Composition methods in the presence of small parameters

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Abstract

We derive numerical methods for arbitrary small perturbations of exactly solvable differential equations. The methods, based in one instance on Gaussian quadrature, are symplectic if the system is Hamiltonian and are asymptotically more accurate than previously known methods.

1 Introduction

Composition methods are numerical integrators for ordinary differential equations which compose certain elementary flows to build an approximation of high order. For a vector field X with flow $\exp(tX)$ (i.e., $\dot{x} = X(x) \Rightarrow x(t) = \exp(tX)(x(0))$), a popular special case is when X can be split as $X = A + B$ where the vector fields A and B can both be integrated explicitly. The advantage of doing this is that geometric properties of the true flow are easily preserved: if X, A, and B are Hamiltonian then the flow and the method are symplectic; if divergence free, then volume preserving, and so on. It is annoying, however, that these special properties of X are never taken advantage of in deriving the composition. In fact, it is shown in [6] that these methods are equivalent to those formed by composing an *arbitrary* first-order method and its inverse, so it seems that even the fact that one is solving the constituent vector fields A and B exactly is not used.

Here we consider one case in which this information can be used to advantage. Suppose the system is a small perturbation of one that can be solved exactly—i.e., X is near-integrable—and is split accordingly:

$$X = A + \varepsilon B.$$

We now have two small parameters, ε and the time step t. Although for convergence one must take ε fixed and $t \to 0$, in practice ε may be very small and

t is taken as large as one can get away with—such as one does with symplectic integrators in their popular "quick and dirty" mode. In this case it may make sense to preferentially eliminate error terms in ε rather than in t. The primary application we have in mind is to large, weakly-coupled systems, such as weakly nonlinear systems and the solar system [9].

In fact, this work was motivated by that of Saha and Tremaine [7] on symplectic integrators for the solar system. They show that in this case the leading-order frequency errors are eliminated, without changing the method, for certain initial conditions. Our approach, altering the method so as to eliminate these and other errors explicitly, is more general and more robust, although of course the new methods do do slightly more work. A detailed comparison remains to be undertaken. We also encourage the reader to consult the recent work of Wisdom et al. [10], who take a different approach to this same problem.

Take a composition of the flows of A and B and write it as the flow of some vector field:

$$\prod_i \exp(b_i t\varepsilon B)\exp(a_i tA) = \exp(\widehat{X}). \tag{1}$$

By the Baker-Campbell-Hausdorff theorem, $\widehat{X} \in L(\{A, B\})$, the free Lie algebra generated by A and B, and can be expanded as a double asymptotic series in t and ε:

$$\widehat{X} = tp_1 A + \varepsilon t p_2 B + \varepsilon t^2 p_3 [A, B] + \varepsilon t^3 p_4 [A, [A, B]] + \varepsilon^2 t^3 p_5 [B, [B, A]] + \dots$$

where the coefficients p_i are polynomials in the a_i and b_i. (See [6] and references therein for a more detailed discussion of this approach to numerical integration, or [1] for some early work; for background on numerical and symplectic integration, see [4].) In this instance, the Lie bracket $[\cdot, \cdot]$ is the vector field commutator. For a method of order s, one requires $\widehat{X} = t(A + \varepsilon B) + \mathcal{O}(t^{s+1})$. The canonical example is the second-order leapfrog method [11]:

$$\exp\left(\frac{1}{2}tA\right)\exp\left(t\varepsilon B\right)\exp\left(\frac{1}{2}tA\right) = \exp\left(t(A + \varepsilon B) - \frac{1}{24}\varepsilon t^3 [A, A, B]] + \frac{1}{12}\varepsilon^2 t^3 [B, [B, A]] + \dots\right).$$

In general, there are a finite number of terms in $\widehat{X}$ at each order in t, but an infinite number at each order in ε. At order $\varepsilon^j t^s$ there are [6]

$$\frac{1}{s}\sum_{\substack{d|j \\ d|(s-j)}} \frac{(s/d)!}{(j/d)!((s-j)/d)!}$$

independent Lie brackets of A and B, tabulated in the following matrix:

$$
\begin{array}{c} \\ t^2 \\ t^3 \\ t^4 \\ t^5 \\ t^6 \\ t^7 \\ \\ \end{array}
\begin{array}{c}
\begin{array}{cccccc} \varepsilon^1 & \varepsilon^2 & \varepsilon^3 & \varepsilon^4 & \varepsilon^5 & \varepsilon^6 \end{array} \\
\left(\begin{array}{cccccc}
1 & & & & & \\
1 & 1 & & & & \\
1 & 1 & 1 & & & \\
1 & 2 & 2 & 1 & & \\
1 & 2 & 3 & 2 & 1 & \\
1 & 3 & 5 & 5 & 3 & 1 \\
\vdots & & & & & \ddots
\end{array}\right)
\end{array}
\tag{2}
$$

We shall say a method has order $(s_1, s_2, \ldots)$ if $\widehat{X} - t(A + \varepsilon B)$ is of order $\mathcal{O}(\sum \varepsilon^j t^{s_j+1})$. It is only sensible to take $s_{i+1} \leq s_i$. A rational expansion would take $\varepsilon = \mathcal{O}(t^r)$, say, and eliminate error terms up to each total order, implying that the s_i should be taken in arithmetic progression. But since the demand is for the simplest possible methods—the competition from leapfrog is strong—we shall give stick to orders $(2s, 2)$ for each s and orders $(6, 4)$ and $(8, 4)$. To find the number of stages (the number of factors in (1)) needed, one can start by matching the number of determining equations from (2) to the the number of free parameters a_i, b_i in (1); there is still the question, addressed in [5], of whether the suggested number of stages is too large (because some of the determining equations are redundant) or too small (because the nonlinear determining equations have no solution). This is of course the fundamental question addressed by algebraic Runge-Kutta theory [4]. Here the suggested number turns out to be correct for order $(2s, 2)$, showing that there are no redundancies, but too small in one case for order (6,4).

2 Methods of order (2s,2).

First note that if $s_1 \geq 2$ then $s_2 \geq 2$ automatically—the only $\mathcal{O}(t^2)$ term is $[A, B]$, which is eliminated by assumption. More generally, if $s_i \geq i + 1$ then the method is of order $i+1$. It is particularly easy to eliminate errors of order ε because there is only one such term for each order in t, namely, $[A, \ldots, [A, B] \ldots]$ (n A's). For a method of order $(2s, 2)$ these must be eliminated for all $n < 2s$. Consider first a method based on the pattern "ABA," with $A(z)$ abbreviating $\exp(ztA)$, etc:

$$A(a_{m+1})B(b_m)A(a_m)\ldots B(b_1)A(a_1) \tag{3}$$

Counting determining equations and unknowns suggests that solutions should be isolated for $m = s$. We now show that this is the case, and that moreover there is then a unique solution with $a_i,\ b_i > 0$ for all i.

Temporarily set $\varepsilon = 1$ and consider the differential equation $\dot{x} = 1$, $\dot{y} = f(x)$ with $A = \partial_x$ and $B = f(x)\partial_y$. The only nonzero Lie brackets of A and B are $[A, \ldots, [A, B] \ldots] = f^{(n)}(x)\partial_y$ (n A's). So a method of order $(2s, 2)$ for $s \geq 1$ must actually be of order $2s$ when applied to this differential equation. Doing so gives the map $(x_0, y_0) \mapsto (x_{m+1}, y_m)$, where

$$\begin{aligned} x_i &= x_{i-1} + ta_i, & i = 1, \ldots, m+1 \\ y_i &= y_{i-1} + tb_i f(x_i), & i = 1, \ldots, m \end{aligned}$$

or

$$y_m = y_0 + t\sum_{j=1}^{m} b_i f(x_i), \quad x_i = x_0 + tc_i, \quad c_i = \sum_{j=1}^{i} a_i.$$

The exact solution is $x(t) = x_0 + t$, $y(t) = \int_{x_0}^{x_0+t} f(x)\,dx$. So the method is of order $2s$ if and only if $c_{m+1} = 1$ and the c_i are the nodes and b_i the weights of a quadrature formula on $[0,1]$ of order $2s$. This requires $m \geq s$ and there is a unique solution, namely, Gaussian quadrature, if $m = s$.

Because the Lie brackets $[A,\ldots,[A,B]\ldots]$ are independent in this example, there are no further determining equations, and the quadrature determines all possible methods of this form of order $(2s,2)$. The nodes c_i may be taken in any order, however, so that there are in fact $m!$ solutions of the determining equations; we take them in ascending order so that $a_i = c_i - c_{i-1}$ is positive for all i. (It is a standard result that the nodes for Gaussian quadrature all lie in the domain of integration $[0,1]$ and that the weights are all positive.) Furthermore the coefficients are symmetric about $1/2$ so the resulting method $\varphi(t)$ is also symmetric, $\varphi(t) = \varphi^{-1}(-t)$. The nodes c_i are the roots of $P_m((x+1)/2)$, where P_m is the Legendre polynomial of degree m, and the weights b_i are given by $b_i^{-1} = 4c_i(1-c_i)P_m'(2c_i-1)^2$. Only quadratics need to be solved to find these for $m \leq 5$, so we reproduce them in Table 1. Although these coefficients also arise in implicit Gaussian Runge-Kutta, there seems to be no connection between it and the method (3).

If A is more complicated than B then one might also need a method with a "BAB" pattern:

$$B(b_m)A(a_m)\ldots B(b_1)A(a_1)B(b_0)$$

as it has one fewer applications of A. This can be reduced to the previous case by adding a dummy stage on the right with $a_0 = 0$. Once again the $c_i = \sum_{j=1}^{i} a_i$ and the b_i, $0 \leq i \leq m$, are the nodes and weights, respectively, of a quadrature formula. This time it has $m+1$ nodes, two of which are fixed at $c_0 = 0$ (by the dummy stage) and $c_m = 1$ (by consistency). This is Gauss-Lobatto quadrature, so order $(2s,2)$ is achieved with $m = s$. Again there is a unique solution with positive a_i and b_i, and it is symmetric. The nodes c_i, $1 \leq i < m$, are the roots of $P_m'((x+1)/2)$, and the weights are $b_0^{-1} = b_m^{-1} = m(m+1)$, $b_i^{-1} = m(m+1)P_m(2c_i-1)^2$ for $1 \leq i < m$. They can be found by solving quadratics for $m \leq 6$, see Table 1.

We write out the two order $(4,2)$—that is, their global truncation errors are $\varepsilon^2 t^2 X_2 + \varepsilon t^4 X_4 + \ldots$— methods:

$$A\Big(\frac{3-\sqrt{3}}{6}\Big)B\Big(\frac{1}{2}\Big)A\Big(\frac{1}{\sqrt{3}}\Big)B\Big(\frac{1}{2}\Big)A\Big(\frac{3-\sqrt{3}}{6}\Big)$$

and

$$B\Big(\frac{1}{6}\Big)A\Big(\frac{1}{2}\Big)B\Big(\frac{2}{3}\Big)A\Big(\frac{1}{2}\Big)B\Big(\frac{1}{6}\Big).$$

These methods are all of order 2 because of the $\mathcal{O}(\varepsilon^2 t^3)$ term in $[B,[B,A]]$ which is still present in $\widehat{X}$. To make sure that this term has not been degraded while our attention was on order ε, we check its coefficient. This is proportional

to the residual in its determining equation which is related to a quadrature condition as above: for the ABA pattern it is

$$\sum_{j=2}^{m+1} a_i \Big(\sum_{i=1}^{j-1} b_i \Big)^2 = \frac{1}{3}, \tag{4a}$$

and for BAB,

$$\sum_{j=1}^{m} a_i \Big(\sum_{i=1}^{j} b_i \Big)^2 = \frac{1}{3}. \tag{4b}$$

The residuals are given in Table 2. They decrease as m increases, perhaps due to the nice placing of the nodes in Gaussian integration, and if we scale them by $(2m+1)^2$—appropriate for a comparison to leapfrog with time step t/m—are roughly constant. Even if $\varepsilon \sim 1$ these methods are all about 3 times more accurate (at constant work) than leapfrog.

What can we do if the flow $\exp(t\varepsilon bB)$ is not available? Suppose we only have $\widehat{B}(b)$, an arbitrary smooth first-order approximation to $\exp(t\varepsilon bB)$. Then

$$\widehat{B}(b) = \exp(\varepsilon tbB + (\varepsilon tb)^2 B_2 + \ldots)$$

for some vector fields B_i, and

$$\widehat{B}^*(b) \equiv \widehat{B}^{-1}(-b) = \exp(\varepsilon tbB - (\varepsilon tb)^2 B_2 + \ldots).$$

The only new error term affecting the order of the method is that due to B_2. This can be eliminated by replacing each $B(b)$, $B(b)$ pair in (3) by the pair $\widehat{B}(b)$, $\widehat{B}^*(b)$. Unpaired terms, such as the central $B(1)$ in leapfrog, must be split. For example, we have the order (4,2) method

$$\widehat{B}\Big(\frac{1}{6}\Big) A\Big(\frac{1}{2}\Big) \widehat{B}\Big(\frac{1}{3}\Big) \widehat{B}^*\Big(\frac{1}{3}\Big) A\Big(\frac{1}{2}\Big) \widehat{B}^*\Big(\frac{1}{6}\Big).$$

The other new error terms, such as $[A, B_2]$ and B_3, are all of the same or higher order than those already present.

The main application here is if the $\mathcal{O}(\varepsilon)$ terms in the vector field X cannot be integrated explicitly but has to be split further. If $X = A + \varepsilon \sum C_i$, say, then we can use the approximation $\exp(t\varepsilon \sum C_i) \approx \prod \exp(t\varepsilon C_i)$ without further alteration. Unfortunately there seems to be no way to apply the idea of this paper if $\exp(tA)$ is not available.

Instead of progressing term-by-term in t, is it possible to eliminate all errors of order ε at once? One way would be to ask, for which vector field $\widetilde{B}$ does

$$\exp(\varepsilon t\widetilde{B}) \exp(tA) = \exp(t(A + \varepsilon B) + \mathcal{O}(\varepsilon^2))?$$

This is a standard problem in Lie theory; the answer, a variant on the Zassenhaus formula, is

$$\widetilde{B} = \int_0^1 B \circ \exp(-\tau tA)\, d\tau.$$

For a proof we note that this formula is exact for the quadrature problem considered above. But, although the flow of A is available, it seems unlikely that one find both $\widetilde{B}$ and its flow analytically.

Table 1: Coefficients of order $(2s, 2)$ methods

Pattern ABA, $m = s$.

$s = 2$: $a_1 = a_3 = (3 - \sqrt{3})/6$, $a_2 = 1/\sqrt{3}$; $b_1 = b_2 = 1/2$.

$s = 3$: $a_1 = a_4 = 1/2 - a_2$, $a_2 = a_3 = \sqrt{3/20}$; $b_1 = b_3 = 5/18$, $b_2 = 4/9$.

$s = 4$: $a_1 = a_5 = (1 - w_1)/2$, $a_2 = a_4 = (w_1 - a_3)/2$, $a_3 = \sqrt{(15 - 2\sqrt{30})/35}$, $w_1 = \sqrt{(15 + 2\sqrt{30})/35}$; $b_1 = b_4 = (18 - \sqrt{30})/72$, $b_2 = b_3 = (18 + \sqrt{30})/72$.

$s = 5$: $a_1 = a_6 = 1/2 - w_2$, $a_2 = a_5 = w_2 - a_3$, $a_3 = a_4 = \sqrt{5 - \sqrt{40/7}}/6$, $w_2 = \sqrt{5 + \sqrt{40/7}}/6$; $b_1 = b_5 = (322 - 13\sqrt{70})/1800$, $b_2 = b_4 = (322 + 13\sqrt{70})/1800$, $b_3 = 64/225$.

Pattern BAB, $m = s$.

$s = 2$: $a_1 = a_2 = 1/2$; $b_1 = b_3 = 1/6$, $b_2 = 2/3$.

$s = 3$: $a_1 = a_3 = (5 - \sqrt{5})/10$, $a_2 = 1/\sqrt{5}$; $b_1 = b_4 = 1/12$, $b_2 = b_3 = 5/12$.

$s = 4$: $a_1 = a_4 = 1/2 - a_2$, $a_2 = a_3 = \sqrt{3/28}$; $b_1 = b_5 = 1/20$, $b_2 = b_4 = 49/180$, $b_3 = 16/45$.

$s = 5$: $a_1 = a_5 = (1 - w_3)/2$, $a_2 = a_4 = (w_3 - a_3)/2$, $a_3 = \sqrt{(1 - 2/\sqrt{7})/3}$, $w_3 = \sqrt{(1 + 2/\sqrt{7})/3}$; $b_1 = b_6 = 1/30$, $b_2 = b_5 = (14 - \sqrt{7})/60$, $b_3 = b_4 = (14 + \sqrt{7})/60$.

Table 2: Error constants and stability of order $(2s, 2)$ methods

s	Error constant (scaled)		Stability limit		
	ABA	BAB	ABA	BAB	Leapfrog
1	0.1863 (1.677)		2		
2	0.0223 (0.558)	0.0278 (0.694)	2.632	2.449	2.828
3	0.0113 (0.552)	0.0126 (0.619)	2.887	2.931	3
4	0.0068 (0.550)	0.0073 (0.590)	3.010	2.997	3.061
5	0.0045 (0.550)	0.0048 (0.576)	3.051	3.048	3.090

3 Methods of order (6,4) and (8,4).

Probably the above methods will prove the most useful, but we explore the determining equations a little further anyway. To decrease the system size so that it will be amenable to algebraic reduction we consider only symmetric methods. Then only terms of odd order in t need be considered [11]. For order (6,4) we have the quadrature conditions conditions corresponding to $[A,[A,B]]$ and $[A,[A,[A,[A,B]]]]$,

$$\sum_{i=1}^{m} b_i c_i^{q-1} = \frac{1}{q} \quad \text{for } q = 3, 5,$$

together with either (4a) (for ABA) or (4b) (for BAB). Adding $\sum a_i = \sum b_i = 1$ suggests that taking $m = 4$, with five parameters, should be sufficient. Working with c_i instead of a_i is simpler. For type ABA, the three determining equations for b_1, c_1, and c_2 may be algebraically reduced to, among others,

$$\begin{aligned} 71 - 2022\,c_2 + 26286\,c_2^2 - 206040\,c_2^3 + 1080360\,c_2^4 - 3972600\,c_2^5 &+ \\ 10461240\,c_2^6 - 19828800\,c_2^7 + 26827200\,c_2^8 - 25272000\,c_2^9 &+ \\ 15746400\,c_2^{10} - 5832000\,c_2^{11} + 972000\,c_2^{12} &= 0. \end{aligned}$$

But this polynomial has no real roots. We conclude that there are no symmetric, $m = 4$, order $(6,4)$ ABA methods.

For type BAB there are solutions so we give more details. The symmetry assumption and $\sum a_i = \sum b_i = 1$ give $b_4 = b_0$, $b_3 = b_1$, $b_2 = 1 - 2(b_0 + b_1)$, $c_4 = 1$, $c_3 = 1 - c_1$, and $c_2 = 1/2$. This leaves three equations in b_0, b_1, and c_1; solving the two quadrature conditions for b_0 and b_1 and substituting into (4b) gives

$$\begin{aligned} b_0 &= \frac{-10c_1^2 + 10c_1 - 1}{60c_1(1 - c_1)} \\ b_1 &= \frac{1}{60c_1(1 - c_1)(2c_1 - 1)^2} \\ 400c_1^6 &- 1400c_1^5 + 1740c_1^4 - 930c_1^3 + 204c_1^2 - 12c_1 - 1 = 0 \end{aligned}$$

The roots of the last polynomial are $c_1 \approx -0.0438$, $0.2378 \pm 0.0786i$, 0.6275, 1.0264, and 1.4142. Thus there are precisely four symmetric, $m = 4$, order $(6,4)$ BAB methods; they have $(b_1, b_2, b_3, a_1, a_2) =$

$$\begin{array}{lccccc} & (0.531639, & -0.308602, & 0.553927, & -0.043751, & 0.543751), \\ & (0.095365, & 1.09677, & -1.38426, & 0.627487, & -0.127487), \\ & (0.780842, & -0.554037, & 0.546389, & 1.02644, & -0.526438), \\ \text{and} & (0.195117, & -0.008510, & 0.626785, & 1.41423, & -0.914229). \end{array}$$

The first has the smallest maximum and largest minimum coefficients, so we give some more digits for it: $c_1 = -0.043751421917374113 74$.

For higher-order methods the determining equations cannot be reduced to polynomials. For order (8,4) ABA with $m = 5$, eliminating the b_i leaves two polynomials of degree 4 and 9, respectively, in c_1 and c_2; a numerical search found 6 real solutions, of which a good one has $(b_1, b_2, b_3, a_1, a_2, a_3)=$

$(0.19022593937367661925, 0.84652407044352625706, -1.07350001963440575260,$
$0.07534696026989288842, 0.51791685468825678230, -0.09326381495814967072)$.

There is a similar situation for order (8,4) BAB methods: again $m = 5$ is sufficient, and a numerical search found 12 real solutions, of which a good one has $(b_1, b_2, b_3, a_1, a_2, a_3)=$

$(0.81186273854451628884, -0.67748039953216912289, 0.36561766098765283405,$
$-0.00758691311877447385, 0.31721827797316981388, 0.38073727029120931994)$.

So it seems that the nonexistence of a symmetric (6,4) ABA method with $m = 4$ was just a fluke. In the same way we expect that there exist order (8,6,4) methods with $m = 7$ and order (8,8,4) with $m = 10$. But these seem unlikely to be useful.

4 Stability

There is no universal characterisation of stability for composition methods, nor do we have a criterion particularly adapted to our case of $\varepsilon \ll 1$. The simplest case would be when A and B are two noncommuting linear vector fields, say $A = y\partial_x$ and $B = -x\partial_y$—the harmonic oscillator. Its period for $\varepsilon = 1$ is 2π and there is a natural obstacle to stability at $t = \pi$, where the two eigenvalues of $\exp(t(A + B))$, namely, $\exp(\pm it)$, meet at -1. Leapfrog is stable for $t < 2$; the order $(2s, 2)$ methods are all more stable (see Table 2) and are not much worse than obtained with s applications of leapfrog with time step t/s (last column of Table 2). For $\varepsilon \neq 1$ the stability limit is larger by a factor $1/\sqrt{\varepsilon}$, corresponding to the period of the oscillator.

The $m = 4$ order (6,4) BAB method is stable for $t < 2.700$, the $m = 5$ (8,4) BAB for $t < 2.974$, and the $m = 5$ (8,4) ABA, strangely, for $t < 3.350$. In the latter case the eigenvalues briefly reverse direction near $t = 2.5$.

It's nice that the order $(2s, 2)$ methods have all coefficients positive [1]. (This would not be possible for a method of more than second order [3].) If one of $\exp(tA)$ and $\exp(tB)$ (or its approximation $\widehat{B}$) is strongly stable for all t, and the other is weakly stable, then the composition method is unconditionally stable. This follows merely from $\|(\alpha\beta)^n\| \leq \|\alpha^n\|\|\beta\|^n$ where $\|\alpha^n\|$ is bounded and $\|\beta\| < 1$. This makes these methods attractive for slightly dissipative systems; for example, the solution of $\dot{u} = \varepsilon\nabla^2 u$ in n dimensions could be approximated by $\prod_i CN(\varepsilon\partial_{ii}u)$, where CN is Crank-Nicolson. But if both operators are only weakly stable, as would be the best possible in a Hamiltonian system, then stability is not guaranteed, as the example $\alpha = \left(\begin{smallmatrix} 1 & -1 \\ 1 & 0 \end{smallmatrix}\right)$ (with eigenvalues $\frac{1}{2} \pm \frac{\sqrt{3}}{2}i$) and $\beta = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$ (with eigenvalues $\pm i$) shows: $\alpha\beta = \left(\begin{smallmatrix} 1 & 1 \\ 0 & 1 \end{smallmatrix}\right)$ is weakly unstable. In the harmonic oscillator considered above, neither operator is stable by itself.

5 Examples

If a system is only weakly nonlinear, a standard second-order numerical method methods will have global truncation errors of $\mathcal{O}(t^2)$. Solving the linear part exactly in a splitting method reduces the errors to $\mathcal{O}(\varepsilon t^2)$; using the $(2s, 2)$ methods introduced here will lead to errors of $\mathcal{O}(\varepsilon^2 t^2 + \varepsilon t^{2s})$. For small t the error is thus reduced by an extra factor of ε; for large t the error decreases more rapidly, like t^{2s}, the switchover taking place at $t \sim \varepsilon^{1/(2s-2)}$. In general it should pay to use larger s as ε decreases, although of course there is no universal criterion here.

An example is the Boussinesq partial differential equation

$$\begin{aligned} \dot{q} &= p_x \\ \dot{p} &= (q - q_{xx} + q^2)_x \end{aligned}$$

The small parameter is the relative size of the nonlinear and nonlinear terms, roughly $\|q\|$. With periodic boundary conditions and a Fourier spatial truncation the linear part can be solved exactly, so the smaller q is the better the new methods should be.

A generalisation is to any weakly coupled system which can be solved exactly when the coupling is zero, such as the solar system. Here ε is ratio of planetary to solar mass, less than 10^{-3}. At $\varepsilon = 0$ we have a set of decoupled two-body Kepler problems. We expect that these methods, particularly the order $(4, 2)$ BAB one (A involves solving the two-body problem and is slower than B if there are not too many planets [7]) should be very useful in solar system studies. One has the same situation in averaged or model equations: in [8], essentially a symplectic integration based on $\exp(\sum A_i) \approx \prod \exp(A_i)$ (i.e., the time step was implicitly taken as 1), one term was $\mathcal{O}(1)$ and 12 were $\approx 10^{-4}$. This time an ABA method would be advantageous.

We test the methods on a simple Hamiltonian system, the one-degree-of-freedom quartic oscillator with Hamiltonian $H = (p^2 + q^2)/2 - q^4/4$. (This anharmonic oscillator is also studied numerically in [2], but a direct comparison is not possible.) The primary piece A is a harmonic oscillator and the perturbation B is a shear. The small parameter is q^2. The results for the relative energy (action) error are shown in the Figure. We compare leapfrog, three order $(2s, 2)$ BAB methods, and a standard fourth order method, $S(zt)^2 S((1-4z)t) S(zt)^2$, where S is leapfrog and $z = 1/(4 - 4^{1/3})$.

For strong nonlinearities (initial condition $(q, p) = (0.95, 0)$), the new methods are little better. As q decreases the expected dependence on order and ε is borne out: for t small enough, all $(2s, 2)$ methods are roughly equal, and $\mathcal{O}(\varepsilon)$ more accurate than leapfrog; but those with larger s reach this state with less work. Also notice the order (4,2) method for $q = 0.1$: even when its behaviour is $\mathcal{O}(\varepsilon t^4)$, formally the same as the fourth order method, its error is about 50 times smaller. This is because the of "nice" coefficients of the methods based on Gaussian integration as compared to those of higher-order methods.

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Figure. Efficiency of order $(2s, 2)$ methods for the anharmonic oscillator. Five different methods and three initial conditions $(q, 0)$ are compared.