Space Charge Modelling of Long Bunches and Data Driven Approaches

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ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION ATAP

Outline

- Two and a half dimensional space-charge solver for long bunches
- Neural network surrogate model for space-charge effects
- Differentiable space-charge model
- This session's talks

Space-Charge Model: from Maxwell Equations to Poisson Equations

Maxwell Equation with Lorenz Gauge

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial s^2}-\frac{1}{c^2}\frac{\partial^2\phi}{\partial t^2} = -\frac{\rho(x,y,s,t)}{\epsilon_0}$$

$$\frac{\partial^2 A_s}{\partial x^2}+\frac{\partial^2 A_s}{\partial y^2}+\frac{\partial^2 A_s}{\partial s^2}-\frac{1}{c^2}\frac{\partial^2 A_x}{\partial t^2} = -\frac{J_s(x,y,s,t)}{c^2\epsilon_0}$$

$$\rho=\rho(x,y,s-v_0t), \qquad \mathbf{J}=\mathbf{J}(x,y,s-v_0t) \qquad z=s-v_0t,$$

Space-Charge Model: Poisson-like Equation

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{1}{\gamma^2}\frac{\partial^2\phi}{\partial z^2} = -\frac{\rho(x,y,z)}{\epsilon_0}$$

$$\frac{\partial^2 A_s}{\partial x^2}+\frac{\partial^2 A_s}{\partial y^2}+\frac{1}{\gamma^2}\frac{\partial^2 A_s}{\partial z^2} = -\frac{J_s(x,y,z)}{c^2\epsilon_0}$$

$$A_s(x,y,z)=\frac{\beta}{c}\phi(x,y,z)$$

2.5D Space-Charge Model for Long Bunch

long bunch: $\frac{\partial^2\phi}{\partial x^2} \gg \frac{1}{\gamma^2}\frac{\partial^2\phi}{\partial z^2}$ and $\frac{\partial^2\phi}{\partial y^2} \gg \frac{1}{\gamma^2}\frac{\partial^2\phi}{\partial z^2}$

zeroth-order solution:

$$\frac{\partial^2\phi_0}{\partial x^2} + \frac{\partial^2\phi_0}{\partial y^2} = -\frac{\rho(x,y,z)}{\epsilon_0} \qquad \rho(x,y,z) = n(x,y)\lambda(z).$$

$$\boxed{\frac{\partial^2\phi_0}{\partial x^2} + \frac{\partial^2\phi_0}{\partial y^2} = -\frac{n(x,y)\lambda(z)}{\epsilon}}$$

for a transverse Gaussian density distribution, the electric potential:

$$\phi_0(x,y,z) = (\varphi(x,y) + \varphi_{00})\lambda(z)$$

$$\varphi(x,y) = \frac{1}{4\pi\epsilon_0}\int_0^\infty dt \frac{\exp[-\frac{x^2}{2(\sigma_x^2+t)} - \frac{y^2}{2(\sigma_y^2+t)}] - 1}{\sqrt{(\sigma_x^2+t)(\sigma_y^2+t)}}$$

$$\varphi_{00} = \frac{-1}{4\pi\epsilon_0}\int\int log((x^2+y^2)/r_0^2)n(x,y)dxdy \qquad \varphi_{00} = \frac{-1}{4\pi\epsilon_0}(\log 2 - \gamma_{em} + 2\log(\frac{\sigma_x+\sigma_y}{2r_0}))$$

r_0 is reference length

Ji Qiang, Two-and-a-half dimensional symplectic space-charge solver, https://arxiv.org/pdf/2606.26484

Reference Length

$$D(r_0) = \int^{\infty} \left(E_z^{2.5D}(0,0,z;r_0) - E_z^{3D}(0,0,z)\right)^2 dz.$$

$$E_z^{2.5D}(0,0,z;r_0) = \varphi_{00}(r_0)\frac{Qz}{\sqrt{2\pi}\sigma_z^3}\exp\left(-\frac{z^2}{2\sigma_z^2}\right),$$

$$E_z^{3D}(0,0,z) = \frac{Qz}{4\pi\epsilon_0\sqrt{2\pi}}\int_0^{\infty} dt\,\frac{\exp\left[-\frac{z^2}{2(\sigma_z^2+t/\gamma^2)}\right]}{(\sigma_z^2+t/\gamma^2)\sqrt{(\sigma_x^2+t)(\sigma_y^2+t)(\sigma_z^2+t/\gamma^2)}}.$$

After minimizing $D(r_0)$ with respect to r_0, one obtains

$$\log(r_0) = \log\left(\frac{\sqrt{2}(\sigma_x+\sigma_y)}{2}\right) - \frac{1}{2}\gamma_{em} + \sqrt{2}\sigma_z^3\gamma^3\int_0^{\infty} dt\,\frac{1}{(2\sigma_z^2\gamma^2+t)^{3/2}\sqrt{(\sigma_x^2+t)(\sigma_y^2+t)}}.$$

Transverse open: $\boxed{r_0 = 4e^{(-0.5\gamma_{em}-1)}\gamma\sigma_z \sim 1.1\,\gamma\sigma_z.}$

Transverse conducting pipe: $\boxed{r_0 = a.}$ $\varphi_{00} \approx \frac{-1}{4\pi\epsilon_0}\left(\log 2 - \gamma_{em} + 2\log\left(\frac{\sigma}{a}\right)\right)$

Symplectic 2.5D Space-Charge Model for a Transverse Gaussian Density Function

$$p_x(\tau) = p_x(0) + \tau K \frac{\lambda(z)}{4\pi\epsilon_0} \int_0^\infty dt \frac{x \exp[-\frac{x^2}{2(\sigma_x^2+t)} - \frac{y^2}{2(\sigma_y^2+t)}]}{(\sigma_x^2+t)\sqrt{(\sigma_x^2+t)(\sigma_y^2+t)}}$$

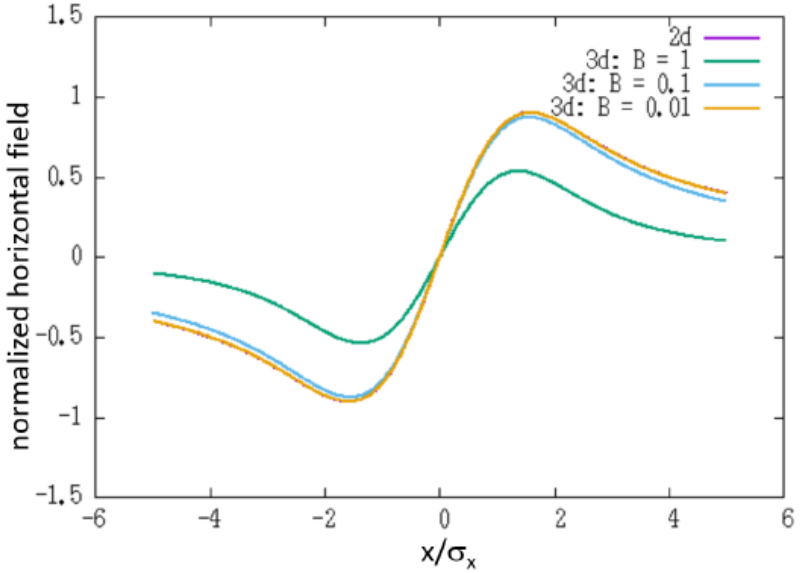
$$p_y(\tau) = p_y(0) + \tau K \frac{\lambda(z)}{4\pi\epsilon_0} \int_0^\infty dt \frac{y \exp[-\frac{x^2}{2(\sigma_x^2+t)} - \frac{y^2}{2(\sigma_y^2+t)}]}{(\sigma_y^2+t)\sqrt{(\sigma_x^2+t)(\sigma_y^2+t)}}$$

$$p_z(\tau) = p_z(0) - \tau K(\varphi(x,y) + \varphi_{00}) \frac{\partial \lambda(z)}{\partial z}$$

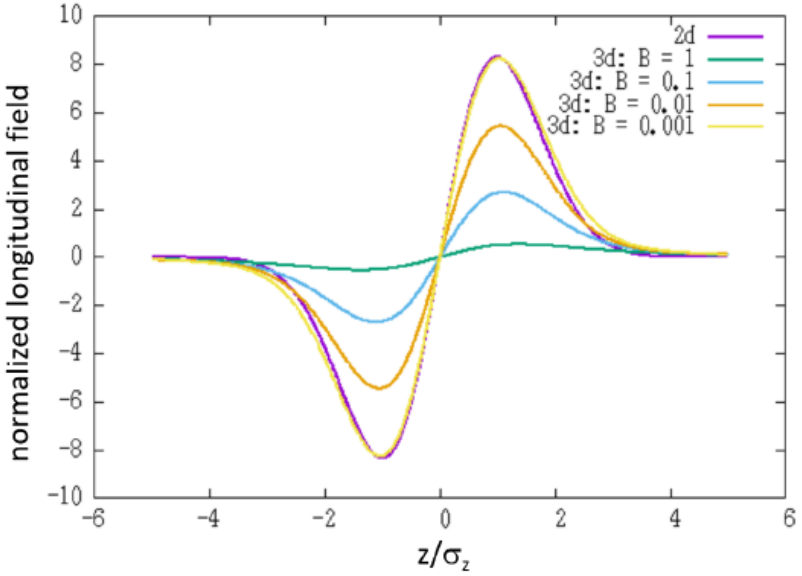
- Symplectic 2.5D space-charge model differs from previous 2.5D model by including the longitudinal space-charge kick

Comparison of Electric Fields from the 3D Gaussian and the 2.5D Gaussian Solvers

horizontal electric field

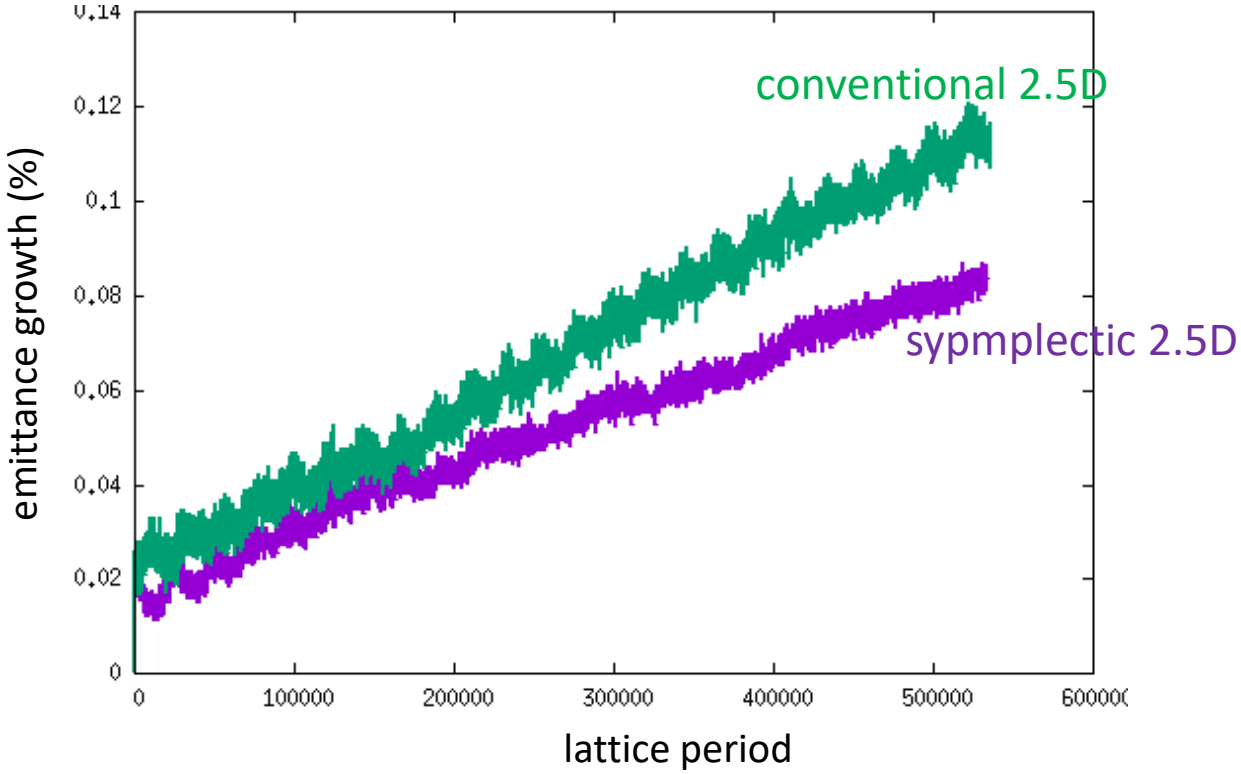


longitudinal electric field



- For a short bunch length (large transverse to longitudinal ratio), there exists significant discrepancy between the 3D and the 2.5D solver
- For a long bunch (small transverse to longitudinal ratio), the 2.5D solver agrees with the 3D solver quite well

Four Dimensional Emittance Growth from the symplectic 2.5D and conventional 2.5D Space-Charge Gaussian Model



- Symplectic 2.5D space-charge solver shows slower emittance growth.

2.5D Symplectic Space-Charge Model with Arbitrary Open Transverse Density Function

$$\varphi(x,y) = \frac{1}{2\pi\epsilon_0}\int\int G(x-x',y-y')n(x',y')dx'dy' \qquad G(x,y) = -\frac{1}{2}log(x^2+y^2)$$

$$\bar{G}(x_i - x_{i'}, y_j - y_{j'}) = \int_{x_{i'}-h_x/2}^{x_{i'}+h_x/2} dx' \int_{y_{j'}-h_y/2}^{y_{j'}+h_y/2} dy' G(x_i - x', y_j - y')$$

$$\varphi(x_i, y_j) = \frac{1}{2\pi\epsilon_0}\sum_{i'=1}^{N_x}\sum_{j'=1}^{N_y} \bar{G}(x_i - x_{i'}, y_j - y_{j'})n(x_{i'}, y_{j'})$$

$$p_x(\tau) = p_x(0) - \tau K\lambda(z)\sum_i\sum_j \frac{\partial S(x_i - x)}{\partial x} S(y_j - y)\varphi(x_i, y_j)$$

$$p_y(\tau) = p_y(0) - \tau K\lambda(z)\sum_i\sum_j S(x_i - x)\frac{\partial S(y_j - y)}{\partial y}\varphi(x_i, y_j)$$

$$p_z(\tau) = p_z(0) - \tau K\frac{\partial\lambda(z)}{\partial z}\sum_i\sum_j S(x_i - x)S(y_j - y)\varphi(x_i, y_j)$$

2.5D Symplectic Space-Charge Model with Arbitrary Transverse Density Function in Rectangular Pipe

$$p_x(\tau) = p_x(0) - \tau K \lambda(z) \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \varphi^{lm} \alpha_l \cos(\alpha_l x) \sin(\beta_m y)$$

$$p_y(\tau) = p_y(0) - \tau K \lambda(z) \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \varphi^{lm} \beta_m \sin(\alpha_l x) \cos(\beta_m y)$$

$$p_z(\tau) = p_z(0) - \tau K \frac{\partial \lambda(z)}{\partial z} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \varphi^{lm} \sin(\alpha_l x) \sin(\beta_m y)$$

$$\varphi^{lm} = \frac{n^{lm}}{\epsilon_0 \gamma_{lm}^2}$$

$$n^{lm} = \frac{4}{ab} \int_0^a \int_0^b n(x,y) \sin(\alpha_l x) \sin(\beta_m y) \; dxdy$$

$$\text{where } \gamma_{lm}^2 = \alpha_l^2 + \beta_m^2$$

2.5D Symplectic Space-Charge Model with Arbitrary Transverse Density Function in Round Pipe

$$p_x(\tau) = p_x(0) - \tau K \lambda(z) \sum_{m=-N_m/2}^{N_m/2-1} \sum_{l=1}^{N_l} \varphi^{lm} (\gamma_{lm} J'_m(\gamma_{lm} r) \frac{x}{r} + i\ m \frac{y}{r^2} J_m(\gamma_{lm} r)) \exp(-im\theta),$$

$$p_y(\tau) = p_y(0) - \tau K \lambda(z) \sum_{m=-N_m/2}^{N_m/2-1} \sum_{l=1}^{N_l} \varphi^{lm} (\gamma_{lm} J'_m(\gamma_{lm} r) \frac{y}{r} - i\ m \frac{x}{r^2} J_m(\gamma_{lm} r)) \exp(-im\theta),$$

$$p_z(\tau) = p_z(0) - \tau K \frac{\partial \lambda(z)}{\partial z} \sum_{m=-N_m/2}^{N_m/2-1} \sum_{l=1}^{N_l} \varphi^{lm} J_m(\gamma_{lm} r) \exp(-im\theta)$$

$$\varphi^{lm} = \frac{n^{lm}}{\epsilon_0 \gamma_{lm}^2}$$

$$n^{lm} = \frac{1}{\pi J'^2_m(\gamma_{lm})} \int_0^{2\pi} \int_0^a n(r,\theta) \exp(im\theta) r J_m(\gamma_{lm} r) dr d\theta$$

$$J_m(\gamma_{lm} a) = 0.$$

2.5D Symplectic Space-Charge Model in FS Coordinate

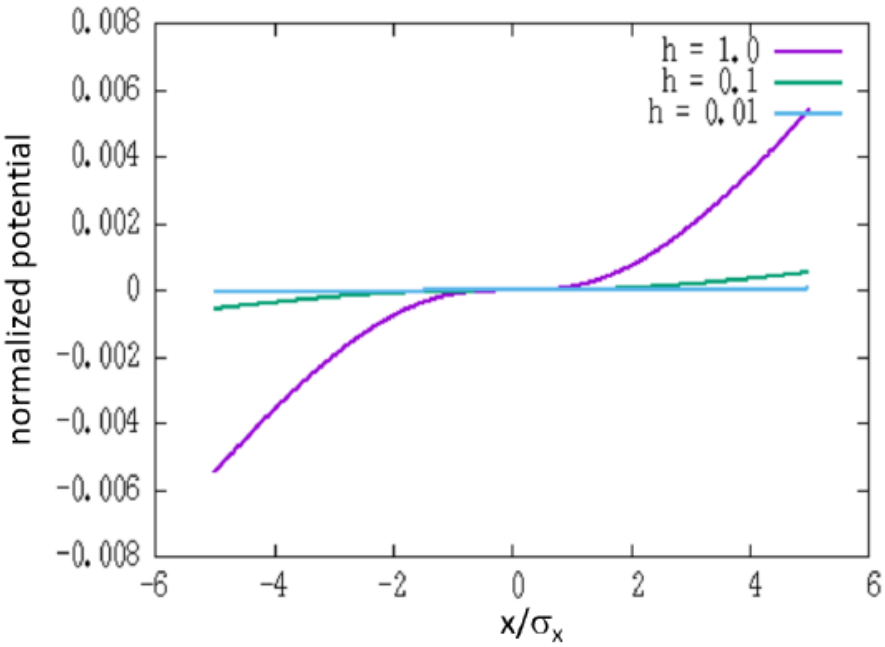
$$\frac{\partial^2\phi}{\partial x^2}+\frac{h}{1+hx}\frac{\partial\phi}{\partial x}+\frac{\partial^2\phi}{\partial y^2}+\frac{1}{\gamma^2(1+hx)^2}\frac{\partial^2\phi}{\partial z^2}=-\frac{\rho}{\epsilon_0}$$

$$\frac{h}{1+hx}\frac{\partial\phi}{\partial x}\ll\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2},\ \text{and}\ \frac{1}{\gamma^2(1+hx)^2}\frac{\partial^2\phi}{\partial z^2}\ll\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}$$

$$\frac{\partial^2\phi_0}{\partial x^2}+\frac{\partial^2\phi_0}{\partial y^2}=-\frac{\rho(x,y,z)}{\epsilon_0}$$

$$\frac{\partial^2\phi_1}{\partial x^2}+\frac{\partial^2\phi_1}{\partial y^2}=-\frac{\rho(x,y,z)}{\epsilon_0}-h\frac{\partial\phi_0}{\partial x}$$

first order horizontal electric potential



- For a ring with radius > 100 m, the effect of curvature might be negligible.

Neural Network Surrogate Space-Charge Model

$$H_2 = 4\pi \frac{K}{ab} \frac{1}{N_p} \sum_{i=1}^{N_P} \sum_{j=1}^{N_P} \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \frac{1}{\gamma_{lm}^2} \sin(\alpha_l x_j) \sin(\beta_m y_j) \sin(\alpha_l x_i) \sin(\beta_m y_i)$$

particle distribution in x-y space

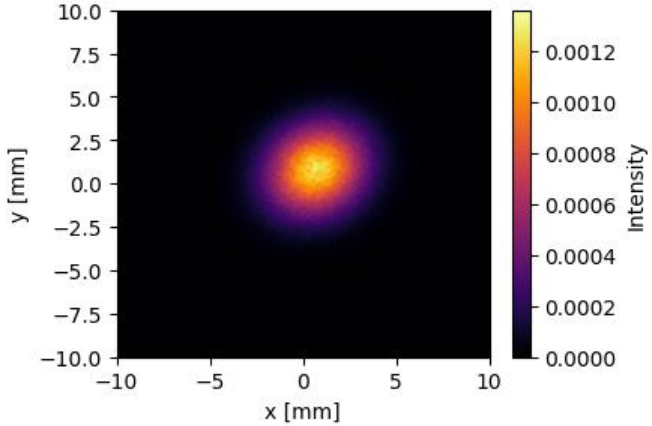
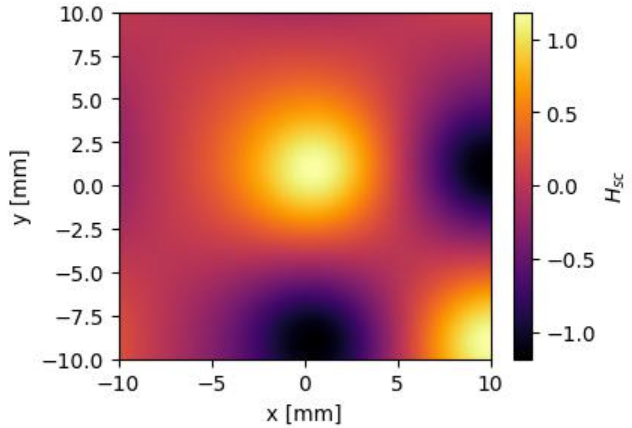


Image to image

space-charge H_{sc}



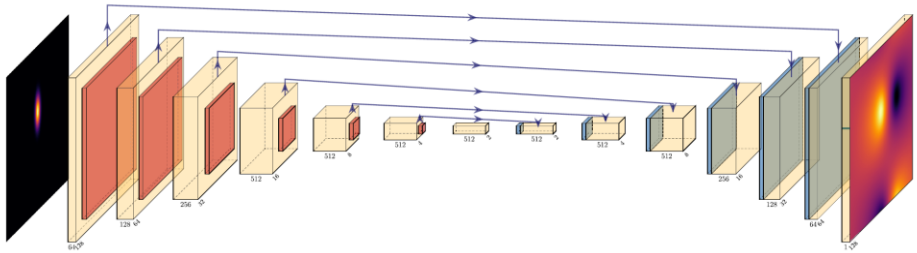
- Space-charge model computes the Hamiltonian associated with the space-charge potential by solving the Poisson equation

- A machine learning model can be used to speed up the calculation of H_{sc} w/o solving the Poisson equation directly

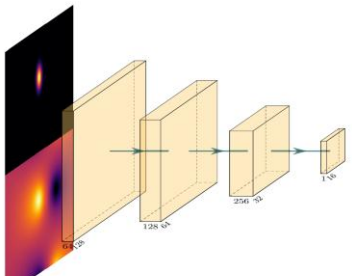
J. Wan, J. Qiang, Y. Hao, "Symplectic machine learning model for fast simulation of space-charge effects", Phys. Rev. Accel. Beams 28, 074602 (2025).

A neural network based ML model enables fast space-charge simulation

schematic diagram of the generator



schematic diagram of the discriminator

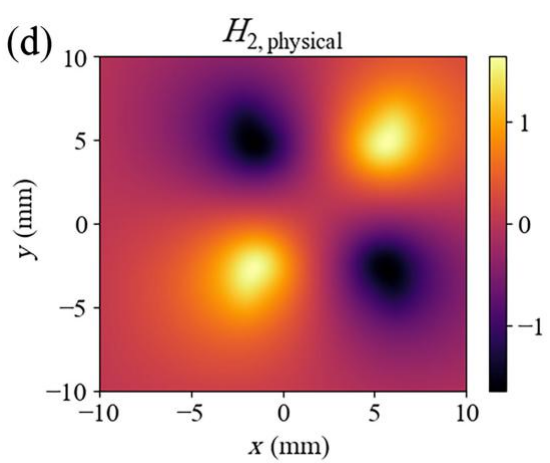


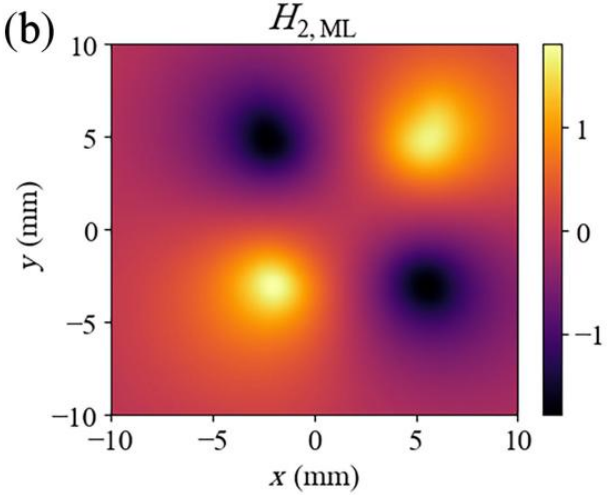
$$\mathcal{L}_G = -\frac{1}{N}\sum_{i=1}^{N}\{y_i \log[D(x_i, G(x_i))] + (1-y_i)\log[1 - D(x_i, G(x_i))]\} + \lambda\frac{1}{N}\sum_{i=1}^{N}|G(x_i) - Y_i|$$

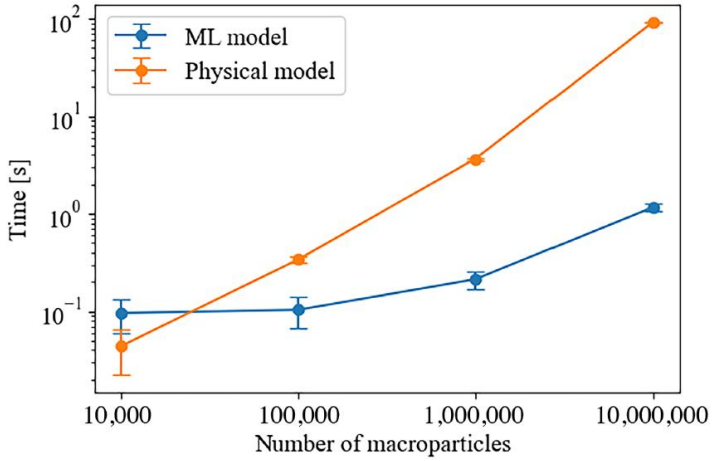
$$\mathcal{L}_D = -\frac{1}{N}\sum_{i=1}^{N}[y_i \log(D(x_i, y_i))] - \frac{1}{N}\sum_{i=1}^{N}\{(1-y_i)\log[1 - D(x_i, G(x_i))]\}$$

- x_i is the input data of the i^{th} training sample, y_i represents its label (1 for real samples and 0 for fake samples), G represents the fake data generated by the generator based on the input x, D represents the discriminator's output, and Y represents the real target image.
- The first term in L_G is the adversarial loss that encourages the generator to produce images as realistic as possible to fool the discriminator, and the second term in L_G is the L1 loss measuring the pixelwise similarity between the target and generated images. Based on a systematic parameter search, the coefficient of the L1 loss λ is set to be 1. The first and second terms in L_D represent the loss function for evaluating the real and fake samples, which encourage the discriminator to output 1 for real images and 0 for fake images.

ML Based Surrogate Model Reproduces the Physical Model Well but Is More Computational Efficient







Differentiable Space-Charge Modeling

- The differentiable simulation is a simulation that can automatically compute derivatives of the simulation result with respect to its input parameters.
- Differentiable space-charge modeling is to include space-charge effects in the differentiable simulation.

- Differentiable simulation can be used to study:
  - -- sensitivity of target physical quantities w.r.t. design or initial parameters
  - -- included in fast gradient-based optimizer

J. Qiang, "Differentiable self-consistent space-charge simulation for accelerator design," Phys. Rev. Accel. Beams 26, 024601 (2023).

Forward Mode Differentiable Simulation Using DA/TPSA

- Conventional graphic representation of a complex function/code might not be easy.
- DA/TPSA has been used to calculate high-order transfer maps in accelerator beam dynamics.
- The same library can be used to calculate derivatives w.r.t. design parameters.
- DA/TPSA changes the calculation derivatives of a function w.r.p. variables into the calculation of function evaluation of DA vector like variables.

Forward AD Based on First Derivatives of DA/TPSA

https://github.com/qianglbl/mAD

Given a function $f(x_1, x_2, \cdots, x_n)$

find its derivatives w.r.p. variable $x_1, x_2, \cdots, x_n$

Define a DA/TPSA vector like variable $F = (f, f_{x_1}, f_{x_2}, \cdots, f_{x_n})$

Addition Rule: $F + G = (f + g, f_{x_1} + g_{x_1}, f_{x2} + g_{x_2}, \cdots, f_{x_n} + g_{x_n})$

Multiplication Rule: $FG = (fg, gf_{x_1} + fg_{x_1}, gf_{x_2} + fg_{x_2}, \cdots, gf_{x_n} + fg_{x_n})$

Division Rule: $\frac{F}{G} = (\frac{f}{g}, \frac{f_{x_1}g - g_{x_1}f}{g^2}, \frac{f_{x_2}g - g_{x_2}f}{g^2} \cdots, \frac{f_{x_n}g - g_{x_n}f}{g^2})$

Function Rule: $h(F) = (h(f), h_f f_{x_1}, h_f f_{x_2}, \cdots, h_f f_{x_n})$

Emittance and Its Derivatives w.r.p. Seven Lattice Param. from the Use of a TPSA Library and the mAD Module

Emittance and its 7 derivatives from the use of a TPSA library

Emx 1.061687927800431E-006 9.404478867221511E-008 -1.812609047369974E-009 -4.761253438860015E-007
-1.763704718594396E-008 2.345272532436834E-011 -1.977599625054010E-008 -1.196832248156261E-008

Emy 1.009205402120444E-006 6.725695553868752E-008 1.304519894794864E-009 4.491663448734034E-007
7.826349966999831E-008 2.017384176315016E-010 -4.701173761686457E-009 3.276319957786300E-008

computing time: 858.41 seconds

Emittance and its 7 derivatives from the use of the mAD module

Emx 1.061687927800431E-006 9.404478867221511E-008 -1.812609047369819E-009 -4.761253438860811E-007
-1.763704718594396E-008 2.345272532436833E-011 -1.977599625054010E-008 -1.196832248156509E-008

Emy 1.009205402120444E-006 6.725695553868883E-008 1.304519894794905E-009 4.491663448734086E-007
7.826349967000353E-008 2.017384176313790E-010 -4.701173761675994E-009 3.276319957786431E-008

computing time: 4.16 seconds

More than a factor of 200 reduction of computing time by using the fast mAD module!

Differentiable Space-Charge Simulation through a FODO Lattice

$$\mathcal{M}_1(\tau) = \begin{pmatrix} \cos(\sqrt{Dk}D\tau) & \frac{1}{\sqrt{Dk}}\sin(\sqrt{Dk}D\tau) \\ -\sqrt{Dk}\sin(\sqrt{Dk}D\tau) & \cos(\sqrt{Dk}D\tau) \end{pmatrix}$$

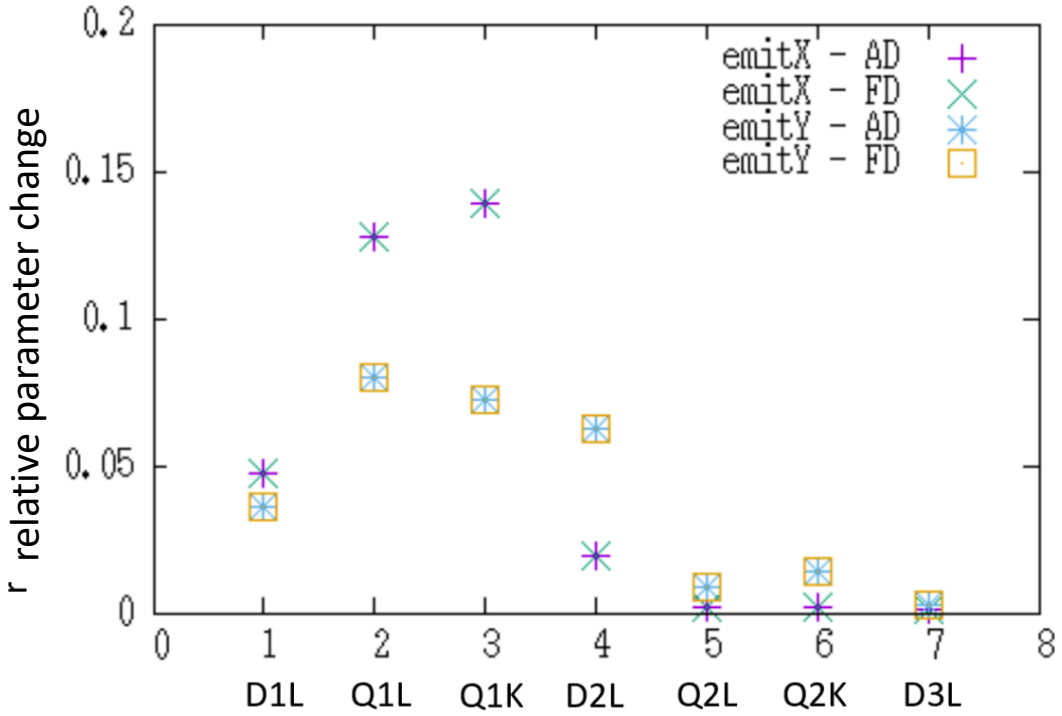
$$Dp_{xi}(\tau) = Dp_{xi}(0) - D\tau\frac{K}{2}\sum_{l=1}^{N_l}\sum_{m=1}^{N_m} D\phi^{lm}\alpha_l\cos(\alpha_l Dx_i)\sin(\beta_m Dy_i)$$

$$Dp_{yi}(\tau) = Dp_{yi}(0) - D\tau\frac{K}{2}\sum_{l=1}^{N_l}\sum_{m=1}^{N_m} D\phi^{lm}\beta_m\sin(\alpha_l Dx_i)\cos(\beta_m Dy_i)$$

$$D\phi^{lm} = 4\pi\frac{4}{ab}\frac{1}{N_p}\sum_{j=1}^{N_p}\frac{1}{\gamma_{lm}^2}\sin(\alpha_l Dx_j)\sin(\beta_m Dy_j)$$

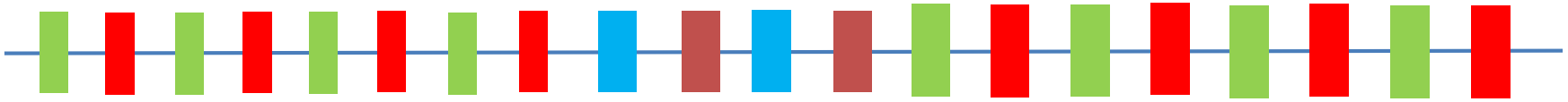
$$D\epsilon_x = \sqrt{D<x^2>D<p_x^2>-(D<xp_x>)^2}$$

Relative emittance changes w.r.p lattice parameters from a single AD simulation and from the FD approximation using 14 simulations



- Excellent agreement between the AD and the FD approximation.

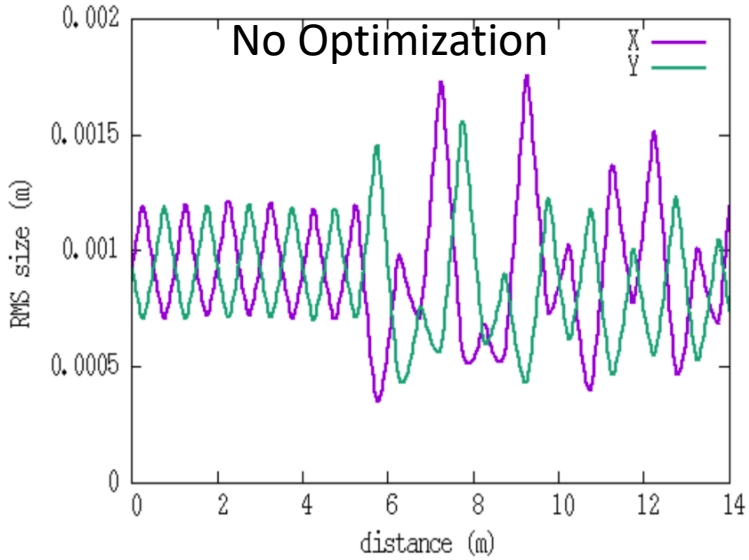
Evolution of the transverse RMS beam size through the FODO lattice w/o optimization (left) and with gradient-based optimization using the auto-differentiable parallel PIC simulation

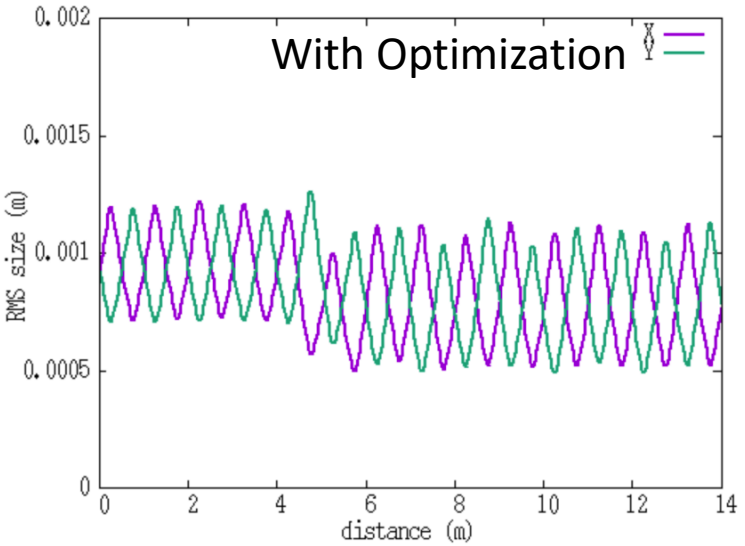


periodic FODO lattice matching lattice periodic FODO lattice

$$f(\mathbf{k}) = \frac{(\beta_x(\mathbf{k}) - \beta_{xt})^2}{\beta_{xt}^2} + (\alpha_x(\mathbf{k}) - \alpha_{xt})^2 + \frac{(\beta_y(\mathbf{k}) - \beta_{yt})^2}{\beta_{yt}^2} + (\alpha_y(\mathbf{k}) - \alpha_{yt})^2$$

- 4 control knobs (quadrupoles) in the matching lattice section





- Optimized matching solution yields more regular envelope oscillation including space-charge effects.

Study of the fully coupled 3D envelope instability using AD

3D Coupled Envelope Equation of 6x6 Covariance Matrix

$$\frac{d\Sigma}{ds} = F\,\Sigma + (F\,\Sigma)^T \qquad F(s) = \begin{pmatrix} 0 & \frac{\delta}{lp_0} & 0 & 0 & 0 & 0 \\ F_{21}(s) & 0 & F_{23}(s) & 0 & F_{25}(s) & 0 \\ 0 & 0 & 0 & \frac{\delta}{lp_0} & 0 & 0 \\ F_{41}(s) & 0 & F_{43}(s) & 0 & F_{45}(s) & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{\delta}{lp_0} \\ F_{61}(s) & 0 & F_{63}(s) & 0 & F_{65}(s) & 0 \end{pmatrix}$$

$$\Sigma(s) = \Sigma_m(s) + \tilde{\Sigma}(s) \qquad \xi = \left(\tilde{\Sigma}_{11}, \tilde{\Sigma}_{12}, \ldots, \tilde{\Sigma}_{66}\right)^T$$

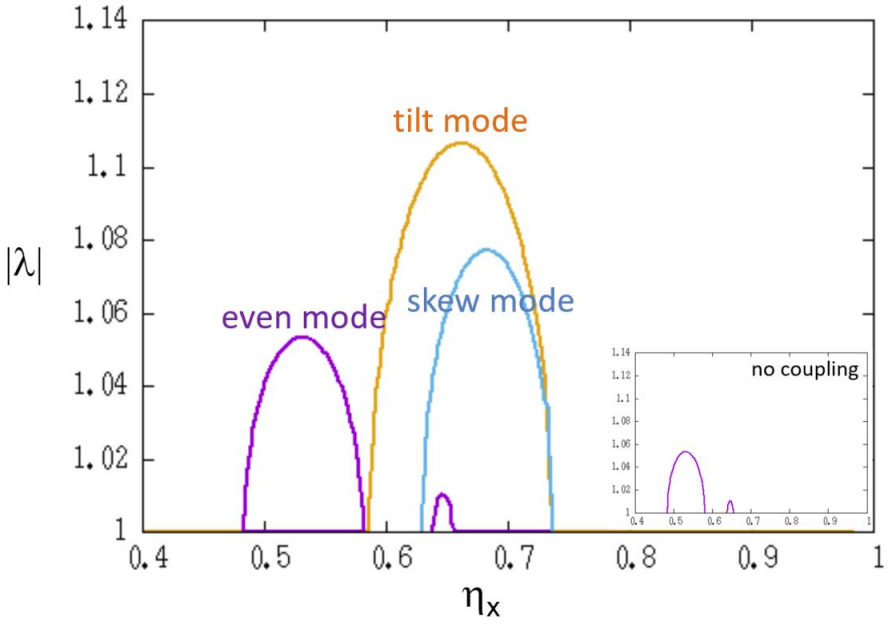
$$\frac{d\xi}{ds} = D(\Sigma_m, s)\,\xi(s) \qquad \xi(s) = M(s)\,\xi(0)$$

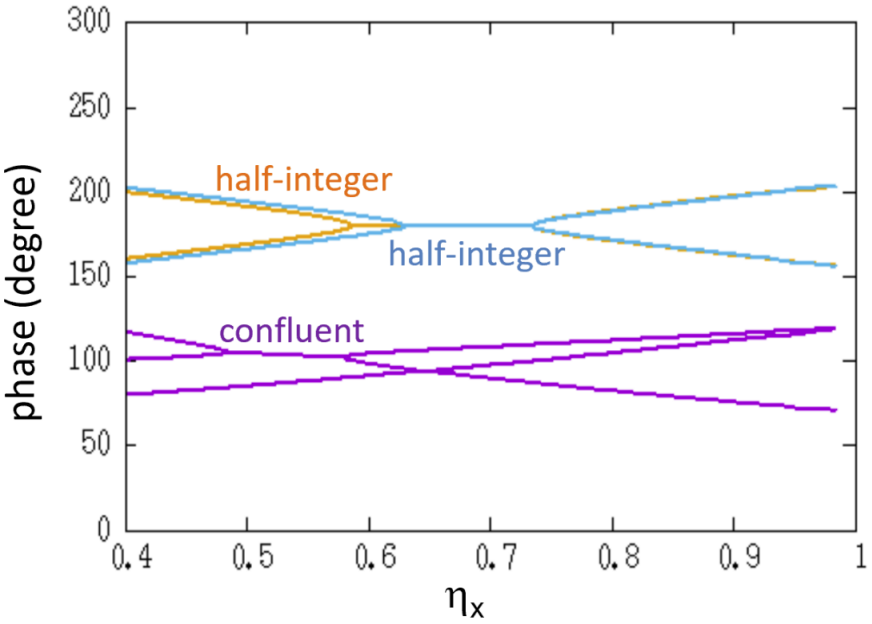
$$\frac{dM(s)}{ds} = D(\Sigma_m, s)\,M(s) \longrightarrow \text{441 coupled ODEs}$$

- Reduction of the number of ODEs from 441 to 21 using AD!

J. Qiang, Study of fully coupled 3D envelope instability using automatic differentiation, Phys. Rev. Accel. Beams, L024201, (2026).

Growth rate amplitudes and phases of unstable envelope modes as a function of the horizontal tune depression





- Including SC induced coupling in the envelope equation shows new instability stopbands

Introducing this session's talks

- Performance-Portable Space-Charge Methods in OPALX for Hadron and Lepton Accelerator Modelling – Michail Zampetakis
- Fast-Tracking Space Charge tool for Nonlinear Dynamics study in Realistic Collider Lattices – Helena Alamprese
- Longitudinal Phase-Space Reconstruction Using Differentiable Space-Charge Solvers – Sergei Sherstiuk
- Space Charge Physics in the Code ImpactX – Chad Mitchell

Thank You for Your Attention!