

## Optimal Symplectic Approximation of Hamiltonian Flows

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Long term simulations of Hamiltonian dynamical systems benefit from enforcing the symplectic symmetry. One of the several available methods to perform this symplectification is provided by the recently developed theory of extended generating functions. The theory offers an infinite supply of generator types that can be used for symplectification. Using Hofer's metric, a condition for optimal symplectification is given. In the weakly nonlinear case, the condition provides a generator type that, based on the limited information available on the system, in general gives optimal results.

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Among many systems of practical interest, hadron colliders in the single particle approximation can be modeled as Hamiltonian systems. It is well known that flows of Hamiltonian systems are characterized by their symplecticity [1]. One of the fundamental quantities in Hamiltonian dynamics in general and accelerator physics in particular is the dynamic aperture (DA), which, roughly, is the region of space containing stable particle orbits over long times. Since usually the systems are so complex that an exact solution is not within reach, simulations are needed to estimate the DA [2,3]. This can be achieved by iteration of the so-called one-turn map, i.e., Poincaré section map, of the system. Unfortunately, only some approximation of the one-turn map, as, for example, the order  $n$  truncation of its Taylor series, is available [4]. While the Taylor map preserves the symplecticity up to order  $n$  terms in the expansion, in general it fails to be exactly symplectic. Numerical simulations show that the truncation often generates inaccurate results [5]. Therefore, restoration of the exact symplecticity of the one-turn map is desirable [6].

There are several symplectification methods [5,7,8]. In beam physics, symplectic tracking to order three was first implemented in the code MARYLIE [9], and to arbitrary order it was first implemented in COSY INFINITY [4]. While every method produces exactly symplectic maps, the results are not equivalent. The symplectified maps depend on the specifics of the methods. Several examples are presented in [5] using the formalism of generating functions of canonical transformations. For some generators, the results are not satisfactory. Therefore, it is not only important to symplectify, but also to symplectify the right way. The purpose of this Letter is to give a precise meaning for how to symplectify "the right way."

As with any approximation method, a criterion for closeness is needed; mathematically speaking, a suitable metric is necessary. In our case, the metric should provide a way to measure distances between Hamiltonian symplectic maps, and should have some desirable properties, namely, (1) the symplectification should work well for every particle in a given Poincaré section, (2) the outcome of

the symplectification should not depend on the specific Poincaré section used, (3) the symplectification should work just as well after any  $N > 1$  turns as after one turn, and (4) based on the previous three conditions, the assessment of the optimality of the symplectification should be unambiguous.

These conditions can be captured by the requirement that if a symplectification method yields the best result, say  $\mathcal{M}$ , with respect to the metric, then the same symplectification gives the same result for the map  $\mathcal{A} \circ \mathcal{M} \circ \mathcal{A}^{-1}$ , the map  $\mathcal{M}$  subjected to any symplectic similarity transform  $\mathcal{A}$ . Thus, we desire coordinate independence of the metric. It is hoped that such special purpose metrics would better capture the details of the dynamics than general purpose metrics (as, for example, the well-known  $C^0$  metric), and would give an as unambiguous as possible way to measure distances. Therefore, mathematically speaking, we would like to have a bi-invariant metric for Hamiltonian symplectic maps. The importance of bi-invariant metrics has been pointed out also in [10]. The question is whether such a metric exists at all. Indeed, existence of such a metric is highly nontrivial over an infinite dimensional noncompact Lie group, similar to the Lie group of symplectic maps. A negative example from the field of motion planning for robotic systems is provided by [11], where it is shown that over the relevant Lie group, i.e.,  $SE(3)$ , no such "natural and univocal concept of distance" exists. Hence the results are task or designer biased.

Fortunately, there exists an outstanding metric that satisfies our needs. It has been introduced by Hofer [12], and has been applied in the fields of symplectic geometry and topology [13,14]. Hofer's metric is an essentially unique intrinsic bi-invariant Finsler metric for compactly supported Hamiltonian symplectic maps. Let us formalize the definition of this metric. A symplectic map is called Hamiltonian if it is the time one map of the flow of some function defined on phase space. A map is said to be compactly supported if it is the identity outside a compact subset. Denote the space of compactly supported Hamiltonian symplectic maps of  $\mathbb{R}^{2n}$  with its standard symplectic

structure by  $\text{Ham}^c(\mathbb{R}^{2n})$ . Then for any two  $\theta, \psi \in \text{Ham}^c(\mathbb{R}^{2n})$ , the Hofer distance between them is defined as

$$\rho(\theta, \psi) = \inf_{\phi_0=\theta, \phi_1=\psi} \int_0^1 \|H_t\| dt. \quad (1)$$

Here the infimum is taken over all smooth paths  $\{\phi_t\}$ ,  $t \in [0, 1]$ , in  $\text{Ham}^c(\mathbb{R}^{2n})$  from  $\theta$  to  $\psi$ . The norm  $\|H_t\| = \sup H_t(z) - \inf H_t(z)$ ,  $z \in \mathbb{R}^{2n}$  is called the oscillation norm, and the functions  $H_t$  are the, possibly time-dependent, Hamiltonians generating the paths  $\{\phi_t\}$ . It is a deep and remarkable result [12] that Hofer's metric is a genuine bi-invariant metric, i.e., it satisfies the positive definiteness, separation and symmetry axioms, the triangle inequality, and for all  $\phi, \theta, \psi \in \text{Ham}^c(\mathbb{R}^{2n})$  the following holds:

$$\rho(\phi \circ \theta, \phi \circ \psi) = \rho(\theta, \psi) = \rho(\theta \circ \phi, \psi \circ \phi). \quad (2)$$

Thus it satisfies all the conditions that we wanted to obey and can be used for our purposes.

Therefore, optimal symplectification can be characterized as a symplectification method that minimizes the distance in Hofer's metric between the exact map and the symplectified maps. That is, if the set of all possible symplectification methods is denoted by  $\Sigma$ , the best result is achieved by any symplectic map  $\mathcal{N}_{\text{opt}}$  which satisfies

$$\rho(\mathcal{M}, \mathcal{N}_{\text{opt}}) = \inf_{i \in \Sigma} \rho(\mathcal{M}, \mathcal{N}_i). \quad (3)$$

While being very general, there is a problem with this formulation of the optimal symplectification, because it is not very useful for practical computations. The reason is that in general it is not known yet how to compute the Hofer distance between two arbitrary maps in  $\text{Ham}^c(\mathbb{R}^{2n})$ . The difficulty lies in the necessity of consideration of all the Hamiltonians generating the two maps, or equivalently, the paths in  $\text{Ham}^c(\mathbb{R}^{2n})$  from  $\mathcal{M}$  to  $\mathcal{N}_i$ . However, by the nature of our optimality condition, we are interested only in the maps  $\mathcal{N}_i$  that are already close to  $\mathcal{M}$  in some sense. Obviously, this necessary condition can be achieved by sufficiently increasing the degree  $n$  of the Taylor polynomials  $\mathcal{M}_n$  with which the exact maps are initially approximated. Thus it would be sufficient if a suitable neighborhood of  $\mathcal{M}$  can be parametrized in such a way that (3) becomes computable.

Indeed, this is possible in the  $C^1$  topology, utilizing the theory of generating functions of canonical transformations, here used synonymously with symplectic transformations, symplectic maps, and symplectomorphisms. The first results in this direction have been obtained in [15] for Hamiltonian maps  $C^1$  close to identity and Poincaré's generating function, and then it was extended to Hamiltonian maps  $C^1$  close to identity and all compactly supported generating functions in [16] and [13]. While the approach of [16] is more general, as it holds on any symplectic manifold, we are interested only in  $\mathbb{R}^{2n}$ , and the method of [15] lends itself more easily to generalizations. The main idea is

to replace the Hamiltonian maps by their generating functions and try to express Hofer's metric between two maps as some norm of the difference of their generating functions. In [15] this was proven to be possible. However, in the recently developed extended theory of generating functions [5,17] it was shown that in fact there exist uncountably many generator types for any symplectic map. To give a precise definition, we need to introduce some notations. Denote the unit matrix of appropriate dimension by  $I$ , the identity map by  $I$ , and the matrix of the standard symplectic form by

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \quad (4)$$

A scalar function  $F$  is called the generating function of type  $\alpha$  of a given symplectic map  $\mathcal{M}$  if

$$(\nabla F)^T = \left[ \alpha_1 \circ \begin{pmatrix} \mathcal{M} \\ I \end{pmatrix} \right] \circ \left[ \alpha_2 \circ \begin{pmatrix} \mathcal{M} \\ I \end{pmatrix} \right]^{-1}, \quad (5)$$

where  $\alpha = (\alpha_1, \alpha_2)^T$  satisfies

$$(\text{Jac}(\alpha))^T \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} (\text{Jac}(\alpha)) = \mu \begin{pmatrix} J & 0 \\ 0 & -J \end{pmatrix}, \quad (6)$$

and  $\mu$  is some nonzero real constant. It can be shown [5] that if (5) is solved for  $\mathcal{M}$ , any arbitrary sufficiently smooth  $F$  yields a symplectic map. Furthermore, it also can be shown that the time evolution of each generator type is given by the following generalized Hamilton-Jacobi equation [17,18]:

$$\frac{\partial}{\partial t} F_t \circ \alpha_2 \circ \begin{pmatrix} \mathcal{M}_t \\ I \end{pmatrix} = \mu H_t \circ \mathcal{M}_t. \quad (7)$$

Finally, using the main result of [19], and introducing a map  $\Phi_\alpha$  that sends a symplectic map into its generating function  $F$  of type  $\alpha$ , we proved that  $\Phi_\alpha$  is an isometry. That is,

$$\begin{aligned} \rho(\mathcal{M}, \mathcal{N}) &= \frac{1}{|\mu|} \|\Phi_\alpha(\mathcal{M}) - \Phi_\alpha(\mathcal{N})\| \\ &= \frac{1}{|\mu|} \|F - G\|, \end{aligned} \quad (8)$$

for any type  $\alpha$ , as long as the generating function of type  $\alpha$  exists for both symplectic maps [17]. This is a local statement in the sense that, although global generators exist for any symplectic map, the same type of generators exists for symplectic maps that are close enough to each other [17].

Now we are ready to transfer the problem of solving (3) to solving

$$\rho(\mathcal{M}, \mathcal{N}_{\text{opt}}) = \inf_{i \in \Sigma} \frac{1}{|\mu|} \|\Phi_\alpha(\mathcal{M}) - \Phi_\alpha(\mathcal{N}_i)\|. \quad (9)$$

Denote  $\Phi_\alpha(\mathcal{M}) = F^\alpha$ . Unfortunately,  $F^\alpha$  is unknown, and to minimize the right-hand side of (9), a good approximation of  $F^\alpha$  is needed. All the information about the system that is available in practice is contained in  $\mathcal{M}_n$ . This entails that, with some *a priori* fixed  $\alpha$ , the best

approximation for  $F^\alpha$  is obtained by solving as accurately as possible (5). The necessary operations of truncated map computation, map composition and order  $m$  inversion, and integration are readily available in the code COSY INFINITY [4], and, as a consequence, the order  $m$  Taylor expansion of  $F^\alpha$ ,  $F_m^\alpha$ , can be easily obtained. Then, it follows that the best result is achieved by the symplectic map  $\mathcal{N}_{\text{opt}}$  which satisfies

$$\rho(\mathcal{M}, \mathcal{N}_{\text{opt}}) = \inf_{\alpha \in \Sigma} \frac{1}{|\mu|} \|F^\alpha - F_m^\alpha\|, \quad (10)$$

where  $\Phi_\alpha(\mathcal{N}_i) = F_m^\alpha$ . Apparently, minimization of the right-hand side of (10) is equivalent to the choice of the generating function type that achieves this minimization. It is worthwhile to note that, due to the one-to-one correspondence between generating functions of a fixed type and symplectic maps,  $\rho(\mathcal{M}, \mathcal{N}_{\text{opt}}) > 0$  always, which means that the true solution can never be recovered by symplectification. Therefore, the differences among symplectification methods are caused by the truncation of the generating functions. However,  $F_m^\alpha$  is the most that can be computed in practice. The remaining question is that, based on this limited information, which generator type will give the best results in general? To answer this question we need to pick a generator type, or equivalently an  $\alpha$ , that minimizes  $\|F^\alpha - F_m^\alpha\|/\mu$ . Again, for an arbitrary  $\mathcal{M}$  this turns out to be a difficult problem, because in general nonlinear  $\alpha$ 's would be required, and it is difficult to construct nonlinear maps that satisfy (6). For weakly nonlinear systems, such as accelerator physics applications, this turns out to not be a problem since the maps of interest are in general weakly nonlinear maps around equilibrium points. For these types of maps linear choices of  $\alpha$  are sufficient, which simplifies the construction of generating functions. Also, in principle any nonlinear Hamiltonian map can be split into a composition of Hamiltonian maps which are only weakly nonlinear. Therefore, the final step is to find the linear  $\alpha$ , such that  $\|F^\alpha - F_m^\alpha\|/\mu$  is minimized in general.

One of the main results of [5] is that the set of linear maps satisfying (6) can be organized into equivalence classes, meaning that for symplectification purposes the following are the only independent generator types:

$$\alpha = \begin{pmatrix} -JM^{-1} & J \\ \frac{1}{2}(I + JS)M^{-1} & \frac{1}{2}(I - JS) \end{pmatrix}, \quad (11)$$

where  $M$  is the linear part of  $\mathcal{M}$ , and  $S$  represent arbitrary symmetric matrices. For a given  $\mathcal{M}$  with linear part  $M$ , the classes characterized by some symmetric matrix  $S$  is denoted by  $[S]$ . We note that  $M$  is known from  $\mathcal{M}_n$ , and  $\mu = 1$  for every  $\alpha$  from (11). Thus optimal symplectification is map dependent; that is, there is a different optimal symplectification for every symplectic map having a different linear part. Then, which class  $[S]$  gives the optimal symplectification for symplectic maps having the same linear part? To answer the question, it is observed that for the requirement of minimization of  $\|F^\alpha - F_m^\alpha\|$ ,

minimization of  $\|F^\alpha\|$  is sufficient. Indeed, if we require  $F^\alpha$  to be small, it follows that the tail  $F^\alpha - F_m^\alpha$  will also be small, because otherwise there must be cancellation of large terms in the Taylor expansion of  $F^\alpha$ . However, as will be shown now, this cannot happen due to the fact that  $C^0$  smallness implies  $C^1$  smallness.

To this end, notice that, with the notations  $\hat{z} = \mathcal{M}(z)$  and  $w = \alpha_2(\hat{z}, z)$ , (5) can be expressed as

$$\nabla_w F^\alpha(w) = \alpha_1(\hat{z}, z). \quad (12)$$

Integration, which can be along an arbitrary path according to Stokes' theorem, gives

$$F^\alpha(w) = \int_0^w \alpha_1(\hat{z}, z) \cdot dw'. \quad (13)$$

Taking norms on both sides of the equation the following estimate is obtained:

$$\begin{aligned} \|F^\alpha\| &\leq \max_{z \in \mathbb{R}^{2n}} |\alpha_1(\hat{z}, z)| \cdot \max_{z \in \mathbb{R}^{2n}} |\alpha_2(\hat{z}, z)| \\ &= \left\| \alpha_1 \circ \begin{pmatrix} \mathcal{M} \\ I \end{pmatrix} \right\| \cdot \left\| \alpha_2 \circ \begin{pmatrix} \mathcal{M} \\ I \end{pmatrix} \right\|. \end{aligned} \quad (14)$$

It is rather straightforward to check from (5) and (11) that

$$\alpha_1(\hat{z}, z) = 0 + \mathcal{O}(z^2), \quad (15)$$

$$\alpha_2(\hat{z}, z) = I \cdot z + \frac{1}{2}(I + JS) \cdot \mathcal{O}(z^2). \quad (16)$$

From these equations it can be inferred that indeed  $C^0$  smallness implies  $C^1$  smallness.

Therefore,  $\alpha_1(\hat{z}, z)$  is already small if  $\mathcal{M}$  is weakly nonlinear, and its norm does not depend on the type of generating function. Hence, minimization of  $\|F^\alpha\|$  in the end is equivalent to minimization of  $I + (I + JS)/2 \cdot \mathcal{O}(z^2)$ . The only free parameter is the symmetric matrix  $S$ . Because the  $\mathcal{O}(z^2)$  comes from the nonlinear part of the symplectic map  $\mathcal{M}$ , a simple calculation shows that  $S = 0$  is the best choice if  $\mathcal{M}$  is allowed to be free [17]. With this result, it can be concluded that the optimal symplectification is achieved by the class of generators  $[S]$  obeying  $S = 0$ , and associated with the following  $\alpha$ :

$$\alpha_{\text{opt}} = \begin{pmatrix} -JM^{-1} & J \\ \frac{1}{2}M^{-1} & \frac{1}{2}I \end{pmatrix}. \quad (17)$$

Interestingly enough, it turns out that if in  $\alpha_{\text{opt}}$  the linear part  $M$  is replaced with the unit matrix  $I$ , the resulting matrix gives a valid generator type, which exists for symplectic maps close enough to identity. It was first used by Poincaré in the restricted three body problem for a completely different purpose [20], and is hence called the Poincaré generating function. Our  $\alpha_{\text{opt}}$  can be regarded as a dynamically adjusted Poincaré generator, to symplectic maps not having identity as linear parts. That is why we call it the extended Poincaré (EXPO for short) generating function type. Finally, the best symplectified map  $\mathcal{N}_{\text{opt}}$ , in the sense presented in this Letter, is obtained if the

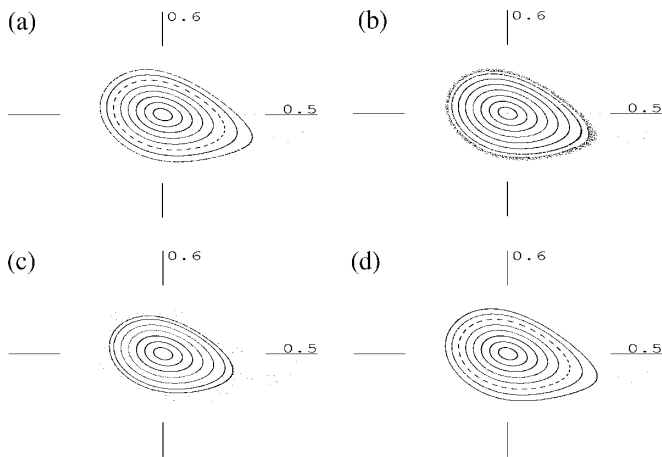


FIG. 1. 1000 turn tracking of a random two dimensional symplectic map with (a) the 19th order Taylor map (considered to be essentially the exact result), (b) with the 11th order Taylor map, (c) with the symplectified map obtained by symplectifying the 11th order Taylor map with  $F_1$ , and (d) with the symplectified map obtained by symplectifying the 11th order Taylor map with EXPO.

symplectification is performed using the EXPO generator type, i.e.,

$$\mathcal{N}_{\text{opt}} \equiv \mathcal{N}_{\text{EXPO}}. \quad (18)$$

The method for optimal symplectic tracking (EXPO) has been implemented in the code COSY INFINITY [5]. A few examples of EXPO can be found in [2,3,5,21]: specifically, muon accelerators, and the standard test problem of an anharmonic oscillator. Here another example is presented to illustrate its performance. To test EXPO, various random two dimensional truncated symplectic maps have been generated from random functions taken as Hamiltonians. The maps have been computed to very high orders (around 20); so for practical purposes they can be considered as the “exact” solutions. Then, using EXPO, the symplectified map has been computed from lower order approximations. In Fig. 1 a typical seed is presented. It is apparent that EXPO predicts the behavior of the exact map under iteration already at order 11, while the order 11 truncated Taylor map and the best of the conventional generator types ( $F_1$  in this case) fail to do that. Similar conclusions can be drawn from other random seeds too.

In summary, using Hofer’s metric, a condition for optimal symplectification was given. After a few manipulations, Hofer’s metric for Hamiltonian symplectic maps was expressed in terms of associated generating functions. Therefore, finding the best symplectified map turned out to be equivalent to finding the appropriate generator type. It was shown that the generator type which satisfies the optimality condition in general is given by (17), and it was called the EXPO type. Consequently, the symplectic

map  $\mathcal{N}_{\text{EXPO}}$ , obtained by symplectification of  $\mathcal{M}_n$  using EXPO, will give the best results in general. We mention that this result does not exclude the existence of custom tailored generator types that give better results for *specific* symplectic maps. Finally, while the results obtained in this Letter have been derived with accelerator physics motivation in mind, their relevance goes beyond beam physics and directly applies to any other weakly nonlinear problem in Hamiltonian dynamics.

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- [1] M. Berz, *Modern Map Methods in Particle Beam Physics* (Academic Press, San Diego, 1999), also available at <http://bt.nsl.msu.edu/papers/cgi/display.pl?name=AIEP108book>.
- [2] M. Berz, B. Erdelyi, and K. Makino, *Phys. Rev. ST Accel. Beams* **3**, 124001 (2000).
- [3] M. Berz, K. Makino, and B. Erdelyi (to be published).
- [4] K. Makino and M. Berz, *Nucl. Instrum. Methods Phys. Res., Sect. A* **427**, 338 (1999).
- [5] B. Erdelyi and M. Berz (to be published), preliminary version available at <http://130.83.124.174/frames/index.htm>.
- [6] M. Berz, in *Nonlinear Problems in Future Particle Accelerators* (World Scientific, Singapore, 1991), p. 288.
- [7] D. Abell, Ph.D. thesis, University of Maryland, 1995.
- [8] J. Shi and P. Suwannakoon, *Phys. Rev. E* **58**, 7868 (1998).
- [9] A. J. Dragt, L. M. Healy, F. Neri, and R. Ryne, *IEEE Trans. Nucl. Sci.* **3**, 2311 (1985).
- [10] G. Rangarajan, A. Dragt, and F. Neri, in *Proceedings of the 1991 Particle Accelerator Conference* (IEEE, San Francisco, 1991).
- [11] C. Altafini, in *Nonlinear Control in Year 2000*, edited by A. Isidori, F. Lamnabhi-Lagarrigue, and W. Respondek (Springer-Verlag, Berlin, 2000).
- [12] H. Hofer, *Proc. R. Soc. London A* **115**, 25 (1990).
- [13] D. McDuff and D. Salamon, *Introduction to Symplectic Topology* (Oxford University Press, New York, 1995).
- [14] H. Hofer and E. Zehnder, *Symplectic Invariants and Hamiltonian Dynamics* (Birkhauser, Basel, 1994).
- [15] M. Bialy and L. Polterovich, *Duke Math. J.* **76**, 273 (1994).
- [16] F. Lalonde and D. McDuff, *Invent. Math.* **122**, 1 (1995).
- [17] B. Erdelyi, Ph.D. thesis (to be published).
- [18] K. Feng, H. Wu, M. Quin, and D. Wang, *J. Comp. Math.* **7**, 71 (1989).
- [19] K. Siburg, *Calc. Var.* **3**, 299 (1995).
- [20] H. Poincare, *New Methods of Celestial Mechanics* (American Institute of Physics, New York, 1893/1993), Vol. 3, Chap. XXVIII.
- [21] B. Erdelyi and M. Berz, in *Proceedings of the 6th International Computational Accelerator Physics Conference* (TU Darmstadt, Darmstadt, Germany, 2000), <http://130.83.124.174/frames/index.htm>.