

EXTRACTING SYMPLECTIC MAPS FOR SPACE CHARGE DOMINATED BEAMS

N. Bachhawat*, V. N. Litvinenko^{†,1}, Stony Brook University, Stony Brook, NY, USA

¹also at Brookhaven National Laboratory, Upton, NY, USA

Abstract

Symplecticity of transfer maps is important for reliable evaluation of space-charge dominated beams in accelerators. Unfortunately, most simulation codes that include collective effects, such as space charge, do not use canonical phase-space variables and therefore are not symplectic in the presence of electromagnetic fields. In this paper, we present a numerical method to extract local linear symplectic transfer maps using particle tracking simulation code IMPACT-T for space-charge dominated beams. We demonstrate this method for the photo-injector (113 MHz SRF gun) section of the Coherent electron Cooling (CeC) Proof of Principle (POP) experiment.

INTRODUCTION

There is a need for rigorous analytical methods to study beam dynamics in accelerator lattices, which frequently involve solving 3D Maxwell-Vlasov equation [1]. Symplecticity of the local linearized maps is critically important for finding analytically tractable solution (i.e. linear integral equation) for microscopic instabilities, which could be otherwise missed even by the most sophisticated codes. An example of this is the discovery of Plasma Cascade instability (PCI), which was first seen experimentally [2, 3], but was not observed in IMPACT-T simulation data. The analytical treatment of PCI [4], subsequently allowed the IMPACT-T model to be updated and to correctly reproduce this phenomenon.

However, most of the commonly used particle codes which include collective effects (CE), including popular Particle-In-Cell (PIC) codes such as IMPACT-T [5], WARP [6], ASTRA [7] and PARMELA [8], track mechanical momenta instead of canonical momenta and generate accurate but non-symplectic transfer maps.

Since most CE particle-tracking codes are non-symplectic and symplectic tracking codes usually have limited functionality for start-to-end simulation that include guns and injectors, we propose a general numerical post-processing method to extract local linear symplectic maps (in the vicinity of a chosen phase-space trajectory) from any non-symplectic particle tracking codes.

METHOD

For codes using time as the independent variable, the extraction of symplectic transfer maps requires knowledge of the geometric transfer map, M_g as well as the vector

* nikhil.bachhawat@stonybrook.edu

[†] vladimir.litvinenko@stonybrook.edu

potential at both initial and final times¹. Then, we can solve the r.h.s. equation:

$$\{\vec{r}(t), \vec{p}(t)\} = M_g : \{\vec{r}(t_0), \vec{p}(t_0)\}, \quad (1)$$

where, $\vec{p}(t) = \vec{P}(t) - \frac{e}{c} \vec{A}(t, \vec{r}(t))$. A solution can be found by linearization of the map around the phase-space trajectories. Let us introduce 6-vectors to denote mechanical (Y) and canonical (X) phase-space coordinates:

$$\begin{aligned} Y &= \begin{bmatrix} \vec{r} \\ \vec{p} \end{bmatrix} \Rightarrow Y(t) = \mathbf{M}_g : Y(t_0); \\ X &= \begin{bmatrix} \vec{r} \\ \vec{P} \end{bmatrix} = Y + \frac{e}{c} \cdot \begin{bmatrix} 0 \\ \vec{A}^T(t, \vec{r}) \end{bmatrix} \Rightarrow X(t) = \mathbf{M}_s : X(t_0), \end{aligned} \quad (2)$$

where \mathbf{M}_s is the desirable, but unknown, symplectic transfer map. Let us pick one of the allowed space-phase trajectories (indicated by the subscript o):

$$Y_o(t) \equiv \begin{bmatrix} \vec{r}_o(t) \\ \vec{p}_o(t) \end{bmatrix} = \mathbf{M}_g : Y_o(t_0), \quad (3)$$

and expand map around it,

$$\begin{aligned} Y &= Y_o + \nu; \quad \nu = \begin{bmatrix} \vec{\rho} \\ \vec{\pi} \end{bmatrix}; \quad \nu(t) = \mathbb{M}_g \cdot \nu(t_0) + O(|\nu|^2); \\ \mathbb{M}_g &= \left. \frac{\partial(\mathbf{M}_g : Y)}{\partial Y} \right|_{Y=Y_o(t)}; \\ X &= X_o + \xi; \quad \xi = \begin{bmatrix} \vec{\rho} \\ \vec{\Pi} \end{bmatrix}; \quad \xi(t) = \mathbb{M}_s \cdot \xi(t_0) + O(|\xi|^2); \\ \vec{\Pi} &= \vec{\pi} + \mathbf{V}(t) \cdot \vec{\rho}; \quad \mathbf{V}(t) = \frac{e}{c} \cdot \left. \frac{\partial(\vec{A}(t, \vec{r}))}{\partial \vec{r}} \right|_{r=r_o(t)} \end{aligned} \quad (4)$$

where the local 6×6 matrix \mathbb{M}_g is defined by the geometric transfer map M_g and the chosen trajectory. The 3×3 matrix \mathbf{V} is defined by the vector potential, and the symplectic 6×6 matrix, \mathbb{M}_s , still needs to be determined. For the rest of the paper, we will also neglect higher order terms identified as $O(\varepsilon^2)$, where ε is the expansion parameter.

Unfortunately, particle tracking codes typically do not provide full information about the vector potential, including self-field contributions, and the user needs to define the necessary components of the EM 4-potential themselves.

¹ For codes using coordinates along the reference trajectory, s , one would need to know transverse components of the vector potential and scalar potential at initial and final azimuth to extract symplectic transfer map for (x,y,-ct, Px,Py, H/c). While technically it is different for the above description, the idea of the method is the same.

In addition, the user needs to be aware of approximations used in the code, such as the type of the field expansions used. Otherwise, there will be additional errors caused by difference between potentials used for tracking and that for extraction of the symplectic map.

In this paper, we provide the specific example of how to use the well-benchmarked code, IMPACT-T [5] to extract the symplectic map for a space-charge dominated electron beam generated in an SRF gun and focused by a solenoid.

First, we need to extract the geometric map, \mathbb{M}_g using IMPACT-T tracking data. We use small deviations in the initial 6D phase-space coordinates of tracked set of particles relative to the reference particle to ensure the linearity of the map given in Eq. 4. We use a set sized $\sim 4\%$ of the RMS values in each of 6 phase-space directions. This choice is specific to our accelerator as well as choice of mesh size and time step in IMPACT-T. Results can differ for other accelerators and tracking program.

To find \mathbb{M}_g , let us first introduce the $6 \times n$ matrix, $\mathbf{Y} = [Y_1, Y_2, \dots, Y_n]$ where n is the number of tracked particles. Each 6-vector, $Y_k = \begin{bmatrix} \vec{r}_k \\ \vec{p}_k \end{bmatrix}$, with $k = 1, 2, \dots, n$, corresponds to the 6D phase-space coordinates of the tracked particles. For \mathbf{Y}_i and \mathbf{Y}_f defined at the chosen initial and final times of the IMPACT-T simulation respectively, we get using Eq. 2,

$$Y_{kf} = \mathbb{M}_g \cdot Y_{ki} \Rightarrow \mathbf{Y}_f = \mathbb{M}_g \cdot \mathbf{Y}_i, \quad (5)$$

where the subscripts i and f denote at the initial and final. Now, we can proceed using the standard ‘‘method of least-squares’’, which requires that we minimize the quantity,

$$\Phi = |\mathbf{Y}_f - \mathbb{M}_g \cdot \mathbf{Y}_i|^2 \quad (6)$$

The solution to this is given by,

$$\begin{aligned} (\mathbf{Y}_f - \mathbb{M}_g \cdot \mathbf{Y}_i) \cdot \mathbf{Y}_i^T &= 0 \\ \Rightarrow \mathbb{M}_g &= (\mathbf{Y}_f \cdot \mathbf{Y}_i^T) \cdot (\mathbf{Y}_i \cdot \mathbf{Y}_i^T)^{-1} \end{aligned} \quad (7)$$

Here, it is not necessary that an inverse of $\mathbf{Y}_i \cdot \mathbf{Y}_i^T$ exists. However, since $\mathbf{Y}_i \cdot \mathbf{Y}_i^T$ is a 6×6 matrix, there is a high probability for an inverse to exist if we have $n \gg 6$ particles. We find that even with ~ 10 particles, we are able to obtain a solution for \mathbb{M}_g using this method. In our analysis, we typically use $n \sim 1000$. We would like to note that this linearization method can be used for both symplectic and non-symplectic tracking codes.

Vector Potential due to External EM Fields

Here, we describe the EM 4-potential for the example of the 113 MHz Superconducting RF (SRF) gun used in the CeC POP experiment [9].

The CeC gun system [2, 9, 10] comprises of two main elements: the 1.25 MV SRF gun and the focusing solenoid. Figure 1 shows profiles of the on-axis accelerating field (E_z) in the gun and the longitudinal magnetic field (B_z) in the solenoid.

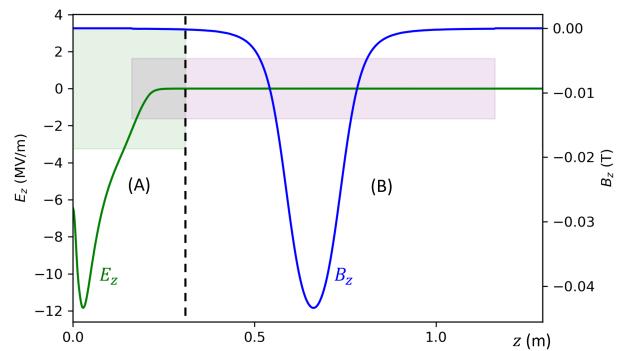


Figure 1: On-axis accelerating E_z field (green curve) of the 113 MHz SRF gun and the B_z field (blue curve) in the gun solenoid.

SRF Gun Since we are interested in local linear maps, it is sufficient to use a truncated expression for the vector potential [11, 12],

$$\begin{aligned} A_x &= \frac{1}{\omega} x \sum_{n=0}^{\infty} \frac{1}{2(n+1)} e'_n(z) r^{2n} \sin(\omega t + \theta) \\ A_y &= \frac{1}{\omega} y \sum_{n=0}^{\infty} \frac{1}{2(n+1)} e'_n(z) r^{2n} \sin(\omega t + \theta) \\ A_z &= -\frac{1}{\omega} \sum_{n=0}^{\infty} e_n(z) r^{2n} \sin(\omega t + \theta) \end{aligned} \quad (8)$$

where $r^2 = x^2 + y^2$ and

$$e_{n+1}(z) = -\frac{1}{4(n+1)^2} \left(e''_n(z) + \frac{\omega^2}{c^2} e_n(z) \right). \quad (9)$$

where $e_0(z)$ is the on-axis RF \mathbf{E} field, ω is the RF frequency (113 MHz), θ is the RF phase, and we only keep terms up to $n = 1$.

Gun Solenoid The vector potential associated with the focusing gun solenoid field is given by,

$$\begin{aligned} A_x(z, r) &= -\frac{B_z y}{2} + \frac{B''_z y r^2}{16} \\ A_y(z, r) &= \frac{B_z x}{2} - \frac{B''_z x r^2}{16} \end{aligned} \quad (10)$$

where B_z is the on-axis solenoid field. Since there is no current along the z direction in the gun solenoid, we have $A_z = 0$.

Correcting for Space-Charge Effects

In IMPACT-T, the space-charge field is assumed to have the form of an electrostatic field in the co-moving frame. For the quasi-static space-charge model in IMPACT-T, the electrostatic potential due to space-charge forces for a localized set of trajectories in a co-moving frame can be approximated by,

$$\vec{A}_c = 0, \quad \varphi_c(x_c, y_c, z_c) \neq 0 \quad (11)$$

where the subscript c denotes co-moving frame. In the lab frame, this field is given by,

$$\begin{aligned} x &= x_c; \quad y = y_c; \quad z = \gamma \cdot (z_c + vt_c); \\ A_{x,y} &= 0; \quad A_z = \beta\varphi; \quad \varphi = \gamma\varphi_c(x, y, z_c) \end{aligned} \quad (12)$$

For local linear maps extracted using IMPACT-T tracking data, the error in the space-charge vector potential due to such a “frozen-charge” approximation is expected to be much smaller than numerical PIC tracking errors as long as the space-charge distribution does not change very significantly. The numerical errors associated with the frozen-charge approximation is included in the symplecticity errors associated with the extracted transfer maps (reported in Table 1 for the CeC photo-injector).

Now, we need expressions for vector potentials, including both external and internal EM fields, to define 3×3 matrix \mathbf{V} at both initial (t_i) and final (t_f) times. Then, we can transform the extracted geometric matrix \mathbb{M}_g into a symplectic one,

$$\mathbb{M}_s = \begin{bmatrix} \mathbf{I} & 0 \\ \mathbf{V}_f & \mathbf{I} \end{bmatrix} \cdot \mathbb{M}_g \cdot \begin{bmatrix} \mathbf{I} & 0 \\ -\mathbf{V}_i & \mathbf{I} \end{bmatrix}. \quad (13)$$

Linearity of the EM field implies that the matrix \mathbf{V} is a direct sum of the contributions from the external and internal components of the EM field,

$$\begin{aligned} \vec{\mathbf{A}} &= \vec{\mathbf{A}}_{gun} + \vec{\mathbf{A}}_{sol} + \vec{\mathbf{A}}_{sc} \\ \Rightarrow \mathbf{V} &= \mathbf{V}_{gun} + \mathbf{V}_{sol} + \mathbf{V}_{sc}, \end{aligned} \quad (14)$$

which in our case comprises of three components: from the gun, the solenoid and the space charge indicated by subscript sc .

We have specific expressions for the gun and solenoid vector potentials, however, we only know the form of the vector potential due to space charge,

$$\mathbf{V}_{sc} = \frac{e}{c} \cdot \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{\partial A_z}{\partial x} & \frac{\partial A_z}{\partial y} & \frac{\partial A_z}{\partial z} \end{bmatrix}, \quad (15)$$

This means that there are three undetermined parameters in each of the initial ($V_{i sc}$) and final ($V_{f sc}$) vector potentials due to space-charge, which must be determined. Fortunately, the nature of extraction of the symplectic matrix from the geometric one allows us to apply the transformation given in Eq. 13 piece-wise.

This allows us to calculate the intermediate matrix (\mathbb{M}_{ext}),

$$\begin{aligned} \mathbb{M}_{ext} &= \begin{bmatrix} \mathbf{I} & 0 \\ \mathbf{V}_{f(gun+sol)} & \mathbf{I} \end{bmatrix} \cdot \mathbb{M}_g \cdot \begin{bmatrix} \mathbf{I} & 0 \\ -\mathbf{V}_{i(gun+sol)} & \mathbf{I} \end{bmatrix}; \\ \mathbb{M}_s &= \begin{bmatrix} \mathbf{I} & 0 \\ \mathbf{V}_{f sc} & \mathbf{I} \end{bmatrix} \cdot \mathbb{M}_{ext} \cdot \begin{bmatrix} \mathbf{I} & 0 \\ -\mathbf{V}_{i sc} & \mathbf{I} \end{bmatrix} \end{aligned} \quad (16)$$

and use the symplectic condition,

$$\mathbb{M}_s^T \mathbf{S} \mathbb{M}_s = \mathbb{M}_s, \quad (17)$$

Table 1: Symplecticity Errors, ϵ_{sym} for Transfer Maps for the CeC Photo-injector Model

Gun Region	$\epsilon_{sym}(\mathbb{M}_{ext})$	$\epsilon_{sym}(\mathbb{M}_s)$
A	0.11	0.031
B	0.084	0.0018

to determine the six unknown coefficients m_1, \dots, m_6 in the expressions for the initial and final space-charge vector potential (Eq. 15). Equation 17 is an over-determined system of 15 equations in six variables. Hence, the six coefficients can be found using the best fit estimate method to determine the final form of the extracted matrix \mathbb{M}_s .

EXAMPLE: CEC PHOTO-INJECTOR

Using the method described in Sec. Method, we extract \mathbb{M}_{ext} and \mathbb{M}_s from IMPACT-T tracking data by adding the 4-potential associated with external EM fields and space-charge forces. Here, it is useful to define “symplecticity error”, $\epsilon_{sym}(\mathbb{M})$ of a matrix \mathbb{M} [13, 14],

$$\epsilon_{sym}(\mathbb{M}) = \|\mathbb{M}^T \mathbf{S} \mathbb{M} - \mathbf{S}\|, \quad (18)$$

where $\|\mathbf{A}\| = \sqrt{\sum_{ij} |a_{ij}|^2}$ is the Frobenius norm of the matrix \mathbf{A} .

The “symplecticity errors” ϵ_{sym} for the geometric and canonical transfer maps are summarized in Table 1.

Finally, we can use a “symplectification algorithm” [15, 16] to eliminate the remaining tracking errors (listed in Table 1) and obtain a symplectic map, \mathbb{M}_{ps} , that is numerically close to \mathbb{M}_s .

Applying this symplectification algorithm [15, 16] on $\mathbb{M}_{s(A)}$, we obtain the symplectic matrix, $\mathbb{M}_{ps(A)}$ with $\epsilon_{sym}(\mathbb{M}_{ps(A)}) = 0$ (to numerical precision, $< 10^{-15}$)

A useful measure for how “close” the symplectic maps (\mathbb{M}_{ps}) are to the canonical transfer maps (\mathbb{M}_s) is,

$$\Delta_s = \frac{\|\mathbb{M}_{ps} - \mathbb{M}_s\|}{\|\mathbb{M}_s\|} \quad (19)$$

We find that $\Delta_s(A) = 0.006$ and $\Delta_s(B) = 0.0004$ for regions A and B of the photoinjector model (Fig. 1). Hence, the symplectification algorithm used only “tweaks” the canonical 6×6 map, which are obtained after adding vector potential contributions from external fields and space-charge forces, by 0.6% and 0.04% (combined for all 36 entries in the map) for regions A and B of the CeC photo-injector respectively.

ACKNOWLEDGEMENTS

We would like to acknowledge the continued support provided by J. Qiang with IMPACT-T. We would also like to thank K. Shih and Y. Jing for useful discussions.

REFERENCES

- [1] A. A. Vlasov, “The Vibrational Properties Of an Electron Gas”, *Soviet Physics Uspekhi*, vol. 10, no. 6, p. 721, Jun. 1968.
doi:10.1070/PU1968v010n06ABEH003709

- [2] I. Petrushina, "The Chilling Recount of an Unexpected Discovery: First Observations of the Plasma-Cascade Instability in the Coherent Electron Cooling Experiment", Ph.D. thesis, SUNY Stony Brook, New York, NY, USA, Jan. 2019.
- [3] V. N. Litvinenko *et al.*, "Plasma-cascade instability", *Phys. Rev. Accel. Beams*, vol. 24, p. 014402, Jan. 2021.
doi:10.1103/PhysRevAccelBeams.24.014402
- [4] V. N. Litvinenko *et al.*, "3D theory of microscopic instabilities driven by space-charge forces", *Phys. Rev. Accel. Beams*, vol. 26, p. 054402, May 2023.
doi:10.1103/PhysRevAccelBeams.26.054402
- [5] J. Qiang, S. M. Lidia, C. Limborg-Deprey, and R. D. Ryne, "A 3D Parallel Beam Dynamics Code for Modeling High Brightness Beams in Photoinjectors", in *Proc. PAC'05*, Knoxville, TN, USA, May 2005, paper WPAP055, pp. 3316–3318.
doi:10.1109/PAC.2005.1591453
- [6] A. Friedman, D. P. Grote, and I. Haber, "Three-dimensional particle simulation of heavy-ion fusion beams", *Phys. Fluids B: Plasma Phys.*, vol. 4, no. 7, pp. 2203–2210, Jul. 1992.
doi:10.1063/1.860024
- [7] K. Floettmann, *ASTRA, A Space Charge Tracking Algorithm*, DESY, 2000.
https://www.desy.de/~mpyflo/Astra_manual
- [8] L. M. Young and J. Billen, "The Particle Tracking Code PARMELA", in *Proc. PAC'03*, Portland, OR, USA, May 2003, paper FPAG029, pp. 3521–3523.
doi:10.1109/PAC.2003.1289968
- [9] I. Pinayev *et al.*, "High Charge High Current Beam From BNL 113 MHz SRF Gun", in *Proc. ERL'19*, Berlin, Germany, Sep. 2019, pp. 145–149.
doi:10.18429/JACoW-ERL2019-THCOYBS02
- [10] K. Shih, "Intelligent Control of Instabilities in Space-Charge Dominated Beams", Ph.D. thesis, SUNY Stony Brook, New York, NY, USA, May 2023.
- [11] P. L. Morton, "Particle dynamics in linear accelerators", Ph.D. thesis, The Ohio State University, Columbus, OH, USA, Dec. 1963.
- [12] J. Qiang, *IMPACT-T User Document Version 2.2*, Lawrence Berkeley National Laboratory, Nov. 2022.
https://github.com/impact-lbl/IMPACT-T/blob/master/doc/ImpactT_v2.pdf
- [13] L. E. Cook *et al.*, "Which Algorithm Best Propagates the Meyer–Miller–Stock–Thoss Mapping Hamiltonian for Non-Adiabatic Dynamics?", *J. Chem. Theory Comput.*, vol. 19, pp. 6109–6125, 2023.
doi:10.1021/acs.jctc.3c00709
- [14] A. N. Ivanov, S. N. Andrianov, N. V. Kulabukhova, R. Maier, Y. Senichev, and D. Zyuzin, "Testing of Symplectic Integrator of Spin-orbit Motion Based on Matrix Formalism", in *Proc. IPAC'13*, Shanghai, China, May 2013, paper WEPEA037, pp. 2582–2584.
- [15] L. M. Healy, "Lie-algebraic methods for treating lattice parameter errors in particle accelerators", Ph.D. thesis, Univ. of Maryland, College Park, MD, USA, Dec. 1985.
<https://www.osti.gov/biblio/6796986>
- [16] W. W. MacKay, "Comment on Healy's Symplectification Algorithm", in *Proc. EPAC'06*, Edinburgh, UK, Jun. 2006, paper WEPCH152, pp. 2281–2283.