Massively Parallel Simulation of Radiation Phenomena using a Lienard-Wiechert Approach

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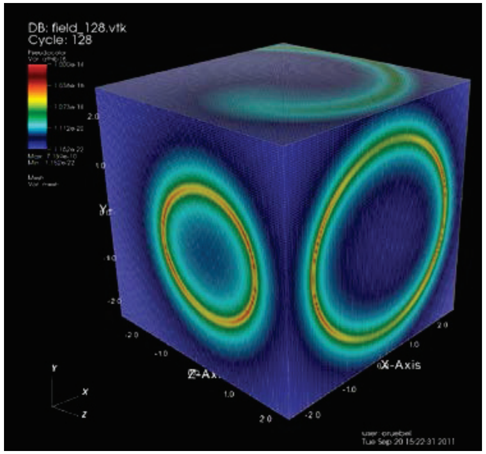
Outline

- Motivation
- Brief code overview
- Applications
- Conclusions

Why develop a massively parallel Lienard-Wiechert code?

- A tool of discovery
  - explore radiative phenomena
  - test novel concepts
- A benchmarking tool
  - explore limits of simplified models and validity of new algorithms
- An enabling tool
  - simulate things that existing codes cannot
- A design tool
  - optimize beamlines for next-generation accelerators



Dipole CSR (O. Ruebel and R. Ryne, LBNL)

L-W codes have been developed before. What's new?

- Massive parallelism enables
  - real-world # of particles
    - shot noise effects
  - 3D effects
  - very high resolution
    - microns to sub-nanoscale

Massive Parallelism
+
Advanced Algorithms

→

transformative tool for multi-physics modeling including radiation

Overview of the parallel L-W solver

- Given N particles whose coordinates $\zeta_j=(x,\gamma\beta_x,y,\gamma\beta_y,z,\gamma\beta_z)$ are known at a number of previous times, t_k
- Find the EM fields produced by the particles at time t

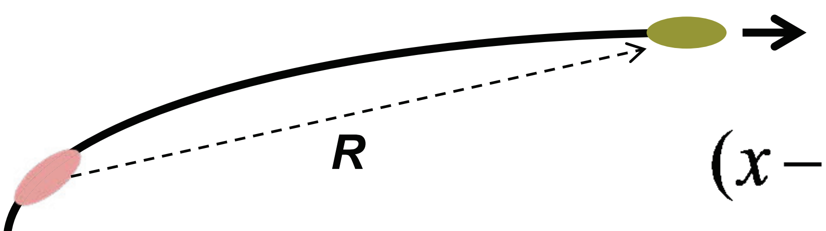
$$\boldsymbol{E}=\frac{1}{4\pi\varepsilon_0}\left[\frac{q}{\gamma^2\kappa^3R^2}(\boldsymbol{n}-\boldsymbol{\beta})+\frac{q}{\kappa^3Rc}\boldsymbol{n}\times\left((\boldsymbol{n}-\boldsymbol{\beta})\times\frac{\partial\boldsymbol{\beta}}{\partial t}\right)\right]$$

$$\boldsymbol{B}=\frac{1}{c}\boldsymbol{n}\times\boldsymbol{E}$$

$$\boldsymbol{\beta}=\mathbf{v}/c$$

$$\boldsymbol{n}=\boldsymbol{R}/|\boldsymbol{R}|$$

$$\kappa=1-\boldsymbol{n}\cdot\boldsymbol{\beta}$$



[…] denotes quantities evaluated at the retarded time

$$(x-x_r)^2+(y-y_r)^2+(z-z_r)^2=c^2(t-t_r)^2$$

R points from the radiating particle's position at the retarded time to the observation point at the observation time

L-W solver:
Key numerical/computational ingredients

For each observation point, retarded quantities of every particle are found through bisection, tracking & iteration

- Parallel implementation to handle $O(10^9)$ particles & their history
- Robust numerical integrator w/ adaptive step size (dop853, E. Hairer, G. Wanner)
- Brent's method
- Occasional double-double precision (D. Bailey)

Strictly particle-based approach:

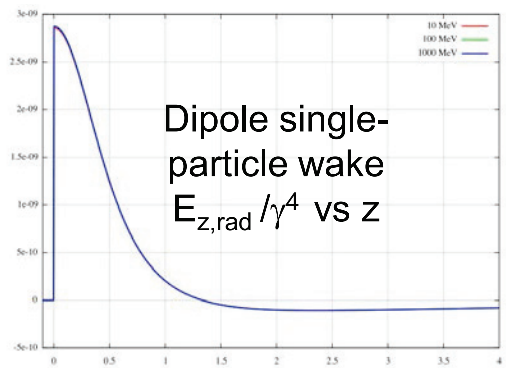
- For each observation point, $$\sum_{\substack{\text{all particles}\\\text{on all cores}}} \frac{1}{4\pi\varepsilon_0}\left[\frac{q}{\gamma^2\kappa^3R^2}(\boldsymbol{n}-\boldsymbol{\beta})+\frac{q}{\kappa^3Rc}\boldsymbol{n}\times\left((\boldsymbol{n}-\boldsymbol{\beta})\times\frac{\partial\boldsymbol{\beta}}{\partial t}\right)\right]$$

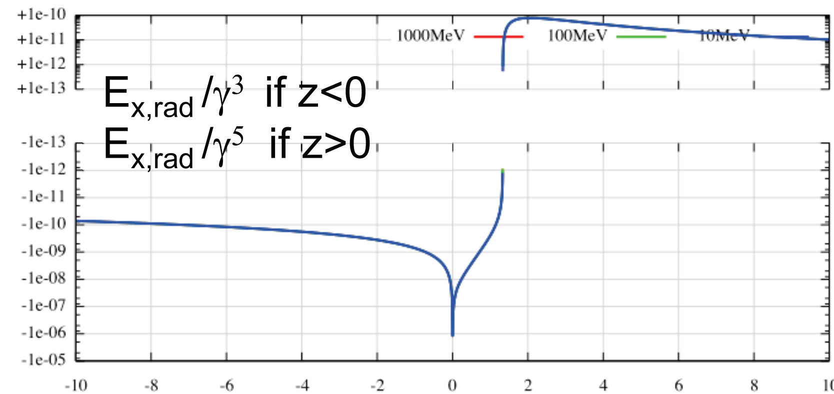
Convolution-based method:

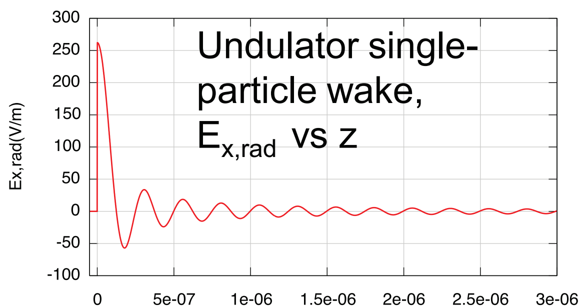
- Parallel FFT (S. Plimpton)
- Domain decomposition
- serial FFT

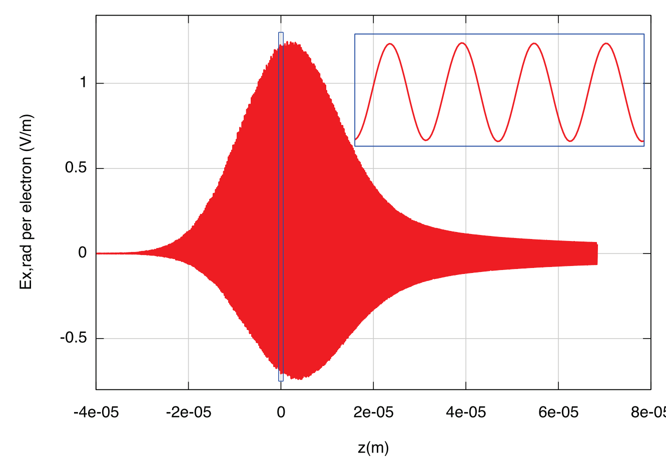
Status of the 3D Lienard-Wiechert Code (CSR3D)

- Run on Hopper, Edison (NERSC), Mustang (LANL), Mira (ANL)
- Compared w/ theory & codes
- Initial focus on dipole CSR
- Now able to model general beamlines, e.g undulators
- Starting to add dynamics







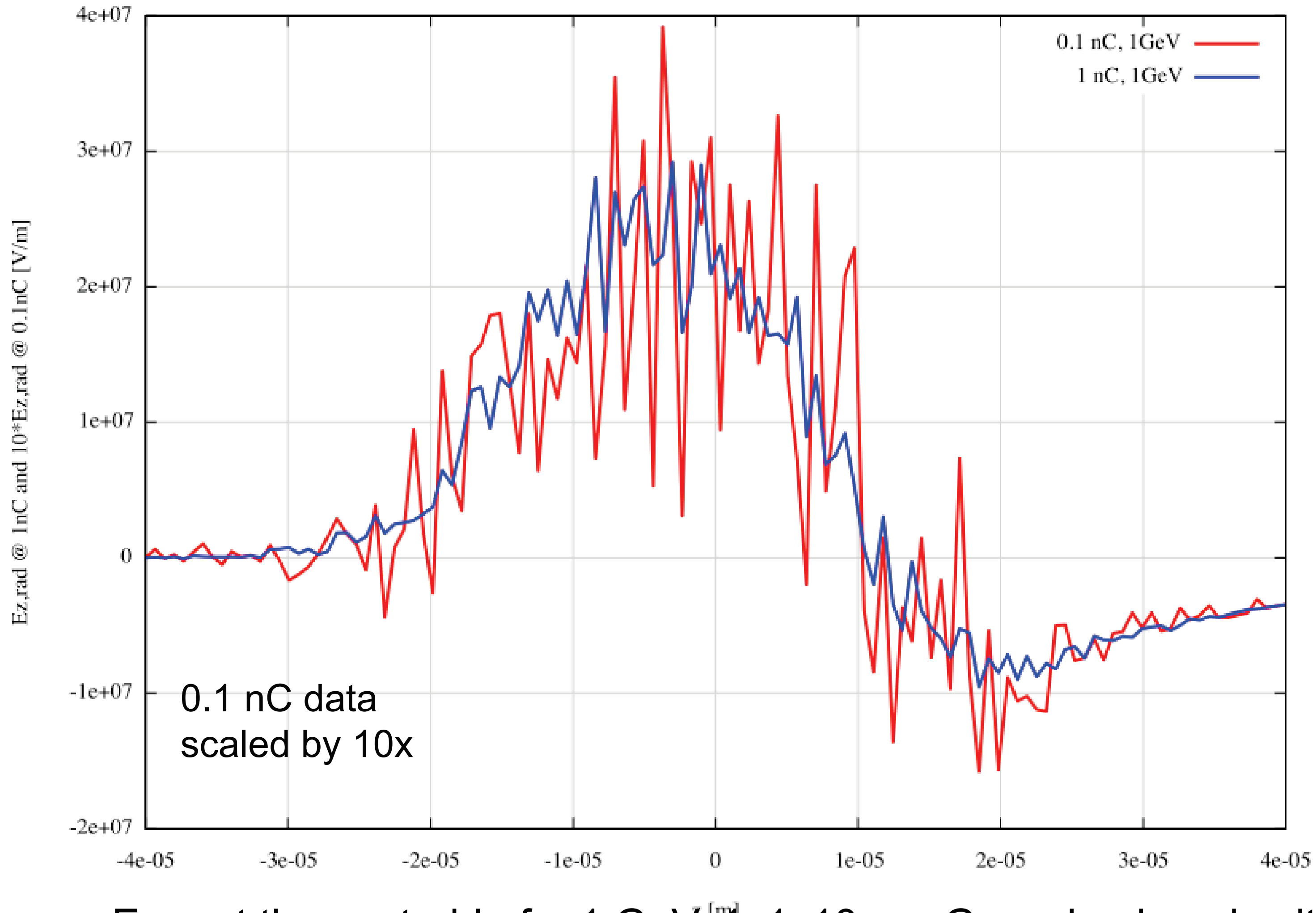


Undulator radiation from a modulated Gaussian bunch

Selected Applications

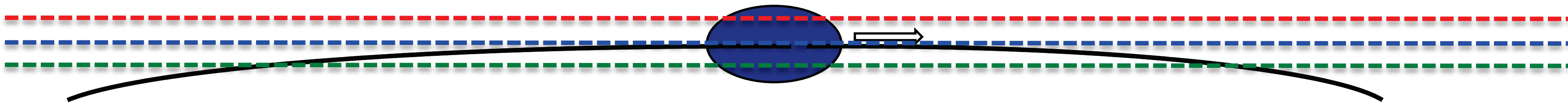
- Steady-state CSR in dipoles
  - Shot noise
  - Microbunching enhancement
  - 3D effects
  - Dynamics: Energy diffusion
- Undulator radiation
  - single-particle wake
  - multi-particle simulation results

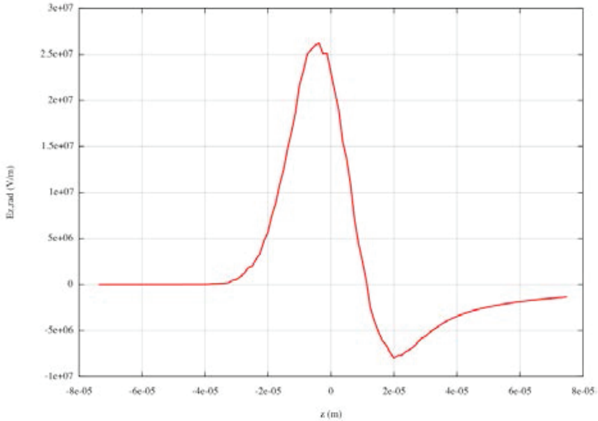
CSR shot noise in dipoles (ρ=1 m) 0.1–1 nC @ 1GeV : Large physical fluctuations



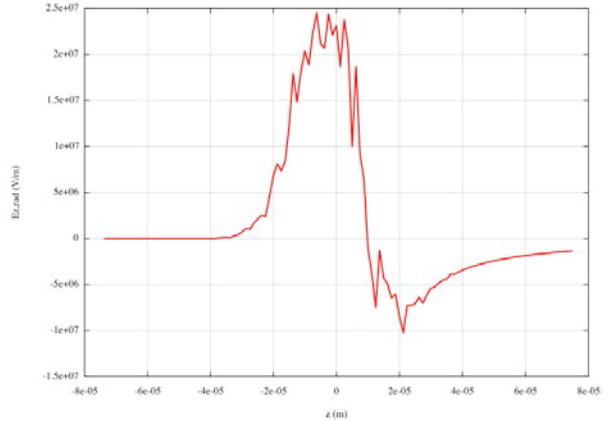
$E_{z,rad}$ at the centroid of a 1 GeV, 1x1x10 μm Gaussian bunch with # electrons = 624 million (0.1nC) and 6.24 billion (1 nC)

We discovered that CSR dipole fluctuations are position-dependent

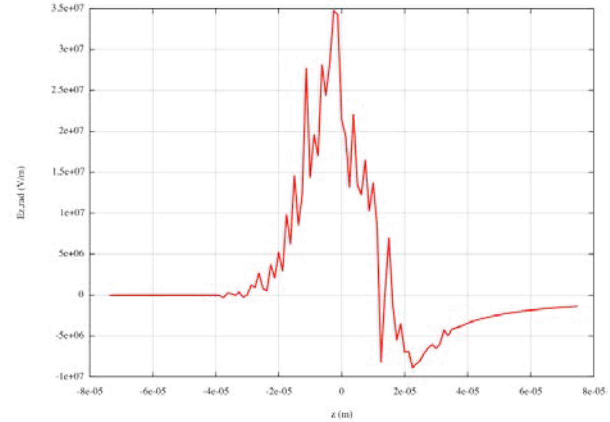




lineout at x=-2 σ_x

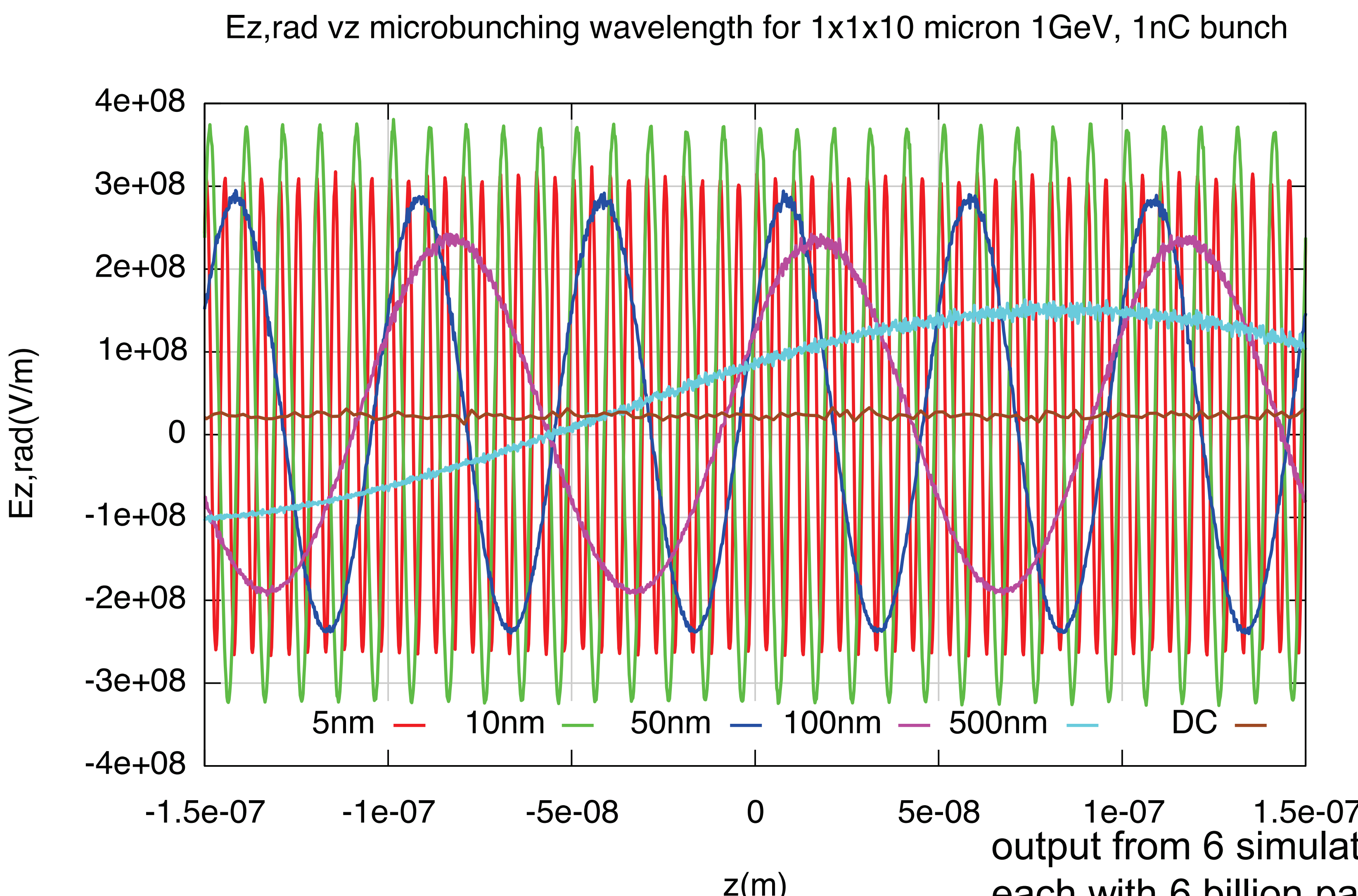


lineout at x=0



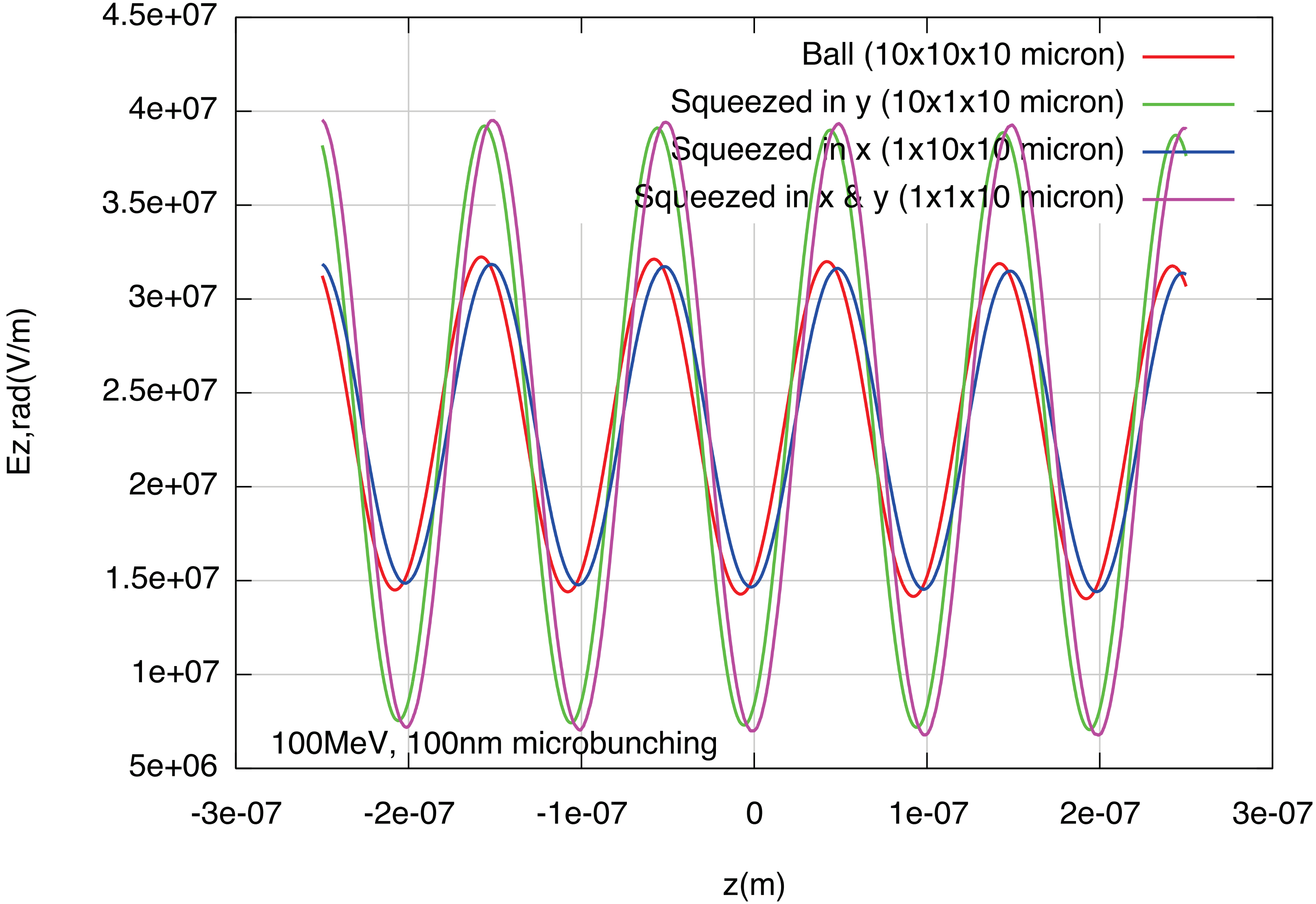
lineout at x=+2 σ_x

CSR enhancement in bunches with a microbunched modulation

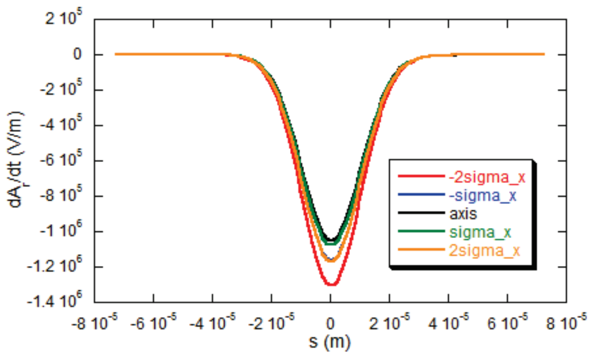


output from 6 simulations, each with 6 billion particles

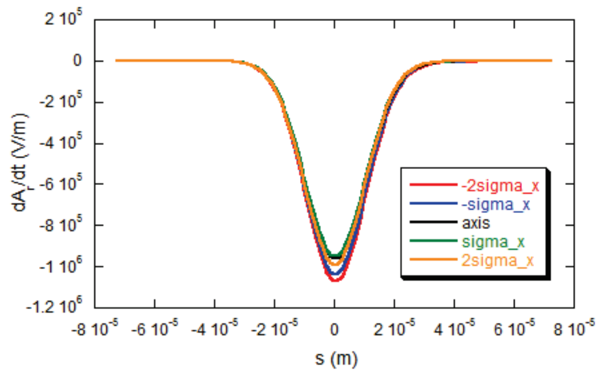
3D effects: sensitivity to vertical bunch size



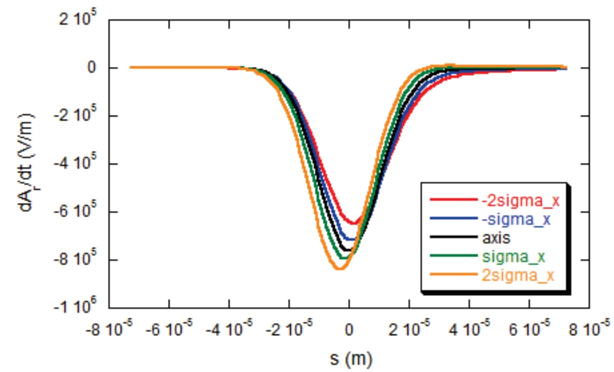
First ever calculation of convective derivative term; can produce significant emittance growth comparable to that from CSR



cigar



ball



disk

$$-e\frac{dA_r}{dt} = \left(F_{r,rad} - e\frac{v_\theta}{r}A_\theta\right)$$

$$\Delta\varepsilon_n = \frac{F_{net,rms}\alpha R}{mc^2}\sigma_x \qquad \Delta\varepsilon_n = \frac{F_{z,rms}\alpha^2 R}{2mc^2}\sigma_x$$

$$\ddot{x} = -\frac{v_\theta^2 x}{R^2} + \frac{e}{\gamma_0 Rm}\left(\left(-\beta_\theta^2\phi + v_\theta A_\theta\right) + \beta_\theta^2\int\left(\dot{\phi} - v_\theta\dot{A}_\theta\right)dt + R\frac{\partial}{\partial x}\left(-\phi + v_\theta A_\theta\right) - R\frac{dA_r}{dt}\right)$$

geometrical focusing

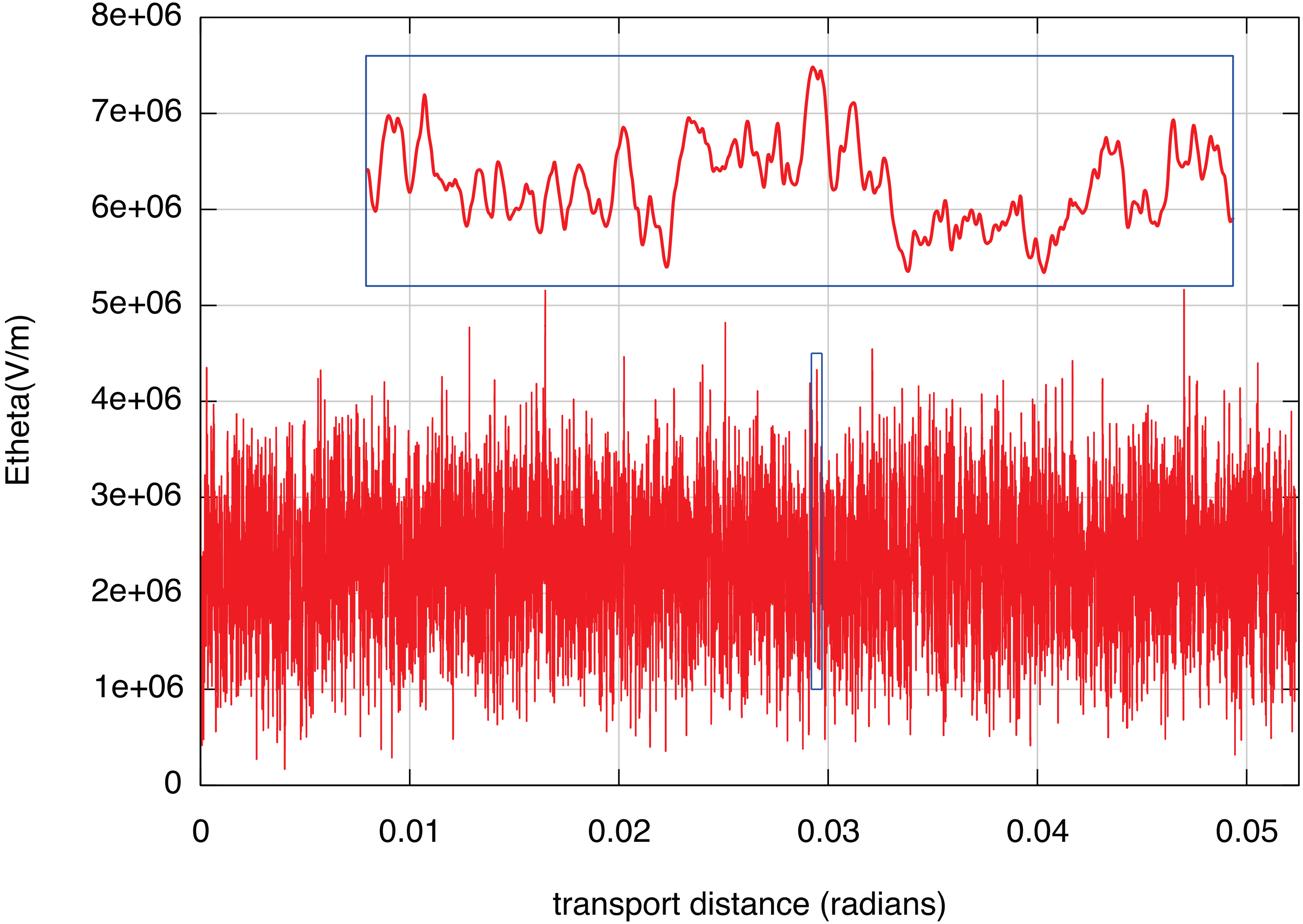
Cancelation of CSCF and potential depression

CSR term from potential depression

“usual” space-charge forces

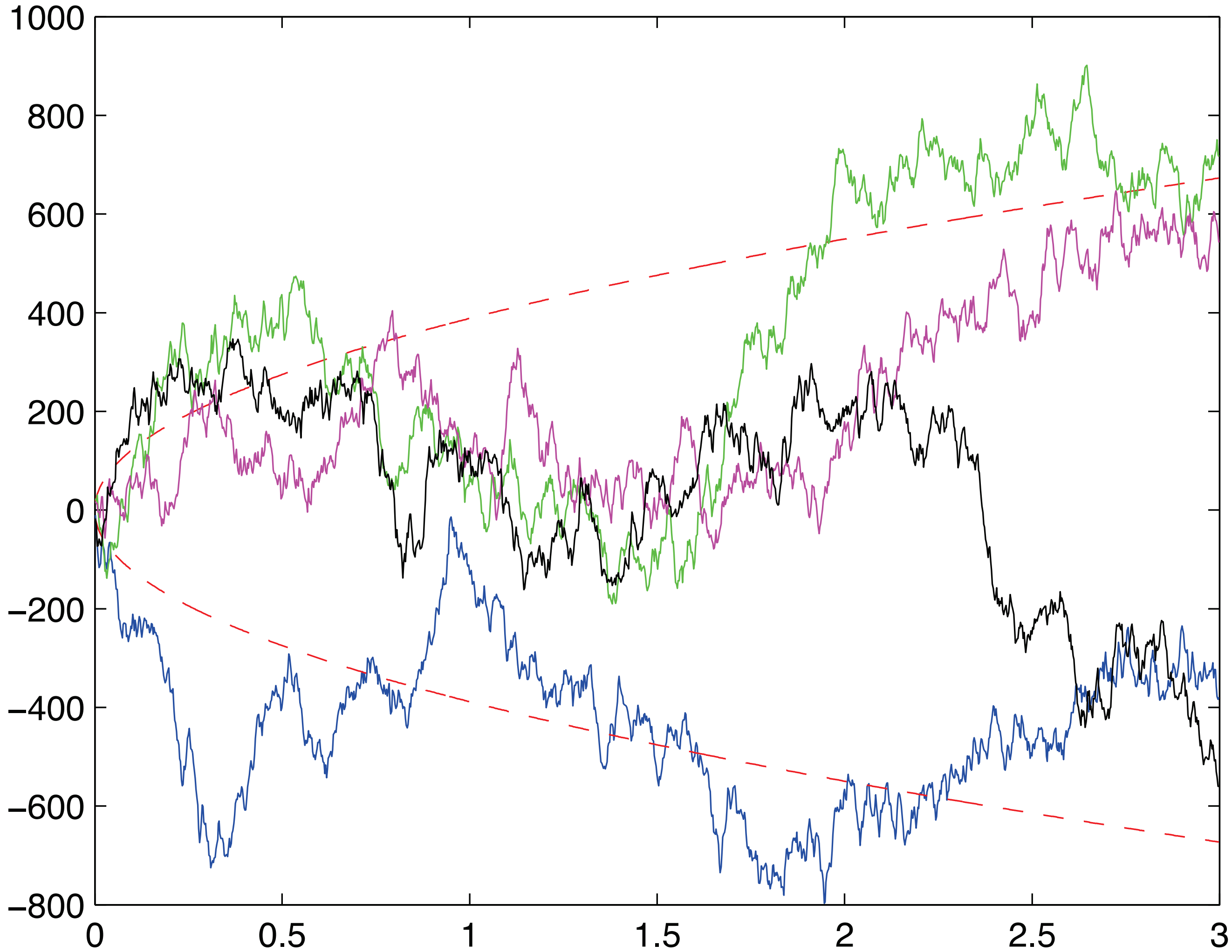
Convective radiation term

Influence of shot noise on energy diffusion



E_θ at the center of Gaussian bunch w/ 6 billion particles

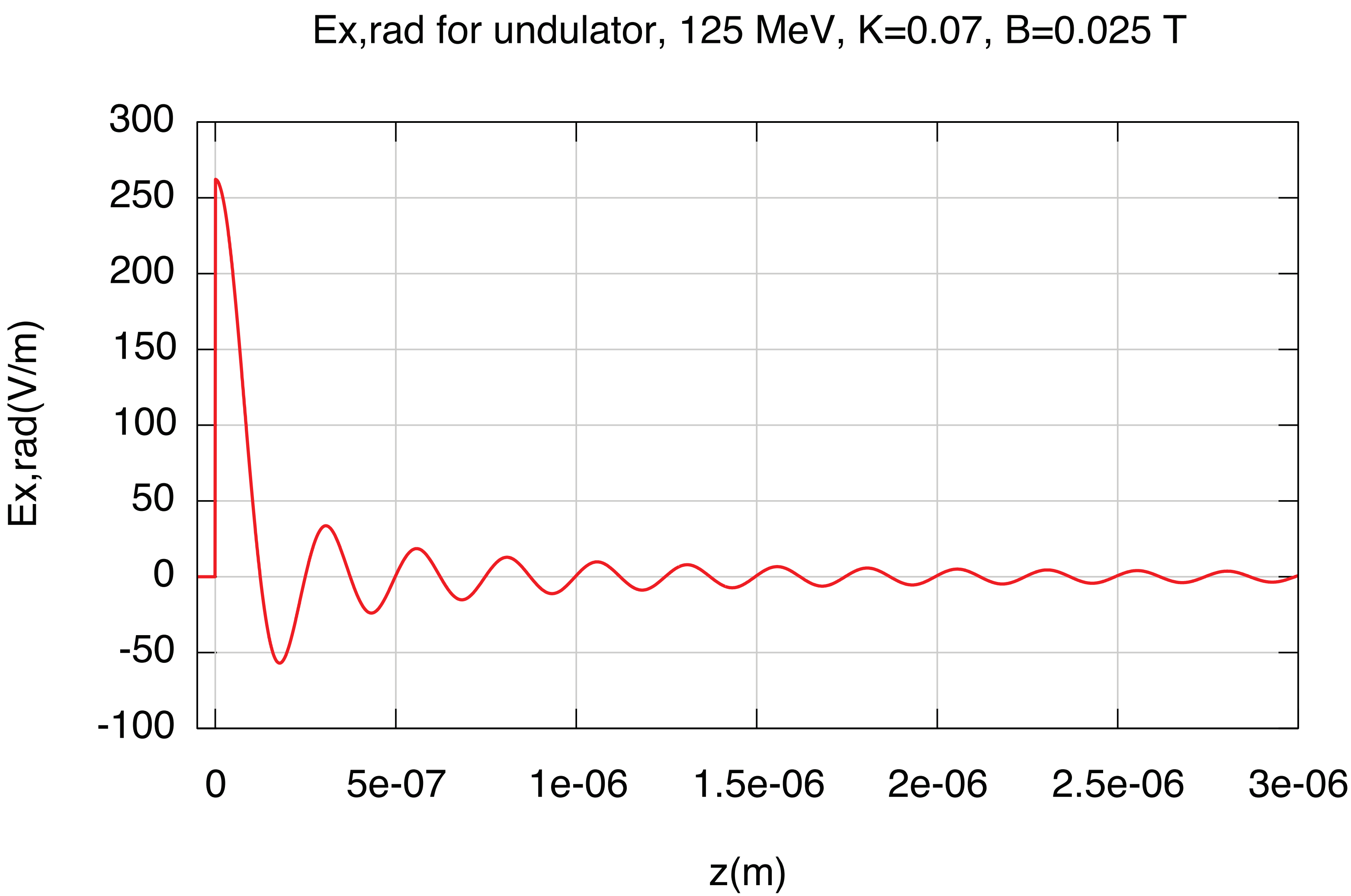
Energy diffusion, cont.



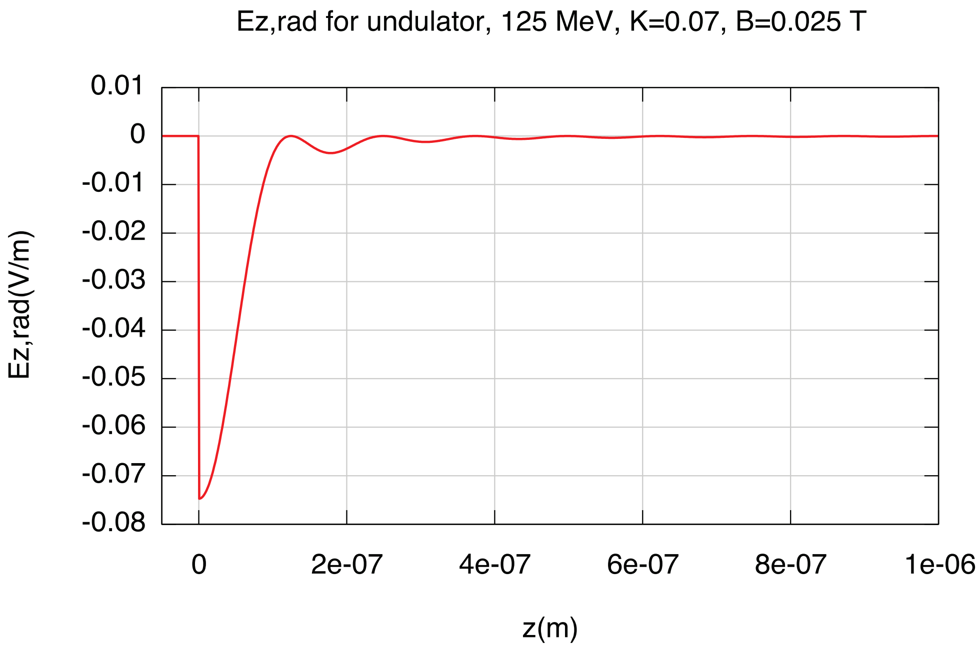
Example: Radiation in a Planar Undulator

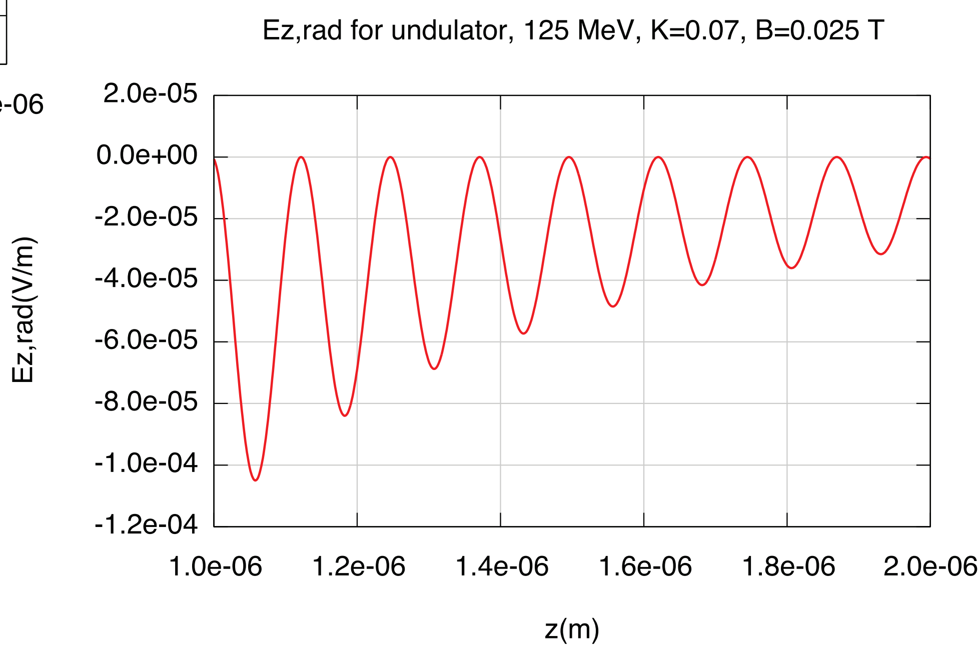
- $B = B_0 \sin(k_{wig}\, z)$
- $\lambda_{wig} = 3$ cm
- Two cases:
  – E=125 MeV, $B_0 = 0.025$ T ➔ $K_{und}=0.07$, $\lambda_{rad}=0.25\mu m$
  – E=14 GeV, $B_0 = 1.4$ T ➔ $K_{und}=3.64$, $\lambda_{rad}=0.15nm$

Transverse single-particle radiation wake (K=0.07): Ex,rad tabulated on the z-axis

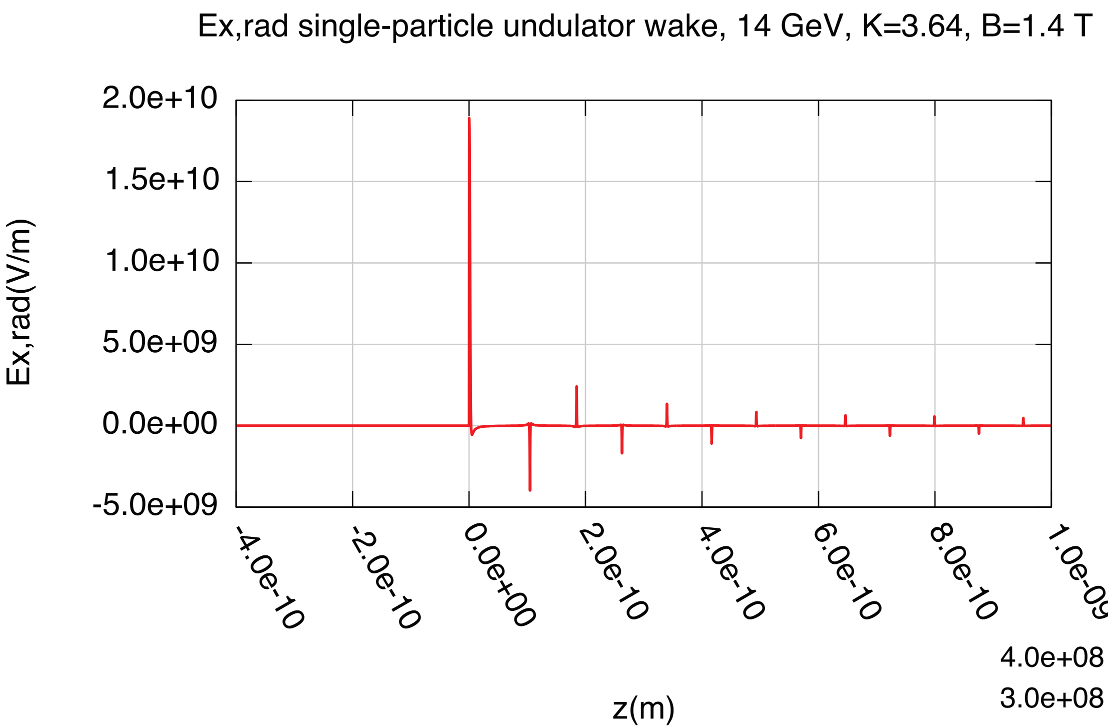


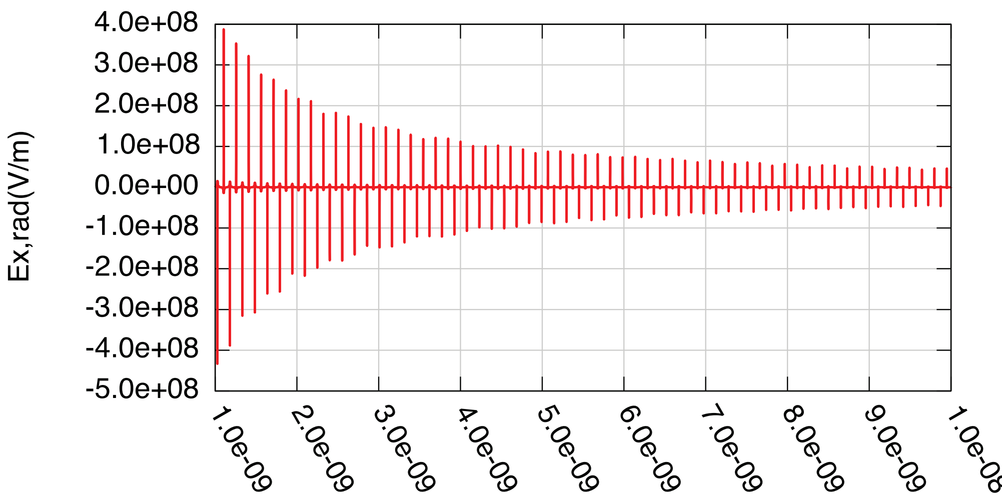
Longitudinal single-particle radiation wake (K=0.07): Ez,rad tabulated on the z-axis



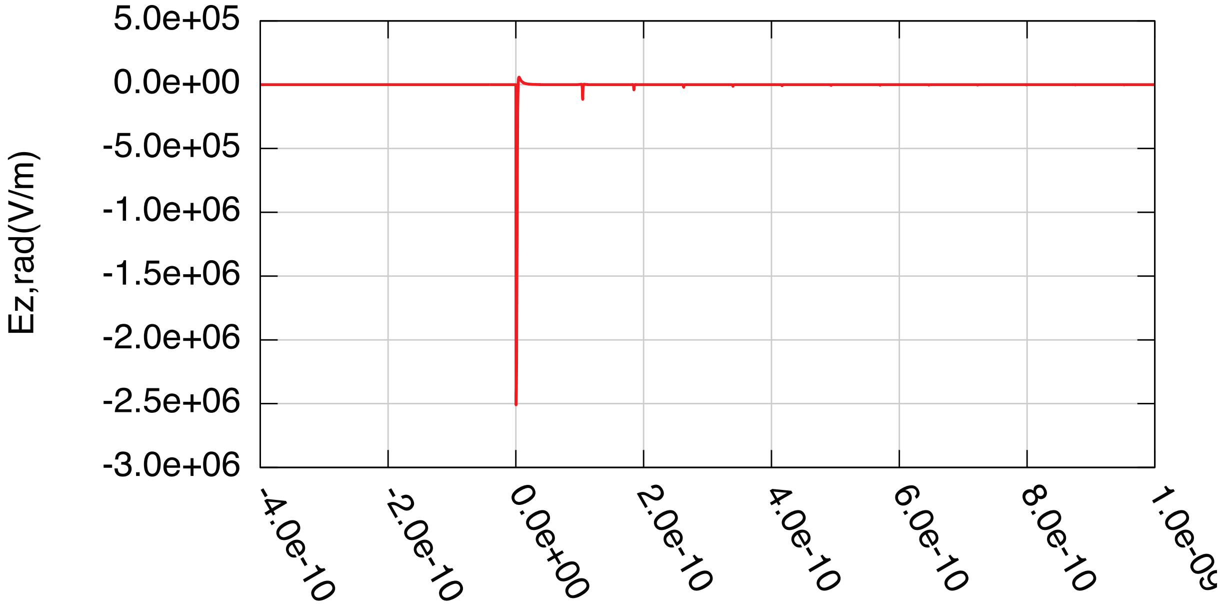


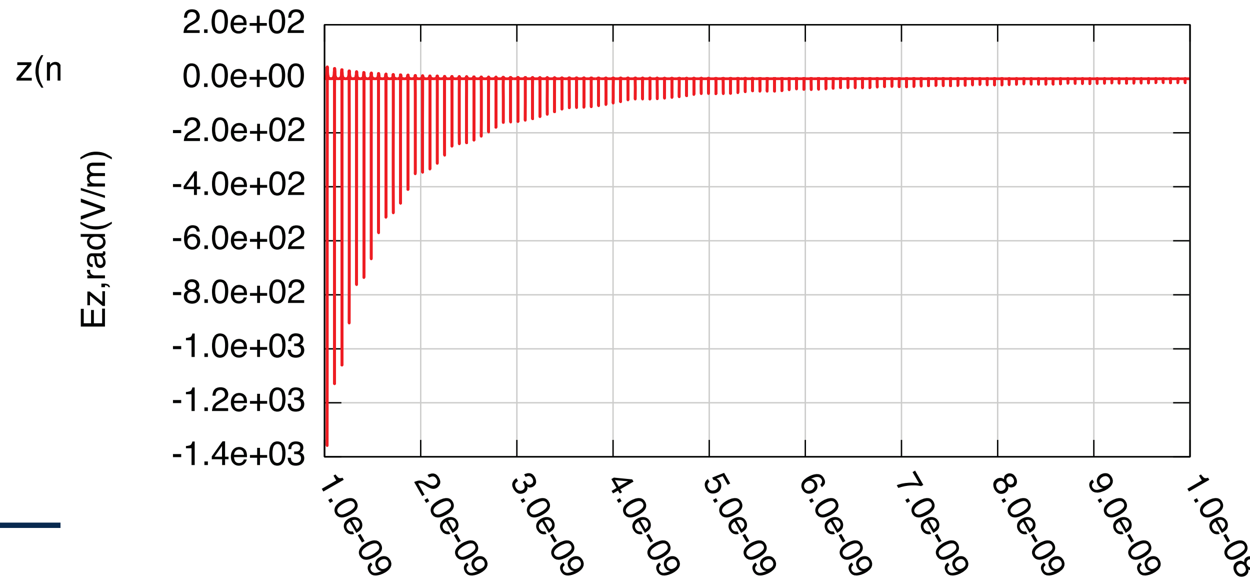
Transverse single-particle radiation wake (K=3.64): Ex,rad tabulated on the z-axis





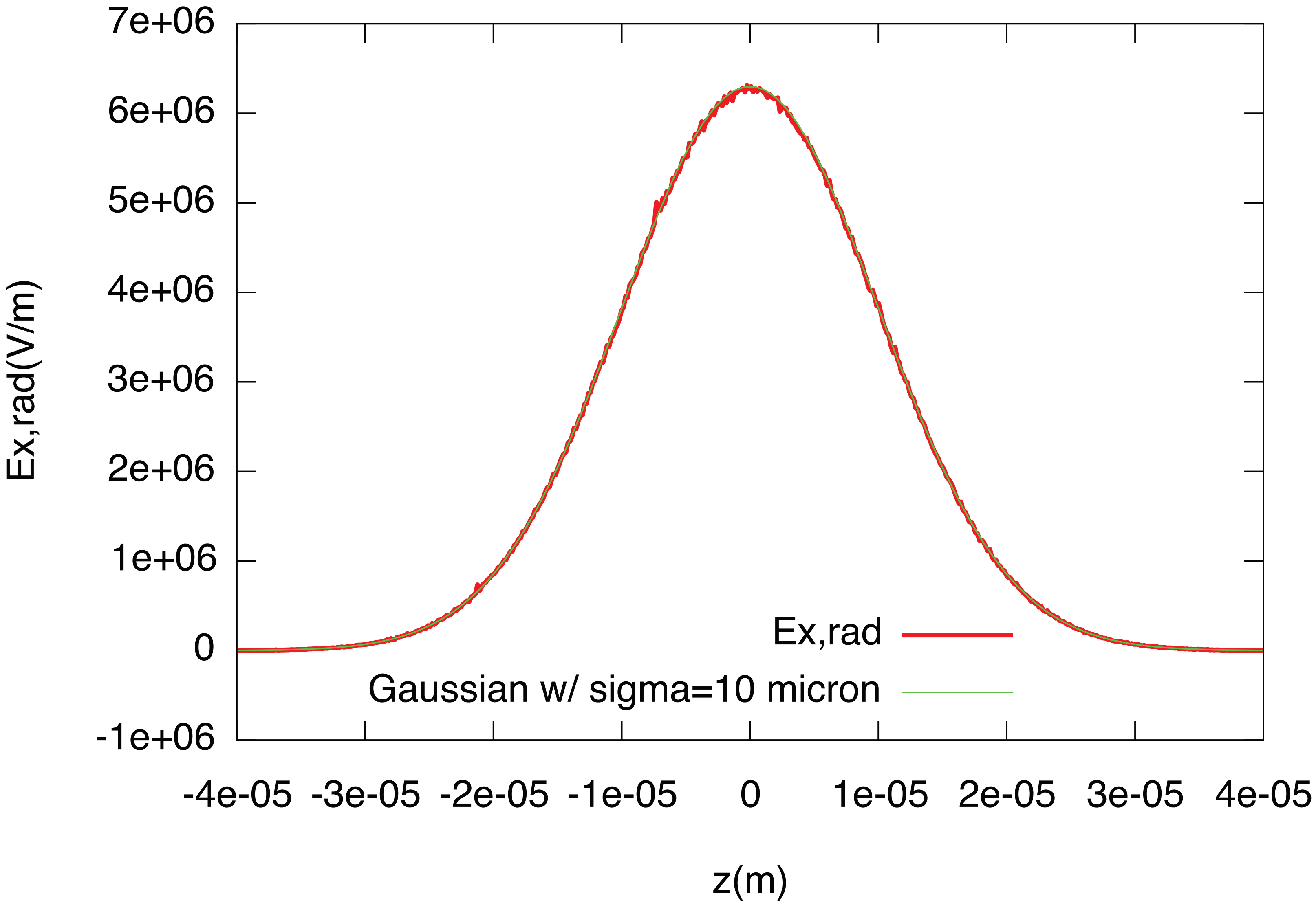
Longitudinal single-particle radiation wake (K=3.64): Ez,rad tabulated on the z-axis



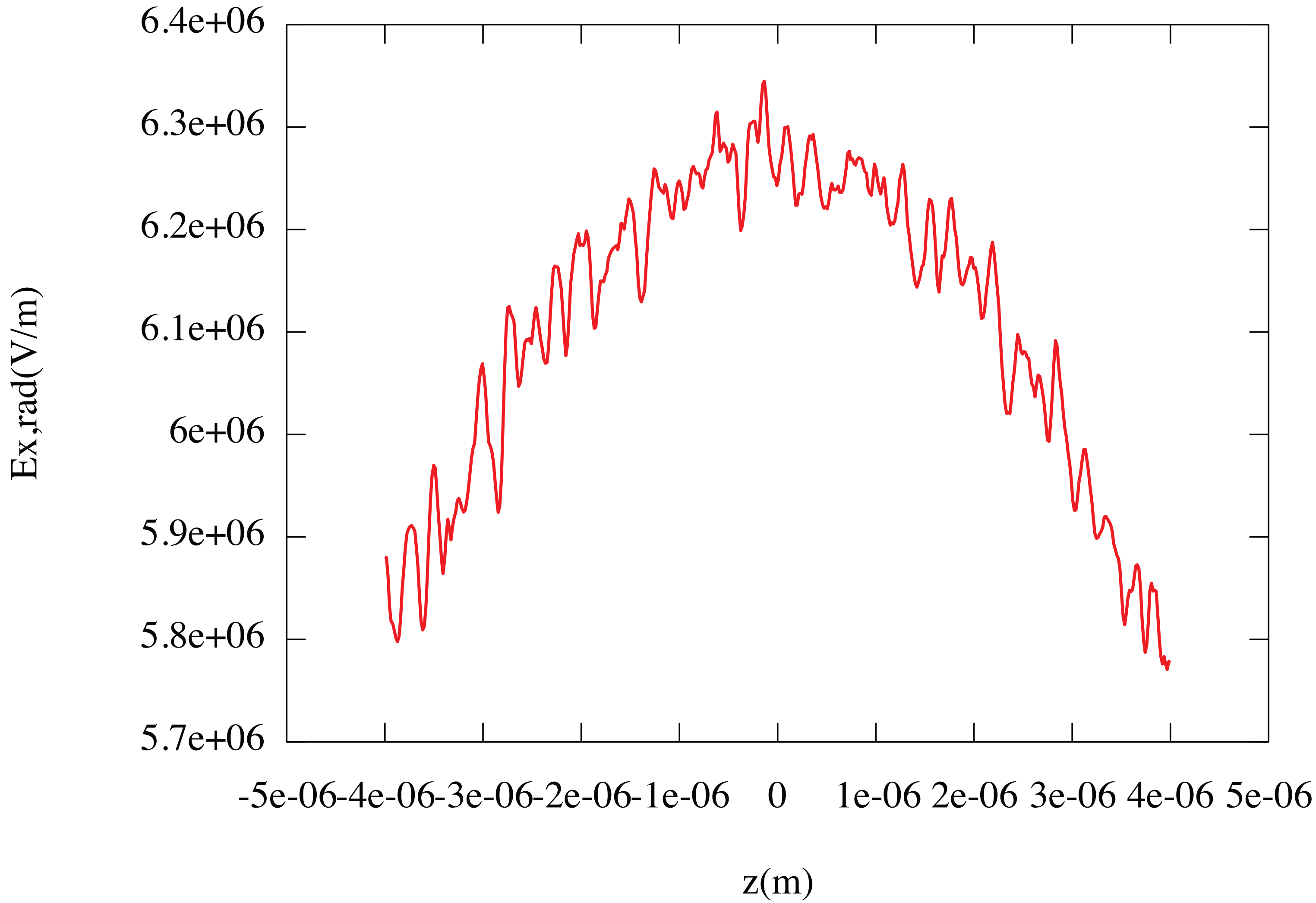


Longitudinal single-particle radiation wake (K=3.64): Longitudinal Poynting vector in y-z plane

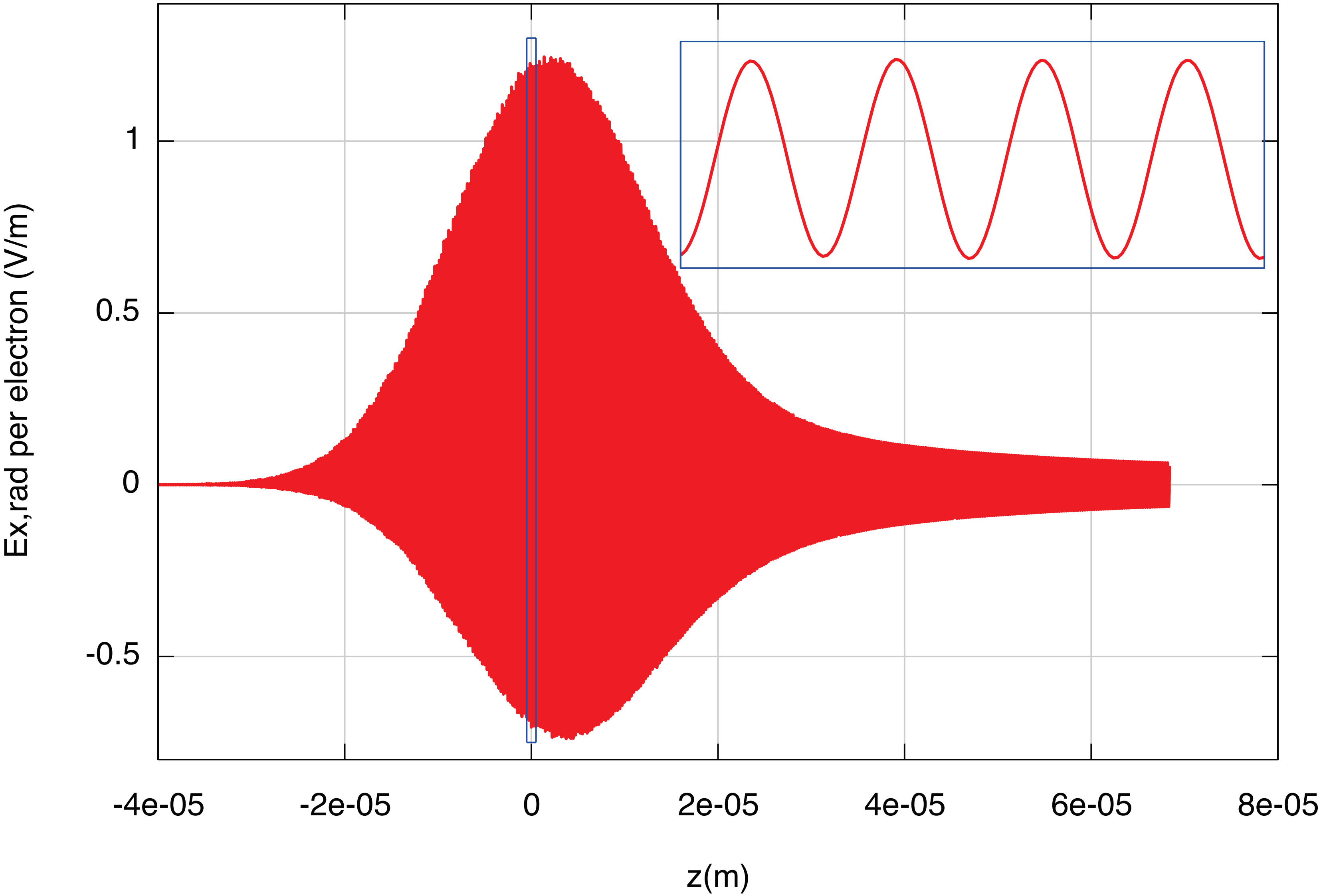
10x10x10 μm Gaussian bunch, E=125 MeV, K=.07: No obvious FEL radiation ahead of the bunch



But there is small amplitude microstructure due to sampling with a small # of particles (24 million)



10x10x10 μm modulated Gaussian (λ_{mod}=0.24 μm): Now there *is* FEL radiation evident ahead of the bunch

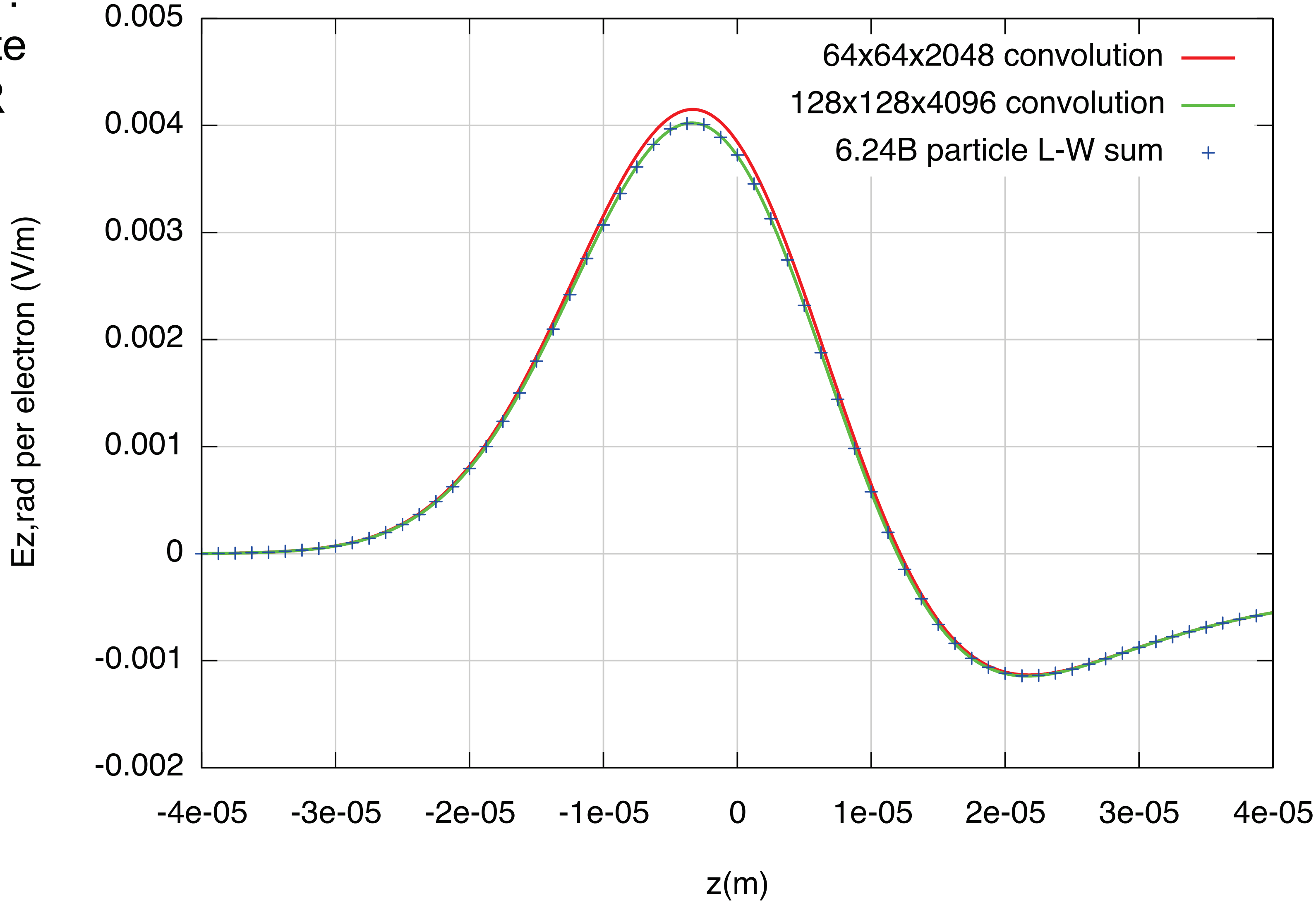


Lienard-Wiechert Particle-Mesh (LWPM)

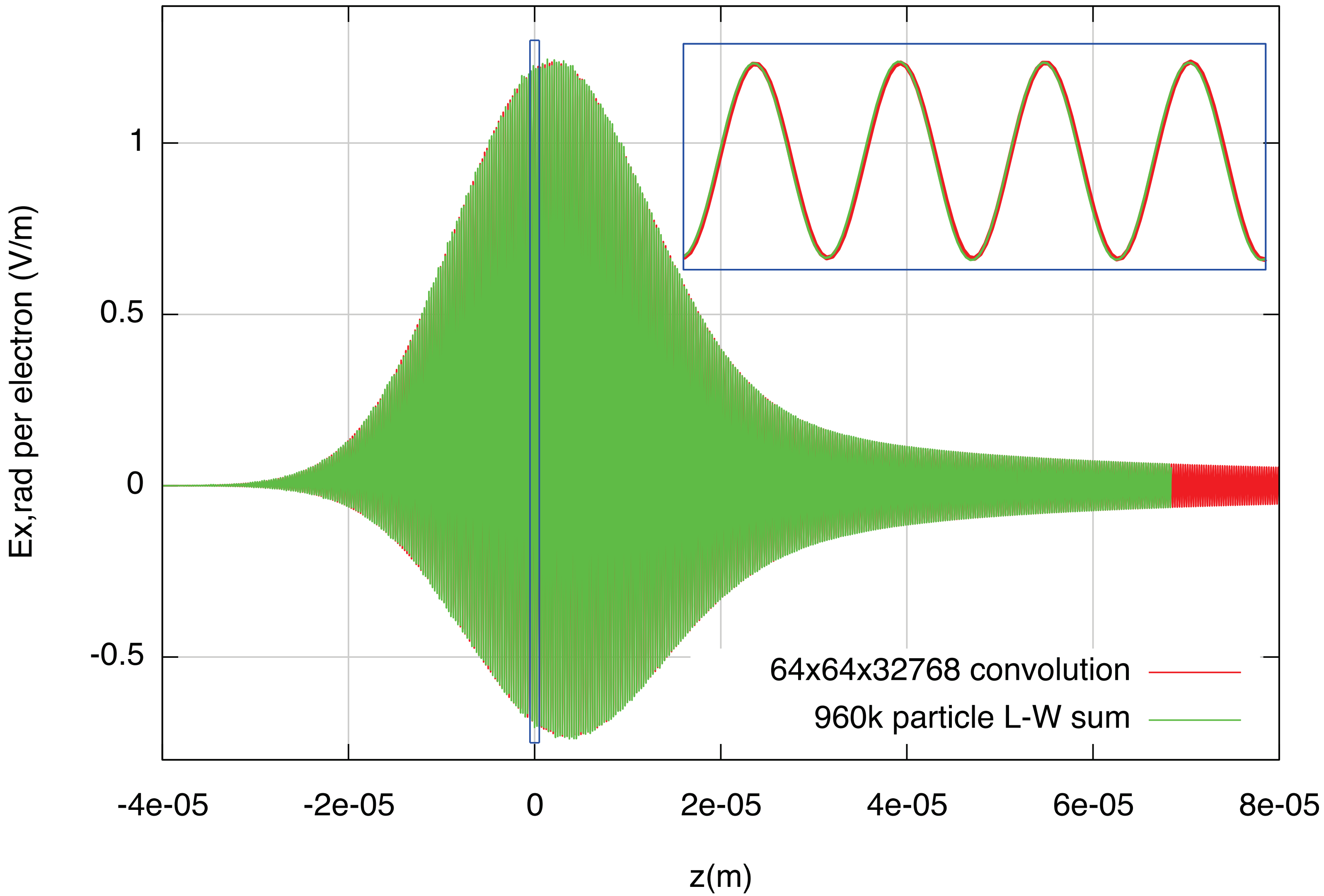
- These calculations are slow. How to speed up?
- Adapt techniques from parallel "space-charge" codes:
  - We don't normally compute the field at a point exactly by summing from all particles
  - Instead of summing N single-particle Green functions, we use ONE Green function, then convolve with ρ on a grid
    - This approximation usually is valid, but not always
      - When it doesn't there is usually a work-around, e.g. when ΔE is large, we do energy binning
- 3D L-W convolution-based approach:
  - Calculate G_{LW} on a 3D grid for 1 particle
  - Zero pad the charge density
  - Use parallel FFT to convolve, scales as M logM

Can we use convolution methods in a L-W code? Yes. Here are 2 examples

Example #1: Steady State Dipole CSR



Convolution-Based L-W solver example #2: Undulator radiation from a modulated bunch



Parallel light source simulation: Status and future prospects

- This year: S2E IMPACT-Z + IMPACT-T + GENESIS run on Hopper@NERSC: 2B particles, 2000 cores, 10 hours (MOPSO66 by J. Qiang et al.)
- Parallel multi-physics light source modeling w/ 3D space-charge, 1D CSR, and wakes is maturing
- 10x performance in computing power is becoming more ubiquitous, soon "routine" simulations will use ~10K cores, "big" will use > 1M cores
- Ultra-high resolution modeling, and 3D CSR self-consistent modeling are around the corner

New tools for modeling 3D radiative phenomena – using advanced algorithms on supercomputers – will transform our ability to design, explore, understand, and advance future light sources and new accelerator concepts

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- Gennady Stupakov
  - energy diffusion, two-particle model
- Computational resources provided by
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