# METHODS OF STABILITY ANALYSIS IN NONLINEAR MECHANICS* 

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ABSTRACT
We review our recent work on methods to study stability in nonlinear mechanics, especially for the problems of particle accelerators, and compare our ideas to those of other authors. We emphasize methods that (a) show promise as practical design tools, (b) are effective when the nonlinearity is large, and (c) have a strong theoretical basis.

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## 1. INTRODUCTION

Emerging problems of nonlinear mechanics in accelerators are taking on a new order of difficulty. Low emittance damping rings and synchrotron light sources have strongly nonlinear lattices and complications due to wigglers and undulators. Large hadron rings are hard to analyze because of their sheer size and the presence of high multipoles, random and systematic, in superconducting magnets. Largeaperture antiproton collectors and conventional-magnet boosters for hadron colliders have prominent nonlinear effects. As the problems become more difficult. the shortcomings of traditional analysis become more apparent.

The traditional methods are based on tracking of single particles and perturbation theory. We first comment on efforts to extend and improve these established methods.

## 2. TRACKING

Tracking is the only method that is generally applicable, in that it gives results in any region of phase space. Its drawbacks are (i) computational expense, and (ii) the difficulty of interpreting the results.

To minimize expense while maintaining accuracy, it is important that the method used to integrate Hamilton's equations generate a symplectic time evolution map. (This is true at least for circular machines; for single-pass beam transport the symplectic condition is less important.) Thin-element "kick codes" generate symplectic time evolutions. By putting together sufficiently many thinelement kicks, one can approximate the effect of a thick element to any desired accuracy. There exist more sophisticated symplectic integrators, ${ }^{1,2,3,4}$ analogous to standard numerical integration schemes for general differential equations. Ruth's fourth-order explicit integrator ${ }^{5}$ has been tested with good results in a skeleton tracking code. A general purpose tracking code using a high order explicit symplectic integrator remains to be written. Also, the "numerical analysis" of symplectic integrators should be developed; i.e., the various algorithms should be compared through rigorous error analysis and experimental tests, as in the established theory of numerical integration of differential equations. We hope that the subject of symplectic integrators will thrive, since we see an important role for it in the general approach to stability questions outlined below. Fortunately, there is increasing interest on the part of mathematicians and physicists in various fields. ${ }^{6}$

In another approach to reduction of cost, one tries to construct an explicit map to describe propagation through a segment of an accelerator, the segment being anything from a single lattice element to the whole lattice. We consider this idea in Section 6.

The problem of how to interpret tracking data is sometimes easy and sometimes difficult. If the computed trajectory leaves the desired physical aperture, we have the obvious conclusion that the motion is effectively unstable. To verify the conclusion, we need only provide a proof that there is no problem of numerical error, which often can be done by backtracking to the initial conditions. On the other hand, if the trajectory stays within the required aperture for many thousands of turns, we do not know what to conclude, since the number of possible turns in a computation is always very small compared to the number achieved by a real beam. In fact, there are examples of tracking runs in which the orbit appeared to be stable for $10^{5}$ turns or so, and then suddenly became unstable.

In view of this ambiguity, it is interesting to examine tracking data in ways that go beyond the simple requirement of confinement to a defined aperture. One possiblity is to judge the data for degree of deviation from linear motion. The degree of deviation, which may be defined in several similar ways, is called the "smear". ${ }^{7}$ Through experience and intuition one tries to set a safe limit for the smear. In Ref. 8 we gave an example, a two-resonance model, in which the smear was quite small even though the system was near the onset of large-scale chaotic motion. This and other considerations suggest that a rule-of-thumb for maximum allowed smear is not likely to be universal. A correct rule might depend strongly on the tune and be different for different kinds of lattices. Nevertheless, optimizing the lattice to reduce the smear is clearly a worthwhile aim.

An idea with a stronger motivation is to test for confinement of the orbit to an invariant surface. On an invariant surface the action $\mathbf{I}$ is a function of the angle variable $\boldsymbol{\Phi}$ and the orbital position $s$ which may be written as

$$
\begin{equation*}
\mathbf{I}=\mathbf{J}+G_{\boldsymbol{\Phi}}(\mathbf{J}, \boldsymbol{\Phi}, s) \tag{2.1}
\end{equation*}
$$

Here $\mathbf{J}$ is the invariant action, and $G$ is the Hamilton-Jacobi generating function which solves the Hamilton-Jacobi equation,

$$
\begin{equation*}
H\left(\mathbf{J}+G_{\boldsymbol{\Phi}}, \boldsymbol{\Phi}, s\right)+G_{s}=H^{(1)}(\mathbf{J}) \tag{2.2}
\end{equation*}
$$

The solution $G$ generates the canonical transformation $(\mathbf{I}, \mathbf{\Phi}) \rightarrow(\mathbf{J}, \mathbf{\Psi})$ which is defined by (2.1) together with the following equation:

$$
\begin{equation*}
\boldsymbol{\Psi}=\boldsymbol{\Phi}+G_{\mathbf{J}}(\mathbf{J}, \boldsymbol{\Phi}, s) \tag{2.3}
\end{equation*}
$$

Bold-faced quantities are vectors with dimension equal to the number of degrees of freedom, and subscripts denote partial derivatives. The generator $G$ is periodic in $\boldsymbol{\Phi}$ with period $2 \pi$, and periodic in $s$ with period $C$.

The set of points on an orbit with $s=0, C, 2 C, \cdots$ are said to lie in a Poincaré surface of section. If the motion is regular and non-resonant, those points lie on a torus $\mathbf{I}=\mathbf{I}(\boldsymbol{\Phi} ; s=0)$, which may be expressed in the form (2.1). Each torus is labeled by a value of the invariant $\mathbf{J}$, which is the average of $\mathbf{I}(\boldsymbol{\Phi} ; s=0)$ over $\boldsymbol{\Phi}$. We can approximate the torus, when it exists, by fitting tracking data to a smooth surface. For instance, for betatron motion in two degrees of freedom we can determine two smooth, two-dimensional surfaces to pass through the points $\left(I_{1}, \Phi_{1}, \Phi_{2}\right)(s)$ and $\left(I_{2}, \Phi_{1}, \Phi_{2}\right)(s), s=0, C, 2 C, \cdots$ which all lie on a single orbit. Since the angle coordinates ( $\Phi_{1}, \Phi_{2}$ ) do not lie on a regular grid, one must have a surface fitting program which can handle scattered data. We have used the IMSL program IQHSCV, which produces a piece-wise polynomial surface which passes through the given points and has continuous first derivatives.

In Figures 1 and 2 we show results for the North Damping Ring of the SLC. Normalizing to the invariants, we plot $I_{1} / J_{1}$ and $I_{2} / J_{2}$ versus ( $\Phi_{1}, \Phi_{2}$ ), with the origin at zero. Each of the surfaces was fitted to 8000 points obtained from 8000 turns of a fourth order symplectic tracking code. Linear motion would correspond to flat surfaces, $I_{i} / J_{i}=1$. The initial displacements of the orbit correspond to about 3.7 mm (horizontal) and 2.6 mm (vertical) at the septum magnet. These are large but sustainable injection offsets for the ring considered. The smear is impressively large.

To gain more insight it is useful to compute the two-dimensional Fourier transform of $\mathbf{I}(\boldsymbol{\Phi} ; s=0)$, which gives us the Fourier coefficients of $G_{\boldsymbol{\Phi}}$ :

$$
\begin{equation*}
\mathbf{I}=\mathbf{J}+\sum_{\mathbf{m}} i \mathbf{m} g_{\mathbf{m}}(0) e^{i \mathbf{m} \cdot \mathbf{\Phi}} \tag{2.4}
\end{equation*}
$$

It is to be emphasized that we are making a Fourier analysis of the invariant surface, not an analysis of the time series $\mathbf{I}(s), s=0, C, 2 C, \cdots$. Although the latter is also of some interest, in that it can be compared to experiment, it is relatively difficult to interpret. The coefficients $\left.g_{\mathbf{m}}(s)\right|_{s=0}$ of (2.4) are the familiar Fourier coefficients of the generating function, which may also be computed in perturbation theory or by direct solution of the Hamilton-Jacobi equation. If $\boldsymbol{\nu}=\left(\nu_{1}, \nu_{2}\right)$ is the tune and $\mathbf{m} \cdot \boldsymbol{\nu}$ is close to an integer, the consequent resonance shows up as a relatively large value of $\mathbf{m} g_{\mathbf{m}}$ in (2.4), since, as is well known, the latter is amplified by a small divisor $\sin (\pi \mathbf{m} \cdot \nu)$. Thus, (2.4) analyzes the motion according to nonlinear resonances in a most direct and elementary way.

Taking an FFT of the surface in Fig. 1 or Fig.2, and retaining modes for $\left|m_{1}\right|,\left|m_{2}\right| \leq 15$, we obtain a Fourier series representation of the surface which agrees well with the original (piecewise-polynomial) surface computed by IQHSCV, and also agrees well with tracking beyond the original 8000 turns. Defining an appropriate metric $\Delta I$ for the difference between the tracked orbit and the


Figure 1 : Invariant surface for SLC North Damping Ring, obtained by a fit to tracking data. $I_{1}\left(\Phi_{1}, \Phi_{2}\right) / J_{1}$ plotted as function of $\Phi_{1}, \Phi_{2}$. Invariant action $J_{1}=2.489 \cdot 10^{-6} \mathrm{~m}$


Figure 2 : Invariant surface for SLC North Damping Ring, obtained by a fit to tracking data. $I_{2}\left(\Phi_{1}, \Phi_{2}\right) / J_{2}$ plotted as function of $\Phi_{1}, \Phi_{2}$. Invariant action $J_{2}=1.508 \cdot 10^{-6} m$

Fourier series (2.4) (the sum of the deviations divided by the number of orbit points) we find $\Delta I_{1} / J_{1}=1.4 \cdot 10^{-4}, \Delta I_{2} / J_{2}=2.2 \cdot 10^{-4}$ for the first 8000 turns, and then very similar values for an additional 8000 turns. On using more than 8000 turns to find the piece-wise polynomial surface and more modes in (2.4), we did not see much decrease of $\Delta I_{i} / J_{i}$. We did, however, maintain values less than $2 \cdot 10^{-4}$ for $\Delta I_{i} / J_{i}$ for 32000 turns. In Table 1 we give the ten largest Fourier coefficients of $I_{1}$, divided by $J_{1}$.

Table 1: Fourier Amplitudes of $G_{\Phi_{1}}$

| $\mathrm{m}_{1}$ | $\mathrm{~m}_{2}$ | $\operatorname{Re}\left(\mathrm{im}_{1} \mathrm{gm}_{\mathrm{m}}\right)$ | $\operatorname{Im}\left(\mathrm{im} \mathrm{g}_{\mathrm{m}}\right)$ |
| :---: | :---: | :---: | :---: |
| 2 | -2 | $-2.06 \cdot 10^{-7}$ | $-9.54 \cdot 10^{-9}$ |
| 1 | 0 | $6.76 \cdot 10^{-8}$ | $-1.91 \cdot 10^{-9}$ |
| 3 | 0 | $-6.61 \cdot 10^{-8}$ | $2.40 \cdot 10^{-10}$ |
| 4 | -4 | $-4.12 \cdot 10^{-8}$ | $-3.77 \cdot 10^{-9}$ |
| 2 | 2 | $1.21 \cdot 10^{-8}$ | $-9.57 \cdot 10^{-11}$ |
| 5 | -2 | $1.17 \cdot 10^{-8}$ | $5.09 \cdot 10^{-10}$ |
| 6 | -6 | $-1.16 \cdot 10^{-8}$ | $-1.59 \cdot 10^{-9}$ |
| 1 | 2 | $-9.34 \cdot 10^{-9}$ | $4.48 \cdot 10^{-10}$ |
| 8 | -8 | $-4.15 \cdot 10^{-9}$ | $-7.64 \cdot 10^{-10}$ |
| 7 | -4 | $2.98 \cdot 10^{-9}$ | $2.62 \cdot 10^{-10}$ |

Thus, we have a surface in the form (2.4) which appears to approximate an invariant surface. We comment presently on means to improve the approximation, but first remark that we have already obtained very reliable information on the important resonances, by means of a modest and convenient computation. Such information might be used to optimize the lattice. For instance, one might try to adjust sextupoles so as to minimize a "figure of demerit" such as the following:

$$
\begin{equation*}
\sum_{i} \frac{1}{J_{i}} \sum_{\mathbf{m}}\left|m_{i} g_{\mathrm{m}}(0)\right| \tag{2.5}
\end{equation*}
$$

The approximate invariant surface in the form (2.4) for $s=0$ can be extended to all s by integration of the Hamilton-Jacobi equation. One then has a generator which can be refined in accuracy through further iterations of the Hamilton-Jacobi
equation, possibly on a bigger mode set. This is a possible starting point for a thorough stability study, as is explained in Sections 4 and 5.

At large amplitudes, or even at small amplitudes with bad tunes, one encounters resonant structures associated with periodic orbits, which preclude the presence of invariant surfaces. In one degree of freedom the resonant structures are the familiar island chains, which can be graphed in a two-dimensional surface of section. In two degrees of freedom the resonant structures can be projected onto a section in which $s$ and one of the angles, say $\Phi_{1}$, are constant. In tracking through a finite number of turns we get essentially zero population of such a section. In a thin slice, $\left|\Phi_{1}\right|<\delta$, we might hope to get enough points to see a structure (slightly smeared out), provided that we can do very long tracking runs. This might be an interesting application of full-turn maps, which have the potential of greatly reducing computation times; see Section 6.

## 3. PERTURBATION THEORY

Perturbation theory ${ }^{9}$ is used primarily to find approximations to invariant surfaces and related quantities such as tune shifts, although it may be used as well to discuss time dependence. ${ }^{10}$ It is an excellent method for situations in which nonlinear effects are weak. Those situations may be defined as cases in which the first term of the perturbation series, or at most the first and second terms, provide a good approximation. Unfortunately, there is no such case in the region of phase space near the dynamic aperture of an accelerator. In the example of the previous section low order perturbation theory would fail drastically, as can be seen immediately from the rich mode spectrum of Table 1 . There are many appreciable modes that simply do not appear in low orders.

There have been attempts to estimate the dynamic aperture using perturbation theory and certain recipes, but the recipes lack theoretical foundation and may be unreliable. ${ }^{10}$

One might hope to save the day by going to higher orders in the perturbation series, but in our view there is little motivation for doing so. Higher order computations require symbol manipulation on a computer. The result is an analytic form for a higher order term, but so complicated as to have little intuitive value. Remembering also that convergence is in doubt, and that only a few terms of the series can be handled, one is better advised to seek a nonperturbative numerical method.

One non-perturbative approach is the simple surface-fitting method of the previous section, which may well turn out to be the most practical technique for getting a good first approximation in cases of strong nonlinearity. Another useful approach is iterative numerical solution of the Hamilton-Jacobi equation, as outlined in Section 4.

Forest and collaborators ${ }^{11}$, extending earlier work of Dragt and Finn, have developed an improvement to perturbation theory, which depends on prior construction of a full-turn map for propagation in the lattice. The map is transformed to a certain normal form by a perturbative technique, thereby providing an analysis according to resonances, and giving an approximate invariant surface in implicit form. The advantage of this approach is that repeated integrations over the lattice are avoided, making it feasible for large lattices. The Hamiltonian and equations of motion are used only once, in construction of the map. The normal form analysis is still basically perturbative, however, and is probably no more effective than usual perturbation theory when nonlinearities are strong. We should reserve judgment on this point, however, until nontrivial results with comparisons to tracking are published.

## 4. HAMILTON-JACOBI METHOD

Perturbation theory is a method for approximate solution of the HamiltonJacobi equation (2.2), based on expansion in powers of the perturbation strength. There are other methods to find approximate solutions which are superior with respect to accuracy, region of convergence, and simplicity of programming. We have in mind iterative methods, ${ }^{8,12}$ which depend on writing the Hamilton-Jacobi equation as a fixed-point problem,

$$
\begin{equation*}
g=A(g) \tag{4.1}
\end{equation*}
$$

Here $g=\left[g_{\mathrm{m}}\right]$ is a vector made up of the Fourier coefficients of the generating function. The only approximation arises from truncation of the Fourier scrics. We have considered various formulations leading to different realizations of the nonlinear operator $A^{8,13,14}$ The best formulation to date for accelerator problems is that of Ref. 14 , in which the periodicity of $g_{\mathrm{m}}(s)$ in $s$ is achieved by a shooting method. In many cases the equation (4.1) can be solved by simple iteration,

$$
\begin{equation*}
g^{(n+1)}=A\left(g^{(n)}\right) \tag{4.2}
\end{equation*}
$$

With $g^{(o)}=0$, the first iterate $g^{(1)}$ is identical with the result of lowest order perturbation theory; on the other hand $g^{(2)}$ entails all orders in the perturbation strength. In difficult cases, for instance strongly nonlinear lattices near the dynamic aperture, the iteration (4.2) diverges unless the set of allowed modes is rather small. For such cases we can resort to the more powerful Newton iteration and recover convergence even on relatively large mode sets. We refer the reader to Ref. 14 for details.

If Newton's method must be used, and the lattice contains more than a few nonlinear cells, the computations become expensive. We are considering several promising ways to reduce the expense, which we can only list briefly:
(i) Use the approximate generator, obtained by a fit to tracking data as in Section 2, as the first guess for a Newton iteration.
(ii) Use Broyden's formula ${ }^{15}$ in place of the full Jacobian matrix after the first iterate of Newton's method.
(iii) Use plain iteration (4.2) on a small mode set, perform a canonical transformation with the resultant generator, and again do plain iteration on the new Hamilton-Jacobi equation in the new variables, but now on a bigger mode set. This is possible because the number of modes allowed in a convergent iteration increases when the perturbation decreases in strength.

If the step of item (iii) is repeated indefinitely, one has an accelerated version of the K.-A.-M. algorithm, which leads to an invariant surface of arbitrary accuracy. ${ }^{16}$ Although Newton's method as such is not used, the iteration will have supcrexponential convergence. In the past it has been awkward to carry out such a program, because of the nonlinear character of the equation (2.3) relating old and new angle variables. In Ref. 8 we introduced an effective nonperturbative method of solving (2.3), which is based on the Fourier expansion

$$
\begin{equation*}
\mathbf{\Phi}=\mathbf{\Psi}+\sum_{\mathbf{m}} \mathbf{A}_{\mathbf{m}}(\mathbf{J}, s) c^{i \mathbf{m} \cdot \mathbf{\Psi}} \tag{4.3}
\end{equation*}
$$

It is easy to calculate the coefficients $\mathbf{A}_{\mathbf{m}}$ numerically, in terms of the generator $G$. We represent the $\mathbf{J}$-dependence of $G$ by polynomial interpolation of solutions $G\left(\mathbf{J}_{i}, \mathbf{\Phi}, s\right)$ computed at a few values $\mathbf{J}_{i}, i=1,2, \cdots, r$. The new Hamiltonian, $H^{(1)}(\mathbf{J}, \boldsymbol{\Psi}, s)$, may be represented similarly as a Fourier series in $\boldsymbol{\Psi}$.

The advent of a compact and manageable method for successive canonical transformations should open up new possibilities for precise results on stability, as explained in the following section.

For large lattices it may be advantageous to work with a functional equation for the invariant surface at a fixed value of $s$, in lieu of the Hamilton-Jacobi equation. Such an equation can be formulated in terms of a full-turn map, as is indicated in Section 7.

## 5. CANONICAL TRANSFORMATIONS AND BOUNDS ON THE MOTION FOR TIME $T$

We have mentioned several ways to approximate invariant surfaces (equivalently, periodic solutions $G$ of the Hamilton-Jacobi equation). Although the approximations that we obtain in practice seem rather close, in the sense that they agree with tracking to about 1 part in $10^{5}$ for several thousand turns, one should ask about their real value in settling the stability question. Mathematical analysis (K.-A.-M. theory) assures the existence of exact invariant surfaces only on a strange set of Cantor type in action space, and such surfaces cannot be represented in terms of a finite number of Fourier modes. Also, the invariant surfaces do not divide phase space into disjoint regions if the number of degrees of freedom is sufficiently large ( $\geq 2$ for our case of a periodic time-dependent Hamiltonian, $\geq 3$ for autonomous systems). This allows Arnol'd Diffusion, a slow drift from one region of phase space to a far removed region. In view of this apparently discouraging theoretical situation, what is the meaning or value of an "approximate invariant surface" ?

One answer is provided by the line of argument used in the Nekhoroshev Theorem. ${ }^{17}$ An approximate invariant surface is associated with a generator of a canonical transformation. Whatever the genesis or pedigree of this transformation, it has the property of reducing the perturbation term in the Hamiltonian, so that the motion in the new variable is closer to being linear. For instance, in Ref. 8 the transformation obtained from an approximate iterative solution of the HamiltonJacobi equation reduced the perturbation by a factor of $10^{7}$, even in a region not too far from the onset of chaos. As in the final step of Nekhoroshev's argument (a trivial but important step) one can make a simple estimate using Hamilton's equations in the new variables. This estimate gives a lower bound on the time $T$ during which an orbit will stay in a chosen region of phase space. This rigorous bound allows for the complications mentioned above, Cantor sets and Arnol'd Diffusion.

The better the canonical transformation, i.e., the smaller the residual dependence of the transformed Hamiltonian on $(\boldsymbol{\Phi}, s)$, the larger the lower bound on $T$. This impels research in the direction of finding highly accurate approximations to invariant surfaces, using if necessary the method of successive canonical transformations as outlined in the previous section. We anticipate much better bounds on $T$ than those of Nekhoroshev, since to prove a theorem he had to make analytical estimates, necessarily very crude, on a canonical transformation obtained from high-order perturbation theory. Since we compute our transformation numerically, we have a closer knowledge of what it actually accomplishes. Moreover, there is no important lapse of rigor in resorting to numerical methods in this context, since the only source of error is in the problem of numerical determination
of an upper bound for a well-defined function of a few variables. It is easy to show that the new action $J(t)$ will be confined to a strip

$$
\begin{equation*}
|J(t)-J(0)|<\Delta J \tag{5.1}
\end{equation*}
$$

for $0<t<T$,

$$
\begin{equation*}
T \geq \frac{\Delta J}{\substack{\left.\left|J \sup _{\begin{subarray}{c}{ \\
0<\Phi \mid(0)<\Delta J \\
0<t<\tau} }}\right| \frac{1}{1+G_{J \Phi}} \frac{\partial}{\partial \Phi}\left[I I\left(J+G_{\Phi}, \Phi, t\right)+G_{t}\right] \right\rvert\,}} \tag{5.2}
\end{equation*}
$$

$\tau$ being the time for one revolution. (We state the formula for one degree of freedom; it is easily generalized). However $G$ was obtained, by fair means or foul, it is a precisely defined function given by a truncated Fourier series, and we should be able to evaluate the denominator of (5.2), or an upper bound to that denominator, without appreciable error.

## 6. FULL TURN MAPS

Maps to describe propagation through one or more nonlinear elements of an accelerator or beam transport line have been utilized for a long time, for instance in the code TRANSPORT since the early 1960 's. ${ }^{18}$ The map

$$
\begin{equation*}
\mathbf{M}\left(\mathbf{z} ; s, s^{\prime}\right)=\mathbf{z}^{\prime} \tag{6.1}
\end{equation*}
$$

takes a phase space point $\mathbf{z}$ at orbital location $s$ into a point $\mathbf{z}^{\prime}$ at orbital location $s^{\prime}$. It has been usual to represent $\mathbf{M}$ as a power series in the components of z. Until recently only the first few Taylor coefficients could be computed in the case of a realistic full-turn map, even with the help of a Lie-algebraic formalism and symbol manipulation codes. By applying a technique for automatic differentiation ${ }^{19}$, which encodes the rules for differentiation of functions composed of truncated power series, one can go to much higher order. This technique is to be distinguished from derivative evaluation by symbol manipulation or by divided differences. It provides values that are exact to machine precision. Berz ${ }^{19}$ has implemented the method in codes which allow one to find the Taylor coefficients of the map defined by an arbitrary tracking program. In principle, derivatives of any order can be handled, but in practice there are restrictions due to limited computer power.

Although Berz's work certainly advances the art of Taylor series maps, we are not convinced that Taylor series provide the most efficient representation of the map M. Taylor series are rarely used in modern numerical analysis for global approximation of functions. The reason is elementary: interpolation through multiple points is usually more accurate and more convenient than extrapolation by Taylor series from a single point. Orthogonal expansions, in particular Fourier series, also provide a tool with a much wider range of validity than Taylor expansions. The practice and theory of interpolation and orthogonal cxpansions arc highly developed ${ }^{20}$, and necessary software is readily available.

We have implemented a representation of maps using a combination of interpolation and Fourier developments. The data required to construct the maps are merely the values of $\mathbf{M}\left(\mathbf{z} ; s, s^{\prime}\right)$ on some set of initial points $\mathbf{z}=\mathbf{z}_{i}$; the values can be taken from any tracking code by running it from $s$ to $s^{\prime}$ for each $\mathbf{z}_{i}$. In contrast to Berz's method, we need not deal with the mathematical operations within the code. We write the map in terms of angle-action coordinates:

$$
\begin{align*}
& \boldsymbol{\Phi}^{\prime}=\boldsymbol{\Phi}+\mathbf{A}(\mathbf{I}, \boldsymbol{\Phi})  \tag{6.2}\\
& \mathbf{I}^{\prime}=\mathbf{I}+\mathbf{B}(\mathbf{I}, \boldsymbol{\Phi}) \tag{6.3}
\end{align*}
$$

The functions $\mathbf{A}$ and $\mathbf{B}$ are periodic in $\boldsymbol{\Phi}$ with period $2 \pi$. In view of general experience in nonlinear mechanics, it seems natural to expand these functions in Fourier series in $\mathbf{\Phi}$. As in the computation of invariant surfaces, we find that a rather sparse set of Fourier modes is dominant. That is, for a given accuracy we have to include modes up to some maximum mode number, but for many mode numbers below that maximum the Fourier coefficients are negligible. Thus, it is efficient to represent $\mathbf{A}$ and $\mathbf{B}$ in a form such as

$$
\begin{equation*}
\mathbf{A}(\mathbf{I}, \boldsymbol{\Phi})=\sum_{\mathbf{m} \in S} \mathbf{A}_{\mathbf{m}}(\mathbf{I}) e^{\mathbf{i m} \cdot \boldsymbol{\Phi}} \tag{6.4}
\end{equation*}
$$

where the set $S$ includes all $\mathbf{m}$ for which $\left|\mathbf{A}_{\mathbf{m}}\right|$ is greater than some $\epsilon$ times the largest $\left|\mathbf{A}_{\mathbf{m}}\right|$. The Fourier coefficients are calculated by evaluating the map on a rectangular grid of points in $\boldsymbol{\Phi}$ space, then taking an FFT of the values.

By numerical evaluation we find that the Fourier coefficients of (6.4) are smooth, uncventful functions of $\mathbf{I}$, usually monotonic and with small curvature over the region encountered on a typical orbit. We have experimented with two ways to represent these functions: ${ }^{20}$ (a) interpolation by polynomials in the variables $\xi_{i}=I_{i}^{1 / 2}$, the $I_{i}$ being components of the vector $I$, and (b) spline interpolation in the same variables. Here we report results from choice (a), while
noting that choice (b) gives similar results in most cases that we have tried. In one dimension, the polynomial approximation of the Fourier coefficient is given in Lagrange form as

$$
\begin{equation*}
A_{m}(I)=\sum_{s=1}^{n} A_{m}\left(I_{s}\right) \lambda_{s}(\xi) \tag{6.5}
\end{equation*}
$$

where the Lagrange factors $\lambda_{s}(\xi)$ are

$$
\begin{equation*}
\lambda_{s}(\xi)=\prod_{t \neq s} \frac{\left(\xi-\xi_{t}\right)}{\left(\xi_{s}-\xi_{t}\right)} \tag{6.6}
\end{equation*}
$$

For the interpolation points $\xi_{t}$ we take the expanded Chebyshev points, as given in Eq. (2.6e) of de Boor ${ }^{20}$, which in a certain sense make an optimal choice. The denominator of (6.6) is computed once for all, while the numerator is evaluated once for each iteration of the map.

To give an example we construct maps for the SLC North Damping Ring, to cover a region including the orbit that yielded Figures 1 and 2. The interpolation polynomials are sixth degree in each variable $\xi_{i}$, with minimum and maximum interpolation points at the ends of the intervals

$$
\begin{equation*}
1.5 \cdot 10^{-6} \leq I_{1} \leq 3.25 \cdot 10^{-6}, \quad 10^{-6} \leq I_{2} \leq 2.5 \cdot 10^{-6} \tag{6.7}
\end{equation*}
$$

with actions given in meters. The Fourier modes are chosen from an initial set with $\left|m_{1}\right|,\left|m_{2}\right| \leq 11$. For each of the four components of the map we retain all modes with coefficients larger than $10^{-7}$ of the largest coefficient, this selection being made at maximum values of the actions. For a one-turn map this yields a total of 223 coefficients to describe all four components of the map; for a two-turn map there are 246. The initial, unselected set had 972 independent coefficients.

To test accuracy of the $n$-th iterate of the map, we compare its value to the corresponding value obtained from the underlying tracking code (a 4th-order symplectic integrator) that was used to construct the map. We define the discrepancy $\delta$ between the map and the tracking code as

$$
\begin{equation*}
\delta(n)=\frac{1}{4} \sum_{i=1}^{2}\left[\left|\frac{\Phi_{i}-\Phi_{i}^{t}}{\Phi_{i}}\right|+\left|\frac{I_{i}-I_{i}^{t}}{I_{i}}\right|\right]_{n-t h \text { turn }} \tag{6.8}
\end{equation*}
$$

The coordinates from the tracking code have superscript $t$, those from the map do not.

We give results for mapping from initial conditions the same as those of Figure 1: $\Phi_{1}=\Phi_{2}=0, \quad I_{1}=I_{2}=2 \cdot 10^{-6}$. For a one-turn map the discrepancy at one turn was $\delta=5.3 \cdot 10^{-8}$, whereas for a two turn map the discrepancy at two turns was $\delta=2.9 \cdot 10^{-8}$. In Table 2 we give the discrepancies for $10^{p}$ turns, with $p=1, \cdots, 4$. We find it remarkable that the discrepancy is quite small for at least 10000 turns. It is likely that the orbit generated by the map stays close to the correct invariant surface for many turns beyond 10000 , since it is usual for phase error to build up faster than amplitude error. That is, the orbit generated by the map might lie close to the surface, without having the correct angular location $\left(\Phi_{1}, \Phi_{2}\right)$ at a particular turn.

Table 2 : Discrepancy $\delta$ between Map and Tracking Code

| $\mathrm{n}=$ number of turns | $\delta(\mathrm{n})$ | $\delta(\mathrm{n})$ |
| :---: | :---: | :---: |
| One-turn map | Two-turn map |  |
| 10 | $2.2 \cdot 10^{-7}$ | $6.8 \cdot 10^{-8}$ |
| 100 | $1.6 \cdot 10^{-7}$ | $1.3 \cdot 10^{-6}$ |
| 1000 | $7.9 \cdot 10^{-6}$ | $9.9 \cdot 10^{-6}$ |
| 10000 | $5.8 \cdot 10^{-4}$ | $6.2 \cdot 10^{-4}$ |

We have not imposed the symplectic condition, beyond maintaining good agreement with the underlying symplectic tracking code. It is possible to enforce the symplectic condition precisely (modulo round-off error) by constructing a canonical transformation that induces a map nearly the same as the onc we have constructed. We have invented an algorithm, based on a Fourier inversion technique, to derive the generator of such a transformation from the map itself. It is also possible to find the generator by solving the Hamilton-Jacobi equation, later obtaining the explicit (but not exactly symplectic) map by the Fourier inversion method. This latter program, complementary and inverse to the present approach, was implemented in Ref. 23 in one degree of freedom.

Results concerning computation time to iterate the maps are encouraging, especially in view of the fact that we have not yct done much to optimize computing. On the IBM 3081 at SLAC the time for one iteration of the one-turn map described above is about five times greater than the time to track for one turn with the underlying tracking code. Since the ring has 72 sextupoles, the map would go faster than element-by-element tracking in a ring with more than $5 \times 72=360$ sextupoles, provided that a map of the same complexity would suffice. In a ring as big as the SSC, with about 10000 nonlinear elements, one would gain a factor of 28
in speed by this reckoning. Actually, much bigger gains can be anticipated, since iteration of the map is a very simple computational problem which undoubtedly can be handled with great efficiency through better programming and hardware. In particular, it lends itself to vector processing to a much greater degree than ordinary tracking.

The outlook for the cost of constructing maps is perhaps not quitc as favorable, but by no means discouraging. It took the equivalent of 28224 turns of element-by-element tracking to construct the one-turn map described above, and twice that much for the two-turn map. Furthermore, the maps do not cover the full domain of interest in action space. It might take three times as much computing to make maps for the full domain. Once the maps are available, however, they can be used to track economically (for large rings) from any initial condition, and also to study invariant surfaces by the method of the following section. Furthermore, one could make maps for several values of tune, and interpolate between them to explore tune space.

It may very well be that the map of our example is much more accurate than necessary. If the symplectic condition were enforced, a less accurate and less expensive map might suffice. In order to check accuracy while allowing for innocuous phase error, one could calculate the distance between the orbit of a proposed map and an accurate, previously established invariant surface. That is, if the map gave the point $(\mathbf{I}, \boldsymbol{\Phi})$ at some iterate, one could compare $\mathbf{I}$ with the action value on the invariant surface at the same $\boldsymbol{\Phi}$.

The question of whether one should work with a one-turn map or a multi-turn map deserves continued study. In Table 2 we see that the one- and two-turn maps give comparable accuracy at the $n$-th turn. Tracking by the two-turn map goes almost twice as fast (not exactly twice as fast, because it has a few more Fourier modes) but the map takes twice as long to construct. Using the two-turn map, one might be able to study invariant curves in the neighborhood of a closed orbit of period two, by the method of the following section. Also, one could imagine a bootstrap operation in which a one-turn map, say, could be used to generate a map for many turns. Essentially this is what we have already done in going from the single-element maps of the tracking code to full-turn maps.

Talman's ${ }^{21}$ recent study of maps for a simple model (the physical pendulum) led to a more pessimistic outlook than we have attained, but gave one result with which we agree: maps based on interpolation are more promising than those based on the Taylor expansion. Hagel and Zotter, ${ }^{22}$ using slightly more relevant but still very simple models, have reexamined Talman's conclusions. We have demonstrated that one can easily make maps for real accelerators, using any tracking code; it is not necessary, and potentially misleading, to work with over-simplified models.

## 7. FUNCTIONAL EQUATION FOR INVARIANT SURFACES

In his original paper on the K.-A.-M. theorem, Jürgen Moser ${ }^{24}$ studied the invariant curves of area preserving maps of an annulus. He based his analysis on a functional equation for the curve. We seek to generalize Moser's approach, so as to capture its advantages in the case of a general Hamiltonian system.

We begin with an $n$-turn map in the form (6.2), (6.3), where $n$ is an integer, say $n=1$. The map may be represented explicitly, as in the work of the previous section, or may be regarded as the result of applying an element-by-element tracking code for $n$ turns. The desired invariant surface may be parametrized in terms of the angular torus coordinates $\boldsymbol{\Phi}$, and developed in a Fourier series, just as in (2.1) . Replacing the notation of (2.1) we write

$$
\begin{equation*}
\mathbf{I}=\mathbf{u}(\mathbf{\Phi})=\sum_{\mathbf{m}} \mathbf{u}_{\mathbf{m}} e^{i \mathbf{m} \cdot \boldsymbol{\Phi}} \tag{7.1}
\end{equation*}
$$

where $\mathbf{u}_{o}$ is the invariant action $\mathbf{K}$. The requirement that the surface be invariant under the map is

$$
\begin{equation*}
\mathbf{I}=\mathbf{u}(\boldsymbol{\Phi}) \quad \Longrightarrow \quad \mathbf{I}^{\prime}=\mathbf{u}\left(\Phi^{\prime}\right) \tag{7.2}
\end{equation*}
$$

In terms of the functions $\mathbf{A}, \mathbf{B}$ of (6.2), (6.3) this means that

$$
\begin{equation*}
\mathbf{I}+\mathbf{B}(\mathbf{I}, \boldsymbol{\Phi})=\mathbf{u}(\mathbf{\Phi}+\mathbf{A}(\mathbf{I}, \boldsymbol{\Phi})) \tag{7.3}
\end{equation*}
$$

whenever $\mathbf{I}=\mathbf{u}(\mathbf{\Phi})$, which is to say

$$
\begin{equation*}
\mathbf{u}(\boldsymbol{\Phi})=\mathbf{u}(\boldsymbol{\Phi}+\mathbf{A}(\mathbf{u}(\boldsymbol{\Phi}), \boldsymbol{\Phi}))-\mathbf{B}(\mathbf{u}(\boldsymbol{\Phi}), \boldsymbol{\Phi}) \tag{7.4}
\end{equation*}
$$

Eq. (7.4) is the generalized Moser equation. (Actually, Moser used an auxiliary curve parameter rather than the torus coordinate $\boldsymbol{\Phi}$ to parametrize his invariant curve, which led to a pair of equations rather than one).

If we introduce (7.1) in (7.4), then take the Fourier transform of (7.4), we obtain a nonlinear system of equations for the coefficients $\mathbf{u}_{\mathbf{m}}$. After truncation of the Fourier series, the system can be solved by iteration, as in our treatment of the Hamilton-Jacobi equation. There are several possible iteration schemes, including a scheme similar to Moser's method of successive (non-canonical!) coordinate changes, which should allow one to include more and more Fourier modes as the iteration goes on, and thus achieve very high accuracy.

Although we have not yet implemented this method, it seems highly promising in light of our experience with the Hamilton-Jacobi system, which has similar mathematical properties, but is more awkward to handle in a context of successive coordinate changes. The method yields $G_{\boldsymbol{\Phi}}$ at one point in the lattice, say $s=0$, which can be taken as the initial value in an integration of the Hamilton- Jacobi equation with respect to $s$ over the whole lattice, to $s=C$. Thus we obtain the generator for a canonical transformation which can lead to bounds for long term stability, along the lines of Section 5.

As was remarked in Section 3, this approach retains the advantage of Forest's scheme by working with the map rather than the Hamiltonian, but allows precise, non-perturbative solutions.

## 8. CONCLUSION

We have discussed two methods for single-particle tracking: symplectic integration and full-turn maps. These techniques support and complement three methods for determination of invariant surfaces: surface fitting, the HamiltonJacobi method, and the generalized Moser method. Knowledge of approximate invariant surfaces is essentially equivalent to knowledge of an approximate HamiltonJacobi generator, which leads to precise bounds on the motion over a finite time $T$. It is too early to say whether $T$ will be large enough to be interesting; we have mentioned the possibility mainly to point out a long range goal, the ideal completion of the program through definite statements on long term stability.

Numerical work to date has been devoted to assessing the relative advantages of the various approaches. This aspect of the task is still not complete, but results are sufficient to convince us that real advances in the art are possible. As soon as a preferred method comes into focus, we hope to take advantage of advanced programming and hardware, and also produce software for general use.

Finally, we should mention that the methods under study should be of interest beyond accelerator theory, for instance in chemical physics (through semi-classical quantum mechanics) and in celestial mechanics.

## REFERENCES

1. R. De Vogelaere, Dept. of Math., University of Notre Dame, Report 4, 1956.
2. R.D. Ruth, IEEE Trans. Nucl. Sci., 30 (1983) 2669.
3. P. Channell, LANL Tech. Note AT-6:ATN-83-9, Los Alamos National Laboratory,1983
4. P.J. Channell and C. Scovel, LA-UR-88-1828, Los Alamos National Laboratory, 1988, submitted to Nonlinearity.
5. R.D. Ruth, unpublished. The 4th-order program TRACK was written at SLAC by Karl Ecklund.
6. Notes on the Los Alamos Workshop on Symplectic Integration, March 19-21, 1988, Daryl Holm, Ed.
7. D. Edwards, SSC-2 (1985); T. Collins, SSC-26 (1985); Proceedings of the Second Advanced ICFA Beam Dynamics Workshop, CERN 88-04 (1988), working group summaries by S. Chattopadhyay and P. Audy et al.
8. R.L. Warnock and R.D. Ruth, Physica 26D, 1 (1987).
9. L. Michelotti, Particle Accelerators 16 (1985) 233.
10. H. Moshammer and J. Hagel, Proceedings of the Second Advanced ICFA Beam Dynamics Workshop, Lugano, April 11-16, 1988, CERN 88-04.
11. E. Forest and M. Berz, LBL-25069 (1988); E. Forest, M. Berz, and J. Irwin, SSC-166 (1988); E. Forest, Particle Accelerators 22,15 (1987), SSC-29 (1985); A.J. Dragt and E. Forest, J. Math. Phys. 24, 2734 (1983).
12. S. Chapman, B. C. Garrett and W. H. Miller, J. Chem. Phys. 64 (1976) 502.
13. R.I. Warnock and R.D. Ruth,Proceedings of the 1987 IEEE Particle Accelerator Conference, p. 1263 .
14. W.E. Gabella, R.D. Ruth, and R.L. Warnock, Second Advanced ICFA Beam Dynamics Workshop, Lugano, 1988, CERN 88-04.
15. C. G. Broyden, Math. Comp. 19 (1965) 577.
16. R.L. Warnock and R.D. Ruth, in The Physics of Phase Space, Lecture Notes in Physics, No.278, Springer-Verlag, 1987.
17. N. N. Nekhoroshev, Russian Math. Surveys $32: 6$ (1977) 1.
18. K.L. Brown, D.C. Carey, Ch. Iselin, and F. Rothacker, TRANSPORT, a Computer Program for Designing Charged Particle Beam Transport Systems, CERN 80-04, 1980; K.L. Brown, R. Belbeoch, and P. Bounin, Rev. Sci. Instr. 35 (1964) 481.
19. M. Berz, SSC-166, March, 1988. For earlier work on automatic differentiation in the same vein see R. F. Wengert, Commun. of the ACM, 8 (1964) 463; L.B. Rall, Automatic Differentiation: Techniqucs and Applications, Lecture Notes in Computer Science, Vol.120, Springer, Berlin, 1981; H. Kagiwada, R. Kalaba, N. Rasakhoo, and K. Spingarn, Numerical Derivatives and Nonlinear Analysis, Plenum, New York, 1986. See also the review of the latter book by A. Griewank, SIAM Review, 30 (1988) 327. Griewank's review contains references not mentioned in the two monographs.
20. C. de Boor, A Practical Guide to Splines, Springer, Berlin, 1978; T. Rivlin, Approximation of Functions.
21. R.Talman, SSC-117, 1988.
22. J. Hagel and B. Zotter, CERN-LEP report, 1988.
23. R. L. Warnock, R. Ruth, and W. Gabella, Symplectic Maps for Accelerator Lattices, Workshop on Symplectic Integration, Los Alamos National Laboratory, March, 1988, SLAC-PUB 4627.
24. J. Moser, Nachr. Akad. Wiss., Göttingen, Math. Phys. Kl., 1-20, 1962.

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