Computation of Maps for Particle and Light Optics by Scaling, Splitting, and Squaring

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New methods are presented for the integration of autonomous flows, with an emphasis on the Hamiltonian case. The Hamiltonian results are expected to have important applications for charged-particle optics (including accelerator design) and for graded-index light optics.

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A common feature in the treatment of many autonomous dynamical systems problems is the need to evaluate in some fashion maps $\mathcal{M}$ of the form $\mathcal{M} = \exp(tL)$. Here t is a parameter, which may be taken to be the time, and L denotes some linear operator that is typically composed of elements of some Lie algebra. The map $\mathcal{M}$ describes the relation between an initial state at time zero and the resulting final state at time t that arises from following the autonomous flow generated by L. For example, L may be a matrix in the case of coupled first-order ordinary linear differential equations, the operator $-i\mathcal{H}/\hbar$ in the case of quantum mechanical systems, the Hamiltonian Lie operator $-:H:$ in the case of classical Hamiltonian systems, and a general Lie operator in the case of general coupled first-order ordinary nonlinear differential equations. There are analogous operators and maps associated with parabolic partial differential equations.

The purpose of this Letter is to describe a new method for the computation of $\exp(tL)$ in the context of classical Hamiltonian systems. This method has immediate application to problems in charged-particle optics (including accelerator physics) and geometrical light optics (including graded-index media). It is expected that it may have applications in other fields as well.

Where feasible, one might attempt to evaluate $\exp(tL)$ directly by using the series

$$\exp(tL) = \sum_{m=0}^{\infty} (tL)^m/m!\,. \tag{1}$$

However, even in the matrix case, use of the series (1) is known to be the most dubious way of computing the exponential function [1]. Although the series is convergent for all t and L in the matrix case, the convergence is often slow thereby requiring the computation of a large number of terms, depending on the magnitude of t and the spectrum of L, and round-off errors can also be severe. Thus, even in the simplest case, a better method is needed.

Let n be a positive integer. The exponential function satisfies the *scaling* identity

$$\exp(tL) = [\exp(tL/2^n)]^{2^n}. \tag{2}$$

Also, the right-hand side of (2) can be calculated by n successive *squarings*,

$$[\exp(tL/2^n)]^{2^n} = [\cdots[[\exp(tL/2^n)]^2]^2\cdots]^2\ (n \text{ squarings})\,. \tag{3}$$

When n is sufficiently large, the argument $tL/2^n$ is in some sense small. Suppose that there is some method of computing $\exp(tL/2^n)$ to sufficient accuracy when $tL/2^n$ is sufficiently small. Suppose also that there is an efficient procedure for successive squarings as needed in (3). Then we may compute $\exp(tL)$ using the *scaling* and *squaring* formula

$$\exp(tL) = [\cdots[[\exp(tL/2^n)]^2]^2\cdots]^2\ (n \text{ squarings})\,. \tag{4}$$

Sometimes L can be written as a sum of two terms, $L = A + B$, in such a way that both $\exp(\tau A)$ and $\exp(\tau B)$ can be evaluated exactly or have some other desired property. In that case use of *splitting* formulas may be advantageous. The simplest nontrivial splitting formula, accurate through terms of order τ^2, is

$$\begin{aligned}\exp(\tau L) &= \exp[\tau(A + B)] \\ &= \exp(\tau A/2)\exp(\tau B)\exp(\tau A/2)[1 + O(\tau^3)]\,.\end{aligned} \tag{5}$$

A fourth-order splitting formula, accurate through terms of order τ^4, is

$$\begin{aligned}\exp[\tau(A + B)] = {}& \exp(w_1\tau A)\exp(w_2\tau B)\exp(w_3\tau A) \\ &\times \exp(w_4\tau B)\exp(w_5\tau A)\exp(w_6\tau B) \\ &\times \exp(w_7\tau A)[1 + O(\tau^5)]\,,\end{aligned} \tag{6}$$

where the *weights* w_i have the values

$$\begin{aligned}w_1 = w_7 = 1/[2(2 - 2^{1/3})],\ w_2 = w_6 = 2w_1, \\ w_3 = w_5 = (1 - 2^{1/3})w_1,\ w_4 = -2^{1/3}w_2\,.\end{aligned} \tag{7}$$

Still higher-order formulas are known [2,3].

Suppose an mth-order splitting formula is used to evaluate $\exp(\tau L) = \exp[\tau(A + B)]$ with $\tau = t/2^n$, and this result is then employed in (4). Doing so we obtain

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a result for $\exp(tL)$ that is correct up to an error of order $2^n(\lambda t/2^n)^{(m+1)}$, where λ is some number that depends on the spectrum, or perhaps the norm, of L. We see that for rather modest m and n the error can be quite small. We call the use of (4) along with suitable splitting formulas, of which (5) and (6) are examples, the method of *scaling*, *splitting*, and *squaring*.

The method of scaling and squaring, along with splitting formulas such as (5) and (6) and their higher-order generalizations, seems very promising for the treatment of a broad range of problems, and deserves further exploration of its use for specific applications. However, the more accurate fourth-order splitting formula (6) and its still higher-order generalizations involve many factors and the solution of complicated sets of algebraic equations for the weights. For some important areas of Hamiltonian mechanics, and for some purposes, we have found better splitting formulas that have fewer factors and can be obtained relatively easily to very high order.

To discuss Hamiltonian mechanics, it is convenient to treat the collection of phase-space variables q, p on an equal footing, and to denote them by the general symbol $z = (q, p)$. Let $f(z)$ be any function of the phase-space variables z. To every such function we associate a Lie operator, which we denote by the symbols $:f:$. The Lie operator $:f:$ is a differential operator (vector field) defined by the equation

$$:f: = \sum_j (\partial f/\partial q_j)\partial/\partial p_j - (\partial f/\partial p_j)\partial/\partial q_j\,. \tag{8}$$

If $:f:$ acts on any other function g, we get from (8) the result $:f:g = [f,g]$, where $[,]$ denotes the familiar Poisson bracket. A commonly used notation for $:f:$, but considerably more awkward for long computations, is $ad(f)$.

In many cases the classical Hamiltonian H has or can be arranged to have an expansion of the form

$$H = h_2 + h_3 + h_4 + \cdots, \tag{9}$$

where the h_l denote *homogeneous* polynomials of degree l in z. In this case it can be shown that $\exp(\tau : -H :)$ can be written in the factored product form

$$\exp(\tau : -H :) = \cdots \exp(: g_4 :) \exp(: g_3 :) \exp(: g_2 :)\,, \tag{10}$$

where the g_l are also homogeneous polynomials of degree l in z [4,5]. The existence of a representation of this form is key to the Lie algebraic treatment of charged-particle and geometrical light optics [6–8]. The quantity $l - 1$ is often referred to as the *aberration order*. What we are essentially using here is the fact that the Lie algebra of Hamiltonian vector fields can be *graded* according to degree. Analogous factorizations can also be obtained for the non-Hamiltonian case with the aid of a similar grading.

The factored product (10) may be viewed as a kind of generalized splitting formula which, although it makes no assumption about splitting L (or equivalently $-:H:$) save for the general decomposition (9), does write the result as a product of factors having desirable properties. As such, it has three advantages: First, its form is fixed, and potentially exact. Second, it can be concatenated easily with other maps of the same form by use of the Baker-Campbell-Hausdorff formula [4,9]. Consequently, it can be squared repeatedly with relative ease. Third, the exact g_l are entire functions of τ, and have rapidly convergent Taylor expansions. As will be described in detail elsewhere, we find through fifth order in τ, for example, the formulas

$$\begin{aligned}
g_2 &= -\tau h_2\,,\\
g_3 &= \sum_{m=1}^{5} (1/m!)(-\tau)^m :h_2:^{(m-1)} h_3\,,\\
g_4 &= g_4^d + g_4^{\mathrm{fu}},\\
g_4^d &= \sum_{m=1}^{5} (1/m!)(-\tau)^m :h_2:^{(m-1)} h_4\,,\\
g_4^{fu} &= -(1/12)\tau^3[h_3, :h_2: h_3] + (1/24)\tau^4[h_3, :h_2:^2 h_3]\\
&\quad - \tau^5\{(1/80)[h_3, :h_2:^3 h_3] + (1/120)[:h_2: h_3, :h_2:^2 h_3]\}\,.
\end{aligned} \tag{11}$$

Similar formulas can be found for the g_l with larger l. Also, results of still higher order in τ can easily be obtained. Note that g_4 consists of a *direct* term g_4^d driven by h_4 and a *feed up* term g_4^{fu} driven by lower degree terms, in this case h_3. This is a general pattern for the g_l with $l > 3$. By contrast, there are no *feed down* terms. To find a given g_l, it is only necessary to know the $h_{l'}$ with $l' \leq l$. We also observe that the formulas

(11) are all expressible in terms of Poisson brackets. All expressions involve only operations within the Poisson bracket Lie algebra generated by the h_l. Such results are to be expected in general as a consequence of the Baker-Campbell-Hausdorff theorem. Analogous formulas, but involving instead commutators of vector fields, are to be expected in the non-Hamiltonian case. The coefficients in (11) should be universal. Finally, we note that the rate of convergence of the series (11) depends only on the properties of $\tau : h_2 :$ (and hence τh_2), because that is the only term that appears infinitely often in the series.

Suppose $\mathcal{M}$ is written in the factored product form

$$\begin{aligned} \mathcal{M} &= \exp(-t : H :) \\ &= \cdots \exp(: f_4 :) \exp(: f_3 :) \exp(: f_2 :) , \end{aligned} \tag{12}$$

and that we attempt to calculate $\mathcal{M}$ using the splitting formula expansions (11) through fifth order in τ and evaluated for $\tau = t/2^n$, and using the scaling and squaring formula (4). What errors are involved in such an approach? To study this question we may, for example, attempt to estimate the error in f_3 based on the first neglected term in g_3, which is $(1/6!)\,(-\tau)^6 : h_2 :^5 h_3$. By this estimate we expect the error in f_3 to be on the order of $2^n (1/6!)\,(-t/2^n)^6 : h_2 :^5 h_3$. Let us write h_2 in the form

$$h_2 = -\tfrac{1}{2} \sum S_{ab} z_a z_b \,, \tag{13}$$

where S is a symmetric matrix. Also, let J be the fundamental symplectic 2-form given by $J_{ab} = [z_a, z_b]$. Then it can be shown that the operator $(t : h_2 :)^5$, when acting on h_3, is bounded by $(3\lambda)^5$. Here λ is the value of some convenient norm, for example, the maximum column sum norm, of the matrix tJS [10]. Note that we expect f_3 itself to be on the order of th_3. Consequently, we expect the *relative* error in f_3 to be on the order of $(1/6!)\,(3\lambda/2^n)^5$. Suppose, for example, given tH and consequently also th_2, we select n so that

$$\lambda/2^n \simeq 10^{-2}. \tag{14}$$

Then we find that the expected relative error in f_3 is on the order of 10^{-10}. By generalization, we may hope that the computation of all terms in $\mathcal{M}$ in this case should be good to approximately ten significant figures.

We have found that this is indeed the case. We have computed $\mathcal{M}$ for several different Hamiltonians chosen at random (with a random number generator) using (4) and (11) with n selected to satisfy (14), and compared the results with those obtained by careful numerical integration of the exact differential equations for the f_l [5]. In every case we found agreement, through at least ten significant figures, between the scaling, splitting, and squaring results and the exact results. Of course, the value of n required to satisfy (14) varies from Hamiltonian to Hamiltonian. However, we note that the n required to achieve some specified accuracy grows only *logarithmically* with the norm of tJS (which can be and is calculated in advance), and that for any given H the accuracy increases very rapidly with increasing n. Correspondingly, because the number of required operations is relatively small and no cancellations are required to occur between large terms, we found no problems with round-off error. Finally, with regard to computational speed, we found that the method of scaling, splitting, and squaring is far faster than numerical integration. It is also faster and, as expected, far more reliable than direct use of the series (1).

In summary, we have found a new method for evaluating $\exp(-t : H :)$ in the factored product form (12) when H is of the form (9). This method is applicable to arbitrarily large aberration order, has high, controllable, and predictable accuracy with negligible round-off problems, and is very fast. Since Hamiltonians of the form (9) are standard fare in both charged-particle optics and graded-index light optics, we expect this method to become the method of choice for these problems, and that its use will greatly facilitate the treatment of important problems in both accelerator design and optical design. For example, its high speed and high accuracy will make possible the calculation of accurate one-turn maps for large storage rings in a reasonable amount of time. Finally, the general method of scaling, splitting, and squaring shows promise for the treatment of a broad range of problems beyond those described here, and merits further study.

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