Novel parallel in time integrators for ODEs

Sergio Blanes

Instituto Universitario de Matemática Multidisciplinar, Universitat Politècnica de València. Spain

Abstract

We present a novel class of integrators for differential equations that are suitable for parallel in time computation, whose structure can be considered as a generalisation of the extrapolation methods. Starting with a low order integrator (preferably a symmetric second order one) we can build a set of second order schemes by few compositions of this basic scheme that can be computed in parallel. Then, a proper linear combination of the results (obtained from the order conditions associated to the corresponding Lie algebra) allows us to obtain new higher order methods. In this letter we present the structure of the methods, how to obtain several methods, we notice some order barriers that depend on the structure of the compositions used and finally, we show how this analysis can be further carried to obtain new and higher order schemes.

Keywords: Numerical methods for ODEs; parallel in time methods, symmetric second order methods; extrapolation; composition methods

1. Introduction

We consider the numerical integration of the ODE

$$x' = f(t,x), \qquad x(t_0) = x_0, \tag{1}$$

with $x \in \mathbb{C}^d$ and formal solution given by $x(t) = \phi_t(x_0)$ by using a novel class of methods that are suitable for parallel computation and whose structure can be considered as a generalisation of extrapolation methods. Extrapolation methods are among the most efficient schemes when highly accurate results are required [7, 11, 12, 16] and, in addition, they can be computed in parallel.

If there is not a constraint in the number of processors, we show that a generalisation of the extrapolation process (leading to a novel class of methods) can improve their accuracy while keeping the sequential cost per step. Different classes of parallel methods for ODEs have been frequently considered in the literature (see [11] or the most recent review work [8]), and in this work we only consider the parallel in time integration [5, 6, 13].

In this letter we illustrate this novel procedure in very simple cases and we present new 4th and 6th-order methods. Closely related schemes with complex coefficients and with the goal to preserve time-symmetry and other qualitative properties to higher order is considered in [5]. Let us denote by S_h a symmetric second order integrator in the time step, h, i.e. $S_h = \phi_h + \mathcal{O}(h^3)$ and $S_h \circ S_{-h} = I$, the identity map (explicit or implicit symmetric second order schemes can be easily built [1, 9, 11, 12, 15]). A 4th-order extrapolation method is given by the linear combination

$$\Phi_h^{[4]} = \frac{4}{3} S_{h/2} \circ S_{h/2} - \frac{1}{3} S_h. \tag{2}$$

To compute x_{n+1} from x_n, with $x_k \simeq x(t_k),\ t_k = t_0 + kh$, each processor computes $y_i = \prod_{j=1}^{i} S_{h/2^{j-1}}(x_n),\ i = 1,2$ and the results are combined to get $x_{n+1} = \frac{4}{3}y_2 - \frac{1}{3}y_1$. The cost is dominated by the evaluation of the most costly process, y_2, i.e. two maps S_h per step (see [7, 11]). If the map S_h is a geometric integrator that preserves

Email address: serblaza@imm.upv.es (Sergio Blanes)

some of the qualitative properties of the exact solution then, these properties are preserved by composition leading to integrators with high performance when medium to long time integrations are considered [2, 10, 14]. However, the linear combination in the extrapolation methods destroy these qualitative properties, although this can happen at a higher orders than the order of the method [3, 4]. In addition, a variable time step procedure can be implemented if one compares the accurate 4th-order approximation, x_{n+1} with the second order one y_2 (see [11]).

Notice that, at the same computational cost, the following more general scheme

$$\Psi_h^{[4]} = b_2 S_{(1-a_2)h} \circ S_{a_2 h} + b_1 S_{(1-a_1)h} \circ S_{a_1 h} \tag{3}$$

(which contains the previous one as a particular case: $a_1 = 0, a_2 = \frac{1}{2}, b_1 = -\frac{1}{3}, b_2 = \frac{4}{3}$) could provide more accurate results for appropriate choices of the coefficients a_1, a_2, b_1, b_2. This scheme can be further generalised to the case in which we have k available processors, as follows

$$\Psi_h^{[m,2]} = \sum_{j=1}^{k} b_j S_{(1-a_j)h} \circ S_{a_j h}.$$

The accuracy of the method will depend on how much the map $\Psi_h^{[m,2]}$ approaches the exact solution ϕ_h, and this depends on the number of order conditions the coefficients a_i, b_isatisfy. Given a value of k we can choose a set of values for the coefficients $a_i,\ i = 1, \ldots, k$ (with $a_i \neq a_j,\ i \neq j$ and taking into account that the choice $a_i = 0$ is equivalent to $a_i = 1$) and then the coefficients b_i have to solve a linear system of equations. In some cases, it is possible to solve the same set of equations with a reduced value of k by allowing some of the coefficients a_i to satisfy non-linear order conditions.

We will show that this class of methods has an order barrier. One of the conditions at order h^5 is not independent. It is possible to obtain 4th-order methods that are optimised in the sense that contributions at higher orders can be vanished leading to superior methods to (2) for a number of problems but, in general, 5th-order methods can not be obtained. In addition, once the coefficients a_i are fixed, it is also possible to find another set of values for the coefficients b_i such that the embedded method is of order three, allowing for sharper error estimators than the estimators for extrapolation methods.

To get higher order methods one has to add another map. We illustrate the procedure by considering combinations of symmetric schemes (to consider symmetric schemes simplify the analysis, but a non-symmetric sequence could be considered) as, for example

$$\Psi_h^{[m,3]} = \sum_{j=1}^{k} b_j S_{a_j h} \circ S_{(1-2a_j)h} \circ S_{a_j h} \tag{4}$$

whose performance has to be compared with the 6th-order extrapolation method

$$\Phi_h^{[6]} = \frac{81}{40} S_{h/3} \circ S_{h/3} \circ S_{h/3} - \frac{16}{15} S_{h/2} \circ S_{h/2} + \frac{1}{24} S_h \tag{5}$$

that uses the more economical harmonic sequence (other sequences for extrapolation methods would require more than three maps per step and usually show slightly worst performance [11]).

2. Fourth and sixth-order methods

The goal of this section is not to obtain the most efficient 4th and 6th-order methods of this class but to illustrate that the performance of the extrapolation methods can be further raised, and we illustrate it with the following schemes:

- An optimised 2-stage 4th-order method

$$\Psi_h^{[4,2]} = b_3 S_{(1-a_3)h} S_{a_3 h} + b_2 S_{(1-a_2)h} S_{a_2 h} + b_1 S_{(1-a_1)h} S_{a_1 h}, \tag{6}$$

with

$$\begin{array}{lll} a_1 = 0.185083473675167899, & a_2 = -\frac{1}{10} & a_3 = \frac{1}{10}, \\ b_1 = 8.200177124779414591, & b_2 = 1.277318043040618944, & b_3 = 1 - b_1 - b_2, \\ \hat{b}_1 = 1, & \hat{b}_2 = -0.912528759429160013, & \hat{b}_3 = 1 - \hat{b}_1 - \hat{b}_2. \end{array}$$

The embedded method, say $\hat{\Psi}_h^{[3,2]}$ is of order three and corresponds to an scheme similar to $\Psi_h^{[4,2]}$ but replacing the coefficients b_i by $\hat{b}_i$.

- An optimised 3-stage 6th-order method

$$\Psi_h^{[6,3]} = \sum_{i=1}^{5} b_i S_{a_i h}\, S_{(1-2a_i)h}\, S_{a_i h} \tag{7}$$

with an embedded method of order five

$$\begin{array}{lll}
a_1 = 1.128520493860176762 & b_1 = -0.031183710241561175 & \hat{b}_1 = -1/10 \\
a_2 = 0.790595004758162983 & b_2 = 0.587534847838132073 & \hat{b}_2 = 0.722848812595572664 \\
a_3 = 0.604432933065477058 & b_3 = -1.141887280735286118 & \hat{b}_3 = -1.177391519427465008 \\
a_4 = -0.022021631480667294 & b_4 = -0.116862322614714864 & \hat{b}_4 = -0.143395596461239863 \\
a_5 = \frac{33}{100} & b_5 = 1 - b_1 - b_2 - b_3 - b_4 & \hat{b}_4 = 1 - \hat{b}_1 - \hat{b}_2 - \hat{b}_3 - \hat{b}_4.
\end{array}$$

2.1. Numerical example

Let us consider the two-dimensional Kepler problem with Hamiltonian

$$H(q,p) = T(p) + V(q) = \frac{1}{2}p^T p - \frac{1}{r}.$$

Here $q = (q_1, q_2), p = (p_1, p_2)$, and we take initial conditions $q_1(0) = 1-e,\ q_2(0) = 0,\ p_1(0) = 0,\ p_2(0) = \sqrt{\frac{1+e}{1-e}}$, so that the trajectory corresponds to an ellipse of eccentricity e and period $T = 2\pi$. We integrate until $t_f = 30$ with the 4th- and 6th-order methods, and compute the maximum error in the vector (q,p) along the whole integration (we compare with a highly accurate numerical solution). Figure 1 shows the maximum error versus the highest number of force evaluations of any of the processors (two and three evaluations per step for the 4th and 6th-order methods, respectively). Solid lines correspond to the new methods and dashed lines to extrapolation methods. Similar lines with circles show the results if the whole integration was carried out with the associated embedded methods. The left picture shows the results of the 4th-order methods and the right picture for the 6th-order ones. The embedded methods also provide sharper error bounds.

We clearly observe that, while the new 4th-order methods is only slightly superior to the extrapolation method, the improvement of the new 6th-order method is significant, and this is due to the fact that one has more parameters available for optimisation purposes.

3. Order conditions

Let us consider, for simplicity in the presentation, the autonomous equation (the results remain also valid for the non-autonomous case too)

$$x' = f(x) = Y_1 x, \qquad Y_1 \equiv f(x)\frac{\partial}{\partial x}$$

whose solution can formally be written as $x(t) = \phi_t(x_0) = \mathrm{e}^{tY_1}x_0$. A symmetric second order scheme, S_h, can be seen as the exact solution of a perturbed differential equation (backward error analysis [10]) where the perturbed vector field only has even powers of h, i.e.

$$x' = f_h(x) = f(x) + h^2 f_3(x) + h^4 f_5(x) + \ldots, \qquad \mathit{or} \qquad x' = (Y_1 + h^2 Y_3 + h^4 Y_5 + \ldots)x,$$

where $f_3, f_5, \ldots$ and their associated operators, $Y_3, Y_5, \ldots$ depend on the particular method, and formally we can writte

$$S_h = \mathrm{e}^{hY_1 + h^3 Y_3 + h^5 Y_5 + \cdots}, \qquad \mathit{so} \qquad S_{ah} = \mathrm{e}^{ahY_1 + a^3h^3Y_3 + a^5h^5Y_5 + \cdots}.$$

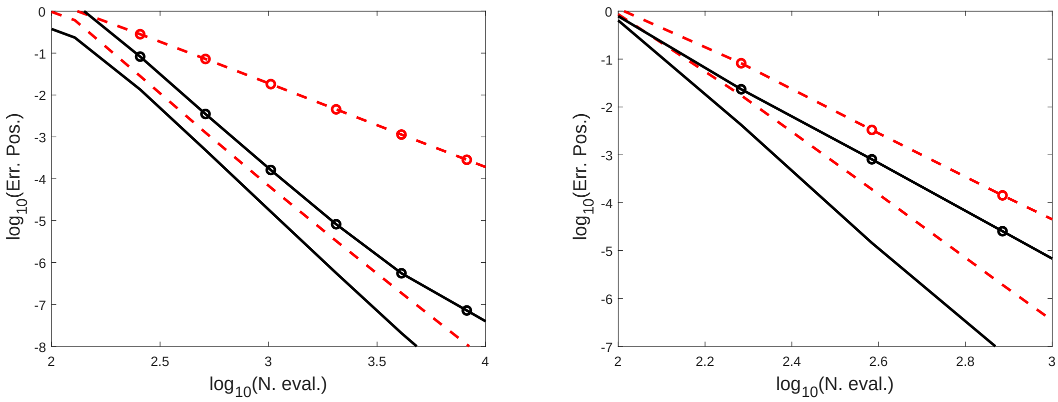

Figure 1: Maximum error in positions vs. the number of evaluations of the basic $\mathcal{S}_h^{[2]}$ scheme for the Kepler problem. Solid lines correspond to the novel 4th- and 6th-order methods and the dashed lines correspond to the extrapolation ones, and with circles are the results if integrated only with the associated embedded methods. Left figure show the results for the 4th-order methods while the right figure shows the results for the 6th-order ones.

Taking into account the BCH formula for non-commuting operators

$$\mathrm{e}^X\mathrm{e}^Y = \mathrm{e}^{X+Y+\frac{1}{12}([X,[X,Y]]+[Y,[Y,X]])+\dots}$$

where $[X,Y]=XY-YX$, and the symmetric BCH formula

$$\mathrm{e}^X\mathrm{e}^Y\mathrm{e}^X = \mathrm{e}^{2X+Y-\frac{1}{6}[X,[X,Y]]+\frac{1}{6}[Y,[Y,X]]+\dots}$$

we obtain that

$$S_{(1-a)h}S_{ah} = \exp\Big(hY_1+g_{3,1}h^3Y_3+g_{4,1}h^3[Y_1,Y_3]+g_{5,1}h^5Y_5+g_{5,2}h^5[Y_1,[Y_1,Y_3]]\dots\Big),$$

with

$$\begin{array}{ll} g_{3,1}=a^3+(1-a)^3, & g_{4,1}=\frac{1}{2}(a^3(1-a)-a(1-a)^3), \\ g_{5,1}=a^5+(1-a)^5, & g_{5,2}=\frac{1}{12}(1-2a)(a^3(1-a)-a(1-a)^3). \end{array} \tag{8}$$

If we now consider the symmetric BCH formula and the Taylor expansion of the exponential we have

$$\begin{aligned} & S_{(1-a)h}S_{ah} \\ = \;& \exp\Big(\frac{1}{2}hY_1\Big)\exp\Big(g_{3,1}h^3Y_3+g_{4,1}h^3[Y_1,Y_3]+g_{5,1}h^5Y_5+\bar{g}_{5,2}h^5[Y_1,[Y_1,Y_3]]+\mathcal{O}(h^6)\Big)\exp\Big(\frac{1}{2}hY_1\Big) \\ = \;& \exp\Big(\frac{1}{2}hY_1\Big)\Big(I+g_{3,1}h^3Y_3+g_{4,1}h^3[Y_1,Y_3]+g_{5,1}h^5Y_5+\bar{g}_{5,2}h^5[Y_1,[Y_1,Y_3]]+\mathcal{O}(h^6)\Big)\exp\Big(\frac{1}{2}hY_1\Big), \end{aligned}$$

where $\bar{g}_{5,2}=g_{5,2}+\frac{1}{6}g_{3,1}$. Then, we can write

$$\begin{aligned} & \Psi_h^{[m,2]} = \sum_{j=1}^k b_j S_{(1-a_j)h}\circ S_{a_jh} \\ = \;& \exp\Big(\frac{1}{2}hY_1\Big)\Big(I+G_{3,1}h^3Y_3+G_{4,1}h^3[Y_1,Y_3]+G_{5,1}h^5Y_5+\bar{G}_{5,2}h^5[Y_1,[Y_1,Y_3]]+\mathcal{O}(h^6)\Big)\exp\Big(\frac{1}{2}hY_1\Big), \end{aligned}$$

(we always assume the consistency condition is satisfied, $\sum_{j=1}^k b_j=1$) and

$$G_{\ell,n}=\sum_{j=1}^k b_j g_{\ell,n}^j$$

where $g_{\ell,n}^j$ denotes $g_{\ell,n}$ when a is replaced by a_j and $\bar{G}_{5,2} = G_{5,2} - \frac{1}{6}G_{3,1}$. Then the 4th-order extrapolation method (2) satisfies

$$G_{3,1} = G_{4,1} = G_{5,2} = 0, \qquad G_{5,1} = \frac{1}{4}.$$

The goal with the new methods is to look for a set of coefficients a_i, b_i such that $G_{5,1} = 0$ is also satisfied, leading to a 5th-order method. Unfortunately, it happens that

$$G_{5,2} = \frac{1}{60} - \frac{1}{12}G_{3,1} + \frac{1}{15}G_{5,1}$$

and $G_{5,2}, G_{3,1}, G_{5,1}$ can not be simultaneously vanished. We considered the scheme (6) that allows to get a method with

$$G_{3,1} = G_{4,1} = G_{5,1} = 0, \qquad G_{5,2} = \frac{1}{60}$$

(we leave two free parameters among the coefficients a_i) that, in general, leads to more accurate results. In addition, we can easily find another set of values for the coefficients b_i with the same values of a_i that lead to a third-order method as an embedded method, i.e. to consider a set of coefficients $\hat{b}_i, 1 = 1, \ldots, k$ such that $\sum_{i=1}^k \hat{b}_i = 1$ and $G_{3,1} = 0$. We have taken one solution, as an illustration, that is not necessarily the optimal one.

Similarly, we have that

$$S_{ah}S_{(1-2a)h}S_{ah} = \exp\Big(hY_1 + f_{3,1}h^3Y_3 + f_{5,1}h^5Y_5 + f_{5,2}h^5[Y_1,[Y_1,Y_3]]\ldots\Big) = \exp\Big(\frac{1}{2}hY_1\Big)$$
$$\Big(I + f_{3,1}h^3Y_3 + f_{5,1}h^5Y_5 + \bar{f}_{5,2}h^5[Y_1,[Y_1,Y_3]] + \frac{1}{2}f_{3,1}^2h^6Y_3^2 + f_{7,1}h^7Y_7 + \mathcal{O}(h^7)\Big)\exp\Big(\frac{1}{2}hY_1\Big),$$

with

$$\begin{array}{ll} f_{3,1} = 2a^3 + (1-2a)^3, & f_{5,1} = 2a^5 + (1-2a)^5, \\ f_{7,1} = 2a^7 + (1-2a)^7, & f_{5,2} = \frac{1}{12}(1-a)(1-2a)a(a^2 - (1-2a)^2). \end{array} \tag{9}$$

If we denote (as previously, $f_{\ell,n}^j$ corresponds to $f_{\ell,n}$ when a is replaced by a_j)

$$F_{\ell,n} = \sum_{j=1}^k b_j f_{\ell,n}^j, \qquad with \qquad F_{6,1} = \sum_{j=1}^k b_j (f_{3,n}^j)^2, \qquad F_{8,1} = \sum_{j=1}^k b_j (f_{3,n}^j f_{5,n}^j)$$

then the 6th-order extrapolation method (5) satisfies

$$F_{3,1} = F_{5,1} = F_{5,2} = F_{6,1} = 0, \qquad F_{7,1} = 0.0277.$$

The scheme $\Psi_h^{[6,3]}$ in (7) has 10 parameters to satisfy the 5 order conditions to reach order six (including consistency). Three processors would suffice to have enough parameters, for example, by taking $b_4 = b_5 = 0$, and there would still have one free parameter. Such free parameter could be used, for example, to vanish $F_{7,1}$ but even in this case the methods we obtain did not show in practice a higher performance that the extrapolation method. We have added two extra processes in order to vanish higher order error contributions as well as to have enough parameters $\hat{b}_i$ to build a 5th-order embedded method that is different from the method itself.

At order seven there are four independent terms, $Y_7, [Y_1,[Y_1,Y_5]], [Y_1,[Y_1,[Y_1,[Y_1,Y_3]]]], [Y_3,[Y_1,Y_3]]$ whose coefficients can not be canceled with linear combinations of this family of 3-map symmetric compositions. Notice that each function $f_{n,i}^j$ is a polynomial function of degree n in the variable a_j, and we can write it as follows

$$f_{n,i}^j = \sum_{\ell=0}^n A_\ell a_j^\ell \qquad so \qquad F_{n,i} = \sum_{j=1}^k b_j f_{n,i}^j = \sum_{\ell=0}^n A_\ell \left(\sum_{j=1}^k b_j a_j^\ell\right)$$

and only n independent conditions $F_{m,i} = 0$ can be satisfied (the same number as independent equations, $\sum_{j=1}^k b_j a_j^\ell = 0, \ell = 1,2,\ldots,n$). This introduces a limit in the highest degree we can reach with the scheme (10), but still allows to choose which conditions at order seven or higher can be convenient to vanish for different classes of problems.

We took a_5 as a free parameter and used the remaining four extra parameters to vanish the coefficients of $Y_7, [Y_1, [Y_1, [Y_1, [Y_1, Y_3]]]]$ at order seven, $Y_3 Y_5$ at order eight and Y_9 at order nine. Different optimisation criterion could be used for different purposes that will depend on each problem with its particular algebra. Once the values a_i are fixed, we took $\hat{b}_1$ as a free parameter and got the remaining coefficients $\hat{b}_i, i = 2, 3, 4, 5$ such that the resulting embedded method satisfies $F_{3,1} = F_{5,1} = F_{5,2} = 0$ in addition to consistency, i.e. it is of order five (instead of four as it happens for extrapolation).

We have shown that this new family of methods can provide highly efficient methods and the next step is to carry a deep analysis of the order conditions and optimisation procedures in order to obtain the most efficient schemes with a moderately low number of processors. Once we have identified the problem to reach methods of order higher than six with the composition (7), it is then natural to consider the more general composition

$$\Psi_h^{[m,3]} = \sum_{j=1}^{k} c_j S_{(1-a_j-b_j)h} S_{b_j h} S_{a_j h}. \tag{10}$$

The number of order conditions increase due to the loss of symmetry of the compositions but there are more free parameters that could circumvent the order barrier we found in the previous symmetric compositions. This long and elaborated analysis will be carried and published elsewhere.

If one is interested in forward integration, we can fix the values of the coefficients a_i, b_i to guarantee forward integration, and then to solve the linear equations with the coefficients c_i (with some few more processors). Methods with complex coefficients as well as preservation of time-symmetry and other qualitative properties to higher orders than the order of the method can also analysed [5].

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