VUV and X-ray Free-Electron Lasers

Injector Beam Dynamics

Dinh Nguyen,[1] Christopher Mayes,[1] Nicole Neveu[2], Colwyn Gulliford[3]

[1] xLight Inc.

[2] SLAC National Accelerator Laboratory

[3] Xelera

xLight

SLAC NATIONAL ACCELERATOR LABORATORY

XELERA

Injector Dynamics Motivation

- Create beam at cathode (sets initial beam quality)
- Accelerate beam to injection energy
- Take care to preserve emittances and LPS

Equations of Motion

Lorentz Force Law for single electron:

$$\dot{\vec{p}} = \vec{F} = e(\vec{E} + \vec{v} \times \vec{B})$$

$$d/dt \rightarrow c\beta_z d/dz \qquad \vec{p}\,' = \vec{F}/c\beta_z = e(\vec{E} + \vec{v} \times \vec{B})/c\beta_z$$

For a bunch of electrons, also care about evolution of the moments of the distributions:

$$\sigma_x = \langle x^2 \rangle^{1/2} \qquad \sigma_x' = \frac{\langle xx' \rangle}{\sigma_x} \qquad x' = p_x/p_z$$

$$\sigma_x'' = \frac{1}{\sigma_x^3}\left[\langle x^2 \rangle \langle (x')^2 \rangle + \langle xx' \rangle^2\right] + \frac{\langle xx'' \rangle}{\sigma_x}$$

$$\sigma_x'' = \frac{1}{\sigma_x^3}\left(\frac{mc\epsilon_{n,x}}{pz}\right)^2 + \frac{\langle xx'' \rangle}{\sigma_x} \qquad \epsilon_{n,x} = \frac{1}{mc}\sqrt{\langle x^2 \rangle \langle p_x^2 \rangle - \langle xp_x \rangle^2}$$

Emittance pressure term

Force term (external and self)

Intuitively, we want the emittance to be constant

$$\epsilon_{n,x}' \propto \frac{d}{dz}\epsilon_{n,x}^2 \propto \left[\langle xx' \rangle \langle p_x^2 \rangle + \langle x^2 \rangle \langle p_x p_x' \rangle - \langle xp_x \rangle (\langle x' p_x \rangle + \langle xp_x' \rangle)\right]$$

$$p_x' = F_x/c\beta_z$$

$$\epsilon_{n,x}' \propto \left[\langle x^2 \rangle \langle p_x F_x \rangle - \langle xp_x \rangle \langle xF_x \rangle\right]$$

$F_x = \alpha x(z)$, then $\epsilon_{n,x}' = 0$

RMS Emittance will only be preserved if forces are linear!

Fields from Beamline Elements

Most injectors feature cylindrical symmetry and are made up of RF Cavities & Solenoids

$$\begin{aligned} \nabla \cdot \mathbf{E} &= 0, \\ \nabla \cdot \mathbf{B} &= 0, \\ \nabla \times \mathbf{E} &= -i\omega \mathbf{B}, \\ \nabla \times \mathbf{B} &= i\frac{\omega}{c^2}\mathbf{E}. \end{aligned}$$

$$\begin{aligned} E_r(r,z) &= \sum_{n=1}^{\infty} E_r^{(n)}(z) r^n, \\ E_z(r,z) &= \sum_{n=0}^{\infty} E_z^{(n)}(z) r^n, \\ B_\theta(r,z) &= \sum_{n=1}^{\infty} B_\theta^{(n)}(z) r^n. \end{aligned}$$

$$\begin{aligned} E_r^{(2n+1)} &= -\frac{1}{2n+2}\frac{d}{dz}E_z^{(2n)} \\ B_\theta^{(2n+1)} &= \frac{1}{2n+2}\frac{i\omega}{c^2}E_z^{(2n)} \\ E_z^{(2n+2)} &= -\frac{1}{(2n+2)^2}\left(\frac{d^2}{dz^2}E_z^{(2n)} + \frac{\omega}{c^2}E_z^{(2n)}\right) \end{aligned}$$

$$\begin{aligned} E_r(r,z) &\approx -\frac{r}{2}\frac{d}{dz}E_z^{(0)} + \frac{r^3}{16}\left(\frac{d^3}{dz^3} + \frac{\omega}{c^2}\frac{d}{dz}\right)E_z^{(0)} \\ B_\theta(r,z) &\approx \frac{i\omega}{c^2}\left[\frac{r}{2}E_z^{(0)} - \frac{r^3}{16}\left(\frac{d^2}{dz^2} + \frac{\omega}{c^2}\right)E_z^{(0)}\right] \\ E_z(r,z) &\approx E_z^{(0)} - \frac{r^2}{4}\left(\frac{d^2}{dz^2} + \frac{\omega}{c^2}\right)E_z^{(0)}. \end{aligned}$$

For DC gun, let $\omega = 0$

$$E_r(r,z) \approx -\frac{r}{2}\frac{dE_z^{(0)}}{dz} + \frac{r^3}{16}\frac{d^3E_z^{(0)}}{dz^3}$$

$$E_r(r,z) \approx E_z^{0)} - \frac{r^2}{4}\frac{d^2E_z^{0)}}{dz^2}$$

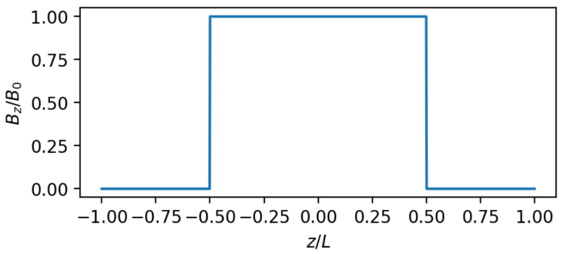
For solenoid:

$$B_r(r,z) \approx -\frac{r}{2}\frac{dB_z^{(0)}}{dz} + \frac{r^3}{16}\frac{d^3B_z^{(0)}}{dz^3}$$

$$B_r(r,z) \approx B_z^{0)} - \frac{r^2}{4}\frac{d^2B_z^{0)}}{dz^2}$$

Knowledge of the field on-axis in principle defines field everywhere

Solenoid Dynamics: Larmor Angle



$$B_z = B_0\left(\theta(z - z_i) - \theta(z - z_f)\right)$$

$$B_r = -\frac{r}{2}B_0\left(\delta(z - z_i) - \delta(z - z_f)\right)$$

At field entrance:

$$\frac{d\vec{p}}{dz} = \frac{e}{c\beta_z}(\vec{v} \times \vec{B}) \qquad \frac{dp_\theta}{dz} = \frac{e}{c\beta_z}(\vec{v} \times \vec{B})_\theta = \frac{e}{c\beta_z}(v_z B_r - v_r Bz)$$

$$\Delta p_\theta = \lim_{\epsilon \to 0} \int_{z_i - \epsilon}^{z_i + \epsilon} \frac{e}{c\beta_z}(v_z B_r - v_r B_z)dz = \frac{1}{2}eB_0 r_i = m\gamma r_i \dot{\theta}$$

$$\dot{\theta} = \frac{eB_0}{2m\gamma}$$

Particles rotating at common frequency

Inside field: $$\frac{dp_r}{dz} = \frac{e}{c\beta_z}(v_\theta B_r - v_z B_\theta) = \frac{e}{c\beta_z} v_\theta B_z = \frac{e}{p_z} p_\theta B_0$$

In Cartesian coordinates: $$p_x' = \frac{d}{dz}(p_z x') \approx p_z x''$$

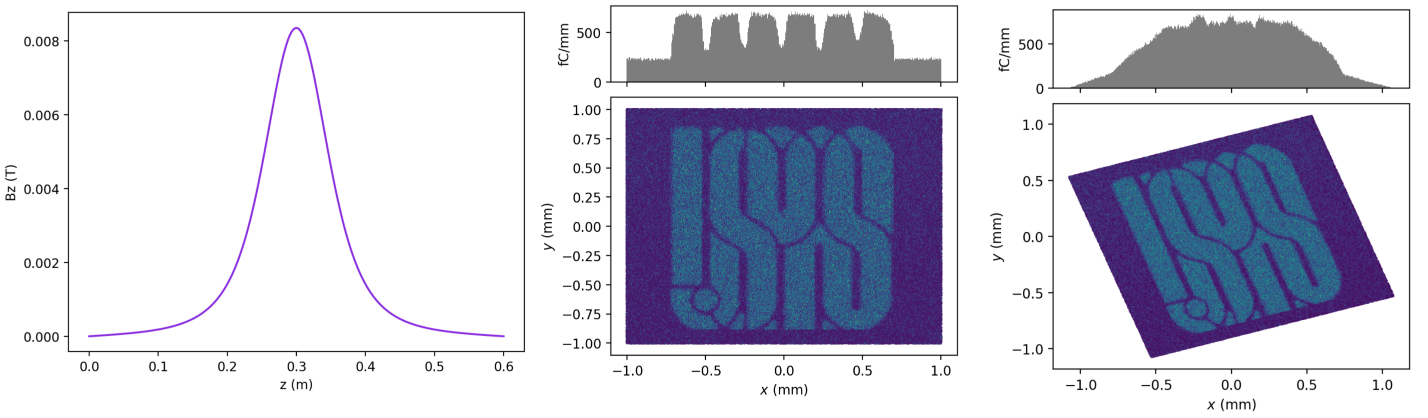
$$x'' - \left(\frac{eB_z}{p_z}\right)y' + \left(\frac{eB_z'}{2p_z}\right)y = 0 \qquad y'' + \left(\frac{eB_z}{p_z}\right)x' + \left(\frac{eB_z'}{2p_z}\right)x = 0$$

Define Larmor angle: $\theta_L' = \dfrac{eB_z}{2p_z}$ $\qquad \theta_L = \displaystyle\int \frac{eB_z}{2p_z} dz$

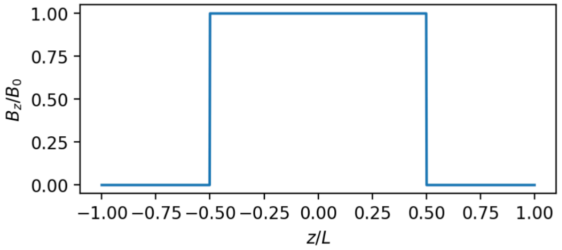
Define Larmor coordinate: $\eta_L = (x + iy)e^{i\theta_L}$

Decoupled motion: $\eta_L'' + (\theta_L')^2 \eta_L = 0$

$p = 500$ keV/c, $\theta_L = -18.75$ deg



Solenoid Dynamics: Larmor Angle



$$B_z = B_0\left(\theta(z-z_i) - \theta(z-z_f)\right)$$

$$B_r = -\frac{r}{2}B_0\left(\delta(z-z_i) - \delta(z-z_f)\right)$$

At field entrance:

$$\frac{d\vec{p}}{dz} = \frac{e}{c\beta_z}(\vec{v}\times\vec{B}) \qquad \frac{dp_\theta}{dz} = \frac{e}{c\beta_z}(\vec{v}\times\vec{B})_\theta = \frac{e}{c\beta_z}(v_z B_r - v_r Bz)$$

$$\Delta p_\theta = \lim_{\epsilon\to 0}\int_{z_i-\epsilon}^{z_i+\epsilon}\frac{e}{c\beta_z}(v_z B_r - v_r B_z)dz = \frac{1}{2}eB_0 r_i = m\gamma r_i\dot{\theta}$$

$$\dot{\theta} = \frac{eB_0}{2m\gamma}$$ Particles rotating at common frequency

Inside field: $$\frac{dp_r}{dz} = \frac{e}{c\beta_z}(v_\theta B_r - v_z B_\theta) = \frac{e}{c\beta_z}v_\theta B_z = \frac{e}{p_z}p_\theta B_0$$

In Cartesian coordinates: $$p'_x = \frac{d}{dz}(p_z x') \approx p_z x''$$

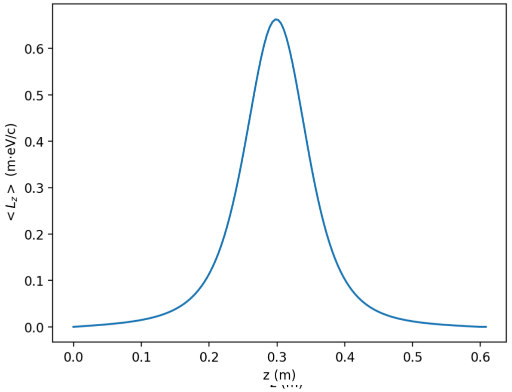
$$x'' - \left(\frac{eB_z}{p_z}\right)y' + \left(\frac{eB'_z}{2p_z}\right)y = 0 \qquad y'' + \left(\frac{eB_z}{p_z}\right)x' + \left(\frac{eB'_z}{2p_z}\right)x = 0$$

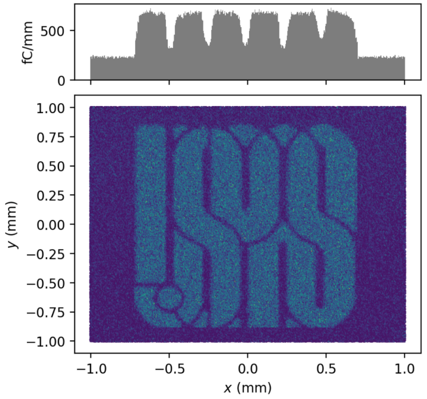
Define Larmor angle: $\theta'_L = \frac{eB_z}{2p_z}$ $\qquad \theta_L = \int \frac{eB_z}{2p_z}dz$

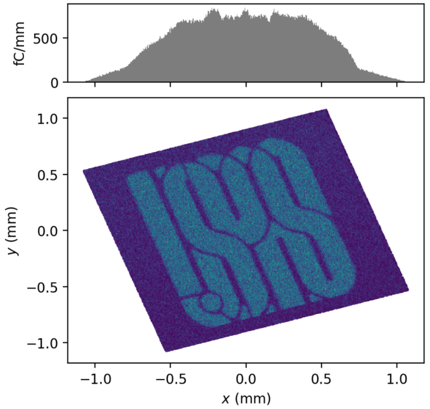
Define Larmor coordinate: $\eta_L = (x+iy)e^{i\theta_L}$

Decoupled motion: $\eta''_L + (\theta'_L)^2\eta_L = 0$

$p = 500$ keV/c, $\theta_L = -18.75$ deg







Misalignments, Aberrations, RF Focusing

The form of the higher order terms for the forces can be used to derive formulas for the geometric and chromatic aberrations in these elements

For Solenoid:

$$\epsilon_x^2 = 4\alpha^2\sigma_x^6(5x_0^2 + 2\sigma_x^2) \quad \text{for Gaussian,}$$

$$\epsilon_x^2 = \tfrac{8}{9}\alpha^2\sigma_x^6(9x_0^2 + \sigma_x^2) \quad \text{for elliptical,}$$

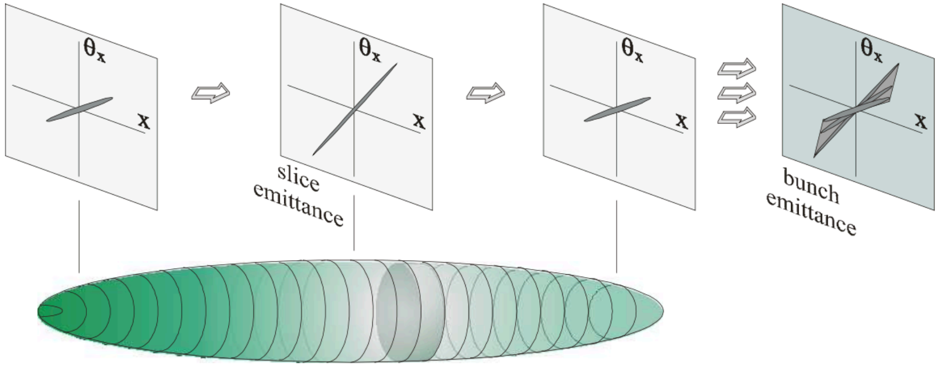
$$\epsilon_x^2 = \frac{4}{147}\alpha^2\sigma_x^6(357x_0^2 + 50\sigma_x^2) \quad \text{for uniform.}$$

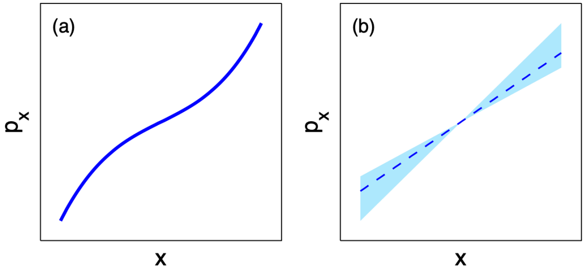
Here x_0 is a position offset of the beam entering the solenoid

Chromatic aberration: $$\epsilon_{nx} = 2\left(\frac{1}{f}\right)_{\text{sol}}\sigma_x\sqrt{\sigma_x^2 + x_0^2}\,\frac{\sigma_p}{mc}$$

Similar expressions for accelerating elements: $$\epsilon_{nx} = \kappa\sigma_x^4\frac{\alpha_p}{mc}.$$

Concept of slice emittance:





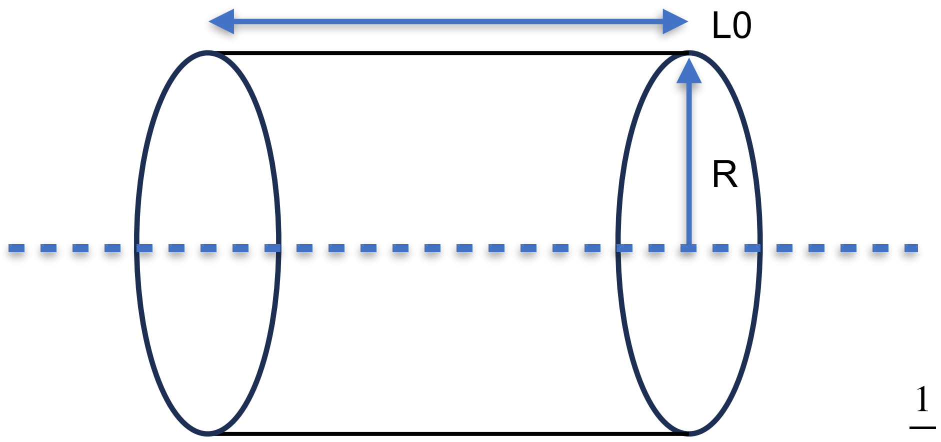
$$\epsilon_{nx} = \frac{1}{mc}\left|\frac{\partial^2 p_x}{\partial x \partial t}\right|\sigma_t\sigma_x\sqrt{\sigma_x^2 + x_0^2},$$

https://journals.aps.org/prab/pdf/10.1103/PhysRevSTAB.14.072001

Space Charge

Space Charge: Simple Analytic Model

Beam rest frame



Uniform cylinder of charge at rest

Integrate up field from finite disks on z-axis:

$$E_z(r=0, z, L_0, R) = \frac{Q}{2\pi\epsilon_0 R^2}\left[\sqrt{\left(1-\frac{z}{L_0}\right)^2+\frac{R^2}{L_0^2}} - \left|1-\frac{z}{L_0}\right| - \sqrt{\frac{z^2}{L_0^2}+\frac{R^2}{L_0^2}} + \left|\frac{z}{L_0}\right|\right]$$

Plug into Gauss's Law

$$\frac{1}{r}\frac{\partial}{\partial r}(rE_r) + \frac{\partial E_z}{\partial z} = \frac{\rho}{\epsilon_0} \qquad E_r^{(1)} = \frac{Qr}{4\pi\epsilon_0 R^2 L_0}\left(\frac{1-z/L_0}{\sqrt{\left(1-\frac{z}{L_0}\right)^2 + R^2/L_0^2}} + \frac{z/L_0}{\sqrt{(z/L_0)^2 + R^2/L_0^2}}\right)$$

Lab frame

Fields transform to lab frame via:

$$\mathbf{E} = \gamma(\mathbf{E}' - \vec{\beta}\times c\mathbf{B}') - \frac{\gamma^2}{1+\gamma}\vec{\beta}(\vec{\beta}\cdot\mathbf{E}'),$$

$$\mathbf{B} = \gamma(\mathbf{B}' + \vec{\beta}\times \mathbf{E}'/c) - \frac{\gamma^2}{1+\gamma}\vec{\beta}(\vec{\beta}\cdot\mathbf{B}'),$$

Note: $L_0 \rightarrow \gamma L$

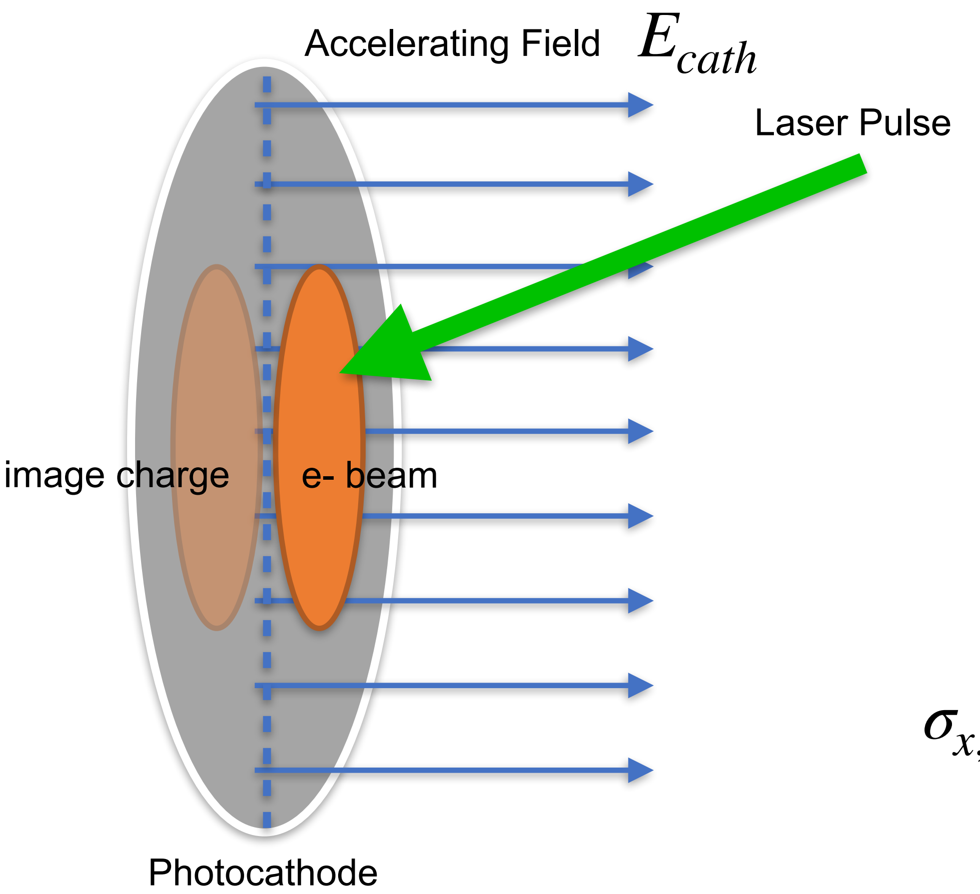
$$E_{r,lab} = \gamma E_r(\gamma L),\ B_{\theta,lab} = \gamma\beta E_r(\gamma L),\ E_{z,lab} = E_z(\gamma L)$$

$$F_{r,lab} = E_r(\gamma L)/\gamma^2$$

Both transverse and longitudinal fields vanish as $\gamma \rightarrow \infty$, getting beam up to high energy as fast as possible reduces effects

Space Charge Limited Emission

Consider a very short bunch being emitted from a photocathode:



Maximum amount of charge extraction occurs when space charge field from beam + image cancel the accelerating field

$$E_z^{SC} = 2 \times \frac{\sigma}{2\epsilon_0} = E_{cath}$$

$$\sigma = \frac{q}{\pi R^2} = \epsilon_0 E_{cath}$$

$$\sigma_{x,y} \propto \sqrt{\frac{q}{\epsilon_0 E_{cath}}} \qquad \epsilon_{n,x,y} \propto \sqrt{\frac{q}{\epsilon_0 E_{cath}} \frac{MTE}{mc^2}}$$

Pancake regime ONLY!

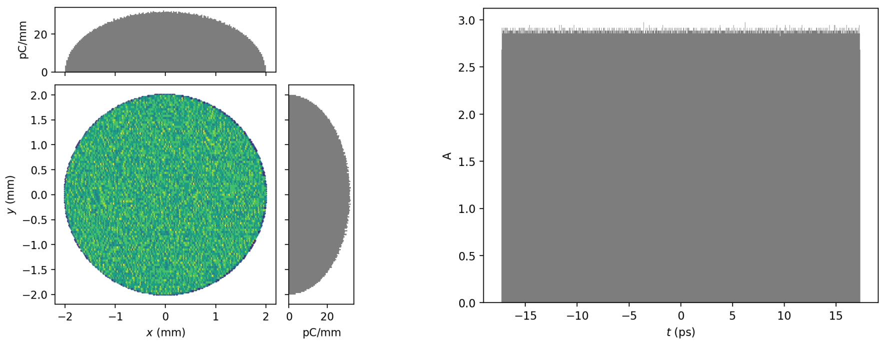
https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.102.104801

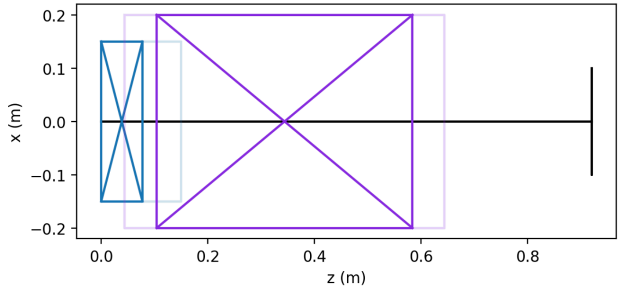
Space Charge Limited Emission

More careful analysis using the uniform cylinder of charge:

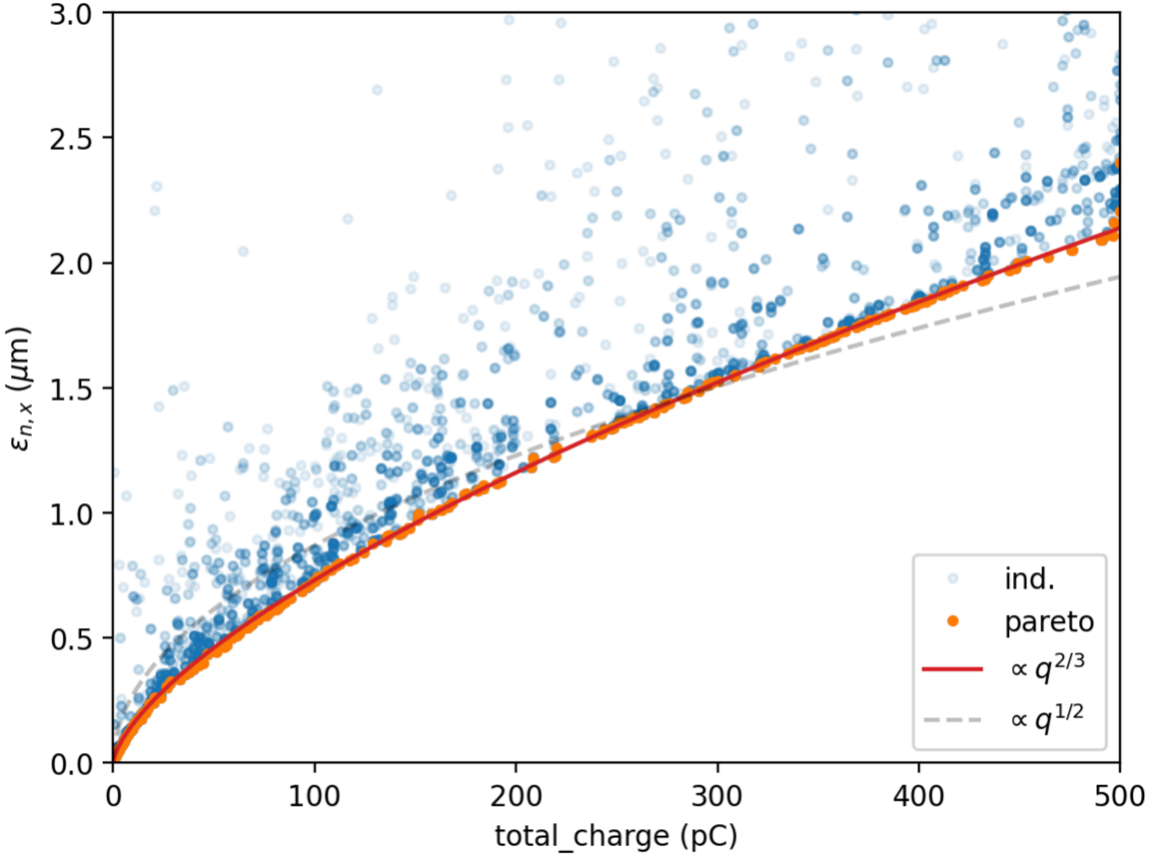
$$\epsilon_{n,x,y} \propto \left(\frac{q}{\epsilon_0 E_{cath}}\right)^{2/3} \sqrt{\frac{MTE}{mc^2}}$$

Test case: DC Gun + Solenoid, Uniform cylinder of charge:





Minimize emittance and maximize bunch charge:
Variables: laser spot size, solenoid strength



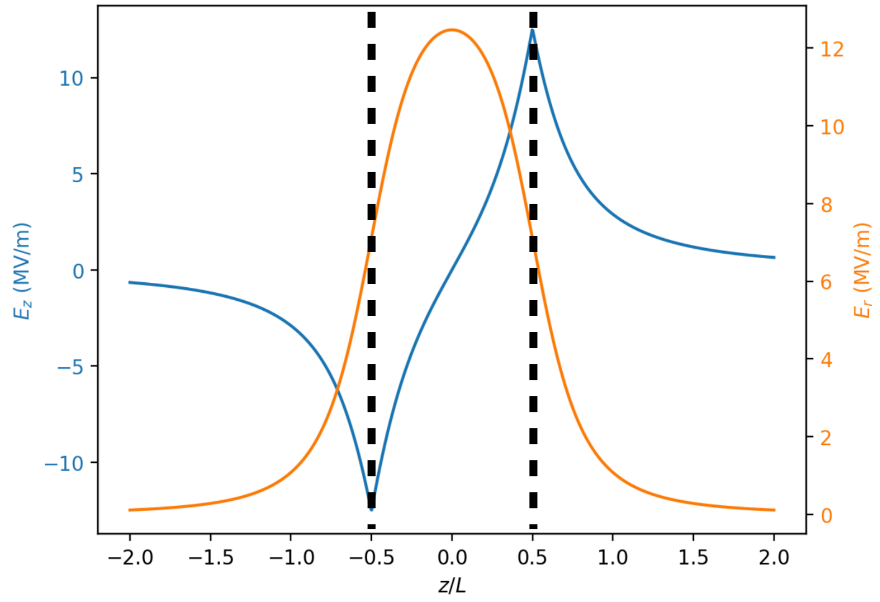
https://journals.aps.org/prab/abstract/10.1103/PhysRevSTAB.17.024201

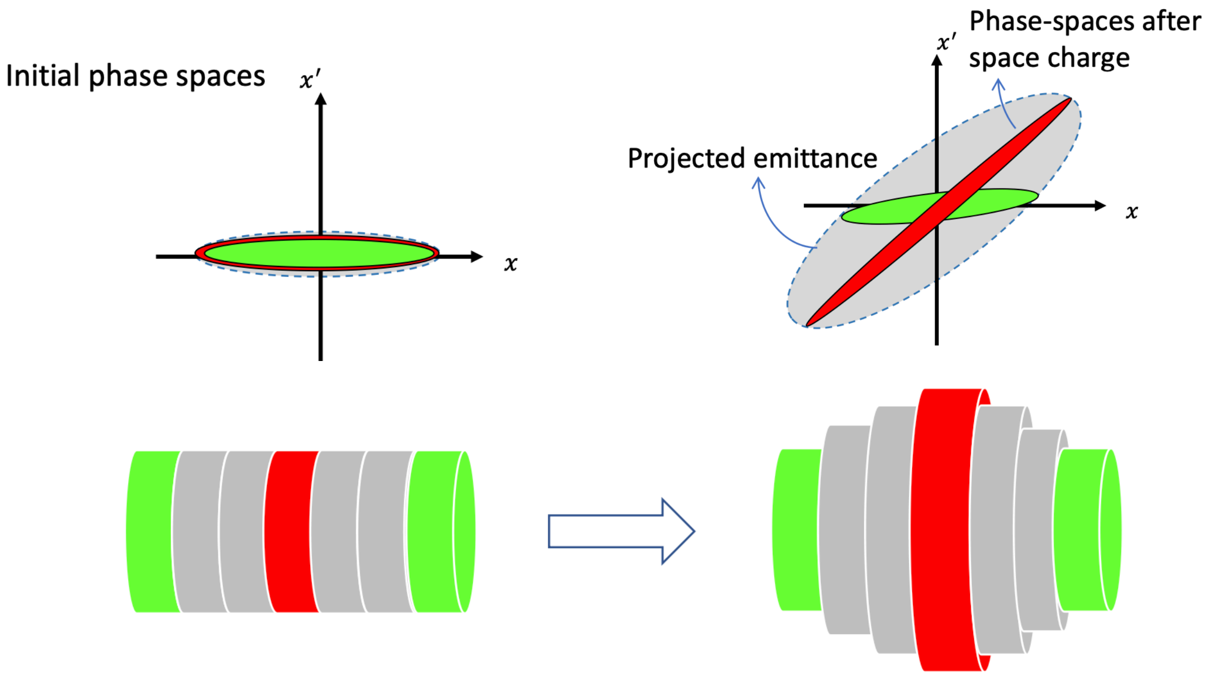
Space Charge Emittance Growth

Space charge has the potential to cause emittance growth in mainly two ways:

1. Non-linearity of the space charge fields (geometric aberration)

2. Fields which depend on the longitudinal coordinate in the bunch (similar to RF focusing)



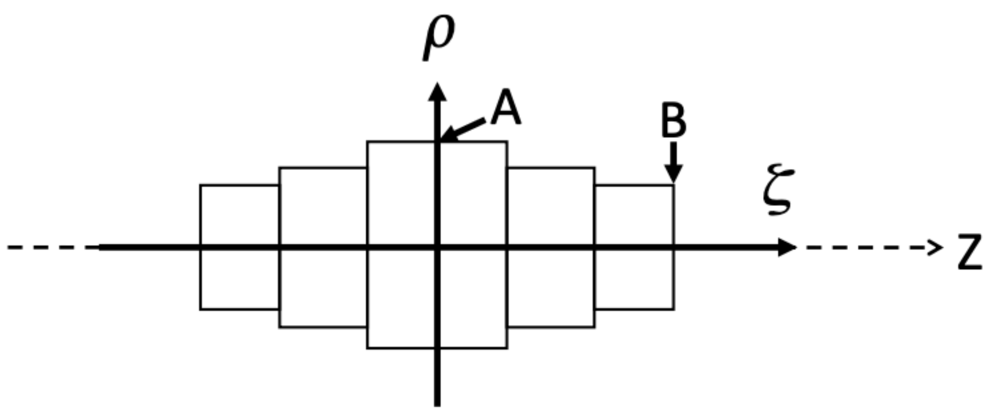


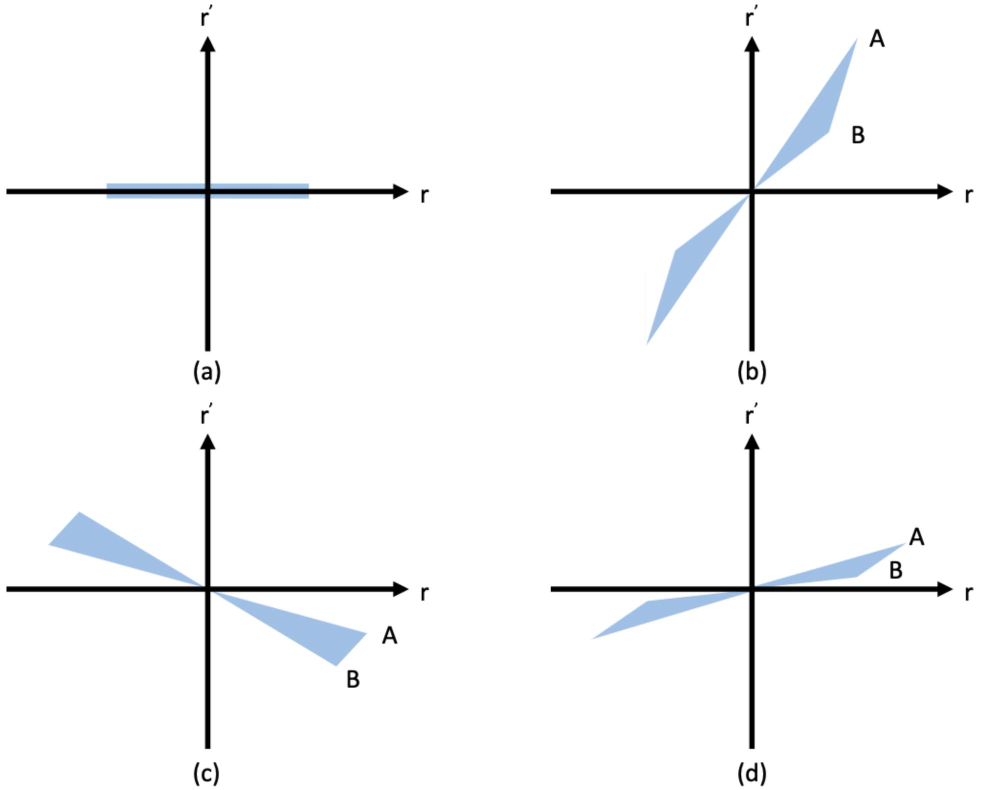
Electron bunch with N slices initially generated at cathode

Same bunch after drifting under space charge force

Emittance Compensation

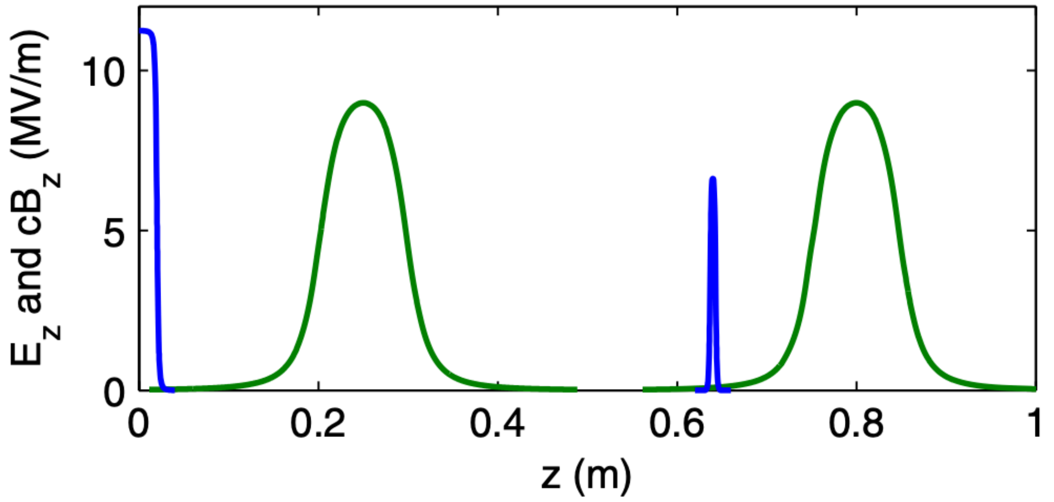
- Theory which explains emittance changes coming from slice alignment/misalignment
- First treatment by Carlsten (1989), show his simplified model here
- Expanded on by Serafini and Rosenzweig

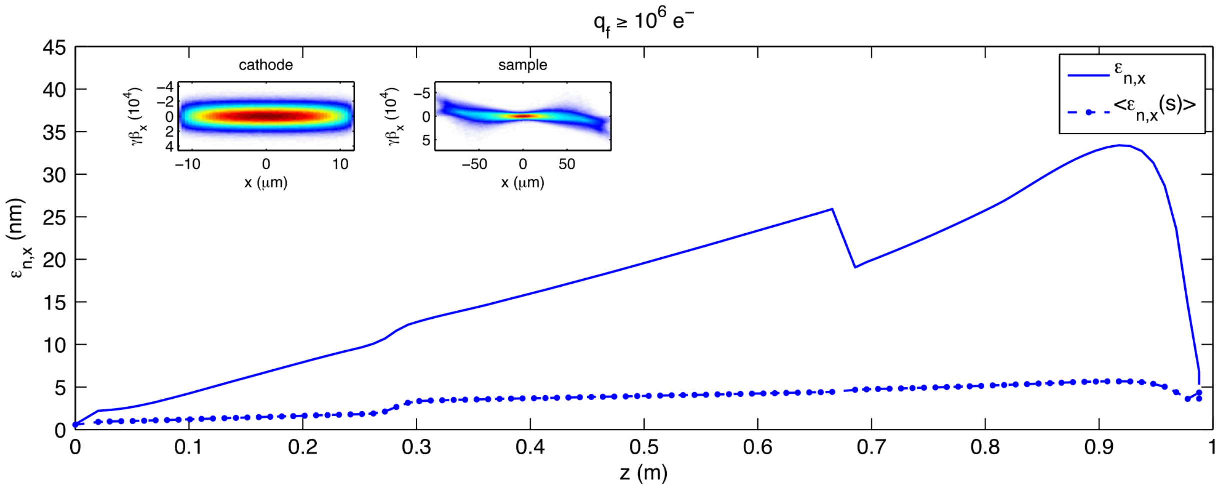




Emittance Compensation

Example from an optimized UED beam line:





Emittance Compensation

Theory makes use of envelope equation we saw before, assuming a long beam

$$\sigma'' + \left(\frac{\gamma'}{\beta^2\gamma}\right)\sigma' + K_r\sigma - \left(\frac{\kappa_s}{\beta^3\gamma^3}\right)\frac{1}{\sigma} - \left(\frac{\epsilon_n}{\beta\gamma}\right)^2\frac{1}{\sigma^3} = 0.$$

$$K_r \equiv -(dF_r/dr)/\beta^2\gamma m_e c^2. \qquad \kappa_s = I/2I_0$$

We know the emittance isn't constant (slice misalignment) and we used pulsed beams…

Assume there is an envelope equation of the form above for each slice: $\kappa_s \to \kappa_s(\zeta)$,

To handle acceleration, move to reduced variable $\hat{\sigma} = \sqrt{\gamma\beta}\sigma$

$$\hat{\sigma}'' + \left(K_r - \frac{(\sqrt{\beta\gamma})''}{\sqrt{\beta\gamma}}\right)\hat{\sigma} - \left(\frac{\kappa_s}{\beta^2\gamma^2}\right)\frac{1}{\hat{\sigma}} - \frac{\epsilon_n^2}{\hat{\sigma}^3} = 0,$$

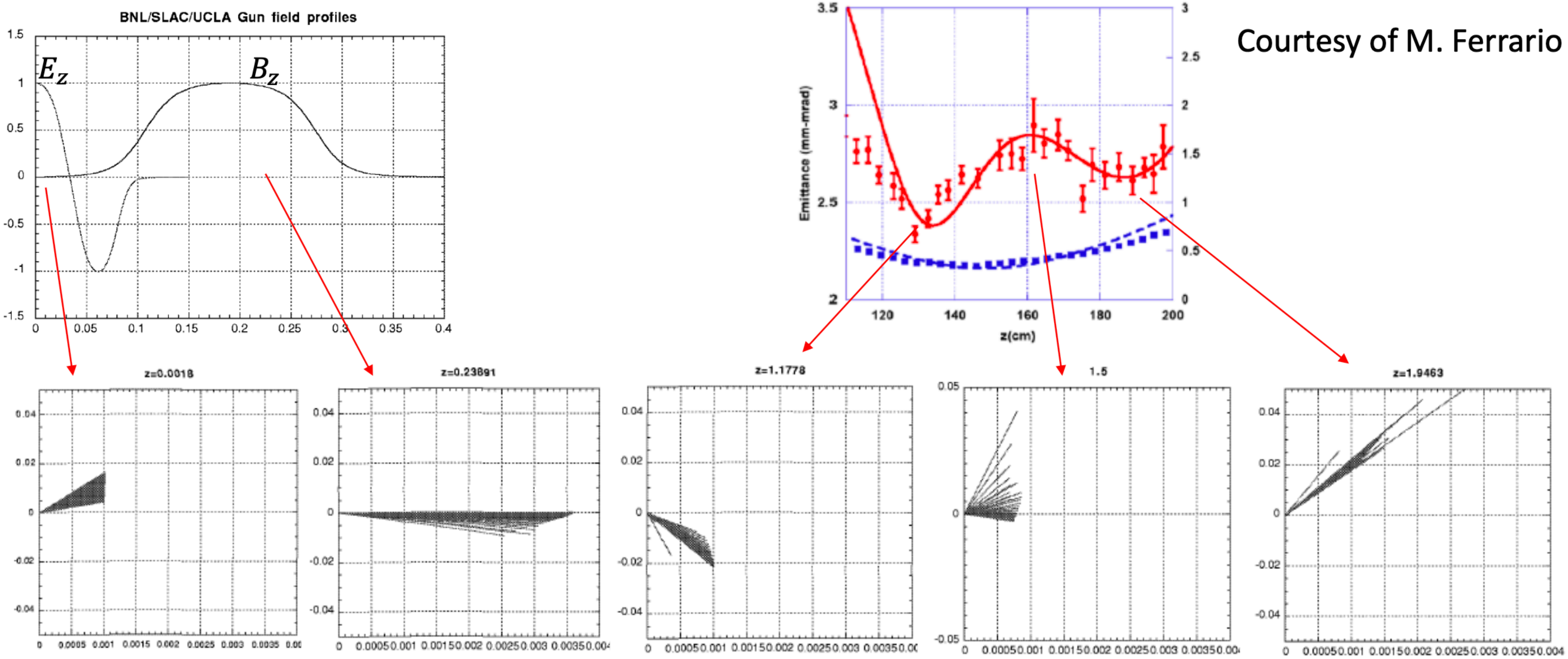
$$\hat{\sigma}'' + \left(\frac{\kappa}{\beta^2\gamma^2}\right)\hat{\sigma} - \left(\frac{\kappa_s}{\beta^2\gamma^2}\right)\frac{1}{\hat{\sigma}} - \frac{\epsilon_n^2}{\hat{\sigma}^3} = 0$$

Assume constant acceleration and radial focusing, can find equilibrium solution known as invariant envelope

$$\hat{\sigma}_{\text{inv}} = \sqrt{\frac{\kappa_s}{\kappa}}, \qquad \hat{\sigma}'_{\text{inv}} = 0.$$

Emittance will oscillate due to plasma oscillations around equilibrium solution

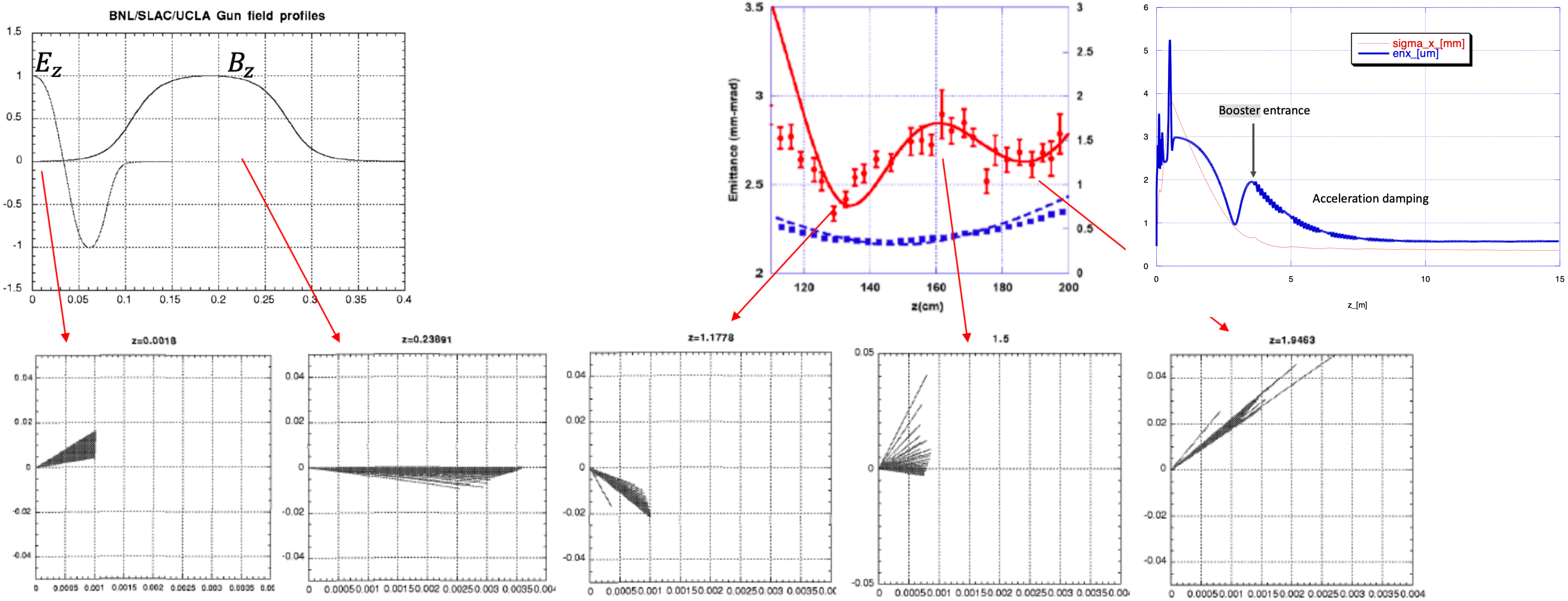
Emittance Compensation with a Short Solenoid



Courtesy of M. Ferrario

Transverse phase space at 5 different z (in m) as shown above the plots. The individual slices have zero emittance.

Emittance Compensation with a Short Solenoid



Transverse phase space at 5 different z (in m) as shown above the plots. The individual slices have zero emittance.

Injector Beam Dynamics In Practice

Field Solvers and Space Charge Codes:

RF and Magnet Design Codes: These codes model the gun cavities via time and frequency domain solvers, as well as designing the solenoid magnets.

- SUPERFISH-POISSON: free codes from LANL; 2D
- MicroWave Studio: commercial code from CST; 3D

Particle Tracking Codes: These codes integrate the macroparticle trajectories under Lorentz forces, including space charge.

- IMPACT-t: particle tracking code from LBNL
- OPAL: free parallel code from PSI
- GPT: Commercial code from Pulsar Physics
- PARMELA: free code from LANL (also commercially available as T-STEP)

Accelerator Codes:

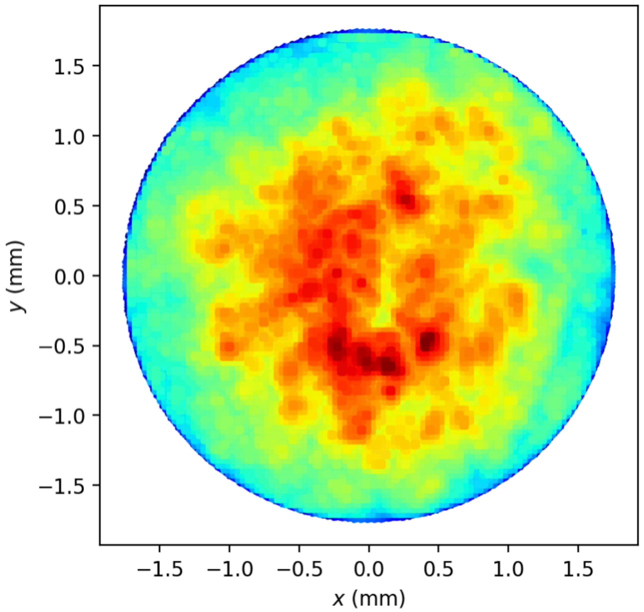
- elegant: free code from ANL
- B-MAD
- IMPACT-z

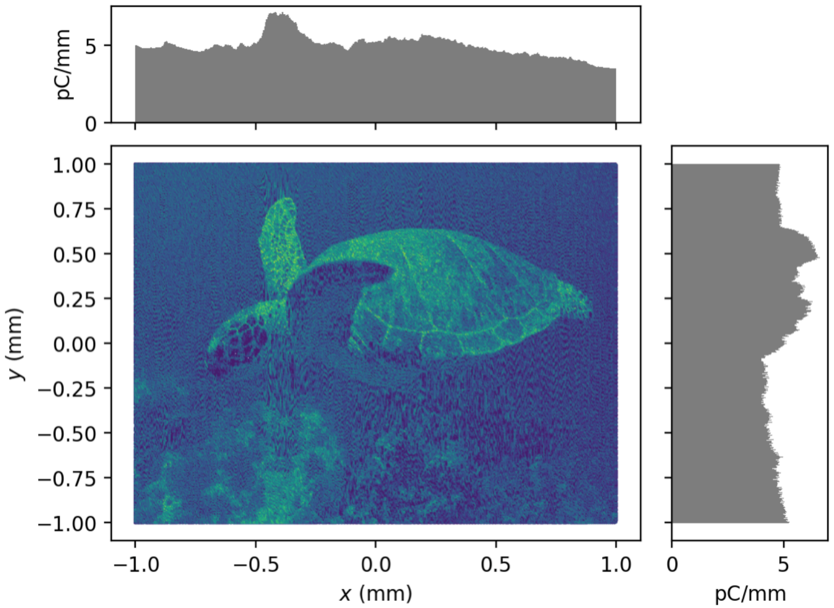
Particle Generation: Distgen

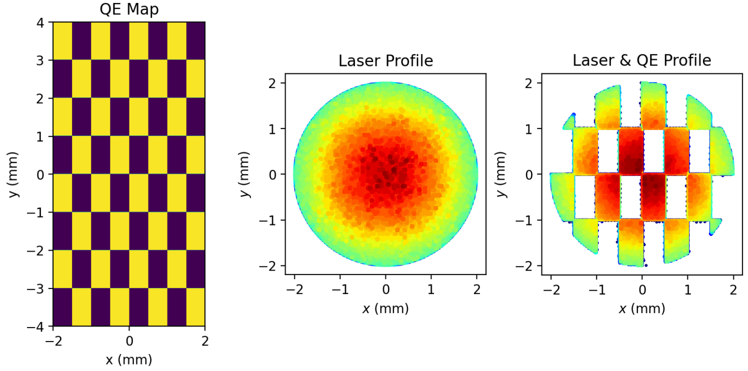
Python Package for generating wide array of useful initial particle distributions

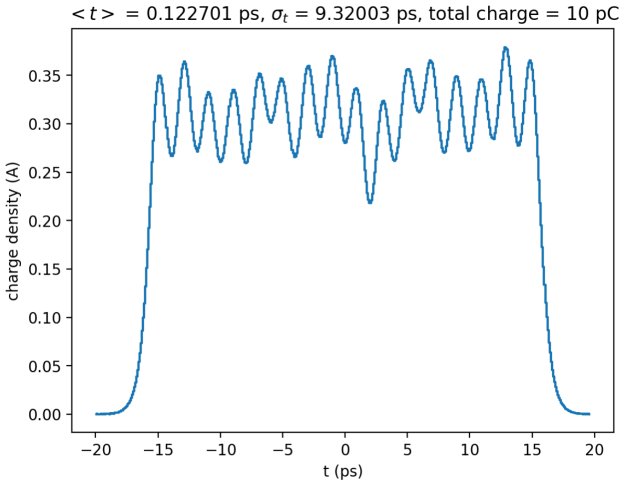
1. Many standard distribution shapes (uniform, Gaussian, etc)
2. Generate distributions from 2d images
3. User can fold in QE maps
4. Simple syntax
5. Parallelization for generating lot's of particles (>= 100M)
6. Interfaces for writing input particle files for
    1. Bmad
    2. GPT
    3. Impact-T
    4. Astra
    5. SimION

https://github.com/ColwynGulliford/distgen



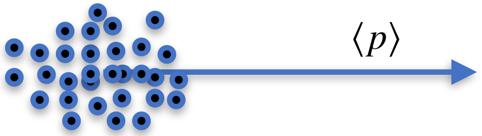




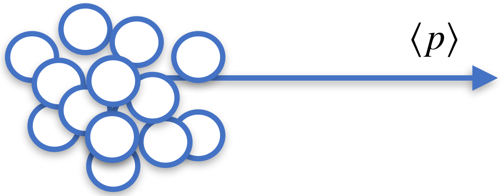


Space Charge: Simulation Basics

N interacting e- (100 pC = 625M e-)

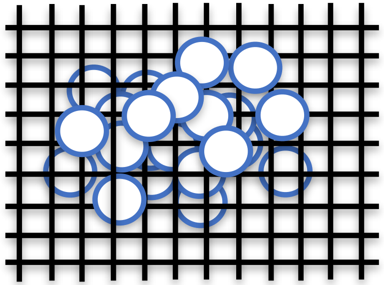


Represent with $n \ll N$ macro particles (charge:mass ratio = e/m_e)



Boost to center of momentum frame, neglect remaining velocities

Bin particles to compute charge density ρ on (3D) grid



$$-\nabla^2 \Phi = \frac{\rho}{\epsilon_0}$$

$$\vec{E} = -\vec{\nabla}\Phi$$

Boost fields back to rest frame

$$\mathbf{E} = \gamma(\mathbf{E}' - \vec{\beta} \times c\mathbf{B}') - \frac{\gamma^2}{1+\gamma}\vec{\beta}(\vec{\beta} \cdot \mathbf{E}'),$$

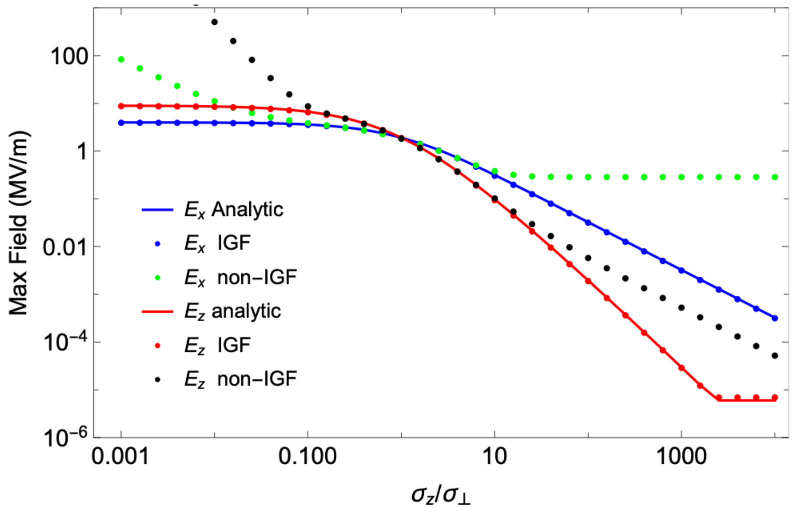
$$\mathbf{B} = \gamma(\mathbf{B}' + \vec{\beta} \times \mathbf{E}'/c) - \frac{\gamma^2}{1+\gamma}\vec{\beta}(\vec{\beta} \cdot \mathbf{B}'),$$

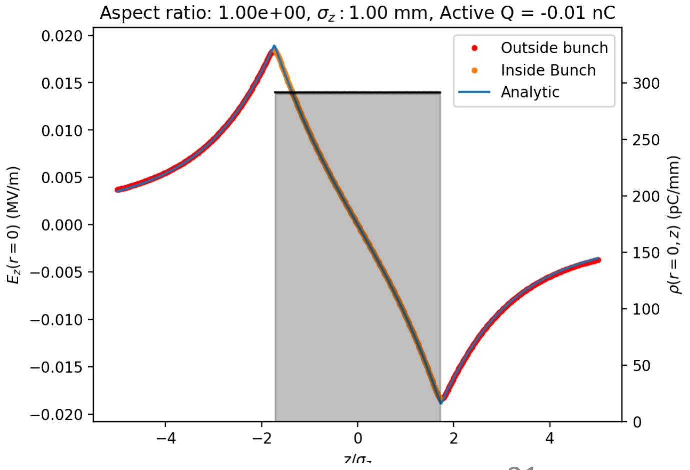
Solution often makes use of integral form of Poisson Equation, rough speaking:

$$\Phi = \int \frac{\rho(\vec{r}')dV}{|\vec{r} - \vec{r}'|} \approx \sum_{i,j,k} \frac{\rho_{ijk} dV}{|\vec{r} - \vec{r}'_{ijk}|}$$

Exploit speed of FFT!

https://journals.aps.org/prab/pdf/10.1103/PhysRevSTAB.9.044204





Multi-objective Genetic Algorithm Optimization

The dynamics in the injector are complicated:

- Cathode materials/emission models
- Non-linear collective forces from Space charge
- Solenoid dynamics, Acceleration, RF focusing
- Longitudinal dynamics
- Laser shaping

We can phrase trying to maximize the performance of the injector for an FEL a multi-objective optimization:

Given the settings of the injector (laser shape, solenoids, cavity voltages)

- Minimize transverse emittance(s)
- Maximize the bunch charge

→ Maximize brightness: $\mathscr{B} \propto \frac{I}{\epsilon_x \epsilon_y}$

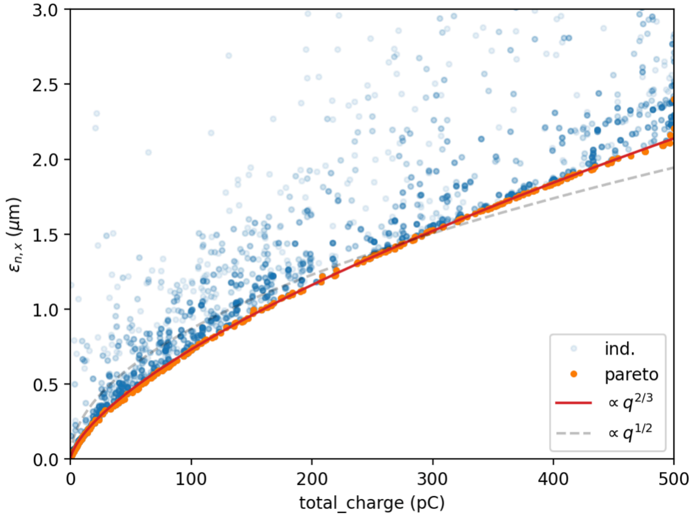
- Minimize (or constrain) bunch length
- Minimize negative effects to longitudinal phase space

Subject to the limits of the input variable and constraints like no particle loss

https://journals.aps.org/prab/abstract/10.1103/PhysRevSTAB.8.034202

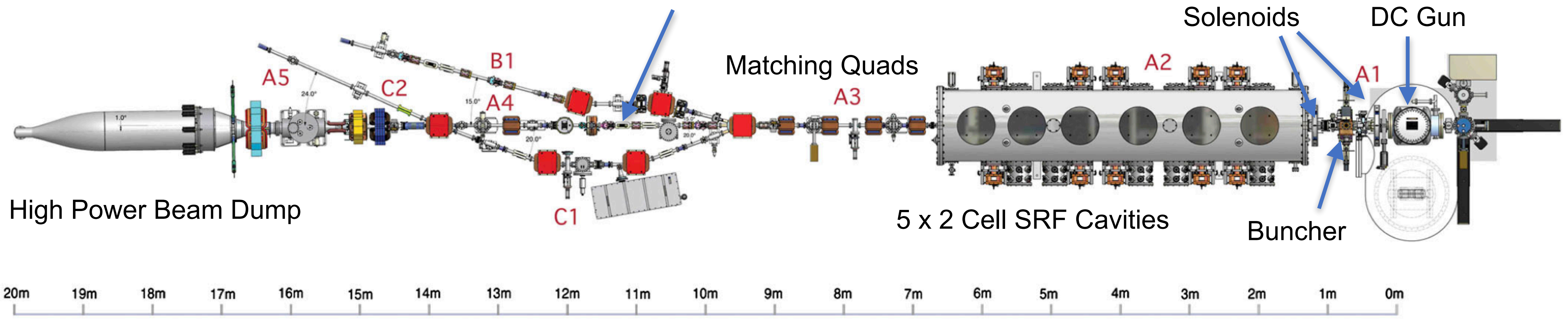
Well suited for Multi-objective Genetic Algorithms:

- Population based approach - implicit parallelization
- No derivative information necessary (direct search)
- Stochastic operators used for selection and variation of members in population to produce new solutions to try
- Map out tradeoffs between competing objectives

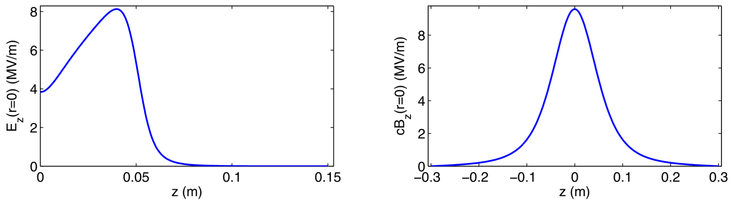


Simulation vs. Experiment

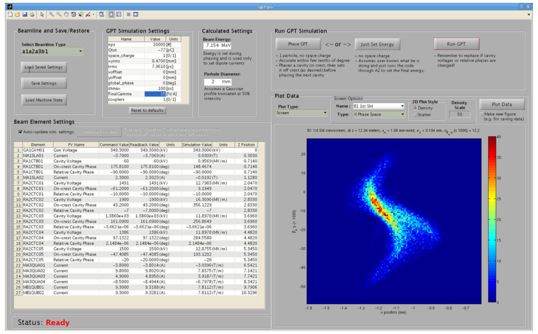
Cornell Photoinjector



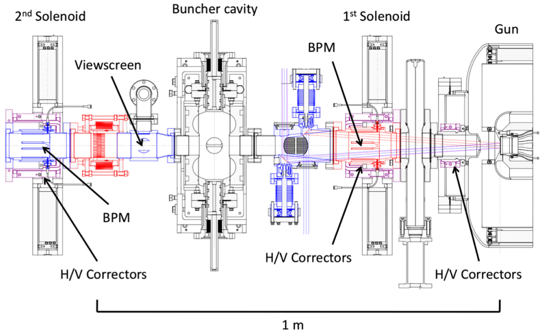
High Quality Field Map Data



Integrated Online Model



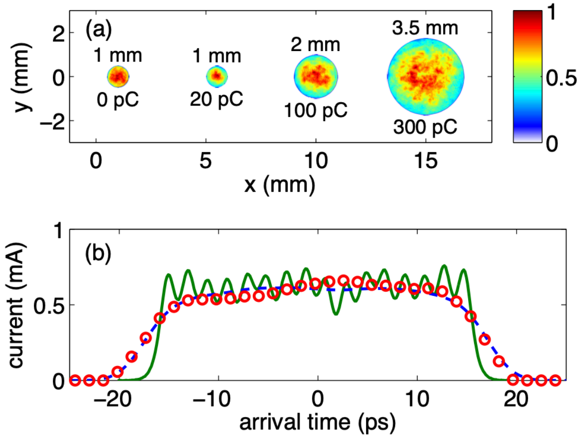
Careful calibration and alignment of optical elements

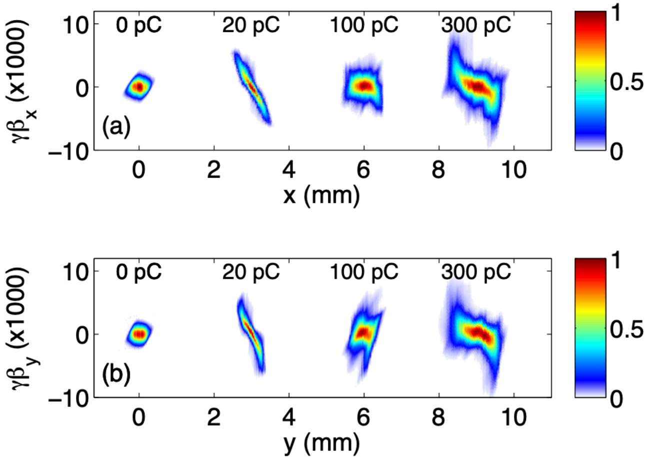


https://pubs.aip.org/aip/apl/article-abstract/106/9/094101/985161/Demonstration-of-cathode-emittance-dominated-high?redirectedFrom=fulltext

Simulation vs. Experiment

xLight SLAC XELERA

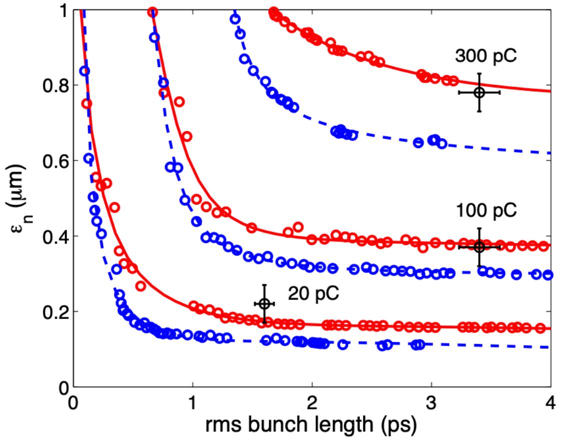


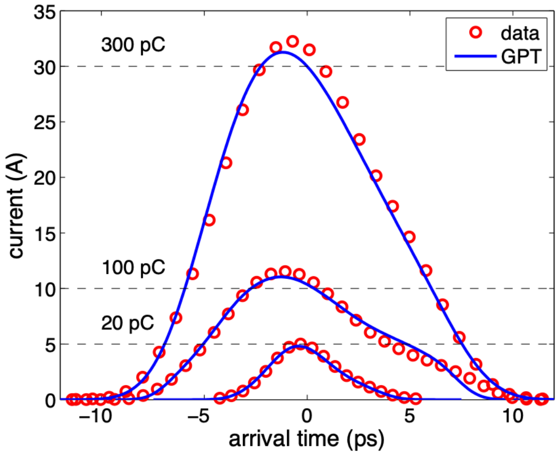


Beam Energy 9 - 9.5 MeV

(a) Horizontal (vertical) projected emittance data.

Charge	Thermal ϵ_n (μm)	95% ϵ_n (μm)	Ratio (%)
20 pC	0.12 (0.11)	0.18 (0.19)	67 (58)
100 pC	0.24 (0.23)	0.30 (0.32)	80 (72)
300 pC	0.42 (0.41)	0.62 (0.60)	67 (68)





(b) Horizontal (vertical) projected core emittance data.

Charge	Cathode $\epsilon_{n,\mathrm{core}}$ (μm)	EMS $\epsilon_{n,\mathrm{core}}$ (μm)	Ratio (%)
20 pC	0.06 (0.06)	0.09 (0.08)	67 (75)
100 pC	0.14 (0.13)	0.16 (0.16)	85 (79)
300 pC	0.26 (0.24)	0.30 (0.28)	87 (87)

https://pubs.aip.org/aip/apl/article-abstract/106/9/094101/985161/Demonstration-of-cathode-emittance-dominated-high?redirectedFrom=fulltext

Summary

- FELs want low emittance, “high charge”, short pulses

- Emittance in the injector initially set by cathode, can be further diluted
- Linear forces help preserve emittance
- Proper alignment can reduce effects aberrations
- RF focusing can cause slice emittance mismatch

- Space charge forces scale strongly with beam energy - bring beam to high energy as quick as possible
- High-brightness injector emittance is limited by space charge forces during charge extraction
- Space charge can cause emittance degradation (non-linearity and longitudinally dependent transverse focusing)
- Emittance compensation - theory for handling slice emittance mismatch due to longitudinally dependent transverse focusing from SC and RF

- In practice use high fidelity models of beam line + modern SC codes and do detailed optimizations to map out trade offs between emittance, bunch length, and energy spread
- Can achieve high quality beams, with beam emittance dominated by cathode emittance component

Outline

1. Review injector requirements - motivate emittance preservation
2. Basic Equations of Motion
3. Beam line Element Fields
    i. Off-axis expansion
    ii. Misalignment, aberrations, RF-focusing
4. Space charge
    i. Analytic model
    ii. Space charge limited emittance
5. Envelope equation and emittance compensation
6. A word on longitudinal dynamics
7. Putting it all together in practice