ORNL/TM-2017/358

Preserving Symplecticity in the Numerical Integration of Linear Beam Optics

Christopher K. Allen
July 11, 2017

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ORNL/TM-2017/358

Research Accelerator Division

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Date Published: July 11, 2017

Prepared by
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, TN 37831-6283
managed by
UT-BATTELLE, LLC
for the
US DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

CONTENTS

ABSTRACT

Presented are mathematical tools and methods for the development of numerical integration techniques that preserve the symplectic condition inherent to mechanics. The intended audience is for beam physicists with backgrounds in numerical modeling and simulation with particular attention to beam optics applications. The paper focuses on Lie methods that are inherently symplectic regardless of the integration accuracy order. Section 2 provides the mathematically tools used in the sequel and necessary for the reader to extend the covered techniques. Section 3 places those tools in the context of charged-particle beam optics; in particular linear beam optics is presented in terms of a Lie algebraic matrix representation. Section 4 presents numerical stepping techniques with particular emphasis on a third-order leapfrog method. Section 5 discusses the modeling of field imperfections with particular attention to the fringe fields of quadrupole focusing magnets. The direct computation of a third order transfer matrix for a fringe field is shown.

1. INTRODUCTION

In the simulation of charged particle dynamics, preservation of the symplectic condition often takes precedence over numerical accuracy. Typically these applications are concerned more with particle ensemble behavior rather than individual behavior, for example, in storage rings where particles may traverse many orders of magnitude of time or distance scales. Preserving the symplectic relationship of the motion is necessary to ensure that it is physical and, thus, quantities such as energy and emittance are meaningful over large time scales. A simulation may be accurate to a numeric degree, but if the symplectic condition is violated the results are suspect. Since simulation codes typically have tuning parameters for increasing accuracy, it is beneficial to ensure that the simulation is always symplectic regardless of the prescribed accuracy.

The objective is to present techniques for designing and developing algorithms that respect symplecticity; these techniques are based upon Lie group and Lie algebraic methods. Since the material here is intended as a resource in the development of symplectic integration methods rather than to solely present individual procedures, basic Lie theoretic background and some useful mathematical theorems are provided. The focus of the Lie theory is on matrix representations and the exponential map, which is more applicable to beam optics applications and linear systems in general. This approach differs from that of Dragt where the focus is on non-linear symplectic maps and is more suited to nonlinear tracking applications [1][2].

In addition to general Lie algorithmic development, the paper presents two concrete applications: a leapfrog technique for including space charge in the dynamics calculations, and methods for adding field imperfections (e.g., fringe fields, pole faces, etc.). One specific leapfrog technique is demonstrated which is third-order accurate and symplectic. The methods for representing field imperfections are symplectic with variable integration accuracy. The material is presented in the context of Lie groups and algebras in order to demonstrate symplecticity of the methods. Thus, a basic background on Lie methods is included as it applies to beam dynamics. Also covered are some more general facts on matrix theory and differential equations that are needed for the development. The idea here is that the material is somewhat self-contained and can be extended at a later date.

The scope here is linear beam dynamics including space charge effects, thus, the usual beam optics matrix techniques for "integrating" the dynamics equations are valid. However, the material is presented in the context the symplectic group $Sp(2n,\mathbb{R})$ composed of real $2n \times 2n$ symplectic matrices, and its Lie algebra $sp(2n,\mathbb{R})$, also represented by real $2n \times 2n$ matrices. For clarity examples are in $Sp(2,\mathbb{R})$ but easily extended to the general case.

2. MATHEMATICS BACKGROUND

2.1 MATRIX EXPONENTIAL MAP

For any square matrix $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ the matrix exponent $e^{\mathbf{A}} \in \mathbb{R}^{n\times n}$ is defined by its Taylor series

$$e^{\mathbf{A}} \triangleq \mathbf{I} + \mathbf{A} + \frac{1}{2}\mathbf{A}^2 + \frac{1}{2\cdot 3}\mathbf{A}^3 + \cdots . \tag{1}$$

If $\|\cdot\|$ is any matrix norm then it is straightforward to show $\left\|e^{\mathbf{A}}\right\| \le e^{\|\mathbf{A}\|}$ and, consequently, the series converges in $\|\cdot\|$ (for more information on matrix norms see, for example, [3]). Also, if λ is an eigenvalue of $\mathbf{A}$ then e^{λ} is an eigenvalue of $e^{\mathbf{A}}$. Using these facts it is often possible to compute $e^{\mathbf{A}}$ symbolically and, indeed, symbolic computing environments such as Mathematica have such capabilities [4].

It is always possible to compute matrix exponential $e^{\mathbf{A}}$ numerically using formula (1), since it is convergent for all $\mathbf{A}$ such that $\|\mathbf{A}\| < \infty$. However, it is best to condition $\mathbf{A}$ before doing so. For

example, first find the smallest integer m such that $\frac{1}{2^m}\|\mathbf{A}\| < 1$, or $m = \lceil \log\|\mathbf{A}\| / \log 2 \rceil$. Next we compute the exponential of $\frac{1}{2^m}\mathbf{A}$ using formula (1) to achieve $e^{\frac{1}{2^m}\mathbf{A}}$. The formula will converge rapidly and can be further expedited by accumulating the term $\frac{2^{-mn}}{n!}\mathbf{A}^n$ by multiplication with $\frac{2^{-m}}{n}\mathbf{A}$. Matrix $e^{\mathbf{A}}$ is then found by squaring $e^{\frac{1}{2^m}\mathbf{A}}$ m times.

2.2 THE SYMPLECTIC GROUP OF MATRICES

For simplicity we start with the set $\mathbb{R}^{2\times 2}$ of real, 2×2 matrices (more precisely the general linear group $GL(n, \mathbb{R})$). Define the matrix $\mathbf{J} \in \mathbb{R}^{2\times 2}$ as

$$\mathbf{J} \triangleq \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{2}$$

Then a matrix $\mathbf{A} \in \mathbb{R}^{2\times 2}$ is *symplectic* if

$$\mathbf{A}^T\mathbf{J}\mathbf{A} = \mathbf{J}\,. \tag{3}$$

The set of symplectic matrices in $\mathbb{R}^{2\times 2}$ is denoted $Sp(2, \mathbb{R})$. It is straightforward to show that the set of symplectic matrices form a group; that is if $\mathbf{A}$ and $\mathbf{B}$ are both in $Sp(2, \mathbb{R})$, then so is $\mathbf{AB}$. It can also be shown that $\det \mathbf{A} = 1 \;\; \forall \mathbf{A} \in Sp(2, \mathbb{R})$. For the special case of 2×2 matrices the symplectic group is also the special linear group $SL(2, \mathbb{R})$.

Larger symplectic groups have similar properties, but are embedded in some $\mathbb{R}^{2n\times 2n}$ where n is an integer greater than 1. The general n-dimensional symplectic group is denoted $Sp(2n, \mathbb{R})$. For any $\mathbf{A} \in Sp(2n, \mathbb{R})$ the relation (3) still holds, however, the symplectic matrix $\mathbf{J}$ has the form

$$\mathbf{J} \triangleq \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & 0 \end{pmatrix}, \tag{4}$$

where $\mathbf{I}$ is the $n \times n$ identity matrix. The symplectic group is important because linear transforms $\mathbf{A}, \mathbf{B} \in Sp(2n, \mathbb{R})$ respect the inner product $<\cdot\,|\,\cdot>$ on phase space vectors $\mathbf{x}, \boldsymbol{y} \in \mathbb{R}^{2n}$ given by $\langle \mathbf{x}|\mathbf{y}\rangle = \mathbf{x}^T\mathbf{J}\mathbf{y}$ which is the primary geometric structure of Hamiltonian systems.

2.3 LIE GROUPS AND LIE ALGEBRAS

A *Lie group* is a differentiable manifold that is also a mathematical group. For example, the group of symplectic matrices is a Lie group where the calculus of smooth matrix functions is the differentiable structure and matrix multiplication is the group operation. The Lie group operation respects the differentiable structure of the manifold; this is the important fact when constructing the Lie algebra of a Lie group from matrices as done in the sequel. A *Lie algebra* is a vector space with the additional binary operation given by *commutation* (see below). With every Lie group there is an associated Lie algebra. However the correspondence is not unique, multiple Lie groups may project (locally) to the same Lie algebra. In the context of differentiable manifolds, the Lie algebra of a Lie group is the tangent bundle. For a more complete presentation see [5].

To make these ideas clear consider the matrix representation of a Lie group, specifically a matrix representation in $\mathbb{R}^{n\times n}$. Let L be a Lie group embedded in $\mathbb{R}^{n\times n}$ and denote $\mathfrak{L}$ as its Lie algebra. The Lie algebraic $\mathfrak{L}$ is identified as the tangent plane of L (as a differentiable manifold) at the identity element $\mathbf{I} \in \mathbb{R}^{n\times n}$. Specifically, if $\mathbf{\Phi}(\cdot)$ is any smooth curve in $L \subset \mathbb{R}^{n\times n}$ such that $\mathbf{\Phi}(0) = \mathbf{I}$, then $\mathbf{\Phi}'(0) \triangleq \lim_{s\to 0}\frac{1}{s}[\mathbf{\Phi}(s) - \mathbf{I}] \in \mathbb{R}^{n\times n}$ is in the tangent plane of L at $\mathbf{I}$, and thus, in $\mathfrak{L}$. The algebra of $\mathfrak{L}$ is formed by adding, as the algebraic multiplicative operation, the matrix commutator $[\cdot,\cdot]$ where $[\mathbf{A}, \boldsymbol{B}] = \mathbf{AB} - \mathbf{BA}$. The properties of $[\cdot,\cdot]$ are what differentiate Lie algebras from ordinary algebras. This representation is also known as the infinitesimal Lie group representation.

As shown above one can identify the set of all smooth curves passing through **I** in L with the set of all elements in the Lie algebra $\mathfrak{L}$. Conversely, if $\mathbf{A} \in \mathfrak{L} \subset \mathbb{R}^{n\times n}$ is constant then the matrix exponential

$$\mathbf{\Phi}_{\mathbf{A}}(s) \triangleq e^{s\mathbf{A}} \tag{5}$$

is a smooth curve in $\mathbb{R}^{n\times n}$ for $s \in \mathbb{R}$. It is then easy to show that $\{\mathbf{\Phi}_{\mathbf{A}}(s) | \, s \in \mathbb{R}\}$ is a one-parameter subgroup of L where **A** is the generator of this subgroup. Moreover, $\mathbf{\Phi}_{\mathbf{A}}(\cdot) \subset L$ is the solution to the linear, first-order differential system

$$\begin{aligned} \mathbf{\Phi}_{\mathbf{A}}'(s) &= \mathbf{A}\mathbf{\Phi}_{\mathbf{A}}(s)\,, \\ \mathbf{\Phi}_{\mathbf{A}}(0) &= \mathbf{I}\,. \end{aligned} \tag{6}$$

Every **A** in a Lie algebra $\mathfrak{L}$ generates a solution $\mathbf{\Phi}_{\mathbf{A}}$ to the above differential equation that is contained in the corresponding Lie group L. The image of $\exp \mathfrak{L} \to L$ for small s is called the *lift* of $\mathfrak{L}$ in L. As mentioned before multiple Lie groups can project down to the same Lie algebra; likewise, a single Lie algebra may lift to multiple Lie groups.

If a Lie group L is defined by some conservation property, then that property manifests itself in the Lie algebra $\mathfrak{L}$. Specifically, consider the symplectic group $Sp(2n, \mathbb{R})$. If $\mathbf{\Phi}(\cdot)$ is a curve in $Sp(2n, \mathbb{R})$ passing through the identity at $s = 0$ with $\mathbf{A} \triangleq \mathbf{\Phi}'(0)$ in $sp(2n, \mathbb{R})$ the Lie algebra of $Sp(2n, \mathbb{R})$, then the symplectic group condition (3) implies

$$\frac{d}{ds}[\mathbf{\Phi}^T(s)\mathbf{J}\mathbf{\Phi}(s) = \mathbf{J}]_{s=0} \Longrightarrow \mathbf{\Phi}^{T\prime}(0)\mathbf{J}\mathbf{\Phi}(0) + \mathbf{\Phi}^T(0)\mathbf{J}\mathbf{\Phi}'(0) = 0\,, \tag{7}$$

or

$$\mathbf{A}^T\mathbf{J} + \mathbf{J}\mathbf{A} = 0\,. \tag{8}$$

Since the choice of $\mathbf{\Phi}(\cdot)$ was arbitrary, the above must be a necessary condition for every **A** in $sp(2n, \mathbb{R})$. Further, note that $\mathbf{J}^T = -\mathbf{J}$ so that $\mathbf{A}^T\mathbf{J} = -(\mathbf{J}\mathbf{A})^T$ and the above relation becomes $(\mathbf{J}\mathbf{A})^T = \mathbf{J}\mathbf{A}$. This fact means that $\mathbf{J}\mathbf{A}$ is a symmetric matrix in $\mathbb{R}^{2n\times 2n}$. Or put another way, for every $\mathbf{\Sigma}$ in the symmetric group of matrices $Sym(\mathbb{R}^{2n\times 2n})$ the matrix $\mathbf{J}\mathbf{\Sigma}$ is in the symplectic lie algebra $sp(2n, \mathbb{R}) \subset \mathbb{R}^{2n\times 2n}$.

Using the matrix exponential definition it is possible to show that the commutator in the Lie algebra can be interpreted as "loop deficiencies" in Lie group flows. Explicitly, for any constant $\mathbf{A}, \mathbf{B} \in \mathfrak{L} \subset \mathbb{R}^{n\times n}$ and small $h > 0$, consider the path c in L defined by $c = e^{h\mathbf{A}}e^{h\mathbf{B}}e^{-h\mathbf{A}}e^{-h\mathbf{B}}$ starting at the identity. This path first follows the flows of vector –**B** a distance h, then an equal distance in the –**A** direction (note that $e^{-h\mathbf{A}} = [e^{h\mathbf{A}}]^{-1}$). The path then winds back following the **B** and **A** tangent vectors, respectively. After expanding, the terminal location of the path is

$$\begin{aligned} c &= e^{h\mathbf{A}}e^{h\mathbf{B}}e^{-h\mathbf{A}}e^{-h\mathbf{B}}\,, \\ &= \left[\mathbf{I} + h\mathbf{A} + \frac{h^2}{2}\mathbf{A}^2 + \cdots\right]\left[\mathbf{I} + h\mathbf{B} + \frac{h^2}{2}\mathbf{B}^2 + \cdots\right]\left[\mathbf{I} - h\mathbf{A} + \frac{h^2}{2}\mathbf{A}^2 - \cdots\right] \\ &\qquad \cdot \left[\mathbf{I} - h\mathbf{B} + \frac{h^2}{2}\mathbf{B}^2 - \cdots\right]\,, \\ &= \mathbf{I} + h^2[\mathbf{A}, \mathbf{B}] + O(h^4)\,. \end{aligned} \tag{9}$$

Thus, the commutator in $\mathfrak{L}$ indicates the "energy" lost or gained when traversing loops in the group flows; it is analogous to the outer product of vector mechanics (actually, Euclidean 3-space with outer product is a Lie algebra).

2.4 SOME MATHEMATICAL FACTS

Here we state some mathematical facts that are needed in the sequel and useful when expanding the results to other applications. The following theorem on the matrix exponential has particular relevance to Lie groups and the treatment of "non-ideal" elements in beam optics:

Theorem 1 (Campbell-Baker-Hausdorff): Given two matrices $\mathbf{A}, \mathbf{B} \in \mathbb{C}^{n\times n}$ sufficiently close to the origin $\mathbf{0}$, there is a well-defined matrix $\mathbf{C} \in \mathbb{C}^{n\times n}$ such that

$$e^{\mathbf{A}} e^{\mathbf{B}} = e^{\mathbf{C}}. \tag{10}$$

The first few terms of the expansion for $\mathbf{C}$ are

$$\mathbf{C} = \mathbf{A} + \mathbf{B} + \frac{1}{2}[\mathbf{A}, \mathbf{B}] + \frac{1}{12}\big([\mathbf{A}, [\mathbf{A}, \mathbf{B}]] - [\mathbf{B}, [\mathbf{B}, \mathbf{A}]]\big) + \cdots \tag{11}$$

Proof: See [6].

Remark: The smooth mapping $\exp \mathfrak{L} \to L$ does not respect the vector addition of $\mathfrak{L}$; that is, $\exp(\mathbf{A} + \mathbf{B}) \neq (\exp \mathbf{A})(\exp \mathbf{B})$ in general. However, the multiplication $[\cdot,\cdot]$ on $\mathfrak{L}$ provides the degree by which it is violated. Thus, the Campbell-Baker-Hausdorff formula (11) can be used to compute corrections.

The next fact concerns the solutions of linear matrix differential equations with variable coefficients.

Theorem 2 (Peano-Baker): Given the linear differential system

$$\begin{aligned} \mathbf{\Phi}'(s) &= \mathbf{A}(s)\mathbf{\Phi}(s)\,, \\ \mathbf{\Phi}(0) &= \mathbf{I}\,, \end{aligned} \tag{12}$$

where $\mathbf{A}(\cdot)$ is an integrable curve on $\mathbb{R}^{n\times n}$, that is, $\mathbf{A}(\cdot) \in L_p(\mathbb{R} \to \mathbb{R}^{n\times n})$, then the solution $\mathbf{\Phi}(\cdot)$ can be represented by the series

$$\begin{aligned} \mathbf{\Phi}(s) = \mathbf{I} + \int_0^s \mathbf{A}(s_1)ds_1 + \int_0^s \int_0^{s_1} \mathbf{A}(s_1)\mathbf{A}(s_2)ds_2 ds_1 \\ + \int_0^s \int_0^{s_1} \int_0^{s_2} \mathbf{A}(s_1)\mathbf{A}(s_2)\mathbf{A}(s_3)\, ds_3 ds_2 ds_1 + \cdots \end{aligned} \tag{13}$$

where the series continues *ad infinitum*.

Proof: Direct differentiation of the above.

Remark: It is readily shown that the above formula reduces to the usual matrix exponential when **A** is a constant.

Remark: The matrix function $\mathbf{\Phi}(\cdot)$ in the above is known as the *transfer matrix* for system (12).

Another standard result concerning transfer matrices is the following:

Theorem 3 (Semi-group property): Let $\mathbf{\Phi}(s, s_0)$ denote the solution to Eqs. (12) starting at some $s_0 \geq 0$ so that $\mathbf{\Phi}(s_0, s_0) = \mathbf{I}$. Then for any $s > s_0 > 0$

$$\mathbf{\Phi}(s, 0) = \mathbf{\Phi}(s, s_0)\mathbf{\Phi}(s_0, 0). \tag{14}$$

Proof: See [7].

Remark: Note that the above relation can be applied multiple times. For example, if we divide the interval $[0, s]$ into subintervals at locations $0 < s_0 < s_1 < \cdots < s_N < s$ then $\mathbf{\Phi}(s, 0) = \mathbf{\Phi}(s, s_N)\mathbf{\Phi}(s_N, s_{N-1}) \ldots \mathbf{\Phi}(s_1, s_0)\mathbf{\Phi}(s_0, 0)$. In other words, the mapping $s \mapsto \mathbf{\Phi}(s, 0)$ respects addition on the real line. Specifically, $(s_1 - s_0) + (s_0 - 0) \mapsto \mathbf{\Phi}(s_1, s_0)\mathbf{\Phi}(s_0, 0)$.

The next lemma follows from the Peano-Baker series and a commutator requirement.

Lemma 4: Let $\mathbf{A}(\cdot): \mathbb{R}_+ \to \mathbb{R}^{n \times n}$ be an integrable matrix function and denote its (Riemann) integral by $\aleph(s)$, specifically,

$$\aleph(s) \triangleq \int_0^s \mathbf{A}(\sigma) d\sigma \,. \tag{15}$$

If $\mathbf{A}(s)$ and $\aleph(s)$ commute for all s, that is, $[\mathbf{A}(s), \aleph(s)] = 0 \; \forall s \in \mathbb{R}_+$, then the solution to system (12) is

$$\mathbf{\Phi}(s) = e^{\aleph(s)} = e^{\int_0^s \mathbf{A}(\sigma) d\sigma}. \tag{16}$$

Proof (Sketch): The proof is inductive, applied to each successive term in (13). First consider

$$\int_0^s [\aleph^2(s_1)]' ds_1 = \int_0^s [\mathbf{A}(s_1)\aleph(s_1) + \aleph(s_1)\mathbf{A}(s_1)] \, ds_1 = 2 \int_0^s \int_0^{s_1} \mathbf{A}(s_1)\mathbf{A}(s_2) ds_2 ds_1,$$

where the last equality follows from the condition $[\mathbf{A}(s), \aleph(s)] = 0$ and the definition of $\aleph$. From the above we can identify the third term in the Peano-Baker series (13)

$$\int_0^s \int_0^{s_1} \mathbf{A}(s_1)\mathbf{A}(s_2) ds_s ds_1 = \frac{1}{2!}\aleph^2(s) \,. \tag{17}$$

Likewise, for the fourth term in series (13) consider

$$\begin{aligned}\int_0^s [\aleph^3(s_1)]' ds_1 &= \int_0^s [\mathbf{A}(s_1)\aleph^2(s_1) + \aleph(s_1)\boldsymbol{A}(s_1)\aleph(s_1) + \aleph^2(s_1)\boldsymbol{A}(s_1)] ds_1 \,, \\ &= 3\int_0^s \mathbf{A}(s_1)\aleph^2(s_1) ds_1 \,, \\ &= 3 \cdot 2 \int_0^s \int_0^{s_1} \int_0^{s_2} \mathbf{A}(s_1)\mathbf{A}(s_2)\mathbf{A}(s_3) ds_3 ds_2 ds_1 \,.\end{aligned}$$

where the second line follows from the commutator relationship and the third line upon substituting the previous result (17). Analogously each term in the Peano-Baker series is generated from the previous. The resulting general formula for the n^{th} repeated integral is

$$\int_0^s \dots \int_0^{s_{n-1}} \mathbf{A}(s_1) \dots \mathbf{A}(s_n) ds_1 \dots ds_n = \frac{1}{n!}\aleph^n(s) \,,$$

which, when substituted into (13), yields

$$\begin{aligned}\boldsymbol{\Phi}(s) &= \mathbf{I} + \aleph(s) + \frac{1}{2}\aleph^2(s) + \frac{1}{3!}\aleph^3(s) + \cdots \\ &= e^{\aleph(s)} \,,\end{aligned}$$

completing the proof.

Remark: Solution (16) is the direct matrix analogue of the scalar case where $\boldsymbol{A}(s) = a(s) \in \mathbb{R}$ and $\int a(\sigma) d\sigma$ always commute.

Remark: The condition $[\mathbf{A}(s), \aleph(s)] = 0$ in the above lemma is very restrictive. The most common application is when $\mathbf{A}(s) = k(s)\mathbf{G}$ where $k(\cdot)$ is an integrable function and $\mathbf{G} \in \mathbb{R}^{n \times n}$ is a constant matrix.

The following lemma is somewhat technical and concerns the "adjoint representation" operator for a Lie algebra.

Definition (Adjoint representation): Given any $\mathbf{A}$ in the Lie algebra $\mathfrak{L}$, the *adjoint representation* $\operatorname{ad}\mathbf{A}\colon \mathfrak{L} \to \mathfrak{L}$ is defined as $\operatorname{ad}\mathbf{A}(\mathbf{B}) \triangleq [\mathbf{A},\mathbf{B}]$. That is, given any $\mathbf{A} \in \mathfrak{L}$ the operator $\operatorname{ad}\mathbf{A}$ takes elements $\mathbf{B} \in \mathfrak{L}$ to elements $[\mathbf{A},\mathbf{B}] \in \mathfrak{L}$. Note that other authors (such as Dragt) use the notation $:\mathbf{A}:$ to signify the adjoint representation.

Lemma 5 (Adjoint flow): Consider the adjoint representation operator $\operatorname{ad}\mathbf{A}\colon \mathfrak{L} \to \mathfrak{L}$ defined as $\operatorname{ad}\mathbf{A}(\mathbf{B}) \triangleq [\mathbf{A},\mathbf{B}]$. Let $\mathbf{A}\colon \mathbb{R}_+ \to \mathbb{R}^{n\times n}$ be a smooth matrix function and consider the matrix exponential $\boldsymbol{\Psi}(s) \triangleq \exp\mathbf{A}(s)$. Then

$$\begin{aligned}\boldsymbol{\Psi}'(s)\boldsymbol{\Psi}^{-1}(s) &= \mathbf{A}'(s) + \frac{1}{2!}[\mathbf{A}(s),\mathbf{A}'(s)] + \frac{1}{3!}\big[\mathbf{A}(s),[\mathbf{A}(s),\mathbf{A}'(s)]\big] + \cdots \\ &= e^{\operatorname{ad}\mathbf{A}}\mathbf{A}'(s)\,,\end{aligned} \tag{18}$$

or

$$\boldsymbol{\Psi}'(s) = \mathbf{A}'(s)\boldsymbol{\Psi}(s) + \left(\frac{1}{2!}[\mathbf{A}(s),\mathbf{A}'(s)] + \frac{1}{3!}\big[\mathbf{A}(s),[\mathbf{A}(s),\mathbf{A}'(s)]\big] + \cdots\right)\boldsymbol{\Psi}(s) \tag{19}$$

where $\boldsymbol{\Psi}^{-1}(s) = \exp -\mathbf{A}(s)$.

Proof (sketch): This follows from the Campbell-Baker-Hausdorff theorem and a judicious choice of flow involving the adjoint representation operator $\operatorname{ad}\mathbf{A}$. For a complete proof see [6].

Remark: The lemma can be considered the compliment of **Theorem 2** providing an estimate to which $\boldsymbol{\Psi}$ differs from characteristic matrix $\boldsymbol{\Phi}$.

Let $\boldsymbol{\Phi}(s) \in \mathbb{R}^{2n\times 2n}$ be the flow generated by the matrix function element $\mathbf{A}(\cdot)$; that is, $\boldsymbol{\Phi}(\cdot)$ solves Eqs. (12). The final theorem is a procedure for calculating an order-by-order approximation of the matrix element $\mathbf{G}(s) \in \mathbb{R}^{2n\times 2n}$ which lifts to $\boldsymbol{\Phi}(s)$ via the exponential map.

Theorem 6 (Magnus Expansion): Let $\boldsymbol{\Phi}(\cdot)$ be the matrix solution to Eq. (12) and let

$$\mathbf{G}(s) = \log\boldsymbol{\Phi}(s). \tag{20}$$

(The fact that $\boldsymbol{\Phi}$ has a logarithm is beyond the scope.) Then $\mathbf{G}(s)$ has the following expansion:

$$\mathbf{G}(s) = \sum_{n=1}^{\infty}\mathbf{G}_{(n)}(s). \tag{21}$$

where

$$
\begin{aligned}
\mathbf{G}_{(1)}(s) &= \int_0^s \mathbf{A}(s_1)ds_1 \ , \\
\mathbf{G}_{(2)}(s) &= \frac{1}{2!}\int_{\mathbf{0}}^{\boldsymbol{s}}\int_{\mathbf{0}}^{\boldsymbol{s_1}} [\mathbf{A}(s_1),\mathbf{A}(s_2)]ds_2 ds_1 \ , \\
\mathbf{G}_{(3)}(s) &= \frac{1}{3!}\int_0^s\int_0^{s_1}\int_0^{s_2} \Big(\big[\mathbf{A}(s_1),[\mathbf{A}(s_2),\mathbf{A}(s_3)]\big] - \big[[\mathbf{A}(s_1),\mathbf{A}(s_2)],\mathbf{A}(s_3)\big]\Big)ds_3\, ds_2\, ds_3 \ , \\
\mathbf{G}_{(4)}(s) &= \frac{1}{4!}\int_0^s\int_0^{s_1}\int_0^{s_2}\int_0^{s_3} \Big(\Big[\big[[\mathbf{A}(s_1),\mathbf{A}(s_2)],\mathbf{A}(s_3)\big],\mathbf{A}(s_4)\Big] \\
&\qquad + \Big[\mathbf{A}(s_1),\big[[\mathbf{A}(s_2),\mathbf{A}(s_3)],\mathbf{A}(s_4)\big]\Big] \\
&\qquad + \Big[\mathbf{A}(s_2),\big[\mathbf{A}(s_3),[\mathbf{A}(s_4),\mathbf{A}(s_1)]\big]\Big]\Big)\, ds_4\, ds_3\, ds_2\, ds_1 \, , \\
&\ \ \vdots
\end{aligned}
\tag{22}
$$

Proof: This follows from Campbell-Baker-Hausdorff, the Peano-Baker series, and the adjoint flow. For a complete proof see [8].

Remark: This fact has clear implications when $\mathbf{A}(s)$ is in a Lie algebra $\mathfrak{L}$ of some Lie group L for every s. The theorem gives us an order-by-order expansion of the flow $\mathbf{\Phi}(s)$ in the Lie group L. The truncated flow $\mathbf{\Phi}_{(n)}(s) \triangleq \exp \mathbf{G}_{(1)}(s) + \cdots + \mathbf{G}_{(n)}(s)$ is guaranteed to be in the Lie group L regardless of the order of truncation n.

3. MECHANICS

3.1 LINEAR BEAM OPTICS

Linear beam optics, whether derived from the equations of motion or Hamiltonian formalism, can be represented as a first-order, matrix-vector differential equation (e.g., see [9][10]). For simplicity consider only the horizontal phase plane. We have

$$
\begin{aligned}
\mathbf{x}'(s) &= \mathbf{G}(s)\mathbf{x}(s) \, , \\
\mathbf{x}(0) &= \mathbf{x}_0 \, ,
\end{aligned}
\tag{23}
$$

where $\mathbf{x} \triangleq (x, x')^T$ is the particle phase vector, $\mathbf{G}(s) \in \mathbb{R}^{2\times 2}$ describes the dynamics, and $\mathbf{x}_0$ is the initial condition of the particle at $s = 0$. The matrix $\mathbf{G}$ is termed the *generator matrix* for the dynamics and for physical systems this matrix must be an element of the symplectic algebra $sp(2, \mathbb{R})$. The solution to (23) is

$$
\mathbf{x}(s) = \mathbf{\Phi}_{\mathbf{G}}(s)\mathbf{x}_0 \, , \tag{24}
$$

where $\mathbf{\Phi}_{\mathbf{G}}(s) = e^{s\mathbf{G}}$ when $\mathbf{G}$ is constant and given by the Peano-Baker series (13) when not. The matrix $\mathbf{\Phi}_{\mathbf{G}}(\mathrm{s})$ is the *transfer matrix* for system (23). For beam envelope simulation where $\boldsymbol{\sigma}$ is the symmetric matrix of second order-moments (given by $\boldsymbol{\sigma} = \langle \mathbf{x}\mathbf{x}^T \rangle$), the dynamics are

$$\boldsymbol{\sigma}(s) = \boldsymbol{\Phi}_{\mathbf{G}}(s)\boldsymbol{\sigma}_0\boldsymbol{\Phi}_{\mathbf{G}}^T(s)\,, \tag{25}$$

where $\boldsymbol{\sigma}_0$ is the initial value.

3.2 THE LIE ALGEBRA OF CONSTANT FOCUSING

When dynamics matrix **G** is independent of axial position *s* it typically has one of the following forms (in a single phase plane):

$$\mathbf{G}_0 \triangleq \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},\ \mathbf{G}_K \triangleq \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},\ \mathbf{G}_F(k) \triangleq \begin{pmatrix} 0 & 1 \\ -k^2 & 0 \end{pmatrix},\ \mathbf{G}_D(k) \triangleq \begin{pmatrix} 0 & 1 \\ k^2 & 0 \end{pmatrix}, \tag{26}$$

where k is the "focusing constant." The subscripts 0, *K*, *F*, and *D* refer to "drift", "kick", "focus", and "defocus", respectively. It can be confirmed that $\mathbf{G}_0, \mathbf{G}_K, \mathbf{G}_F, \mathbf{G}_D$ all satisfy the symplectic algebra condition (8) thus they belong in $sp(2,\mathbb{R})$. With the addition of matrix

$$\mathbf{E} \triangleq \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{27}$$

the set $\mathrm{span}\{\mathbf{G}_0, \mathbf{G}_K, \mathbf{G}_F, \mathbf{G}_D, \mathbf{E}\}$ is complete under the commutator $[\cdot,\cdot]$ and generates the symplectic Lie algebra $sp(2,\mathbb{R})$. Since the focusing and defocusing matrices decompose as $\mathbf{G}_F(k) = \mathbf{G}_0 - k^2\mathbf{G}_K$ and $\mathbf{G}_D(k) = \mathbf{G}_0 + k^2\mathbf{G}_K$, the set $\{\mathbf{G}_0, \mathbf{G}_K, \mathbf{E}\}$ is really all that is needed to generate the algebra. The algebra generator relations are

$$[\mathbf{G}_0, \mathbf{G}_K] = \mathbf{E}\,, \qquad [\mathbf{E}, \mathbf{G}_0] = 2\mathbf{G}_0\,, \quad [\mathbf{E}, \mathbf{G}_K] = -2\mathbf{G}_K\,, \tag{28}$$

which yields

$$\begin{aligned} &[\mathbf{G}_F(k), \mathbf{G}_0] = +k^2\mathbf{E}, \quad [\mathbf{G}_F(k), \mathbf{G}_K] = \mathbf{E}, \quad [\mathbf{E}, \mathbf{G}_F(k)] = 2\mathbf{G}_F(k), \\ &[\mathbf{G}_D(k), \mathbf{G}_0] = -k^2\mathbf{E}, \quad [\mathbf{G}_D(k), \mathbf{G}_K] = \mathbf{E}, \quad [\mathbf{E}, \mathbf{G}_D(k)] = 2\mathbf{G}_D(k). \end{aligned} \tag{29}$$

Finally,

$$[\mathbf{G}_F(k_F), \mathbf{G}_D(k_D)] = (k_F^2 + k_D^2)\mathbf{E}\,. \tag{30}$$

Equations (28) are all that is necessary to define the algebra $sp(2,\mathbb{R})$, the rest are listed for the sake of completeness.

The Lie group elements corresponding to the Lie algebra generators are the one-parameter flows $\boldsymbol{\Phi}(\cdot)$ produced by the exponential map $\exp: sp(2,\mathbb{R}) \to Sp(2,\mathbb{R})$. For the constant focusing generators $\{\mathbf{G}_0, \mathbf{G}_K, \mathbf{G}_F, \mathbf{G}_D, \mathbf{E}\}$ we have

$$\begin{aligned} \boldsymbol{\Phi}_0(s) &\triangleq e^{s\mathbf{G}_0} = \begin{pmatrix} 1 & s \\ 0 & 1 \end{pmatrix}, \\ \boldsymbol{\Phi}_K(s) &\triangleq e^{s\mathbf{G}_K} = \begin{pmatrix} 1 & 0 \\ s & 1 \end{pmatrix}, \\ \boldsymbol{\Phi}_F(s) &\triangleq e^{s\mathbf{G}_F} = \begin{pmatrix} \cos ks & \dfrac{\sin ks}{k} \\ -k\sin ks & \cos ks \end{pmatrix}, \\ \boldsymbol{\Phi}_D(s) &\triangleq e^{s\mathbf{G}_D} = \begin{pmatrix} \cosh ks & \dfrac{\sinh ks}{k} \\ -k\sinh ks & \cosh ks \end{pmatrix}, \\ \boldsymbol{\Phi}_E(s) &\triangleq e^{s\mathbf{E}} = \begin{pmatrix} e^s & 0 \\ 0 & e^{-s} \end{pmatrix}, \end{aligned} \tag{31}$$

which are the usual optics transfer matrices for drifts, kicks, focusing quadrupoles, defocusing quadrupoles, and the "error" matrix.

4. APPLICATIONS: NUMERICAL INTEGRATION

Consider a stepping procedure for the numerical solution of dynamics equations (23). To solve the dynamics over a distance L we divide the path $[s_0, s_{N-1}]$ into N subsections of length $h_n \triangleq s_{n+1} - s_n$ each (lengths h_n need not be the same size). In the cases where the subsections $[s_n, s_{n+1}]$ correspond naturally to the boundaries of beam optics devices we have what is commonly referred to as *beam optics* [9]. There the generator matrices **G** are typically constant so that the "optics" refers to the transfer matrices of defined in (31); dynamics equations (23) are "integrated" element-by-element using these transfer matrices. However, when the generator matrix is not constant additional techniques are required. This section considers methods that are strictly numeric where the accuracy is based upon the step length h_n. The next section concerns techniques that attempt to maintain the beam optics paradigm when treating the non-ideal situation where the generator matrices are not constant.

4.1 A STRAIGHTFORWRAD STEPPING PROCEDURE

One general integration method that is simple yet still has practical use is to assume the generator matrix is constant over a given subinterval. Typically the generator matrix **G** is a function of path length *s*. But by choosing the interval $I_n \triangleq [s_n, s_{n+1}]$ small enough the matrix function $\mathbf{G}(s)$ does not change significantly enough on $[s_n, s_{n+1}]$ to affect the dynamics past a given order *K* and one can approximate $\mathbf{G}(s) = \mathbf{G}(s_n) + O(h_n^K)$ for $s \in [s_n, s_{n+1}]$ and some $K > 0$. We select h_n small enough to hold the error term $O(h_n^K)$ in the above approximation below a predetermined error tolerance ϵ. The integration then proceeds in steps

$$\mathbf{x}_{n+1} = \mathbf{\Phi}_n \mathbf{x}_n \ , \tag{32}$$

where, since **G** is approximately constant over the interval $[s_n, s_{n+1}]$,

$$\begin{aligned} \mathbf{x}_n &\triangleq \mathbf{x}(s_n), \\ \mathbf{\Phi}_n &\triangleq e^{h_n \mathbf{G}(s_n)} \ . \end{aligned} \tag{33}$$

Thus we have a set of discrete transfer matrices $\{\mathbf{\Phi}_n\}$ which transport the beam in steps $\{h_n\}$ down the beamline. So long as each $\mathbf{G}(s_n) \in sp(2n, \mathbb{R})$ the technique is guaranteed to be symplectic. The accuracy order *K* is typically determined by the choice of particular integration technique. That is, how accurately does the "sampled" transfer matrix $\mathbf{\Phi}_n = \exp h_n \mathbf{G}(s_n)$ approximate the exact transfer matrix $\mathbf{\Phi}(s_{n+1}, s_n)$. One of the most simple would be a Taylor expansion of $\mathbf{G}(s)$ at s_n; in this case the order *K* is 1 and we have a first-order stepping procedure.

Computing the matrix exponent $e^{h_n \mathbf{G}(s_n)}$ for each *n* can be an expensive procedure if done numerically. However, for most practical applications the dynamics generator **G**(*s*) varies between one of a handful of known constant matrices $\{\mathbf{G}_1, \mathbf{G}_2, \ldots\}$ representing different beamline elements [9][10]. Thus, the transfer matrices $\{\mathbf{\Phi}_1(h), \mathbf{\Phi}_2(h), \ldots\}$ are known analytically *a priori* and can be quickly computed as necessary.

4.2 SPACE CHARGE

Space charge can be modeled as a defocusing force that is dependent upon the size and shape of the beam (computing the magnitude of this force is beyond our scope). Thus, space charge forces can be represented with the generator matrix $\mathbf{G}_D\big(k_{sc}(s)\big)$ where $k_{sc}(\cdot)$ is the defocusing "constant" originating from the beam's self forces. However, the beam typically experiences external forces in addition to space charge forces such as focusing and defocusing from quadrupole magnets. Thus, space charge forces are more often modeled as variable forces within a constant (ideal) element. The resultant effect is a series of kicks with amplitude $k_{sc,n}$ computed at selected steps h_n within the ideal element.

The beam dynamics generator matrix **G**(*s*) in the presence of space charge can be written in the form

$$\mathbf{G}(s) = \mathbf{G}_{ext}(\mathrm{s}) + k_{sc}^2(s)\mathbf{G}_K\,, \tag{34}$$

where $\mathbf{G}_{ext}$ is the generator matrix for external forces and $k_{sc}(\cdot)$ is the defocusing function arising from space charge. We can assume that $\mathbf{G}_{ext}$ is one of the $sp(2n,\mathbb{R})$ generator matrices $\{\boldsymbol{G}_1, \mathbf{G}_2, \ldots\}$ and has the transfer matrix function $\boldsymbol{\Phi}_{ext}(s)$ that is know a priori. The *space charge transfer matrix* $\boldsymbol{\Phi}_{sc}(s)$ for generator $k_{sc}^2(s)\mathbf{G}_K$ is trivially computed from Eq. (1) since $\mathbf{G}_K^2 = 0$ (known as *idempotency*). By **Lemma 4** with $\mathbf{A}(s) = k_{sc}^2(s)\mathbf{G}_K$ we have

$$\boldsymbol{\Phi}_{sc}(s, s_n) = e^{\int_{s_n}^{s} k_{sc}^2(\sigma)d\sigma\, \mathbf{G}_K}, \tag{35}$$

for any $s \in [s_n, s_{n+1}]$. Expanding the above exponential and invoking the idempotency $\mathbf{G}_K^2 = 0$ leaves us with

$$\boldsymbol{\Phi}_{sc}(s, s_n) = \mathbf{I} + \mathbf{G}_K \int_{s_n}^{s} k_{sc}^2(\sigma)d\sigma, \tag{36}$$

Now that we have the known independent transfer matrix $\boldsymbol{\Phi}_{ext}(s, s_n)$ for external forces and the above transfer matrix $\boldsymbol{\Phi}_{sc}(s, s_n)$ for internal forces we need to create a form for the exact transfer matrix $\boldsymbol{\Phi}_n \triangleq \boldsymbol{\Phi}(s_{n+1}, s_n)$ that includes both forces simultaneously over the region $[s_n, s_{n+1}]$. Specifically, we wish an approximation for transfer matrix

$$\boldsymbol{\Phi}_n \triangleq \boldsymbol{\Phi}(s_{n+1}, s_n)\,, \tag{37}$$

where is the solution to the dynamics equations

$$\begin{aligned} &\boldsymbol{\Phi}'(s, s_n) = [\mathbf{G}_{ext}(\mathrm{s}) + k_{sc}^2(s)\mathbf{G}_K]\boldsymbol{\Phi}(s, s_n)\,, \\ &\boldsymbol{\Phi}(s_n, s_n) = \mathbf{I}\,, \end{aligned} \tag{38}$$

which include both internal and external forces.

First, consider the approximation $\widetilde{\boldsymbol{\Phi}}_n^{(1)}$ for transfer matrix $\boldsymbol{\Phi}_n$ at integration step *n*

$$\widetilde{\boldsymbol{\Phi}}_n^{(1)} \triangleq \boldsymbol{\Phi}_{sc}(s_{n+1}, s_n)\boldsymbol{\Phi}_{ext}(s_{n+1}, s_n). \tag{39}$$

Assume that external forces $\mathbf{G}_{ext}$ are constant and for convenience set

$$\kappa_{sc,n} \triangleq \int_{s_n}^{s_{n+1}} k_{sc}^2(s)ds\,. \tag{40}$$

Using Campbell-Baker-Hausdorff (11)

$$\begin{aligned} \widetilde{\boldsymbol{\Phi}}_n^{(1)} &= \exp\left\{\kappa_{sc,n}\mathbf{G}_K + h_n\mathbf{G}_{ext} + \frac{1}{2}h_n\kappa_{sc,n}[\mathbf{G}_K, \mathbf{G}_{ext}] + O(h_n^3)\right\}\,, \\ &= \boldsymbol{\Phi}_n \otimes \boldsymbol{O}\big(h_n\kappa_{sc,n}\big)\,, \end{aligned} \tag{41}$$

where $\boldsymbol{O}\big(h_n\kappa_{sc,n}\big)$ is some element in $Sp(2n,\mathbb{R})$ a distance $h_n\bar{k}_{sc}^2$ from identity element. In the special case $[\mathbf{G}_K, \mathbf{G}_{ext}] = 0$ then $\boldsymbol{O}\big(h_n\kappa_{sc,n}\big) = 0$ and the approximation is exact. However, in the general case $\widetilde{\boldsymbol{\Phi}}_n^{(1)}$ is only a first-order accurate approximate for $\boldsymbol{\Phi}_n$; that is, the error term is of order $h_n\kappa_{sc,n}$. Note that the accuracy is dependent upon both the space charge effect $\kappa_{sc,n}$ incurred over $[s_n, s_{n+1}]$ and the stepping distance h_n.

Consider now the alternate approximation $\widetilde{\boldsymbol{\Phi}}_n^{(3)}$ defined as

$$\widetilde{\boldsymbol{\Phi}}_n^{(3)} \triangleq \boldsymbol{\Phi}_{ext}(s_{n+1}, \bar{s}_n)\boldsymbol{\Phi}_{sc}(s_{n+1}, s_n)\boldsymbol{\Phi}_{ext}(\bar{s}_n, s_n)\,, \tag{42}$$

where $\bar{s}_n = s_n + h_n/2$ is the midpoint of $[s_n, s_{n+1}]$. Applying Campbell-Baker-Hausdorff as before and collecting we have

$$\begin{aligned}\widetilde{\boldsymbol{\Phi}}_n^{(3)} &= e^{h_n\left(\bar{k}_{sc}^2\mathbf{G}_K+\mathbf{G}_{ext}(\bar{s})\right)+O\left(h_n^4\right)}, \\ &= \boldsymbol{\Phi}_n \otimes \boldsymbol{O}(4),\end{aligned} \tag{43}$$

where $\boldsymbol{O}(4)$ indicates coefficients in $sp(2n,\mathbb{R})$ which are fourth-degree or greater polynomials in h_n and $\kappa_{sc,n}$. Thus we have gained two orders of accuracy in the computation of transfer matrix $\boldsymbol{\Phi}_n$ by adding the extra matrix multiplication.

Using an abuse of notation let us rewrite the definition of $\widetilde{\boldsymbol{\Phi}}_n^{(3)}$ as

$$\widetilde{\boldsymbol{\Phi}}_n^{(3)} = \boldsymbol{\Phi}_{ext}\left(\frac{h_n}{2}\right)\boldsymbol{\Phi}_{sc}(h_n)\boldsymbol{\Phi}_{ext}\left(\frac{h_n}{2}\right), \tag{44}$$

where $\boldsymbol{\Phi}_{sc}(h_n)$ indicates a space charge step of length h_n at s_n, and $\boldsymbol{\Phi}_{ext}\left(\frac{h_n}{2}\right)$ indicates a an external force step of length $h_n/2$ at either $s = s_n$ or $s = \bar{s}_n$ depending upon the context. Now consider the composite transfer matrix $\widetilde{\boldsymbol{\Phi}}_{n+1}^{(3)}\widetilde{\boldsymbol{\Phi}}_n^{(3)}$ which propagates the phase coordinates over the intervals $[s_n, s_{n+1}]$ and $[s_{n+1}, s_{n+2}]$ equal to $[s_n, s_{n+2}]$. If $\mathbf{G}_{ext}$ is constant and equal over the extended interval $[s_n, s_{n+2}]$ then $\boldsymbol{\Phi}_{ext}\left(\frac{h_n}{2}\right)\boldsymbol{\Phi}_{ext}\left(\frac{h_n}{2}\right) = \boldsymbol{\Phi}_{ext}(h_n)$ so that all internal multiplications are actually of full step length. This form suggests the idea of "leapfrog integration."

4.3 LEAPFROG INTEGRATION

The above result suggests the use of a leapfrog method when traversing a finite-length beamline element. This technique first steps a distance $h/2$ into the element using the external force matrix $\boldsymbol{\Phi}_{ext}(h/2)$. The method then begins stepping alternately between $\boldsymbol{\Phi}_{sc}(h)$ and $\boldsymbol{\Phi}_{ext}(h)$ until the element is traversed finally by $\boldsymbol{\Phi}_{ext}(h/2)$. For example, say $h = h_n$ is a constant for each *n* and consider two consecutive steps of formula (44). The resulting transfer matrix $\boldsymbol{\Phi}(2h)$ is given by

$$\begin{aligned}\boldsymbol{\Phi}(2h) &= \boldsymbol{\Phi}_{ext}\left(\frac{h}{2}\right)\boldsymbol{\Phi}_{sc}(h)\boldsymbol{\Phi}_{ext}\left(\frac{h}{2}\right)\boldsymbol{\Phi}_{ext}\left(\frac{h}{2}\right)\boldsymbol{\Phi}_{sc}(h)\boldsymbol{\Phi}_{ext}\left(\frac{h}{2}\right), \\ &= \boldsymbol{\Phi}_{ext}\left(\frac{h}{2}\right)\boldsymbol{\Phi}_{sc}(h)\boldsymbol{\Phi}_{\mathrm{ext}}(h)\boldsymbol{\Phi}_{sc}(h)\boldsymbol{\Phi}_{ext}\left(\frac{h}{2}\right).\end{aligned} \tag{45}$$

Multiplying by $\boldsymbol{\Phi}_{ext}(h)$ and $\boldsymbol{\Phi}_{sc}(h)$ throughout the element gives an integration scheme that is both symplectic and third-order accurate, so long as one applies $\boldsymbol{\Phi}_{ext}\left(\frac{h}{2}\right)$ at the entrance and exit. This scheme is a similar to the trapezoidal rule for function integration.

Note we have assumed that $\boldsymbol{G}_{ext}$ is constant so the transfer matrix $\boldsymbol{\Phi}_{ext}$ only depends upon distance *h* and not position *s*. It is possible to include external field variations and is described in Section 5.

4.4 ADAPTIVE STEPPING

Although outside the scope, briefly described here is the notion of adaptive step-size integration. Specifically, the step lengths $\{h_n\}$ are computed dynamically, during the integration, according to a prescribed error tolerance. Adaptive stepping can provide substantial gains in computational efficiency along with guaranteed solution errors (i.e., rather than an observed error given a prescribed step length). The a priori knowledge of integration accuracy allows for the implementation of adaptive stepping techniques and motivates the inclusion here. See reference [11] for more details.

Suppose we have a given allowable error tolerance ϵ_{max} for the solution accuracy, that is, for every step *n*

$$\left\|\widetilde{\boldsymbol{\Phi}}_n(h) - \boldsymbol{\Phi}_n(h)\right\| \le \epsilon_{max}\,, \tag{46}$$

where $\widetilde{\boldsymbol{\Phi}}_n(h)$ is the computed approximation for exact transfer matrix $\boldsymbol{\Phi}_n(h)$ at step n and $\|\cdot\|$ is a matrix norm. Suppose also that our stepping technique is K-order accurate. Clearly we do not know $\boldsymbol{\Phi}_n(h)$ but we do have the following relationship from the previous arguments:

$$\widetilde{\boldsymbol{\Phi}}_n(h) = \boldsymbol{\Phi}_n(h)e^{h^K\widetilde{\mathbf{G}}_n}\,, \tag{47}$$

where $\widetilde{\mathbf{G}}_n$ is some constant in $sp(2n,\mathbb{R}) \subset \mathbb{R}^{2n\times 2n}$. Now consider the effects of step doubling, taking two integration steps of size h compared with one step of size $2h$. Specifically, consider the residual error $res_n(h)$ between two such transfer matrices

$$res_n(h) \triangleq \left\|\widetilde{\boldsymbol{\Phi}}_{n+1}(h)\widetilde{\boldsymbol{\Phi}}_n(h) - \widetilde{\boldsymbol{\Phi}}_n(2h)\right\|. \tag{48}$$

Substituting Eq. (47)

$$\begin{aligned} res_n(h) &= \left\|\widetilde{\boldsymbol{\Phi}}_{n+1}(h)e^{h^K\widetilde{\mathbf{A}}_n}\widetilde{\boldsymbol{\Phi}}_n(h)e^{h^K\widetilde{\mathbf{B}}_n} - \widetilde{\boldsymbol{\Phi}}_n(2h)e^{2^Kh^K\tilde{\mathbf{C}}_n}\right\|, \\ &= \|\boldsymbol{\Phi}_n(2h)\|\left\|e^{h^K\widetilde{\mathbf{A}}_n + h^K\widetilde{\mathbf{B}}_n + O(h^{2K})} - e^{2^Kh^K\tilde{\mathbf{C}}_n}\right\|, \\ &= (2^K-2)h^K\|\boldsymbol{\Phi}_n(2h)\| + O(h^{2K}), \end{aligned} \tag{49}$$

where $\widetilde{\mathbf{A}}_n, \widetilde{\mathbf{B}}_n, \widetilde{\boldsymbol{C}}_n$ are constants of $sp(2n,\mathbb{R})$, the second line follows from Campbell-Baker-Hausdorff, and the third line from the expansion of the matrix exponential function. Although the above value is an estimate we can expect it to be relatively tight since the error is of order h^{2K}, significantly smaller than our requirements. Consider the relationship between step h_n and the following step h_{n+1}:

$$\begin{aligned} \frac{res_{n+1}(h_{n+1})}{res_n(h_n)} &\approx \frac{(2^K-2)h_{n+1}^K\|\boldsymbol{\Phi}_{n+1}(2h_{n+1})\|}{(2^K-2)h_n^K\|\boldsymbol{\Phi}_n(2h_n)\|}\,, \\ &\approx \left(\frac{h_{n+1}}{h_n}\right)^K. \end{aligned} \tag{50}$$

Note that $res_n(h_n)$ is something we can calculate directly from definition (48) provided we do the extra double-step computation $\widetilde{\boldsymbol{\Phi}}_n(2h)$. Assume we pick h_{n+1} so that $res_{n+1}(h_{n+1}) \to \epsilon_{max}$, the maximum allowable error. Then the above approximation suggests the step size update formula

$$h_{n+1} \leftarrow h_n\left[\frac{(2^K-2)\epsilon_{max}}{res_n(h_n)}\right]^{\frac{1}{K}}. \tag{51}$$

That is, given a maximum allowable error tolerance ϵ_{max}, a current step size h_n, and a current residual error of $res_n(h_n)$, the next step size h_{n+1} should be given by formula (51). It is the largest step size that still accommodates the error tolerances.

An important point to make is that if $h_{n+1} < h_n$ then the previous integration at step n must be recomputed with the smaller step h_{n+1}, since the tolerance condition has been violated. Another practical point is that one may not want to update the step size for small changes if re-computing the transfer matrices is expensive.

5. APPLICATIONS: FIELD IMPERFECTIONS

Fringe fields are magnetic fields that deviate from the ideal flat top situation. Instead of falling abruptly to zero, there is a finite region of fall-off at the edge of a magnet. Typically the fringe field is completely contained within an adjacent drift space. However, *leakage* fields occur when the fringing effect is so dramatic that the fields of one magnet actually interact with the fields of an adjacent magnet. We refer to both fringe fields and leakage fields as *field imperfections*.

We have a set of transfer matrices $\{\mathbf{\Phi}_m(s)\}$ for the ideal modeling elements $\{m\}$ and we want to include field imperfections. Denote by $\boldsymbol{G}_\delta(s) \in sp(2n,\mathbb{R})$ the generator matrix for these field imperfections at each position *s*; that is, $\mathbf{G}_\delta(s)$ is the deviation of real-world fields from the ideal fields. For example, $\mathbf{G}_\delta(s)$ could represent the fringe fields in a drift space beyond the hard edge of an ideal magnet and the error field within the magnet. The generator matrix **G**(*s*) for the real-world fields is then given by

$$\mathbf{G}(s) = \mathbf{G}_\delta(s) + \mathbf{G}_m(s)\,, \tag{52}$$

where $\mathbf{G}_m(s)$ is the generator matrix for the ideal beamline element (i.e., the model element). The prescription that most naturally fits into this representation is

$$\mathbf{G}_\delta(s) = k_\delta^2(s)\mathbf{G}_K\ , \tag{53}$$

where $k_\delta^2(\cdot)$ is the focusing function for the field deviation. Let $k_Q^2(s)$ be the true focusing profile for a quadrupole (i.e., with fringing). For example, if we wish to model the situation as an ideal (hard-edge) quadrupole *Q* with focusing strength k_F and a field imperfection represented by δ, then $k_\delta^2(s) = k_F^2 - k_Q^2(s)$ within the quadrupole. Thus, the quadrupole generator once decomposed into ideal and non-idea components is $\mathbf{G}_Q(s) = k_\delta^2(s)\mathbf{G}_K + \mathbf{G}_F(k_F)$ inside the quadrupole region. A drift space *D* adjacent to quadrupole *Q* and containing fringe fields would be modeled with generator $\mathbf{G}_D(s) = k_Q^2(s)\mathbf{G}_K + \mathbf{G}_0$.

5.1 FIRST-ORDER TECHNIQUE

To get an appreciation for the field imperfection idea consider a simple first-order technique that can be easily demonstrated and analyzed. It would be convenient to treat field imperfections as a separate modeling element $\mathbf{\Phi}_\delta$. Define

$$\mathbf{\Gamma}_\delta(s) \triangleq \int_0^s \mathbf{G}_\delta(s_1)ds_1 = \int_0^s k_\delta^2(s_1)ds_1\,\mathbf{G}_K\ , \tag{54}$$

then $[\mathbf{G}_\delta(s), \mathbf{\Gamma}_\delta(s)] = 0$ for all *s*, so by **Lemma 4**

$$\begin{aligned}\mathbf{\Phi}_\delta(s) &= \exp\left[\int_0^s k_\delta^2(s_1)ds_1\,\mathbf{G}_K\right]\ ,\\ &= \mathbf{I} + \int_0^s k_\delta^2(s_1)ds_1\,\mathbf{G}_K\,,\end{aligned} \tag{55}$$

where the second line follows from expansion (1) and the idempotency of $\mathbf{G}_K$. By defining

$$\kappa_\delta(s) \triangleq \int_0^s k_\delta^2(s_1)ds_1\ , \tag{56}$$

The modeling element has the convenient representation

$$\mathbf{\Phi}_\delta(s) = \mathbf{I} + \kappa_\delta(s)\mathbf{G}_K\ . \tag{57}$$

Let us now find an error estimate when modeling the real-world transfer matrix $\mathbf{\Phi}(s)$ by the composite approximation

$$\widetilde{\mathbf{\Phi}}(s) \triangleq \mathbf{\Phi}_\delta(s)\mathbf{\Phi}_m(s)\ . \tag{58}$$

This is a convenient model since we can approximate the action of the exact transfer matrix $\mathbf{\Phi}(s)$ by propagation with the ideal element $\mathbf{\Phi}_m(s)$, after which we include the field imperfections through

multiplication by $\boldsymbol{\Phi}_\delta(s)$. Assume that the ideal beamline element generator $\mathbf{G}_m$ is constant (this is not unreasonable since the term "ideal" usually refers to exactly this condition). Applying Eqs. (11), (55), (58) and expanding everything in site yields

$$\begin{aligned}\widetilde{\boldsymbol{\Phi}}(s) &= \left(e^{s\mathbf{G}_m}\right)\left(e^{\kappa_\delta(s)\mathbf{G}_K}\right), \\ &= e^{s\mathbf{G}_m+\kappa_\delta(s)\mathbf{G}_K+\frac{1}{2}s\kappa_\delta(s)[\mathbf{G}_m,\mathbf{G}_K]+O(3)},\end{aligned} \tag{59}$$

where $O(3)$ refer to terms of third order and higher in Lie product $[\cdot,\cdot]$ and, consequently, s and $\kappa_\delta(s)$. From **Theorem 6** the matrix

$$\boldsymbol{\Phi}_{(1)}(s) = e^{s\mathbf{G}_m+\kappa_\delta(s)\mathbf{G}_K} \tag{60}$$

is a first-order approximation to the exact transfer matrix $\boldsymbol{\Phi}(\mathrm{s})$. Thus, inclusion of the field imperfections via (58) results in a first-order approximation $\widetilde{\boldsymbol{\Phi}}(s)$ for $\boldsymbol{\Phi}(\mathrm{s})$, that is, the error is of second order.

Let $\boldsymbol{\chi}_{(1)}(s)$ be the *corrector* (or *conditioning*) matrix defined as

$$\boldsymbol{\chi}_{(1)}(s) \triangleq e^{\frac{1}{2}s\kappa_\delta(s)[\mathbf{G}_m,\mathbf{G}_K]}. \tag{61}$$

Then

$$\boldsymbol{\chi}_{(1)}(s)\widetilde{\boldsymbol{\Phi}}(s) = \boldsymbol{\Phi}_{(1)}(s)\otimes\boldsymbol{O}(3), \tag{62}$$

by Campbell-Baker-Hausdorff and so represents a loose form of error (note to get true second-order accuracy we need to start with the second-order Magnus expansion $\boldsymbol{\Phi}_{(2)}$). The direction of this error is $[\mathbf{G}_m, \mathbf{G}_K]$ and the magnitude of the error is $\frac{1}{2}s\kappa_\delta(s)$.

5.2 FIRST-ORDER EXAMPLE

Let us work out the example of a quadrupole magnet fringe field impinging into a drift space using the above first-order correction. Let the quadrupole exit location be $s = 0$ and let the fringe field extend into the drift region which is given by $s > 0$. In this case the model element generator matrix is that of the drift, that is, $\mathbf{G}_m = \mathbf{G}_0$, and with reference to definitions (31) we get

$$\begin{aligned}\boldsymbol{\Phi}_m(s) &= \boldsymbol{\Phi}_0(s) = \begin{pmatrix}1 & s\\ 0 & 1\end{pmatrix}, \\ \boldsymbol{\Phi}_\delta(s) &= \begin{pmatrix}1 & 0\\ \kappa_\delta(s) & 1\end{pmatrix}.\end{aligned} \tag{63}$$

These expressions are directly verified by matrix expansion and the idempotency of $\mathbf{G}_0$ and $\mathbf{G}_K$. Assume a simple linear profile $k_\delta^2(s)$ with field magnitude B_0 and fringe field length l, that is

$$k_\delta^2(s) = \begin{cases} B_0\left(1-\dfrac{\sigma}{l}\right) & \text{for} \quad s < l, \\ 0 & \text{for} \quad s > l. \end{cases} \tag{64}$$

Then

$$\kappa_\delta(s) = \begin{cases} \displaystyle\int_0^s B_0\left(1-\frac{\sigma}{l}\right)d\sigma & \text{for} \quad s < l \\ \\ \displaystyle\int_0^l B_0\left(1-\frac{\sigma}{l}\right)d\sigma & \text{for} \quad s > l \end{cases} \tag{65}$$

$$= \begin{cases} \frac{sB_0}{2}\left(2 - \frac{s}{l}\right) & \text{for} \quad s < l \\ \frac{lB_0}{2} & \text{for} \quad s > l \end{cases}$$

From here we get

$$\boldsymbol{\chi}_{(1)}(s) = \begin{cases} e^{\frac{s^2 B_0}{4}\left(2-\frac{s}{l}\right)\mathbf{E}} & \text{for} \quad s < l \\ e^{\frac{slB_0}{4}\mathbf{E}} & \text{for} \quad s > l \end{cases}$$

$$= \begin{cases} \begin{pmatrix} e^{\frac{s^2 B_0}{4}\left(2-\frac{s}{l}\right)} & 0 \\ 0 & e^{-\frac{s^2 B_0}{4}\left(2-\frac{s}{l}\right)} \end{pmatrix} & \text{for} \quad s < l \\ \begin{pmatrix} e^{\frac{slB_0}{4}} & 0 \\ 0 & e^{-\frac{slB_0}{4}} \end{pmatrix} & \text{for} \quad s > l \end{cases} \tag{66}$$

We see the correction involves increasing the magnitude of particle position and decreasing the magnitude of particle momentum. Thus, the approximation $\boldsymbol{\Phi}_\delta(s)\boldsymbol{\Phi}_m(s)$ for $\boldsymbol{\Phi}(s)$ tends to under-represent the position coordinate and over-represent the momentum coordinate. We can also see that $\boldsymbol{\Phi}_\delta(s)\boldsymbol{\Phi}_m(s)$ is, in general, not an overly accurate model for the true fields. For example, if we add the effects of a fringe field after a drift of length L, then the magnitude of the error in $\boldsymbol{\Phi}_\delta(L)\boldsymbol{\Phi}_0(L)$ is $e^{\frac{lLB_0}{4}} - 1$, which could be quite large depending upon the leakage l and field strength B_0. This is, however, a worst-case scenario since field imperfections are generally hyper-linear, meaning $k_\delta^2(\cdot)$ is usually convex. However, first-order techniques are generally not suitable for this type of beam optics modeling (i.e., without stepping).

5.3 COMPUTATION TO THIRD-ORDER

The field imperfection model can be refined using the Magnus expansion of **Theorem 6**. To make the process clear consider the fringe field $k_Q^2(s)$ within a drift space. In the nomenclature of the theorem this situation can be represented with the generator matrix **A** given by

$$\mathbf{A}(s) = \mathbf{G}_0 + k_Q^2(s)\mathbf{G}_K \ . \tag{67}$$

Denote by $\boldsymbol{\Phi}_{(n)}(s)$ the transfer matrix for this system to n^{th} order. By the Magnus expansion the third-order transfer matrix is

$$\boldsymbol{\Phi}_{(3)}(s) = e^{\mathbf{G}_{(1)}(s)+\mathbf{G}_{(2)}(s)+\mathbf{G}_{(3)}(s)} , \tag{68}$$

where the ordered generator matrices $\mathbf{G}_{(n)}(s)$ can be expanded into the Lie algebraic basis vectors $\{\mathbf{G}_0, \mathbf{G}_K, \mathbf{E}\}$ as

$$\begin{aligned} \mathbf{G}_{(1)}(s) &= g_{(1,0)}(s)\mathbf{G}_0 + g_{(1,K)}(s)\mathbf{G}_K + g_{(1,E)}(s)\mathbf{E} , \\ \mathbf{G}_{(2)}(s) &= g_{(2,0)}(s)\mathbf{G}_0 + g_{(2,K)}(s)\mathbf{G}_K + g_{(2,E)}(s)\mathbf{E} , \\ \mathbf{G}_{(3)}(s) &= g_{(3,0)}(s)\mathbf{G}_0 + g_{(3,K)}(s)\mathbf{G}_K + g_{(3,E)}(s)\mathbf{E} . \end{aligned} \tag{69}$$

The functions $g_{(n,\alpha)}(s)$ are computed from the formulas (22)

$$
\begin{aligned}
&g_{(1,0)}(s) = s, \qquad g_{(1,K)}(s) = \int_0^s k_Q^2(s_1)ds_1\,, \qquad g_{(1,E)}(s) = 0\,,\\
&g_{(2,0)}(s) = 0, \qquad g_{(2,K)}(s) = 0, \qquad g_{(2,E)}(s) = \frac{1}{2}\int_0^s\int_0^{s_1}\left(k_Q^2(s_2) - k_Q^2(s_1)\right)ds_2\,ds_1\,,\\
&g_{(3,0)}(s) = \frac{1}{3}\int_0^s\int_0^{s_1}\int_0^{s_2}\left(k_Q^2(s_1) - k_Q^2(s_3)\right)ds_3\,ds_2\,ds_1\,,\\
&g_{(3,K)}(s) = \frac{1}{3}\int_0^s\int_0^{s_1}\int_0^{s_2}\left(k_Q^2(s_2)k_Q^2(s_3) - k_Q^2(s_1)k_Q^2(s_3)\right)ds_3\,ds_2\,ds_1\,,\\
&g_{(3,E)}(s) = 0\,.
\end{aligned}
\tag{70}
$$

Thus, the transfer matrix $\mathbf{\Phi}_{(3)}(s)$ can be written

$$\mathbf{\Phi}_{(3)}(s) = e^{\left(s+g_{(3,0)}(s)\right)\mathbf{G}_0+\left(g_{(1,K)}(s)+g_{(3,K)}(s)\right)\mathbf{G}_K+g_{(2,K)}(s)\mathbf{E}}\,. \tag{71}$$

It is the quadrupole fringe field transfer matrix that is third-order accurate in distance *s* and guaranteed symplectic by virtue of its construction. Of course $\mathbf{\Phi}_{(3)}(s)$ would represent a special element of a beam optics simulation, that is, one for which the quadrupole field profile $k_Q^2(s)$ is known a priori. Or rather, as seen above, where the functions $g_{(n,\alpha)}(s)$ are known. If so, then $\mathbf{\Phi}_{(3)}$ can be used as a third-order approximation for a drift-with-fringe transfer matrix.

Return now to the alternative model of ideal transport/correction; that is, multiplication by $\mathbf{\Phi}_m(s)$/multiplication by $\mathbf{\Phi}_\delta(s)$. Equation (71) suggests a new form for the field imperfection matrix $\mathbf{\Phi}_\delta(s)$. Consider the following fringe field correction matrix for the drift space

$$\mathbf{\Phi}_\delta(s) = e^{g_{(3,0)}(s)\mathbf{G}_0+\left(g_{(1,K)}(s)+g_{(3,K)}(s)\right)\mathbf{G}_K+g_{(2,K)}(s)\mathbf{E}}\,. \tag{72}$$

Then the result from a drift $\mathbf{\Phi}_D(s)$ followed by the correction $\mathbf{\Phi}_\delta(s)$ is

$$
\begin{aligned}
\mathbf{\Phi}_\delta(s)\mathbf{\Phi}_D(s) &= e^{s\mathbf{G}_0}e^{g_{(3,0)}(s)\mathbf{G}_0+\left(g_{(1,K)}(s)+g_{(3,K)}(s)\right)\mathbf{G}_K+g_{(2,K)}(s)\mathbf{E}}\\
&= e^{(s+g_{(3,0)}(s))\mathbf{G}_0+\left(g_{(1,K)}(s)+g_{(3,K)}(s)\right)\mathbf{G}_K+g_{(2,K)}(s)\mathbf{E}+\frac{s}{2}\left(g_{(1,K)}(s)+g_{(3,K)}(s)\right)\mathbf{E}+O(3)}\,,
\end{aligned}
\tag{73}
$$

where the second line follows from Campbell-Baker-Hausdorff and *O*(3) indicates terms of third order and higher in commutation. The above formula shows that the term $\frac{1}{2}sg_{(1,K)}(s)\mathbf{E}$ is unfortunately polluting the transfer matrix at the second order. Thus, we are back at first-order accuracy. This fact can be circumvented via pre-conditioning.

5.4 BALANCING TO SECOND ORDER

The accuracy of the Magnus expansion to third order can be preserved using a balancing technique based upon the Campbell-Baker-Hausdorff relation, and which is analogous to the leapfrog integration. Let us return to the general-case field imperfection of Eq. (52) and recap the previous procedure. Converting to the notation of **Theorem 6**

$$\mathbf{A}(s) = k_\delta^2(s)\mathbf{G}_K + \mathbf{G}_m\,, \tag{74}$$

where $\mathbf{G}_m$ is the generator matrix for the ideal element without field imperfections (assumed a constant matrix). Again denote by $\mathbf{\Phi}_{(3)}(s)$ the third-order transfer matrix computed with the above procedure for

the given ideal (constant) generator $\mathbf{G}_m$ and having the expansion given by Eq. (68). Define the field-imperfection generator $\mathbf{G}_{(\delta)}(s)$

$$\mathbf{G}_{(\delta)}(s) \triangleq -s\mathbf{G}_m + \mathbf{G}_{(1)}(s) + \mathbf{G}_{(2)}(s) + \mathbf{G}_{(3)}(s)\,, \tag{75}$$

The field imperfection transfer matrix $\mathbf{\Phi}_\delta(s)$, the ideal element transfer matrix $\mathbf{\Phi}_m(s)$, and the third-order transfer matrix $\mathbf{\Phi}_{(3)}(s)$ can all be expressed

$$\begin{aligned} \mathbf{\Phi}_\delta(s) &= e^{\mathbf{G}_{(\delta)}(s)}\,, \\ \mathbf{\Phi}_m(s) &= e^{s\mathbf{G}_m}\,, \\ \mathbf{\Phi}_{(3)}(s) &= e^{s\mathbf{G}_m + \mathbf{G}_{(\delta)}(s)}\,. \end{aligned} \tag{76}$$

Now consider the square root of the field-imperfection matrix $\mathbf{\Phi}_\delta^{1/2}(s)$, which is

$$\mathbf{\Phi}_\delta^{\frac{1}{2}}(s) = e^{\frac{1}{2}\mathbf{G}_{(\delta)}(s)}\,. \tag{77}$$

Rather than integrating the field imperfection as $\mathbf{\Phi}_\delta(s)\mathbf{\Phi}_m(s)$, consider the following approximation:

$$\begin{aligned} \widetilde{\mathbf{\Phi}}(s) &= \mathbf{\Phi}_\delta^{\frac{1}{2}}(s)\mathbf{\Phi}_m(s)\mathbf{\Phi}_\delta^{\frac{1}{2}}(s)\mathbf{\Phi}_m(s)\,, \\ &= e^{\frac{1}{2}\mathbf{G}_{(\delta)}(s)} e^{s\mathbf{G}_m}\, e^{\frac{1}{2}\mathbf{G}_{(\delta)}(s)}. \end{aligned} \tag{78}$$

Applying the Campbell-Baker-Hausdorff theorem yields

$$\widetilde{\mathbf{\Phi}}(s) = e^{s\mathbf{G}_m + \mathbf{G}_{(\delta)}(s) - \frac{s}{16}[\mathbf{G}_\delta(s),[\mathbf{G}_\delta(s),\mathbf{G}_m]] + O(4)}\,. \tag{79}$$

The first error term in the exponent, that is $\frac{s}{16}\left[\mathbf{G}_\delta(s),[\mathbf{G}_\delta(s),\mathbf{G}_m]\right]$, is of order three so that $\widetilde{\mathbf{\Phi}}(s)$ is the second-order approximation to $\mathbf{\Phi}_{(3)}(s)$, which is the third-order approximation to the true transfer function $\mathbf{\Phi}(s)$.

5.5 PRE-/POST-CONDITIONING TO THIRD-ORDER

Continuing from the previous subsection and motivated by Eq. (79) define the *conditioning* matrix $\boldsymbol{\chi}_{(3)}(s)$ as

$$\boldsymbol{\chi}_{(3)}(s) \triangleq e^{\frac{s}{16}[\mathbf{G}_\delta(s),[\mathbf{G}_\delta(s),\mathbf{G}_m]]}\,. \tag{80}$$

Matrix $\boldsymbol{\chi}(s)$ can be used to pre-condition (or post-condition) $\widetilde{\mathbf{\Phi}}(s)$ to achieve the full third-order accuracy. This is clear to see with direct multiplication

$$\begin{aligned} \boldsymbol{\chi}_{(3)}(s)\widetilde{\mathbf{\Phi}}(s) &= \left(e^{\frac{s}{16}[\mathbf{G}_\delta(s),[\mathbf{G}_\delta(s),\mathbf{G}_m]]}\right)\left(e^{s\mathbf{G}_m + \mathbf{G}_{(\delta)}(s) - \frac{s}{16}[\mathbf{G}_\delta(s),[\mathbf{G}_\delta(s),\mathbf{G}_m]] + O(4)}\right)\,, \\ &= e^{s\mathbf{G}_m + \mathbf{G}_{(\delta)}(s) + O(4)}\,, \end{aligned} \tag{81}$$

where the second line follows from application of the Campbell-Baker-Hausdorff theorem. The same result is achieved when pre-conditioning as $\widetilde{\mathbf{\Phi}}(s)\boldsymbol{\chi}_{(3)}(s)$. Although convenient, this technique has the drawback in that matrix $\boldsymbol{\chi}_{(3)}(s)$ is dependent on both the ideal element and the field imperfection as seen in the definition (80). Thus, some abstraction is lost in the simulation and special conditioning matrices must be computed according to which element $\mathbf{G}_m$ is adjacent to field imperfection $\mathbf{G}_\delta(s)$. This situation may or may not be advantageous to direct computation of $\mathbf{\Phi}_{(3)}(s)$ depending upon the simulation architecture.

5.6 LEAPFROG INTEGRATION TO THIRD ORDER

As with space charge, a simple, third order method for including the field imperfections is to apply a leapfrog integration technique using the decomposition of Eq. (58). The technique is straightforward as described in Subsection 4.3. The problem is once again in the bookkeeping required for maintaining a special field imperfection profile $k_\delta^2(s)$. We must assign a k_δ^2 to an element m that is generated by an adjacent element, say m+1. For example, consider the leakage fields in one quadrupole magnet that originate from another quadrupole magnetic. If such profiles are available, however, this technique is completely viable due to the simple form of $\mathbf{\Phi}_\delta(\cdot)$, the field imperfection transfer matrix. The approach requires that we compute $\mathbf{\Phi}_{\delta,n} \triangleq \mathbf{I} + \int_{s_n}^{s_{n+1}} k_\delta^2(\sigma) d\sigma \, \mathbf{G}_K$ for each step each position s_n. Now the value of the field imperfection matrix is first order accurate with error given by $e^{\frac{B_0}{4}h_n^2} - 1 = \frac{B_0}{4}h_n^2 + \frac{B_0^2}{32}h_n^4 + O(h_n^6)$ where B_0 is the magnitude of the leakage field and h_n is the step length at n. Thus, the computation of $\mathbf{\Phi}_{\delta,n}$ is first-order accurate and the integration technique is third-order accurate.

6. CONCLUSION

The matrix representation of Lie groups from Lie algebras can be used to formulate integration techniques that preserve symplecticity in linear beam optics simulations. By working within the symplectic algebra of matrices to integrate the equations of motion the symplectic condition is maintained regardless of the final order of accuracy. The matrix exponential function and its computation are central to the realization of a transfer matrix from the Lie algebra representation. The Magnus expansion is a mathematical tool by which transfer matrices can be computed to any given order; it is a re-expression of the Peano-Baker series in term of the matrix commutator. The Magnus expansion takes special significance when the generator matrix is in the symplectic algebra, then all transfer matrices computed via these formulae are guaranteed symplectic. The Campbell-Baker-Hausdorff theorem is the tool by which we can determine the accuracy order of the integration technique itself and formulate additional techniques that, in turn, may improve accuracy.

In addition to demonstrating the general process of symplectic integration, several notable results are presented. It is seen that leapfrog integration has the potential for third-order accuracy whenever the transfer matrices themselves are at least third order accurate. In particular, a technique for including space charge effects in the beam optics simulation is shown through the Campbell-Baker-Hausdorff formula to be third order accurate so long as half steps are taken at the initial and final stage (the trapezoid rule). It was found, however, that a simple ideal step/correction step could only be first order accurate. There are methods within the beam optics paradigm to improve accuracy though. By combining integration techniques such as balancing and preconditioning one can achieve differing overall integration accuracies. Another specific result is the computation of a third-order accurate transfer matrix including field imperfections using the Magnus expansion. If we have direct knowledge of the field profile for a quadrupole we compute a dynamic transfer matrix for it to third order.

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