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MODELING OF NONLINEAR BEAM DYNAMICS VIA A NOVEL PARTICLE-MESH METHOD AND SURROGATE MODELS WITH SYMPLECTIC NEURAL NETWORKS*

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Abstract

The self-consistent nonlinear dynamics of a relativistic charged particle beam, particularly through the interaction with its complete self-fields, is a fundamental problem underpinning many accelerator design issues in high brightness beam applications, as well as the development of advanced accelerators. A novel self-consistent particle-mesh code, CoSyR, is developed based on a Lagrangian method for the calculation of the beam particles' radiation near-fields and associated beam dynamics. Our recent simulations reveal the slice emittance growth in a bend and complex interplay between the longitudinal and transverse dynamics that are not captured in the 1D longitudinal static-state Coherent Synchrotron Radiation (CSR) model. We further show that surrogate models with symplectic neural networks can be trained from simulation data with significant time-savings for the modeling of nonlinear beam dynamics effects. Possibility to extend such surrogate models for the study of spin-orbital coupling is also briefly discussed.

CSR MODELING WITH PARTICLE MESH METHOD

Nonlinear beam dynamics can arise from the nonlinearity of the lattice or the self-fields in an intense beam. These nonlinear dynamics are challenging to be modelled accurately and efficiently, especially over long term evolution. In Ref. [1], we have implemented a particle-mesh method for the self-consistent calculation of the self-fields of a high brightness beam, using wavefront/wavelet meshes following the characteristic of the Green's function of the Maxwell equations. Based on the time scale of field propagation, these self-fields are either calculated exactly from the particle trajectory or approximated due to the close proximity of the emission. The former leads to retarded interactions among the beam particles that are typically paraxial but sensitive to model/numerical errors, while the latter describes close-by interactions for which the usual static-state model is applicable. For an emitting particle, both retarded and close-by contributions to the beam self-fields are then interpolated from the particle's wavefront/wavelet meshes onto a moving mesh for dynamic update of the beam. This method allows radiation co-propagation and self-consistent interaction with the beam in 2D/3D simulations at greatly reduced numerical errors. Multiple levels of parallelisms are inherent in this method and implemented in our code CoSyR to enable at-scale simulations of nonlinear beam dynamics on modern computing platforms using MPI, multi-threading, and GPUs.

Beam Dynamics in Chicane Compressor

For high brightness beam applications, such as free electron lasers, the transverse dynamics are of importance. Recently, there is interest to develop the understanding of the transverse effects of CSR beyond the 1D models, e.g., in Refs. [2, 3]. We have shown that the longitudinal and transverse beam dynamics in a bend happen in a complex manner [1], which is not captured in the 1D longitudinal CSR model. To further elucidate their role and interplay for a chirped beam in a chicane compressor, we simulated an initial beam of 50 MeV, 0.6 kA in a chicane with a compression ratio of about 3. CoSyR is used only for the first bend for 3 cases: without CSR, or with only longitudinal or full 2D steady-state CSR effect. The rest of the chicane is modeled with linear beam optics. The final beam slice emittance and current are compared in Fig. 1. The longitudinal CSR field introduces a large distortion of the current profile and slice emittance. However, much lower slice emittance growth is observed when the transverse field is also included in the simulation, and the beam profile is closed to the case without CSR.

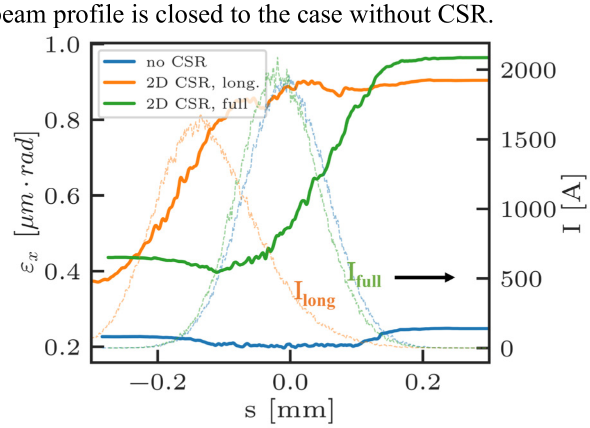

Figure 1: Beam slice remittances (left) and current profiles (right) without CSR, or with only longitudinal or full 2D steady-state CSR effect.

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BEAM DYNAMIC MODELING WITH NEURAL NETWORKS

The existing software for modeling particle beam dynamics is either limited to linear analysis or only provides the preliminary lattice design evaluation, while first-principle codes for spot-checking are too expensive for tackling inverse problems, parameter optimization and data-intensive applications. The successful deployment of a robust machine-learning (ML) based surrogate that embeds fundamental physical constraints to the interaction and evolution of such beams may significantly help the design and optimization of large scale accelerators. We explore the design of HenonNet [4] for a multi-physics nonlinear beam dynamic surrogate modeling capability that can be orders of magnitude faster than first-principle codes. Two examples are the nonlinear radiative effects of high brightness electron beams in linacs and transfer lines, and the stochastic spin dynamics in high energy polarized electron storage rings. For the former, the CSR fields can disrupt the beam transport in a complex manner as shown above. In spin dynamics, our interest is the study of the polarization in electron-positron storage rings.

Network Architectures and Training

In this work we propose several structure-preserving neural networks as a surrogate to approximate the flow maps corresponding to Hamiltonian beam dynamics. The most critical property of the flow maps Φ of Hamiltonian is the symplecticity, i.e., its Jacobian satisfies $(D\Phi)^T J\, D\Phi = J$, where J is the skew-symmetric matrix with zero diagonal blocks and $\pm I$ off-diagonal blocks. Note that all the linear symplectic matrices form a real Lie group $Sp(2n, R)$. This Lie group has been commonly used in accelerator physics to describe the dynamics, although a general flow map is nonlinear, which has not been fully explored yet in data-driven applications due to the lack of approximation tools. In this work, we will fill in the gap and propose two network architectures that can approximate linear or nonlinear symplectic maps.

G-reflectors for Linear Symplectic Matrices The optimization on $Sp(2n, R)$ has been recently explored in [5]. However, the approach therein is cumbersome to realise in a machine learning framework. In this work we propose a simple but very effective alternative approach that is naturally compatible with any ML framework. The idea is to first parameterize any symplectic matrix and then perform its optimization in the parameterized space. In particular, we define a G-reflector of $G := I + \beta u u^T J$ where β is scalar and u is a vector in R^{2n}. It is easy to show G is a symplectic matrix and its inverse is $G^{-1} = I - \beta u u^T J$, which is also symplectic. Note that any G is parameterized by $2n$ parameters (assume u is normalised). The theorem in [6] says that any real symplectic matrix can be expressed as a product of at most $4n$ G-reflectors. Therefore, by simply compositing 4n different G-reflectors, we obtain a general parameterization of a symplectic matrix. This general architecture is called **SympMat**. It is well known that the symplectic group has a dimension of $n(2n+1)$ while the total parameterization in our SympMat architecture is $8n^2$, which is sup-optimal. However, since the beam dynamics is low-dimensional, SympMats work very well.

HenonNets for Nonlinear Symplectic Maps Our previous work [4] proposed a symplectic neural network–HenonNets–that is a general symplectic nonlinear map and has a provable symplectic universal approximation property. However, the previous work only considered a low dimensional case of 2D Hamiltonians that is used to describe a divergence-free magnetic field in tokamaks. We generalise the previous network to 6D beam dynamics in this work. The basic building block of HenonNets is a Henon layer, which is defined as a map from $(x, y) \to (\underline{x}, \underline{y})$ such that $\underline{x} = y + \eta$, $\underline{y} = -x + \partial\psi(y)$ and η is a bias and $\psi(\cdot)$ is a scalar potential function represented as a neural network. Here both η and $\psi(\cdot)$ are learned in a ML framework in a supervised fashion. The Henon layer is then composited $4N$ times to become a HenonNet, which is thus symplectic by design. We note that when $\eta = 0$ and $\psi(\cdot) = 0$, a HenonNet represents a trivial identity map. Since we rely on a HenonNet as a correction of a trained linear SympMat in this work, the HenonNet is typically initialised as an identity map using the above property.

Network Implementation and Training Our networks are deployed using Tensorflow. Both SympMats and HenonNets are implemented as custom models (and layers). The overall model is composed of a SympMat followed by a HenonNet. The general training workflow follows the standard procedure of transfer learning and fine tuning. We start with learning the SympMat for given data for linear beam dynamics and follow by learning the HenonNet with the learned SympMat being fixed. The final fine tuning stage uses a small learning rate to train the network. The training uses a loss of a standard mean-squared error and it is supervised. The training data uses the particle trajectory data for one or several beams with different initial phase space, collected through tracking simulations of a chicane or of several turns in a ring.

Application to Nonlinear Beam Dynamics

In our preliminary study (Fig. 2), we have applied SympMat and HenonNet to the beam dynamics in a chicane bunch compressor. As discussed above, the electron beam brightness can be disrupted in a complex manner in self-consistent simulation beyond 1D model prediction, however, an accurate first-principle simulation requires $\sim 10^4$ core-hours due to the ultrawide bandwidth of synchrotron radiation. As a first step, we focus on the nonlinear dynamics from the chicane itself and use particle tracking simulation data for training.

The model is trained from the 4D phase space data (i.e., in the bending plane) of a nonlinear tracking simulation for a beam with 5% energy chirp at 130MeV designed for the compressor. Then the trained ML surrogate model is used to predict the dynamics of two beams with 10% energy chirp (i.e., unseen data). One beam has the same length

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(leading to over compression) and the other beam is 2 times longer (so that the compression ratio remains the same). Figure 2 shows that both beam distributions are predicted reasonably well by the surrogate model. We note that the curved shape of the phase space in Fig. 2 is due to 2nd order nonlinearity of the chicane. It is also captured by our ML model and can be improved via better training procedures. This result indicates that such a physics-based surrogate model has the ability to extrapolate the learned 2nd order lattice nonlinearity on a trained dataset to that with another beam distribution.

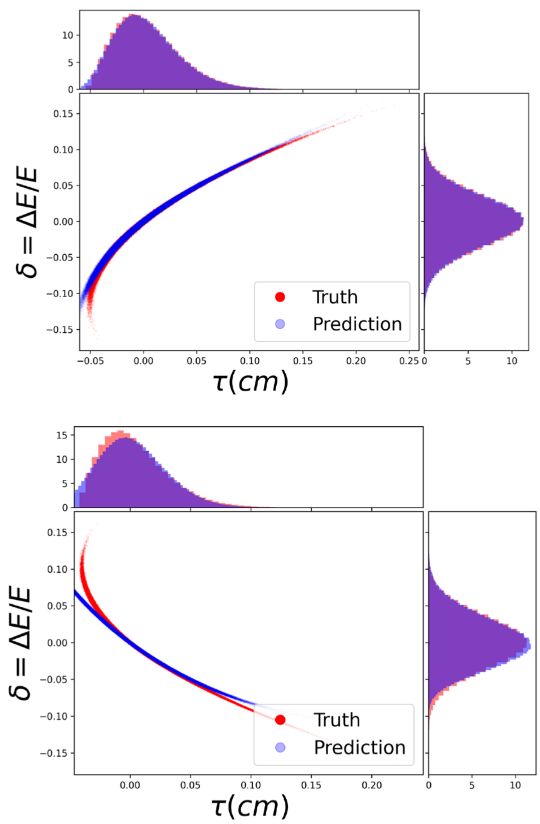

Figure 2: Preliminary HenonNet model prediction of the longitudinal phase space (δ=ΔE/E, τ: bunch length in cm) of electron beams with 10% initial energy chirp after a chicane compressor with length: (top) 2x longer, (bottom) same as the beam in the training data.

Application to Spin Dynamics

The electric and magnetic fields in a storage ring couple to the magnetic moments of electrons and exert a torque on the intrinsic angular momenta, causing the spins to precess. The spin precession is described by the Thomas-Bargmann-Michel-Telegdi equation (Thomas-BMT) [7]. The photon emission in synchrotron radiation affects the orbital motion of electrons in a storage ring and this can lead to an equilibrium particle distribution in phase space of a bunch. This is modelled by adding noise and damping to the particle motion [8, 9] in Monte-Carlo simulations. The photon emission also affects the spin motion and this can lead to the build-up of spin polarization which can reach an equilibrium resulting from a balance of three factors, namely the Sokolov-Ternov process, depolarization and the so-called kinetic polarization effect. One of the ways to study spin depolarization that avoids the long term Monte-Carlo simulations is the analysis of the lattice's *invariant spin field (ISF)* - a spin field which is periodic and size one at every point of phase space. The ISF $\hat{n}(s,r)$, satisfies

$$\partial_s \hat{n} = -\sum_{i=1}^{6} \partial_{r_i} A(s,r) + \Omega(s,r) \times \hat{n}, \tag{1}$$

$$\hat{n}(s,r) = \hat{n}(s+L,r), \ |\hat{n}| = 1, \forall\, s,r. \tag{2}$$

Here, $r \in \mathbb{R}^{2d}$ $(d = 1{,}2,$ or $3)$ is the phase space variable, and s is accelerator azimuth. The ML algorithm seeking the approximation to the ISF using the tracking data can be summarised as follows:

- Train the SympMat/HenonNet for the orbital dynamics as explained in earlier sections.
- Approximate the ISF by minimising the residual of Eq. (1) under constraints Eq. (2), or alternatively minimize the residual of
  $$R(r)\hat{n}(s_0,r) = \hat{n}(s_0, M(r)),$$

where M and R are orbit and spin transport maps and s_0 is a fixed azimuth.

CONCLUSION

Self-consistent simulation indicates that transverse CSR fields can lead to slice emittance growth in a chicane. A physics-based ML surrogate model is also developed for the nonlinear beam dynamics and will be extended to collective and spin dynamics in future work.

REFERENCES

[1] C.-K. Huang *et al.*, "CoSyR: A novel beam dynamics code for the modeling of synchrotron radiation effects", *Nucl. Instr. Meth. Phys. Res. Sect. A,* vol. 1034, p. 166808, 2022. doi:10.1016/j.nima.2022.166808

[2] Y. Cai and Y. Ding, "Three-dimensional effects of coherent synchrotron radiation by electrons in a bunch compressor", *Phys. Rev. Accel. Beams,* vol. 23, p. 014402, 2020. doi:10.1103/PhysRevAccelBeams.23.014402

[3] A. D. Brynes *et al.*, "Beyond the limits of 1D coherent synchrotron radiation", *New J. Phys.,* vol. 20, no. 7, p. 073035, 2018. doi:10.1088/1367-2630/aad21d

[4] J. W. Burby, Q. Tang, and R. Maulik, "Fast neural Poincaré maps for toroidal magnetic fields", *Plasma Phys. Controlled Fusion,* vol. 63, no. 2, p. 024001, 2020. doi:10.1088/1361-6587/abcbaa

[5] P. Birtea, I. Cașu, and D. Comănescu, "Optimization on the real symplectic group", *Monatsh Math,* vol. 191, pp. 465–485, 2020. doi.org/10.1007/s00605-020-01369-9

[6] D. S. Mackey and N. Mackey, "On the determinant of symplectic matrices", Numerical Analysis Report No. 422, Manchester Centre for Computational Mathematics, Manchester, England, 2003.

[7] J. Jackson, *Classical Electrodynamics, 3rd Ed.*, New York, NY, Wiley, 1999.

[8] M. Sands, "The Physics of Electron Storage Rings: An Introduction," SLAC Rep. No. SLAC-121, 1970.

[9] J. A. Ellison, H. Mais, and G. Ripken, "Orbital eigen-analysis for electron storage rings," *Handbook of Accelerator Physics and Engineering, 2nd Ed.*, World Scientific, pp. 68-71, 2013.