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Raising the order of geometric numerical integrators by composition and extrapolation

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We analyse composition and polynomial extrapolation as procedures to raise the order of a geometric integrator for solving numerically differential equations. Methods up to order sixteen are constructed starting with basic symmetric schemes of order six and eight. If these are geometric integrators, then the new methods obtained by extrapolation preserve the geometric properties up to a higher order than the order of the method itself. We show that, for a number of problems, this is a very efficient procedure to obtain high accuracy. The relative performance of the different algorithms is examined on several numerical experiments.

Keywords: geometric integration, composition methods, processing, extrapolation

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1. Introduction

In this paper we analyse several procedures to build high order one-step numerical integrators for the ordinary differential equation

$$y' = f(y), \qquad y(0) = y_0 \in \mathbb{R}^d, \tag{1}$$

with $f : \mathbb{R}^d \to \mathbb{R}^d$ and associated vector field (or Lie operator associated with f)

$$F = \sum_{i=1}^{d} f_i(y) \frac{\partial}{\partial y_i}. \tag{2}$$

We focus our attention, in particular, on integration methods which preserve some geometric properties of the vector field F, the so-called *geometric integrators* (for example, symplectic integrators). It is widely recognized that this class of discretization algorithms provide a better description of the original systems, even with respect to the accumulation of numerical errors along the integration process [14,21,25].

Generally speaking, the vector field F of each family of differential equations arising in different branches of physics, chemistry, biology, etc., has a very specific geomet-

ric structure which is advantageous to preserve under discretization. Thus, geometric integrators of moderate order for several families of problems have been constructed during the last few years. However, building up efficient high order algorithms for problems where high accuracy is required is a task whose complexity grows enormously with the order. For this reason, a widely used technique in geometric integration is to compose one or more low order basic methods (usually first or second order) with appropriately chosen weights to achieve a higher order scheme. For instance, if the map $\mathcal{S}_h^{[2]}: \mathbb{R}^d \to \mathbb{R}^d$ denotes a self-adjoint (or time-symmetric) second order method in the time step h, an integrator of order $q > 2$ can be obtained with the composition

$$\mathcal{S}_h^{[q]} \equiv \mathcal{S}_{\alpha_k h}^{[2]} \circ \mathcal{S}_{\alpha_{k-1} h}^{[2]} \circ \cdots \circ \mathcal{S}_{\alpha_1 h}^{[2]}, \tag{3}$$

where k has to be sufficiently large and the coefficients α_i, $i = 1, \ldots, k$, must satisfy a system of nonlinear equations (the order conditions). In this way $\mathcal{S}_h^{[q]}$ inherits the relevant geometric properties the basic scheme $\mathcal{S}_h^{[2]}$ shares with the exact flow. In particular, if $\mathcal{S}_h^{[2]}$ is a symplectic integrator then $\mathcal{S}_h^{[q]}$ is also a symplectic integrator. This procedure has several drawbacks, however: (i) low order methods rarely take advantage of the simplifying conditions that the specific structure of the vector field F introduces in some particular problems; (ii) the number and complexity of the order conditions grow very rapidly with the order and it is difficult to find all their possible solutions and eventually determine the optimal one; (iii) the methods constructed in this way usually involve a large number of function evaluations and thus the balance between accuracy and computational cost is not very good when high accuracy is desired.

Alternatively, one could also consider a basic method of moderate order (typically four or six) and construct higher order schemes by composition. As we will show, this can turn into very efficient algorithms for a number of problems.

On the other hand, the processing technique has proved to be very useful in this context. In essence, it consists in taking a composition of the form

$$\widehat{\mathcal{S}}_h \equiv \pi_h \circ \mathcal{S}_h \circ \pi_h^{-1}. \tag{4}$$

Here $\mathcal{S}_h$ is referred to as the kernel and the map $\pi_h: \mathbb{R}^d \to \mathbb{R}^d$ as the post-processor or corrector. The method $\mathcal{S}_h$ is said to be of effective order q if a post-processor π_h exists for which $\widehat{\mathcal{S}}_h$ is of (conventional) order q. Application of $\widehat{\mathcal{S}}_h$ over p steps with constant time step h leads to $\widehat{\mathcal{S}}_h^p = \pi_h \circ \mathcal{S}_h^p \circ \pi_h^{-1}$: the computation of the pre-processor π_h^{-1} is done once at the beginning of the integration, then the kernel $\mathcal{S}_h$ acts once per step and finally π_h is evaluated only when output is desired. The analysis of the order conditions of the processed method $\widehat{\mathcal{S}}_h$ has shown that many of them can be satisfied by using π_h and so $\mathcal{S}_h$ must fulfill a much reduced set of restrictions. Thus one may consider kernels of effective order q involving less evaluations than conventional integrators of order q. This has allowed, in particular, to construct highly efficient processed geometric integrators when both the kernel and the post-processor are taken as compositions of low order basic schemes [2–7].

Composition is not the only way, however, to achieve high order numerical integrators starting from a low order basic scheme. For instance, the extrapolation technique can also be used with this purpose. As it is well known, in extrapolation one starts with a basic low order method of order n (typically, a time-symmetric 2nd order integrator, $n = 2$) which is applied with different values of h. Then, by an appropriate combination of the results, one obtains a new method which approximates the exact solution to a higher order. This procedure has the advantage that not only the step size can be changed at each step, but also the order of the method itself [15].

Recently, the question of what happens when the basic method used in extrapolation is a geometric integrator of order n has been analysed [6,10]. The answer is that, although the resulting scheme of order $q > n$ is no longer geometric in character, still preserves geometric properties of the system up to an order higher than q. If $n < q < 2n$ then it is possible to preserve the geometric properties up to order $2q + 1$, with $2n + 1 < 2q + 1 < 4n + 1$. Thus, the undesired effects of non-geometric schemes will finally show up but, in general, this will happen at very long times, and its effect can be neglected in most cases if the order n of the basic method is taken sufficiently high. In practice, extrapolation is used in geometric integration starting with a basic time-symmetric method of order six or eight, at variance with the situation in standard numerical integration of ODEs.

It is the purpose of this paper to construct high order geometric integrators (up to order 14 or 16) to carry out very accurate numerical calculations starting with a basic time-symmetric method of order 6 or 8 and applying composition with processing and polynomial extrapolation. The basic methods considered preserve the geometric structure of the exact solution and in some cases they are especially adapted to the particular structure of F. The interest of the integration schemes thus constructed is illustrated on the important class of differential equations $y'' = g(y, t)$ and the Schrödinger equation. Finally, several numerical examples show the performance on some problems such that very efficient geometric integrators up to order 8 are known.

2. Composition methods

2.1. Standard technique

If φ_h denotes the exact h-flow of the system (1), i.e., $y(h) = \varphi_h(y_0)$, then for each inifinitely differentiable map $g : \mathbb{R}^d \to \mathbb{R}$, $g(\varphi_h(y))$ admits an expansion of the form

$$g\big(\varphi_h(y)\big) = \exp(hF)[g](y) = g(y) + \sum_{k\geqslant 1} \frac{h^k}{k!} F^k[g](y), \quad y \in \mathbb{R}^d,$$

where F is the vector field (2). Let us consider a time-symmetric integrator of order $2n$, $\mathcal{S}_h^{[2n]}$, such that there exists a series of differential operators $S_h^{[2n]}$ verifying $g \circ \mathcal{S}_h^{[2n]}(y) =$

$S_h^{[2n]}[g](y)$ for any function g and $y \in \mathbb{R}^d$. This series can be written as $S_h^{[2n]} = \exp(Y_h)$, with

$$Y_h = hY_1 + h^{2n+1}Y_{2n+1} + h^{2n+3}Y_{2n+3} + \cdots \tag{5}$$

and, for consistency, $Y_1 = F$. In other words, $\mathcal{S}_h^{[2n]}$ is formally the exact 1-flow of the vector field Y_h. As it is well known, by composition of this basic method one can build integration methods of arbitrarily high order. For instance, the composition [12,27]

$$\mathcal{S}_h^{[2n+2]} \equiv \left(\mathcal{S}_{\alpha_1 h}^{[2n]}\right)^p \circ \mathcal{S}_{\alpha_0 h}^{[2n]} \circ \left(\mathcal{S}_{\alpha_1 h}^{[2n]}\right)^p, \tag{6}$$

with $(\mathcal{S}_h^{[2n]})^p = \mathcal{S}_h^{[2n]} \circ \cdots \circ \mathcal{S}_h^{[2n]}$ p-times, provides a time-symmetric method of order $2(n+1)$ if $\alpha_1 = 1/(2p - (2p)^{1/(2n+1)})$, $\alpha_0 = 1 - 2p\alpha_1$. Since $\mathcal{S}_h^{[2n+2]}$ is again a time-symmetric scheme, it can be used as the basic method in the composition (6) to get a new integrator of order $2n+4$ and so on. A method of order $2(n+m)$ obtained in this way requires $(1+2p)^m$ evaluations of the basic scheme $\mathcal{S}_h^{[2n]}$, and this number grows too fast with m and p to be competitive for $m > 1$.

One could also consider the more general composition [2,22]

$$\psi_h^{[2(n+m)]} \equiv \mathcal{S}_{\alpha_s h}^{[2n]} \circ \mathcal{S}_{\alpha_{s-1} h}^{[2n]} \circ \cdots \circ \mathcal{S}_{\alpha_2 h}^{[2n]} \circ \mathcal{S}_{\alpha_1 h}^{[2n]} \tag{7}$$

with appropriately chosen weights α_i and a sufficiently large s. With (7) the number of stages to attain a given order grows more slowly and therefore more efficient integrators can be obtained. Similarly to the basic method $\mathcal{S}_h^{[2n]}$, for the map $\psi_h^{[2(n+m)]}$ one has

$$g\left(\psi_h^{[2(n+m)]}(y)\right) = \exp(F_h)[g](y),$$

i.e., $\psi_h^{[2(n+m)]}$ is formally the exact 1-flow of the series of vector fields F_h and

$$\exp(F_h) = \exp(Y_{h\alpha_1}) \exp(Y_{h\alpha_2}) \cdots \exp(Y_{h\alpha_{s-1}}) \exp(Y_{h\alpha_s}). \tag{8}$$

Now F_h can be obtained by repeated application of the Baker–Campbell–Hausdorff formula [29], which shows that $F_h = hF_1 + h^{2n+1}F_{2n+1} + h^{2n+2}F_{2n+2} + \cdots$ belongs to the graded free Lie algebra $\mathcal{L}$ generated by $\{hY_1, h^{2n+1}Y_{2n+1}, h^{2n+3}Y_{2n+3}, \ldots\}$. In fact, $\mathcal{L} = \mathcal{L}_1 \oplus \mathcal{L}_{2n+1} \oplus \mathcal{L}_{2n+2} \oplus \cdots$ is such that $hY_1 = hF \in \mathcal{L}_1$, $h^k F_k \in \mathcal{L}_k$ for $k \geqslant 2n+1$ and $[\mathcal{L}_k, \mathcal{L}_m] \subset \mathcal{L}_{k+m}$. Each $\mathcal{L}_k$ is the subspace of $\mathcal{L}$ of vector fields affected by a kth power of h, and we denote $l_k = \dim \mathcal{L}_k$. Since the grade corresponds to the power of h, we will usually refer to it as the order.

In this work we choose in $\mathcal{L}_k$ the particular basis $\{E_{k,i}\}_{i=1}^{l_k}$ collected in table 1. Observe that, in particular, the element $[Y_{2n+1}, [Y_1, Y_{2n+1}]] \in \mathcal{L}_{4n+3}$ is not included because for $2n \geqslant 6$ it is true that $4n+3 > 2n+8$, which is the highest order considered here. Then, from (8) we get explicitly

$$F_h = hf_{1,1}E_{1,1} + \sum_{k \geqslant 2n+1} h^k \sum_{i=1}^{l_k} f_{k,i}E_{k,i},$$

Table 1
Basis of $\mathcal{L}_k$ ($k = 1, 2n+1 \leqslant k \leqslant 2(n+4)$ and $2n \geqslant 6$).

$\mathcal{L}_i$	Basis of $\mathcal{L}_i$	
$\mathcal{L}_1$	$E_{1,1} = Y_1 = F$	
$\mathcal{L}_{2n+1}$	$E_{2n+1,1} = Y_{2n+1}$	
$\mathcal{L}_{2n+2}$	$E_{2(n+1),1} = [F, E_{2n+1,1}]$	
$\mathcal{L}_{2n+3}$	$E_{2(n+1)+1,1} = Y_{2n+3}, \quad E_{2(n+1)+1,2} = [F, E_{2(n+1),1}]$	
$\mathcal{L}_{2n+4}$	$E_{2(n+2),i} = [F, E_{2(n+1)+1,i}]$,	$i = 1, 2$
$\mathcal{L}_{2n+5}$	$E_{2(n+2)+1,1} = Y_{2n+5}, \quad E_{2(n+2)+1,1+i} = [F, E_{2(n+2),i}]$,	$i = 1, 2$
$\mathcal{L}_{2n+6}$	$E_{2(n+3),i+1} = [F, E_{2(n+2)+1,i}]$,	$i = 1, 2, 3$
$\mathcal{L}_{2n+7}$	$E_{2(n+3)+1,1} = Y_{2n+7}, \quad E_{2(n+3)+1,i+1} = [F, E_{2(n+3),i}]$,	$i = 1, 2, 3$
$\mathcal{L}_{2n+8}$	$E_{2(n+4),i} = [F, E_{2(n+3)+1,j}]$,	$j = 1, \ldots, 4$

where the $f_{k,i}$ are homogeneous polynomials of degree k in the coefficients α_j, $j = 1, \ldots, s$. In particular,

$$f_{1,1} = \sum_{i=1}^{s} \alpha_i, \qquad f_{2j+1,1} = \sum_{i=1}^{s} \alpha_i^{2j+1}, \quad j \geqslant n.$$

Since we are considering a graded free Lie algebra, the number of order conditions $\mathcal{N}_{2(n+m)}$ to be satisfied by the coefficients α_j in the composition (7) to get an integrator of order $2(n+m)$ out of a basic method of order $2n$ is just

$$\mathcal{N}_{2(n+m)} = 1 + \sum_{k=2n+1}^{2(n+m)} l_k. \tag{9}$$

If the composition (7) is symmetric, i.e., $\alpha_{s+1-i} = \alpha_i$ for $i = 1, \ldots, s$, those conditions at even orders are automatically satisfied. In addition, time-symmetry is an important feature to be preserved for many problems and efficient methods are also obtained by imposing this symmetry, so that usually only symmetric compositions are considered in the literature. For instance, methods up to orden 10 have been constructed starting with a basic method of order 2 [14,16,19,27,30], whereas in [22] new composition schemes up to order 12, 14 and 16 have been proposed starting with basic methods of order 4, 6 and 8 ($n = 2, 3, 4$), respectively.

2.2. Composition with processing

As we pointed out in the introduction, one could also consider constructing integration methods of order $2(n+m)$ of the form

$$\hat{\psi}_h^{[2(n+m)]} = \pi_h \circ \psi_{h,K}^{[2(n+m)]} \circ \pi_h^{-1},$$

where both the post-processor π_h and the kernel $\psi_{h,K}^{[2(n+m)]}$ are themselves compositions of the basic scheme $\mathcal{S}_h^{[2n]}$, as in (7). The computational cost of the method corresponds essentially to the cost of the kernel and the coefficients of the post-processor can be used

to solve a number of order conditions. As a result, highly efficient processed integrators up to order 10 and 12 have been presented in [4] by taking compositions of $\mathcal{S}_h^{[2n]}$ with $n = 1, 2$.

In the following, by applying similar techniques, we propose new composition methods up to order $2(n + m) = 14, 16$ by taking basic integrators of order 6 and 8, respectively. Specifically, we consider a kernel of the form

$$\psi_{h,K}^{[2(n+m)]} = \mathcal{S}_{\beta_s h}^{[2n]} \circ \mathcal{S}_{\beta_{s-1} h}^{[2n]} \circ \cdots \circ \mathcal{S}_{\beta_2 h}^{[2n]} \circ \mathcal{S}_{\beta_1 h}^{[2n]} \tag{10}$$

so that, as before, it can be seen as the exact 1-flow of a vector field G_h such that

$$G_h = h g_{1,1} E_{1,1} + \sum_{k \geqslant 2n+1} h^k \sum_{i=1}^{l_k} g_{k,i} E_{k,i}, \tag{11}$$

where now the $g_{k,i}$ are homogeneous polynomials of degree k in the β_j, $j = 1, \ldots, s$. The number of effective order conditions, i.e., the number of equations to be satisfied by the β_j so that the kernel has effective order $2(n + m)$, is precisely [4]

$$\widehat{\mathcal{N}}_{2(n+m)} = 1 + l_{2(n+m)}. \tag{12}$$

In fact, all the terms $g_{k,i}$ in (11) such that their corresponding basis element in table 1 is of the form $E_{k,i} = [F, E_{k-1,j}]$ can be cancelled out with the processor. Therefore, if $m \leqslant 4$ and $2n \geqslant 6$, the kernel has only to satisfy the order conditions associated with the coefficients of $E_{1,1}$ and $E_{2(n+j)-1,1}$, $j = 1, \ldots, m$, which in explicit form are

$$g_{1,1} \equiv \sum_{i=1}^{s} \beta_i = 1, \qquad g_{2(n+j)-1,1} \equiv \sum_{i=1}^{s} \beta_i^{2(n+j)-1} = 0, \tag{13}$$

$j = 1, \ldots, m$, $m \leqslant 4$. Due to their very simple structure, these equations can be solved numerically in a trivial way with all the desired accuracy. In contrast with standard composition schemes now it is quite easy to find and analyse all the possible numerical solutions for the kernel and select the most appropriate one to get an efficient scheme, even if some free parameters are included in the composition.

The remaining order conditions take a much more complicated form, but they can be solved by using the post-processor. The search of numerical solutions of these equations is more difficult and the resulting composition for π_h requires typically at least as many basic integrators as the kernel. On the other hand, most of the real solutions found are valid, since their differences only contribute to higher order error terms.

Notice that if the kernel $\psi_{h,K}^{[2(n+m)]}$ is a symmetric composition of $\mathcal{S}_h^{[2n]}$ with $2n \geqslant 6$ and $m \leqslant 4$ there is no reduction in the number of effective order conditions: it has to solve exactly the same equations (13). Even so, this number is significantly smaller than the corresponding to symmetric non-processed schemes. For the sake of illustration, in table 2 we show these numbers when $2n = 2, 4, 6, 8$ and several values of m. The results for $\mathcal{S}_h^{[6]}$ and $\mathcal{S}_h^{[8]}$ follow readily from table 1 and the preceding discussion, whereas for $\mathcal{S}_h^{[2]}$ and $\mathcal{S}_h^{[4]}$ we refer to [4], where these cases are treated in detail.

Table 2
Number of order conditions for symmetric standard composition methods, $\mathcal{N}_q^{(s)}$, and number of effective order conditions for processed composition methods of order $q = 2(n+m)$, $\widehat{\mathcal{N}}_q^{(s)}$, if the basic method is $\mathcal{S}_h^{[2n]}$ with $n = 1, 2, 3, 4$.

	$\mathcal{S}_h^{[2]}$		$\mathcal{S}_h^{[4]}$		$\mathcal{S}_h^{[6]}$		$\mathcal{S}_h^{[8]}$	
q	$\mathcal{N}_q^{(s)}$	$\widehat{\mathcal{N}}_q^{(s)}$	$\mathcal{N}_q^{(s)}$	$\widehat{\mathcal{N}}_q^{(s)}$	$\mathcal{N}_q^{(s)}$	$\widehat{\mathcal{N}}_q^{(s)}$	$\mathcal{N}_q^{(s)}$	$\widehat{\mathcal{N}}_q^{(s)}$
4	2	2	–	–	–	–	–	–
6	4	3	2	2	–	–	–	–
8	8	5	4	3	2	2	–	–
10	16	8	7	4	4	3	2	2
12			12	6	7	4	4	3
14					11	5	7	4
16							11	5

Among the different solutions obtained for the effective order conditions, one is interested in those that minimize the non-correctable terms at order $2(n+m)+1$ according to some criterion previously adopted, such as the minimization of a certain objective function. Unfortunately there is not a universal measure of the performance of integration methods of this class, since for different problems the dominant error terms are not necessarily the same. Here, as in [4], we consider two different objective functions:

$$E_1(\beta) = \sum_{i=1}^{s} |\beta_i| \quad \text{and} \quad E_2(\beta) = s|g_{2(n+m)+1,1}|^{1/(2n+2m)}. \tag{14}$$

Here s is the number of stages, which can be considered as a measure of the cost and thus E_2 may be seen as an effective error, since $g_{2(n+m)+1,1}$ is the only non-vanishing error term at order $2(n+m)+1$ for $2n \geqslant 6$ and $m < 4$. A method whose coefficients lead to a small value of E_1 usually has good stability properties and small error terms, whereas E_2 is the dominant error term in the limit $h \to 0$. Both of them contain obvious limitations, however. E_1 is not useful to compare the efficiency of schemes with different number of stages. For instance, one can find a family of solutions for different values of s with values $E_1^{(s)}$ such that $E_1^{(s+1)} < E_1^{(s)}$ and $\lim_{s\to\infty} E_1^{(s)} = 1$. This is the case, in particular, for the composition (6) with $s = 2p+1$. On the other hand, if one considers E_2 as the only objective function to be minimized and some free parameters are incorporated in the composition, then it is possible to attain the global minimum $E_2 = 0$. This is not necessarily the optimal solution, however, because then the higher order error terms are dominant and they can take very large values. For these reasons we try to find local minima of both $E_1(\beta)$ and $E_2(\beta)$ which in this particular problem it is possible, as shown in [20].

As it was mentioned before, to get efficient methods one usually considers symmetric compositions with more stages than the number of effective order conditions, so that there are l free parameters, say $\beta_1, \beta_2, \ldots, \beta_l$. Recently, McLachlan [20] has proposed

as a rule of thumb to choose these free parameters equal to the first (and last) coefficient β_{l+1} of the symmetric composition with the minimum number of stages necessary to satisfy the order conditions. This gives, in a simple way, isolated solutions which correspond to simultaneous local minima of E_1 and E_2 [20], being just the case we are looking for. To construct specific kernels by following this approach, we take different values of l and analyse all the numerical solutions obtained. We stop when, increasing the value of l, the values of E_1 and E_2 are not significantly reduced. This stopping criterion is adopted to avoid methods with too many stages which in some cases could lead to stability problems.

The new schemes are denoted by $\hat{\psi}_h^{[2(n+m)]}(2n; s)$: a processed method of order $2n + 2m$ built with an s-stage symmetric kernel composition of a basic method of order $2n$. In other words,

$$\hat{\psi}_h^{[2(n+m)]}(2n; s) = \pi_h \circ \psi_{h,K}^{[2(n+m)]} \circ \pi_h^{-1}$$

with

$$\psi_{h,K}^{[2(n+m)]} = \mathcal{S}_{\beta_1 h}^{[2n]} \circ \cdots \circ \mathcal{S}_{\beta_{r-1} h}^{[2n]} \circ \mathcal{S}_{\beta_r h}^{[2n]} \circ \mathcal{S}_{\beta_{r-1} h}^{[2n]} \circ \cdots \circ \mathcal{S}_{\beta_1 h}^{[2n]} \tag{15}$$

and $s = 2r - 1$. The best solutions obtained from $2n = 6, 8$ are presented in table 3.

In a similar way as for the post-processor, we take a similar composition, so that the algorithm employed to compute the kernel can also be used. In particular, we construct π_h as a composition of the form $\pi_h = w_h \circ w_{-h}$, with [4]

$$w_h = \mathcal{S}_{\gamma_1 h}^{[2n]} \circ \cdots \circ \mathcal{S}_{\gamma_p h}^{[2n]} \tag{16}$$

because with this special structure several order conditions at odd orders are automatically satisfied. For $m = 2, 3$ the post-processor is built with additional stages to cancel the non-correctable terms at order $2(n+m)+1$. This is not done for $m = 4$, because the number of stages required to solve the equations increases drastically and the improvement in the accuracy of the resulting method is not so clear [4].

Contrarily to the kernel, for the processor it is not necessary to carry out a rigorous numerical search of all the solutions and, as mentioned, only one solution with moderately small coefficients is required. Nevertheless, as it can be observed in table 3, the post-processor usually involves as many stages as the kernel, so that its computational cost could decrease the performance of the overall method when output is frequently required. In those cases it can be safely replaced by an approximated post-processor obtained at essentially cost free from intermediate values in the computation of the kernel following the procedure presented in [4]. Thus the cost of the processed method corresponds essentially to the cost of the kernel.

3. Extrapolation of geometric integrators

Extrapolation constitutes a very useful technique for raising the order of an integrator. Nevertheless, if the basic scheme $\mathcal{S}_h^{[2n]}$ is a geometric integrator, the final method

Table 3
Coefficients for the most efficient kernels obtained (15) and one solution for their post-processor $\pi_h = w_h \circ w_{-h}$ with w_h given by (16) when the time-symmetric basic method is of order $2n = 6$ ($\mathcal{S}_h^{[6]}$) and $2n = 8$ ($\mathcal{S}_h^{[8]}$).

$\psi_{h,K}^{[10]}(6;9)$	$\psi_{h,K}^{[12]}(6;13)$	$\psi_{h,K}^{[14]}(6;15)$
$\beta_1 = \beta_2 = \beta_3$	$\beta_1 = \beta_2 = \beta_3 = \beta_4$	$\beta_1 = \beta_2 = \beta_3 = \beta_4$
$\beta_3 = 0.2157264116709669$	$\beta_4 = 0.1530960766803307$	$\beta_4 = 0.1536532739869463$
$\beta_4 = -0.3157867596148055$	$\beta_5 = -0.2489473170424535$	$\beta_5 = -0.3335622906088959$
$\beta_5 = 1 - 2(3\beta_3 + \beta_4)$	$\beta_6 = 0.2847405643878192$	$\beta_6 = 0.3057149938043347$
	$\beta_7 = 1 - 2(4\beta_4 + \beta_5 + \beta_6)$	$\beta_7 = -0.2581741612607714$
		$\beta_8 = 1 - 2(4\beta_4 + \beta_5 + \beta_6 + \beta_7)$
π_h	π_h	π_h
$\gamma_5 = 0.1$	$\gamma_7 = -0.1633802595635479$	$\gamma_7 = 0.1006758986148266$
$\gamma_4 = 0.1295705841112265$	$\gamma_6 = -0.2444257593717152$	$\gamma_6 = -0.3297793266038176$
$\gamma_3 = 0.2303276447320048$	$\gamma_5 = 0.1936296323692213$	$\gamma_5 = 0.2808380505843029$
$\gamma_2 = -0.2156727681577507$	$\gamma_4 = -0.04498272119682715$	$\gamma_4 = 0.2934568294346022$
$\gamma_1 = -(\gamma_2 + \gamma_3 + \gamma_4 + \gamma_5)$	$\gamma_3 = -0.2212625977608340$	$\gamma_3 = 0.1420049625018795$
	$\gamma_2 = 0.2389306909257556$	$\gamma_2 = -0.1700510812262375$
	$\gamma_1 = -(\gamma_2 + \cdots + \gamma_7)$	$\gamma_1 = -(\gamma_2 + \cdots + \gamma_7)$
$\psi_{h,K}^{[12]}(8;11)$	$\psi_{h,K}^{[14]}(8;13)$	$\psi_{h,K}^{[16]}(8;17)$
$\beta_1 = \beta_2 = \beta_3 = \beta_4$	$\beta_1 = \beta_2 = \beta_3 = \beta_4$	$\beta_1 = \beta_2 = \beta_3 = \beta_4 = \beta_5$
$\beta_4 = 0.1498593540118365$	$\beta_4 = 0.1506611476621996$	$\beta_5 = 0.1166307052906320$
$\beta_5 = -0.2105425094814418$	$\beta_5 = -0.2228762186169689$	$\beta_6 = -0.1834320793720009$
$\beta_6 = 1 - 2(4\beta_4 + \beta_5)$	$\beta_6 = 0.2487696922765247$	$\beta_7 = 0.2113185016765999$
	$\beta_7 = 1 - 2(4\beta_4 + \beta_5 + \beta_6)$	$\beta_8 = -0.2273787494663681$
		$\beta_9 = 1 - 2(5\beta_5 + \beta_6 + \beta_7 + \beta_8)$
π_h	π_h	π_h
$\gamma_5 = 0.1$	$\gamma_7 = 0.1821172669208845$	$\gamma_7 = -0.1555359247536682$
$\gamma_4 = 0.0751545688344758$	$\gamma_6 = 0.2104488571749604$	$\gamma_6 = -0.1787323715816782$
$\gamma_3 = 0.1780626762617966$	$\gamma_5 = 0.2233377718718366$	$\gamma_5 = -0.1865310629258911$
$\gamma_2 = -0.1691819618963899$	$\gamma_4 = -0.2239174891060533$	$\gamma_4 = 0.1872216121810449$
$\gamma_1 = -(\gamma_2 + \gamma_3 + \gamma_4 + \gamma_5)$	$\gamma_3 = -0.2017261987431234$	$\gamma_3 = 0.1700937755102425$
	$\gamma_2 = 0.01913915279278383$	$\gamma_2 = -0.01559173224766973$
	$\gamma_1 = -(\gamma_2 + \cdots + \gamma_7)$	$\gamma_1 = -(\gamma_2 + \cdots + \gamma_7)$

obtained by polynomial extrapolation does not preserve, in general, the geometric properties of the exact solution, so that this procedure does not generate geometric integrators. In spite of this situation, it has been proved that, under certain conditions, it is in fact possible to build by extrapolation high order schemes which nearly preserve the main qualitative properties of the exact flow [6,10]. Usually these methods possess very small error terms and, for most practical purposes, the preservation of the geometric properties they provide is sufficiently accurate. In this sense extrapolation could be considered as an alternative procedure to composition.

We summarize next the main features of the polynomial extrapolation technique in the geometric integration setting and refer the reader to [6,10], where it is treated in more detail.

In a similar way as for composition, we start with a time-symmetric integrator of order $2n$, $\mathcal{S}_h^{[2n]}$, with associated vector field Y_h given by (5). If the time step h is divided in k substeps and the method is applied k times, then the resulting map $(\mathcal{S}_{h/k}^{[2n]})^k$ is formally the exact 1-flow of the series of vector fields

$$kY_{h/k} = hF + h\left(\frac{h}{k}\right)^{2n}\left(\sum_{i=0}^{\infty}\left(\frac{h}{k}\right)^{2i} Y_{2n+1+2i}\right) \in \mathcal{L}.$$

Taking different values of k we get different approximate solutions after one step. Now we consider a linear combination of all of them,

$$\psi_{E,h} = \sum_{j=1}^{l} \alpha_j \big(\mathcal{S}_{h/k_j}^{[2n]}\big)^{k_j} \tag{17}$$

where we fix the l integers k_j and determine the coefficients α_j so as to eliminate the lowest order terms in the corresponding asymptotic expansion of the local error and thus obtain a higher order integrator. This procedure involves $s = k_1 + \cdots + k_l$ evaluations of $\mathcal{S}_h^{[2n]}$. In terms of the corresponding series of differential operators one has

$$\Psi_{E,h} = \sum_{j=1}^{l} \alpha_j \big(S_{h/k_j}^{[2n]}\big)^{k_j}$$

and $S_{h/k_j}^{[2n]} = \exp(Y_{h/k_j})$, so that formally $g \circ \psi_{E,h} = \Psi_{E,h}[g]$.

Observe that $\psi_{E,h}$ cannot be interpreted as the exact 1-flow of a formal vector field in the Lie algebra $\mathcal{L}$, that is, $\log(\Psi_{E,h}) \notin \mathcal{L}$, since $\Psi_{E,h}$ is a linear combination of exponentials of vector fields in $\mathcal{L}$. This being the case, however, it is not difficult to show that we can still write the formal series $\Psi_{E,h}$ with $m = 1, \ldots, n$, as [6]

$$\Psi_{E,h} = \exp\left(\frac{h}{2}F\right) Y \exp\left(\frac{h}{2}F\right), \tag{18}$$

where

$$\begin{aligned} Y = \exp\big(h^{2(n+m)+1}Z\big) + \frac{1}{2}h^{4n+2}\big(r_{4n}R_1 + h^2 r_{4n+2}R_2 + \cdots \\ + h^{4m}\big(r_{4n+4m}R_3 - r_{2n+2m}^2 R_4\big) + \mathcal{O}\big(h^{4m+2}\big)\big) + \mathcal{O}\big(h^{6n+3}\big), \end{aligned} \tag{19}$$

if $l = m + 1$ and the coefficients α_j satisfy the linear system of equations

$$\begin{aligned} r_0 &\equiv \sum_{j=1}^{l} \alpha_j = 1, \\ r_{2(n+p)} &\equiv \sum_{j=1}^{l} \frac{\alpha_j}{k_j^{2(n+p)}} = 0 \quad \text{for } p = 0, \ldots, m-1. \end{aligned} \tag{20}$$

In (19), $Z = \sum_{j=0}^{\infty} h^{2j} Z_{2(n+m)+2j+1} \in \mathcal{L}$ and $R_j \notin \mathcal{L}$ (in particular, $R_1 = Y_{2n+1}^2 \notin \mathcal{L}$).

Notice that the resulting method $\psi_{E,h}$ is of order $2(n+m)$ and, according to (19), it can be considered as the flow of a vector field in $\mathcal{L}$ up to order $r = 4n+1$. Observe also that the lowest error term, R_1, which does not belong to $\mathcal{L}$ appears at order $4n+2$. If, for instance, $\mathcal{S}_h^{[2n]}$ is a symplectic integrator, then $\psi_{E,h}$ is a pseudo-symplectic method [1]. We will denote this class of methods as $\psi_{E,h}^{[2(n+m)]}(2n; s; r)$: an integrator of order $2(n+m)$ obtained by extrapolation from a basic scheme of order $2n$, evaluated s times, and which preserves the geometric character of the solution up to order r. In fact, it is possible to build methods of order $2(n+m)$ which preserve geometric properties up to order $4(n+m)+1$ simply by canceling r_{4n+2j} for $j = 0, 1, \ldots, 2m-1$. One could try to rise even more the value of r, but then the condition $r_{2n+2m}^2 = 0$ has to be satisfied so the order of consistency of the method increases and efficiency could be degraded. Obviously, l has to be larger to solve all the necessary equations.

According to this result, if the order $2n$ of the basic method is sufficiently high ($2n \geqslant 6$), with a proper choice of the coefficients it is possible to construct integrators such that their 'non-geometric' error terms R_j do not contribute significantly to the global error, even for very long time integrations. For instance, if $2n = 6$ it is possible to build a 10th-order ($m = 2$) integrator which preserves the geometric properties up to order h^{21} ($4(n+m)+1 = 21$).

Example. Let us consider equation (1) with $f(y) = A(y)y$, where $A(y)$ is a skew-symmetric matrix. Then the exact flow is given by an orthogonal transformation. Suppose that $\mathcal{S}_h^{[2n]}$ is a (matrix) map preserving orthogonality and consider the linear combination (17) with $k_1 = 1$, $k_2 = 2$ and coefficients $\alpha_1 = -1/(2^{2n}-1)$, $\alpha_2 = 1-\alpha_1$. Then the resulting extrapolation scheme

$$\psi_{E,h} = \frac{1}{2^{2n}-1}\left[2^{2n}\left(\mathcal{S}_{h/2}^{[2n]}\right)^2 - \mathcal{S}_h^{[2n]}\right] \tag{21}$$

is of order $2n+2$, requires three evaluations of the basic method per step and verifies

$$(\psi_{E,h})^{\mathrm{T}} \circ \psi_{E,h} = I + \mathcal{O}\left(h^{4n+2}\right),$$

where I is the identity matrix. In other words, it preserves orthonogality up to order $4n+1$, so that we can denote it by $\psi_{E,h}^{[2n+2]}(2n; 3; 4n+1)$. In this sense it could be considered as a pseudo-orthogonal integrator.

Several sequences $\{k_j\}$ are used in the literature (see [15] and references therein). The choice of a particular sequence does not affect the values of $2(n+m)$ and r which can be attained. Nevertheless, the computational cost of the algorithm as well as the magnitude of the leading error terms $Z_{2(n+m)+1}$ and the coefficients multiplying R_j depend on that particular election. We have analysed different sequences and observed that for large values of l in (17) the 'harmonic sequence' $k_j = j$ is the most economic one. This is in fact the case if a symmetric second order method is taken as basic integrator and a high order (12 or higher) is desired but the sensitivity to round-off increases with the order. However, since we are mainly interested in methods with $2n \geqslant 6$, we only

Table 4
Coefficients α_j in (17) for different values of m, r and s using as basic integrators symmetric compositions of order six and eight and the sequence $k_j = j$. For simplicity it is written $D\alpha_i$, where $D = \sum_i D\alpha_i$ because $\sum_i \alpha_i = 1$.

	$D\alpha_5$	$D\alpha_4$	$D\alpha_3$	$D\alpha_2$	$D\alpha_1$
$\psi^{[8]}_{E,h}(6;3;13)$				2^6	-1
$\psi^{[10]}_{E,h}(6;6;13)$			19683	-2048	5
$\psi^{[12]}_{E,h}(6;10;13)$		2097152	-531441	14336	-7
$\psi^{[14]}_{E,h}(6;15;15)$	1220703125	-536870912	43046721	-393216	42
$\psi^{[10]}_{E,h}(8;3;17)$				2^8	-1
$\psi^{[12]}_{E,h}(8;6;17)$			177147	-8192	5
$\psi^{[14]}_{E,h}(8;10;17)$		33554432	-4782969	57344	-7
$\psi^{[16]}_{E,h}(8;15;17)$	30517578125	-8589934592	387420489	-1572864	42

require moderately small values of l and thus both the specific sequence and this source of round-off error are not particularly relevant.

In table 4 we collect the coefficients α_j in (17) for different values of m, s and r with symmetric basic integrators of order $2n = 6, 8$ and the harmonic sequence. These are the solutions of the linear equations (20).

From this table it is clear that, with respect to the preservation of geometric properties, methods $\psi^{[12]}_{E,h}(6;10;13)$, $\psi^{[14]}_{E,h}(6;15;15)$ and $\psi^{[16]}_{E,h}(8;15;17)$ behave as standard extrapolation schemes, whereas the value r of the remaining methods can be increased by considering larger values of l. For instance, a method $\psi^{[12]}_{E,h}(8;s;21)$ can be constructed with $l = 5$ (i.e., $s = 15$ using the harmonic sequence).

4. Particular classes of problems

To illustrate the interest of the new procedures to raise the order of integrators we analyse two families of problems which frequently appear in classical and quantum mechanics. For those particular problems, highly efficient (geometric) integrators exist in the literature up to moderate orders (fourth, sixth and eighth-order).

4.1. The equation $x'' = g(x, t)$

Let us consider the second order differential equation

$$x'' = g(x,t), \qquad x(0) = x_0 \in \mathbb{R}^D, \qquad x'(0) = x_0' \in \mathbb{R}^D, \tag{22}$$

which is suitable to be integrated with Runge–Kutta–Nyström (RKN) methods. If we denote $y = (x, x', y_t)$, where the time is considered as a new coordinate, $y_t = t$, then (22)

can be written as the first order system

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{Bmatrix} x \\ x' \\ y_t \end{Bmatrix} = \underbrace{\begin{Bmatrix} x' \\ 0 \\ 1 \end{Bmatrix}}_{f_A(y)} + \underbrace{\begin{Bmatrix} 0 \\ g(x, y_t) \\ 0 \end{Bmatrix}}_{f_B(y)}, \tag{23}$$

with associated vector fields

$$F_A \equiv \sum_{i=1}^{D} x_i' \frac{\partial}{\partial x_i} + \frac{\partial}{\partial y_t}, \qquad F_B \equiv \sum_{i=1}^{D} g_i(x, y_t) \frac{\partial}{\partial x_i'}, \tag{24}$$

and flows associated to each part

$$\varphi_h^{[A]}(y) = \begin{Bmatrix} x + hx' \\ x' \\ y_t + h \end{Bmatrix}, \qquad \varphi_h^{[B]}(y) = \begin{Bmatrix} x \\ x' + hg(x, y_t) \\ y_t \end{Bmatrix}. \tag{25}$$

This system is separable and the time-symmetric second order Störmer/leapfrog/ Verlet integrator

$$\mathcal{S}_h^{[2]} = \varphi_{h/2}^{[A]} \circ \varphi_h^{[B]} \circ \varphi_{h/2}^{[A]} \tag{26}$$

can be used. As mentioned, methods up to order ten obtained by composition of (26) are available in the literature (see [14,21] and references therein). This method is essentially equivalent to the basic method proposed by Gragg (see [15, p. 294]) to be used with extrapolation for this problem. This method, in our notation, would correspond to n evaluations with time-step $2h$ of the basic method $\bar{\mathcal{S}}_h^{[2]} = \varphi_{h/2}^{[B]} \circ \varphi_h^{[A]} \circ \varphi_{h/2}^{[B]}$. But, for the numerical examples carried out in this paper, the basic method $\mathcal{S}_h^{[2]}$ in (26) gave more accurate results being the method used.

However, this problem has a very specific structure (not fully exploited by (26)) which could allow to build more efficient integrators. For instance:

1. It is easy to check that $[F_B, [F_B, [F_B, F_A]]] = 0$, simplifying the Lie algebra of this problem. Then it seems more convenient to consider instead the composition

$$\mathcal{S}_h^{[r]} = \varphi_{b_s h}^{[B]} \circ \varphi_{a_s h}^{[A]} \circ \cdots \circ \varphi_{b_1 h}^{[B]} \circ \varphi_{a_1 h}^{[A]} \tag{27}$$

   with a proper choice of s and coefficients a_i, b_i. In [8] symmetric methods up to order six are obtained which clearly outperform composition methods (3) of similar order and using (26).

2. For this problem we have that

$$F_C = \big[F_B, [F_A, F_B]\big] = \sum_{i=1}^{D} 2\big(g^{\mathrm{T}} \cdot \nabla_x g\big)_i \frac{\partial}{\partial x_i'}. \tag{28}$$

We will refer to F_C as a modified vector field. We then observe that the flow associated to F_B and F_C can be computed together. For this reason, we can consider the more general composition

$$\mathcal{S}_h^{[r]} = \varphi^{[\widehat{B}]}_{b_s h, c_s h^3} \circ \varphi^{[A]}_{a_s h} \circ \cdots \circ \varphi^{[\widehat{B}]}_{b_1 h, c_1 h^3} \circ \varphi^{[A]}_{a_1 h} \tag{29}$$

with

$$\varphi^{[\widehat{B}]}_{b_i h, c_i h^3}(y) = \left\{ \begin{array}{c} x \\ x' + h\big(b_i I + 2c_i h^2 \nabla_x g^{\mathrm{T}}\big) g \\ y_t \end{array} \right\} \tag{30}$$

and I is the identity matrix. Methods up to order eight with a relatively small number of stages and low error terms are given in [5,7,11,17,18,22–24,28]. These methods can be used as basic integrators to obtain higher order methods. They are interesting in several situations:

- Each stage requires also the computation of $\nabla_x g$ which, in general, is computationally expensive. However, in some cases, the evaluations done for the computation of g can be reused to compute the most expensive parts of $\nabla_x g$, making the additional cost not significant.
- For some problems with a different splitting but similar Lie algebra structure, the most costly part of the method comes from the evaluation of $\varphi_h^{[A]}(y)$. Then, the extra cost due to the modified vector fields does not contribute considerably to the overall cost of the method.
- It is possible to find especially well suited solutions for the coefficients $\{a_i, b_i, c_i\}$; for instance, contrarily to the composition (27), there exists fourth order methods with all coefficients $\{a_i, b_i, c_i\}$ positive. Then, schemes with very small error terms can be found which compensate the additional cost.

4.2. The Schrödinger equation

Let us consider the time-dependent Schrödinger equation

$$\mathrm{i}\,\frac{\partial}{\partial t}\psi = -\frac{1}{2}\nabla^2\psi + V(x,t)\psi, \qquad \psi(x,0) = \phi(x), \tag{31}$$

where $\psi(x,t)$ is the wave function associated with the system.

For numerically solving this equation, it is usual to consider a spatial semidiscretisation. Suppose the system is one-dimensional, defined in the interval $x \in [x_0, x_N]$, and we split this interval in N parts of length $\Delta x = (x_N - x_0)/N$. Next, consider $u_n = \psi(x_n, t)$, where $x_n = x_0 + n\Delta x$, $n = 1, \ldots, N$, thus obtaining the finite-dimensional linear equation

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}u = \big(A + B(t)\big)u, \qquad u(0) = u_0, \tag{32}$$

where $u = (u_1, \ldots, u_N)^{\mathrm{T}} \in \mathbb{C}^N$ and $A, B \in \mathbb{C}^{N\times N}$ are Hermitian matrices. The potential energy B is a diagonal matrix with diagonal elements $V(x_i, t)$ and the kinetic energy A is a full matrix which can be diagonalised using Fourier transforms, $A = \mathcal{F}^{-1} D_A \mathcal{F}$, where $\mathcal{F}$ and $\mathcal{F}^{-1}$ correspond to the forward and backward Fourier transform and D_A is a diagonal matrix. Then the computations of $\mathrm{e}^{-\mathrm{i}tA}u_0$ and $\mathrm{e}^{-\mathrm{i}tB}u_0$ can be done using fast Fourier transforms (FFTs) and splitting methods can be used efficiently.

On the other hand, it is easy to check that $[B, [B, [B, A]]] = 0$. It has the same algebraic structure as the previous second order differential equation and the same splitting Nyström integrators in the form (27) can be used. In addition, $C = [B, [A, B]]$ is a diagonal matrix with diagonal elements $C_i = -(V'(x_i, t))^2$, where V' is the derivative with respect to x. Then the composition with modified potentials (29) can be used. The FFTs are usually the most time consuming part and the additional computational cost due to the modified potentials can be neglected. This is therefore another important problem for which highly efficient geometric integrators up to moderate order are available.

5. Numerical examples

In the following we test numerically the main properties of the new high-order methods based on the extrapolation of geometric integrators. We also check their efficiency in comparison with strictly geometric composition methods, both standard and processed, when they are implemented with constant step size. We use the following basic integrators for the comparisons:

- *Sixth order.* M6 (the 9-stage scheme (3) of [19]); BM6 (the 11-stage RKN scheme (27) of [8]); OMF6 (the 5-stage RKN scheme (29) of [22]).
- *Eighth order.* M8 (the 17-stage scheme (3) of [19]); OMF8 (the 11-stage RKN scheme (29) of [22]).
- *Tenth order.* G10 (the 33-stage scheme (3) of [14]).

For the standard extrapolation we consider as the basic second order symmetric integrator the composition (26).

Reduction of round-off errors. In this paper we consider high order methods to obtain very accurate results and then round-off errors can be significant, so it seems appropriate to consider some techniques to reduce those rounding errors. Given y_n, the numerical solution at t_n, the intermediate stages for most integrators take the form (for an m-stage method)

$$y^{(i)} = y_n + \delta^{(i)}, \quad i = 1, \ldots, m, \tag{33}$$

with $\delta^{(i)} = \mathcal{O}(h)$ and $y_{n+1} = y^{(m)}$. If we define the increments $\Delta y^{(i)} = y^{(i)} - y_n$, with $\Delta y^{(0)} = 0$, this equation can be written in the more convenient form

$$\Delta y^{(i)} = \Delta y^{(i-1)} + \delta^{(i)}, \quad i = 1, \ldots, m, \tag{34}$$

where $\Delta y^{(i)} = \mathcal{O}(h)$ and $y_{n+1} = y_n + \Delta y^{(m)}$. In general, working with increments reduces round-off errors. This technique can also be used with extrapolation [13]. There each integration with a substep $h_i = h/k_i$ can be written as (33) and we can extrapolate for the increments $\delta^{(i)}$ to get δ_{extr}, where $y_{n+1} = y_n + \delta_{\text{extr}}$.

In addition, each full time step by composition as well as by extrapolation takes the form $y_{n+1} = y_n + \Delta y_n$ and compensated summation can be used. This corresponds to the following algorithm for N steps (see [26] and references therein):

$y_{\text{err}} = 0$
for $n = 1$ **to** N
  $\Delta y = \Delta y_n + y_{\text{err}}$
  $y_{\text{new}} = y_n + \Delta y$
  $y_{\text{err}} = (y_n - y_{\text{new}}) + \Delta y$
  $y_{n+1} = y_{\text{new}}$.

Numerical experiments carried out by us in double precision indicate that the round-off errors are reduced, approximately, between one and two orders of magnitude using the previous techniques. They can be considered as computational cost free since no additional evaluations of the vector field are required and then they are recommended to be used in general.

Example 1. Let us consider the equation studied in [9]

$$x'' + x = -\varepsilon \sum_{j=1}^{k} \sin(x - \omega_j t), \quad x \in \mathbb{R}. \tag{35}$$

It describes the motion of a charged particle in a constant magnetic field perturbed by k electrostatic plane waves, each with the same wavenumber and amplitude, but with different temporal frequencies ω_j. This equation can be derived from the Hamiltonian

$$H(q, p, t) = \frac{1}{2}\left(p^2 + q^2\right) + \varepsilon \cos(q) g_1(t) + \varepsilon \sin(q) g_2(t) \tag{36}$$

with $g_1(t) = \sum_{j=1}^{k} \cos(w_j t)$, $g_2(t) = \sum_{j=1}^{k} \sin(w_j t)$. We take the following values for the initial conditions and parameters [9]: $q_0 = 0$, $p_0 = 11.2075$, $\varepsilon = 1$, $\omega_j = j\omega_0$, with $\omega_0 = 7$ and $k = 3$.

The system is separable in different ways. We consider the splitting (harmonic oscillator)–(perturbation), where Nyström methods can also be used. Notice that modified potentials are evaluated at essentially cost free because the most expensive computations can be reused, and this problem is suitable to be integrated with the composition (29).

To illustrate the strong influence of the choice of the basic method in the performance of the final integrator, we consider three different sixth-order methods: M6, BM6 and OMF6. We compare their performances as sixth-order methods as well as when used as basic methods to get pseudo-symplectic 8th-, 10th- and 12th-order integrators

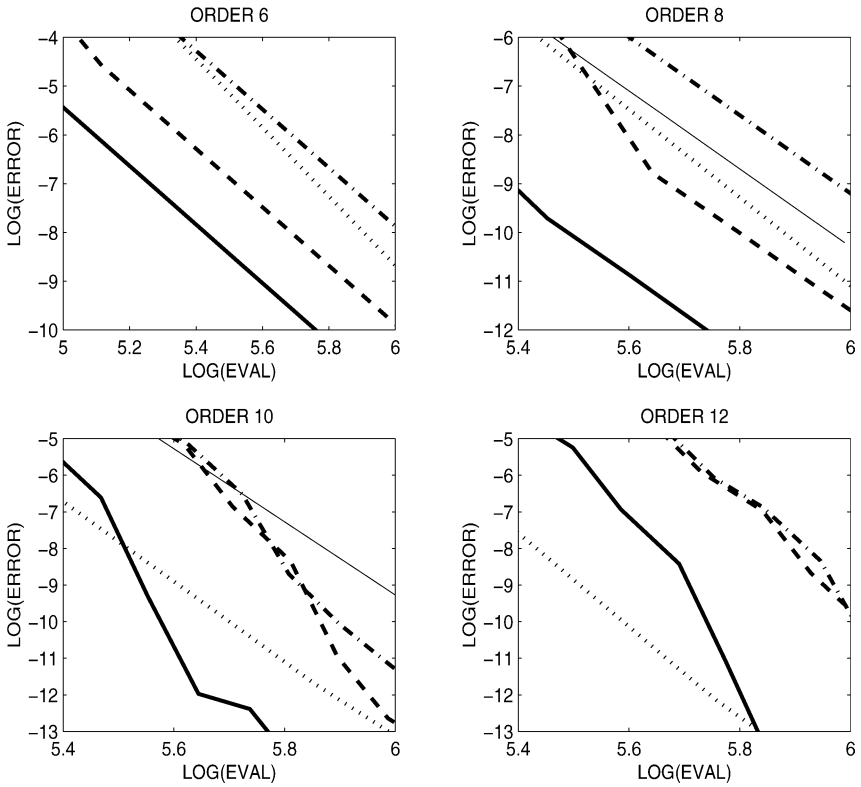

Figure 1. Work-accuracy curves for methods of order six, eight, ten and twelve obtained by extrapolation with the harmonic sequence and using as basic methods the symmetric second order scheme (dotted lines) and the sixth-order schemes: M6 (dotted broken lines), BMF6 (broken lines) and OMF6 (solid lines). For illustration, the eighth- and tenth-order symmetric–symmetric schemes M8 and G10 are also included as thin solid lines in their corresponding figures.

as given in table 4. We also consider integrators of the same order, but obtained using standard extrapolation with (26) as the basic method. In the figures for the 8th- and 10th-order methods we also include the symplectic integrators M8 and G10. We integrate the system up to $t_f = 100 \cdot 2\pi$ and measured the average error in (q, p) during the last period. The *exact* solution was obtained taking a very small time step.

Figure 1 shows the results obtained. We observe significant differences in the performance of the integrators as well as the fact that it is possible to outperform standard extrapolation using an efficient sixth-order method, but this superiority is reduced as the order increases. Notice that OMF6 is not necessarily the most efficient sixth-order integrator for this problem (more efficient methods could exist). We then conclude that for some problems it is possible to build high-order pseudo-symplectic integrators which can be competitive with standard extrapolation (considered as one of the most efficient integrators to attain very high accuracies). Then, contrarily to what is usually claimed, for some problems geometric integrators can also be competitive for relatively short integrations and high accuracies.

Example 2. We consider now the two-body problem of classical mechanics, defined by the equations

$$x_i'' = -\frac{x_i}{(x_1^2 + x_2^2)^{3/2}}, \quad i = 1, 2, \tag{37}$$

which can be rephrased as (1) with $y = (x_1, x_2, x_1', x_2')$, and is generated by the Hamiltonian function

$$H = T(p) + V(q) = \frac{1}{2}\|p\|^2 - \frac{1}{\|q\|}. \tag{38}$$

Here $q = (x_1, x_2)$, $p = (x_1', x_2')$ are the coordinates and momenta, respectively.

Now the flows $\varphi_{ah}^{[A]}$ and $\varphi_{bh,ch^3}^{[\widehat{B}]}$ are given by ($G \equiv h/(x_1^2 + x_2^2)^{3/2}$)

$$\varphi_{ah}^{[A]}(x_i) = x_i + ahx_i', \qquad \varphi_{bh,ch^3}^{[\widehat{B}]}(x_i') = x_i' - x_i G(b + 4chG), \quad i = 1, 2, \tag{39}$$

where the extra cost due to the modified potential can be neglected. In all the numerical experiments we take as initial condition $x_1(0) = 1 - e$, $x_2(0) = x_1'(0) = 0$, $x_2'(0) = [(1 + e)/(1 - e)]^{1/2}$, which produces an orbit with eccentricity e.

On the preservation of symplecticity. To illustrate the different behaviour of integration methods built by polynomial extrapolation with respect to the preservation of the symplectic character of the exact solution, we consider two 10th-order integrators obtained with the harmonic sequence from S2 and OMF6. Specifically, we take $k_j = 1, 2, 3, 4, 5$ for S2 to construct $\psi_{E,h}^{[10]}(2; 15; 11)$ (requiring 15 force evaluations per step) and $k_j = 1, 2, 3$ for OMF6 to build $\psi_{E,h}^{[10]}(6; 6; 13)$ (which requires 6 evaluations of OMF6, i.e., 30 force evaluations per step). Clearly, it is more economical to start with S2, but one has also to analyse the magnitude of the error and how it is propagated along the integration. With this goal in mind, we compute the average relative error in position E_r for $T = 10$ and $T = 1000$ periods. Let us denote by N_e the number of force evaluations. It is know that the average error in positions for this problem grows linearly when using symplectic integrators, instead of quadratically for standard integrators [25]. Then, if we plot E_r/T as a function of N_e/T we should find:

(i) if the integrator is symplectic then the same curve has to be obtained with independence of the number of periods, i.e., it has to be essentially invariant;

(ii) if the integrator is not symplectic, the error will grow linearly with the number of periods.

Figure 2 shows the results achieved with $\psi_{E,h}^{[10]}(2; 15; 11)$ (broken lines) and $\psi_{E,h}^{[10]}(6; 6; 13)$ (solid lines) when $T = 10$ (thick curves) and $T = 1000$ (thin curves). As a reference, we also include the results obtained with the symplectic integrator G10 (dash-dotted lines). The effect of preserving symplecticity at higher orders than the order of the method itself is clear in this example: $\psi_{E,h}^{[10]}(2; 15; 11)$ is more efficient, but

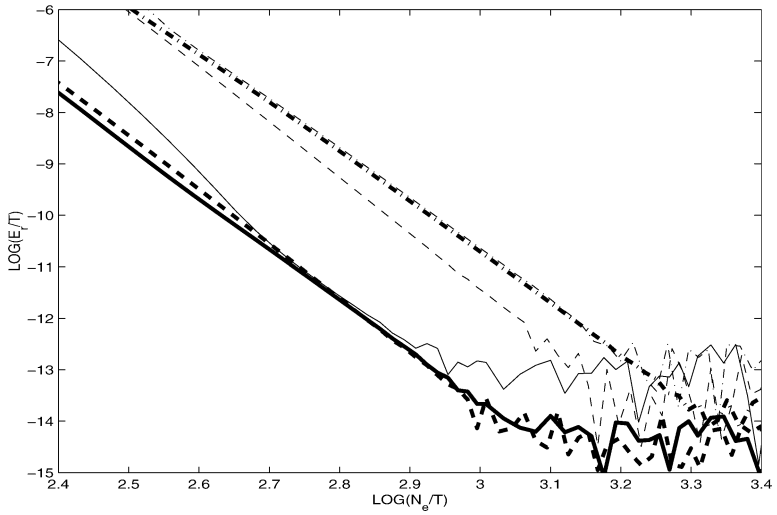

Figure 2. Average relative error in position vs. number of evaluations per period for two 10th order extrapolation methods using as basic integrators: S2 (broken lines) and OMF6 (solid lines), and the 10th-order symplectic integrator G10 (dash-dotted lines). We compare the average error per period vs. the number of evaluations per period after 10 periods (thick lines) and after 1000 periods (thin lines).

only for the first few periods. For large values of h we can observe in the figure that the non-symplectic error terms in $\psi^{[10]}_{E,h}(6;6;13)$ (of order $\mathcal{O}(h^{14})$) start to be significant after a long number of periods. Nevertheless, we should remark that these high-order integrators are employed typically when one requires very accurate results and so only moderately small time steps are used, otherwise lower order integrators are more efficient. On the other hand, it is known that round-off can be an important problem for extrapolation. However, if we consider both extrapolation for the increments and compensated summation as previously mentioned, the round-off error for all extrapolated and composition methods are of similar magnitude. We repeated the computation with the 12th- and 14th-order methods obtained with OMF6 and also a round-off error of similar magnitude for this problem was found.

Several additional remarks are in order. First, as we mentioned in section 3, it is, in fact, possible to build methods $\psi^{[10]}_{E,h}(6;s;r)$ with $r > 13$ simply by taking $l > 3$ in (17), i.e., $s > 6$, and then the harmonic sequence is more appropriate. Second, it can be shown that if we start with a 6th order basic scheme, the highest order method we can achieve with $r > 2(n+m)+1$ is precisely 10 (i.e., $m = 2$, where the symplecticity can be preserved up to order $r = 21$). Therefore, methods of order 12 and higher possess the same qualitative properties as the standard extrapolation methods. Third, similar results are obtained if we repeat the same experiment taking OMF8 as the basic integrators. The main difference is that symplecticity is now preserved at a considerably higher order because we are starting with a higher order symplectic integrator.

Extrapolation versus standard and processed composition. Finally, we compare the relative performance of high-order integrators obtained by composition (both standard

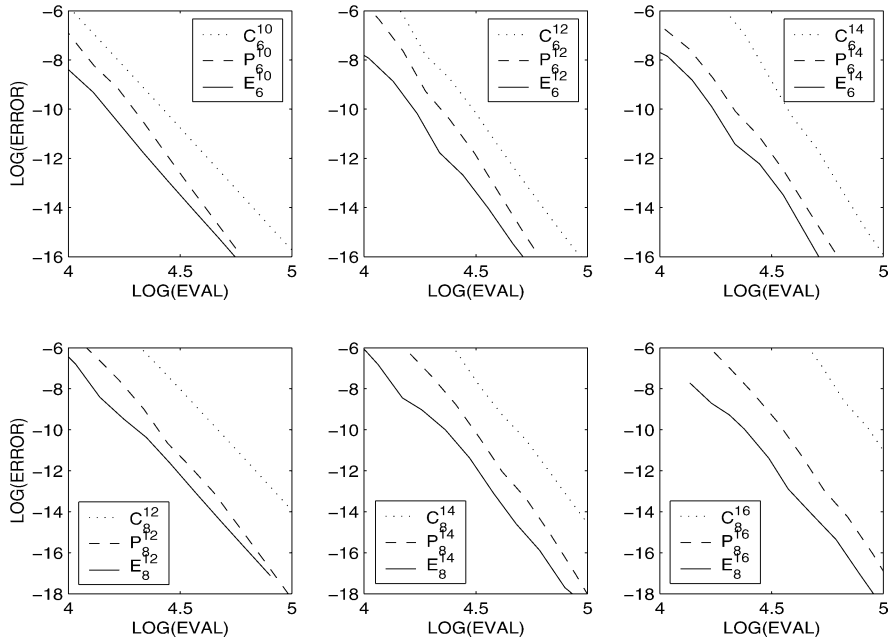

Figure 3. Work-accuracy curves taking a sixth-order and an eighth-order method as the basic integrators to get methods up to order fourteen and sixteen, respectively.

and processed) and extrapolation starting from the basic methods OMF6 and OMF8. In particular, with OMF6 we analyse schemes of order 10, 12 and 14, whereas for the basic integrator OMF8 we test methods of order 12, 14 and 16. In all cases we integrate for 10 periods an orbit with eccentricity $e = 1/2$ and measure the average error in position versus the number of potential evaluations (the computations are done with quadruple precision). Figure 3 shows the results obtained. There, for simplicity, the following notation has been used: the recently obtained [22] standard composition methods $\psi_h^{[2(n+m)]}(2n; s)$ are denoted by $\mathrm{C}_{2n}^{2(n+m)}$; $\mathrm{P}_{2n}^{[2(n+m)]}$ stands for the processed method $\hat{\psi}_h^{[2(n+m)]}(2n; s)$ and $\mathrm{E}_{2n}^{2(n+m)}$ corresponds to the extrapolation scheme $\psi_{E,h}^{[2(n+m)]}(2n; s; r)$, with $r = \max\{13, 2(n+m)+1\}$ for $2n = 6$ (OMF6) and $r = 17$ for $2n = 8$ (OMF8).

In all cases, extrapolation methods seem to be slightly more efficient than processed composition schemes, and both of them are clearly superior to standard composition algorithms for this example. Nevertheless, one has also to take into account the pseudo-symplectic property of extrapolation schemes: according to figure 2, the error of E_6^{12}, E_6^{14} and E_8^{16} will grow always faster than for composition methods of the same order.

6. Concluding remarks

We have analysed composition and polynomial extrapolation as procedures to raise the order of geometric integrators. From basic integrators of order six or eight we have

presented new processed composition and extrapolation methods up to order sixteen. The results achieved by all these methods on the numerical examples analysed allow us to conclude that geometric and pseudo-geometric integrators can also be competitive with standard integrators for high accuracies and short time integrations for certain problems. Notice that it is usually claimed that the interest of geometric integrators is only for low accuracies and very long time integrations. This result is in our opinion worth to be emphasized and it leaves the following open questions with respect to the final choice of an efficient integrator for a given problem:

- Which basic integrator of a given order will produce the most efficient integrator?
- Given several integrators of different orders, which one will produce the most efficient integrator by composition and/or extrapolation (taking into account the order at which the geometric properties are lost in the last case)?
- How to build basic integrators which produce efficient high order integrators?
- Is it reasonable to build a variable order and variable step algorithm using a high order basic integrator in spite of the loose of the *nice* pseudo-geometric properties?

These questions are at present under investigation for the Schrödinger equation as well as for some other second order differential equations.

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