SLAC–PUB–7638
DESY 97–163
August, 1997

From Symplectic Integrator to Poincaré Map: Spline Expansion of a Map Generator in Cartesian Coordinates *

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Abstract

Data from orbits of a symplectic integrator can be interpolated so as to construct an approximation to the generating function of a Poincaré map. The time required to compute an orbit of the symplectic map induced by the generator can be much less than the time to follow the same orbit by symplectic integration. The construction has been carried out previously for full-turn maps of large particle accelerators, and a big saving in time (for instance a factor of 60) has been demonstrated. A shortcoming of our work to date arose from the use of canonical polar coordinates, which precluded map construction in small regions of phase space near coordinate singularities. This paper shows that Cartesian coordinates can also be used, thus avoiding singularities. The generator is represented in a basis of tensor product B-splines. Under weak conditions the spline expansion converges uniformly as the mesh is refined, approaching the exact generator of the Poincaré map as defined by the symplectic integrator, in some parallelepiped of phase space centered at the origin.

Invited paper at the *NSF/CBMS Regional Conference on Numerical Analysis of Hamiltonian Systems*, Colorado School of Mines, Golden, Colorado, June 2–6, 1997. Proceedings of the conference to be published in *Applied Numerical Mathematics*.

*Work supported in part by Department of Energy contract DE–AC03–76SF00515 and the Deutsches Elektronen-Synchrotron (DESY), Hamburg.

1 Introduction

Questions of stability in Hamiltonian systems can usually be addressed by restricting attention to a *Poincaré section* Σ, which has dimension one less than the effective dimension of phase space [1]. (For an autonomous system in d degrees of freedom the effective dimension is that of the energy surface, namely $2d-1$; for a non-autonomous system in d degrees of freedom and Hamiltonian periodic in the time the effective dimension is $2d+1$, the dimension of the so-called extended phase space.) In the autonomous case suppose that there is a T-periodic orbit Γ, and choose Σ so that it intersects Γ transversely at z_0. Then a point z in a sufficiently small neighborhood $U \subset \Sigma$ of z_0 will return to Σ in a time $t(z)$ close to T. If $\Phi(z;t)$ is the time evolution map that takes $z = z(0)$ into $z(t)$, then the *Poincaré return map* is $M = \Phi(z;t(z))$ with z restricted to U. In the non-autonomous case with $T-$periodic Hamiltonian, a convenient choice for Σ consists of the entire $2d-$dimensional phase space. Then the Poincaré map is simply $M = \Phi(z,T)$. The full-turn map of particle accelerator theory is a Poincaré map under this definition, but in that theory the independent variable t is not actually the time, but rather arc-length s along a closed reference orbit [2,3]. Thus, the map describes the change in phase space coordinates when the particle makes a full turn around the accelerator ring.

The Poincaré section is a convenient arena in which to study stability by methods such as long-term mapping and construction of quasi-invariants, or to study resonance structure [4]. Its lower dimension in comparison to effective phase space can be critical in making it easier to compute and visualize quantities of interest such as quasi-invariant surfaces.

In numerical work on non-integrable flows, the basic dynamical model is often provided by a *symplectic integrator* [5–8]. The orbits of the integrator, the *numerical flow*, define a *numerical Poincaré map* M. (In the case of an autonomous system, part of the algorithm to determine M consists of locating the intersection of the orbit with the Poincaré section [9,10]. Since it is easy to locate the intersection approximately, some iterative procedure or a local change of variable will suffice to locate it exactly.) The use of M, defined in this way as the result of numerical integration, is fairly common in the literature of dynamical systems. Another idea is to devise an approximate closed formula for M. If the approximation $\tilde{M}$ could be evaluated much more quickly than M itself, one might be able to follow much longer orbits and make better estimates of long-term stability than would otherwise be possible. This approach has been pursued seriously by authors in accelerator theory, because something of the sort provides the only hope of following orbits over the long times that are involved in high-energy hadronic storage rings. The particle beams are stored for the order of one day, during which time there may be

about 10^{11} interactions with localized non-linear magnetic fields [11]. It is far too expensive to follow such long orbits by symplectic integration through each of the nonlinear regions, even though it is considered adequate to use only a few integration steps per region.

In early work, $\tilde{M}$ was represented by a truncated power series [12,13]. Although that worked quite well at small oscillation amplitudes, it was doubtful at large amplitudes near the effective border of stability (the "dynamic aperture"), because the violation of the symplectic condition was too large (for feasible orders of truncation)[14]. One response to the requirement of symplecticity, the one that we pursue, is to construct in closed form the canonical, mixed-variable generator of a map $\tilde{M}$, rather than $\tilde{M}$ itself. The resulting implicit definition of $\tilde{M}$ adds only moderately to the cost of iterating the map. Another idea, due to Irwin [15] and pursued by Dragt and Abell [16,17], results in a map $\tilde{M}$ that is both explicit and symplectic, but the approximation theory of that technique is difficult to manage, and the prospects of a practical advantage still uncertain. By contrast, the approximation theory for the generating function is rather simple, as was shown in [18] and will be shown again here in a different framework.

In prior work by the authors and their collaborators [19,18,4] the generator was expressed in canonical polar coordinates. It was given as a Fourier series in angles, the Fourier coefficients being spline functions of actions. An advantage of this approach is that the Fourier coefficients can be represented explicitly in terms of the map M. A disadvantage is that coordinate singularities arise in problems with more than one degree of freedom, at points in phase space where just one action variable vanishes. No such singularities occur in Cartesian coordinates. Cartesian coordinates have been used by other authors [20–22], but only in schemes in which the generator is given as a truncated power series. Since the generator in any coordinate system has singularities at large phase-space amplitudes (possibly complex), the power series may show poor convergence at large amplitudes. We are therefore led to examine a spline expansion, which is likely to be more robust in the large-amplitude regime, and in any case should allow quicker map iteration. Quicker iteration arises from the fact that one has only to evaluate the local, low-order polynomial components of the splines, rather than all terms of a multidimensional power series.

As far as we know, maps $\tilde{M}$ giving a close approximation to M for non-trivial flows have been used only in accelerator physics. It seems likely that the method could be valuable in other Hamiltonian problems with a few degrees of freedom, in subjects such as plasma physics, models of galactic dynamics, and semi-classical quantization of small molecules. The construction of quasi-invariant surfaces [24], as well as computation of long orbits, is aided by fast mapping.

2 Generating Function as a Line Integral

For simplicity in notation we consider a system in one degree of freedom. The generalization to two or more degrees of freedom will be obvious, at least when the motions are decoupled at the linear level as in the case studied in Ref.[18]. The map M defined by a symplectic integrator will be denoted in Cartesian coordinates (x, p) as follows. If $M : (x, p) \mapsto (x', p')$ then

$$x' = \cos(2\pi\nu)\ x + \sin(2\pi\nu)\ p + X(x, p)\ , \tag{1}$$
$$p' = -\sin(2\pi\nu)\ x + \cos(2\pi\nu)\ p + P(x, p)\ . \tag{2}$$

or, in terms of the rotation matrix R for angle $2\pi\nu$,

$$z' = Rz + N(z)\ , \tag{3}$$

where $z = (x, p)^T$ and $N(z) = (X(x, p), P(x, p))^T$ are column vectors. The positive constant ν is the tune or winding number. We suppose that X and P have the forms

$$X(x, p) = \sum_{q=2}^{n} X_q(x, p)\ , \quad P(x, p) = \sum_{q=2}^{n} P_q(x, p)\ , \tag{4}$$

where X_q and P_q are homogeneous polynomials of degree q and n is finite. A typical symplectic integrator [5,6], applied to the Hamiltonian $H(x, p, s)$ of an accelerator model, produces such a map. Here the independent time-like variable is s, the arc length along a closed reference orbit, and H is periodic in s with period equal to the circumference C of the reference orbit. The Poincaré section Σ is the two-dimensional phase space. Each step of the integrator produces a polynomial map representing transport through a simple magnetic element or a fraction of such an element. A composition of a finite number of steps corresponding to a full turn around the accelerator yields a map of form (3)-(4), with n for a typical magnetic lattice being quite large (as much as several thousand). The integrator may represent the effect of linear magnetic elements as exact rotations. Some codes follow that procedure, while others use similar algorithms for linear and nonlinear elements.

In defining the generating function we have to distinguish two domains of the tune parameter ν, one in which $\cos(2\pi\nu)$ does not vanish, and one in which $\sin(2\pi\nu)$ does not vanish. Any ν falls into one of the two cases

$$(i): \qquad |\cos(2\pi\nu)| > 1/\sqrt{2}\ , \tag{5}$$
$$(ii): \qquad |\sin(2\pi\nu)| \geq 1/\sqrt{2}\ . \tag{6}$$

For convenience we choose this division of ν-space, while remarking that a less symmetric division could sometimes be better in higher dimensional problems in which ν is a vector. Now suppose for the moment that the nonlinear term N in Eq.(3) were absent. Then in case (i) we could solve (1) for x as a function of p and x' and, correspondingly, we could represent the map by means of a generating function $L(p, x')$ and the equations

$$p' = L_{x'}(p, x') \ , \qquad x = L_p(p, x') \ , \tag{7}$$

where subscripts denote partial derivatives. From the linear map and integration of (7) one finds

$$L(p, x') = \frac{1}{\cos(2\pi\nu)} p x' - \frac{\tan(2\pi\nu)}{2}(p^2 + x'^2) \ , \tag{8}$$

a result that is unique up to a constant addend. On the other hand, in case (ii) we can solve Eq.(1) for p as a function of x and x', and represent the map through a different generating function $L(x, x')$ and the equations

$$p' = -L_{x'}(x, x') \ , \qquad p = L_x(x, x') \ , \tag{9}$$

with

$$L(x, x') = \frac{1}{\sin(2\pi\nu)} x x' - \frac{\cot(2\pi\nu)}{2}(x^2 + x'^2) \ . \tag{10}$$

In a region of phase space sufficiently close to the origin, we expect that the full nonlinear equation (1) will behave like the linear equation as far as solving for x or p is concerned, thanks to the fact that X begins with quadratic terms. Thus we look for a generator depending on (p, x') in case (i), but one depending on (x, x') in case (ii). Henceforth we deal only with case (i), since (ii) can be treated similarly.

We write the full generator as

$$S(p, x') = L(p, x') + G(p, x') \ , \tag{11}$$

where L is the generator of the linear map as given by Eq.(8). The map (3) is to be defined implicitly by the equations

$$p' = p/\cos(2\pi\nu) - x' \tan(2\pi\nu) + G_{x'}(p, x') \ , \tag{12}$$

$$x \ = x'/\cos(2\pi\nu) - p \ \tan(2\pi\nu) + G_p(p, x') \ . \tag{13}$$

It is well known, and easy to verify by direct computation, that a map defined by (12) and (13) is symplectic, for any $G \in C^2$. The existence of G such that these equations do indeed define the map (3) is implied by the existence of a suitable solution $x(p, x')$ of Eq.(1), provided that the map is symplectic. This argument was outlined by Berz in the framework of formal Taylor expansions [21]. We repeat his argument with more detail and without appeal to expansions.

Let us define $I(r)$ to be the open interval $(-r, r)$ and assume the following:

- (A) There exists a unique solution $x(p, x')$ of (1) of the form

$$x = -p\ \tan(2\pi\nu) + x'/\cos(2\pi\nu) + F(p, x') \tag{14}$$

  for $(p, x') \in I(r) \times I(r) = S(r)$, with $F \in C^1[S(r)]$.
- (B) The Jacobian of the transformation $x \mapsto x'$ at fixed p, namely $\partial x'/\partial x = \cos 2\pi\nu + X_x(x, p)$ from Eq.(1), is non-zero in the image of $S(r)$ under the transformation $x(p, x')$.
- (C) The map (3) is symplectic.

Under assumption (A) we can express the gradient of G as a function $\gamma(p, x')$. Defining the vector $\zeta = (p, x')$ we have

$$G_\zeta = \gamma(\zeta)\ , \tag{15}$$

where $\gamma \in C^1[S(r)]$ and

$$\gamma_1 = F(p, x')\ , \tag{16}$$

$$\gamma_2 = -\sin(2\pi\nu)F(p, x') + P(-p\ \tan(2\pi\nu) + x'/\cos(2\pi\nu) + F(p, x'), p)\ . \tag{17}$$

These expressions are obtained by comparing Eqs. (1) and (2) with Eqs. (12) and (13), using assumption (A) to express functions of (x, p) in terms of (p, x').

In order that Eq.(15) have a C^2 solution it is clearly necessary that curl $\gamma = \partial\gamma_2/\partial\zeta_1 - \partial\gamma_1/\partial\zeta_2 = 0$. Conversely, Stokes's theorem ensures that if curl $\gamma = 0$ in $S(r)$, then (15) has a C^2 solution in $S(r)$ given by the path-independent line integral

$$G(\zeta) = \int_{\zeta_0}^{\zeta} \omega\ , \qquad \omega = \gamma_1 d\zeta_1 + \gamma_2 d\zeta_2\ . \tag{18}$$

A solution of (15) is obviously unique up to a constant addend.

It is a matter of calculation to show that assumptions (B) and (C) above imply that curl $\gamma = 0$, hence that a solution of (15) exists. In calculating curl γ we encounter derivatives of F which may be obtained in terms of the function $X(x,p)$ by differentiating the equation that defines F, namely

$$F(p,x') = -X(-p\ \tan(2\pi\nu) + x'/\cos(2\pi\nu) + F(p,x'),p)/\cos(2\pi\nu)\ , \quad (19)$$

which results from substituting the assumed form (14) in (1). The resulting expressions have a divisor $\cos(2\pi\nu) + X_x$, which is non-zero by assumption (B). In this two-dimensional example the symplectic condition on the Jacobian matrix D of the map is equivalent to $\det D = 1$, or

$$\cos(2\pi\nu)(X_x + P_p) + \sin(2\pi\nu)(X_p - P_x) + X_x P_p - X_p P_x = 0\ . \quad (20)$$

Now by using the derivatives of F and Eq.(20) one can verify that curl $\gamma = 0$. In two or more degrees of freedom the steps of the computation follow the same lines but are less obvious; see Ref.[18].

Finally we show that assumptions (A) and (B) hold if the square $S(r)$ is sufficiently small by applying the contraction mapping theorem to Eq.(1) written in the form

$$x = A(x;p,x') = [x' - p\ \sin(2\pi\nu) - X(x,p)]/\cos(2\pi\nu)\ . \quad (21)$$

We look for a solution x in the complete metric space $\bar{I}(s)$, the closure of $I(s)$. If $x \in \bar{I}(s)$ and $(p,x') \in S(r)$, then $A(x;p,x') = O(r) + O(sr) + O(s^2) + O(r^2)$ by Eq.(4); hence A as a function of x takes $\bar{I}(s)$ into itself if s and r are sufficiently small. Also, for $x_1, x_2 \in \bar{I}(s)$, the mean value theorem and (4) give

$$\begin{aligned} |A(x_1;p,x') - A(x_2;p,x')| &\le \frac{1}{|\cos(2\pi\nu)|} \sup_{\xi \in \bar{I}(s), p \in I(r)} |X_x(\xi,p)||x_1 - x_2| \\ &= (O(r) + O(s))|x_1 - x_2| \le \beta |x_1 - x_2|\ , \end{aligned} \quad (22)$$

with $\beta < 1$ for r and s small. Thus the contraction mapping principle implies that there is a unique solution of Eq.(1) in $\bar{I}(s)$ for r sufficiently small. Moreover, we have already demanded that $\sup |X_x|/|\cos(2\pi\nu)| < 1$, so that assumption (B) holds. It remains to show that $x(p,x') \in C^1[S(r)]$, but that follows immediately from an appropriate form of the implicit function theorem [23] (or from a simple direct argument using (19)) since $x - A(x;p,x')$ is a polynomial in all three variables. In fact, x has continuous derivatives of all orders, as does the generator G as given by Eq.(18).

3 Construction of the Generator from Numerical Values of the Symplectic Map

We now turn to the question of how to represent and determine the generator G in a numerical setting. Our plan is to represent the γ_i of Eqs.(16),(17) in a spline basis, then carry out the integral (18) analytically to obtain the desired approximation $\tilde{G}$ to G. When $\tilde{G}$ is used in place of G to define a map implicitly through (12) and (13), it is important that the derivatives $\tilde{G}_{x'}$ and $\tilde{G}_p$ be evaluated exactly, since otherwise we cannot expect the implicit map to be exactly symplectic. Accordingly, we shall take the derivatives analytically, by differentiating the splines and integrals of splines that will serve to represent $\tilde{G}$.

We first look for the values of γ_i on a mesh $\{p_i, x'_j\}$, then do spline interpolation to approximate the function off the mesh. Thus we require the function $F(p, x')$, which expresses the solution of (1) through (14), at the mesh points. We have seen that this function can be obtained by the simple iteration used in the proof of the contraction mapping principle, for (p, x') near the origin. By using instead a Newton iteration or one of its variants, one has a chance to extend the solution to a larger region of the parameter (p, x'). Here one might use a linear extrapolation from the last good solution to obtain a first guess for an iteration at the next larger value of the parameter, or use a more sophisticated continuation method based on a differential equation with p or x' as independent variable. In any case the iteration will involve several evaluations of the map function $X(x, p)$ and possibly its derivatives, which can be an excessive expense in the case of complicated systems such as particle accelerators.

To reduce cost we suggest that $X(x, p)$ first be evaluated on a mesh, with the mesh points in p being the same as the p_i above, and the resulting values interpolated by splines in x to give an approximation $\tilde{X}(x, p_i)$ for all x and all i. Now $\tilde{X}$ can be used in a Newton iteration, to determine an approximation $\tilde{F}(p_i, x'_j) \approx F(p_i, x'_j)$, all i, j. The derivative required in Newton's method is obtained analytically by differentiating splines. If the mesh is sufficiently fine, $\tilde{F}$ will be a close approximation to the exact F, and it can be used as a first guess in a final Newton iteration using the exact X to determine the exact F on the mesh. It should be possible to get a solution after relatively few iterations, using a modified Newton method (not quadratically convergent) based on the approximate derivative $\tilde{X}_x$ given by splines. Notice that the evaluation of P in Eq.(17) at the final value of x is free, since X and P are always evaluated together by the symplectic integrator. The final iteration gives directly the exact values of γ on the mesh, modulo round-off error, if the iteration is carried to machine precision.

In practice it may turn out that $\tilde{F}$ gives an adequate approximation without refinement, or that it is more economical to improve $\tilde{F}$ by refining the mesh rather than by the final iteration described. To simplify the approximation theory let us assume, however, that F and γ are given exactly on the mesh.

Let us digress a moment to give another motivation for the initial interpolation of map functions. At little extra expense the interpolation of values of $X(x,p)$ on a mesh can be augmented with an interpolation of $P(x,p)$ to give explicit, approximate map functions $\tilde{X}(x,p), \tilde{P}(x,p)$. This explicit map should be quite useful, in at least two ways. First, it can give a close first guess for a Newton solution of Eq.(13), the latter being a necessary step in iterating the map defined by the generator. Second, the explicit map can save time in the construction of quasi-invariant tori, an important application of maps in which exact symplecticity is not essential [24].

Now that γ is given on the mesh, it remains to interpolate the values on the mesh and then carry out the integral (18). We denote the interpolation by $\tilde{\gamma}$ and represent it in a tensor-product B-spline basis [25]. Taking spline knots and end conditions the same in both dimensions we can write

$$\tilde{\gamma}(p,x') = \sum_{i,j} g^{ij} B_i(p) B_j(x') \ , \tag{23}$$

where $g^{ij} = (g_1^{ij}, g_2^{ij})$ is a vector and the B_i are one-dimensional B-splines of order k with maximum smoothness allowed for that k; i.e., they are made up of polynomials of degree not greater than $k-1$, and have $k-2$ continuous derivatives. A convenient choice of path for the integral (18) in the (p,x')-plane consists of the straight line from $(0,0)$ to $(0,x')$, followed by the straight line from $(0,x')$ to (p,x'). Then our approximation $\tilde{G}$ to the exact G is

$$\tilde{G}(p,x') = \int_0^{x'} \tilde{\gamma}_2(0,u)du + \int_0^{p} \tilde{\gamma}_1(u,x')du \ . \tag{24}$$

Introducing (23) and defining the constant $g_2^j = \sum_i g_2^{ij} B_i(0)$ we have

$$\tilde{G}_p(p,x') = \tilde{\gamma}_1(p,x') = \sum_{i,j} g_1^{ij} B_i(p) B_j(x') \ , \tag{25}$$

$$\begin{aligned} \tilde{G}_{x'}(p,x') &= \tilde{\gamma}_2(0,x') + \int_0^{p} \frac{\partial \tilde{\gamma}_1}{\partial x'}(u,x')du \\ &= \sum_j g_2^j B_j(x') + \sum_{ij} g_1^{ij} B_j'(x') \int_0^{p} B_i(u)du \ . \end{aligned} \tag{26}$$

In iterating the implicit map defined by Eqs. (12) and (13), we have to solve (13) for x' by Newton's method. For that reason it is expedient to require that $G_p(p, x')$ have a continuous second derivative with respect to x', so that the standard sufficient conditions for convergence of Newton's method can be applied [26]. If we take the spline order $k \geq 4$ we can provide such smoothness in the formula (25).

The formula (25) is quite suitable as it stands for numerical evaluation. One can use de Boor's stable recursive algorithm for B-spline evaluation, and take advantage of the fact that the B_i are locally supported; i.e., only k of the $B_i(x)$ are non-zero at any x. Thus for $k = 4$ only sixteen terms in the sum (25) will be non-zero at any (p, x'). For evaluation of (26) we have to deal with integrals of B-splines, which are not locally supported. Most of the cost of non-local support can be avoided by computing and storing, once for all, the integrals over complete inter-knot intervals. Suppose that the knots are at points p_r, with $p_{r+1} \geq p_r$, and define $\chi_r(p)$ to be the characteristic function of the half-open interval $[p_r, p_{r+1})$;(for the largest value of $r+1$ make this the closed interval). Then

$$\sum_i g_1^{ij} \int_0^p B_i(u)du = \sum_i g_1^{ij} \sum_r \chi_r(p) \Big[\int_0^{p_r} + \int_{p_r}^p \Big] B_i(u)du \ . \tag{27}$$

After defining the constants

$$C_r^j = \sum_i g_1^{ij} \int_0^{p_r} B_i(u)du \ , \tag{28}$$

we can write (26) as

$$\begin{aligned} \tilde{G}_{x'}(p, x') = & \sum_j g_2^j B_j(x') + \\ & \sum_j B_j'(x') \sum_r \chi_r(p) \Big[C_r^j + \sum_i g_1^{ij} \int_{p_r}^p B_i(u)du \Big] \ . \end{aligned} \tag{29}$$

The remaining integral involves only one of the polynomial components of B_i. Suppose that (p, x') is fixed. Then at most k values of j contribute non-zero terms to this formula, and for a given j, only one value of r and at most k values of i contribute. As in the case of (25), the full sum is "mostly empty", and we have a formulation that seems suitable for fast iteration of the map.

One could avoid integrals of splines and simplify coding by representing $\tilde{G}$ directly in the tensor product basis, by interpolating values of (24). It seems

worthwhile, however, to avoid an extra layer of approximation by working with Eq.(29).

4 Convergence of the Spline Approximation

We wish to show that our spline approximation to the gradient of the generator, $(\tilde{G}_p, \tilde{G}_{x'})$, converges to the exact gradient, $(G_p, G_{x'})$, when the mesh $\{p_i, x'_j\}$ is refined indefinitely. Since we have already treated the nonlinear part of the problem in passing from the given map to the function γ, this is simply a matter of applying known convergence results for spline interpolation to Eqs.(25) and (26). As an example, we apply a theorem of Carlson and Hall [27] on bicubic spline interpolation in a rectangle. Those authors use a tensor product basis of cubic splines ($k = 4$) with continuous second derivatives at the knots and Hermite end conditions; i.e., the value of the partial derivative of the function at the endpoints in either variable is specified, as is the mixed second derivative at each of the four corners. Let $f(x_1, x_2)$ be any function in $C^4(D)$, where D is a rectangle in the (x_1, x_2)-plane, and let h_i be the maximum mesh step in the x_i-direction. If $s(x_1, x_2)$ is the bicubic spline interpolant with Hermite end conditions, then the theorem of Carlson and Hall is that for all $(x_1, x_2) \in D$,

$$\begin{aligned} \|(f-s)^{(i,j)}\| \le{}& \epsilon_{4-j,i}\, h_1^{4-i} \|f^{(4-j,j)}\| + \epsilon_{2i}\epsilon_{2j} h_1^{2-i} h_2^{2-j} \|f^{(2,2)}\| \\ &+ \epsilon_{4-i,j}\, h_2^{4-j} \|f^{(i,4-i)}\| \ , \qquad 0 \le i,j \le 2 \ , \end{aligned} \tag{30}$$

where $f^{(i,j)} = \partial^{i+j} f / \partial x_i \partial x_j$ and $\|\cdot\|$ is the supremum norm. The constants $\epsilon_{i,j}$ are given in Table 1 of Ref.[27].

Since γ has continuous fourth derivatives in some rectangle D centered at the origin (in fact is in $C^\infty(D)$), this can be applied to Eqs.(25), (26) to get the following error bounds:

$$\begin{aligned} |G_p(p,x') - \tilde{G}_p(p,x')| &= |\gamma_1(p,x') - \tilde{\gamma}_1(p,x')| \\ &\le \epsilon_{40} h_1^4 \|\gamma_1^{(4,0)}\| + \epsilon_{20}^2 h_1^2 h_2^2 \|\gamma_1^{(2,2)}\| + \epsilon_{40} h_2^4 \|\gamma_1^{(0,4)}\| \ , \end{aligned} \tag{31}$$

$$\begin{aligned} |G_{x'}(p,x') - \tilde{G}_{x'}(p,x')| &\le |\gamma_2(0,x') - \tilde{\gamma}_2(0,x')| + \left| \int_0^p \left[\frac{\partial \gamma_1(u,x')}{\partial x'} - \frac{\partial \tilde{\gamma}_1(u,x')}{\partial x'} \right] du \right| \\ &\le \epsilon_{40} h_1^4 \|\gamma_2^{(4,0)}\| + \epsilon_{20}^2 h_1^2 h_2^2 \|\gamma_2^{(2,2)}\| + \epsilon_{40} h_2^4 \|\gamma_2^{(0,4)}\| \\ &\quad + |p| \left[\epsilon_{30} h_1^4 \|\gamma_1^{(3,1)}\| + \epsilon_{20}\epsilon_{21} h_1^2 h_2 \|\gamma_1^{(2,2)}\| + \epsilon_{41} h_2^3 \|\gamma_1^{(0,4)}\| \right] \ . \end{aligned} \tag{32}$$

With $h_1 = h_2 = h$ we have $O(h^4)$ uniform convergence of one derivative, but only $O(h^3)$ for the other, in the rectangle D.

To provide derivatives of γ at the endpoints for the Hermite boundary condition, one would have to know derivatives of the map function $N(z)$ of Eq.(3). Those can be obtained by automatic differentiation [28,29,13] of the symplectic integration algorithm, a technique that is available in some accelerator tracking codes. Alternatively, the derivatives might be approximated by using one-sided numerical differentiation from function values on the basic mesh alone. Szeto reports $O(h^4)$ convergence for cubic spline interpolation in that scheme, at least in one dimension, if numerical differentiation of appropriately high order is used [30]. For not-a-knot boundary conditions, requiring no derivatives, he finds $O(h^3)$.

5 Acknowledgment

R. Warnock wishes to thank Graeme Fairweather and Erik Van Vleck for generous hospitality and support at the Colorado School of Mines during the NSF/CBMS Regional Conference on Numerical Analysis of Hamiltonian Systems. J. Ellison acknowledges partial support for this work from the Deutsches Elektronen-Synchrotron (DESY) in Hamburg.

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