Simulation advances in Coherent Synchrotron Radiation modeling

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#### https://github.com/lanl/cosyr.git [1]Huang et al., NIMA 1034 (2022) 166808





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#### Outline

- Challenge: modeling/understanding of high brightness beams dynamics at the most detailed level and with fast turn-around time
- A new particle-mesh beam dynamics tool and neural surrogate models
- Some understandings from first beam dynamic simulations with accurate Coherent Synchrotron Radiation (CSR) treatment



# Near-field SR plays an important role in the dynamics of high-current beams

#### Far field SR (x-ray) is generated in 3<sup>rd</sup> and 4<sup>th</sup> generation light sources



### The quest for brighter beams with better control



# Increasing importance of collective beam dynamic effects from radiative interaction

- Beam brightness cannot be improved once generated from the source
- As a non-neutral plasma, the collective effects of a high brightness beam in the transport is critical for accelerator applications
  - Space charge (electrostatic interaction)
  - o Intra-beam scattering (collisional interaction)
  - Wakefield (boundary interaction)
  - Coherent and incoherent synchrotron radiation (radiative interaction)



Degradation of brightness due to beam compression



S. Di Mitri et al., Phys. Rep., vol. 539, no. 1, 2014.

# PIC simulation of beam dynamics from coherent synchrotron radiation : high resolution needed to reduce numerical errors









- High cost at fine resolution due to Courant condition
- Yee or high order solver
- Need moving window and proper PML
- Difficult to find suitable boosted frame
- > Error in field cancellation from staggered grids (esp. for transverse force  $\propto \gamma^{-2}$ )

2D analytical steadystate model (LW-CSR)

### **CSR** simulation models

- 1D steady-state models
- 2D/3D steady-state models: pyCSR
- 2D self-similarity model based on Liénard-Wiechert (LW) equation
- 2D sub-bunch model: CSRtrack
- 3D model with prescribed particle trajectories: LW3D
- Particle-In-Cell (PIC) based on FDTD (Finite Difference Time Domain)
- Jefimenko's equation





(e) Longitudinal wake at x = 0, y = 0, parameter set A

(f) Longitudinal wake at x = 0, y = 0, parameter set B



(a) Horizontal wake at x = 0, y = 0, parameter set A



<sup>(</sup>b) Horizontal wake at x = 0, y = 0, parameter set B

G. Bassi, T. Agoh, M. Dohlus, L. Giannessi, R. Hajima, A. Kabel, T. Limberg, and M. Quattromini, Overview of CSR Codes, Nucl. Instruments Methods Phys. Res. Sect. A Accel. Spectrometers, Detect. Assoc. Equip. 557, 189 (2006).

C. E. Mayes, Computational Approaches to Coherent Synchrotron Radiation in Two and Three Dimensions, J. Instrum. 16, P10010 (2021).

# The need of a beam dynamics simulation tool for the extreme scale

- Modeling near-field SR accurately & efficiently is critical to understand the self-consistent dynamics of high brightness beams, e.g., for hard x-ray FELs.
- For CSR modeling, many methods and simulation tools have been developed. Yet self-consistent multi-dimensional simulation is lacking.
- We are developing a self-consistent Green's function-based dispersion-free particle-mesh method for the exascale inspired by Shintake's idea.



# A Lagrangian method that enables near-field radiation calculation by tracing wavefronts



#### Radiation field on an adaptive mesh from acceleration



Electric fields can be calculated in instantaneous electron rest frame

$$\vec{E}'_{vel} = -e \frac{\hat{n}}{r'^2}$$

$$\vec{E}'_{acc} = e \frac{\hat{n} \times (\hat{n} \times \vec{a}')}{r'} \longrightarrow \text{Missing term}$$

$$\text{Li et al., Proc. 10th Int.}$$
Particle Accelerator Conf.  
207-309 (2010)

Lorentz transformation

$$\vec{E} = \frac{e\left(\hat{n} - \overrightarrow{\beta'}\right)}{\gamma^2 \rho^2 \left(1 - \hat{n} \cdot \overrightarrow{\beta'}\right)^3} + \frac{e\hat{n} \times \left[\left(\hat{n} - \overrightarrow{\beta'}\right) \times \dot{\overrightarrow{\beta'}}\right]}{c\rho \left(1 - n \cdot \overrightarrow{\beta'}\right)^3}$$

#### Design of CoSyR: algorithm



time scale

-200

-100

 $\alpha \gamma^3$ 

-2

-300

- The retarded Green's functions are collocated in this wavefront-wavelet approach
- General for other Green's functions, e.g., for the Jefimenko equation.

0.05

300

slow time s

200

100

#### Los Alamos National Laboratory

#### **Combining subcycle and dynamic wavelets**

- Wavelets are generated at past dt's up to t=0 or up to the point the emitted wavefront outruns the mesh, whichever comes first
- Take left region as subcycle area (owing to their small retardation) defined by

 $dt_{sub} \sim \frac{\Delta x'_m}{4} + \frac{\Delta {y'_m}^2}{2\Delta x'_m}$ 

- Pre-calculate mesh points (from LW-CSR) with retarded angle(time) satisfying  $\psi \leq dt_{sub}$  as subcycle wavelets, and shift according to particle's offset to mesh center (i.e., discrete convolution)
- Self-generated wavelets and shifted subcycle wavelets are interpolated to mesh





C.-K. Huang, et al., NIM A, 1034, 166808, 2022

## **Mesh remapping with Portage**

#### https://laristra.github.io/portage/



- remap steps:
  - 1. redistribute points (optional)
  - 2. search: retrieve wavelet neighbors of a mesh point.
  - 3. accumulate: evaluate weight functions on each mesh point.
  - 4. estimate: do field estimation on mesh points.



#### **Tailoring the search step for wavelets**

- create dedicated search kernel in Portage:
  - assign a box to each mesh point based on the smoothing length.
  - create a helper grid that encloses those boxes (GPU-friendly).
  - bin wavelet points into cells by coordinates hashing.
  - -queries: retrieve and scan cells that overlap with the box of the mesh point.



•  $h_{ij}$ : radius of  $p_i$  for  $j^{th}$  axis.

• mean radius: 
$$h_j = \frac{\alpha}{n} \sum_{i=1}^n |h_{ij}|$$
,  $\alpha > 0$ .

• sides: 
$$s_j = \min\left[\frac{x_{Mj} - x_{mj}}{h_j}, s_M\right]$$
 cached

• number of bins:  $n_{bins} = s_1 s_2$  cached

• point: 
$$p_i = (x_{i1}, \dots, x_{id})$$

• cell: 
$$c_{ij} = \min \left[ s_j * \frac{x_{ij} - x_{mj}}{x_{Mj} - x_{mj}}, s_j - 1 \right]$$

• bin: 
$$b_i = c_{i1} + c_{i2}s_1$$

#### Field remapping from wavelets



#### **Design of CoSyR: parallelization**

#### **Parallelization**

#### **CoSyR** weak scaling





Kokkos, CoPA-Cabana are DOE ECP projects supporting major platforms (CPU/GPU/KNL/ROCm)

### Single-particle kernel field benchmark ( $\gamma$ =10,3000x200um)





#### Benchmark and new understanding of beam CSR fields



#### Benchmark and new understanding of beam CSR fields

γ=100, 0.01nC, 200x200um



Large cancellation in transverse force, however, this force plays an important role in transverse dynamics and offsetting longitudinal energy loss

#### Benchmark and new understanding of beam CSR fields

Comparison between results with subcycle only and subcycle + dynamic wavelets



Dynamic components with slower time scale

Comparison between results with subcycle only and subcycle + dynamic wavelets



γ=500, 0.01nC, 10x10um

### **CSR effects in a bending magnet**

Comparison of beam dynamics from longitudinal and transverse CSR fields



#### **CSR** effects in a chicane compressor

Comparison of beam dynamics from longitudinal and transverse CSR fields



 $\gamma$ =100, I=0.6kA, compression rate ~3

Full 2D CSR simulation shows slice emittance growth, but substantially less than from the case with longitudinal field only

### **CSR shielding: Impressed Currents and Moving Mesh**



 $t_{\rm transit}$  can be swept so that all intersections at  $t_R$  can be found

We validated the method by considering a bigaussian bunch (0.01 nC, gamma=500, 10 micron spot) being bent through a magnetic dipole.

We compare the longitudinal wake against CoSyR

- To compute the CSR shielding effect, we employ an approach similar to a boundary element method (BEM).
- On all shielding walls, surface currents are computed in response to the moving bunch.
- The resulting radiating fields can be computed through a convolution.
- For parallel plates, this surface current can be computed analytically using image theory.
- Our eventual goal is to implement a complete BEM to generalize the method to arbitrary shielding surfaces.





### **1D Shielding Results**



- Next, we considered CSR shielding on a 1D Gaussian bunch moving through a dipole magnet.
- 1 nC, 0.3 mm length, 10 m bending radius
- We considered the steady state longitudinal field along the length of the bunch for different gap sizes.
- In each case, we see good agreement against the results from Sagan et al. 2008.
- We are currently working on validating shielding for a 2D bunch against CSRtrack.



- An interesting observation we made was that having image charges for each physical particle seems to be unnecessary.
- We note in the plot above that having 4 macroparticles approximating the image bunch gives use a virtually identical result.

#### Symplectic neutral surrogate model based on HenonNet

Basic idea: Hamiltonian dynamic of charge particle is symplectic, surrogate model can employ such constraint for robustness

The basic building block

Symplectic universal approximation theorem

#### Definition (Hénon layer)

Let  $V_W : \mathbb{R}^N \to \mathbb{R}$ ,  $W \in \mathcal{W}$ , be a feed-forward neural network. The **Hénon layer** with potential  $V_W$  and bias  $\eta \in \mathbb{R}^N$  is the layer  $HL_{(W,\eta)} : \mathbb{R}^{2N} \to \mathbb{R}^{2N}$  given by

$$\mathit{HL}_{(W,\eta)} = \mathit{H}_{(W,\eta)} \circ \mathit{H}_{(W,\eta)} \circ \mathit{H}_{(W,\eta)} \circ \mathit{H}_{(W,\eta)}$$

where  $H_{(W,\eta)}: (x,y) \mapsto (\overline{x},\overline{y})$  is given by

 $\overline{x} = y + \eta$  $\overline{y} = -x + \nabla V_W(y).$ 

 $HL_{(W,\eta)}$  is a symplectic map for any  $(W,\eta)!$ 

$$|H[V,\eta]^{4N} - \mathcal{F}|_{C'(U)} < \epsilon$$

Dmitry Turaev. Nonlinearity 16.1 (2002): 123.



J. Burby J, Q. Tang Q and R. Maulik, Plasma Phys. Control. Fusion 63 024001, 2020

### Symplectic neural surrogate for RF cavities

C.-K.Huang et al. 2022 Proc. North American Particle Accelerator Conference pp.462–464



Synchronous particle defined by the average of the matched beam

#### Training and test on mismatched beams in CCL



Analytic transfer matrix

ML learned transfer matrix

	1.2821 0.09569	6.729 1.2821	0 0	0 0	0 0	0 0	$ \begin{vmatrix} x \\ x \\ p \end{vmatrix} $
=	0	0	1.2821	6.729	0	0	2
	0	0	0.09569	1.2821	0	0	P
	0	0	0	0	0.4955	4.108	
	0	0	0	0	- 0.18355	0.4955	ll p

у

[1.256 6.659 -0.003 0.034 -0.003 0.022] [0.084 1.241 0.000 -0.004 0.000 -0.000] [0.013 0.120 1.245 6.663 -0.005 -0.012] [0.001 0.013 0.085 1.259 -0.000 0.000] [0.014 0.178 -0.000 0.053 0.576 4.338] [-0.001 -0.012 0.002 0.028 -0.159 0.540]

- Demonstrated ~10% level accuracy
- Accuracy may be impacted by the nonlinear part of the beam
- We are exploring other techniques to improve this accuracy.

# Parametric HenonNet can learn parameter-dependentcollective beam dynamicsC.-K. Huang, et al., J. Phys. Conf. Ser. 2687, 062026 (2024)

A single **P-HenonNet** learns longitude dynamics parameterized by beam current. I=0mA I=10mA I=20mA



- Each plot predicts the dynamics of a LANSCE beam from 100 MeV to 800 MeV under various space charge conditions and only takes 0.015s on one GPU! (Data from each BEAMPATH simulation is generated in 20 hours using a high-end workstation)
- Error <~10% after transfer learning and fine tuning even for the most challenging case (I=20mA)

#### Parametric HenonNet can handle multiple parameters







#### Symplectic neutral surrogate for beam dynamics in chicane



### Symplectic neutral surrogate for beam dynamics in chicane



#### Symplectic neutral surrogate for beam dynamics in chicane

Linear chicane beam dynamics + CSR



Possible explanation: the network learns two maps, one for  $\delta - \tau$ , and the other one is the linear map of the chicane without self-field

#### Summary

- Challenge: modeling/understanding of high brightness beams dynamics at the most detailed level and with fast turn-around time
- Development and verification of a unique beam dynamics code (CoSyR) and ML model (HenonNet)
- First beam dynamic simulations with accurate CSR treatment, more to come!



• Future development: incoherent synchrotron radiation model; performance improvement for high beam energy and on Exascale platforms; neural surrogate models

### **Backup slides**

### Improving the weights computation



red: mesh point  $p_i$ blue: wavelet points  $q_{1 \le j \le n}$ 

basis vector: b<sub>i</sub> = (1, x, x<sup>2</sup>/2, ..., x<sup>n</sup>/n!) in 1D
moment vector: m<sub>ij</sub> = (b<sub>i</sub>, ∇b<sub>i</sub>, ...)<sup>-1</sup> b<sub>j</sub>
scalar weight: w<sub>ij</sub> = K(d<sub>ij</sub>)/K(0) with kernel K.
n<sub>basis</sub> : number of components of b<sub>i</sub> and m<sub>ij</sub>.

- normal algorithm for each mesh point  $p_i$ :
  - build moment matrix  $A_i = (a_{\tilde{i}\tilde{j}})_{0 \leq \tilde{i}, \tilde{j} \leq n_{basis} = 1}$  with each  $a_{\tilde{i}\tilde{j}} = \sum_{j=1}^n m_{ij|\tilde{i}} m_{ij|\tilde{j}} w_{ij}$
  - for each wavelet neighbor  $q_j$ , solve  $A_i X_{ij} = m_{ij}$ , then deduce  $\omega_{ij} = X_{ij} w_{ij}$ .
- optimize it since field derivatives are not needed:

-cache scalars 
$$s_{ij} = m_{ij|0}$$
 and  $a_i = \sum_{j=1}^n s_{ij}^2 w_{ij}$ 

- for each wavelet neighbor  $q_j$ , compute  $\omega_{ij} = \frac{s_{ij}w_{ij}}{a_i}$ 

#### Neural network as universal function approximator



#### HenonNets have some good properties

- Collection of all HénonNets forms a group
- Closure of that set is the symplectomorphism group
- HénonNet is an invertible network. Inverse of a HénonNet is a HénonNet. Its inverse is easy to construct and fast to evaluate.
- Derivatives of a HénonNet are easy to compute using automatic differentiation (sensitivity analysis)
- HénonNet is a type of ResNet. We can prove each Hénon layer fits into the ResNet framework of

$$\overline{\mathbf{x}} = \mathbf{x} + \mathcal{F}(\mathbf{x}).$$

#### Symplectic neutral surrogate of Hamiltonian dynamics

Consider a perturbed pendulum

$$H_{\rm pp}(x, y, \phi) = \frac{1}{2}y^2 - \omega_0^2 \cos x - \epsilon \left[ 0.3 \, xy \sin(2\phi) + 0.7 \, xy \sin(3\phi) \right],$$

with 
$$\omega_0=$$
 0.5 and  $\epsilon=$  0.5.



J. W. Burby, Q. Tang, and R. Maulik. ``Fast neural Poincaré maps for toroidal magnetic fields." Plasma Physics and Controlled Fusion 63.2 (2020): 024001.