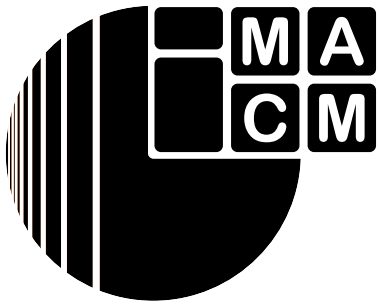

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Abstract

Force-gradient decomposition methods are used to improve the energy preservation of symplectic schemes applied to Hamiltonian systems. If the potential is composed of different parts with strongly varying dynamics, this multirate potential can be exploited by coupling force-gradient decomposition methods with splitting techniques for multi-time scale problems to further increase the accuracy of the scheme and reduce the computational costs. In this paper, we derive novel force-gradient nested methods and test them numerically. We apply them on the three-body problem, modified for a better observation of the advantageous properties, needed for the future research.

Keywords: numerical geometric integration, decomposition methods, energy conservation, force-gradient, nested algorithms, multirate schemes, operator splitting
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1. Introduction

For classical mechanical systems, the equation of motion can be written as

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = [\rho \circ H] \equiv \mathcal{L}(t)\rho(t), \tag{1}$$

where ρ is the set of phase variables, $[\ \circ\ ]$ denotes the Poisson bracket, H represents the Hamiltonian function, and $\mathcal{L}$ denotes the Liouville operator. For the case of N particles, located in a spatially inhomogeneous time-dependent external field $u(\mathbf{r}_i, t)$ and interacting through the pair-wise potential $\varphi(r_{ij}) \equiv \varphi(|\mathbf{r}_i - \mathbf{r}_j|)$, the *Hamiltonian* reads

$$H = \sum_{i=1}^{N} \frac{m_i \mathbf{v}_i^2}{2} + \frac{1}{2}\sum_{i\neq j}^{N} \varphi(r_{ij}) + \sum_{i=1}^{N} u(\mathbf{r}_i,\ t) \equiv T(\mathbf{v}) + V(\mathbf{r}, t). \tag{2}$$

Here $\mathbf{r}_i$ represents the position of particle i $(i = 1, 2, \ldots, N)$ moving with velocity $\mathbf{v}_i = \mathrm{d}\mathbf{r}_i/\mathrm{d}t$ and carrying the mass m_i, so that T and V are the total kinetic and potential energies, respectively. Then $\rho = \{\mathbf{r}_i,\ \mathbf{v}_i\} \equiv \{\mathbf{r},\ \mathbf{v}\}$, and the *Liouville operator* of the system takes the form

$$\mathcal{L}(t) = \sum_{i=1}^{N} \left(\mathbf{v}_i \cdot \frac{\partial}{\partial \mathbf{r}_i} + \frac{\mathbf{f}_i(t)}{m_i} \cdot \frac{\partial}{\partial \mathbf{v}_i} \right), \tag{3}$$

where

$$\mathbf{f}_i(t) = \sum_{j(j\neq i)}^{N} \frac{\varphi'(r_{ij})\mathbf{r_{ij}}}{r_{ij}} - \frac{\partial u(\mathbf{r}_i, t)}{\partial \mathbf{r}_i}$$

are forces acting on the particles due to their interactions.

If the initial configuration $\rho(0)$ is specified, the unique solution to the problem of Eqn. (1) can be presented by the *time propagator operator* as

$$\rho(t) = \left[\mathrm{e}^{(\mathcal{D}+\mathcal{L})h}\right]^l \rho(0), \tag{4}$$

where h is a temporal step size and $l = t/h$ the total number of steps. $\mathcal{D} = \overleftarrow{\partial}/\partial t$ denotes the time derivative operator acting on the left of time-dependent functions. If $\mathcal{L}$ does not depend explicitly on time we set $\mathcal{D} = 0$. In case of many-particle systems $(N > 2)$ the time propagator cannot be computed exactly even in the absence of time dependent potentials. Hence one

has to apply numerical integration methods such as decomposition schemes, which both preserve the physical properties of the Hamiltonian system (4) (symplecticity, time reversibility) and are computationally efficient [11].

The basic idea of a decomposition approach is to factor out the exponential propagator $e^{(\mathcal{D}+\mathcal{L})h}$ in (4), such that $\mathcal{D}+\mathcal{L} = \hat{T}+\hat{V}$, where the differential operators $\hat{T} = \mathbf{v} \cdot \partial/\partial\mathbf{r}$ and $\hat{V} = \mathbf{a} \cdot \partial/\partial\mathbf{v}$ represent the kinetic and potential energies with the acceleration $\mathbf{a} = \{\mathbf{a}_i\} = \{\mathbf{f}_i/m_i\}$. In our case the operator (3) does not depend on time explicitly, hence $\mathcal{D} = 0$.

In Section 2 we will discuss two well-known approaches to increase the accuracy of decomposition schemes: force-gradient schemes and nested multirate algorithms, which are both based on decomposition techniques. For both methods, computing the shadow Hamiltonian is the suitable tool for deriving the order of the numerical integration scheme. In Section 3 both approaches are combined to obtain a more efficient scheme. Finally, numerical results for a three body problem confirm the theoretical findings in Section 4.

2. Methods for obtaining higher order schemes

In this section we will briefly recapitulate two well-known schemes (force-gradient and nested multirate schemes) for reducing the computational costs. As both approaches are based on decomposition, the computation of the shadow Hamiltonian can be used to determine the order of the numerical scheme.

2.1. Shadow Hamiltonians

When transferring the well-known concept of modified equations to Hamiltonian systems one ends up with the Hamiltonian if and only if the integrator is symplectic [14]. The motivation for studying numerically the conservation properties of these 'modified Hamiltonians' are multifaceted [14], e.g. numerical evidence for the existence of a Hamiltonian for a particular calculation, exposure of energy drifts caused by numerical instability, etc.. Skeel and Hardy [14] proposed a simple strategy for deriving highly accurate estimates for modified Hamiltonians. Since these modified Hamiltonians approximate well the true Hamiltonian, they are referred as "shadow" Hamiltonians $\tilde{H}$, cf. [5]. The existence of these shadow Hamiltonians guarantees the boundedness of the error in the symplectic map, in fact we have $\tilde{H}(\mathbf{r}, \mathbf{v}, h) \to H(\mathbf{r}, \mathbf{v})$ for $h \to 0$.

Conversely, if one starts from a given numerical solver then it is well known that any symplectic integrator different from the Hamiltonian flow itself does not preserve the Hamiltonian however a nearby system, the so-called *shadow Hamiltonian* $\tilde{H}$ is conserved. The energy computed from the shadow Hamiltonian of a symplectic integrators differs by $H(\mathbf{r},\mathbf{v}) - \tilde{H}(\mathbf{r},\mathbf{v},h) = \mathcal{O}(h^p)$ from the true Hamiltonian [7], with p being the order of the integration scheme. Hence, computing the shadow Hamiltonian of a symplectic integrator is equivalent to determining the order of the integrator.

To compute a shadow Hamiltonian it is necessary to expand an exponential map to a *Hausdorff series*. To do so, we need to use the *Baker-Cambell-Hausdorf (BCH) formula* [9].

$$\ln(\mathrm{e}^T\,\mathrm{e}^V) = \sum_{n=1}^{\infty} c_n(T,V), \tag{5}$$

where the coefficients c_n are recursively determined from the relations $c_1 = T + V$ and

$$(n+1)c_{n+1} = \sum_{m=1}^{\lfloor n/2\rfloor} \frac{B_{2m}}{(2m)!} \sum_{k_1,\ldots,k_{2m}\geq 1} \mathrm{ad}c_{k_1}\ldots\mathrm{ad}c_{k_{2m}}(T+V) - \frac{1}{2}(\mathrm{ad}c_n)(T-V),$$

for $n \geq 0$, where $\mathrm{ad}a : b \mapsto [a,b]$ and B_n denote the Bernoulli numbers. For example, the shadow Hamiltonian of the leap-frog method $\mathrm{e}^{h\frac{\hat{T}}{2}}\,\mathrm{e}^{h\hat{V}}\,\mathrm{e}^{h\frac{\hat{T}}{2}}$ is given by

$$\tilde{H} = H - \frac{h^2}{24}\Big(2\big[V,[T,V]\big] + \big[T,[T,V]\big]\Big) + \mathcal{O}(h^4),$$

which is of second order accuracy.

2.2. Force-gradient schemes

Force-gradient schemes are based on the fact that the total propagator in Eqn. (4) can be split in the following way:

$$\mathrm{e}^{(\hat{T}+\hat{V})h+\mathcal{O}(h^{K+1})} = \prod_{p=1}^{P} \mathrm{e}^{\hat{T}a_p h}\,\mathrm{e}^{\hat{V}b_p h+\mathcal{C}c_p h^3}, \tag{6}$$

where $\mathcal{C} = [V,[T,V]]$ and [,] denotes the commutator of two operators.

$$\mathcal{C} \equiv \big[V,[T,V]\big] = \sum_{i=1}^{N} \frac{\mathbf{g}_i}{m_i} \cdot \frac{\partial}{\partial \mathbf{v}} \equiv \mathbf{G} \cdot \frac{\partial}{\partial \mathbf{v}},$$

where

$$\mathbf{g}_{i\alpha} = 2 \sum_{j\beta} \frac{\mathbf{f}_{j\beta}}{m_j} \frac{\partial \mathbf{f}_{i\alpha}}{\partial \mathbf{r}_{j\beta}},$$

α and β denote the Cartesian components of the vectors. The force-gradient evaluations $\partial \mathbf{f}_{i\alpha}/\partial \mathbf{r}_{j\beta}$ can be explicitly represented taking into account that

$$\mathbf{f}_{i\alpha} = m_i \mathbf{w}_{i\alpha} - \frac{\partial u(\mathbf{r}_i, t)}{\partial \mathbf{r}_{i\alpha}},$$

where

$$\mathbf{w}_{i\alpha} = -\frac{1}{m_i} \sum_{j(j\neq i)} \varphi'(r_{ij}) \, \frac{(\mathbf{r}_{i\alpha} - \mathbf{r}_{j\alpha})}{r_{ij}}$$

is the inter-particle part of the acceleration. The result is

$$\mathbf{g}_i = -2 \sum_{j(j\neq i)}^{N} \Big[(\mathbf{w}_i - \mathbf{w}_j) \frac{\varphi'_{ij}}{r_{ij}} + \frac{\mathbf{r}_{ij}}{r_{ij}^3} \left(r_{ij}\varphi''_{ij} - \varphi'_{ij} \right) \left(\mathbf{r}_i \cdot (\mathbf{w}_i - \mathbf{w}_j) \right) \Big] + \mathbf{h}_i, \quad (7)$$

where

$$\mathbf{h}_i = \frac{2}{m_i} \sum_{\beta} \frac{\partial u}{\partial \mathbf{r}_{i\beta}} \frac{\partial^2 u}{\partial \mathbf{r}_{i\alpha} \partial \mathbf{r}_{i\beta}}.$$

The coefficients a_p, b_p and c_p in (6) have to be chosen in such way to obtain the highest possible order $K \geq 1$ for a given integer $P \geq 1$. Eqn. (6) represents the general form of the decomposition, while for $c_p \equiv 0$ the decomposition reduces to the standard non-gradient factorization. The force-gradient method is defined by using the value of c_p which reduces the difference between the true Hamiltonian and shadow Hamiltonian $\tilde{H}$ which is conserved by the method. We will show how to determine the shadow Hamiltonian $\tilde{H}$ in the next section.

Basically the evolution operators $\mathrm{e}^{Ta_p h}$ and $\mathrm{e}^{Vb_p h + \mathcal{C}c_p h^3}$ displace $\mathbf{v}$ and $\mathbf{r}$ forward in time with

$$\mathbf{v} \to \mathbf{v} + b_p \mathbf{a} h + c_p \mathbf{G} h^3 \qquad \text{and } \mathbf{r} \to \mathbf{r} + a_p \mathbf{v} h. \quad (8)$$

The decomposition integration of Eqn. (6) conserves the symplectic map of flow of the particles in phase space, because the separate shifts of Eqn. (8) of positions and velocities do not change the phase volume. Time-reversibility can be ensured by imposing two conditions, namely $a_1 = 0$, $a_{p+1} = a_{P-p+1}$, $b_p = b_{P-p+1}$, $c_p = c_{P-p+1}$, as well as $a_p = a_{P-p+1}$, $b_p = b_{P-p}$, $c_p = c_{P-p}$ with $b_P = 0$ and $c_P = 0$.

Next we deal with numerical integrators of the form given in Eqn. (6), the most efficient version of which is due to Omelyan [11]. Adding the force-gradient term $\mathcal{C}$ in the leap-frog scheme does not increase the order of the method as one cannot cancel the commutator $\big[T,[T,V]\big]$. However, the second-order five-stage method

$$\Delta(h)_5 = \mathrm{e}^{\frac{1}{6}h\hat{V}}\,\mathrm{e}^{\frac{1}{2}h\hat{T}}\,\mathrm{e}^{\frac{2}{3}h\hat{V}}\,\mathrm{e}^{\frac{1}{2}h\hat{T}}\,\mathrm{e}^{\frac{1}{6}h\hat{V}},$$

conserves the shadow Hamiltonian [2]

$$\tilde{H}_5 = H - \big[V,[T,V]\big]\frac{h^2}{72} + \mathcal{O}(h^4),$$

where the leading error coefficient is a scalar multiple of the force-gradient term $\mathcal{C}$. Thus adding a proper amount of the shadow Hamiltonian defines the force-gradient scheme

$$\Delta(h)_{5C} = \mathrm{e}^{\frac{1}{6}h\hat{V}}\,\mathrm{e}^{\frac{1}{2}h\hat{T}}\,\mathrm{e}^{\frac{2}{3}h\hat{V}+\frac{1}{72}h^3\mathcal{C}}\,\mathrm{e}^{\frac{1}{2}h\hat{T}}\,\mathrm{e}^{\frac{1}{6}h\hat{V}}.$$

This scheme conserves the shadow Hamiltonian [8]

$$\tilde{H}_{5C} = H + \left(41\Big[V,\Big[V,\big[V,[V,T]\big]\Big]\Big] + \ldots \right.$$
$$\left. +54\Big[T,\Big[T,\big[T,[V,T]\big]\Big]\Big]\right)\frac{h^4}{155520} + \mathcal{O}(h^6),$$

which gains two orders of accuracy.

2.3. Nested integrators for multirate systems

In order to reduce the computational effort to evaluate an evolution operator for one part of the action, we use a *nested integrator* with a small step-size to evaluate the inner cheap part [13]. An example of such class of problems can be the multi-time scale problems.

Let us consider a Hamiltonian which can be represented in the following form

$$H = T + V_1 + V_2, \tag{9}$$

where T represents the kinetic part, V_1 is the potential energy of the small (fast) scale part of the system and V_2 corresponds to the potential energy of the large (slow) scale part.

We choose the following integrator to compute the inner part $H = T + V_1$

$$\Delta(h)_M = \left[\mathrm{e}^{\frac{h}{2M}\hat{V}_1} \, \mathrm{e}^{\frac{h}{M}\hat{T}} \, \mathrm{e}^{\frac{h}{2M}\hat{V}_1} \right]^M .$$

Therefore we define $\Delta\,(h)$ a nested integrator to solve the split problem of Eqn. (9), it yields

$$\hat{\Delta}(h) = \left[\mathrm{e}^{\frac{h}{2}\hat{V}_2} \, \Delta\,(h)_M \, \mathrm{e}^{\frac{h}{2}\hat{V}_2} \right]^l . \tag{10}$$

This method, called *nested leap-frog*, conserves the shadow Hamiltonian [13]

$$\begin{aligned} \tilde{H}_M = H + \Bigg(& -\frac{1}{24}\big[V_2,[V_2,T]\big] + \frac{1}{12}\big[V_1,[V_2,T]\big] + \frac{1}{12}\big[T,[V_2,T]\big] \\ & + \frac{1}{M^2}\Big(-\frac{1}{24}\big[V_1,[V_1,T]\big] + \frac{1}{12}\big[T,[V_1,T]\big]\Big)\Bigg) h^2 + \mathcal{O}(h^4). \end{aligned}$$

3. Combining force-gradient and multirate splitting technique

Our idea is to combine both the force-gradient and the nested algorithm approaches in order to obtain a higher energy conservation rate. To do so, let us first take a look at the following *alike 5-stage nested integrator*

$$\Delta(h) = \left[\mathrm{e}^{\lambda h \hat{V}_2} \, \Delta\left(\frac{h}{2}\right)_M \mathrm{e}^{(1-2\lambda) h \hat{V}_2} \, \Delta\left(\frac{h}{2}\right)_M \mathrm{e}^{\lambda h \hat{V}_2} \right]^l , \tag{11}$$

where

$$\Delta\left(\frac{h}{2}\right)_M = \left[\mathrm{e}^{\frac{h}{4M}\hat{V}_1} \, \mathrm{e}^{\frac{h}{2M}\hat{T}} \, \mathrm{e}^{\frac{h}{4M}\hat{V}_1} \right]^M .$$

We have chosen the 5-stage numerical integrator, since it has an optimal number of steps, necessary for increasing its order. To analyze the energy conservation of this integrator we have to determine its shadow Hamiltonian.

In order to do so, we use the BCH formula (5). To simplify this task we consider the limit of the integrator of Eqn. (11), as M tends to infinity. We obtain

$$\Delta(h) = \left[\mathrm{e}^{\lambda h \hat{V}_2}\, \mathrm{e}^{\frac{h}{2}(\hat{V}_1+T)}\, \mathrm{e}^{(1-2\lambda)h\hat{V}_2}\, \mathrm{e}^{\frac{h}{2}(\hat{V}_1+\hat{T})}\, \mathrm{e}^{\lambda h \hat{V}_2}\right]^l. \tag{12}$$

Theorem 1 (Shadow Hamiltonian of (12))**.** *The shadow Hamiltonian of the nested multirate integrator* (12) *is given by*

$$\begin{aligned}\tilde{H} = H + \Big(&\frac{-1+6\lambda-6\lambda^2}{12}\big[V_2,[T,V_2]\big] \\ &+ \frac{-1+6\lambda}{24}\big[V_1,[T,V_2]\big] + \frac{-1+6\lambda}{24}\big[T,[T,V_2]\big]\Big)h^2 + \mathcal{O}(h^4). \end{aligned}\tag{13}$$

Proof: We apply the BCH formula to the first two evolution operators

$$X = \ln\left(\mathrm{e}^{\lambda h \hat{V}_2}\, \mathrm{e}^{h\frac{\hat{V}_1+\hat{T}}{2}}\right) = c_1 h + c_2 h^2 + c_3 h^3 + \mathcal{O}(h^5),$$

where

$$\begin{aligned}
\mathbf{c_1} &= \lambda V_2 + \frac{V_1+T}{2},\\
2c_2 &= \frac{B_2}{2!}\mathrm{ad}c_1\left(\lambda V_2 + \frac{V_1+T}{2}\right) - \frac{1}{2}\mathrm{ad}c_1\left(\lambda V_2 - \frac{V_1+T}{2}\right),\\
\mathbf{c_2} &= -\frac{1}{4}\left[\lambda V_2 + \frac{V_1+T}{2},\ \lambda V_2 - \frac{V_1+T}{2}\right] = -\frac{\lambda}{4}[V_1,V_2] - \frac{\lambda}{4}[T,V_2],\\
3c_3 &= \frac{B_3}{3!}\mathrm{ad}c_1\mathrm{ad}c_1\left(\lambda V_2 + \frac{V_1+T}{2}\right) - \frac{1}{2}\mathrm{ad}c_2\left(\lambda V_2 - \frac{V_1+T}{2}\right),\\
\mathbf{c_3} &= -\frac{1}{6}\left[-\frac{\lambda}{4}[V_1,V_2] - \frac{\lambda}{4}[T,V_2],\ \lambda V_2 - \frac{V_1+T}{2}\right]\\
&= -\frac{\lambda^2}{24}\big[V_2,[V_1,V_2]\big] - \frac{\lambda^2}{24}\big[V_2,[T,V_2]\big] + \frac{\lambda}{48}\big[V_1,[V_1,V_2]\big]\\
&\quad + \frac{\lambda}{48}\big[V_1,[T,V_2]\big] + \frac{\lambda}{48}\big[T,[V_1,V_2]\big] + \frac{\lambda}{48}\big[T,[T,V_2]\big].
\end{aligned}$$

Then we have the result for our first two operators

$$X = \left(\lambda V_2 + \frac{V_1+T}{2}\right) h + \left(-\frac{\lambda}{4}[V_1,V_2] - \frac{\lambda}{4}[T,V_2]\right) h^2 \\ + \left(-\frac{\lambda^2}{24}\big[V_2,[V_1,V_2]\big] - \frac{\lambda^2}{24}\big[T,[T,V_2]\big] + \frac{\lambda}{48}\big[V_1,[V_1,V_2]\big] \right. \\ \left. + \frac{\lambda}{48}\big[V_1,[T,V_2]\big] + \frac{\lambda}{48}\big[T,[V_1,V_2]\big] + \frac{\lambda}{48}\big[T,[T,V_2]\big]\right) h^3 + \mathcal{O}(h^5).$$

The next step is to apply the BCH formula on the following operators

$$Y = \ln\left(\mathrm{e}^X\, \mathrm{e}^{(1-2\lambda)h\hat{V}_2}\right) = c_1 + c_2 + c_3 + \mathcal{O}(h^5)$$

and coefficients

$$\mathbf{c_1} = X + (1-2\lambda)hV_2 = \left((1-\lambda)V_2 + \frac{V_1+T}{2}\right) h + (\ldots)h^2 + (\ldots)h^3,$$

$$2c_2 = \frac{B_2}{2!}\mathrm{ad}c_1\big(X + (1-2\lambda)hV_2\big) - \frac{1}{2}\mathrm{ad}c_1\big(X - (1-2\lambda)hV_2\big),$$

$$\mathbf{c_2} = -\frac{1}{4}\big[X + (1-2\lambda)hV_2,\ X - (1-2\lambda)hV_2\big] \\ = \left(\frac{1-2\lambda}{4}[V_1,V_2] + \frac{1-2\lambda}{4}[T,\ V_2]\right) h^2 \\ + \left(\frac{\lambda-2\lambda^2}{8}\big[V_2,[V_1,V_2]\big] + \frac{\lambda-2\lambda^2}{8}\big[V_2,[T,V_2]\big]\right) h^3$$

$$3c_3 = \frac{B_3}{3!}\mathrm{ad}c_1\mathrm{ad}c_1\big(X + (1-2\lambda)hV_2\big) - \frac{1}{2}\mathrm{ad}c_2\big(X - (1-2\lambda)hV_2\big),$$

$$\mathbf{c_3} = -\frac{1}{6}\big[c_2,\ X - (1-2\lambda)hV_2\big] \\ = \left(-\frac{(1-2\lambda)(1-3\lambda)}{24}\big[V_2,[V_1,V_2]\big] - \frac{(1-2\lambda)(1-3\lambda)}{24}\big[V_2,[T,V_2]\big] \right. \\ + \frac{(1-2\lambda)}{48}\big[V_1,[V_1,V_2]\big] + \frac{(1-2\lambda)}{48}\big[V_1,[T,V_2]\big] + \frac{(1-2\lambda)}{48}\big[T,[V_1,V_2]\big] \\ \left. + \frac{(1-2\lambda)}{48}\big[T,[T,V_2]\big]\right) h^3,$$

and we obtain the following expansion

$$
\begin{aligned}
Y = &\left((1-\lambda)V_2 + \frac{V_1+T}{2}\right)h + \left(\frac{1-3\lambda}{4}[V_1,V_2] + \frac{1-3\lambda}{4}[T,V_2]\right)h^2 \\
&+\left(\frac{-1+8\lambda-13\lambda^2}{24}\big[V_2,[V_1,V_2]\big] + \frac{-1+8\lambda-13\lambda^2}{24}\big[T,[T,V_2]\big]\right. \\
&+\frac{1-\lambda}{48}\big[V_1,[V_1,V_2]\big] + \frac{1-\lambda}{48}\big[V_1,[T,V_2]\big] + \frac{1-\lambda}{48}\big[T,[V_1,V_2]\big] \\
&\left.+\frac{1-\lambda}{48}\big[T,[T,V_2]\big]\right)h^3 + \mathcal{O}(h^5),
\end{aligned}
$$

The next step would be to repeat the previous procedures to find

$$
Z = \ln\left(\mathrm{e}^{Y}\,\mathrm{e}^{h\frac{\hat{V}_1+\hat{T}}{2}}\right) = c_1 + c_2 + c_3 + \mathcal{O}(h^5).
$$

Using the BCH formula we obtain

$$
\begin{aligned}
\mathbf{c_1} &= Y + h\frac{V_1+T}{2} = ((1-\lambda)V_2 + V_1 + T)h + (\ldots)h^2 + (\ldots)h^3, \\
2c_2 &= \frac{B_2}{2!}\mathrm{ad}c_1\left(Y + h\frac{V_1+T}{2}\right) - \frac{1}{2}\mathrm{ad}c_1\left(Y - h\frac{V_1+T}{2}\right), \\
\mathbf{c_2} &= -\frac{1}{4}\left[Y + h\frac{V_1+T}{2},\ Y - h\frac{V_1+T}{2}\right] \\
&= \left(-\frac{1-\lambda}{4}[V_1,\ V_2] - \frac{1-\lambda}{4}[T,\ V_2]\right)h^2 \\
&\quad + \left(-\frac{1-3\lambda}{16}\big[V_1,[V_1,V_2]\big] - \frac{1-3\lambda}{16}\big[V_1,[T,V_2]\big]\right. \\
&\qquad \left. -\frac{1-3\lambda}{16}\big[T,[V_1,V_2]\big] - \frac{1-3\lambda}{16}\big[T,[T,V_2]\big]\right)h^3, \\
3c_3 &= \frac{B_3}{3!}\mathrm{ad}c_1\mathrm{ad}c_1\left(Y + h\frac{V_1+T}{2}\right) - \frac{1}{2}\mathrm{ad}c_2\left(Y - h\frac{V_1+T}{2}\right) \\
\mathbf{c_3} &= -\frac{1}{6}\left[c_2,\ Y - h\frac{V_1+T}{2}\right], \\
&= \left(-\frac{(1-\lambda)^2}{24}\big[V_2,[V_1,V_2]\big] - \frac{(1-\lambda)^2}{24}\big[V_2,[T,V_2]\big]\right)h^3.
\end{aligned}
$$

Therefore we obtain

$$\begin{aligned}
Z = \big((1-\lambda)V_2 + V_1 + T\big)h + \Big(\frac{-\lambda}{2}[V_1,V_2] + \frac{-2\lambda}{2}[T,V_2]\Big)h^2 \\
+ \bigg(\frac{-1+5\lambda-7\lambda^2}{12}\big[V_2,[V_1,V_2]\big] + \frac{-1+5\lambda-7\lambda^2}{12}\big[T,[T,V_2]\big] \\
+\frac{-1+4\lambda}{48}\big[V_1,[V_1,V_2]\big] + \frac{-1+4\lambda}{48}\big[V_1,[T,V_2]\big] \\
+\frac{-1+4\lambda}{48}\big[T,[V_1,V_2]\big] + \frac{-1+4\lambda}{48}\big[T,[T,V_2]\big]\bigg)h^3 + O(h^4).
\end{aligned}$$

Applying the BCH formula for a last time we obtain the shadow Hamiltonian

$$\tilde{H} = \ln\left(\mathrm{e}^{Z}\,\mathrm{e}^{\lambda\hat{V}_2 h}\right) = c_1 + c_2 + c_3 + \mathcal{O}(h^5),$$

with the coefficients

$$\begin{aligned}
\mathbf{c_1} &= Z + \lambda V_2 h = (V_2 + V_1 + T)h + (\ldots)h^2 + (\ldots)h^3, \\
2c_2 &= \frac{B_2}{2!}\mathrm{ad}c_1\left(Z + \lambda V_2 h\right) - \frac{1}{2}\mathrm{ad}c_1\left(Z - \lambda V_2 h\right), \\
\mathbf{c_2} &= -\frac{1}{4}\left[Z + \lambda V_2 h,\ Z - \lambda V_2 h\right] \\
&= \left(\frac{\lambda}{2}[V_1,\ V_2] + \frac{\lambda}{2}[T,\ V_2]\right)h^2 + \left(\frac{\lambda^2}{4}\big[V_2,[V_1,V_2]\big] + \frac{\lambda^2}{4}\big[V_2,[T,V_2]\big]\right)h^3, \\
3c_3 &= \frac{B_3}{3!}\mathrm{ad}c_1\mathrm{ad}c_1\left(Z + \lambda V_2 h\right) - \frac{1}{2}\mathrm{ad}c_2\left(Z - \lambda V_2 h\right), \\
\mathbf{c_3} &= -\frac{1}{6}\left[c_2,\ Z - \lambda V_2 h\right] \\
&= \bigg(\frac{\lambda(1-2\lambda)^2}{12}\big[V_2,[V_1,V_2]\big] + \frac{\lambda(1-2\lambda)^2}{12}\big[V_2,[T,V_2]\big] + \frac{\lambda}{12}\big[V_1,[V_1,V_2]\big] \\
&\quad + \frac{\lambda}{12}\big[V_1,[T,V_2]\big] + \frac{\lambda}{12}\big[T,[V_1,V_2]\big] + \frac{\lambda}{12}\big[T,[T,V_2]\big]\bigg)h^3,
\end{aligned}$$

and finally

$$\begin{aligned}
\tilde{H} = H + \bigg(\frac{-1+6\lambda-6\lambda^2}{12}\big[V_2,[V_1,V_2]\big] + \frac{-1+6\lambda}{24}\big[V_1,[T,V_2]\big] \\
+\frac{-1+6\lambda-6\lambda^2}{12}\big[V_2,[T,V_2]\big] + \frac{-1+6\lambda}{24}\big[V_1,[V_1,V_2]\big] \\
+\frac{-1+6\lambda}{24}\big[T,[V_1,V_2]\big] + \frac{-1+6\lambda}{24}\big[T,[T,V_2]\big]\bigg)h^2 + \mathcal{O}(h^4).
\end{aligned}$$

Finally, taking into account that $[V_1, V_2] = 0$, hence $\big[V_2, [V_1, V_2]\big]$, $\big[V_1, [V_1, V_2]\big]$ and $\big[T, [V_1, V_2]\big]$ are equal to zero, we obtain (13). □

We can eliminate a couple of terms by choosing $\lambda = 1/6$, thus

$$\tilde{H} = H - \frac{1}{72}\big[V_2, [T, V_2]\big]h^2 + \mathcal{O}(h^4).$$

We would like to increase the order of the method (11) by adding the force-gradient term, but first we consider the force-gradient itself. Due to the splitting (9) it can be represented as

$$\begin{aligned} C = \big[V, [T, V]\big] &= \big[V_2 + V_1, [T, V_2 + V_1]\big] \\ &= \big[V_2, [T, V_2]\big] + \big[V_1, [T, V_1]\big] + \big[V_1, [T, V_2]\big] + \big[V_2, [T, V_1]\big]. \end{aligned}$$

Then we can tune the original algorithm (11) by adding the first term of the force gradient $\big[V_2, [T, V_2]\big]$ and neglect the last three terms:

$$\Delta(h) = \left[\mathrm{e}^{\frac{1}{6}h\hat{V}_2}\,\Delta\left(\frac{h}{2}\right)_M \mathrm{e}^{\frac{2}{3}h\hat{V}_2 + \frac{1}{72}h^3\left[V_2,[T,V_2]\right]}\,\Delta\left(\frac{h}{2}\right)_M \mathrm{e}^{\frac{1}{6}h\hat{V}_2}\right]^l, \qquad (14)$$

which preserves the fourth-order accurate shadow Hamiltonian

$$\tilde{H} = H + \mathcal{O}(h^4).$$

4. Numerical experiments

In order to estimate the performance of the integrator of Eqn. (14) we compare it with the other algorithms mentioned above. Let us consider the three body problem [6] and a particular case of it, the *Sun-Earth-Moon problem*. The given system has the energy

$$E = \sum_{i=0}^{2} \frac{m_i v_i^2}{2} - G\sum_{i=1}^{2}\sum_{j=0}^{i-1} \frac{m_i m_j}{r_{ij}},$$

where $r_{ij} = \|\mathbf{r_i} - \mathbf{r_j}\|$, m_0, m_1 and m_2 represent the masses of the Sun, the Earth and the Moon, respectively and G is the gravitational constant. The equations of motion are then

$$\begin{aligned} \frac{\mathrm{d}\mathbf{r}_0}{\mathrm{d}t} &= \mathbf{v}_0, & \frac{\mathrm{d}\mathbf{v}_0}{\mathrm{d}t} &= -m_1 G\,\frac{\mathbf{r}_0 - \mathbf{r}_1}{r_{01}^3} - m_2 G\,\frac{\mathbf{r}_0 - \mathbf{r}_2}{r_{02}^3}, \\ \frac{\mathrm{d}\mathbf{r}_1}{\mathrm{d}t} &= \mathbf{v}_1, & \frac{\mathrm{d}\mathbf{v}_1}{\mathrm{d}t} &= -m_0 G\,\frac{\mathbf{r}_1 - \mathbf{r}_0}{r_{10}^3} - m_2 G\,\frac{\mathbf{r}_1 - \mathbf{r}_2}{r_{12}^3}, \\ \frac{\mathrm{d}\mathbf{r}_2}{\mathrm{d}t} &= \mathbf{v}_2, & \frac{\mathrm{d}\mathbf{v}_2}{\mathrm{d}t} &= -m_0 G\,\frac{\mathbf{r}_2 - \mathbf{r}_0}{r_{20}^3} - m_1 G\,\frac{\mathbf{r}_2 - \mathbf{r}_1}{r_{21}^3}. \end{aligned} \qquad (15)$$

Gravitational constant (G)	6.67384×10^{-11},m^3/kg s	0.2662 AU^3/SU mo
Mass of the Sun (m_0)	1.9891×10^{30}, kg	1 SU
Mass of the Earth (m_1)	5.9736×10^{24}, kg	3×10^{-6} SU
Mass of the Moon (m_2)	7.3477×10^{22}, kg	0.0369×10^{-6} SU
Initial position of the Sun ($\mathbf{r}_0$)	(0, 0), m	(0, 0), AU
Initial position of the Earth ($\mathbf{r}_1$)	(0, 1.52098×10^{11}), m	(0, 1.0167138), AU
Initial position of the Moon ($\mathbf{r}_2$)	(0, 1.52504×10^{11}), m	(0, 1.0191138), AU
Initial velocity of the Sun ($\mathbf{v}_0$)	(0, 0), m/s	(0, 0), AU/mo
Initial velocity of the Earth ($\mathbf{v}_1$)	(0, 29.78×10^3), m/s	(0, 0.5160), AU/mo
Initial velocity of the Moon ($\mathbf{v}_2$)	(0, 30.802×10^3), m/s	(0, 0.5337), AU/mo

Table 1: Physical parameters of the Sun-Earth-Moon problem.

The force-gradient terms can be obtained from (7) for this case, using the external field potential $u(r_{ij}) = 0$ and the pair-wise potentials

$$\varphi(r_{ij}) = -G\frac{m_i m_j}{r_{ij}},$$

respectively for each interaction, with the *fast* V_1 and the *slow* V_2 potentials are given

$$V_1 = -G\frac{m_1 m_2}{r_{12}}, \qquad V_2 = -G\frac{m_0 m_1}{r_{01}} - G\frac{m_0 m_2}{r_{02}}.$$

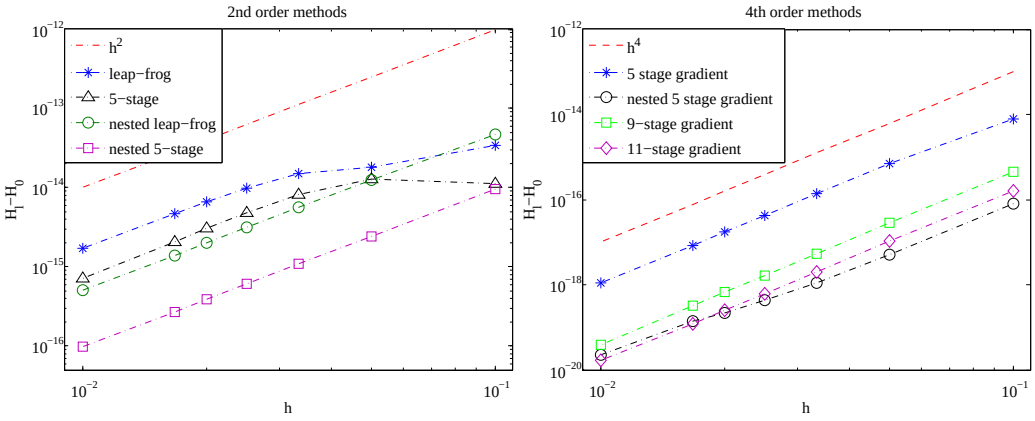

Figure 1: Sun-Moon-Earth problem: absolute error for different integrators

Figure 1 presents a comparison between the standard numerical algorithms, nested approaches, the force-gradient and our combined method.

The proposed integrator of Eqn. (14) with $M = 30$, which combines nested and force-gradient ideas, yields a better energy conservation even compared with 9-stage and 11-stage force-gradient numerical schemes. These numerical results correspond to our analytical observations.

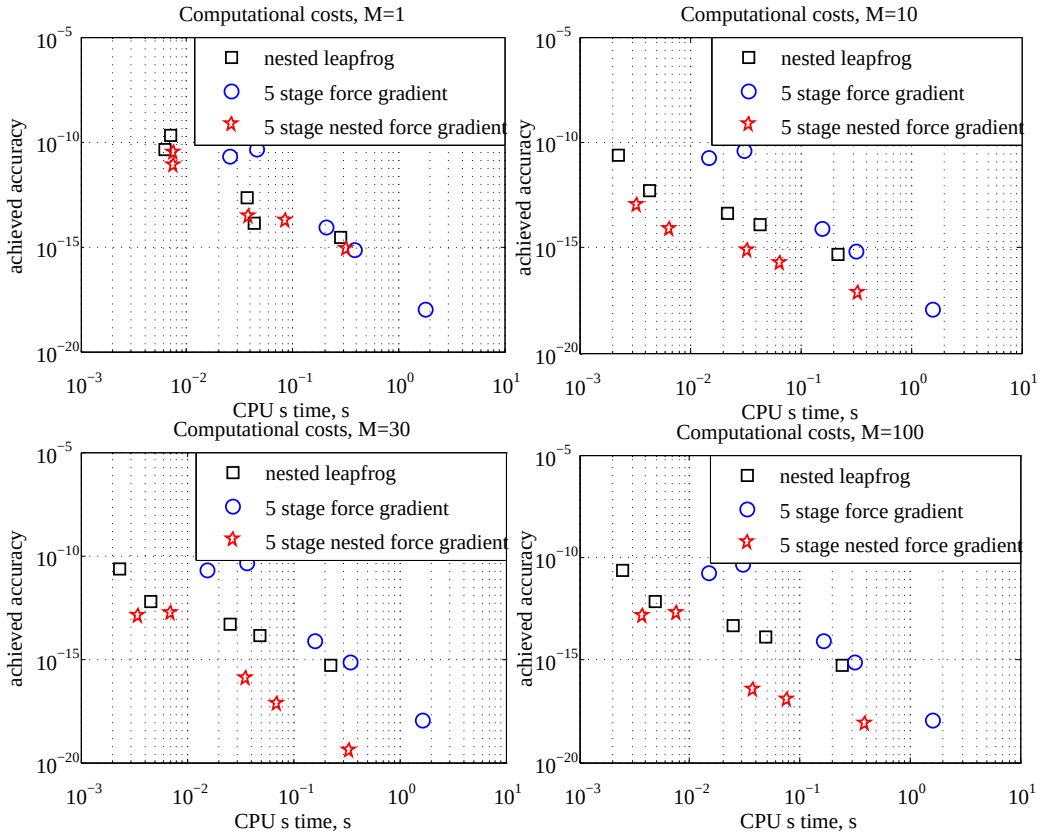

Figure 2: Sun-Moon-Earth problem: CPUs time vs. achieved accuracy for different integrators

Figure 2 presents the CPU time, required for the three different integrators against the achieved accuracy. Here we scale the time needed for the computation of the fast part by a factor of 0.001, since we assume that the computation of the fast scale functions is very cheap compared to the slow scale function evaluations. We can see that in general our nested force-gradient method (14) requires less CPU time and performs more accurate than the standard schemes, presented in Figure 2.

Thus we can argue that, if the evaluation of fast function is significantly cheaper than the *slow* function, computational costs decrease. This is exactly the case found in our long-term goal applications in lattice quantum chromodynamics (LQCD), where the action can be split into two parts: the gauge action (whose force evaluations are cheap) and the fermion action (expensive).

5. Conclusions and outlook

We have introduced a new decomposition scheme for Hamiltonian systems, which combines the idea of the force-gradient time-reversible and symplectic integrators and the splitting approach of nested algorithms. The new method of Eqn. (14) is fourth-order accurate. Compared to other fourth-order schemes, the leading error coefficient is smaller and computational costs are lower.

Our future work will apply this approach in the Hybrid Monte Carlo [3] (HMC) algorithm for numerical integration of the lattice path-integral of quantum chromodynamics (QCD), which describes the strong interactions between quarks and gluons inside the nucleons. In this case, the Hamiltonian dynamics are defined on curved manifolds and one has to take into account the non-commutativity of the operators $\hat{T}$ and $\hat{V}$.

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