition is satisfied, $\gamma^* \leq \gamma$ and $\nu^* > \nu + d + 1$. For a precise statement of this result, we refer to Lemma 6.3. in Chapter X of [5] (see also [10]).

Theorem 2 *Assume that the conditions of Theorem* 1 *and condition* (25) *are satisfied and let* $T = nh > 0$ *for a given integer* $n \geq 2$. *Let us further define the Riemann sums corresponding to the* continuous time-*average*

$$\langle A \rangle^{\mathrm{Rie}}(T) := \frac{1}{n} \sum_{j=0}^{n-1} A(q(jh), p(jh)),$$

and the filtered *time-average*

$$\langle A \rangle_\varphi^{\mathrm{Rie}}(T) := \frac{\sum_{j=0}^{n-1} \varphi(\frac{j}{n}) A(q(jh), p(jh))}{\sum_{j=0}^{n-1} \varphi(\frac{j}{n})},$$

where $\varphi \in C^0(0,1)$ *is the* filter *function. Then we have the following convergence estimates:*

1. *If* A *is real analytic on* $\mathbb{R}^d \times \mathbb{R}^d$, *then there exists a constant* c^* *depending on* A, d, ν^* *and* γ^* *such that*

$$\left| \langle A \rangle^{\mathrm{Rie}}(T) - \langle A \rangle \right| \leq \frac{c^*}{T}.$$

2. *If* φ *is* $C^{k+1}(0,1)$ *with* $\varphi^{(j)}(0) = \varphi^{(j)}(1) = 0$ *for all* $j = 0, \ldots, k-1$, *and if* A *is real analytic on* $\mathbb{R}^d \times \mathbb{R}^d$, *then there exist strictly positive constants* c_0^* *and* R^* *depending on* A, φ, d, ν^* *and* γ^*, *such that*

$$\left| \langle A \rangle_\varphi^{\mathrm{Rie}}(T) - \langle A \rangle \right| \leq \frac{c_0^* (R^*)^{k+1} k^k (\nu^*(k+1)+1)!}{T^{k+1}} \frac{\left(|\varphi^{(k)}(0)| + |\varphi^{(k)}(1)| + \|\varphi^{(k+1)}\|_{\mathrm{L}^\infty}\right)}{\|\varphi\|_{\mathrm{L}^1}}.$$

3. *If ξ is taken as the filter function and if A is real analytic on $\mathbb{R}^d \times \mathbb{R}^d$, then there exist strictly positive constants c_1^*, κ^* and ρ^* depending on A, d, ν^* and γ^*, such that*

$$\left|\langle A\rangle_\xi^{\mathrm{Rie}}(T) - \langle A\rangle\right| \le c_1^* e^{-\kappa^* T^{1/\rho^*}}.$$

Remark 2 In the proof of Theorem 2, one gets $c_0^* = 2\varepsilon e^2 C(8C)^d$, $R^* = (2C)^{\nu^*}/\gamma^*$, $c_1^* = \mu c_0^*$, $\kappa^* = -(\delta+1+\tilde{\nu}^*)e^{-1}(\tilde{\nu}^*)^{-\frac{\tilde{\nu}^*}{\tilde{\nu}^*+\delta+1}}$ and $\rho^* = (\delta+1+\tilde{\nu}^*)$, where $\tilde{\nu}^* = \nu^*+1$ and where

$$\varepsilon = \|\varphi\|_{\mathrm{L}^1} \sup_{n\ge 2} \left(\sum_{j=0}^{n-1} (1/n)\varphi(j/n)\right)^{-1}.$$

It is worth noticing that these constants do *not* depend on the step-size h.

Proof. Statement 1. is a special case of Statement 2. with $\varphi \equiv 1$, so that we focus on the error estimate for the filtered average. Expanding $(A\circ\psi)$ in Fourier series as in Theorem 1 and denoting $S_n = \sum_{j=0}^{n-1}(1/n)\varphi(j/n)$, we have:

$$\langle A\rangle_\varphi^{\mathrm{Rie}}(T) - \langle A\rangle = \frac{1}{nS_n} \sum_{\alpha\in\mathbb{Z}^d,\ \alpha\neq 0} \widehat{A\circ\psi}(a_0,\alpha) e^{i(\alpha\cdot\theta_0)}$$
$$\times \sum_{j=0}^{n-1} \varphi\left(\frac{j}{n}\right) e^{i\alpha\cdot jh\omega(a_0)}. \tag{26}$$

We use the following result, whose proof is given in Appendix:

Lemma 2 *For a given* filter-*function φ in $C^{k+1}(0,1)$ with $\varphi^{(j)}(0) = \varphi^{(j)}(1) = 0$ for all $j = 0,\dots,k-1$, and a given integer $n \ge k+2$, let φ_j be the real numbers defined by $\varphi_j = \varphi(j/n)$ for $j = 0,\dots,n$. If $b \neq 1$ is a complex number of modulus 1, then we have the estimate*

$$\left|\sum_{0\le j\le n-1} \varphi_j b^j\right| \le \frac{2e^2 k^k}{n^k |1-b|^{k+1}} \left(|\varphi^{(k)}(0)| + |\varphi^{(k)}(1)| + \|\varphi^{(k+1)}\|_{\mathrm{L}^\infty}\right)$$

Using this lemma with $b = e^{i\alpha\cdot h\omega(a_0)}$, we obtain:

$$\left|\langle A\rangle_\varphi^{\mathrm{Rie}}(T) - \langle A\rangle\right| \le \frac{2e^2k^k}{n^{k+1}S_n} \left(|\varphi^{(k)}(0)| + |\varphi^{(k)}(1)| + \|\varphi^{(k+1)}\|_{\mathrm{L}^\infty}\right)$$
$$\times \sum_{\alpha\in\mathbb{Z}^d,\ \alpha\neq 0} \frac{Ce^{-|\alpha|/C}}{|1-e^{i\alpha\cdot h\omega(a_0)}|^{k+1}}$$

We now use condition (25) and obtain:

$$\sum_{\alpha\in\mathbb{Z}^d,\ \alpha\neq 0} \frac{Ce^{-|\alpha|/C}}{\left|1-e^{i\alpha\cdot h\omega(a_0)}\right|^{k+1}} \leq \frac{C}{h^{k+1}} \sum_{\alpha\in\mathbb{Z}^d,\ \alpha\neq 0} e^{-|\alpha|/C} \frac{|\alpha|^{\nu^*(k+1)}}{(\gamma^*)^{k+1}},$$

$$\leq \frac{C(2C)^{\nu^*(k+1)}(8C)^d}{h^{k+1}(\gamma^*)^{k+1}} (\nu^*(k+1)+1)!.$$

This proves Statement 2. Statement 3. can then be obtained as in Theorem 1. ■

5 Fully discrete averages

We now consider a symplectic discretization of the exact trajectory of (1). Two types of results exist, according to whether we use results on invariant tori of symplectic integrators [6,5] or ultraviolet cut-off theory [1,5]. Given that the strong non-resonance condition (25) already appears for semi-discrete averages, we will only detail results using KAM tori in the spirit of [5,10].

In action-angles variables, the Hamiltonian $H(p,q) = K(a)$ depends only on a. Without loss of generality, we may assume that $a_0 = 0$, so that we can write

$$K(a) = c + \omega \cdot a + \frac{1}{2} a^T M(a) a,$$

where $\omega = \omega(0)$. We assume that M is non degenerate in the sense that

$$\exists\, \alpha > 0, \quad \|M(0)v\| \geq \alpha \|v\| \quad \text{for} \quad v \in \mathbb{R}^d, \tag{27}$$

so that Kolmogorov-Arnold-Moser theory can be applied (see [6,7,1, 8]).

We consider a symplectic integrator Φ_h of order r applied to the problem (1) with a stepsize h. The numerical solution is written $(p_n, q_n) \in \mathbb{R}^d$ for $n \geq 0$. For a function A defined in a neighborhood of $S(p_0, q_0)$ and for $T = nh$, we define the *filtered* numerical time-average

$$\langle A \rangle^{\mathrm{Rie}}_{\varphi,h}(T) := \frac{\sum_{j=0}^{n-1} \varphi(\frac{j}{n}) A(q_j, p_j)}{\sum_{j=0}^{n-1} \varphi(\frac{j}{n})}. \tag{28}$$

Under these conditions, we can apply Theorems 6.1 and 6.2 of [5] (see also [9,10]): For small enough h, there exists a symplectic analytic transformation $\psi_h : (b, \varphi) \mapsto (a, \theta)$, $\mathcal{O}(h^r)$-close to the identity, such that $\psi_h^{-1} \circ \Phi_h \circ \psi_h : (b, \varphi) \mapsto (\widehat{b}, \widehat{\varphi})$ is given by

$$\widehat{b} = b - h\frac{\partial S_h}{\partial \widehat{\varphi}}(b, \widehat{\varphi}) \quad \text{and} \quad \widehat{\varphi} = \varphi + h\frac{\partial S_h}{\partial b}(b, \widehat{\varphi})$$

with

$$S_h(b, \widehat{\varphi}) = c_h + \omega \cdot b + \frac{1}{2}b^T M_h(b, \widehat{\varphi})b,$$

where $c_h \in \mathbb{R}$ and M_h is analytic and bounded with respect to h. In coordinates (b, φ), we thus have

$$\psi_h^{-1} \circ \Phi_h \circ \psi_h : (b, \varphi) \mapsto (b, \varphi + h\omega) + \mathcal{O}(h\|b\|) \tag{29}$$

Based on this transformation, we have the following result:

Theorem 3 *Consider a symplectic integrator Φ_h of order r and of stepsize h applied to* (1) *under the conditions of Theorem* 1*. Assume that* (27) *holds, and suppose that ω and h satisfy the conditions* (12) *and* (25)*. Then we have the following estimates:*

1. *If φ is C^{k+1} with $\varphi^{(j)}(0) = \varphi^{(j)}(1) = 0$ for all $j = 0, \dots, k-1$ and if A is real analytic on $\mathbb{R}^d$, then there exist constants C and h_0 depending on A, γ^*, ν^*, d, k, φ, and there exist $(\tilde{p}_0, \tilde{q}_0)$ in an h^r-neighborhood of (p_0, q_0) such that if the numerical trajectory starts with $(\tilde{p}_0, \tilde{q}_0)$, then we have*

$$\forall h \le h_0 \quad \forall T = nh \ge 0, \quad |\langle A\rangle^{\text{Rie}}_{\varphi,h}(T) - \langle A\rangle| \le C\left(\frac{1}{T^{k+1}} + h^r\right) \tag{30}$$

2. *If ξ is taken as the filter function, if A is real analytic, then there exist constants C, h_0, κ and ρ depending on A, γ^*, ν^*, d, k, and there exist $(\tilde{p}_0, \tilde{q}_0)$ in an h^r-neighborhood of (p_0, q_0) such that if the numerical trajectory starts with $(\tilde{p}_0, \tilde{q}_0)$, then we have*

$$\forall h \le h_0 \quad \forall T = nh \ge 0, \quad |\langle A\rangle^{\text{Rie}}_{\xi,h}(T) - \langle A\rangle| \le C\left(e^{-\kappa T^{1/\rho}} + h^r\right) \tag{31}$$

Proof. Using (29), we have for all n

$$\psi_h^{-1} \circ \Phi_h^n \circ \psi_h : (b, \varphi) \mapsto (b, \varphi + nh\omega) + \mathcal{O}(nh\|b\|)$$

Consider the points $(b_n, \varphi_n) = \psi_h^{-1} \circ \psi^{-1}(p_n, q_n)$, and suppose that the point (p_0, q_0) is such that $b_0 = 0$. Then using the previous formula, we have

$$\forall\, n \ge 0, \quad b_n = b_0 = 0 \quad \text{and} \quad \varphi_n = \varphi_0 + nh\omega.$$

Now we have with $S_n = \sum_{j=0}^{n-1}(1/n)\varphi(j/n)$,

$$\langle A\rangle^{\text{Rie}}_{\varphi,h}(T) := \frac{1}{nS_n}\sum_{j=0}^{n-1}\varphi(\frac{j}{n})A\circ\psi\circ\psi_h(b_j,\varphi_j),$$

and using the Fourier expansion of $A\circ\psi\circ\psi_h$,

$$\langle A\rangle^{\text{Rie}}_{\varphi,h}(T) := \frac{1}{nS_n}\sum_{\alpha\in\mathbb{Z}^d} A\widehat{\circ\psi\circ}\psi_h(0,\alpha)e^{i\alpha\cdot\varphi_0}\sum_{j=0}^{n-1}\varphi(\frac{j}{n})e^{i\alpha\cdot jh\omega}.$$

As ψ_h is an analytic function $\mathcal{O}(h^r)$-close to the identity, we have

$$A\widehat{\circ\psi\circ}\psi_h(0,0) = \langle A\rangle + \mathcal{O}(h^r),$$

and the Fourier coefficients $A\widehat{\circ\psi\circ}\psi_h(0,\alpha)$ decay exponentially with respect to α, uniformly with respect to h. Thus the same proof as in Theorem 2 shows the result. ∎

Remark 3 For the iterated averages, as defined in Section 2:

$$\langle A\rangle^{\text{Rie}}_{k,h}(T) := \frac{1}{n^k}\sum_{j_1=0}^{n-1}\cdots\sum_{j_k=0}^{n-1}A(q_J,p_J),\ \ k\geq 0, \tag{32}$$

where $J = j_1 + \cdots j_k$, we would get, using the result of Section X.4 in [5], and by similar computations as in (16) and (19),

$$|\langle A\rangle^{\text{Rie}}_{k,h}(T) - \langle A\rangle| \leq C\left(\frac{1}{T^k} + h^r\right) \tag{33}$$

over exponentially long time-interval.

6 Remarks on the implementation and numerical experiments

Though optimal with respect to the rate of convergence, the filter function ξ does not seem to allow for the derivation of an error estimate: Given that the values of the constant C in (31) is out of reach, the value of n for which

$$R_n^{\varphi} := \frac{\sum_{j=0}^{n}\varphi(j/n)A_j}{n\|\varphi\|_{\mathrm{L}^1}}$$

becomes sufficiently close (up to user's tolerance) to its limit as n goes to infinity can not be determined in advance. An update formula for R_n^{φ} from n to $n+1$ thus appears of much use and this should guide the choice of φ. In order to get such a formula, we study the dependence in T of

$$a(T) = \int_0^T \varphi\Big(\frac{t}{T}\Big) A(p(t), q(t))dt.$$

Differentiating with respect to T leads to

$$\frac{da(T)}{dT} = \varphi(1)A(p(T), q(T)) - \frac{1}{T}\int_0^T \frac{t}{T}\varphi'\Big(\frac{t}{T}\Big) A(p(t), q(t))dt. \tag{34}$$

To be of practical use, it is thus necessary that $x\varphi'(x)$ is of the form $\alpha\varphi(x)$ (where α is an arbitrary constant) so that (34) becomes an ordinary differential equation for $a(T)$. The only admissible solutions are thus monomials in x. We thus consider the following polynomial filter functions

$$\varphi_p(x) = x^p(1-x)^p,\ p \in \mathbb{N}. \tag{35}$$

Denoting for p and n in $\mathbb{N}$ the *elementary* Riemann sums

$$S_n^p = \sum_{j=0}^{n} \Big(\frac{j}{n}\Big)^p A_j,$$

it is easy to get the desired update formula

$$S_0^p = 0 \text{ and } S_n^p = A_n + (1-1/n)^p S_{n-1}^p, n \geq 1.$$

Now, since

$$\varphi_p(x) = \sum_{k=0}^{p} (-1)^k \binom{p}{k} x^{p+k} \text{ and } \|\varphi_p\|_{\mathrm{L}^1} = \frac{(p!)^2}{(2p+1)!}$$

the approximation we seek for can be obtained as the linear combination

$$R_n^{\varphi_p} = \frac{(2p+1)!}{n(p!)^2} \sum_{k=0}^{p} (-1)^k \binom{p}{k} S_n^{p+k}.$$

We now consider the application of our method to the 3-dimensional Kepler problem with Hamiltonian

$$H(p,q) = p_1^2 + p_2^2 + p_3^2 - \frac{1}{\sqrt{q_1^2 + q_2^2 + q_3^2}}.$$

Besides the Hamiltonian, this system has three other invariants, the so-called angular momenta

$$L_1 = q_2p_3 - q_3p_2,\ L_2 = q_1p_3 - q_3p_1 \text{ and } L_3 = q_2p_1 - q_1p_2,$$

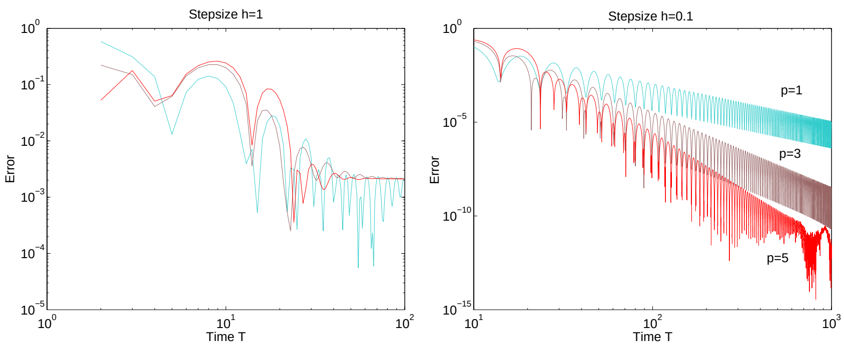

Fig. 1. Error in the averages for $p = 1, 3, 5$ for the 3D-Kepler problem

and we shall denote $L = \sqrt{L_1^2 + L_2^2 + L_3^2}$. Our goal is here to estimate the average over the manifold

$$S = \{(p, q) \in \mathbb{R}^6;\ L_1(p, q) = L_1(p_0, q_0),\ L_2(p, q) = L_2(p_0, q_0),\\ L_3(p, q) = L_3(p_0, q_0),\ H(p, q) = H(p_0, q_0)\}$$

of the quantity $r = \sqrt{q_1^2 + q_2^2 + q_3^2}$, for it is known to have the following analytical expression

$$\langle r \rangle = \frac{3 + 2\,H(p_0, q_0)\,L(p_0, q_0)^2}{4\,|H(p_0, q_0)|}.$$

For $p_0 = (0, 1.1, 0.5)^T$ and $q_0 = (0.9, 0, 0)^T$ this leads to $\langle r \rangle = 1.376630029154519$.

To this aim, we consider the Verlet method as basic step and use the 8^{th}-order 15-stages composition of [11]. On Figure 1 are represented the errors $|\langle r \rangle_{\varphi_p}(T) - \langle r \rangle|$ in logarithmic scale for two different step-sizes. On the left of the figure, the three curves all reach a plateau corresponding to the incompressible h-error term. Refining the step-size removes this plateau (or at least shifts it to the left, see the right graphics). In both cases, the predicted rate of convergence in $1/T^{p+1}$ is clearly observed (it corresponds to a slope of $p + 1$ for φ_p).

Appendix: some technical results

In this appendix section, we collect a few technical results used in the paper.

Lemma 3 *Let ξ be the function defined on $[0,1]$ by $\xi(x) = e^{-\frac{1}{x(1-x)}}$. There exist strictly positive constants $\mu \leq 1$, $\beta \leq (2\sqrt{3}+6)/e^2$ and $\delta \leq 3$ such that the following estimates hold for all $k \in \mathbb{N}^*$:*

$$\|\xi^{(k)}\|_{\mathrm{L}^1} := \int_0^1 |\xi^{(k)}(x)|dx \leq \mu\beta^k k^{\delta k},$$
$$\|\xi^{(k)}\|_{\mathrm{L}^\infty} = \sup_{x\in[0,1]} |\xi^{(k)}(x)| \leq \mu\beta^k k^{\delta k}.$$

Proof. Looking for an expression of $\xi^{(k)}(x)$ of the form

$$\xi^{(k)}(x) = \frac{P_k(x)}{[\Pi(x)]^{2k}} e^{-\frac{1}{x(1-x)}},$$

where $\Pi(x) = x(1-x)$ and where P_k is a polynomial, we easily find the recurrence relation:

$$P_0 \equiv 1 \text{ and } P_{k+1} = \Pi'\,(1-2k\Pi)\,P_k + P_k'\,\Pi^2,\ k \geq 0, \tag{36}$$

We now look for bounds on balls B_r of radius $r > 0$ and center $z = 1/2 + 0\,i \in \mathbb{C}$. The bounds for Π and Π' read

$$\sup_{z\in B_r} |\Pi(z)| \leq (r^2+1/4),\ \sup_{z\in B_r} |\Pi'(z)| \leq r,$$

and the Cauchy integral representation of P_k' leads to

$$\forall\,\varepsilon > 0,\ \sup_{z\in B_r} |P_k'(z)| \leq \frac{r+\varepsilon}{\varepsilon} \sup_{z\in B_{r+\varepsilon}} |P_k(z)|.$$

Inserting these bounds in (36) we get:

$$\begin{aligned}\sup_{z\in B_r} |P_{k+1}(z)| \leq{}& r[k(2r^2-1/2)+1] \sup_{z\in B_r} |P_k(z)| \\ &+ (r^2+1/4)^2 \frac{r+\varepsilon}{\varepsilon} \sup_{z\in B_{r+\varepsilon}} |P_k(z)|, \\ \leq{}& \left(r[k(2r^2-1/2)+1] + \frac{r+\varepsilon}{\varepsilon}(r^2+1/4)^2 \right) \sup_{z\in B_{r+\varepsilon}} |P_k(z)|.\end{aligned}$$

Denoting $C(r,k,\varepsilon) := r[k(2r^2-1/2)+1] + \frac{r+\varepsilon}{\varepsilon}(r^2+1/4)^2$, we finally get

$$\begin{aligned}\sup_{z\in B_r} |P_{k+1}(z)| &\leq C(r,k,\varepsilon) \sup_{z\in B_{r+\varepsilon}} |P_k(z)|, \\ &\leq C(r,k,\varepsilon)C(r+\varepsilon,k-1,\varepsilon) \sup_{z\in B_{r+2\varepsilon}} |P_{k-1}(z)|, \\ &\leq \left(\prod_{i=0}^{k} C(r+i\varepsilon,k-i,\varepsilon) \right) \sup_{z\in B_{r+(k+1)\varepsilon}} |P_0(z)|.\end{aligned}$$

A bound can then be obtained as follows: let $\varepsilon_0 = \frac{-1+\sqrt{3}}{2}$, $\varepsilon = \frac{\varepsilon_0}{k}$ and $r = 1/2$. Then it is easy to check that for all $0 \le i \le k$, we have

$$C(\frac{1}{2} + i\frac{\varepsilon_0}{k}, k-i, \frac{\varepsilon_0}{k}) \le \frac{\sqrt{3}}{2}[k-i+1] + \frac{1}{\sqrt{3}-1}k + i + 1, \\ \le \frac{\sqrt{3}+3}{2}(k+1),$$

and hence,

$$\left(\prod_{i=0}^{k} C(r+i\varepsilon, k-i, \varepsilon)\right) \le [\frac{\sqrt{3}+3}{2}(k+1)]^{k+1}.$$

Taking into account that $P_0 \equiv 1$, we obtain

$$\forall\, k\, \in\, \mathbb{N}^*,\ \sup_{z\in B_{1/2}} |P_k(z)| \le [\frac{\sqrt{3}+3}{2}k]^k.$$

It remains to bound $\frac{1}{[\Pi(x)]^{2k}}e^{-\frac{1}{x(1-x)}}$. Denoting $Y = \frac{1}{x(1-x)}$, we have:

$$\sup_{x\in[0,1]} \frac{1}{[\Pi(x)]^{2k}}e^{-\frac{1}{x(1-x)}} = \sup_{Y\ge 4} e^{-Y}Y^{2k} \\ \le e^{-2k}(2k)! \\ \le \left(\frac{4}{e^2}\right)^k k^{2k}.$$

■

Proof of lemma 2. Let us denote by ∇ the operator of *backward divided differences* defined by:

$$\forall\, j\, \in \{0,\dots,n\},\ \nabla^0\varphi_j = \varphi_j, \\ \forall\, j\, \in \{m+1,\dots,n\},\ \nabla^{m+1}\varphi_j = \nabla^m\varphi_j - \nabla^m\varphi_{j-1}.$$

The sum in the statement can then be written as

$$\sum_{j=0}^{n-1}\varphi_j b^j = \sum_{j=1}^{n-1} b^j \sum_{i=1}^{j}\nabla\varphi_i + \sum_{j=0}^{n-1}\varphi_0 b^j, \\ = \frac{1-b^n}{1-b}\varphi_0 + \sum_{i=1}^{n-1}\nabla\varphi_i\frac{b^i-b^n}{1-b}, \\ = \frac{\varphi_0 - b^n\varphi_{n-1}}{1-b} + \frac{1}{1-b}\sum_{j=1}^{n-1}(\nabla\varphi_j)b^j = \dots, \\ = \sum_{m=0}^{k}\frac{b^m\nabla^m\varphi_m - b^n\nabla^m\varphi_{n-1}}{(1-b)^{m+1}} + \frac{1}{(1-b)^{k+1}}\sum_{j=k+1}^{n-1}(\nabla^{k+1}\varphi_j)b^j.$$

Denoting $h = 1/n$, it is well-known that, for all $n-1 \leq j \geq k+1$, there exists $\zeta_{j,k+1} \in [(j-k-1)h, jh] \subset [0,1]$ such that we have:

$$\nabla^{k+1}\varphi_j = \varphi^{(k+1)}(\zeta_{j,k+1})h^{k+1}$$

Hence, we can bound the second term in (37) as follows:

$$\left|\sum_{j=k+1}^{n-1} (\nabla^{k+1}\varphi_j)b^j\right| \leq \|\varphi^{(k+1)}\|_{\mathrm{L}^\infty}\, h^{k+1}(n-k-2).$$

In order to estimate the first sum, we notice that, for $0 \leq m \leq k \leq n-2$,

$$\nabla^m\varphi_m = \varphi^{(m)}(\zeta_{m,m})h^m$$

for some $\zeta_{m,m} \in [0, mh]$ and a Taylor-Lagrange expansion of $\varphi^{(m)}(\zeta_{m,m})$ at order $k+1-m$ gives

$$\nabla^m\varphi_m = \frac{\zeta_{m,m}^k h^k}{(k-m)!}\varphi^{(k)}(0) + \frac{\zeta_{m,m}^{k+1} h^{k+1}}{(k+1-m)!}\varphi^{(k+1)}(\eta_m)$$

for some $\eta_m \in [0, mh] \subset [0,1]$. Hence, we have:

$$\begin{aligned}\left|\sum_{m=0}^{k} \frac{b^m}{(1-b)^m}\nabla^m\varphi_m\right| &\leq |\varphi^{(k)}(0)|\frac{k^k h^k}{|1-b|^{k+1}}\sum_{m=0}^{k}\frac{|1-b|^m}{(m)!} \\ &\quad+\|\varphi^{(k+1)}\|_{\mathrm{L}^\infty}\frac{k^k h^{k+1}}{|1-b|}\sum_{m=0}^{k}\frac{|1-b|^m}{(m+1)!}, \\ &\leq \frac{e^2 k^k h^k}{|1-b|^{k+1}}\left(|\varphi^{(k)}(0)| + h\|\varphi^{(k+1)}\|_{\mathrm{L}^\infty}\right).\end{aligned}$$

Similarly we have:

$$\nabla^m\varphi_{n-1} = \varphi^{(m)}(\zeta_{n-1,m})h^m$$

for some $\zeta_{n-1,m} \in [1-(m+1)h, 1-h] \subset [0,1]$, so that

$$\left|\sum_{m=0}^{k} \frac{b^n}{(1-b)^m}\nabla^m\varphi_{n-1}\right| \leq \frac{2e^2 k^k h^k}{|1-b|^{k+1}}\left(|\varphi^{(k)}(1)| + h\|\varphi^{(k+1)}\|_{L^\infty}\right).$$

Gathering the contributions of all terms then gives the result. ■

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