COMPUTING TRANSPORT & TURTLE TRANSFER MATRICES FROM MARYLIE & MAD LIE MAPS

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Abstract

Modern optics codes often utilize a Lie algebraic formulation of single particle dynamics. Lie algebra codes such as MARYLIE and MAD offer a number of advantages that makes them particularly suitable for certain applications, such as the study of higher order optics and for particle tracking. Many of the older more traditional optics codes use a matrix formulation of the equations of motion. Matrix codes such as TRANSPORT and TURTLE continue to find useful applications in many areas where the power of the Lie algebra approach is not necessary. Arguably the majority of practical optics applications can be addressed successfully with either Lie algebra or matrix codes, but it is often a tedious exercise to compare results from the two types of codes in any detail. Differences in the dynamic variables used by various codes compounds the comparison difficulties already inherent in the different formulations of the equations of motion. This paper summarizes key relationships that permit the direct numerical comparison of results from MARYLIE or MAD with those from TRANSPORT or TURTLE. Methods that provide for the computation of transfer matrices, which can be used directly in TRANSPORT and TURTLE, from the Lie maps provided by MARYLIE or MAD, are described. The implementation of these methods in a commercially available software package is discussed in a companion paper.

INTRODUCTION

The transfer map M of order n-1 may be written as [1]

$$M = \exp(:f_n:) \ldots \exp(:f_4:) \exp(:f_3:) \exp(:f_2:) \quad , \quad (1)$$

where the f_n are the generating functions for the map, shown explicitly through third-order (n=4) in (1). The Lie operators appearing in (1) are defined by:

$$:f: = \Sigma_i\{(\partial f/\partial q_i)(\partial/\partial p_i) - (\partial f/\partial p_i)(\partial/\partial q_i)\} \quad , \quad (2)$$

where the derivatives are with respect to canonical coordinates q_i and momenta p_i of the system. The sum in (2) runs from 1 to 3. Application of a Lie operator to a function of the coordinates and momenta, $g(q_i, p_i)$, results in a Poisson bracket of the generating function f and g:

$$:f:g = \Sigma_i\{(\partial f/\partial q_i)(\partial g/\partial p_i)-(\partial f/\partial p_i)(\partial g/\partial q_i)\} = [f,g] \ . \ (3)$$

The exponential forms appearing in (1) are to be evaluated via an (eventually truncated) infinite series:

$$\exp(:f:) = \Sigma_m\{(:f:)^m/m!\} \quad , \quad (4)$$

where m runs from 0 to ∞. This exponential Lie operator is referred to as the Lie transformation associated with the generating function f.

It is convenient to define a generalized 6-D phase space coordinate variable Q_k, where k runs from 1 to 6. For example, in equations (2) and (3), the set of $[Q_k] = (q_1, p_1, q_2, p_2, q_3, p_3)$. The generating functions f_2 through f_4 for the map can then be written as:

$$\begin{aligned} f_2 &= \Sigma_{i<j}\, f^{(2)}_{ij}\, [Q_iQ_j] \\ f_3 &= \Sigma_{i<j<k}\, f^{(3)}_{ijk}\, [Q_iQ_jQ_k] \\ f_4 &= \Sigma_{i<j<k<l}\, f^{(4)}_{ijkl}\, [Q_iQ_jQ_kQ_l] \quad . \end{aligned} \quad (5)$$

In equation (5) and elsewhere in this paper, the symbol < is to be interpreted here to mean *less than or equal*. The $f^{(2)}_{ij}$ through $f^{(4)}_{ijkl}$ are the coefficients of the polynomials for the corresponding generating functions, following the conventions of MARYLIE [1]. MAD [2] uses a different convention in which the corresponding $F^{(2)}_{ij}$ through $F^{(4)}_{ijkl}$ are the partial derivatives of the generating functions f_2 through f_4. The $F^{(n)}$ are fully symmetric and there are no < symbols in the expressions corresponding to (5) [3].

Applying a transfer map M that describes a particle beam system to a function of the initial phase space coordinates and momenta $g(Q_k)^{init}$ leads to the final (or output) function $g(Q_k)^{final}$ of those phase space coordinates and momenta. Applying to M to $[Q_k]^{init}$ yields in the equations of motion for the particle beam system. Those equations of motion can be expressed in the form of transfer matrices:

$$\begin{aligned} [Q_i]^{final} = {} & \Sigma_j\, R_{ij}\, [Q_j]^{init} + \Sigma_{j<k}\, T_{ijk}\, [Q_jQ_k]^{init} \\ & + \Sigma_{j<k,k<l}\, U_{ijkl}\, [Q_jQ_kQ_l]^{init} \quad . \end{aligned} \quad (6)$$

R, T, and U are the 1st, 2nd and 3rd order transfer matrices, respectively. The task of computing the transfer matrices appropriate to TRANSPORT [4] and TURTLE [5] from the MARYLIE or MAD maps involves two elements:

1. The R_{ij}, T_{ijk}, U_{ijkl} need to be related to the $f^{(n)}$ or $F^{(n)}$,
2. The different Q_k of each code need to be related.

TRANSFER MATRICES FROM LIE MAPS

The two computational tasks, involved in computing TRANSPORT and TURTLE transfer matrices from MARYLIE or MAD Lie maps, are discussed in the following two sections. Due to the large number of expressions required to include terms through 3rd order, it is not possible give all details here. In this paper the procedure is outlined. A companion paper gives some example numerical results [6].

Matrices from maps in the same coordinates

For 1st order it is generally easier to work with the R-matrix directly, rather than the f_2 generating function. For this reason, both MARYLIE and MAD output 1st order results in terms of the R-matrix. Obtaining the R-matrix in the coordinates used by MARYLIE and MAD is thus provided by those codes themselves. For 2nd order, the T-matrix terms can be derived from the f_3 and R-matrix using the cascade of transformations procedure [7]. Similarly, the U-matrix terms can be derived from the f_4, f_3 and R-matrix. MARYLIE and MAD have implemented this procedure so that the T-matrix and U-matrix elements, in the coordinates used by those codes, can also be obtained directly from those codes. In addition, this procedure has been implemented as an independent computation for the T-matrix and U-matrix elements, so that once a Lie map is obtained the transfer matrices can be computed without recourse to MARYLIE or MAD [6].

Relationships between coordinates

The different optics codes considered here utilize different phase space coordinate variables Q_k. MARYLIE and MAD use a canonical set of variables for Q_k, whereas TRANSPORT and TURTLE use a non-canonical set for Q_k. In order to obtain transfer matrices for TRANSPORT and TURTLE from the MARYLIE or MAD Lie maps, the differences in these phase space coordinates also need to be taken into account.

MARYLIE uses the normalized phase space variables:

$$[Q_k]_M = (x, P_x, y, P_y, \tau, P_\tau) = (x/L, p_x/p_s, y/L, p_y/p_s, c(t-t_s)/L, -[E-E_s]/p_s) \quad , \quad (7)$$

where L is a scale length, c is the speed of light, and the subscripts "s" refer to the reference (or synchronous) trajectory, e.g. $p_s=\beta_s\gamma_s m_o c$. The 6th element in (7) is the negative of the difference between the total energy, E, and the reference trajectory energy, E_s, divided by p_s. MAD also uses canonical coordinates. The MAD coordinates are nearly the same as the MARYLIE coordinates with L=1, except that the 5th and 6th variables differ by a sign [3] from those in (7). Some versions of MAD [2] also permit normalization with respect to an average momentum, rather than the reference momentum p_s. With these differences taken into consideration, results for MARYLIE can be used for MAD as well. In the remainder of this paper, attention is restricted to the relationship between MARYLIE and TRANSPORT, with L=1 in (7).

TRANSPORT and TURTLE use the phase space coordinates:

$$[Q_k]_T = (x, x', y, y', l, \delta) \quad . \quad (8)$$

The TRANSPORT variables x and y are the same as the x and y of MARYLIE, but the x', y', l and δ of TRANSPORT are different from the P_x, P_y, τ and P_τ of MARYLIE. The relationships of x', y' and δ to P_x, P_y and P_τ have been given by Dragt et al [1], and may be written as:

$$x' = P_x/D \quad , \quad (9)$$
$$y' = P_y/D \quad , \quad (10)$$
$$\delta = [1-(2P_\tau/\beta_s)+P_\tau^2]^{1/2} - 1 \quad , \quad (11)$$

with

$$D = [1 - (2P_\tau/\beta_s) + P_\tau^2 - P_x^2 - P_y^2]^{1/2} \quad . \quad (12)$$

The relationship between l and τ is apparently:

$$l = -\beta_s\tau \quad . \quad (13)$$

The inverse relationships are:

$$P_x = D\, x' \quad , \quad (14)$$
$$P_y = D\, y' \quad , \quad (15)$$
$$P_\tau = -(1/\beta_s)\{[1+\delta(2+\delta)\beta_s^2]^{1/2} - 1\} \quad , \quad (16)$$
$$\tau = -\, l/\beta_s \quad . \quad (17)$$

For (14) and (15) it is useful to write D in terms of the TRANSPORT variables:

$$D = \{(1+\delta)^2 - (x'^2+y'^2)[1+\delta(2+\delta)\beta_s^2]\}^{1/2} \quad . \quad (18)$$

To relate the transfer matrices in MARYLIE (or MAD) coordinates, denoted here by $[R_{ij}]_M$, $[T_{ijk}]_M$ and $[U_{ijkl}]_M$, to those of TRANSPORT, $[R_{ij}]_T$, $[T_{ijk}]_T$ and $[U_{ijkl}]_T$, the above relationships are expanded in a power series. The results are used to substitute into Equation (6) for MARYLIE. Comparing term-by-term the corresponding Equation (6) for TRANSPORT yields the desired formulas for converting the MARYLIE matrices to the TRANSPORT matrices.

For relating the x and y terms, i.e. i=1,3 in (6), substituting the relationships (14)-(18) for the *initial coordinates* into the right hand side of the MARYLIE form of (6) is adequate. However, for all other coordinates (i=2,4,5 and 6) one must also substitute the relationships (9)-(13) for the *final coordinates* into the left hand side of (6) and then rearrange. This complicates the analysis somewhat, but is otherwise straightforward. The results of the analysis are summarized next.

TRANSPORT matrices from MARYLIE matrices

The final relationships between the R-matrix for TRANSPORT the R-matrix of MARYLIE can be summarized by:

$$
\begin{aligned}
&[R_{ij}]_T = [R_{ij}]_M \quad \text{for all i,j , except for} \\
&[R_{i5}]_T = -(1/\beta_s)\,[R_{i5}]_M \quad \text{when } i=1,\dots,4\ ; \\
&[R_{i6}]_T = -(\beta_s)\,[R_{i6}]_M \quad \text{when } i=1,\dots,4\ ; \\
&[R_{5j}]_T = -(\beta_s)\,[R_{5j}]_M \quad \text{when } j=1,\dots,4\ ; \\
&[R_{6j}]_T = -(1/\beta_s)\,[R_{6j}]_M \quad \text{when } j=1,\dots,4\ ; \\
&[R_{56}]_T = (\beta_s)^2\,[R_{56}]_M \ ; \text{ and} \\
&[R_{65}]_T = (1/\beta_s)^2\,[R_{65}]_M \quad . \qquad (19)
\end{aligned}
$$

The relationships between the T-matrix for TRANSPORT and the T-matrix of MARYLIE, simplified for the magnetic case where R_{6j}=0 when j=1,…, 5 and R_{66}=1, can be summarized by:

$[T_{ijk}]_T = [T_{ijk}]_M$ for i=1,…, 5 , all j,k, except for
$[T_{ij5}]_T = -(1/\beta_s)\,[T_{ij5}]_M$ when i or j=1,…, 4 ;
$[T_{ij6}]_T = -(\beta_s)\,[T_{ij6}]_M$ when i or j=1,…, 4, except for;
$[T_{i26}]_T = [-(\beta_s)T_{i26} + R_{i2}]_M$ for i = 1 or 3 ;
$[T_{i46}]_T = [-(\beta_s)T_{i26} + R_{i4}]_M$ for i = 1 or 3 ;
$[T_{i66}]_T = [(\beta_s)^2T_{i26} - (1/2)(\beta_s/\gamma_s^2)\,R_{i6}]_M$ for i = 1 or 3 ;
$[T_{i16}]_T = [-(\beta_s)T_{i16} - R_{i1}]_M$ for i = 2 or 4 ;
$[T_{i36}]_T = [-(\beta_s)T_{i36} - R_{i3}]_M$ for i = 2 or 4 ;
$[T_{i56}]_T = [T_{i56} + (1/\beta_s)\,R_{i5}]_M$ for i = 2 or 4 ;
$[T_{i66}]_T = [(\beta_s)^2T_{i26}+(1/2)(\beta_s)(1+\beta_s^2)R_{i6}]_M$ for i = 2 or 4 ;
$[T_{5jk}]_T = -(\beta_s)\,[T_{5jk}]_M$ for all j,k , except for
$[T_{5j6}]_T = (\beta_s)^2\,[T_{5j6}]_M$ for j = 1 or 3 ;
$[T_{5j6}]_T = [(\beta_s)^2T_{5j6} - (\beta_s)\,R_{5j}]_M$ for j = 2 or 4 ; and
$[T_{566}]_T = [-(\beta_s)^3T_{566}+(1/2)(\beta_s^2/\gamma_s^2)\,R_{56}]_M$. (20)

The relationships between the U-matrix for TRANSPORT and the U-matrix of MARYLIE are a little longer to summarize. As with the R-matrix and T-matrix relationships given in (19) and (20) above, many of the $[U_{ijkl}]_T$ are given directly by the $[U_{ijkl}]_M$ *within factors involving powers of* β_s. Those relationships are relatively simple to derive and are not presented here. The relationships that involve the mixing of R- and T-matrix terms into the U-matrix equations are more complex. Those relationships are summarized in equation (20) below for the i=1 cases. The cases for i=3 can be constructed by symmetry. To avoid confusion of the subscript letter "l" with subscript number "1" equation (20) only uses k as a subscript letter for indices appearing in either the 3rd or 4th position.

$[U_{11k6}]_T = [-(\beta_s)U_{11k6} + T_{11k}]_M$ for k = 2 or 4 ;
$[U_{1j66}]_T = [(\beta_s)^2U_{1166} - (1/2)(\beta_s/\gamma_s^2)T_{1j6}]_M$
for j = 1 or 3 ;
$[U_{122k}]_T = [U_{122k} - (1/2)R_{1k}]_M$ for k = 2 or 4 ;
$[U_{12k6}]_T = [-(\beta_s)U_{12k6} + 2T_{12k}]_M$ for k = 2 or 4 ;
$[U_{1236}]_T = [-(\beta_s)U_{1236} + T_{123}]_M$;
$[U_{1j44}]_T = [U_{1j44} - (1/2)R_{1j}]_M$ for j = 2 or 4 ;
$[U_{1j56}]_T = [U_{1j56} - (1/\beta_s)T_{1j5}]_M$ for j = 2 or 4 ;
$[U_{1j66}]_T = [(\beta_s)^2U_{1j66} - (1/2)\beta_s(3-\beta_s)^2T_{1j6}]_M$
for j = 2 or 4 ;
$[U_{1446}]_T = [-(\beta_s)U_{1446} + 2T_{144}]_M$;
$[U_{1566}]_T = [-(\beta_s)U_{1566} + (1/2)(1/\gamma_s^2)\,T_{156}]_M$;
$[U_{1666}]_T = [-(\beta_s)^3U_{1666}+(\beta_s^2/\gamma_s^2)T_{166}+(1/2)(\beta_s^3/\gamma_s^2)R_{16}]_M$;
(20)

For j=2 and 4 every $[U_{ijkl}]_T$ term involves the mixing of R- and T-matrix elements with the $[U_{ijkl}]_M$. Only a few representative examples can be presented in a paper of this length. The results given below for $[U_{2111}]_T$ and $[U_{2112}]_T$ indicate the general structure of the U-matrix expressions.

$$[U_{2111}]_T = [U_{2111}+(1/2)(1/\beta_s^2)(3-\beta_s^2)R_{61}^2R_{21}+(1/2)R_{21}^3 +(1/2)R_{41}^2R_{21}+(1/\beta_s)R_{61}T_{211}]_M \text{ , and}$$
$$[U_{2112}]_T = [U_{2112}+(1/2)(1/\beta_s^2)(3-\beta_s^2)R_{61}^2R_{22} +(1/\beta_s^2)(3-\beta_s^2)R_{61}R_{62}R_{21}+(3/2)R_{21}^2R_{22} +(1/2)R_{41}^2R_{22}+(1/2)R_{41}R_{42}R_{21} +(1/\beta_s)R_{61}T_{212}+(1/\beta_s)R_{62}T_{211}]_M \text{ .} \quad (21)$$

SUMMARY

Formulas have been developed to compute TRANSPORT and TURTLE transfer matrices from either the Lie maps or transfer matrices of MARYLIE and MAD. The general procedure for deriving the formulas is outlined, and selected examples of the results are presented. The formulas obtained are believed to be complete through 3rd order. The formulas have been added as new tools [6] in the Particle Beam Optics Laboratory (PBO Lab) software, where they have been applied to a representative set of magnetic optics elements to compare transfer matrices through 3rd order. The new tools should prove valuable in comparing results from different optics codes.

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