Molecular Dynamics Simulation of Longitudinal Space-Charge Induced Optical Microbunching

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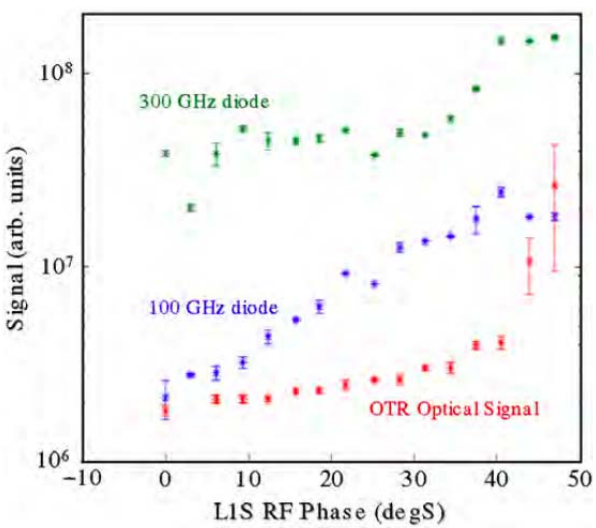
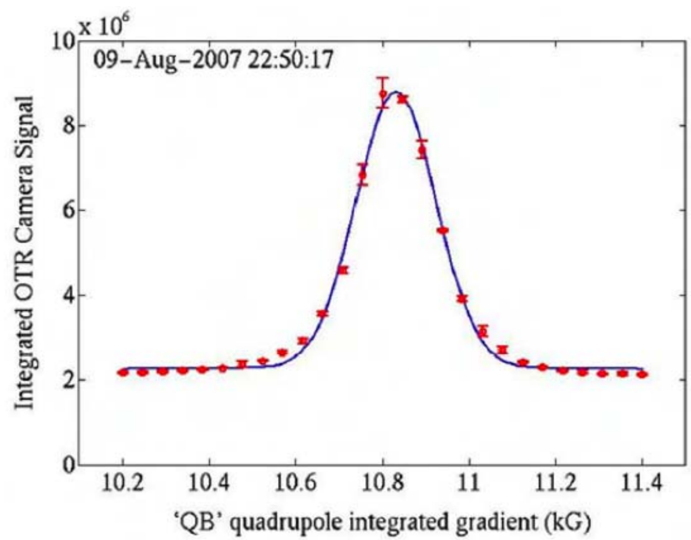
The Problem

- Observed coherent *optical* transition radiation (COTR) from FEL injector beams
- Some structure formation in beam at microscopic (<μm) level; near the mean inter-particle distance. How?
- Phenomenon related to transversal of dispersive sections
- Longitudinal and transverse spectra show stochastic behavior, 3D effects

Boundary Cond'ns: observations

- Data from LCLS, DESY FLASH, ANL, etc…
- *No COTR* upstream of bends
- Large enhancement possible after 1st bends





D. Dowell, *et al. PRST-AB* 11, 030703 (2008)

Spectral information constrains micobunching models: FLASH example

- High resolution COTR exp'ts reported
  - FEL 2008, FEL 2009, by Schmidt, *et al.*
  - Multi-spike spectra
  - Transverse imaging indicates *not* simple 1D bunching

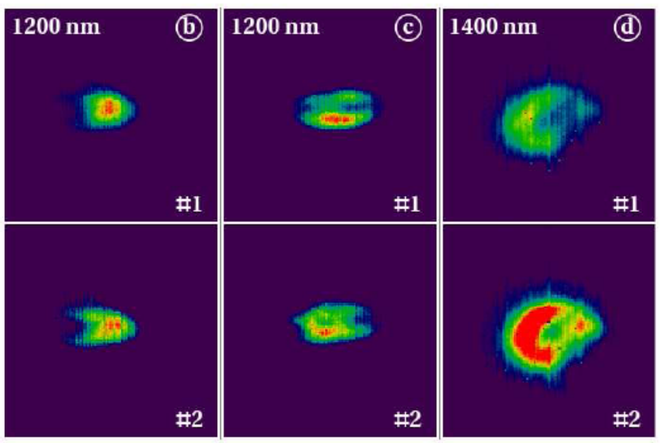


Figure 7: Selection of transverse profiles at different on-crest configurations and various spectral filters. The dimensions of the images are 2×2 mm^2

Schmidt, et al., FEL 2009 (WEPC50)

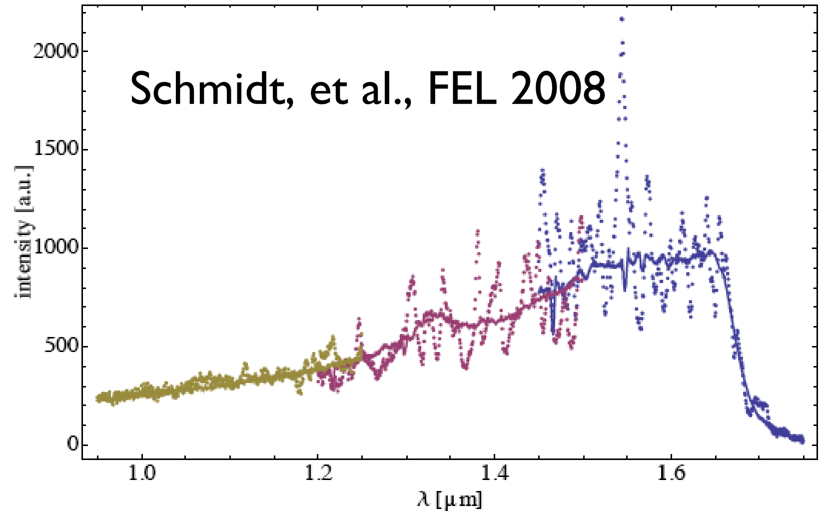
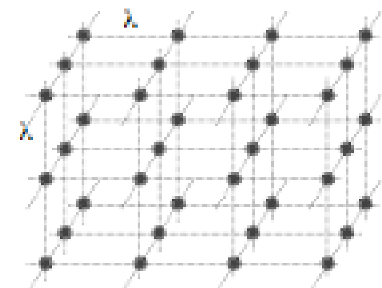


Figure 7: Single shot (dots) and averaged (line) CTR spectrum between 0.95 μm and 1.7 μm measured with a commercial InGaAs spectrograph. The response of the detector is basically flat between 1.0 μm and 1.7 μm.

Interesting limit for beam organization: crystalline beams

- Emittance dominated beam: gas
- Space-charge dominated beam: liquid
- Coulomb (Wigner) crystal: solid
- Density $n = \lambda^{-3}$
- Compare ratio of
  - Potential energy $qV \propto e^2/\lambda = e^2 n^{-1/3}$
  - Kinetic energy $k_B T \propto m_e \omega_p^2 \delta x^2$
- Crystal formed when $\Gamma \equiv qV/k_B T \propto (\lambda/\delta x)^2 >> 1$
- Evaluate in rest frame $\Gamma = \dfrac{e^2 n_b^{1/3}}{k_B T}$



Can we have 1D crystal conditions in photoinjector?

- Transverse focusing gives higher temperatures Γ small and time dependent conditions
  - No transverse crystallization possible
- Longitudinal 1D crystal OK
  - Observed in storage rings
  - Schottky spectral signature: noise suppression, spectral spikes near crystal λ
  - Still have Γ too small at linac entrance
    - Overtaking of particles in ζ possible
  - Acceleration produces rapid cooling
    - In lab frame, $k_B T_z$=2 keV, but at LCLS linac exit, rest frame $k_B T_z$=8 eV…
    - In lab frame: "freezing" of longitudinal motion
    - At linac exit λ ~ 800 nm, rest frame $\Gamma \approx 300$

Analytical Models

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THREE-DIMENSIONAL ANALYSIS OF LONGITUDINAL SPACE CHARGE MICROBUNCHING STARTING FROM SHOT NOISE*

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"Collective-Interaction Control and Reduction of Optical Frequency Shot Noise in Charged-Particle Beams"
A. Gover and E. Dyunin
Phys. Rev. Lett. 102, 154801 (2009)

Quasicrystalline Beam Formation in RF Photoinjectors

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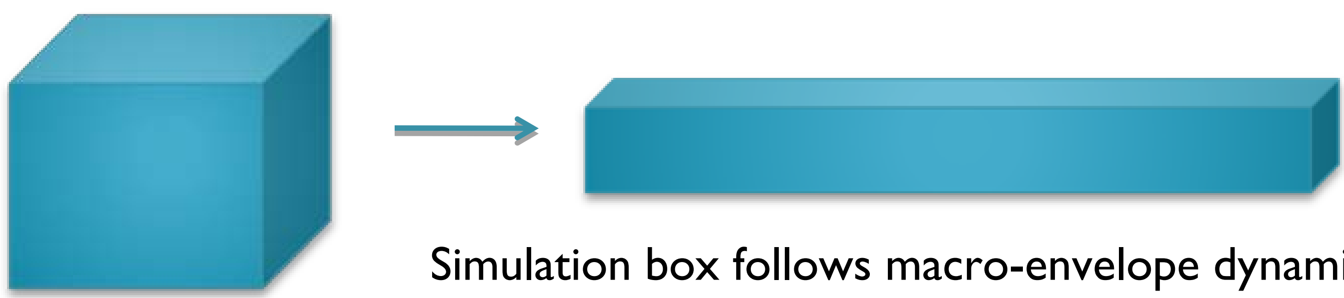
Molecular dynamics simulations

- Resolution well below λ needed
- Like to have full beam 3D geometry
  - Computationally intensive
- "Rest frame" quasi-electrostatic analysis
    - Transverse, longitudinal focusing
    - Macro-space-charge defocusing
    - Longitudinal "stretching" due to acceleration
    - Fourier approach to μ-scopic fields
- 1[st] pass: use deformable box for beam center 1E4 electrons, widths 10-50λ

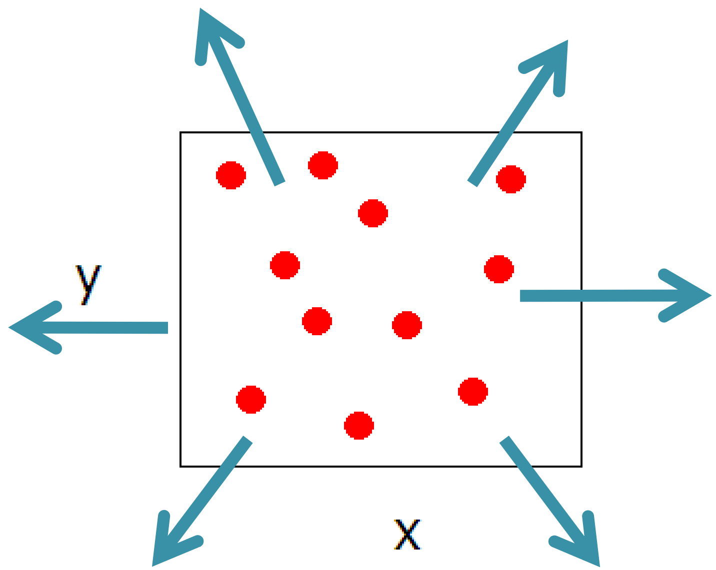


Simulation box follows macro-envelope dynamics

Periodicity in 3D for High Resolution Simulations

We are interested in simulating only a fraction of the beam to obtain high resolution.

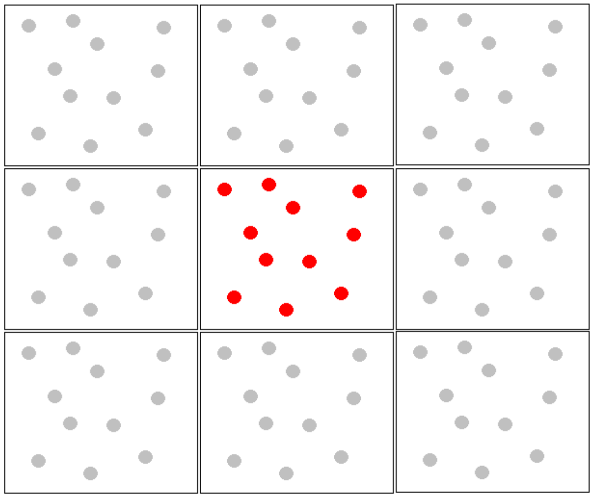
To enforce the right shot-noise statistics and particle to particle coulomb interaction, each particle is associated with a single electron.



An unphysical outward pressure would cause the beam to expand if only a small fraction of the beam was included

Periodicity in 3D for High Resolution Simulations

By imposing periodicity in 3D we avoid beam expansion in transverse dimension. Electrons behave as if they were in the center of the beam!

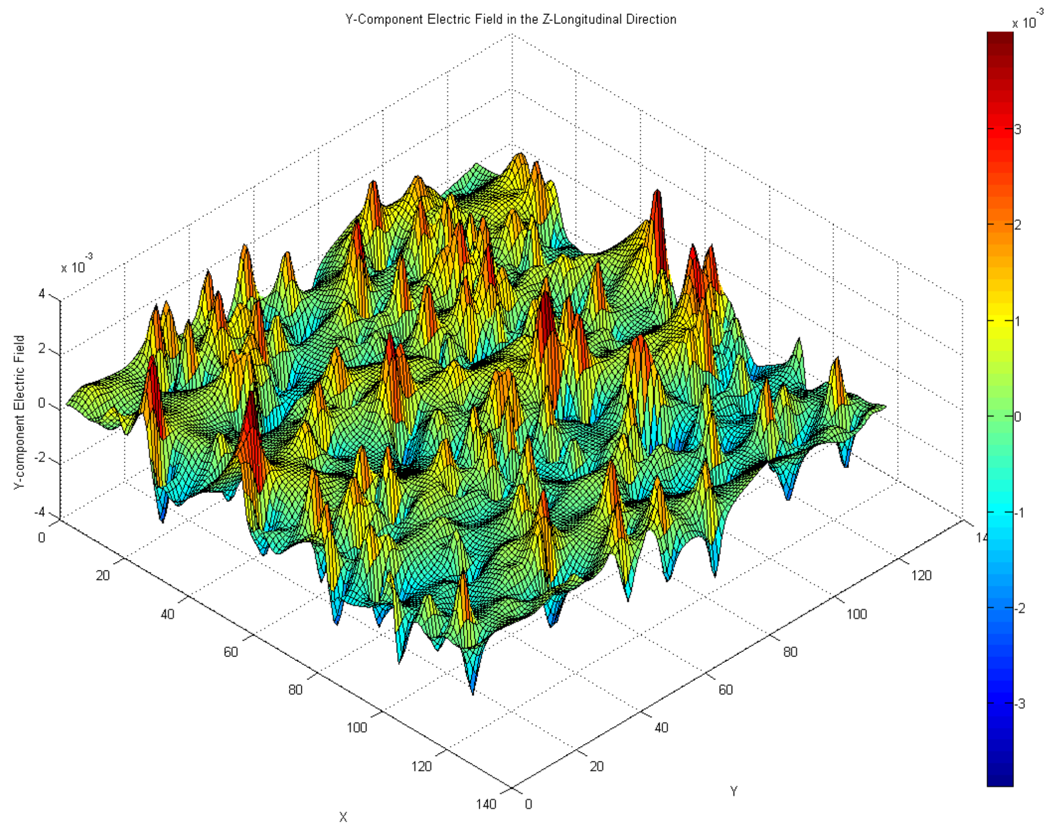


Periodicity arises naturally using Fourier methods for space-charge force calculation.

Field calculated in the rest frame and then Lorentz-transformed back to the Lab Frame

$$\rho\,(\vec{x}) \xrightarrow[\text{FFT}]{} \tilde{\rho}\,(\vec{k}) \longrightarrow \tilde{E}(\vec{k}) = \frac{i\vec{k}\,\tilde{\rho}\,(\vec{k})}{k^2} \xrightarrow[\text{IFFT}]{} \vec{E}\,(\vec{x})$$

Periodic field solver using standard Fourier methods



Example: E_y as a function of x and z

Macroscopic Motion

X and Y sides of the box evolve through the macroscopic envelope equation leaving the ratio of boxSize/σ_x constant:

$$\sigma_r''(\zeta, z) + \left(\frac{\gamma'}{\gamma(z)}\right)\sigma_r'(\zeta, z) + \frac{\eta}{8}\left(\frac{\gamma'}{\gamma(z)}\right)^2 \sigma_r(\zeta, z) = \frac{r_e \lambda(\zeta)}{\gamma(z)^3 \sigma_r(\zeta, z)}$$

Head and tail of the box follow equations of motion in RF bucket.

Solenoid and RF focusing, acceleration as well as macroscopic beam self-force are also included in the equuations of motion of the particles.

Range of Applicability

-Restriction to a small fraction of the beam requires quasi-laminar flow (no transverse mixing).

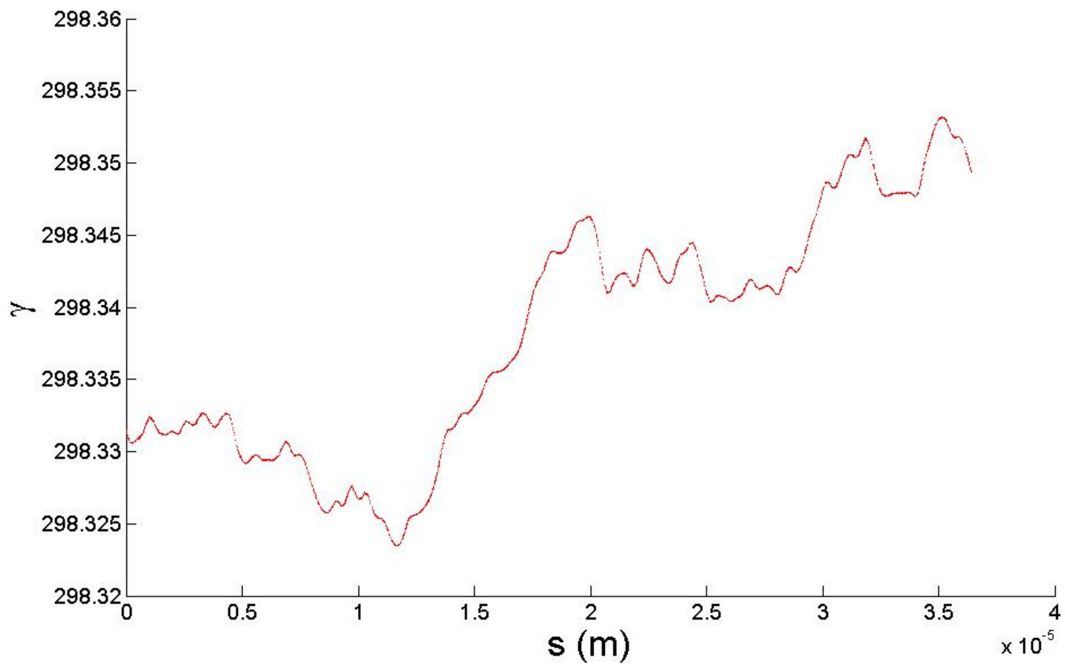
-Periodicity requires observation of wavelengths in the rest-frame smaller than the longitudinal and transverse sizes of the beam. (full-filled for optical and sub-optical microbunching).

Example: SPARC-like (LCLS with solenoid focusing)

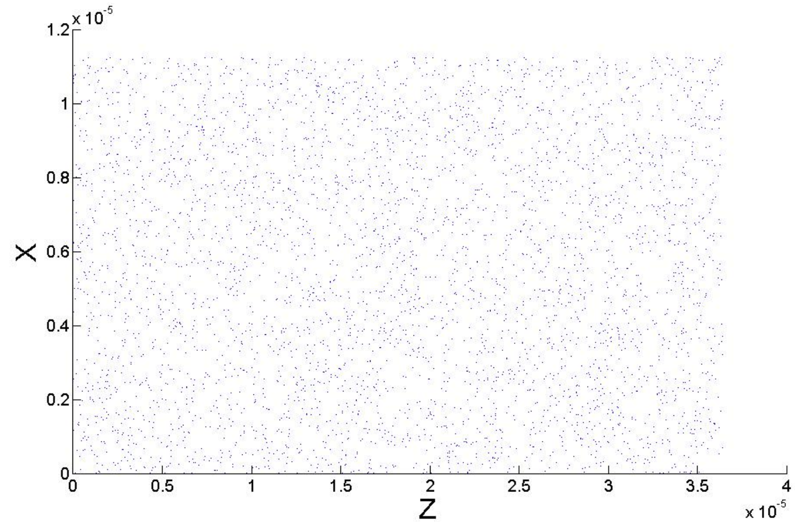
Simulation parameters:

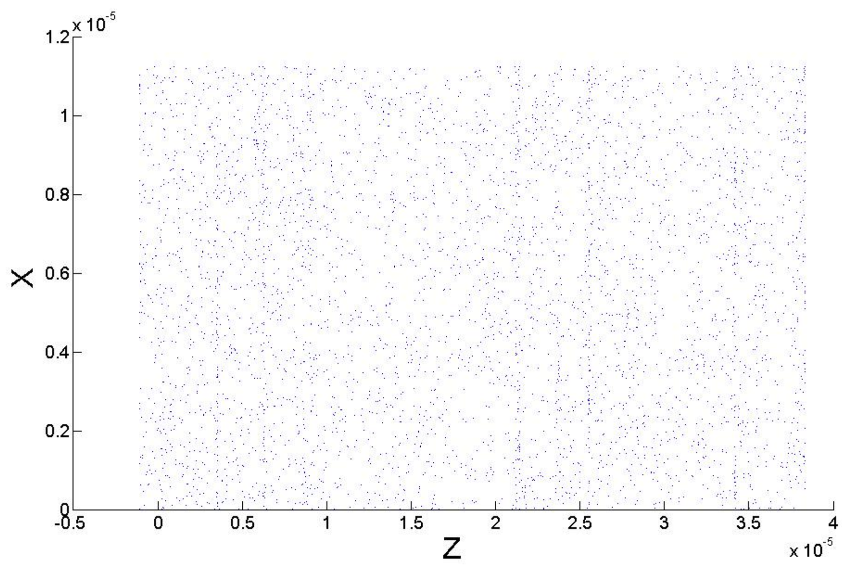
- 1nC, 100 Amps beam,
- Invariant envelope propagation
- No initial energy spread.
- 4000 particles
- 128 x 128 x 512 grid points (260 gridpoints/particle!)

Longitudinal Phase Space After 150 MeV Acceleration



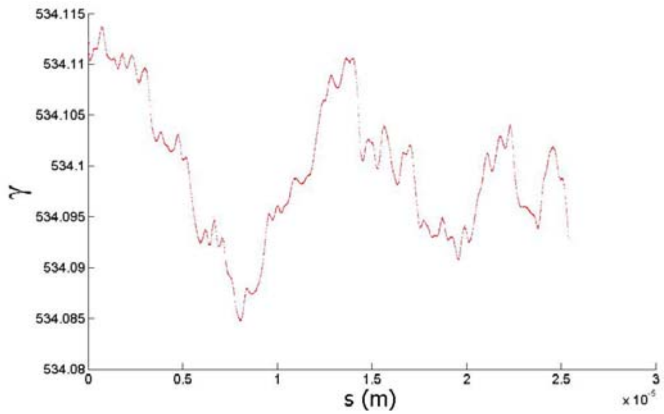
Trace Space Before and After R56

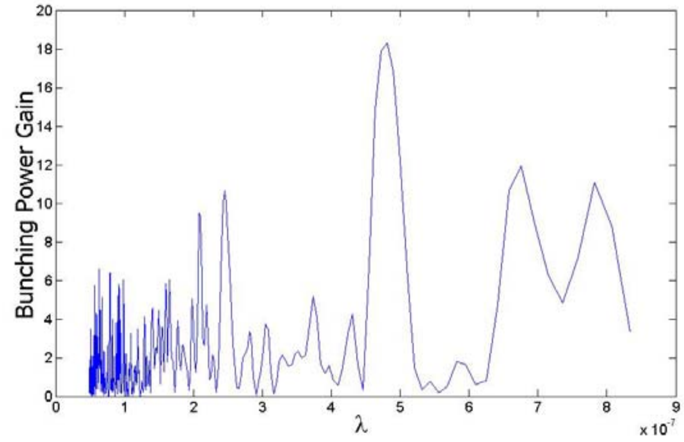


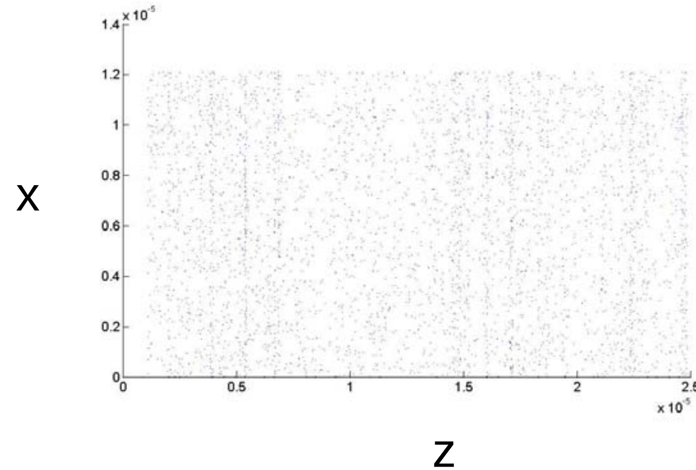


Optical
Microbunching!

LCLS-Like Case, Microbunching After BC1 for the 250 pC Beam



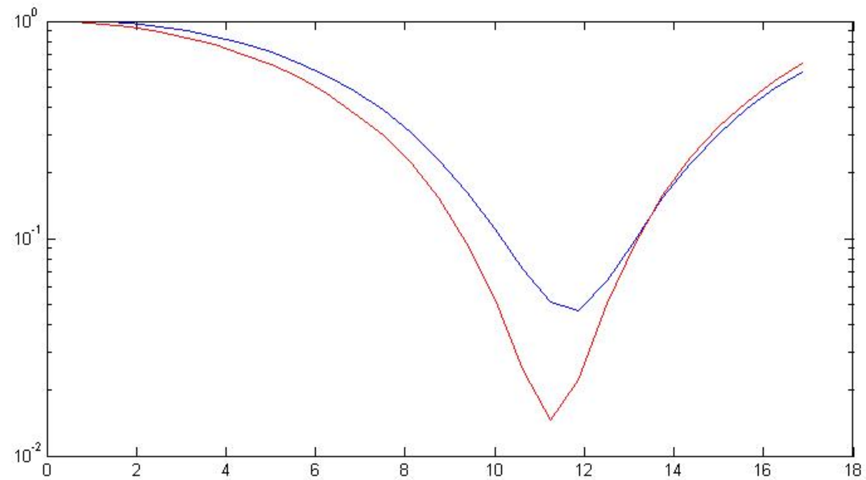




Application of code to noise reduction ?

- The results are in good agreement with the theory for the value of the plasma oscillation period.
- Some macroscopic 3D effects are missing (suppression of collective behaviours at short wavelengths should limit the shot-noise reduction. At optical wavelengths. Abusing starting assumptions for periodicity?).

Normalized noise power within optical bandwidth



z (m)

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Code limitations and extension

- Periodic boundary conditions limit transverse beam structure resolution to box-size
- Need to understand transverse structure
  - Also in COTR data (virtual photon analysis)
- Extend to full beam size transversely
  - Large memory demand for particles
  - Use Hermite-Gaussian mode analysis for fields
  - Implement soon