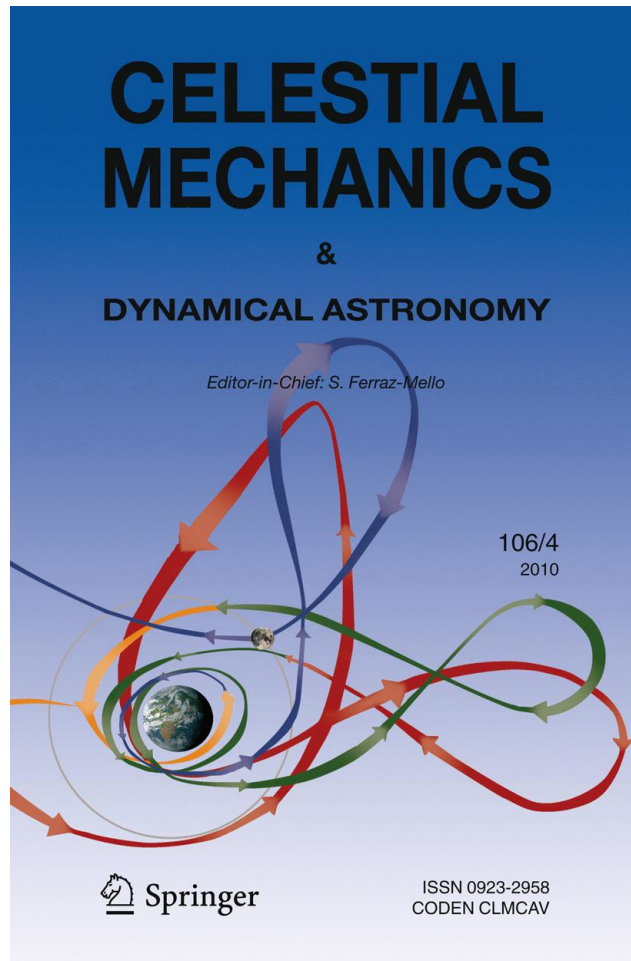


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Multi-product splitting and Runge-Kutta-Nyström integrators

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Abstract The splitting of $e^{h(A+B)}$ into a single product of e^{hA} and e^{hB} results in symplectic integrators when A and B are classical Lie operators. However, at high orders, a single product splitting, with exponentially growing number of operators, is very difficult to derive. This work shows that, if the splitting is generalized to a sum of products, then a simple choice of the basis product reduces the problem to that of extrapolation, with analytically known coefficients and only quadratically growing number of operators. When a multi-product splitting is applied to classical Hamiltonian systems, the resulting algorithm is no longer symplectic but is of the Runge-Kutta-Nyström (RKN) type. Multi-product splitting, in conjunction with a special force-reduction process, explains why at orders $p = 4$ and 6 , RKN integrators only need $p - 1$ force evaluations.

Keywords Runge-Kutta-Nyström integrators · Extrapolated symplectic integrators · Arbitrary high-order integrators

1 Introduction

The approximation of $e^{h(A+B)}$ to any order in h via a single product decomposition

$$e^{h(A+B)} = \prod_i e^{a_i h A} e^{b_i h B} \quad (1)$$

is the basis of the splitting method (McLachlan and Quispel 2002; Hairer et al. 2002; Leimkuhler and Reich 2004) for solving diverse classical (Dragt and Finn 1976; Ruth 1983; Neri 1987; Creutz and Gocksch 1989; Forest and Ruth 1990; Suzuki 1990; Yoshida 1990; Wisdom and Holman 1991; Yoshida 1993), quantum mechanical (Glasner et al. 1991; Bandrauk and Shen 1993; Sanz-Serna and Portillo 1996; Chin and Chen 2001), and stochastic evolution equations (Drozdov and Brey 1998; Forbert and Chin 2001). The resulting

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algorithms are then symplectic, unitary and norm-preserving, respectively. However, at high orders, a single product splitting of the form (1) is very difficult to derive and the number of operators grows exponentially. This is easy to see: the error terms of the decomposition are governed by the fundamental Baker-Campbell-Hausdorff formula,

$$e^{hA}e^{hB} = e^{h(A+B) + \frac{1}{2}h^2[A,B] + \frac{1}{12}h^3([A,[A,B]] - [B,[A,B]]) + \dots} \quad (2)$$

where $[A, B] = AB - BA$ is the commutator bracket. Starting with the first error term $[A, B]$, successive higher order error terms are generated by further commutators of A and B , such as $[A, [A, B]]$, $[B, [A, B]]$, $[A, [A, [A, B]]]$ and $[B, [A, [A, B]]]$, etc. This rapid doubling is moderated somewhat by the Jacobi identity and the special form of operators A and B , but the growth of these error terms is essentially exponential. This implies that high-order symplectic integrators must require many force-evaluations to eliminate these many error terms. For symplectic integrators, the minimum number of force-evaluations necessary at orders 4, 6, 8, 10 has been found empirically to be 3 (Ref. [Creutz and Gocksch 1989](#); [Forest and Ruth 1990](#); [Suzuki 1990](#); [Yoshida 1990](#)), 7 (Ref. [Yoshida 1990](#)), 15 (Ref. [Suzuki and Umeno 1993](#)) and 31 (Ref. [Kahan and Li 1997](#); [Tsitouras 1999](#)), respectively. The doubling trend is clearly visible and seems to be precisely twice plus one.

While symplectic integrators have many desirable conserving properties, such as the exact conservation of Poincaré invariants, they are not immune from the irreversible phase errors ([Kinoshita et al. 1991](#); [Gladman et al. 1991](#); [Chin and Kidwell 2000](#); [Chin 2007a](#)) that directly affects the accuracy of trajectories. Since the accuracy of the trajectory is of paramount importance, regardless of how well some Poincaré invariants are preserved, it is less clear then, given the same number of force-evaluations, that a $2n$ -order symplectic integrator should be preferred over a $2n + 4$ or $2n + 6$ order non-symplectic integrator, even for long-term integrations.

This work shows that if one generalizes the decomposition of $e^{h(A+B)}$ to a sum of products, then for a special choice of the basis product, the problem reduces to that of simple extrapolation and can be solved easily to any even order. When applied to classical Hamiltonian systems, the resulting algorithms are no longer symplectic, but correspond to Runge-Kutta-Nyström (RKN) type integrators. [Blanes et al. \(1999\)](#) and [Blanes and Casas \(2005\)](#) have previously shown that these extrapolated symplectic integrators enjoy better conservation properties than conventional RKN algorithms. Interestingly, multi-product splitting not only reproduces Nyström integrators at orders $p = 4$ and 6 but also explain why they only need $p - 1$ force evaluations. At even higher order, these extrapolated RKN algorithms are surprisingly competitive with symplectic and other RKN integrators found in the literature.

2 Multi-product expansion

If $e^{h(A+B)}$ were to be decomposed into a sum of products

$$e^{h(A+B)} = \sum_k c_k \prod_i e^{a_{k,i}hA} e^{b_{k,i}hB} \quad (3)$$

then there is tremendous freedom in the choice of $\{c_k, a_{k,i}, b_{k,i}\}$. However, for the most general of applications, including solving time-irreversible diffusion type equations ([Drozdov and Brey 1998](#); [Forbert and Chin 2001](#)), one must keep the coefficients $\{a_{k,i}, b_{k,i}\}$ positive. This crucial and deliberate choice distinguishes this work from previous extrapolations, which made no distinction between solving time-reversible and time-irreversible problems.

If $\{a_{k,i}, b_{k,i}\}$ were to be positive, then by Sheng's theorem (1989), any such individual product can at most be second order and some coefficients c_k must be negative. Thus without loss of generality, one can choose the simplest basis product as either one of the following symmetric second-order splittings

$$\mathcal{T}_2(h) = e^{\frac{1}{2}hB} e^{hA} e^{\frac{1}{2}hB} \tag{4}$$

or

$$\mathcal{T}_2(h) = e^{\frac{1}{2}hA} e^{hB} e^{\frac{1}{2}hA}. \tag{5}$$

The choice of a symmetric product is important, because it has only odd powers of h ,

$$\mathcal{T}_2(h) = \exp(h(A + B) + h^3 E_3 + h^5 E_5 + \dots) \tag{6}$$

where E_i are higher order error commutators of A and B . It then follows that the k th power of \mathcal{T}_2 at step size h/k is exactly given by

$$\mathcal{T}_2^k\left(\frac{h}{k}\right) = \exp(h(A + B) + k^{-2}h^3 E_3 + k^{-4}h^5 E_5 + \dots). \tag{7}$$

Thus the set of powers $\mathcal{T}_2^k(h/k)$ has well known error structure and forms a suitable basis for expanding $e^{h(A+B)}$. For example, any two terms with $k = l$ and $k = m$ can approximate $e^{h(A+B)}$ to fourth-order via

$$e^{h(A+B)} = c_l \mathcal{T}_2^l\left(\frac{h}{l}\right) + c_m \mathcal{T}_2^m\left(\frac{h}{m}\right) + e_5(h^5 E_5) \tag{8}$$

with obvious solutions

$$c_l = \frac{l^2}{l^2 - m^2} \quad c_m = \frac{m^2}{m^2 - l^2} \tag{9}$$

and error coefficient

$$e_5 = -\frac{1}{l^2 m^2}. \tag{10}$$

The RHS of (8) can also be written as

$$\mathcal{T}_2^l\left(\frac{h}{l}\right) + \frac{1}{(l/m)^2 - 1} \left[\mathcal{T}_2^l\left(\frac{h}{l}\right) - \mathcal{T}_2^m\left(\frac{h}{m}\right) \right] \tag{11}$$

which coincide with the diagonal elements of the Richardson-Aitken-Neville extrapolation (Hairer et al. 1993) table. Here, we do not do the extrapolation numerically, instead, we give an analytical formula for extrapolating to any even order. More generally, for a given set of n distinct whole numbers $\{k_1, k_2, \dots, k_n\}$, one can form a $2n$ -order approximation of $e^{h(A+B)}$ via

$$e^{h(A+B)} = \sum_{i=1}^n c_i \mathcal{T}_2^{k_i}\left(\frac{h}{k_i}\right) + e_{2n+1}(h^{2n+1} E_{2n+1}). \tag{12}$$

The expansion coefficients c_i are determined by a specially simple Vandermonde equation,

$$\begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ k_1^{-2} & k_2^{-2} & k_3^{-2} & \dots & k_n^{-2} \\ k_1^{-4} & k_2^{-4} & k_3^{-4} & \dots & k_n^{-4} \\ \dots & \dots & \dots & \dots & \dots \\ k_1^{-2(n-1)} & k_2^{-2(n-1)} & k_3^{-2(n-1)} & \dots & k_n^{-2(n-1)} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \dots \\ c_n \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \dots \\ 0 \end{pmatrix} \tag{13}$$

with *closed form* solutions

$$c_i = \prod_{j=1(\neq i)}^n \frac{k_i^2}{k_i^2 - k_j^2} \tag{14}$$

and error coefficient,

$$e_{2n+1} = (-1)^{n-1} \prod_{i=1}^n \frac{1}{k_i^2}. \tag{15}$$

The closed forms (14) and (15) are the key results of this multi-product expansion. All error terms of the same order, rather than be forced to zero individually, are extrapolated to zero simultaneously. The Vandermonde equation (13) is a special case of extrapolated symplectic algorithms considered by [Blanes et al. \(1999\)](#). However, they did not obtain the exact solution given by (14). The proof that (14) is the exact solution is given in ‘‘Appendix A’’. According to [Blanes et al. \(1999\)](#), this class of extrapolated integrator is symplectic to order $2n + 3$, which at higher orders, can easily exceed one’s machine precision. That is, at sufficiently high orders, these extrapolated symplectic algorithms are, up to machine precision, indistinguishable from truly symplectic algorithms.

Since a $2n$ -order expansion is completely characterized by a set of n whole numbers $\{k_1, k_2, \dots, k_n\}$, the resulting algorithm will be referred to as the $\{k_1, k_2, \dots, k_n\}$ -integrator. The error coefficient (15) implies that, if the number of application of \mathcal{T}_2 is fixed,

$$\sum_{i=1}^n k_i = K \tag{16}$$

then the optimal algorithm with the least error is given by a set of n distinct whole numbers $\{k_i\}$ closest to $\text{INT}(K/n)$ satisfying (16). On the other hand, at order $2n$, the minimum number of \mathcal{T}_2 required is given by the natural sequence $\{k_i\} = \{1, 2, 3 \dots n\}$, corresponding to approximating $e^{h(A+B)}$ via

$$e^{h(A+B)} = \sum_{k=1}^n c_k \mathcal{T}_2^k \left(\frac{h}{k} \right) + e_{2n+1} (h^{2n+1} E_{2n+1}) \tag{17}$$

with $n(n + 1)/2$ applications of \mathcal{T}_2 and an error coefficient of

$$e_{2n+1} = (-1)^{n-1} \frac{1}{(n!)^2}. \tag{18}$$

The simplicity of these results make multi-product splitting algorithms extremely easy to analyze and implement.

From (14), the minimum- \mathcal{T}_2 expansions of orders four to ten are given by

$$\mathcal{T}_4(h) = -\frac{1}{3} \mathcal{T}_2(h) + \frac{4}{3} \mathcal{T}_2^2 \left(\frac{h}{2} \right) \tag{19}$$

$$\mathcal{T}_6(h) = \frac{1}{24} \mathcal{T}_2(h) - \frac{16}{15} \mathcal{T}_2^2 \left(\frac{h}{2} \right) + \frac{81}{40} \mathcal{T}_2^3 \left(\frac{h}{3} \right) \tag{20}$$

$$\mathcal{T}_8(h) = -\frac{1}{360} \mathcal{T}_2(h) + \frac{16}{45} \mathcal{T}_2^2 \left(\frac{h}{2} \right) - \frac{729}{280} \mathcal{T}_2^3 \left(\frac{h}{3} \right) + \frac{1024}{315} \mathcal{T}_2^4 \left(\frac{h}{4} \right) \tag{21}$$

$$\begin{aligned} \mathcal{T}_{10}(h) = & \frac{1}{8640} \mathcal{T}_2(h) - \frac{64}{945} \mathcal{T}_2^2\left(\frac{h}{2}\right) + \frac{6561}{4480} \mathcal{T}_2^3\left(\frac{h}{3}\right) \\ & - \frac{16384}{2835} \mathcal{T}_2^4\left(\frac{h}{4}\right) + \frac{390625}{72576} \mathcal{T}_2^5\left(\frac{h}{5}\right). \end{aligned} \quad (22)$$

In contrast to a single product decomposition, whose coefficients $\{a_i, b_i\}$ are generally irrational and must be determined order-by-order numerically with limited precision, the multi-product expansion has only rational coefficients and are given analytically by (14) for all even orders.

The operator extrapolation here is at once more general and simpler than extrapolating solutions of differential equations. First, in the extrapolation of solutions, Gragg (1965) has to first prove that the second-order solution has the error structure (6). In terms of operators (4) and (5), the error structure (6) is a trivial consequence of the symmetric form \mathcal{T}_2 and is the same for any evolution equation with two non-commuting operators. (The left-right symmetric operator form implies time-symmetric integrators. Presumably, any time-symmetric integrators, thought not symplectic, must also have odd order errors and can be extrapolated to higher order according to (12). However, as noted by Blanes et al. (1999) only in extrapolating a $2n$ -order symplectic integrator, can one preserve symplecticity to order $4n + 1$.) Second, the expansion, or extrapolation coefficient c_i , has never been explicitly given before. This is of enormous utility. A simple routine can be written to compute all c_i as a function of n and automatically produces integrator of order $2n$ by repeating calling \mathcal{T}_2 as a sub-routine. The working of a 100th-order algorithm has been recently demonstrated (Chin and Geiser unpublished). Also, as will be shown in the next section, knowing c_i allows fourth- and sixth-order RKN algorithms to be derived as extrapolated symplectic integrators. The simplest fourth-order operator extrapolation (19) is well known and has been used previously (Schmidt and Lee 1995; Schatzman 2002) in different contexts.

3 Deriving RKN integrators

As emphasized in the last section, the multi-product expansion (17) is an extrapolated operator approximation to the evolution operator $e^{h(A+B)}$ and can be applied to many different types of equations. Its applications to quantum (Chin et al. 2009) and stochastic (Zillich et al. 2010) evolution equations have already been proven to be highly successful. Here, we will concentrate on its use in solving classical dynamic problems.

If $e^{h(A+B)}$ is decomposed into a sum of products as in (17), then the resulting algorithm will no longer be symplectic. This is because for more than one product, cross terms will spoil the usual proof of symplecticity (See Ref. Dragt and Finn 1976, Theorem 1). As we will show, multi-product splitting now produces RKN type integrators.

For solving Hamilton's equation in the form,

$$\frac{d\mathbf{q}}{dt} = \mathbf{v} \quad \frac{d\mathbf{v}}{dt} = \mathbf{a}(\mathbf{q}) \quad (23)$$

the operators are

$$A = \sum_i v_i \frac{d}{dq_i} \quad B = \sum_i a_i(\mathbf{q}) \frac{d}{dv_i} \quad (24)$$

and where we have abbreviated $\mathbf{v} = \mathbf{p}/m$ and $\mathbf{a}(\mathbf{q}) = \mathbf{F}(\mathbf{q})/m$. Thus (4) corresponds to the velocity-form of the Verlet algorithm (VV):

$$\begin{aligned} \mathbf{v}_1 &= \mathbf{v}_0 + \frac{h}{2} \mathbf{a}(\mathbf{q}_0) \\ \mathbf{q}_1 &= \mathbf{q}_0 + h \mathbf{v}_1 \\ \mathbf{v}_2 &= \mathbf{v}_1 + \frac{h}{2} \mathbf{a}(\mathbf{q}_1) \end{aligned} \tag{25}$$

and (5) corresponds to the position-form of the Verlet algorithm (PV):

$$\begin{aligned} \mathbf{q}_1 &= \mathbf{q}_0 + \frac{h}{2} \mathbf{v}_0 \\ \mathbf{v}_1 &= \mathbf{v}_0 + h \mathbf{a}(\mathbf{q}_1) \\ \mathbf{q}_2 &= \mathbf{q}_1 + \frac{h}{2} \mathbf{v}_1. \end{aligned} \tag{26}$$

The last numbered variables are the updated variables. Both VV and PV are second order symplectic integrators. The operator $\mathcal{T}_2^k(h/k)$ simply iterates either algorithm k times at step size h/k and is therefore, also symplectic. The PV algorithm uses only one force evaluation per update. If \mathcal{T}_2 is taken to be PV, then the extrapolated integrators of order $2n$, as exemplified by (19)–(22), only require $n(n + 1)/2$ force-evaluations. The minimal integrator of orders 4, 6, 8 and 10 requires only 3, 6, 10, and 15 force evaluations, respectively.

If \mathcal{T}_2 is taken to the VV algorithm, since all products use the same starting force, each $\mathcal{T}_2^k(h/k)$ for $k > 2$ also uses only k force-evaluations. However, $\mathcal{T}_2(h)$ must then evaluate the initial force for the rest of the product and its own final force. Thus $\mathcal{T}_2(h)$ requires two force-evaluations, giving the final force count as $n(n + 1)/2 + 1$.

There are other possible extrapolation methods, such as

$$\mathcal{T}_6(h) = -\frac{1}{15} \mathcal{T}_4(h) + \frac{16}{15} \mathcal{T}_4^2\left(\frac{h}{2}\right) \tag{27}$$

which is similar to the triplet concatenation for symplectic integrators (Creutz and Gocksch 1989; Forest and Ruth 1990; Suzuki 1990; Yoshida 1990). However, such an iterative extrapolation, which triples the number of force-evaluations in going from order $2n$ to $2n + 2$, is not competitive with (17)'s linear increase of only $n + 1$ additional force-evaluations.

To see how the expansion (17) results in RKN integrators, let's takes \mathcal{T}_2 to be VV, then the extrapolation (19) produces the following fourth-order, {1, 2}-integrator

$$\begin{aligned} \mathbf{q} &= \mathbf{q}_0 + h \mathbf{v}_0 + \frac{h^2}{6} (\mathbf{a}_0 + 2\mathbf{a}_{1/2}) \\ \mathbf{v} &= \mathbf{v}_0 + \frac{h}{6} (\mathbf{a}_0 + 4\mathbf{a}_{1/2} + 2\mathbf{a}_{2/2} - \mathbf{a}_{1/1}) \end{aligned} \tag{28}$$

where we have systematically denoted the force evaluation point of $\mathcal{T}_2^k(h/k)$ at the intermediate step $(i/k)h$ as $\mathbf{q}_{i/k}$ and the resulting force as $\mathbf{a}_{i/k} = \mathbf{a}(\mathbf{q}_{i/k})$, with $\mathbf{a}_0 = \mathbf{a}(\mathbf{q}_0)$. The final force evaluation point of $\mathcal{T}_2(h)$, the midpoint of $\mathcal{T}_2^2(h/2)$, and the final position of $\mathcal{T}_2^2(h/2)$ are given by

$$\begin{aligned}
 \mathbf{q}_{1/1} &= \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{2}\mathbf{a}_0 \\
 \mathbf{q}_{1/2} &= \mathbf{q}_0 + \frac{h}{2}\mathbf{v}_0 + \frac{h^2}{8}\mathbf{a}_0 \\
 \mathbf{q}_{2/2} &= \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{4}(\mathbf{a}_0 + \mathbf{a}_{1/2}).
 \end{aligned} \tag{29}$$

The resulting integrator (28) appears to require four force-evaluations, in accordance with the formula $n(n+1)/2+1$. However, a key observation here is that force subtractions at the *same time step* can be combined into a single force evaluation. Let

$$\delta\mathbf{q}_2 = \mathbf{q}_{2/2} - \mathbf{q}_{1/1} = \frac{h^2}{4}(\mathbf{a}_{1/2} - \mathbf{a}_0) \approx O(h^3) \tag{30}$$

then the subtraction of two forces gives,

$$2\mathbf{a}_{2/2} - \mathbf{a}_{1/1} = 2\mathbf{a}(\mathbf{q}_{1/1} + \delta\mathbf{q}_2) - \mathbf{a}(\mathbf{q}_{1/1}) \tag{31}$$

$$\begin{aligned}
 &= \mathbf{a}(\mathbf{q}_{1/1} + 2\delta\mathbf{q}_2) + O(h^6) \\
 &= \mathbf{a}\left(\mathbf{q}_0 + h\mathbf{v}_0 + \frac{1}{2}h^2\mathbf{a}_{1/2}\right) + O(h^6).
 \end{aligned} \tag{32}$$

The total number of force evaluations is reduced from four to three and (28) reproduces Nyström's original fourth-order integrator (Nyström 1925; Battin 1999). Thus we have shown analytically that, the subtraction of two *symplectic* integrators reproduces Nyström's original integrator. This connection between extrapolated symplectic integrators and Nyström's integrators has not been appreciated previously.

If $T_2(h)$ is taken to be PV, the corresponding {1, 2}-integrator with three force-evaluations is given by

$$\begin{aligned}
 \mathbf{x} &= \mathbf{x}_0 + h\mathbf{v}_0 + \frac{h^2}{6}(3\mathbf{a}_{1/4} - \mathbf{a}_{1/2} + \mathbf{a}_{3/4}) \\
 \mathbf{v} &= \mathbf{v}_0 + \frac{h}{3}(2\mathbf{a}_{1/4} - \mathbf{a}_{1/2} + 2\mathbf{a}_{3/4}).
 \end{aligned} \tag{33}$$

Since PV and VV based algorithms have different force-evaluation points, to avoid confusion, we will denote the positions of PV-based integrator as $\mathbf{x}_{i/k}$. Here, the force-evaluation points are

$$\begin{aligned}
 \mathbf{x}_{1/4} &= \mathbf{x}_0 + \frac{h}{4}\mathbf{v}_0 \\
 \mathbf{x}_{1/2} &= \mathbf{x}_0 + \frac{h}{2}\mathbf{v}_0 \\
 \mathbf{x}_{3/4} &= \mathbf{x}_0 + \frac{3}{4}h\mathbf{v}_0 + \frac{h^2}{4}\mathbf{a}_{1/4}.
 \end{aligned} \tag{34}$$

All such PV-based integrators are non-FSAL (First Step As Last) RKN integrators in that the force is never evaluated initially. The explicit force subtraction will be more susceptible to round-off errors. However, this fourth-order integrator is superior to the Nyström integrator when solving Kepler's orbit and concerns for round-off errors are moderated by the wide use of quadruple and multi-precision packages.

To compare the long time integration error of numerical algorithms, it is useful to solve Kepler's orbit in two dimension,

$$a_x = -\frac{q_x}{q^3} \quad a_y = -\frac{q_y}{q^3} \quad q = \sqrt{q_x^2 + q_y^2} \tag{35}$$

with initial conditions

$$v_x = 0 \quad v_y = \sqrt{\frac{1-e}{1+e}} \quad q_x = 1+e \quad q_y = 0 \tag{36}$$

where e is the eccentricity of the orbit. The resulting energy and period are, respectively, $-1/2$ and 2π . This set of initial conditions is chosen (instead of the usual one in the literature) because it is non-singular as $e \rightarrow 1$ and the orbit's semi-major axis is always along the x-axis for all values of e . Both are useful for computing the precession error of Kepler's orbit at high eccentricity.

To gauge the accuracy of the trajectory intrinsically, without any external comparison, we monitor the irreversible phase error (Kinoshita et al. 1991; Gladman et al. 1991) by computing the rotation angle per period, $\Delta\theta$, of the Laplace-Runge-Lenz (LRL) vector (Chin and Kidwell 2000; Chin 2007a):

$$\mathbf{A} = \mathbf{v} \times \mathbf{L} - \frac{\mathbf{q}}{q} \tag{37}$$

with $\mathbf{L} = \mathbf{q} \times \mathbf{v}$. If the orbit is exact, then the LRL vector would remain constant pointing along the semi-major axis of the orbit. If $\Delta\theta \neq 0$, then the orbit will have precessed an angle of $\Delta\theta$ after each period. (This is the advance of the perihelion of solar planets.) Thus $\Delta\theta$ is a much more direct measure of the trajectory's accuracy than the energy error. This precession error grows linearly with time as $m\Delta\theta$, where m is the number of periods, even for symplectic integrators (Kinoshita et al. 1991; Gladman et al. 1991). The corresponding precession error coefficient is extracted by dividing $\Delta\theta$ by h^4 using smaller and smaller h until

$$\lim_{h \rightarrow 0} \frac{\Delta\theta}{h^4} = e_P \tag{38}$$

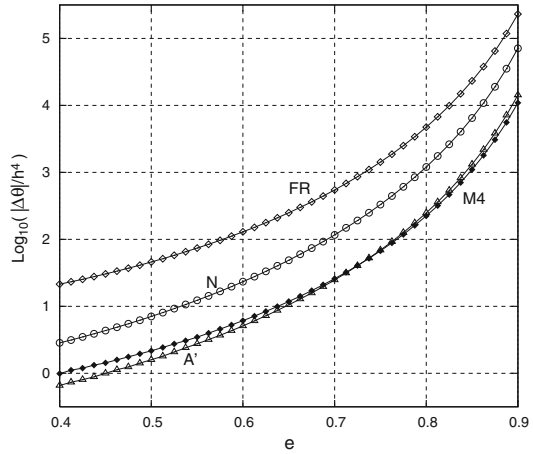
is independent of h . The coefficient e_P as a function of the eccentricity is therefore, a unique error signature of each fourth-order integrator independent of the step size.

In Fig. 1, we compare the precession error coefficient of four distinct fourth-order integrators with only three force evaluations. The symplectic Forest-Ruth (FR) integrator (Forest and Ruth 1990), the forward integrator A' (Omelyan 2006; Chin 2007b), the Nyström integrator (N) given by (28), (32) and the minimal fourth-order {1, 2}-integrator M4, given by (33). The forward integrator A' has only positive splitting coefficients a_i and b_i . The convergence of (38) is seen near $h = 2\pi/3000$; the final value used is $h = 2\pi/5000$. The coefficient e_P grows steeply with e , by four orders of magnitude from $e = 0.4$ to $e = 0.9$, but all integrators showed similar dependence on e . It is well known that the precession error of the symplectic FR integrator is greater than that of RKN algorithms (Kinoshita et al. 1991; Gladman et al. 1991) such as N, but it was not known previously that M4 is so much better than FR and N. The error coefficient e_P at $e = 0.9$ for FR, N, A' and M4 are -23.1×10^4 , 7.1×10^4 , -1.4×10^4 and -1.1×10^4 , respectively.

4 Sixth order RKN integrators

If $T_2(h)$ is taken to be VV, the difference between the two force evaluation points at the same intermediate time step, such as (30), is always of order $O(h^3)$ and the resulting force

Fig. 1 The orbital precession error coefficient as a function of the eccentricity e of the Kepler orbit for four fourth-order integrators which use only three force evaluations per update. FR is the Forest-Ruth symplectic integrator, N is the original Nyström integrator, A' is a forward integrator and M4 is the multi-product splitting integrator (33)



subtraction, such as (32), is of order $O(h^6)$. This immediately suggests that the three final force evaluations in the {1, 2, 3}-integrator can be collapsed into one, yielding a sixth order algorithm with only five force-evaluations. This is indeed the case. The {1, 2, 3}-integrator, according to (20), is given by

$$\mathbf{q} = \mathbf{q}_0 + h \mathbf{v}_0 + \frac{h^2}{120} (11\mathbf{a}_0 + 54\mathbf{a}_{1/3} - 32\mathbf{a}_{1/2} + 27\mathbf{a}_{2/3}), \tag{39}$$

$$\mathbf{v} = \mathbf{v}_0 + \frac{h}{240} (22\mathbf{a}_0 + 162\mathbf{a}_{1/3} - 128\mathbf{a}_{1/2} + 162\mathbf{a}_{2/3} + 81\mathbf{a}_{3/3} - 64\mathbf{a}_{2/2} + 5\mathbf{a}_{1/1}), \tag{40}$$

with three additional force evaluations at:

$$\mathbf{q}_{1/3} = \mathbf{q}_0 + \frac{h}{3}\mathbf{v}_0 + \frac{h^2}{18}\mathbf{a}_0, \tag{41}$$

$$\mathbf{q}_{2/3} = \mathbf{q}_0 + \frac{2}{3}h\mathbf{v}_0 + \frac{h^2}{9}(\mathbf{a}_0 + \mathbf{a}_{1/3}), \tag{42}$$

$$\mathbf{q}_{3/3} = \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{18}(3\mathbf{a}_0 + 4\mathbf{a}_{1/3} + 2\mathbf{a}_{2/3}). \tag{43}$$

Let

$$\delta\mathbf{q}_3 = \mathbf{q}_{3/3} - \mathbf{q}_{1/1} = \frac{1}{9}h^2(2\mathbf{a}_{1/3} + \mathbf{a}_{2/3} - 3\mathbf{a}_0) \approx O(h^3), \tag{44}$$

then the three final-step force-evaluations can be collapsed into one,

$$81\mathbf{a}_{3/3} - 64\mathbf{a}_{2/2} + 5\mathbf{a}_{1/1} = 22\mathbf{a}(\tilde{\mathbf{q}}_1) + O(h^6), \tag{45}$$

with

$$\begin{aligned} \tilde{\mathbf{q}}_1 &= \mathbf{q}_{1/1} + \frac{1}{22}(81\delta\mathbf{q}_3 - 64\delta\mathbf{q}_2) \\ &= \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{22}(18\mathbf{a}_{1/3} - 16\mathbf{a}_{1/2} + 9\mathbf{a}_{2/3}). \end{aligned} \tag{46}$$

The force consolidation (45) now renders (40) symmetric,

$$\mathbf{v} = \mathbf{v}_0 + \frac{h}{240} (22\mathbf{a}_0 + 162\mathbf{a}_{1/3} - 128\mathbf{a}_{1/2} + 162\mathbf{a}_{2/3} + 22\tilde{\mathbf{a}}_1). \tag{47}$$

This sixth order integrator seems not to be known prior to this work. The well known sixth order integrator with five force evaluations due to Albrecht (1955), can be derived from an alternative expansion,

$$\mathcal{T}_6(h) = \frac{1}{45}\mathcal{T}_2(h) - \frac{4}{9}\mathcal{T}_2^2\left(\frac{h}{2}\right) + \frac{64}{45}\mathcal{T}_2^4\left(\frac{h}{4}\right), \tag{48}$$

corresponding to the integrator {1, 2, 4},

$$\mathbf{q} = \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{90} (7\mathbf{a}_0 + 24\mathbf{a}_{1/4} + 16\mathbf{a}_{2/4} - 10\mathbf{a}_{1/2} + 8\mathbf{a}_{3/4}), \tag{49}$$

$$\mathbf{v} = \mathbf{v}_0 + \frac{h}{90} (7\mathbf{a}_0 + 32\mathbf{a}_{1/4} + 32\mathbf{a}_{2/4} - 20\mathbf{a}_{1/2} + 32\mathbf{a}_{3/4} + 16\mathbf{a}_{4/4} - 10\mathbf{a}_{2/2} + \mathbf{a}_{1/1}), \tag{50}$$

with four additional force evaluations at

$$\mathbf{q}_{1/4} = \mathbf{q}_0 + \frac{h}{4}\mathbf{v}_0 + \frac{h^2}{32}\mathbf{a}_0, \tag{51}$$

$$\mathbf{q}_{2/4} = \mathbf{q}_0 + \frac{h}{2}\mathbf{v}_0 + \frac{h^2}{16}(\mathbf{a}_0 + \mathbf{a}_{1/4}), \tag{52}$$

$$\mathbf{q}_{3/4} = \mathbf{q}_0 + \frac{3}{4}h\mathbf{v}_0 + \frac{h^2}{32}(3\mathbf{a}_0 + 4\mathbf{a}_{1/4} + 2\mathbf{a}_{2/4}), \tag{53}$$

$$\mathbf{q}_{4/4} = \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{16}(2\mathbf{a}_0 + 3\mathbf{a}_{1/4} + 2\mathbf{a}_{2/4} + \mathbf{a}_{3/4}). \tag{54}$$

This algorithm nominally requires eight force evaluations, but forces can now be collapsed at $h/2$ and at h . At $h/2$, one has

$$16\mathbf{a}_{2/4} - 10\mathbf{a}_{1/2} = 6\mathbf{a}(\mathbf{q}_{1/2}^*) + O(h^6), \tag{55}$$

where the new half time-step evaluation point is

$$\mathbf{q}_{1/2}^* = \mathbf{q}_0 + \frac{h}{2}\mathbf{v}_0 + \frac{h^2}{24}(4\mathbf{a}_{1/4} - \mathbf{a}_0). \tag{56}$$

Similarly, the three force evaluations at h can be collapsed into one,

$$16\mathbf{a}_{4/4} - 10\mathbf{a}_{2/2} + \mathbf{a}_{1/1} = 7\mathbf{a}(\mathbf{q}_1^\dagger) + O(h^6), \tag{57}$$

where

$$\mathbf{q}_1^\dagger = \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{14}(6\mathbf{a}_{1/4} + 4\mathbf{a}_{2/4} - 5\mathbf{a}_{1/2} + 2\mathbf{a}_{3/4}). \tag{58}$$

The number of force-evaluations can be reduced from eight to five if both $\mathbf{q}_{2/4}$ and $\mathbf{q}_{1/2}$ can be replaced everywhere by $\mathbf{q}_{1/2}^*$. However, replacing $\mathbf{a}_{2/4}$ in $\mathbf{q}_{3/4}$ by $\mathbf{a}_{1/2}^*$, would yield

$$\begin{aligned}\mathbf{q}_{3/4}^* &= \mathbf{q}_0 + \frac{3}{4}h\mathbf{v}_0 + \frac{h^2}{32} \left(3\mathbf{a}_0 + 4\mathbf{a}_{1/4} + 2\mathbf{a}_{1/2}^* \right) \\ &= \mathbf{q}_{3/4} + \frac{h^2}{16} \left(\mathbf{a}_{1/2}^* - \mathbf{a}_{2/4} \right) \\ &= \mathbf{q}_{3/4} + O(h^5),\end{aligned}\quad (59)$$

and the resulting $32\mathbf{a}_{3/4}^*$ term in (50) would produce an error of $O(h^6)$, spoiling the algorithm. Remarkably, replacing $\mathbf{q}_{2/4}$ and $\mathbf{q}_{1/2}$ everywhere by $\mathbf{q}_{1/2}^*$ in (58) defines

$$\begin{aligned}\mathbf{q}_1^* &= \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{14} \left(6\mathbf{a}_{1/4} - \mathbf{a}_{1/2}^* + 2\mathbf{a}_{3/4}^* \right) \\ &= \mathbf{q}_1^\dagger - \frac{h^2}{14} \left(\mathbf{a}_{1/2}^* + 4\mathbf{a}_{2/4} - 5\mathbf{a}_{1/2} \right), \\ &= \mathbf{q}_1^\dagger + O(h^5),\end{aligned}\quad (60)$$

and the resulting $O(h^6)$ error of $7\mathbf{a}_1^*$ in (50) exactly cancels that of $32\mathbf{a}_{3/4}^*$! Thus, one recovers Albrecht's integrator:

$$\mathbf{q} = \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{90} \left(7\mathbf{a}_0 + 24\mathbf{a}_{1/4} + 6\mathbf{a}_{1/2}^* + 8\mathbf{a}_{3/4}^* \right) + O(h^7) \quad (61)$$

$$\mathbf{v} = \mathbf{v}_0 + \frac{h}{90} \left(7\mathbf{a}_0 + 32\mathbf{a}_{1/4} + 12\mathbf{a}_{1/2}^* + 32\mathbf{a}_{3/4}^* + 7\mathbf{a}_1^* \right) + O(h^7). \quad (62)$$

Within the context of multi-product expansion, these are the only two sixth-order integrators possible with only five force evaluations. Again, we have shown analytically that the extrapolation of three second-order symplectic integrators produces sixth-order RKN integrators.

To compare integrators of the same order but with different number of force evaluations, we compute the precession error $\Delta\theta$ at $e = 0.9$ as a function of N , the number of force-evaluations used. The results for four sixth-order algorithms are shown in Fig. 2. Y6 is Yoshida's symplectic algorithm (Yoshida 1990) with the minimum 7 force evaluations. KL6 is a much improved version by Kahan and Li (1997) with 9 force evaluations. A6 and M6 are Albrecht's and the PV-based, minimal {1,2,3}-integrator with 5 and 6 force-evaluations, respectively. While KL6's error is only half of Y6's at 10^5 force-evaluations, their respective error are nearly 50 and 100 times larger than those of RKN integrators A6 and M6. This calculation was carried out in quadruple-precision using the widely available free software by Miller (2002).

5 Higher order comparisons

Since the force reduction process considered is only of $O(h^6)$, this process will no longer be effective for integrators beyond sixth-order. Thus beyond sixth-order, some other force reduction processes must be found if the number of force-evaluation is to be less than $n(n+1)/2$. At higher orders, since the expansion coefficients (14) are known explicitly, it is trivial to write a subroutine for (27) and simply call it according the multi-product expansion (17). Alternatively, one can also construct them from the Aitken-Neville table (Hairer et al. 1993), as done conventionally. It is of interest to compare these extrapolated RKN integrators at high orders with existing symplectic and specially derived RKN integrators found in the literature.

Fig. 2 The orbital precession error of sixth-order integrators as a function of the number of force evaluation N . Y6, KL6 and A6 are integrator of Yoshida, Kahan-Li and Albrecht, respectively. M6 is the minimal extrapolated integrator corresponding to (20)

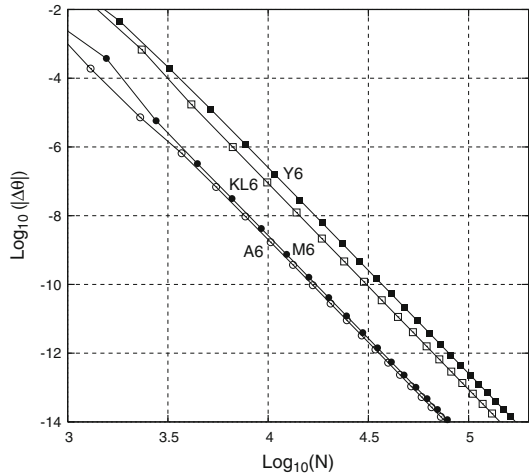
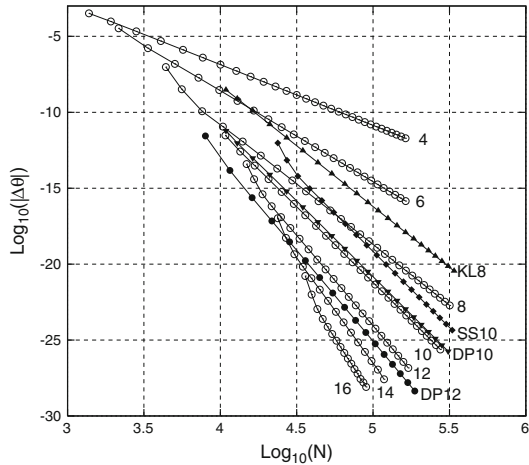


Fig. 3 The orbital precession error as a function of the number of force evaluation N . KL8 and SS10 are Kahan-Li's eighth-order and Sofroniou-Spalletta's tenth-order symplectic integrators, respectively. DP10 and DP12 are the 10th and 12th order RKN pair of Dormand and Prince. The numbers 4, 6, 8, etc., denote the $2n$ -order integrators corresponding to the minimal multi-product expansion (17)



In Fig. 3, we compare some well known higher order integrators with the PV-based, minimal extrapolated integrators (17). KL8 and SS10 are eighth and tenth order symplectic integrators by [Kahan and Li \(1997\)](#) and [Sofroniou and Spaletta \(2005\)](#) with 17 and 35 force evaluations, respectively. Both are recommended by [Hairer et al. \(2002\)](#). Because of their large number of force-evaluations, they are not competitive ([Calvo and Sanz-Serna 1993](#)) in a precision-effort comparison as shown in Fig. 3. At $N = 10^5$, the error of KL8 is more than 300 times that of the PV-based $\{1, 2, 3, 4\}$ -integrator denoted simply as 8 rather than M8. Similarly, the error of SS10 at $N = 10^5$ is about 100 times that of the minimal $\{1, 2, 3, 4, 5\}$ -integrator denoted as 10. DP10 and DP12 are the RKN integrator-pair by [Dormand et al. \(1987\)](#) with 17 force evaluations. The coefficients for this integrators-pair were taken from [Brankin et al. \(1989\)](#) and converted to quadruple precision. DP10 is comparable to 10, which uses 15 force evaluations. DP12's error at $N = 10^5$ is 10 times smaller than 12. However, DP12's superior performance can be quickly matched by going to integrator 14, whose error is then 100 times smaller than DP12 at $N = 10^5$.

Figure 3 implies that the most efficient integrator for attaining a given level of precision is never a fixed order integrator. As one demands greater and greater precision, one must increase the order of the integrator accordingly. In Fig. 3, the error curve of the $2n + 2$ integrator is plotted only when it is below that of the $2n$ integrator. The enveloping error curve is steeper than any fixed order integrator. This maximum efficiency can be achieved only when one has the means of producing an arbitrary high-order integrator at will, as it is done here. The highest order considered in Fig. 3 is 16 because quadruple precision is inadequate for precision below 10^{-30} .

6 Summary and conclusions

In this work, we have generalized the single product decomposition of the evolution operator $e^{h(A+B)}$ to that of a sum of products. By using powers of \mathcal{T}_2 as basis products, the multi-product expansion reduces to that of a simple extrapolation, with analytically known solutions. Because the extrapolation is formulated on the level of operators, it can be applied with great generality in solving diverse evolution equations not only in classical mechanics but also in quantum (Chin et al. 2009) and stochastic (Zillich et al. 2010) dynamics. In particular, for perturbative Hamiltonian of the form

$$H = H_0 + \epsilon H_1, \quad (63)$$

arbitrary higher order algorithms can be derived by defining A and B as the Lie operators corresponding to H_0 and ϵH_1 , respectively. Second-order symplectic integrators for solving (63) were pioneered by Wisdom and Holman (1991). This has led to the later development of “pseudo-higher-order” symplectic algorithms for solving perturbed Hamiltonians by (McLachlan 1995; Chambers and Murison 2000) and (Laskar and Robutel 2001). The work of Laskar and Robutel showed that these “pseudo-higher-order” algorithms greatly improved upon the second-order integrator, but higher accuracy still depends on the elimination of higher order step size errors in h . Such an elimination can be easily done according to the analytical extrapolation method demonstrated in this work.

A multi-product expansion loses some desirable properties, such as not being symplectic, unitary, norm preserving, etc., as compared to a single product decomposition. However, at high orders, it gains in economy, needing only a quadratic, rather than an exponential number of operators. This is a vital consideration when high precision are needed in solving direct N-body problems (Emel'yanenko 2007), simulating Oort Cloud dynamics (Breiter et al. 2007), computing satellite orbits (Hadjifotinou and Gousidou-Koutita 1998; González et al. 1999) and in determining the long term evolution of planets (Milani and Nobili 1988; Gladman et al. 1991).

In applying to classical Hamiltonian dynamics, this work showed that extrapolating symplectic integrators produces RKN integrators. The process of force consolidation provided a simple explanation for why $p - 1$ force evaluations are sufficient for RKN integrators at orders $p = 4$ and 6. An order-barrier then naturally arises when forces can no longer be consolidated at higher p . Moreover, this work showed that, there exists a sequence of easily implemented, $2n$ -order extrapolated RKN integrators, with only $n(n + 1)/2$ force evaluations. Thus any other RKN integrator with fewer force evaluations is special and must embody some unique force consolidation schemes. These extrapolated RKN integrators are surprisingly competitive with existing symplectic and specially devised RKN algorithms in solving the Kepler problem. Since this series of extrapolated RKN integrators can be easily produced by anyone, they can serve as a common benchmark by which more sophisticated

high order integrators can be judged. For example, of all the integrators compared in this work, only DP12 has outperformed its corresponding extrapolated RKN integrator by having fewer force evaluations (17) than $n(n + 1)/2 (=21)$. Thus DP12 must possess some highly nontrivial force consolidation schemes.

Appendix A: Proving the solution

To solve the Vandermonde equation (13) for $\{c_i\}$, let $x_i = k_i^{-2}$ so that (13) reads conventionally

$$\begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ x_1 & x_2 & x_3 & \dots & x_n \\ x_1^2 & x_2^2 & x_3^2 & \dots & x_n^2 \\ \dots & \dots & \dots & \dots & \dots \\ x_1^{(n-1)} & x_2^{(n-1)} & x_3^{(n-1)} & \dots & x_n^{(n-1)} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \dots \\ c_n \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \dots \\ 0 \end{pmatrix} \tag{A1}$$

Consider the usual Lagrange interpolation at n points $\{x_1, x_2, \dots, x_n\}$ with values $\{y_1, y_2, \dots, y_n\}$. The interpolating $n - 1$ degree polynomial is given by

$$f(x) = \sum_{i=1}^n y_i L_i(x), \tag{A2}$$

where $L_i(x)$ are the Lagrange polynomials given by

$$L_i(x) = \prod_{j=1(\neq i)}^n \frac{(x - x_j)}{(x_i - x_j)}. \tag{A3}$$

Since by construction

$$L_i(x_k) = \delta_{ik} \tag{A4}$$

the interpolation polynomial (A2) correctly gives,

$$f(x_k) = \sum_{i=1}^n y_i L_i(x_k) = \sum_{i=1}^n y_i \delta_{ik} = y_k. \tag{A5}$$

Now let $y_i = x_i^m$ for $0 \leq m \leq n - 1$, then the interpolating polynomial

$$f(x) = \sum_{i=1}^n x_i^m L_i(x) \tag{A6}$$

and the function

$$g(x) = x^m \tag{A7}$$

both interpolate the same set of points. Since interpolating polynomials of the same order are unique, we must have $f(x) = g(x)$ and hence

$$\sum_{i=1}^n x_i^m L_i(x) = x^m. \tag{A8}$$

Writing this out in matrix form yields

$$\begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ x_1 & x_2 & x_3 & \dots & x_n \\ x_1^2 & x_2^2 & x_3^2 & \dots & x_n^2 \\ \dots & \dots & \dots & \dots & \dots \\ x_1^{(n-1)} & x_2^{(n-1)} & x_3^{(n-1)} & \dots & x_n^{(n-1)} \end{pmatrix} \begin{pmatrix} L_1(x) \\ L_2(x) \\ L_3(x) \\ \dots \\ L_n(x) \end{pmatrix} = \begin{pmatrix} 1 \\ x \\ x^2 \\ \dots \\ x^{n-1} \end{pmatrix} \quad (\text{A9})$$

Compare this to (A1), we immediately see that the solution is

$$\begin{aligned} c_i &= L_i(0) \\ &= \prod_{j=1(\neq i)}^n \frac{x_j}{x_j - x_i} \\ &= \prod_{j=1(\neq i)}^n \frac{k_i^2}{k_i^2 - k_j^2} \end{aligned} \quad (\text{A10})$$

This proof is a simple application of the more general result of inverting the Vandermonde matrix (El-Mikkawy 2003).

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