FEL SIMULATION USING LIE METHOD Advances in FEL Simulation

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Kilean Hwang

Lawrence Berkeley National Laboratory

Oct 23, 2018

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Advances in FEL simulation

Oct 23, 2018 1 / 37

Outline

Introduction

Generalize WPA

- How?
- Review : Perturbative Lie Map
- Hamiltonian
- Generator
- Effective Hamiltonian
- Improve Shot Noise Modeling
 - Review of shot-noise modeling methods
 - Improved shot-noise modeling methods
 - IMPACT code suit and example

Conclusion

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Conclusion

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- FEL design optimization often involve multiple times simulation including start-to-end.
 - Wiggler-Period-Averaging (WPA) : highly efficient
- Generalize WPA perturbatively using Lie map method
 - Leading order : conventional WPA

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- Next order corrections : coupling between betatron and wiggling motion, field envelope gradients,...
- Improve shot-noise model especailly suited for WPA
 - Further improvement : smoother numerical discretization

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 - leaves small coupling effects between the fast wiggling and slow
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• Split the Hamiltonian H = S + F(z) + V(z)

- $S = \oint H dz / \lambda_u$ represent slow motion
- V(z) is the radiation field potential
- F(z) is the rest : the fast wiggling motion
- Accordingly, Lie map from z = 0 to $z = \lambda_u$ is fatored as

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Magnus Series

Slow

$$\mathscr{G}_{S}(z) = -z:S:$$

• Fast

$$\begin{aligned} \mathscr{G}_{F}(z) &= -\int_{0}^{z} dz_{1} : F^{\text{int}}(z_{1}) : \\ &+ \frac{1}{2!} \int_{0}^{z} dz_{1} \int_{0}^{z_{1}} dz_{2} : \left[F^{\text{int}}(z_{2}), F^{\text{int}}(z_{1}) \right] : \\ &- \frac{1}{3!} \int_{0}^{z} dz_{1} \int_{0}^{z_{1}} dz_{2} \int_{0}^{z_{2}} dz_{3} : \left[F^{\text{int}}(z_{3}), \left[F^{\text{int}}(z_{2}), F^{\text{int}}(z_{1}) \right] \right] \\ &+ \left[\left[F^{\text{int}}(z_{3}), F^{\text{int}}(z_{2}) \right], F^{\text{int}}(z_{1}) \right] : \\ & \text{where } F^{\text{int}}(z_{i}) \equiv \mathscr{S}(z_{i}) F(z_{i}) \end{aligned}$$

• Field Potential

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$$\mathscr{G}_V(z) = -\int_0^z dz : \mathscr{S}(z_i) \mathscr{F}(z_i) V(z_i):$$

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Next leading order

	Leading order (WPA)	Next leading order
GS	integand <i>S</i> is linear	S includes higher order terms
G _F	integrand is F	integrand is \mathscr{SF}
\mathscr{G}_V	integrand is \mathscr{FV}	integrand <i>SFV</i>

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$$H(\mathbf{x}, \mathbf{p}, ct, -\gamma; z) = -\sqrt{\gamma^2 - 1 - (p_x - a_x)^2 - (p_y - a_y)^2}$$

where

$$a_x = K \cosh(k_x x) \cosh(k_y y) \cos(k_u z) + a_r$$

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$$a_r = \Re \sum_{h \ge 1} K_h(x,t;z) e^{ihk_r(z-ct)}$$

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$$H(\mathbf{x}, \mathbf{p}, ct, -\gamma; z) = -\sqrt{\gamma^2 - 1 - (p_x - a_x)^2 - (p_y - a_y)^2}$$

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Example



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$$G_2(ct,\eta) = [k_r(z-ct)+k_u z]\eta$$

New Hamiltonian

$$H = (k_u + k_r) \eta - \sqrt{k_r^2 \eta^2 - 1 - (p_x - a_x)^2 - (p_y - a_y)^2}$$

• New longitudinal conjugate pair

$$\theta \equiv k_r(z-ct)+k_u z, \qquad \eta \equiv \gamma/k_r$$

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Split Hamiltonians

Slow Hamiltonian

$$S \equiv \frac{k_{u}}{k_{s}}\gamma + \frac{1}{2\gamma} \left[1 + p_{x}^{2} + p_{y}^{2} + \frac{K^{2}}{2} \left(1 + k_{x}^{2}x^{2} + k_{y}^{2}y^{2} \right) \right] \\ + \frac{K^{2}}{4\gamma} \left[\frac{1}{3} \left(k_{x}^{4}x^{4} + k_{y}^{4}y^{4} \right) + k_{x}^{2}k_{u}^{2}x^{2}y^{2} \right] \\ + \frac{1}{(2\gamma)^{3}} \left(1 + K^{2} + \frac{3}{8}K^{4} \right) + O\left(\frac{q_{\perp}^{6}}{\gamma}, \frac{q_{\perp}^{2}}{\gamma^{3}}, \frac{1}{\gamma^{5}} \right)$$

• Fast Hamiltonian

$$= \frac{K_{\rm eff}^2}{4\gamma}\cos(2k_u z) + \frac{K_{\rm eff}}{\gamma}p_x\cos(k_u z) + O\left(\frac{q_{\perp}^3}{\gamma}, \frac{1}{\gamma^3}\right)$$

Field Potential

$$V \equiv -\Re \sum_{h} \left[\frac{K_{eff}}{\gamma} \cos(k_{u}z) + \frac{p_{x}}{\gamma} \right] K_{h} e^{ih(\theta - k_{u}z)} + O\left(\frac{K_{h}q_{\perp}^{2}}{\gamma}, \frac{K_{h}}{\gamma^{3}}, \frac{K_{h}^{2}}{\gamma} \right)$$

Split Hamiltonians

Propagated Field Model

Slow Hamiltonian

$$S \equiv \frac{k_{u}}{k_{s}}\gamma + \frac{1}{2\gamma} \left[1 + p_{x}^{2} + p_{y}^{2} + \frac{\kappa^{2}}{2} \left(1 + k_{x}^{2}x^{2} + k_{y}^{2}y^{2} \right) \right] \\ + \frac{\kappa^{2}}{4\gamma} \left[\frac{1}{3} \left(k_{x}^{4}x^{4} + k_{y}^{4}y^{4} \right) + k_{x}^{2}k_{u}^{2}x^{2}y^{2} \right] \\ + \frac{1}{(2\gamma)^{3}} \left(1 + \kappa^{2} + \frac{3}{8}\kappa^{4} \right) + O\left(\frac{q_{\perp}^{6}}{\gamma}, \frac{q_{\perp}^{2}}{\gamma^{3}}, \frac{1}{\gamma^{5}} \right)$$

Fast Hamiltonian

$$F \equiv \frac{K_{\rm eff}^2}{4\gamma}\cos(2k_u z) + \frac{K_{\rm eff}}{\gamma}p_x\cos(k_u z) + O\left(\frac{q_{\perp}^3}{\gamma}, \frac{1}{\gamma^3}\right)$$

where $K_{\rm eff} \equiv K\left(1 + k_x^2\frac{x^2}{2} + k_y^2\frac{y^2}{2}\right)$

Field Potential

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$$V \equiv -\Re \sum_{h} \left[\frac{K_{eff}}{\gamma} \cos(k_{u}z) + \frac{p_{x}}{\gamma} \right] K_{h} e^{ih(\theta - k_{u}z)} + O\left(\frac{K_{h}q_{\perp}^{2}}{\gamma}, \frac{K_{h}}{\gamma^{3}}, \frac{K_{h}^{2}}{\gamma} \right)$$

Split Hamiltonians

Propagated Field Model

Slow Hamiltonian

$$S \equiv \frac{k_{u}}{k_{s}}\gamma + \frac{1}{2\gamma} \left[1 + p_{x}^{2} + p_{y}^{2} + \frac{K^{2}}{2} \left(1 + k_{x}^{2}x^{2} + k_{y}^{2}y^{2} \right) \right] \\ + \frac{K^{2}}{4\gamma} \left[\frac{1}{3} \left(k_{x}^{4}x^{4} + k_{y}^{4}y^{4} \right) + k_{x}^{2}k_{u}^{2}x^{2}y^{2} \right] \\ + \frac{1}{(2\gamma)^{3}} \left(1 + K^{2} + \frac{3}{8}K^{4} \right) + O\left(\frac{q_{\perp}^{6}}{\gamma}, \frac{q_{\perp}^{2}}{\gamma^{3}}, \frac{1}{\gamma^{5}} \right)$$

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Field Potential

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Slow / Fast Map



Slow Map

 $\mathscr{G}_{S}(\lambda_{\mu}) = -\lambda_{\mu}S$

• Fast Map

$$\mathscr{G}_{F}(\lambda_{u}) = -\lambda_{u} rac{K^{4}k_{x}^{2}}{16k_{u}^{2}\gamma^{3}}$$


Slow Map

$$\mathscr{G}_{\mathcal{S}}(\lambda_u) = -\lambda_u S$$

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• coupling b/w slow betatron and fast wiggling motion • small coupling due to large frequency ratio b/w slow and fast motion

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$$\mathscr{G}_V(z) = -\int_0^z dz : \mathscr{S}(z_i) \mathscr{F}(z_i) V(z_i) :$$

• assumning slowly varying, we model the propagated field enverlope by

$$K_h^{\text{int}} \equiv \mathscr{SF} K_h \simeq \mathscr{F} K_h \equiv \mathbb{K}_h + \frac{K_{\text{eff}}}{k_u \gamma} \sin(k_u z) \frac{\partial}{\partial x} \mathbb{K}_h + z \partial_z \mathbb{K}_h$$

• $\mathbb{K}_h = rac{1}{z} \int_0^z K_h dz$: averaged field envelope

• $\partial_z \mathbb{K}_h$: first order longitudinal variation

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• where we used

$$\mathscr{F}(z) x = \frac{K_{eff}}{k_u \gamma} \sin\left(k_u z\right)$$

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$$\mathscr{F}(z)x = \frac{K_{eff}}{k_u\gamma}\sin\left(k_uz\right)$$

Generator

Propagated Potential

Similarly the FEL phase becomes

$$\theta^{\rm int} \equiv \mathscr{SF}\theta = \theta + \dot{\theta}z - \xi\sin\left(2k_{u}z\right) - \zeta\sin\left(k_{u}z\right)$$

where

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$$\dot{\theta} \equiv k_u - \frac{k_r}{2\gamma^2} \left[1 + p_x^2 + p_y^2 + \frac{K_{\text{eff}}^2}{2} \right]$$

$$\xi \equiv \frac{k_r K_{\text{eff}}^2}{8k_u \gamma^2}$$

$$\zeta \equiv \frac{k_r K}{k_u \gamma^2} p_x$$

• Exactly on resonance $\dot{ heta}
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Propagated Potential

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$$\begin{split} \dot{\theta} &\equiv k_u - \frac{k_r}{2\gamma^2} \left[1 + \rho_x^2 + \rho_y^2 + \frac{K_{\text{eff}}^2}{2} \right] \\ \xi &\equiv \frac{k_r K_{\text{eff}}^2}{8k_u \gamma^2} \\ \zeta &\equiv \frac{k_r K}{k_u \gamma^2} \rho_x \end{split}$$

ullet Exactly on resonance $\dot{ heta}
ightarrow 0$. The inclusion of it encompasses small off-resonant effects.

• We can write the propagated field potential by

$$V^{\text{int}} \equiv \mathscr{SF} V = -\Re \sum_{h} \left[\frac{K_{\text{eff}}}{\gamma} \cos(k_{u}z) + \frac{p_{x}}{\gamma} \right] K_{h}^{\text{int}} e^{ih\left(\theta^{\text{int}} - k_{u}z\right)}$$

• Therefore, finally, the generator of the field potential reads,

$$\mathcal{G}_{V} = -\int_{0}^{\lambda_{u}} V^{\text{int}} dz$$
$$= \lambda_{u} \Re \sum_{h} \frac{e^{ih\theta}}{\gamma} \left[K_{\text{eff}} \int_{C}^{h} + p_{x} \int_{1}^{h} + K \int_{zC}^{h} \partial_{z} + \frac{K_{\text{eff}}^{2}}{k_{u} \gamma} \int_{SC}^{h} \partial_{x} \right] \mathbb{K}_{h}$$

where $C \equiv \cos(k_u z)$, $SC \equiv \sin(k_u z)\cos(k_u z)$, and the inegration parameter is, for example,

$$\int_{C}^{h} \equiv \frac{e^{-ih\theta}}{\lambda_{u}} \int_{0}^{\lambda_{u}} \cos(k_{u}z) e^{ih\left(\theta^{int} - k_{u}z\right)} dz$$

explicitly..

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explicitly....



Integration Parameters

To the 1st order of
$$\dot heta$$
, ζ , and $\Delta\xi\equiv\xi-\xi_R$ where $\xi_R\equivrac{k_rK^2}{8k_u\gamma_R^2}$

$$\begin{split} \int_{C}^{h} &= \frac{1}{2} \left(J_{-\frac{h-1}{2}}^{h\xi_{R}} + J_{-\frac{h+1}{2}}^{h\xi_{R}} \right) \left(1 + \frac{ih\dot{\theta}\lambda_{u}}{2} \right) - \frac{1}{2} \frac{h\dot{\theta}}{k_{u}} \left(\sum_{l\neq -\frac{h-1}{2}} \frac{J_{l}^{h\xi_{R}}}{(2l+h-1)} + \sum_{l\neq -\frac{h+1}{2}} \frac{J_{l}^{h\xi_{R}}}{(2l+h+1)} \right) \\ &- \frac{1}{2} \Delta \xi \left(\frac{h-1}{2\xi_{R}} J_{-\frac{h-1}{2}}^{h\xi_{R}} + hJ_{-\frac{h-3}{2}}^{h\xi_{R}} + \frac{h+1}{2\xi_{R}} J_{-\frac{h+1}{2}}^{h\xi_{R}} + hJ_{-\frac{h-1}{2}}^{h\xi_{R}} \right) + \frac{h\zeta}{2} \frac{1}{2} \left(J_{-\frac{h+2}{2}}^{h\xi_{R}} - J_{-\frac{h-2}{2}}^{h\xi_{R}} \right) \\ \int_{1}^{h} &= J_{-\frac{h}{2}}^{h\xi_{R}} \left(1 + \frac{ih\dot{\theta}\lambda_{u}}{2} \right) - \frac{h\dot{\theta}}{k_{u}} \sum_{l\neq -\frac{h}{2}} \frac{J_{l}^{h\xi_{R}}}{(2l+h)} - \Delta \xi \left(\frac{h}{2\xi_{R}} J_{-\frac{h}{2}}^{h\xi_{R}} + hJ_{-\frac{h+1}{2}}^{h\xi_{R}} \right) + \frac{h\zeta}{2} \left(J_{-\frac{h+1}{2}}^{h\xi_{R}} - J_{-\frac{h-1}{2}}^{h\xi_{R}} \right) \\ \int_{zC}^{h} &= \frac{\lambda_{u}}{4} \left(J_{-\frac{h\xi_{R}}{2}}^{h\xi_{R}} + J_{-\frac{h+1}{2}}^{h\xi_{R}} \right) + \frac{i\lambda_{u}}{4\pi} \left(\sum_{l\neq -\frac{h-1}{2}} \frac{J_{l}^{h\xi_{R}}}{(2l+h-1)} + \sum_{l\neq -\frac{h+1}{2}} \frac{J_{l}^{h\xi_{R}}}{(2l+h+1)} \right) \\ \int_{SC}^{h} &= \frac{1}{4i} \left(J_{-\frac{h\xi_{R}}{2}}^{h\xi_{R}} - J_{-\frac{h+2}{2}}^{h\xi_{R}} \right) \end{split}$$

 $J_i^{h\xi_R}$: First kind Bessel function of order *i* and argument $h\xi_R$, only integer *i* allowed. \int_{SC} vanishes for *odd* harmonics but can be large for *even* harmonics.

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Example

Hamiltonian

Figure

- : Pusher Comparison
- $\Delta \theta \equiv |\theta \theta_{\rm ref}|$
- $heta_{
 m ref} \leftarrow {\sf using exact H}$

• Fixed envelope $\mathbb{K}_{1} = A_{0}e^{-x^{2}/\sigma_{x}^{2}}e^{z/L_{G}}$ $\sigma_{x} = 55\,\mu\text{m}$ $L_{G} = 50\lambda_{u}$ • eBeam param

$$\gamma = 1000$$

 $\Delta \gamma / \gamma = 2 \times 10^{-4}$

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Oct 23, 2018 19

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Outline

Introduction

Generalize WPA

- How?
- Review : Perturbative Lie Map
- Hamiltonian
- Generator
- Effective Hamiltonian
- Improve Shot Noise Modeling
 - Review of shot-noise modeling methods
 - Improved shot-noise modeling methods
 - IMPACT code suit and example

Conclusion

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5D mirroring

• Here, we review two 1D methods by Dr. Fawley and Dr. McNeil et.al.



- 1st step : uniform along temporal coordinate ightarrow zero bunching factor
- Next step : add (temporal coordinate / charge weight) perturbations
 - to model physical shot noise : correct RMS bunching factor $\langle b_h b_h^* \rangle = 1/N_e$ at least

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6D extension

• Here, we review two 6D extension methods of the 1D model.



5D mirroring (Fawley) 6D volume division (McNeil et.al.)



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5D mirroring (Fawley)

6D volume division (McNeil et.al.)



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5D mirroring

- same 5D coordinates x, y, p_x, p_y, γ among a set of particles called "beamlet"
 - each beamlet is based on 1D model
- member particles of a beamlet are not statistically independent
 - numerical shot-noise upon particles migration across the numerical mesh

• 6D volume division

- comes with the charge perturnbation \leftarrow Poisson principle
- all particles are statistically indepedent
 - No shot-noise upon particles migration
- requires a lot of particles as division over 6 dimension can be huge

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• We adopt the 5D mirroring strategy

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- Our idea is to interpret one beamlet as one statistically independent entity
 - based on the fact that member particles are not statistically indepedent and
 - > motion of beamlets are macroscopic $(\gtrsim \lambda_r)$
 - \circ -motion of member particles are microscopic ($\lesssim \lambda_r)$
 - phase-space coordinate of a beamlet is given by the average over the member particles in it
 - This allows natural loading method :
 - random number of particle density functions or
 - external uptream tracking code

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 - motion of beamlets are macroscopic $(\gtrsim \lambda_r)$
 - motion of member particles are microscopic ($\lesssim \lambda_r)$
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Particle Loading



• : beamlet

• : member particle

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Migrate all member particles when a beamlet migrate

Smoother numerical discretization

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Figure. Benchmark : Beamlet vs individual particle migration NGLS-like parameters are used.

- Migrate all member particles when a beamlet migrate
- Smoother numerical discretization

weight and shape functions are evaluated at the beamlet position



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Slippage Resolution

- Typical implementation of slippage is to copy the field data from the previous temporal mesh point to the next temporal mesh point
- Beamlet migration enables arbitrary slippage resolution through moving window
 - It also allows natural slippage modeling through arbitrary length of non-resonant tranport like drift

Data Copy from previous slice

```
for i in [0,1,2,...,nt]:
 Fld.data[:,:,nt-i] = Fld.data[:,:,nt-i-1]
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Moving wondow : change of domain

Fld.domain.theta[:]

= Fld.domain.theta[:]+dtheta



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Improved shot-noise modeling methods

Copying Data vs Moving Window



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- integration step size = $5\lambda_{\mu}$
- temporal mesh size = $20\lambda_r$
- One slippage operation every 4 step when copying data is used.

Split and Composition

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Field solver can be split into two operation - diffusion 𝓕_⊥ and slippage 𝓕_{||}
2nd order composition method

$$\mathscr{F}_{\parallel}\left(\frac{\Delta z}{2}\right)\mathscr{F}_{\perp}(\Delta z)\mathscr{F}_{\parallel}\left(\frac{\Delta z}{2}\right)$$

is possbile due to arbitrary slippage resolution.



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IMPACT code suit and example

All the methods presented are implemented in IMPACT code suite. Example:



Outline

Introduction

Generalize WPA

- How?
- Review : Perturbative Lie Map
- Hamiltonian
- Generator
- Effective Hamiltonian
- Improve Shot Noise Modeling
 - Review of shot-noise modeling methods
 - Improved shot-noise modeling methods
 - IMPACT code suit and example

Conclusion

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Advances in numerical methods for FEL simulation under the WPA are presented

- We generalized WPA perturbatively using Lie map method
- We improved numerical shot-noise modeling method
 - supressed artificial shot-noise upon migration
 - enabled smoother numerical descretization
 - arbitrary mesh size, weight/shape function, sippage resolution
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- All these methods are implemented in beam dynamics simulation framework IMPACT code suite

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Appendix

1D Model

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 $\bullet~$ 1st step : uniform along temporal coordinate \rightarrow zero bunching factor

$$b_h^0 = \frac{1}{N_e} \sum_{j=1}^M m_j e^{ih\theta_j} = 0$$

• Next step is to add perturbations to model physical shot noise : $\langle b_h b_h^* \rangle = 1/N_e$

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Appendix

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• Temporal coordinate perturbation (Fawley)

$$\delta heta_{j} \equiv \sum_{h'=1}^{M/2} \xi_{h'} e^{-ih' heta_{j}}$$

Bunching Factor becomes

$$b_h = \frac{1}{N_e} \sum_{j=1}^M m_j e^{ih(\theta_j + \delta \theta_j)} \simeq ih\xi_h$$

• Therefore, RMS becomes

$$\langle b_h b_h^*
angle \simeq h^2 \langle \xi_h \xi_h^*
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 $\langle \xi_h \xi_h^* \rangle = 1/(h^2 N_e)$



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Charge weight perturbation

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• Let $ilde{m}_j \equiv m_j + \delta m_j$ such that

$$\left\langle \tilde{m}_{j} \right\rangle = \left\langle \tilde{m}_{j}^{2} \right\rangle - \left\langle \tilde{m}_{j} \right\rangle^{2} = \frac{N_{e}}{M}$$

• Then, from $b_h = \frac{1}{N_e} \sum_{j=1}^M \tilde{m}_j e^{ih\theta_j}$

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angle &= & rac{1}{N_e^2} \sum_j^M \sum_k^M \left< ilde{m}_j ilde{m}_k
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