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Symplectic integrators from composite operator factorizations

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Abstract

I derive fourth order symplectic integrators by factorizing the exponential of two operators in terms of an additional higher order composite operator with positive coefficients. One algorithm requires only one evaluation of the force and one evaluation of the force and its gradient. When applied to Kepler's problem, the energy error function associated with these algorithms are approximately 10 to 80 times smaller than the fourth order Forest–Ruth, Candy–Rozmus integrator.

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1. Introduction

In recent years, studies of numerical methods for solving both classical [1] and quantum [2] mechanical many-body problems have converged on a common theme of factorizing the general evolution operator

$$e^{\epsilon H} = e^{\epsilon(T+V)} \tag{1}$$

into products of exactly solvable parts. While first and second order factorizations such as

$$\begin{aligned} e^{\epsilon(T+V)} &\approx e^{\epsilon T} e^{\epsilon V}, \\ &\approx e^{\frac{1}{2}\epsilon T} e^{\epsilon V} e^{\frac{1}{2}\epsilon T}, \\ &\approx e^{\frac{1}{2}\epsilon V} e^{\epsilon T} e^{\frac{1}{2}\epsilon V}, \end{aligned} \tag{2}$$

are well known, the systematics of higher order factorization has only been investigated recently [3,4].

In quantum mechanics, ϵ is negative or imaginary and $T = -\frac{1}{2}\sum_i \nabla_i^2$, $V = V(r_i)$ are the usual kinetic and potential energy operators. A quantum state is evolved forward in "time" via

$$|\psi(\epsilon)\rangle = e^{\epsilon(T+V)}|\psi(0)\rangle. \tag{3}$$

When ϵ is negative, this evolution projects out the exact ground state of H. Methods which implement second order factorization schemes (2) are various quadratic diffusion Monte Carlo algorithms [2].

In classical mechanics, the equation of motion for any dynamical variable w without explicit time-dependence is given by the Poisson bracket

$$\frac{dw}{d\tau} = \{w, h\} = -\sum_i \left(\frac{\partial h}{\partial q_i}\frac{\partial}{\partial p_i} - \frac{\partial h}{\partial p_i}\frac{\partial}{\partial q_i} \right) w = Hw, \tag{4}$$

where h is the Hamiltonian function, and H is the Lie operator [5] associated with h defined by the above equation. This equation can also be integrated to give [6]

$$w(\epsilon) = e^{\epsilon(T+V)}w(0), \tag{5}$$

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where T and V are similarly defined Lie operators associated with the kinetic and potential energy functions t and v. For $t = \frac{1}{2}\sum_i p_i^2$ and $v = v(q_i)$, T and V are just first order differential operators

$$T = \sum_i p_i \frac{\partial}{\partial q_i}, \quad V = \sum_i f_i \frac{\partial}{\partial p_i}, \tag{6}$$

where $f_i = -\partial v/\partial q_i$ is the ith component of the force. Their exponentiations, $e^{\epsilon T}$, $e^{\epsilon V}$, are displacement operators which displace q_i and p_i forward in time via

$$q_i \to q_i + \epsilon p_i \quad \text{and} \quad p_i \to p_i + \epsilon f_i. \tag{7}$$

Every decomposition of the evolution operator $e^{\epsilon(T+V)}$ produces a *symplectic* map [5], or algorithm, which exactly conserves all Poincaré invariants. Second order factorizations (2) reproduce the well known velocity-Verlet and leap-frog algorithms.

Until recently, the evolution operator has been factorized only in the form [6,3,4]

$$e^{\epsilon(T+V)} = \prod_i e^{a_i \epsilon T} e^{b_i \epsilon V}, \tag{8}$$

with coefficients $\{a_i, b_i\}$ determined by the required order of accuracy. The resulting algorithm is a sequence of of symplectic maps of the form (7) following the order of the factorized displacement operators. The power of this operator approach is well demonstrated in the work of Yoshida [4], where he has given the simplest derivation of the fourth order Forest–Ruth [6], Candy–Rozmus [7] integrator, and has shown how his method can be generalized to arbitrarily high even orders. However, this way of factorizing the evolution operator has no impact on solving quantum many-body problems. Suzuki [3] has proved that, beyond second order, any factorization of the form (8) must produce some negative coefficients in the set $\{a_i, b_i\}$. In Monte Carlo simulations, the diffusive character of the kinetic energy operator can be exactly simulated by Gaussian random walks. Having a negative coefficient multiplying the time step means that one must simulate the diffusion process backward in time, which is impossible. (Mathematically, the resulting operator becomes unbounded.)

In an effort to produce factorizations with only positive coefficients, Suzuki [8] has recently proposed to include composite operators of the form $[V,[T,V]]$ into the factorized product. In the quantum many-body context, $[V,[T,V]] = \sum_i |\nabla_i V|^2$ and is only slightly more complicated than the potential itself. His suggested fourth order factorization is [8]

$$e^{\epsilon(T+V)} = S_T(\epsilon/3)Q(\epsilon)S_V(\epsilon/3)Q(\epsilon)S_T(\epsilon/3) + O(\epsilon^5), \tag{9}$$

where

$$S_T(\epsilon) = e^{\frac{1}{2}\epsilon T} e^{\epsilon V} e^{\frac{1}{2}\epsilon T},$$
$$S_V(\epsilon) = e^{\frac{1}{2}\epsilon V} e^{\epsilon T} e^{\frac{1}{2}\epsilon V}, \tag{10}$$

and

$$Q(\epsilon) = \exp\{\tfrac{1}{2}(\tfrac{1}{6}\epsilon)^3 [V,[T,V]]\}. \tag{11}$$

This factorization scheme, if implemented as a Monte Carlo simulation, would have required four evaluations of V, two evaluations of $[V,[T,V]]$ and five sampling of Gaussian random variables. For comparison, a second order algorithm only requires one evaluation of of V and two sampling of Gaussian random variables. The computational effort would have been nearly quadrupled.

In this work, I will show that Suzuki's idea can be implemented in a much simpler manner.

2. Composite operator factorizations

By repeated application of the Baker–Campell–Hausdorff formula, a left–right symmetric operator product can be recombined as

$$e^{\epsilon B} e^{\epsilon A} e^{\epsilon B} = e^{\epsilon C}, \tag{12}$$

with

$$C = \epsilon(A + 2B) - \tfrac{1}{6}\epsilon^3 [A,[B,A]] + \tfrac{1}{6}\epsilon^3 [B,[A,B]] + O(\epsilon^5). \tag{13}$$

There are no even order terms in the above expansion. A basic strategy for obtaining a fourth order factorization is to multiply this product symmetrically by more operators so that third order terms in C are eliminated. As mentioned earlier, if no new operators other than A and B are used, this will result in negative coefficients. My implementation of Suzuki's idea is to add just enough old operators to kill off only *one* third order term in C and eliminate the remaining one explicitly by multiplying the product by the latter's inverse.

For example, the following symmetric product has the expansion

$$e^{\epsilon C_2 V} e^{\epsilon C_1 T} e^{\epsilon C_0 V} e^{\epsilon C_1 T} e^{\epsilon C_2 V} = e^{\epsilon W}, \tag{14}$$

with

$$\begin{aligned} W = {} & 2C_1\epsilon T + (C_0 + 2C_2)\epsilon V \\ & - \tfrac{1}{6}C_1(C_0^2 - 2C_0C_2 - 2C_2^2)\epsilon^3[V,[T,V]] \\ & + \tfrac{1}{6}C_1^2(C_0 - 4C_2)\epsilon^3[T,[V,T]] + O(\epsilon^5). \end{aligned} \tag{15}$$

In order for W to match $\epsilon(T+V)$, we must choose $C_1 = 1/2$ and $C_0 + 2C_2 = 1$. The undesirable third order term with operator $[T,[V,T]]$ can be eliminated by setting $C_0 = 4C_2$. This fixes $C_0 = 2/3$, $C_1 = 1/2$, and $C_2 = 1/6$, so that

$$W = \epsilon(T+V) - \tfrac{1}{72}\epsilon^3[V,[T,V]] + O(\epsilon^5). \tag{16}$$

The remaining third order term above can then be "moved" back to the other side, i.e., eliminated by explicitly multiplying the left hand side of (14) on both ends by $e^{(\epsilon^3/144)[V,[T,V]]}$. To minimize the evaluation of $[V,[T,V]]$, we should combine both at the central V. Thus we have effected a fourth order factorization in the form of

$$e^{\epsilon(T+V)} = e^{\epsilon\frac{1}{6}V} e^{\epsilon\frac{1}{2}T} e^{\epsilon\frac{2}{3}\widetilde{V}} e^{\epsilon\frac{1}{2}T} e^{\epsilon\frac{1}{6}V} + O(\epsilon^5), \tag{17}$$

with $\widetilde{V}$ given by

$$\widetilde{V} = V + \tfrac{1}{48}\epsilon^2[V,[T,V]]. \tag{18}$$

We will refer to this as factorization scheme A. If evaluating $[V,[T,V]]$ is not a major problem, then we should distribute this operator more evenly over the three V. We will not bother with this refinement here.

Alternatively, we can consider the symmetric product (14) with T and V interchanged. In this case, the undesirable operator can be eliminated by setting $C_0^2 = 2C_2(C_0 + C_2)$. The positive solutions are $C_0 = 1/\sqrt{3}$, $C_1 = 1/2$ and $C_2 = (1 - 1/\sqrt{3})/2$, yielding

$$W = \epsilon(T+V) - \tfrac{1}{24}(2-\sqrt{3})\epsilon^3[V,[T,V]] + O(\epsilon^5). \tag{19}$$

Adding half of this third order term to the two Vs in the product gives us another fourth order decomposition:

$$\begin{aligned} e^{\epsilon(T+V)} = {} & e^{\epsilon\frac{1}{2}(1-\frac{1}{\sqrt{3}})T} e^{\epsilon\frac{1}{2}\widetilde{V}} e^{\epsilon\frac{1}{\sqrt{3}}T} e^{\epsilon\frac{1}{2}\widetilde{V}} e^{\epsilon\frac{1}{2}(1-\frac{1}{\sqrt{3}})T} \\ & + O(\epsilon^5), \end{aligned} \tag{20}$$

where $\widetilde{V}$ now is given by

$$\widetilde{V} = V + \tfrac{1}{24}(2-\sqrt{3})\epsilon^2[V,[T,V]]. \tag{21}$$

We will refer to this as factorization scheme B. Factorization schemes A and B have been derived by Suzuki in a more recent work [9] based on McLachlan's method of small perturbation [10].

One more fourth order factorization scheme deserves consideration. If bilateral symmetry is not imposed initially, then it can be shown that the following product can be recombined as

$$e^{\epsilon a_1 T} e^{\epsilon b_1 V} e^{\epsilon a_2 T} e^{\epsilon b_2 V} = e^{\epsilon W}, \tag{22}$$

with

$$\begin{aligned} W = {} & (a_1 + a_2)\epsilon T + (b_1 + b_2)\epsilon V \\ & + \tfrac{1}{2}[(a_1+a_2)(b_1+b_2) - 2a_2b_1]\epsilon^2[T,V] \\ & - \tfrac{1}{12}[(a_1+a_2)^2(b_1+b_2) - 6a_1a_2b_1]\epsilon^3[T,[V,T]] \\ & - \tfrac{1}{12}[(a_1+a_2)(b_1+b_2)^2 - 6b_1b_2a_2]\epsilon^3[V,[T,V]] \\ & + O(\epsilon^4). \end{aligned} \tag{23}$$

Since we must have $(a_1 + a_2) = 1$ and $(b_1 + b_2) = 1$, we can eliminate the second order term [11] by setting $2a_2b_1 = 1$ and knock out the undesirable third order term by requiring $6a_1a_2b_1 = 1$. This gives $a_1 = 1/3$, $a_2 = 2/3$, $b_1 = 3/4$, and $b_2 = 1/4$. The remaining third order term can then be removed explicitly as earlier to yield

$$e^{\epsilon(T+V)} = e^{\epsilon\frac{1}{3}T} e^{\epsilon\frac{3}{4}V} e^{\epsilon\frac{2}{3}T} e^{\epsilon\frac{1}{4}\widetilde{V}} + O(\epsilon^4), \tag{24}$$

with

$$\widetilde{V} = V + \tfrac{1}{12}\epsilon^2[V,[T,V]]. \tag{25}$$

Since no even power can occur in a symmetrized product, the fourth order error term in (24) can be eliminated by symmetrization. Thus by taking two products of (24) at half the step size, flip one over and concatenate, one generates a fourth order factorization:

$$e^{\epsilon(T+V)} = e^{\epsilon\frac{1}{6}T} e^{\epsilon\frac{3}{8}V} e^{\epsilon\frac{1}{3}T} e^{\epsilon\frac{1}{4}\widetilde{V}} e^{\epsilon\frac{1}{3}T} e^{\epsilon\frac{3}{8}V} e^{\epsilon\frac{1}{6}T} + O(\epsilon^5). \tag{26}$$

$\widetilde{V}$ here corresponds to

$$\widetilde{V} = V + \tfrac{1}{48}\epsilon^2[V,[T,V]]. \tag{27}$$

We will refer to this as factorization scheme C. Again, we will not bother with refinements such as alternative concatenations or re-distributions of the composite operator.

The applications of these three factorization schemes to quantum many-body problems will be considered elsewhere. Here I will focus on their use in deriving symplectic integrators.

3. Symplectic integrators with force gradients

In the context of classical mechanics where T and V are Lie operators defined by (6),

$$[V,[T,V]] = 2f_j\frac{\partial f_i}{\partial q_j}\frac{\partial}{\partial p_i} = \nabla_i|f|^2\frac{\partial}{\partial p_i}. \tag{28}$$

This composite operator in (18), (21), (25), (27) simply modifies the original force f_i to an effective force

$$\tilde{f}_i = f_i + C\epsilon^2\nabla_i|f|^2, \tag{29}$$

with an appropriate coefficient C. Factorization scheme A (17) thus produces the following fourth order symplectic integrator,

$$\begin{aligned} &p_1 = p_0 + \tfrac{1}{6}\epsilon f_0, \quad q_1 = q_0 + \tfrac{1}{2}\epsilon p_1,\\ &p_2 = p_1 + \tfrac{2}{3}\epsilon(f_1 + \tfrac{1}{48}\epsilon^2\nabla|f_1|^2),\\ &q_2 = q_1 + \tfrac{1}{2}\epsilon p_2, \quad p_3 = p_2 + \tfrac{1}{6}\epsilon f_2, \end{aligned} \tag{30}$$

where $q(0) = q_0$, $p(0) = p_0$, $q(\epsilon) = q_2$, $p(\epsilon) = p_3$ and $f_i = f(q_i)$. It appears that three force evaluations f_0, f_1, f_2 are necessary. This is not the case. Since on the next iteration the new f_0 is just the old f_2, there is never a need to evaluate f_0 separately except at the initial step. Furthermore, if one is only interested in the trajectory, the last step can be combine with the first into a single step of size $\frac{1}{3}\epsilon$. Thus only one evaluation of the force and one evaluation of the force and its gradient are required. This will be referred to as integrator A.

Similarly, factorization scheme B (20) gives

$$\begin{aligned} &q_1 = q_0 + \tfrac{1}{2}(1 - 1/\sqrt{3})\epsilon p_0,\\ &p_1 = p_0 + \tfrac{1}{2}\epsilon[f_1 + \tfrac{1}{24}(2-\sqrt{3})\epsilon^2\nabla|f_1|^2],\\ &q_2 = q_1 + (1/\sqrt{3})\epsilon p_1,\\ &p_2 = p_1 + \tfrac{1}{2}\epsilon[f_2 + \tfrac{1}{24}(2-\sqrt{3})\epsilon^2\nabla|f_2|^2],\\ &q_3 = q_2 + \tfrac{1}{2}(1 - 1/\sqrt{3})\epsilon p_2, \end{aligned} \tag{31}$$

where now $q(\epsilon) = q_3$ and $p(\epsilon) = p_2$. This algorithm requires two evaluations of the force and its gradient and will be referred to as integrator B.

The third order factorization (24) gives

$$\begin{aligned} &p_1 = p_0 + \tfrac{1}{4}\epsilon(f_0 + \tfrac{1}{12}\epsilon^2\nabla|f_0|^2),\\ &q_1 = q_0 + \tfrac{2}{3}\epsilon p_1, \quad p_2 = p_1 + \tfrac{3}{4}\epsilon f_1,\\ &q_2 = q_1 + \tfrac{1}{3}\epsilon p_2, \end{aligned} \tag{32}$$

which is none other than Ruth's [12] original third order integrator found by using canonical transformations. The power of the operator approach is that one sees immediately that this is only half of an integrator. The symmetrized algorithm, corresponding to factorization scheme C is

$$\begin{aligned} &q_1 = q_0 + \tfrac{1}{6}\epsilon p_0, \quad p_1 = p_0 + \tfrac{3}{8}\epsilon f_1,\\ &q_2 = q_1 + \tfrac{1}{3}\epsilon p_1, \quad p_2 = p_1 + \tfrac{1}{4}\epsilon(f_2 + \tfrac{1}{48}\epsilon^2\nabla|f_2|^2),\\ &q_3 = q_2 + \tfrac{1}{3}\epsilon p_2, \quad p_3 = p_2 + \tfrac{3}{8}\epsilon f_3,\\ &q_4 = q_3 + \tfrac{1}{6}\epsilon p_3. \end{aligned} \tag{33}$$

This integrator requires three force evaluations plus one derivative. At first sight, it appears to be less efficient than the standard Forest–Ruth, Candy–Roszmus algorithm, which requires only three force evaluations. However, as we will see in the next section, this integrator is extraordinarily close to being a *sixth* order integrator when solving Kepler's problem. This will be referred to as integrator C.

4. Numerical comparisons

To gauge the numerical effectiveness of these three integrators, I use them to solve the two-body Kepler problem

$$\frac{\mathrm{d}^2\boldsymbol{q}}{\mathrm{d}t^2} = -\frac{\boldsymbol{q}}{q^3} \tag{34}$$

with initial conditions $\boldsymbol{q}_0 = (10,0)$ and $\boldsymbol{p}_0 = (0,1/10)$. The resulting high eccentricity ($e = 0.9$) orbit with widely varying $\boldsymbol{p}(t)$ and $\boldsymbol{q}(t)$ provides a nontrivial testing ground for energy conservation.

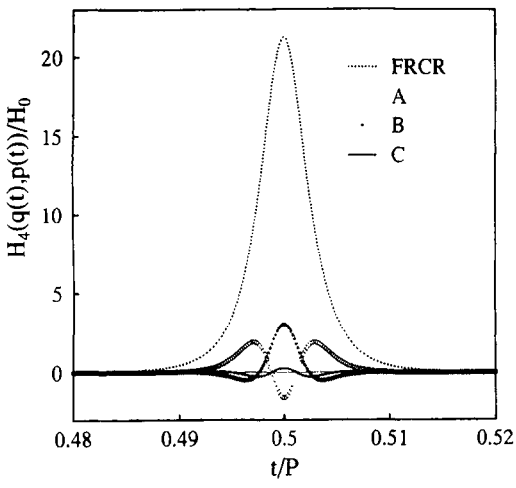

Fig. 1. Various symplectic integrators' normalized, fourth order, energy error coefficient as a function of time when solving Kepler's problem. FRCR is the Forest–Ruth, Candy–Rozmus integrator. A, B, and C are the three force gradient integrators discussed in the text. P is the period of the orbit. The particle is closest to the attractor at mid-period when $t = P/2$.

As discussed in Section 2, a product of operator defining a fourth order integrator, when recombined, will yield a Hamiltonian H' related to the originally Hamiltonian H_0 by

$$H'(\boldsymbol{p}(t),\boldsymbol{q}(t)) = H_0 + \epsilon^4 H_4(\boldsymbol{p}(t),\boldsymbol{q}(t)) + \mathrm{O}(\epsilon^6). \tag{35}$$

The leading error coefficient $H_4(\boldsymbol{p}(t),\boldsymbol{q}(t))$ is difficult to compute analytically, but in a numerical calculation, one can simply extract it via

$$H_4(\boldsymbol{p}(t),\boldsymbol{q}(t)) = \lim_{\epsilon\to 0}\frac{1}{\epsilon^4}[H'(\boldsymbol{p}(t),\boldsymbol{q}(t)) - H_0]. \tag{36}$$

Since the next order contribution to H' is $\mathrm{O}(\epsilon^6)$, the limit sets in quickly and is very stable. I evaluated the right hand side at $\epsilon = P/5000$ using double precision arithmetics. P is the period of the orbit. Fig. 1 shows the normalized error function $H_4(\boldsymbol{p}(t),\boldsymbol{q}(t))/H_0$ for all three gradient integrators as compared to that of the Forest–Ruth, Candy–Rozmus integrator. Time is measured in units of P. The error function is substantial only near mid-period, when the particle is closest to the attractor. The normalized error maxima (absolute values) for integrators A, B and C, are respectively 1.9, 3.0, and 0.27. The normalized error maximum for the Forest–Ruth, Candy–Roszmus integrator is 21. In this problem, integrator C can achieve the same accuracy as FRCR with a step size three times as large. Thus its single gradient evaluation is worth six more force evaluations of FRCR, at least for this simple problem. Its unusually small error coefficient make it very close to being a *sixth* order integrator.

5. Conclusions

In this work I have derived three symplectic algorithms on the basis of factorization schemes designed to solve quantum many-body problems. It is remarkable that the operator approach of quantum mechanics, which grew out of Poisson's bracket, is now used to solve Poisson's equation of motion. These fourth order integrators can easily be used to build higher order algorithms using Yoshida's [4] symmetrized triplet construction. However, this will again lead to negative coefficients. This work suggests that the pursuit of positive coefficients may continue to produce other fruitful methods for solving both classical and quantum many-body problems.

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