Higher order splitting methods with modified integrators for a class of Hamiltonian systems

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Abstract

We discuss systematic extensions of the standard (Störmer-Verlet) splitting method for differential equations of Hamiltonian mechanics, with relative accuracy of order $\tau^2$ for a timestep of length $\tau$, to higher orders in $\tau$. We present some splitting schemes, with all intermediate timesteps real and positive, which increase the relative accuracy to order $\tau^N$ (for $N = 4, 6, \text{and } 8$) for a large class of Hamiltonian systems.

Keywords: Splitting methods, Modified integrators, Higher order methods, Generating function, Fermi-Pasta-Ulam-Tsingou problem

1. Introduction

The Hamilton equations of motion constitute a system of ordinary first order differential equations,

$$ q^a = \frac{\partial H}{\partial p_a}, \quad p_a = -\frac{\partial H}{\partial q^a}, \quad a = 1, \ldots, N, $$

where the \( \cdot \) denotes differentiation with respect to time $t$, and $H = H(q,p)$. They can be viewed as the characteristic equations of the partial differential equation

$$ \frac{\partial}{\partial t} \rho(q,p;t) = \mathcal{L} \rho(q,p;t), $$

with $\mathcal{L}$ the first order differential operator,

$$ \mathcal{L} = \sum_{a=1}^{N} \frac{\partial H}{\partial p_a} \frac{\partial}{\partial q^a} - \frac{\partial H}{\partial q^a} \frac{\partial}{\partial p_a}.$$

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generating a flow on phase space. If $H$ does not depend explicitly on $t$, a formal solution of (2) is
\[ \rho(q, p; t) = e^{t\mathcal{L}} \rho(q, p; 0). \]  
(4)
In most cases this expression remain just formal, but one may often split the Hamiltonian into two parts, $H = H_1 + H_2$, with a corresponding splitting $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$ such that the flows generated by $\mathcal{L}_1$ and $\mathcal{L}_2$ are separately integrable. One may then use the Cambell-Baker-Hausdorff formula to approximate the flow generated by $\mathcal{L}$. By doing this in a symmetric way one obtains the Strang splitting formula [1, 2],
\[ \exp \left[ \frac{1}{2} \tau \mathcal{L}_2 \right] \exp [\tau \mathcal{L}_1] \exp \left[ \frac{1}{2} \tau \mathcal{L}_2 \right] = \exp \left[ \tau \mathcal{L} + \frac{1}{24} \tau^3 [2 \mathcal{L}_1 + \mathcal{L}_2, [\mathcal{L}_1, \mathcal{L}_2]] + \cdots \right], \]  
(5)
which shows that time stepping this expression with a timestep $\tau$ provides an approximation with relative accuracy of order $\tau^2$, exactly preserving the symplectic property of the flow.

This corresponds to the symplectic splitting scheme of iterating the process of solving
\begin{align*}
\dot{q}^a &= \frac{\partial H_2}{\partial p^a}, \quad \dot{p}_a = -\frac{\partial H_2}{\partial q^a}, \quad \text{for a timestep} \quad \frac{1}{2} \tau, \\
\dot{q}^a &= \frac{\partial H_1}{\partial p^a}, \quad \dot{p}_a = -\frac{\partial H_1}{\partial q^a}, \quad \text{for a timestep} \quad \tau, \\
\dot{q}^a &= \frac{\partial H_2}{\partial p^a}, \quad \dot{p}_a = -\frac{\partial H_2}{\partial q^a}, \quad \text{for a timestep} \quad \frac{1}{2} \tau. 
\end{align*}  
(6)
Here the last part of one iteration may be combined with the first part of the next, unless one deals with time dependent systems or wants to register the state of the system at the intermediate times.

There have been several approaches to construct integration schemes which are of higher order in $\tau$, while maintaining the exact symplectic nature of the evolution. Accessible reviews of such approaches have f.i. been given by Yoshida [3], McLachan et. al. [4], and Blanes et.al. [5]. Neri [6] has provided the general idea to construct symplectic integrators for Hamiltonian systems. Forest and Ruth [7] discussed an explicit fourth order method for the integration of Hamiltonian equations for the simplest non-trivial case. Suzuki [8] presented the idea of how recursive construction of successive approximants may be extended to other methods.
Many of the higher order symplectic splitting methods involve an extension of equation (5) to an expression of the form

$$\prod_{i=1}^k \exp[c_i \tau \mathcal{L}_2] \exp[d_i \tau \mathcal{L}_1] = \exp[\tau(\mathcal{L}_1 + \mathcal{L}_2) + \mathcal{O}(\tau^k)],$$

as discussed by Yoshida [9]. It was noted that if one uses a symmetric integrator, such that

$$S(\tau) = \exp[\tau(\mathcal{L}_1 + \mathcal{L}_2) + \tau^\ell R + \mathcal{O}(\tau^k)]$$

for some generator $R$, then

$$S(x_1 \tau) S(x_0 \tau) S(x_1 \tau) = \exp[(x_0 + 2x_1) \tau(\mathcal{L}_1 + \mathcal{L}_2) + (x_0^\ell + 2x_1^\ell) \tau^\ell R + \mathcal{O}(\tau^k)].$$

Hence, by choosing

$$x_0 + 2x_1 = 1,$$
$$x_0^\ell + 2x_1^\ell = 0,$$

one increases the order of the scheme by two or more. However, equations (8, 9) have real solutions only if either $x_0$ or $x_1$ is negative. In fact, it has been proven (cf. Sheng [10], Suzuki [11], Goldman and Kaper [12], Blanes and Casas [13]) that all schemes of the form (7) require at least one $c_i < 0$, and at least one $d_i < 0$. For equations invariant under time reversal, which is often the case for Hamiltonian systems, this may not be a big obstacle (although it seems like an inefficient way of integrating equations forward in time).

Worse, if one wants to use the same code to solve parabolic equations (like a heat type equation, $-\partial_t u(t, x) = [-\Delta + V(x)]u(t, x)$, instead of a Schrödinger equation, $i\partial_t \psi(t, x) = [-\Delta + V(x)]\psi(t, x)$, (which formally corresponds to replacing $t$ by $-it$ in the Schrödinger equation) negative timesteps may have a disastrous effect on numerical stability due to exponentially growing errors. Castella et. al. [14] have proposed to use complex solutions of equations (8, 9). It is possible to find solutions where all timesteps have a positive real part. This can stabilize the scheme, but at the cost of working with complex variables.

In this paper we investigate a different approach, based on our [15] observation that the operators $\mathcal{L}_1, \mathcal{L}_2$ of each step of a splitting scheme don’t need to be exactly the same as those in the sum $\mathcal{L} = \mathcal{L}_1 + \mathcal{L}_2$. Instead, our approach is to construct $\tau$-dependent operators $\mathcal{L}_1, \mathcal{L}_2$ such that

$$\exp[\frac{1}{2} \tau \mathcal{L}_2] \exp[\tau \mathcal{L}_1] \exp[\frac{1}{2} \tau \mathcal{L}_2] = \exp[\tau(\mathcal{L}_1 + \mathcal{L}_2) + \mathcal{O}(\tau^k)].$$

(10)
For Hamiltonians of the form,
\[ H(q,p) = \frac{1}{2} p^T M p + V(q), \]
with \( M \) a symmetric positive definite matrix (the inverse mass matrix), we have constructed explicit expansions,
\[ \tilde{\mathcal{L}}_i = \mathcal{L}_i + \sum_{k=1}^{(N-2)/2} \tau^{2k} \mathcal{L}^{(k)}_i, \]
for \( N = 4, 6, 8 \), leading to schemes with global error of order \( \tau^N \). We denote \( N \) the order of these schemes. Since the operators \( \tilde{\mathcal{L}}_i \) generate flows \( \exp[\tau \tilde{\mathcal{L}}_i] \) which are modifications of those generated by \( \mathcal{L}_i \), we refer to such flows as modified integrators. Chartier et. al. [16] have labeled such schemes as modified differential equations. Thus, the \( N \)’th order scheme is constructed to generate the same flow as
\[ \mathcal{L}' = \mathcal{L} - \tau^N \left( \mathcal{L}^{(N/2)}_1 + \mathcal{L}^{(N/2)}_2 \right) + O(\tau^{N+2}), \]
when averaged over timesteps. I.e., we use modified integrators to generate the unmodified flow better.

One possible restriction on the class of available splitting schemes is the requirement that both of the flows \( \exp[\frac{1}{2} \tau \tilde{\mathcal{L}}_2] \) and \( \exp[\tau \tilde{\mathcal{L}}_1] \) should be explicitly computable. We have relaxed this requirement by demanding both flows to be efficiently computable: I.e., each (short) timestep must be possible to integrate numerically sufficiently fast, while preserving the symplectic structure to sufficient numerical precision.

We have implemented this through the systematic construction of a generating function \( \mathcal{G} \) for an exact symplecting transformation which reproduces the flow over each finite timestep \( \tau \) to sufficient accuracy. For nonlinear dynamics this results in implicit formulas for the evolution
\[ \mathcal{G} : \{q(t), p(t)\} \rightarrow \{q(t + \tau), p(t + \tau)\}. \]
This leads to schemes where each kick step is explicitly computable, while each move step actually involve a small implicitly defined push followed by an explicitly computable move. Here kick and push involve a change in momenta \( p \) with fixed positions \( q \); a move involves a change in positions \( q \) with fixed momenta \( p \).

The rest of this paper is organized as follows: In section 2 we demonstrate the basic idea of the proposed methods on linear systems. Next we develop the
general theory, valid for separable Hamiltonians (11), in section 3. Here we construct the operators \( \hat{L}_i \) explicitly; more precisely the Hamiltonians \( T_{2k} \) and \( V_{2k} \), cf. equation (30) corresponding to these operators. We focus our discussion on the numerical implementation of these methods in section 5 together with investigations of how they work in practice. We have tested these methods on anharmonic oscillators and Fermi-Pasta-Ulam-Tsingou type problems (named as suggested by Dauxois [17]). We close this paper with some brief concluding remarks in section 6.

2. Linear Systems

2.1. Single Harmonic Oscillator

For a simple illustration of our idea consider the Hamiltonian

\[
H(q, p) = \frac{1}{2} (p^2 + q^2),
\]

(15)

whose exact evolution over a time interval \( \tau \) is

\[
\begin{pmatrix}
q_e \\
p_e
\end{pmatrix} =
\begin{pmatrix}
\cos \tau & \sin \tau \\
-\sin \tau & \cos \tau
\end{pmatrix}
\begin{pmatrix}
q \\
p
\end{pmatrix}.
\]

(16)

Compare this with the process of first evolving the system with the Hamiltonian \( H_{\text{kick}} = \frac{1}{2} k q^2 \) for a time \( \frac{1}{2} \tau \), followed by an evolution with \( H_{\text{move}} = \frac{1}{2} m p^2 \) for a time \( \tau \), and ending with an evolution by \( H_{\text{kick}} = \frac{1}{2} k q^2 \) for a time \( \frac{1}{2} \tau \). One such combination gives

\[
\begin{pmatrix}
q_s \\
p_s
\end{pmatrix} =
\begin{pmatrix}
1 - \frac{1}{2} mk \tau^2 & m \tau \\
-(1 - \frac{1}{4} km \tau^2) k \tau & 1 - \frac{1}{2} km \tau^2
\end{pmatrix}
\begin{pmatrix}
q \\
p
\end{pmatrix}.
\]

(17)

We note that by choosing

\[
m = \frac{\sin \tau}{\tau} = 1 - \frac{1}{6} \tau^2 + \frac{1}{120} \tau^4 - \frac{1}{5040} \tau^6 + \cdots,
\]

\[
k = \frac{2}{\tau} \tan \frac{\tau}{2} = 1 + \frac{1}{12} \tau^2 + \frac{1}{120} \tau^4 + \frac{17}{20160} \tau^6 + \cdots,
\]

(18)

the exact evolution is reproduced, provided the timestep is restricted to the interval \( 0 < \tau < \pi \). If we interchange the rôles of \( H_{\text{kick}} \) and \( H_{\text{move}} \) one combination instead gives

\[
\begin{pmatrix}
q_s \\
p_s
\end{pmatrix} =
\begin{pmatrix}
1 - \frac{1}{2} mk \tau^2 & (1 - \frac{1}{4} mk) m \tau \\
-k \tau & 1 - \frac{1}{2} km \tau^2
\end{pmatrix}
\begin{pmatrix}
q \\
p
\end{pmatrix},
\]

(19)
which becomes exact if we choose
\[ m = \frac{2}{\tau} \tan \frac{\tau}{2}, \quad k = \frac{\sin \tau}{\tau}, \tag{20} \]
again provided the timestep is restricted to the interval \( 0 < \tau < \pi \).

2.2. Higher-dimensional linear systems

It should be clear that this idea works for systems of harmonic oscillators in general, i.e. for quadratic Hamiltonians of the form
\[ H(q, p) = \frac{1}{2} (p^T M p + q^T K q), \tag{21} \]
where \( M \) and \( K \) are symmetric matrices. For a chosen splitting scheme and step interval \( \tau \) there are always modified matrices,
\[
M_\tau = M - \frac{\tau^2}{6} M (K M) + \frac{\tau^4}{120} M (K M)^2 - \frac{\tau^6}{5040} M (K M)^3 + \mathcal{O}(\tau^8), \tag{22}
\]
\[
K_\tau = K + \frac{\tau^2}{12} (K M) K + \frac{\tau^4}{120} (K M)^2 K + \frac{17\tau^6}{20160} (K M)^3 K + \mathcal{O}(\tau^8), \tag{23}
\]
generating kick-move-kick flow which reproduces the exact flow up to corrections of order \( \tau^8 \). It should be obvious how this can be extended to arbitrary order in \( \tau^2 \), with coefficients taken from the expansions in equation (18). In principle this can be used to reproduce the exact flow, provided \( \tau \) is not too large. The constraint is the restriction \( 0 < \tau < \pi/\omega_{\text{max}} \), where \( \omega_{\text{max}} \) is the largest frequency of the system.

3. General potentials

For a more general treatment we consider Hamiltonians of the form
\[ H(q, p) = \frac{1}{2} p^T M p + V(q). \tag{24} \]
A series solution of the Hamilton equations in powers of \( \tau \) is
\[
q_\alpha^\tau = q^\alpha + p^\alpha \tau - \frac{1}{2} \partial^\alpha V \tau^2 - \frac{1}{6} \partial^\alpha(DV) \tau^3 + \mathcal{O}(\tau^4),
\]
\[
p_\alpha^\tau = p_\alpha - \partial_\alpha V \tau - \frac{1}{2} \partial_\alpha(DV) \tau^2 + \partial_\alpha \left( \frac{1}{12} \partial V - \frac{1}{6} \partial^2 V \right) \tau^3 + \mathcal{O}(\tau^4).
\]
Here we have introduced notation to shorten expressions,

\[ \partial_a \equiv \frac{\partial}{\partial q^a}, \quad \partial^a \equiv M^{ab} \partial_b, \quad p^a \equiv M^{ab} p_b, \quad D \equiv p_a \partial^a, \quad \dot{D} \equiv (\partial_a V) \partial^a, \]

where we employ the Einstein summation convention: An index which occur twice, once in lower position and once in upper position, are implicitly summed over all available values. I.e., \( M^{ab} \partial_b \equiv \sum_b M^{ab} \partial_b \) (we will generally use the matrix \( M \) to rise an index from lower to upper position).

If we instead use a splitting method to generate the flow, with generators \( H_1 = V(q) \) and \( H_2 = \frac{1}{2} p^T M p \equiv T \) (i.e., a kick-move-kick scheme), we obtain

\[
q^a_s = q^a + p^a \tau - \frac{1}{2} \partial^a V \tau^2 + O(\tau^4),
\]

\[
p^a_s = p_a - \partial_a V \tau - \frac{1}{2} \partial_a (DV) \tau^2 + \partial_a \left( \frac{1}{8} \bar{D} V - \frac{1}{4} D^2 V \right) \tau^3 + O(\tau^4). \tag{25}
\]

As expected the result differs from the exact result in the third order. However, the difference can be corrected by modifying the generators, \( H_1 \to T + T_2 \) and \( H_2 \to V + V_2 \), with

\[
T_2 = -\frac{1}{12} D^2 V \tau^2, \quad V_2 = \frac{1}{24} \bar{D} V \tau^2. \tag{26}
\]

Specialized to a one-dimensional system with potential \( V = \frac{1}{2} q^2 \) this agrees with equation (18). With this correction the kick-move-kick splitting scheme agrees with the exact solution to 4th order in \( \tau \), but differ in the \( \tau^5 \)-terms. We may again correct the difference by introducing fourth order generators, \( H_1 \to T + T_2 + T_4 \) and \( H_2 \to V + V_2 + V_4 \), with

\[
T_4 = \frac{1}{720} (D^4 - 9 \bar{D} D^2 + 3 D \bar{D} D) V \tau^4, \quad V_4 = \frac{1}{480} \bar{D} ^2 V \tau^4. \tag{27}
\]

Specialized to a one-dimensional system with potential \( V = \frac{1}{2} q^2 \) this agrees with equation (18). With this correction the kick-move-kick splitting scheme agrees with the exact solution to 6th order in \( \tau \), but differ in the \( \tau^7 \)-terms. We finally correct this difference by introducing sixth order generators, \( H_1 \to T + T_2 + T_4 + T_6 \) and \( H_2 \to V + V_2 + V_4 + V_6 \), with

\[
T_6 = -\frac{1}{60480} \left( 2 D^6 - 40 \bar{D} D^4 + 46 D \bar{D} D^3 - 15 D^2 \bar{D} D^2 + 54 \bar{D}^2 D^2
\]

\[-9 \bar{D} \bar{D} \bar{D} D - 42 \bar{D} D^2 D + 12 D^2 \bar{D} D \right) V \tau^6
\]

\[
V_6 = \frac{1}{161280} (17 \bar{D}^3 - 10 \bar{D}_3) V \tau^6, \tag{28}
\]
where we have introduced
\[ \bar{D}_3 \equiv (\partial_a V)(\partial_b V)(\partial_c V)\partial^a \partial^b \partial^c. \] (29)

Specialized to a one-dimensional system with potential \( V = \frac{1}{2}q^2 \) this agrees with equation (18). With this correction the kick-move-kick splitting scheme agrees with the exact solution to 8th order in \( \tau \), but differ in the \( \tau^9 \)-terms. The process may be continued to higher orders in \( \tau \),
\[ H_1 \rightarrow T + \sum_{k \geq 1} T_{2k}, \quad H_2 \rightarrow V + \sum_{k \geq 1} V_{2k}. \] (30)

To keep track of the algebraic expressions which occurred during the calculations above, we have represented them graphically in terms of bi-colored tree-diagrams. I.e., these calculations are related to “rooted-tree-type” theories. Our tree-diagrams describing \( T_{2k} \) and \( V_{2k} \), and the generating functions \( G_k \) below, are unrooted (the derivatives of these scalar functions can be represented by rooted trees). It is fairly straightforward to find the general structure of the order \( \tau^N \) correction terms, but more laborious to compute the rational coefficients multiplying each term. They are simplest found by considering enough special cases for unique determination. After the explicit expressions (26, 27) were found we verified them manually for a general Hamiltonian (21) using graphical calculations. The explicit expression (28) has been checked against a general Hamiltonian (21) acting on a four-dimensional phase space (i.e., with two-dimensional \( q \) and \( p \)).

4. Solving the move steps

Addition of extra potential terms \( V \rightarrow V_{\text{eff}} \equiv V + V_2 + V_4 + \ldots \), is in principle unproblematic for solution of the kick steps. The equations,
\[ \dot{q}^a = 0, \quad \dot{p}_a = -\partial_a V_{\text{eff}}(q), \] (31)
can still be integrated exactly, preserving the symplectic structure. The situation is different for the kinetic term \( T \rightarrow T_{\text{eff}} \equiv T + T_2 + T_4 + \cdots \), since it now leads to equations
\[ \dot{q}^a = \frac{\partial}{\partial p_a} T_{\text{eff}}(q, p), \quad \dot{p}_a = -\partial_a T_{\text{eff}}(q, p), \] (32)
which are no longer straightforward to integrate exactly. Although the problematic terms are small one should make sure that the move steps preserve the symplectic structure. Let \( q, p \) denote the positions and momenta just before the move.
step, and $Q, P$ the positions and momenta just after. The relation between $q, p$ and $Q, P$ can be expressed in terms of a generating function (cf. Golstein [22], Arnold [23]),

$$G(q, P; \tau) = q^a p_a + \Delta G(q, P; \tau),$$

(33)
such that the transformation

$$Q^a = \frac{\partial G}{\partial P_a}, \quad p_a = \frac{\partial G}{\partial q^a} = P_a + \frac{\partial \Delta G}{\partial q^a}.$$  

(34)
preserves the symplectic structure exactly. However, note that the relation between $p$ and $P$ in general is a nonlinear equation of the form

$$P_a = p_a - \frac{\partial}{\partial q^a} \Delta G(q, P; \tau),$$

(35)
where the second term on the right is of order $\tau^3$ or higher. We solve this equation by iteration. With $P^{(0)} = p$,

$$P^{(n+1)}_a = p_a - \frac{\partial}{\partial q^a} \Delta G(q, P^{(n)}; \tau).$$

(36)
Writing $P^{(n)} = P + \Delta P^{(n)}$, with $P$ the exact solution, we find to first order in $\Delta P$ that

$$\Delta P^{(n+1)}_a = -\frac{\partial^2}{\partial q^a \partial P_b} \Delta G(q, P; \tau) \Delta P^{(n)}_b = -\Delta G_a^b \Delta P^{(n)}_b.$$  

(37)
Let $\lambda$ be the eigenvalue of $\Delta G_a^b$ with largest magnitude. Then the iteration converges exponentially fast towards the exact solution, with $\Delta P^{(n)}$ decaying like $\lambda^n \sim \tau^{3n}$. Since it is most to gain by a higher order method when the timestep $\tau$ is small, we assume that $\lambda$ is small in cases of practical relevance. Our experience is that the iteration scheme is robust, with 3–4 iterations been sufficient for computations to double precision accuracy.

Some of our theoretical results have already been given in the literature. The generating function formalism has been used earlier by Feng [18] and Feng et.al [19] to construct canonical difference schemes (see also Channell and Scovel [20], Stuchi [21]). They give the result (26), but the actual solution of the resulting implicit equations are not discussed. One can construct a generating function for the full symplectic evolution over a timestep $\tau$, without combination with a
splitting method. However, in that case the resulting nonlinear equations would be more time consuming and/or difficult to solve by direct iteration.

We now explicitly construct \( G \) so that the move step is reproduced to sufficient accuracy. Consider first the case when \( H_1 = T \). The choice \( G = q^a P_a + \frac{1}{2} P^a P_a \tau \) gives

\[
Q^a = q^a + P_a \tau, \quad p_a = P_a, \quad (38)
\]

which is the correct relation. Now add the \( T_2 \)-term to the move step. The exact solution of equation (32) becomes

\[
Q^a = q^a + p_a \tau - \frac{1}{6} \partial^a DV \tau^3 - \frac{1}{24} \partial^a D^2 V \tau^4 + \mathcal{O}(\tau^5),
\]

\[
P_a = p_a + \frac{1}{12} \partial_a D^2 V \tau^3 + \frac{1}{24} \partial_a D^3 V \tau^4 + \mathcal{O}(\tau^5). \quad (39)
\]

Compare this with the result of changing \( G \rightarrow G - \frac{1}{12} \mathcal{D}^2 V \tau^3 - \frac{1}{24} \mathcal{D}^3 V \tau^4 \),

\[
G \rightarrow G - \frac{1}{12} \partial^a D^2 V \tau^3 - \frac{1}{24} \partial^a D^3 V \tau^4, \quad (40)
\]

where \( \mathcal{D} \equiv P_a \partial^a \). The solution of equation (34) change from the relations (38) to

\[
Q^a = q^a + P^a \tau - \frac{1}{6} \partial^a \mathcal{D} V \tau^3 - \frac{1}{8} \partial^a \mathcal{D}^2 V \tau^4 + \mathcal{O}(\tau^5),
\]

\[
p_a = p_a + \frac{1}{12} \partial_a \mathcal{D}^2 V \tau^3 - \frac{1}{24} \partial_a \mathcal{D}^3 V \tau^4 + \mathcal{O}(\tau^5). \quad (41)
\]

Since \( \mathcal{D} \) is linear in \( P \), equation (42) constitute a system of third order algebraic equations which in general must be solved numerically. This should usually be a fast process for small \( \tau \). An exact solution of this equation is required to preserve the symplectic structure, but this solution should also agree with the exact solution of (32) to order \( \tau^4 \). This may be verified by perturbation expansion in \( \tau \). A perturbative solution of equation (42) is

\[
P_a = p_a + \frac{1}{12} \partial_a D^2 V \tau^3 + \frac{1}{24} \partial_a D^3 V \tau^4 + \mathcal{O}(\tau^5),
\]

which inserted into (41) reproduces the full solution (39) to order \( \tau^4 \).

This process can be systematically continued to higher orders. We write the transformation function as

\[
G(\tau) = \sum_{k=0}^{\infty} G_k \tau^k, \quad (43)
\]
and find the first terms in the expansion to be

\[ G_0 = q^4 p^2, \quad G_1 = \frac{1}{2} p^2 p^2, \quad G_2 = 0, \quad G_3 = -\frac{1}{12} q^2 V, \quad G_4 = -\frac{1}{24} q^3 V, \]

\[ G_5 = -\frac{1}{720} \left( 2 q^6 + 8 D^2 q^3 - 5 q^2 D^2 \right) V, \]

\[ G_6 = -\frac{1}{20160} \left( 10 q^6 + 10 D^2 q^4 + 90 D^2 D^2 q^3 - 75 q^2 D^2 q^2 + 18 D^2 D^2 q^2 - 3 D^2 D D - 14 D^2 q^2 + 4 q^2 D^2 \right) V, \]

\[ G_7 = -\frac{1}{30240} \left( 45 D^7 - 87 D^2 q^3 + 231 D^2 D^2 q^3 - 133 q^2 D^2 q^3 + 63 D^2 q^3 - 3 D^2 D^2 q^2 - 21 q^2 D^2 q^2 + 4 q^3 D^2 - 63 D^2 D D^2 + 25 D^2 D D D \right) V. \]

Also in these calculations we represent the algebraic expressions by bi-colored tree diagrams, to better visualise and understand their structure. The possible graphical structures for \( G_n \) is fairly simple to write down. But it is quite laborious to find the rational coefficients multiplying each graph. They are simplest found by considering enough special cases for unique determination. After that we have verified the expressions up to \( G_6 \) manually using graphical calculations, and \( G_7, G_8 \) against a general Hamiltonian (21) acting on a four-dimensional phase space (i.e., with two-dimensional \( q \) and \( p \)) using a computer algebra program.

5. Numerical results on nonlinear systems

5.1. One-dimensional anharmonic oscillator

It remains to demonstrate that our algorithms can be applied to real examples. We have considered the Hamiltonian

\[ H = \frac{1}{2} p^2 + \frac{1}{4} q^4, \quad (44) \]

with initial condition \( q(0) = 0, p(0) = 1 \). The exact motion is a nonlinear oscillation with \( H \) constant equal to \( \frac{1}{2} \), and period

\[ T = 4 \int_0^{2^{1/4}} \frac{\sqrt{2} dq}{\sqrt{2} - q^4} = 2^{1/4} B \left( \frac{1}{4}, \frac{1}{2} \right) \approx 6.236339 \ldots \quad (45) \]

Here \( B(x,y) = \Gamma(x) \Gamma(y) / \Gamma(x+y) \) is the beta function. In Figure [1] we plot the behaviour of \( (H - \frac{1}{2}) / \tau^{2+n} \) during the last half of the 16th oscillation, for various values of \( \tau \) and corrected generators up to order \( \tau^6 \) (corresponding to \( n = 6 \)).
5.2. Fermi-Pasta-Ulam-Tsingou type problems

Here we will consider a one-dimensional closed chain of $d$ particles (as illustrated in Figure [3]) interacting with its nearest neighbours through a potential $U$, and possibly with a local substrate through a potential $V$. The latter will confine the $n$th particle to the vicinity of a position $\mathcal{R}_n = nL/d$, where $L$ is the circumference of the chain.

The class of models for this system include the Fermi-Pasta-Ulam-Tsingou
Figure 2: These figures illustrate the long time behaviour through the last half of the 16th period for the Störmer-Verlet, first half of 257th period for $\tau^2$-corrected, last half of the 4104th period for $\tau^4$-corrected and last half of the 262718th period for $\tau^6$-corrected schemes. Different timesteps $\tau$ have an effect on the period of oscillation, but the preservation of energy remains stable for a very long time.

(FPU) problem introduced in 1953 by Fermi et al. [24] for investigating equipartition of energy among the different degrees of freedom. This study opened up the doors of research in many fields of mathematics and physics. Lot of research is going on in different field of studies to understand the highly unexpected dynamical behaviors. A preview of last 50 years comprehensive study on FPU is provided by G.P. Berman [25].

In the recent papers by E. Hairer and C. Lubich [26] presented a study for FPU by using the modulated Fourier expansions on the chains with large number of particles, and in [27] I. McLachlan and D. Neal have given the good comparison of integrators on FPU. A good analysis of the Störmer-Verlet method applied to
the FPU problem has been given by G. Benettin and A. Ponno [28] by using BCH formula. Numerical methods with some results on FPU are the part of [29].

Here we will demonstrate that our integrators can be implemented and applied in practice to these type of models. There is of course a computational cost per timestep by going to a higher order method, but asymptotically that cost grows linearly with the size of the system. There is also a cost in complexity of code implementation, which we have solved by writing a program for automatic generation of the numerical code [30].

Let \( q_m(t) = r_m(t) - R_m \), where \( r_m(t) \) the position of the \( n^{th} \) particle, and consider the system described by the Hamiltonian

\[
H(q,p) = \frac{1}{2} \sum_{m=0}^{d-1} p_m^2 + \sum_{m=0}^{d-1} V(q_m) + \sum_{m=0}^{d-2} U(s_m),
\]

(46)

where \( d \) is the number of particles, and \( s_m = q_{m+1} - q_m \). A class of model which includes both the linear chain and the FPU model can be obtained by choosing

\[
V(q) = \frac{1}{2} \omega^2 q^2, \quad U(s) = \frac{1}{2} s^2 + \frac{1}{3} \alpha s^3 + \frac{1}{4} \beta s^4,
\]

where \( U \) is describing the interactions between particles. This model has been referred to as the FPU \( \alpha + \beta \) model (with \( \omega^2 = 0 \)). In this example we have used \( \alpha = 0 \) and \( \beta = 1 \). We have tested the methods with respect to (i) energy conservation, (ii) deviation of the generated solution from the exact solution\(^1\) and (iii) efficiency of the methods with respect to CPU time.

In Figure 4 we show the scaled energy error on FPU by using different choices of \( \tau \) of all four methods. For these experiments we consider 9 particles with initial energy \( E(0) = 1.425 \). As can be seen the energy conserved very well for all methods, with the error scaling like \( \tau^N \) for a method of order \( N \). As demonstrated by the long time behaviour in Figure 5 the energy error does not increase noticeably with time.

\(^1\) Actually a numerical solution of the same system computed to very high precision.
Another quantity of interest in a system with many degrees of freedom is the \textit{global error}, i.e. a measure how much the numerical solution deviates from the exact solution. Here an exact solution is not available. Instead we have generated a very accurate solution by use of our 8\textsuperscript{th} order method with timestep $\tau = 5 \cdot 10^{-4}$, calculated with multiprecision (50 decimal digits) floating point accuracy. This is for practical purposes as good as an exact result, and we will refer to it as such. We have investigated several measures of deviation; they all give qualitatively the same results. Here we will only discuss the quantity

\[
\varepsilon(t) \equiv \| (q(t), p(t)) - (q_n, p_n) \|_2 \\
= \left[ \sum_{m=0}^{d-1} (q_m(t) - q_{m,n})^2 + (p_m(t) - p_{m,n})^2 \right]^{1/2}, \tag{47}
\]

Figure 4: Scaled energy error for higher order methods of the FPU
Long time scaled energy error

Figure 5: Long time scaled energy error for a Fermi-Pasta-Ulam-Tsingou type problem, computed with the Störmer-Verlet (A) and higher order corrected integrators (B–D) with timestep $\tau = \frac{1}{12}$ and initial energy $E(0) = 1.425$.

where $q_n$ ($p_n$) denote the positions (momenta) of the numerical solution at a timestep $n$ such that $n\tau = t$, and $q(t)$ ($p(t)$) denote the positions (momenta) of the exact solution at time $t$. As shown in Figure 5, the global error behaves roughly like

$$\varepsilon(t) \sim Ct\tau^N,$$

for relatively short times $t$. Here $C$ is a constant which depends on the order $N$ of the method and the initial conditions. This is in agreement with exact behaviour of integrable systems, cf. Theorem 3.1 in the book [1] by Hairer et. al.
To check the efficiency of our methods in practical use, we have also measured CPU time used to integrate systems with different number \(d\) of particles, with \(d\) ranging from 9 to 50000. All runs have been done on the same system, a workstation equipped with two six-core Opteron 2431 processors, but using code written in NumPy. Hence, the code is not parallellized and run on a single core. Some results, run with timestep \(\tau = 1/12\) for all methods, is shown in Figure 7. Under these conditions we find that the CPU time increases by a factor of about 10 for each step in order. From the left frame of Figure 6 we see that this step also increases the accuracy with a factor of about \(10^{-1/2\tau^2}\) (for \(d = 9\) particles). If we want a prescribed accuracy \(10^{-P}\) for the global error \(\epsilon(t)\) at time \(t\) we may choose to use lower order method with a small timestep (which requires many steps \(n\)), or a higher order method with fewer, but more time-consuming steps. Which choice is best? For the parameters displayed in Figure 6 we estimate the condition

\[
\epsilon(t) \approx 10^{-2-N/2} t \tau^N \approx 10^{-P}.
\]  

(49)

I.e., we must choose a timestep such that

\[
\tau^N \approx \frac{1}{t} \times 10^{2+N/2-P},
\]  

(50)

which requires

\[
n \approx \frac{t}{\tau} \approx \frac{1}{\sqrt{10}} \times t^{(1+1/N)} \times 10^{(P-2)/N}
\]  

(51)
steps, where each step requires a CPU time \( t_{\text{step}} \approx t_0 10^N \) for some constant \( t_0 \) which depends on the computer being used. Hence, we should choose \( N \) to minimize

\[
T_{\text{CPU}} = n t_{\text{step}} \approx t_0 t \frac{10^N}{\sqrt{10}} \times 10^{N/2 + (P + \log_{10} t - 2)/N}.
\]  

(52)

Treating \( N \) as a continuous variable gives the optimal value

\[
N_{\text{opt}} \approx \sqrt{2 (P + \log_{10} t - 2)}.
\]  

(53)

Figure 7: CPU time \( T_{\text{CPU}} \) used to solve a lattice of \( d \) particles for 1000 timesteps (\( \tau = \frac{1}{12} \)) for schemes of different orders \( N \). Asymptotically, \( T_{\text{CPU}} \) grows linearly with \( d \). The penalty for increasing the order \( N \) by 2 is about a factor 10 increase in \( T_{\text{CPU}} \), when \( d \) and the number of timesteps is kept fixed.

6. Concluding remarks

In this paper we have shown that it is possible to systematically extend the standard Störmer-Verlet symplectic integration scheme to higher orders of accuracy, and that the higher order schemes can be applied in practise to physical
systems of interest, including FPU-like lattice problems with many particles (with nearest-neighbour interactions). As illustrated by equation (53), it is advantageous to use a higher order method when one wants a solution of high precision $P$, and also if one wants a solution of moderate accuracy but over a long time interval.

As demonstrated, the theoretical algorithms have been implemented and tested. One rapidly discovers that it is a nightmare to do a correct implementation by hand. The general compact form of these schemes usually expand to very long expressions, which are laborious and error-prone to handle manually. We have therefore developed a set of computer routines which automatically generate the basic numerical integrators for a complete timestep of each specific model.

For the cases we have investigated these integrators perform according to expectations, sometimes even better than expected.

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