Advances in Modeling Space-Charge Effects

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14th International Computational Accelerator Physics Conference

Oct. 3 - Oct. 5, 2024, Lufthansa Seeheim, Germany

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Outline

- **Differentiable space-charge modeling using TPSA**
- **Space-charge simulation using a quantum Schrodinger approach**
- **Future work**

See Prof. Yue Hao's talk on Friday for differentiable simulation with a different auto differentiation package

Truncated Power Series Algebra (TPSA)

- 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.
- TPSA changes the derivatives of a function into a function of DA vector variables.

Solution of Hamilton Equation in Transfer Map

$$\frac{d\zeta}{ds} = -[H,\zeta]$$

$$\zeta_s = f(\zeta_0) = \sum_i^N \mathrm{M}_i \zeta_0{}^i$$

- f can be a very complicated function
- M_i is the i^{th} order transfer map, and is related to the i^{th} derivative of function f

How to attain M_i effectively?

Consider a one-dimensional Taylor approximation:

$$f(x) = f(x_0) + (x-x_0)f'(x_0) + \frac{1}{2!}(x-x_0)^2 f''(x_0) + \frac{1}{3!}(x-x_0)^3 f'''(x_0) + \cdots + \frac{1}{N!}(x-x_0)^N f^{(N)}(x_0)$$

To find the derivative, i.e. Taylor map, one can approximate the derivative numerically:

$$f'(x_0) \approx \frac{f(x_0+\varepsilon) - f(x_0)}{\varepsilon}$$

$$f''(x_0) \approx \frac{f(x_0+\varepsilon) - 2f(x_0) + f(x_0-\varepsilon)}{\varepsilon^2}$$

→ loss of accuracy

Introduction to Truncated Power Series Algebra (TPSA)

Use symbolic calculation from package like Mathematica:

For example: $f(x)=\dfrac{1}{1+x+x^2}$ $f'(x)=\dfrac{-(1+2x)}{(1+x+x^2)^2}$ $f''(x)=\dfrac{6x+6x^2}{(1+x+x^2)^3}$

- very complicated for high order derivatives
- even impossible for some function without closed form (e.g. simulation)

Define a N-dimension function space with bases:

$$\{1,(x-x_0),\frac{1}{2!}(x-x_0)^2,\frac{1}{3!}(x-x_0)^3,\cdots,\frac{1}{N!}(x-x_0)^N\}$$

The derivative up to Nth order can be regarded as a point in that space and represented as a vector:

$$Df_{x_0}=[f(x_0),f'(x_0),f''(x_0),f'''(x_0),\cdots,f^{(N)}(x_0)]$$

For example, a constant c, its representation as $Dc=[c,0,0,0,\cdots,0]$

a variable x as, $Dx=[x,1,0,0,\cdots,0]$

$$x\Rightarrow y=f(x)$$

A point x in number space maps to another point y=f(x) in number space

$$Dx\Rightarrow Df_x=f(Dx)$$

A point Dx in DA vector space maps to another point Df_x in DA vector space

Basic Operations for the TPSA vector

- A complicated function can be broken down as the operations of **addition** and **multiplication**

❖ Rule of addition:

$$Df_{x_0} = [f(x_0), f^{'}(x_0), f^{''}(x_0), f^{'''}(x_0), \cdots, f^{(N)}(x_0)] = [a_0, a_1, a_2, a_3, \cdots a_N]$$

$$Df_{x_1} = [f(x_1), f^{'}(x_1), f^{''}(x_1), f^{'''}(x_1), \cdots, f^{(N)}(x_1)] = [b_0, b_1, b_2, b_3, \cdots b_N]$$

$$Df_{x_0} + Df_{x_1} = [f(x_0) + f(x_1), f^{'}(x_0) + f^{'}(x_1), f^{''}(x_0) + f^{''}(x_1), f^{'''}(x_0) + f^{'''}(x_1), \cdots, f^{(N)}(x_0) + f^{(N)}(x_1)]$$

$$Df_{x_0} + Df_{x_1} = [a_0 + b_0, a_1 + b_1, a_2 + b_2, a_3 + b_3, \cdots, a_N + b_N]$$

❖ Rule of multiplication:

$$Df_{x_0} \times Df_{x_1} = ?$$

$$Df_{x_0} \times Df_{x_1} \neq [f(x_0) \times f(x_1), f^{'}(x_0) \times f^{'}(x_1), f^{''}(x_0) \times f^{''}(x_1), f^{'''}(x_0) \times f^{'''}(x_1), \cdots, f^{(N)}(x_0) \times f^{(N)}(x_1)]$$

Basic Operations for the TPSA vector

- Rule of multiplication:

$$(g(x)\times h(x))' = g(x)h'(x) + g'(x)h(x)$$
$$(g(x)\times h(x))'' = g(x)h''(x) + 2g'(x)h'(x) + g''(x)h(x)$$
$$\cdots$$
$$(g(x)\times h(x))^{(N)} = \sum_{k=0}^{N} \frac{N!}{k!(N-k)!} g^{(k)}(x) h^{(N-k)}(x)$$

$$Df_{x_0} \times Df_{x_1} = [\, f(x_0) f(x_1),\, f(x_0) f'(x_1) + f'(x_0) f(x_1),\, f(x_0) f''(x_1) + 2 f'(x_0) f'(x_1) + f''(x_0) f(x_1), \cdots]$$

$$Df_{x_0} \times Df_{x_1} = [a_0 b_0, a_0 b_1 + a_1 b_0, a_0 b_2 + 2a_1 b_1 + a_2 b_0, \cdots, c_N]$$

$$c_N = \sum_{k=0}^{N} \frac{N!}{k!(N-k)!} a_k b_{N-k}$$

- Operation of TPSA vector in a complicated function can be calculated using the rules of addition and multiplication

An Example of Calculation of Derivatives Using TPSA

For example, inverse of TPSA vector $[a_0, a_1, a_2, a_3, \cdots a_N]^{-1} = [x_0, x_1, x_2, x_3, \cdots x_N]$

$$[a_0, a_1, a_2, a_3, \cdots a_N] \times [x_0, x_1, x_2, x_3, \cdots x_N] = [1,0,0,0,\cdots 0]$$

$$[a_0, a_1, a_2, a_3, \cdots a_N]^{-1} = [\frac{1}{a_0}, -\frac{a_1}{a_0^2}, \frac{2a_1^2}{a_0^3} - \frac{a_2}{a_0^2}, \cdots]$$

Another example: evaluate f'(1) and f''(1) for the following function:

$$f(x) = \frac{1}{1+x+x^2}$$

Analytical function method:

$$f'(x) = \frac{-(1+2x)}{(1+x+x^2)^2} \qquad f''(x) = \frac{6x+6x^2}{(1+x+x^2)^3}$$

$$f'(1) = -\frac{1}{3} \qquad f''(1) = \frac{4}{9}$$

TPSA method:

$$x = 1 \qquad D1 = [1,1,0]$$

$$Df_1 = f(D1) = \frac{1}{1+[1,1,0]+[1,1,0]^2} = \frac{1}{[1,0,0]+[1,1,0]+[1,2,2]} = \frac{1}{[3,3,2]} = [\frac{1}{3}, -\frac{3}{9}, \frac{18-6}{27}] = [\frac{1}{3}, -\frac{1}{3}, \frac{4}{9}]$$

Special Functions of TPSA Vector

- How about special functions such as sin(X), exp(X), log(X), etc

➢ Answer: use Taylor expansion:

$$f(x) = f(x_0) + (x - x_0) f^{'}(x_0) + \frac{1}{2!}(x - x_0)^2 f^{''}(x_0) + \frac{1}{3!}(x - x_0)^3 f^{'''}(x_0) + \cdots + \frac{1}{N!}(x - x_0)^N f^{(N)}(x_0)$$

$$X = [x_0, x_1, x_2, x_3, \cdots x_N] = [x_0, 0,0,0,\cdots 0] + [0, x_1, x_2, x_3, \cdots x_N]$$

$$([x_0, x_1, x_2, x_3, \cdots x_N] - [x_0, 0,0,0,\cdots 0])^m = [0, x_1, x_2, x_3, \cdots x_N]^m = [\underbrace{0,0,0,0,\cdots 0}_{\text{leading m zeros}}, ?, ?]$$

➢ This means $[0,x_1,x_2,x_3,\ldots x_N]$ raised to $(N+1)_{th}$ power is exactly zero in TPSA.

$$f(X) = f([x_0, x_1, x_2, x_3, \cdots x_N]) = f([x_0, 0,0,0,\cdots 0]) + \sum_{m=1}^{N} \frac{[0, x_1, x_2, x_3, \cdots x_N]^m f^{(m)}([0, x_1, x_2, x_3, \cdots x_N])}{m!}$$

Some Special Functions of TPSA Vector

$$
\begin{aligned}
e^{(a_0,a_1,a_2,\dots\, a_\Omega)} &= e^{a_0}\sum_{k=0}^{\Omega}\frac{1}{k!}(0,a_1,a_2,\dots\, a_\Omega)^k \\
\ln(a_0,a_1,a_2,\dots\, a_\Omega) &= (\ln a_0, 0, 0, 0\dots, 0) \\
&\quad + \sum_{k=1}^{\Omega}(-1)^{k+1}\frac{1}{k}(0,\frac{a_1}{a_0},\frac{a_2}{a_0},\dots,\frac{a_\Omega}{a_0})^k \\
\sqrt{(a_0,a_1,a_2,\dots\, a_\Omega)} &= \sqrt{a_0}\Big[(1,0,0,0\dots0)+\frac{1}{2}(0,\frac{a_1}{a_0},\frac{a_2}{a_0},\dots,\frac{a_\Omega}{a_0}) \\
&\quad + \sum_{k=2}^{\Omega}(-1)^k\frac{(2k-3)!!}{(2k)!!}(0,\frac{a_1}{a_0},\frac{a_2}{a_0},\dots,\frac{a_\Omega}{a_0})^k\Big] \\
\sin(a_0,a_1,a_2,\dots\, a_\Omega) &= \sin a_0\sum_{k=0}\frac{(-1)^k}{(2k)!}(0,a_1,a_2,\dots,a_\Omega)^{2k} \\
&\quad + \cos a_0\sum_{k=0}\frac{(-1)^k}{(2k+1)!}(0,a_1,a_2,\dots,a_\Omega)^{2k+1} \\
\cos(a_0,a_1,a_2,\dots\, a_\Omega) &= \cos a_0\sum_{k=0}\frac{(-1)^k}{(2k)!}(0,a_1,a_2,\dots,a_\Omega)^{2k} \\
&\quad - \sin a_0\sum_{k=0}\frac{(-1)^k}{(2k+1)!}(0,a_1,a_2,\dots,a_\Omega)^{2k+1}
\end{aligned}
$$

Differentiable Simulation Enables Sensitivity Study and Fast Design Optimization

- The differentiable simulation is a simulation that can automatically compute derivatives of the simulation result with respect to its input parameters.
- Differentiable simulation can be used to study:
  - sensitivity of target physical quantities w.r.t. design parameters
  - included in fast gradient-based optimizer

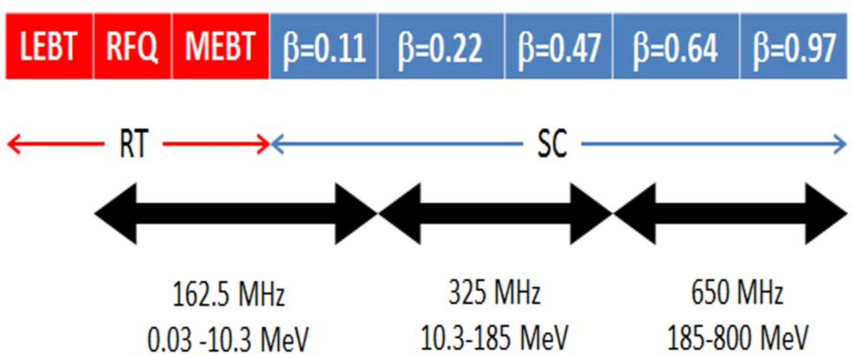


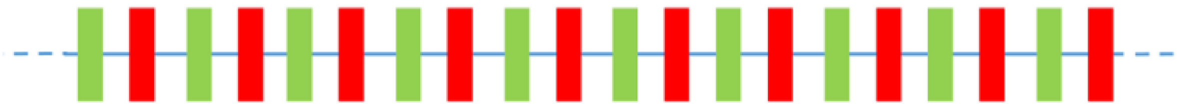
Figure 2.1: The linac technology map.

Table 2.1: SC Linac Parameters

Parameter	Requirement	Units
Particle species	H^-	
Input beam energy (kinetic)	2.1	MeV
Output beam energy (kinetic)	0.8	GeV
Bunch repetition rate	162.5	MHz
RF pulse length	pulsed-to-CW	
Sequence of bunches	Programmable	
Average beam current in SC Linac	2	mA
Final rms norm. transverse emittance, $\varepsilon_x=\varepsilon_y$	≤0.3	mm-mrad
Final rms norm. longitudinal emittance	≤0.35 (1.1)	mm-mrad (keV-ns)
Rms bunch length at the SC Linac end	4	Ps

Ref: PIP-II CDR report 2017.

Differentiable Space-Charge Simulation through a FODO Lattice



A formal single step solution

$$\zeta(\tau) = \exp(-\tau(:H:))\zeta(0)$$

$H = H_1 + H_2$

$$\zeta(\tau) = \exp(-\tau(:H_1: + :H_2:))\zeta(0)$$
$$= \exp(-\frac{1}{2}\tau : H_1 :)\exp(-\tau : H_2 :)\exp(-\frac{1}{2}\tau : H_1 :)\zeta(0) + O(\tau^3)$$

$$\zeta(\tau) = \mathcal{M}(\tau)\zeta(0)$$
$$= \mathcal{M}_1(\tau/2)\mathcal{M}_2(\tau)\mathcal{M}_1(\tau/2)\zeta(0)$$

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

$$\mathbf{r}_i(\tau) = \mathbf{r}_i(0)$$
$$\mathbf{p}_i(\tau) = \mathbf{p}_i(0) - \frac{\partial H_2(\mathbf{r})}{\partial \mathbf{r}_i}\tau$$

J. Qiang, Differentiable self-consistent space-charge simulation for accelerator design, PRAB 26, 024601, 2023

Self-Consistent Space-Charge Transfer Map (1)

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = -\frac{\rho}{\epsilon_0}$$

$$\begin{aligned} \phi(x=0,y) &= 0 \\ \phi(x=a,y) &= 0 \\ \phi(x,y=0) &= 0 \\ \phi(x,y=b) &= 0 \end{aligned}$$

$$\rho(x,y) = \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \rho^{lm} \sin(\alpha_l x) \sin(\beta_m y)$$

$$\phi(x,y) = \sum_{l=1}^{N_l} \sum_{m=1}^{N_m} \phi^{lm} \sin(\alpha_l x) \sin(\beta_m y)$$

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

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

where $\alpha_l = l\pi/a$ and $\beta_m = m\pi/b$

$$\boxed{\phi^{lm} = \frac{\rho^{lm}}{\epsilon_0 \gamma_{lm}^2}}$$

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

Symplectic Gridless Particle Model

$$\rho(x,y) = \sum_{j=1}^{N_p} w\delta(x - x_j)\delta(y - y_j)$$

w is the particle charge weight

$$H_2 = \frac{1}{2\epsilon_0}\frac{4}{ab}w\sum_i\sum_j\sum_l\sum_m\frac{1}{\gamma_{lm}^2}\sin(\alpha_l x_j)\sin(\beta_m y_j)\sin(\alpha_l x_i)\sin(\beta_m y_i)$$

$\mathcal{M}_2$ →

$$\begin{aligned} p_{xi}(\tau) &= p_{xi}(0) - \tau\frac{1}{\epsilon_0}\frac{4}{ab}w\sum_j\sum_l\sum_m\frac{\alpha_l}{\gamma_{lm}^2} \\ &\quad \sin(\alpha_l x_j)\sin(\beta_m y_j)\cos(\alpha_l x_i)\sin(\beta_m y_i) \\ p_{yi}(\tau) &= p_{yi}(0) - \tau\frac{1}{\epsilon_0}\frac{4}{ab}w\sum_j\sum_l\sum_m\frac{\beta_m}{\gamma_{lm}^2} \\ &\quad \sin(\alpha_l x_j)\sin(\beta_m y_j)\sin(\alpha_l x_i)\cos(\beta_m y_i) \end{aligned}$$

Differentiable Space-Charge Simulation through a FODO Lattice

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

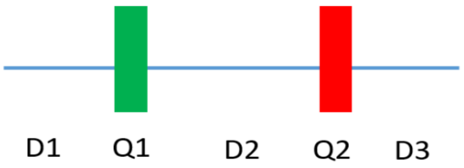
$$Dp_{xi}(\tau) \;=\; Dp_{xi}(0) - D\tau\frac{K}{2}\sum_{l=1}^{N_l}\sum_{m=1}^{N_m} D\phi^{lm}\alpha_l\cos(\alpha_l Dx_i)\sin(\beta_m Dy_i)$$

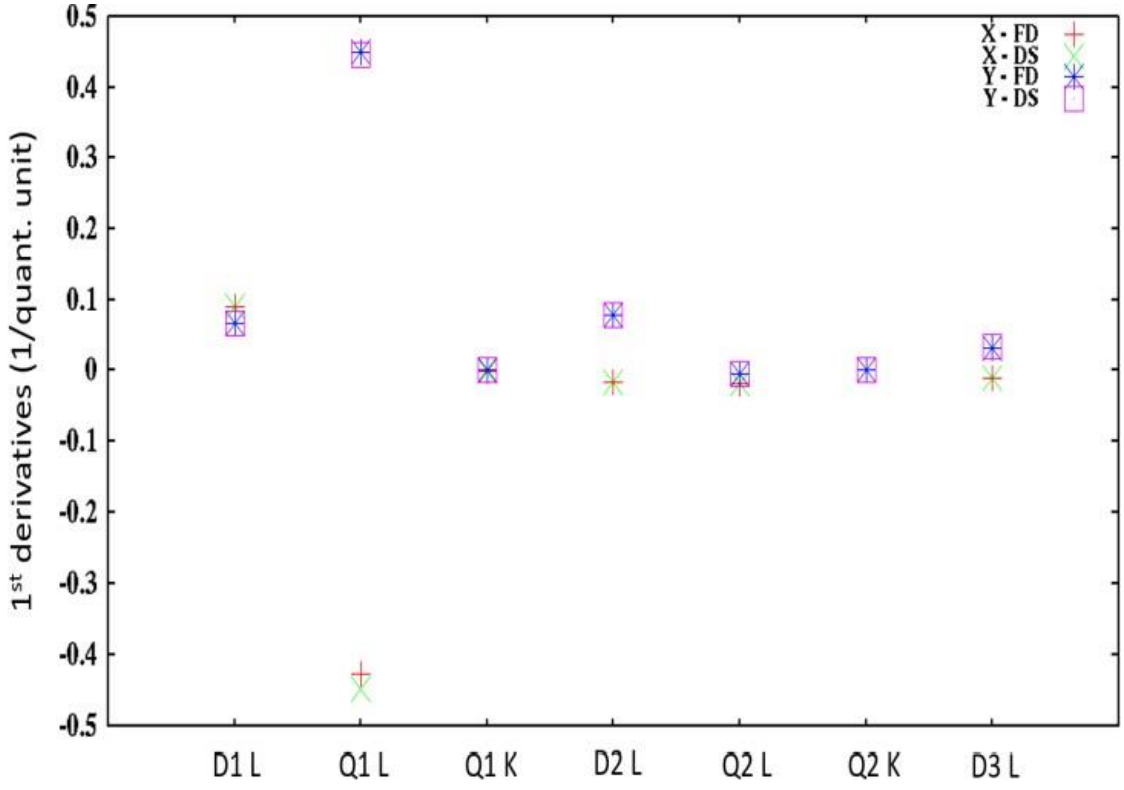
$$Dp_{yi}(\tau) \;=\; Dp_{yi}(0) - D\tau\frac{K}{2}\sum_{l=1}^{N_l}\sum_{m=1}^{N_m} D\phi^{lm}\beta_m\sin(\alpha_l Dx_i)\cos(\beta_m Dy_i)$$

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

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

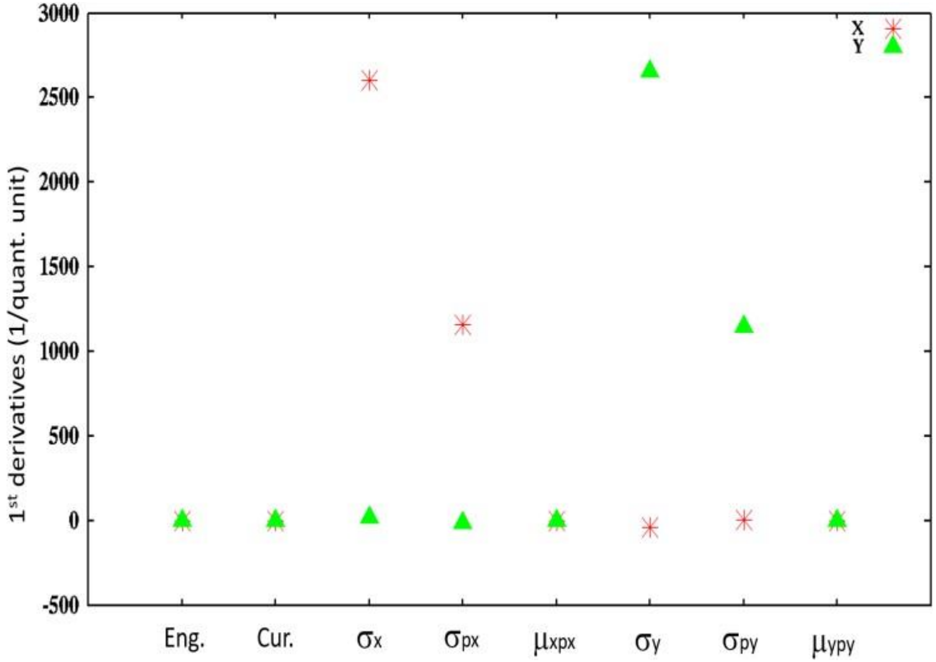
Derivatives of the X and Y Emittances w.r.t. 7 Lattice Parameters from 1 Differentiable Simulation and from Finite Difference Approximation with Multiple Simulations Shows Good Agreement





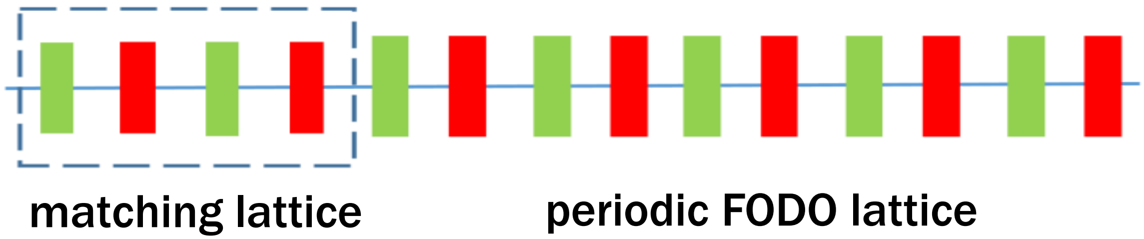
Derivatives of the X and Y Emittances w.r.t. 8 Beam Parameters from 1 Differentiable Simulation

$$f(x,p_x,y,p_y) \propto \exp(-\frac{1}{2}(\frac{x^2}{\sigma_x^2}+2xp_x\frac{\mu_{xp_x}}{\sigma_x\sigma_{p_x}}+\frac{p_x^2}{\sigma_{p_x}^2}))\exp(-\frac{1}{2}(\frac{y^2}{\sigma_y^2}+2yp_y\frac{\mu_{yp_y}}{\sigma_y\sigma_{p_y}}+\frac{p_y^2}{\sigma_{p_y}^2}))$$



- Final emittances are more sensitive to initial beam distribution parameters.

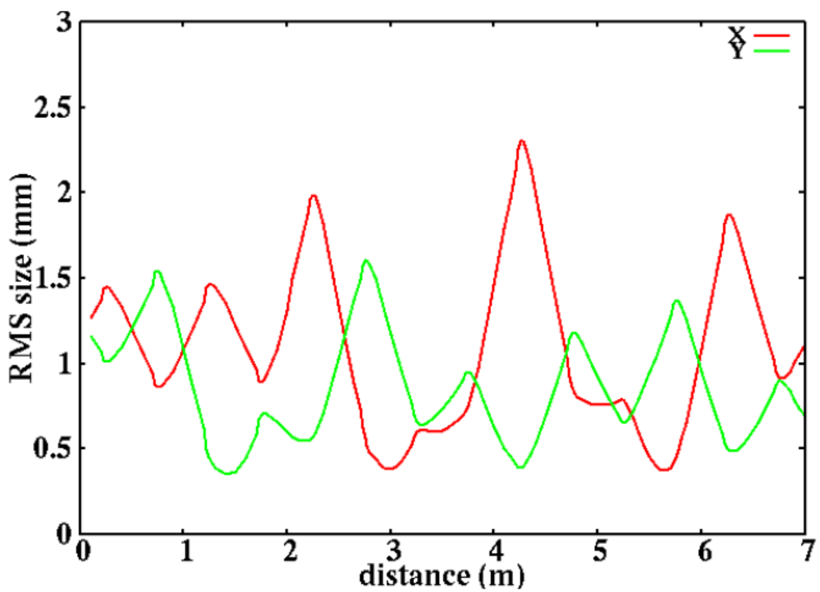
Matching Including Space-Charge Effects Using the Differentiable Simulation with Conjugate Gradient Optimizer

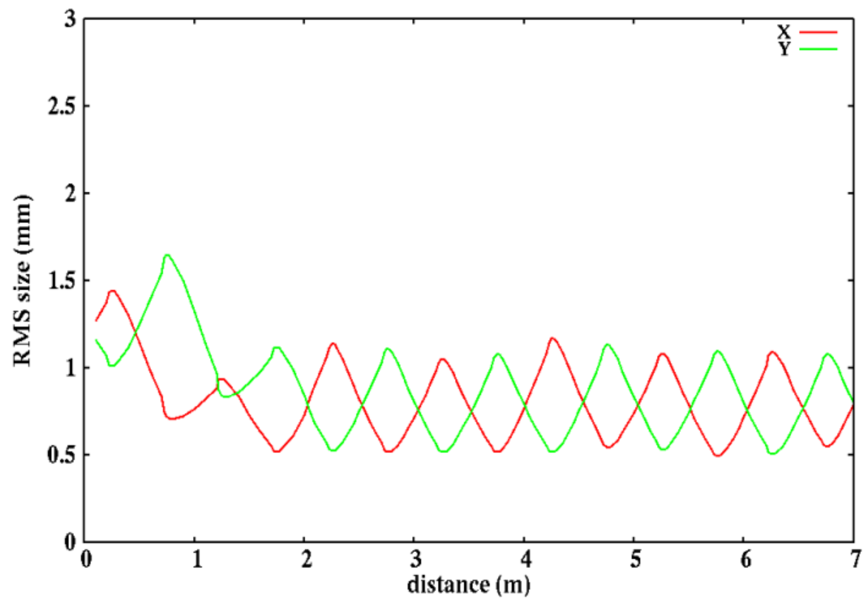


- 4 control knobs in the matching lattice section

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

Differentiable Simulation Enables Gradient Based Optimization (Conjugate Gradient Method)





- Transverse RMS size evolution without the quadrupole matching (left) and with the quadrupole matching including the space-charge effects (right) through the FODO lattice.

Modeling of Space-Charge Effects Involves Solution of 6D Vlasov-Poisson Equations

$$\frac{\partial f}{\partial t} + [f, H] = 0,$$

$$\nabla^2 \phi = -\frac{\rho}{\epsilon_0}, \qquad \rho = \iiint f(r, p, t) d^3 p$$

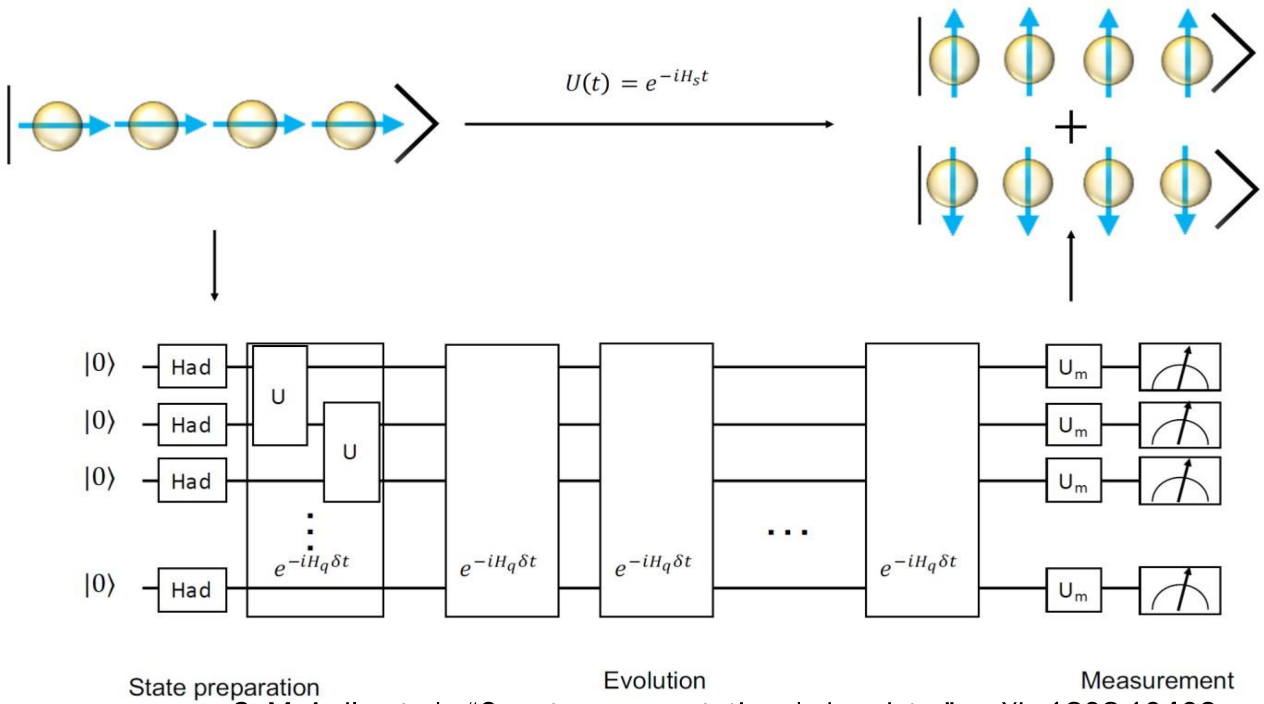
Conventional Solution Methods:

-- Using macroparticle in particle-in-cell method

-- Direct numerical solution of 6D partial differential equation

Simulation of Space-Charge Effects Using a Quantum Approach Involves Lower Dimensions and Enables Potential New Platform

- Reduce the computational domain from 6/4 dimensional classical phase space to 3/2 dimensional spatial space
- Open the possibility to explore the beam physics simulation on quantum computers



S. McArdle et al., “Quantum computational chemistry”, arXiv:1808.10402.

J. Qiang, “Simulation of space-charge effects using a quantum Schrodinger approach,” Phys. Rev. Accel. Beams 25, 034602 (2022).

Husimi Representation of Phase Space Distribution

$$\mathcal{F}(\mathbf{r}, \mathbf{p}, t) = |\bar{\Psi}(\mathbf{r}, \mathbf{p}, t)|^2$$

$$\Psi(\mathbf{r}, \mathbf{p}, t) = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \left(\frac{1}{2\pi\sigma^2}\right)^{3/4} \int d^3x \times \psi(\mathbf{x}, t) \exp\left(-\frac{|\mathbf{r} - \mathbf{x}|^2}{4\sigma^2} - i\frac{\mathbf{p} \cdot \mathbf{x}}{\hbar}\right)$$

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(x, y, z)\psi,$$

$$\frac{\partial\mathcal{F}}{\partial t} + [\mathcal{F}, H] = O(\hbar) + O(\hbar^2) + \cdots.$$

Schrodinger Equation of a Coasting Beam

Start with a z-dependent Hamiltonian of a particle in accelerator:

$$\bar{H}(z) = \frac{1}{2}(\bar{p}_x^2 + \bar{p}_y^2) + V(x, y, z), \quad \bar{p}_{x,y} = p_{x,y}/p_0$$

Rewrite the z-dependent Hamiltonian as t-dependent Hamiltonian:

$$H(t) = \frac{1}{2m\gamma_0}(p_x^2 + p_y^2) + p_0 v_0 V(x, y, z).$$

Replace the energy and momentum with corresponding operators:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m\gamma_0}\nabla^2 \psi + p_0 v_0 V(x, y, z)\psi.$$

Numerical Solution of the Schrodinger Equation (1)

$$i\hbar \frac{\partial \psi}{\partial z} = -\frac{\hbar^2}{2p_0}\nabla^2\psi + p_0 V(x,y,z)\psi$$

Lie-Trotter Splitting-Operator Method for Time Integration:

$$\psi(z+\tau) = e^{\frac{i\hbar\tau}{4p_0}\nabla^2} e^{-i\frac{p_0}{\hbar}V\tau} e^{\frac{i\hbar\tau}{4p_0}\nabla^2}\psi(z),$$

Spectral Method with Sine Function Representation in Spatial Dom.

$$\psi(x,y) = \sum_{l=1}^{N_l}\sum_{m=1}^{N_m} \psi_{lm}\ \sin(\alpha_l x)\ \sin(\beta_m y),$$

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

Numerical Solution of the Schrodinger Equation (2)

Wave Function Evolution for a Single Step:

$$\psi_{lm}(z+\tau/2) = e^{-\frac{i\hbar\tau}{4p_0}\gamma_{lm}^2}\psi_{lm}(z).$$

$$V = \frac{1}{2}k(z)(x^2 - y^2) + \frac{1}{2}K\phi,$$

$$\tilde{\psi}(z+\tau/2) = e^{-i\frac{p_0}{\hbar}V\tau}\psi(z+\tau/2).$$

$$\psi_{lm}(z+\tau) = e^{-\frac{i\hbar\tau}{4p_0}\gamma_{lm}^2}\tilde{\psi}_{lm}(z+\tau/2).$$

Numerical Solution of Poisson's Equation for Space-Charge Effects (1)

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = -4\pi\rho,$$

$$\rho(x,y) = \int\int e^{-\frac{(x-x')^2}{2\sigma_x^2}} e^{-\frac{(y-y')^2}{2\sigma_y^2}} \psi(x',y')\psi^*(x',y')dx'dy',$$

Spectral Method with Sine Function Representation:

$$\rho(x,y) = \sum_{l=1}^{N_l}\sum_{m=1}^{N_m} \rho_{lm} \sin(\alpha_l x)\sin(\beta_m y)$$

$$\phi(x,y) = \sum_{l=1}^{N_l}\sum_{m=1}^{N_m} \phi_{lm} \sin(\alpha_l x)\ \sin(\beta_m y),$$

$$\phi_{lm} = \frac{4\pi\rho_{lm}}{\gamma_{lm}^2},$$

Initial Condition and Diagnostics

Initial condition of wave function:

$$\psi(\mathbf{r},0) \propto \sum_{\mathbf{p}} \sqrt{f(\mathbf{r},\mathbf{p},0)}\, e^{i\mathbf{p}\cdot\mathbf{r}/\hbar + 2\pi\phi_{\mathrm{rand},\mathbf{p}}},$$

Beam properties from wave function:

$$\langle x^2 \rangle = \int\int x'^2 \psi\psi^* dx' dy'$$

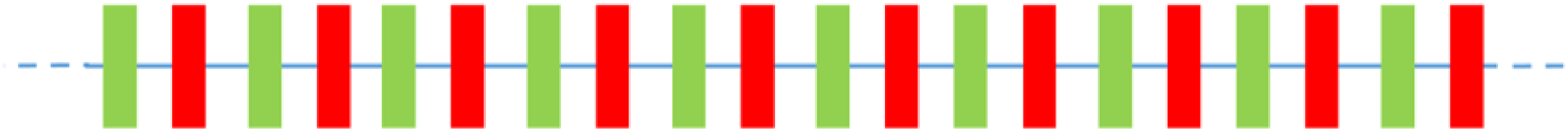
$$\langle p_x^2 \rangle = \hbar^2 \int\int \frac{\partial\psi}{\partial x'}\frac{\partial\psi^*}{\partial x'} dx' dy'$$

$$\langle x p_x \rangle = \hbar\, \mathrm{Im}\left(\int\int x' \frac{\partial\psi}{\partial x'} \psi^* dx' dy' \right),$$

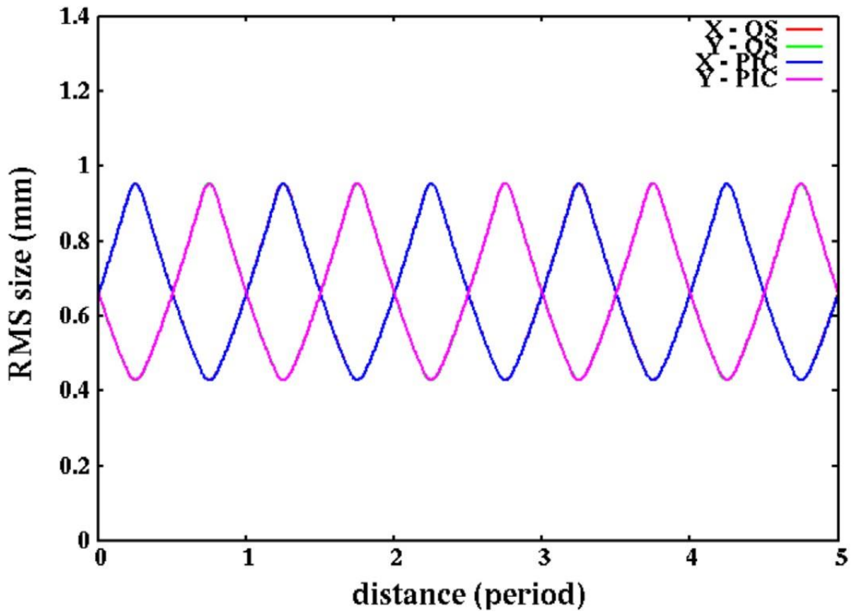
$$\epsilon_x = \sqrt{\langle x^2 \rangle \langle (p_x/p_0)^2 \rangle - \langle x(p_x/p_0) \rangle^2}$$

$$\epsilon_y = \sqrt{\langle y^2 \rangle \langle (p_y/p_0)^2 \rangle - \langle y(p_y/p_0) \rangle^2}.$$

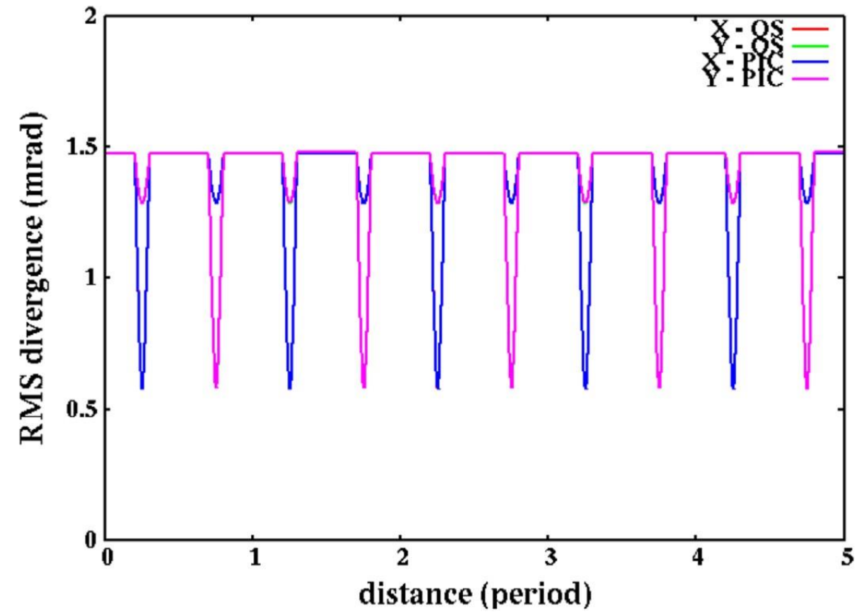
Test Case 1: No Space-Charge Effects (1)



RMS Size Evolution



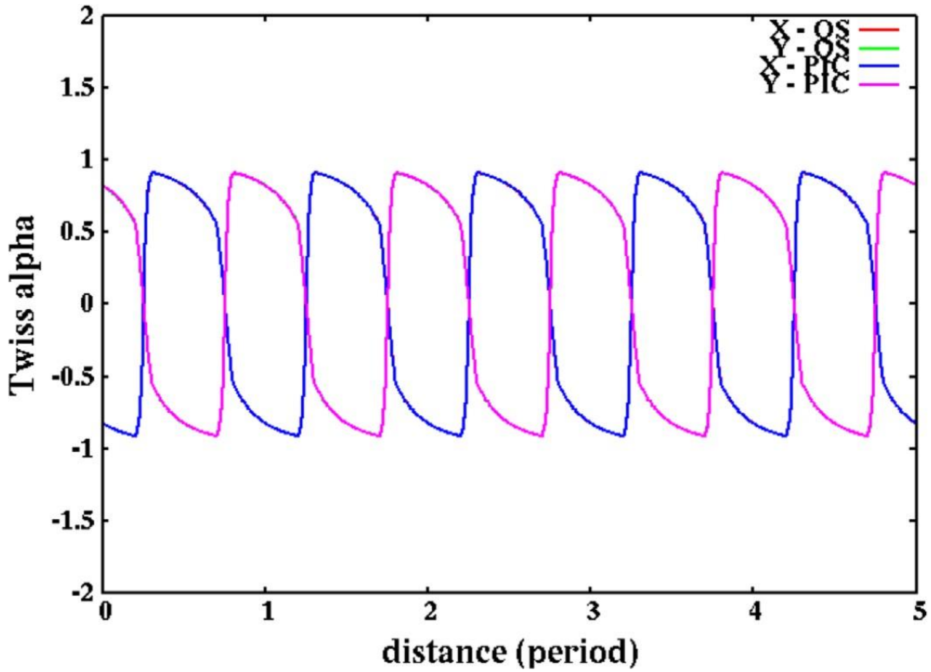
RMS Divergence Evolution



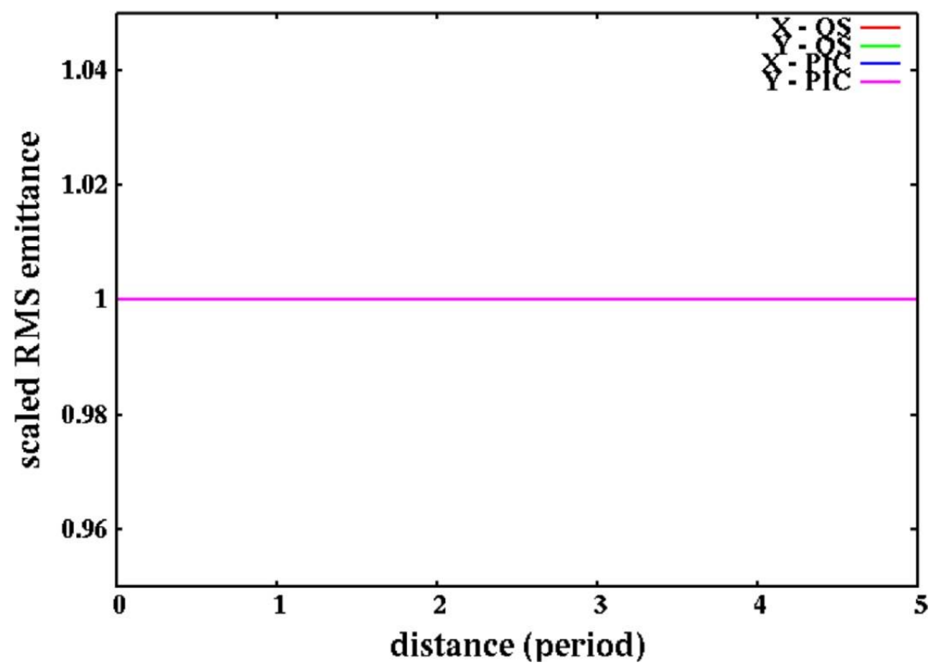
- Good agreement between the PIC simulation and the quantum Schrodinger simulation.

Test Case 1: No Space-Charge Effects (2)

Twiss Parameter Alpha Evolution



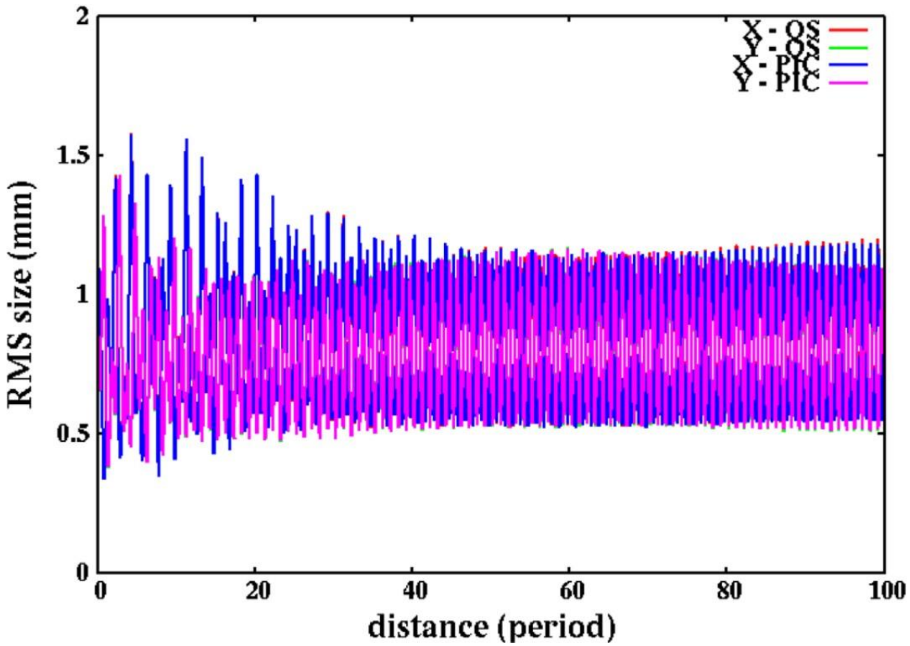
RMS Emittance Evolution



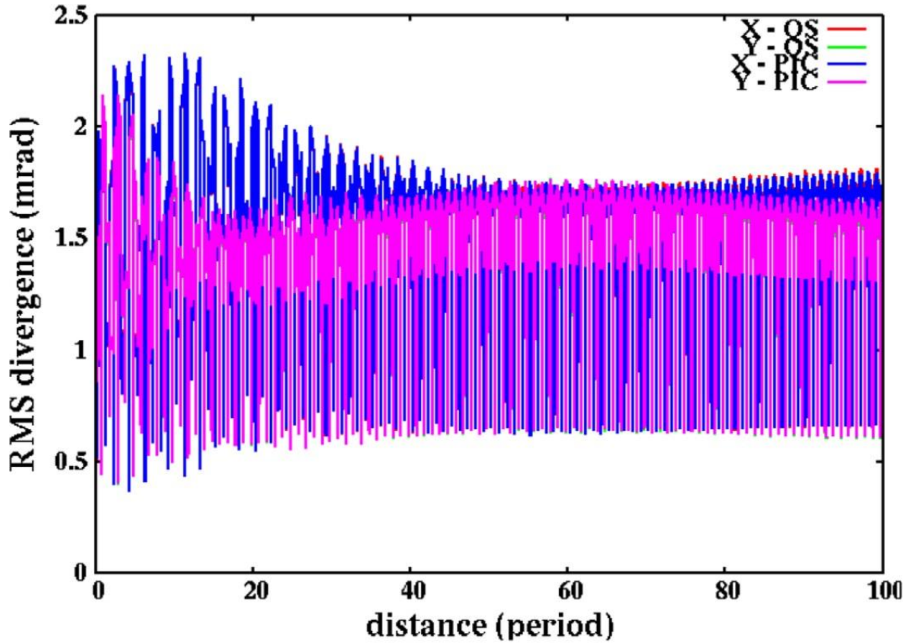
- Both methods agree with each other well and show no emittance growth without the space-charge effects.

Case 2: with Space-Charge and Initial Mismatched Beam (1)

RMS Size Evolution



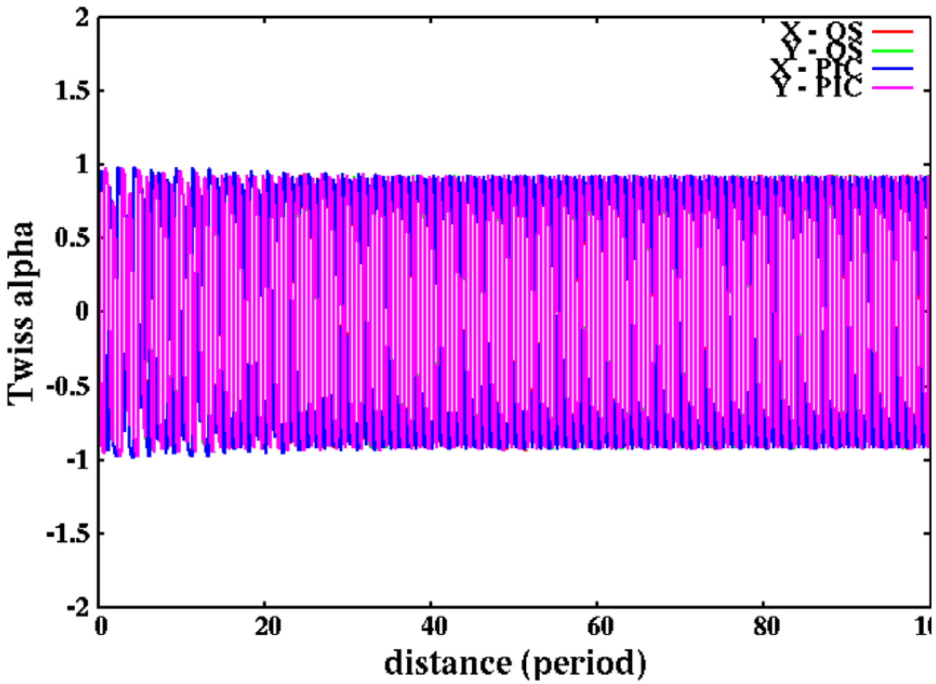
RMS Divergence Evolution



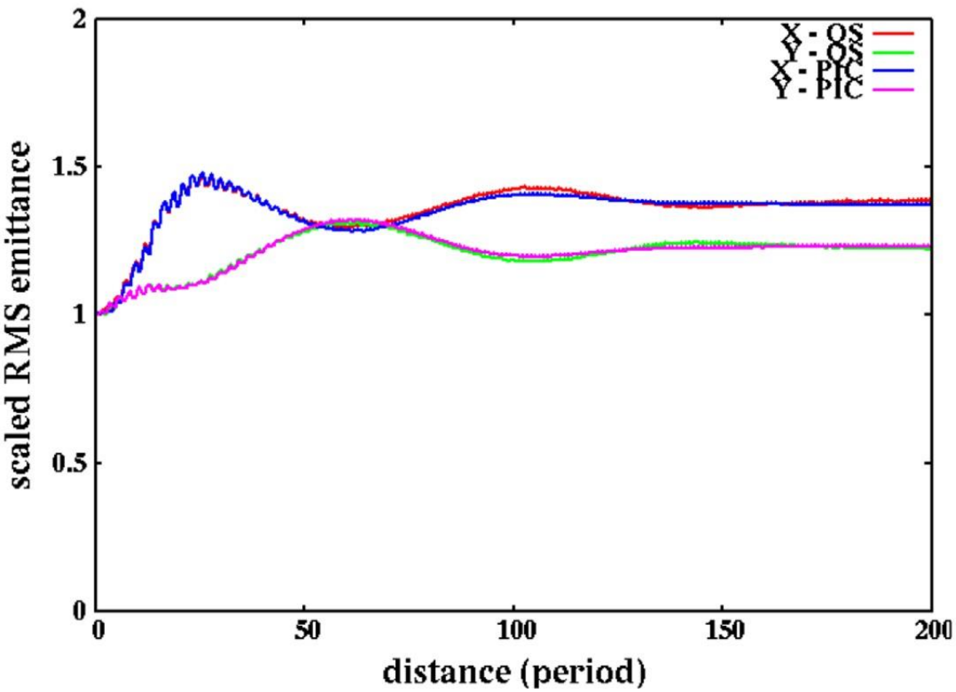
- Both the PIC and the quantum Schrodinger methods show initial beam size growth due to mismatched space-charge effects.

Case 2: with Space-Charge and Initial Mismatched Beam (2)

Twiss Parameter Alpha Evolution



RMS Emittance Evolution



- **Both methods show large emittance growth due the mismatched space-charge effects.**

Future Work

- Improve computational speed in differentiable space-charge modeling
- Extend the quantum Schrodinger approach to 3D space-charge
- Explore potential quantum computing application