Modeling of Accelerators for Next Generation Light Sources Using the IMPACT Code Suite

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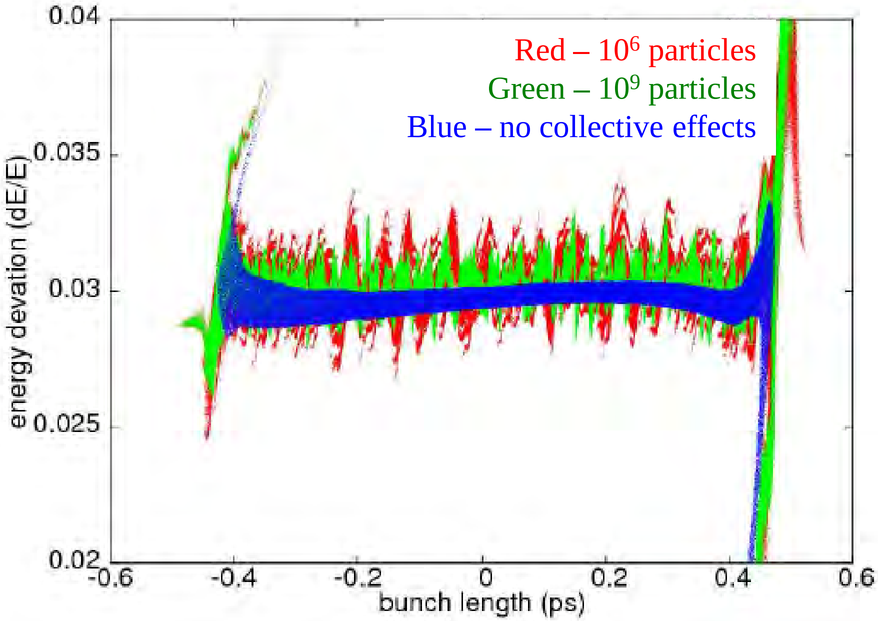
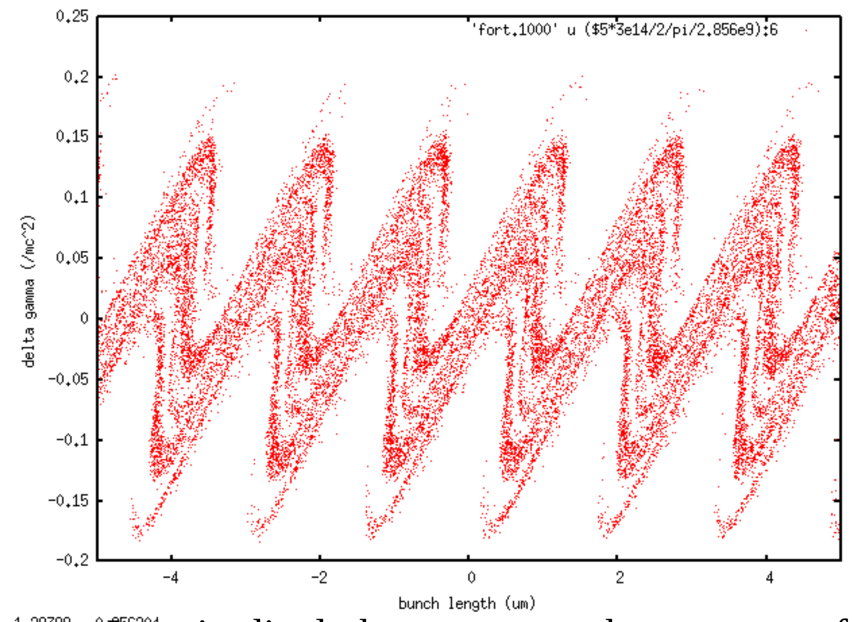
High-resolution multi-physics codes are required for state-of-the-art accelerator design

For example

- The microbunching instability significantly degrades beam quality
- New seeding schemes (e.g. ECHO) demand production and transport of very fine beam structure
- High resolution modeling is needed to accurately model initial shot noise, resolve fine structure, and avoid numerical artifacts



The longitudinal phase space of a beam at the exit of a linac



Longitudinal phase space at the entrance of an ECHO seeded FEL

IMPACT – **I**ntegrated **M**ap and **PA**rti**C**le **T**racking

- A high performance computing tool for large-scale accelerator beam dynamics modeling
  - **Multi-physics**
  - **State-of-the-art numerical algorithms**
  - **Advanced parallel implementation**

- High performance computing plays an important role in accelerator science by optimizing operation performance, minimizing design risk, reducing construction cost, and exploring new physical regimes

- Started in mid-90s under the Computational Accelerator Grand-Challenge

- Developed under the accelerator Scientific Discovery through Advanced Computing project (SciDAC 1 and 2)

- Has been used by about 30 research institutes and universities around the world

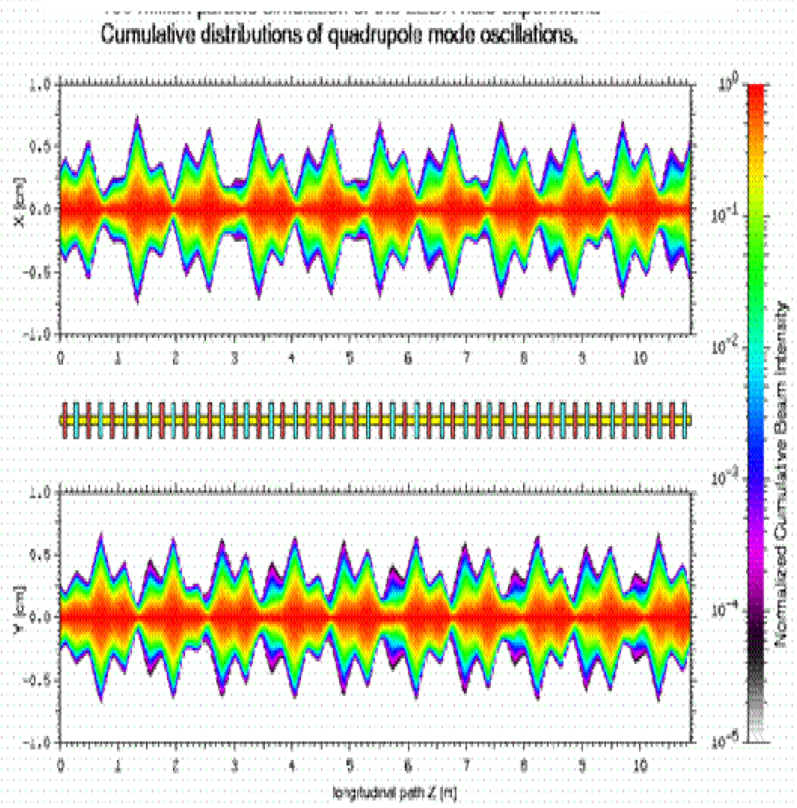
IMPACT: A 3D Parallel Beam Dynamics Code Suite

- IMPACT-Z
  - Parallel particle-in-cell (PIC) code used for electron & ion linacs
- IMPACT-T
  - Parallel PIC code used for space-charge dominated beams (e.g. photoinjectors)
- Fix3D/2D
  - RMS envelope code for optics design, matching
- Pre and Post-Processing
  - Matlab script for parameter optimization with IMPACT code
  - Python script for initial drive phase setting
  - Fourier coefficients field calculation
  - Slice emittances, uncorrelated energy spread

IMPACT-Z

- Parallel PIC code using longitudinal coordinate "z" as the independent variable
- Key Features
  - —Detailed RF accelerating and focusing model
  - —Multiple 3D Poisson solvers
    - Variety of boundary conditions
    - 3D Integrated Green Function
  - —Multi-charge state
  - —Machine error studies and steering
  - —Wakes
  - —CSR (1D)
  - —Run on both serial and multiple processor computers

100 million macroparticle simulation of the LEDA halo experiment

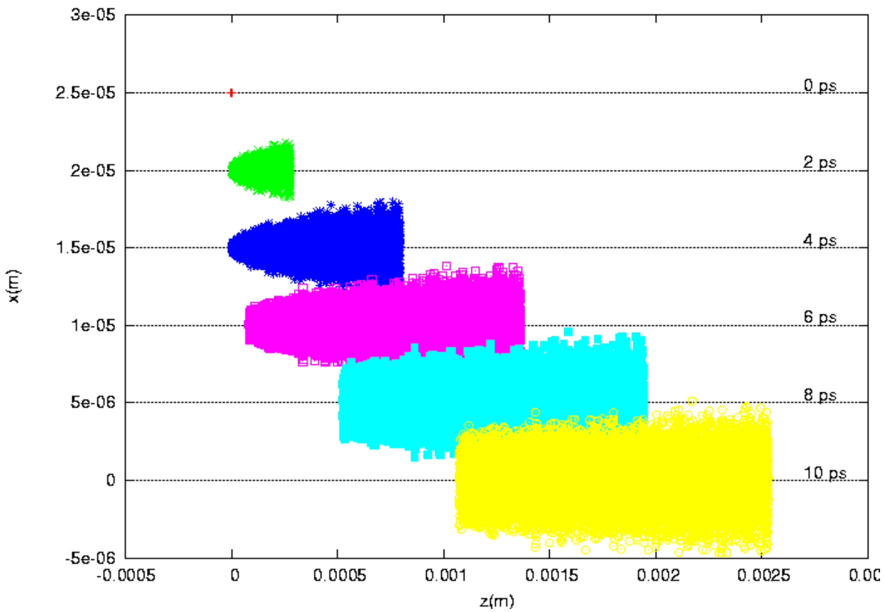


J. Qiang et al., Phys. Rev. ST Accel. Beams, Vol 5, 124201 (2002).

J. Qiang, R. Ryne, S. Habib, V. Decyk, J. Comp. Phys. vol. 163, 434, (2000).

IMPACT-T

- Parallel PIC code using time "t" as the independent variable
- Key Features
  - —Detailed RF accelerating and focusing model
  - —Multiple Poisson solvers
    - 3D Integrated Green Function
    - point-to-point
  - —Multiple species
  - —Monte Carlo gas ionization model
  - —Cathode image effects
  - —Wakes
  - —CSR (1D)
  - —Run on both serial and multiple processor computers



Emission from nano-needle tip including Borsch effect

J. Qiang, S. Lidia, R. D. Ryne, and C. Limborg-Deprey, Phys. Rev. ST Accel. Beams, vol 9, 044204 (2006).

State-of-the-art **numerical algorithms** and **parallel implemenation** are used in the IMPACT code suite to calculate collective effects

Some Algorithm Examples

Space-Charge Calculation Based on Integrated Green Function for Large Aspect Ratio Beams

$$\phi_c(r_i) = \sum_{i'=1}^{2N} G_i(r_i - r_{i'})\rho_c(r_{i'})$$

$$G_i(r,r') = \oint G_s(r,r')\,dr'$$

Integrated Green function

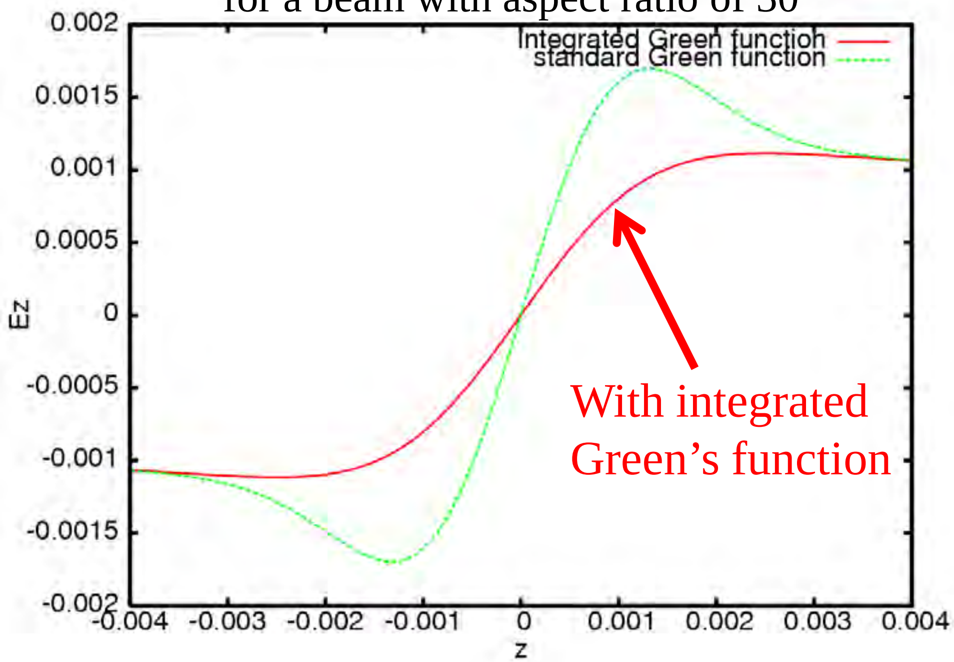
$$G_s(x,y,z) = 1/\sqrt{(x^2+y^2+z^2)}$$

Standard Green function

Integrated Green's function is needed for modeling large aspect ratio beams!

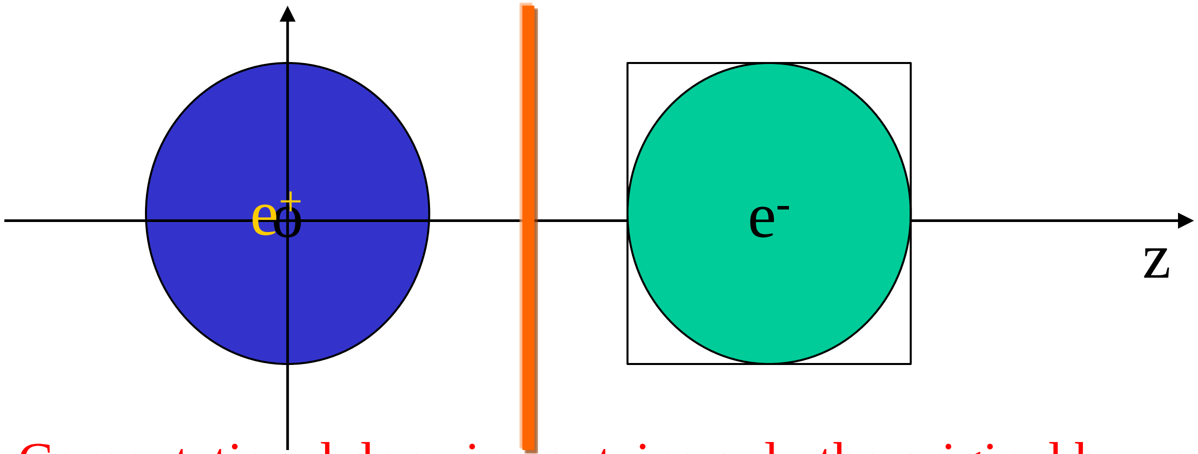
O(N log N) vs O(N^2)

Comparison between the IG and SG for a beam with aspect ratio of 30

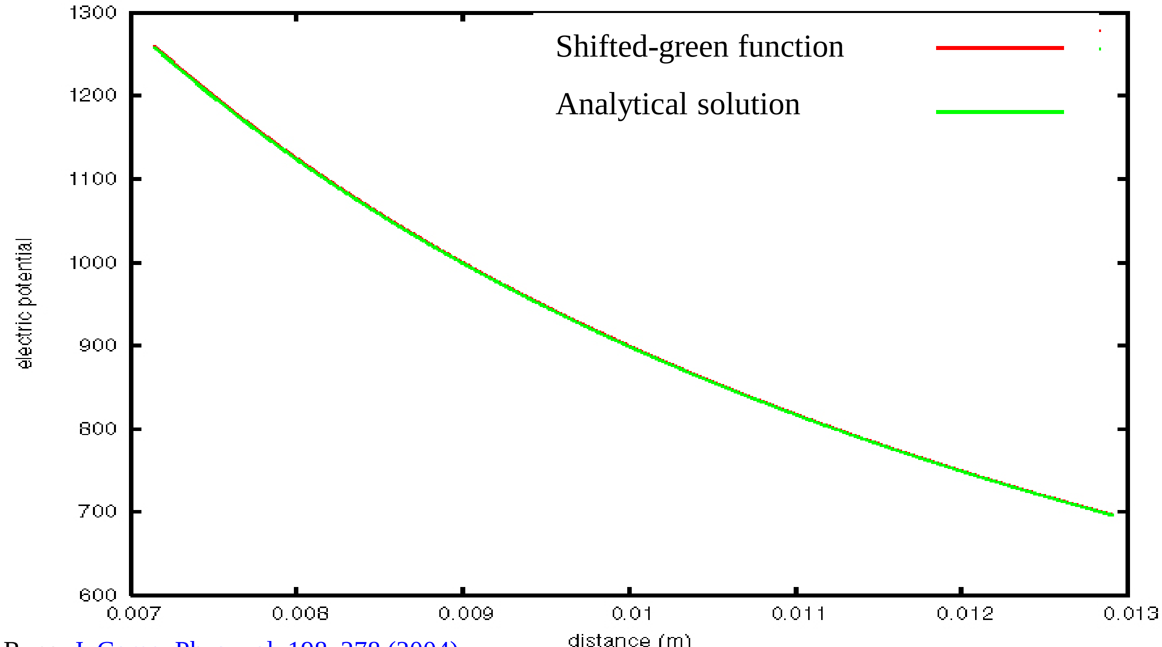


R. D. Ryne, ICFA Beam DynamicsMini Workshop on Space Charge Simulation, Trinity College, Oxford, 2003
J. Qiang, S. Lidia, R. D. Ryne, and C. Limborg-Deprey, Phys. Rev. ST Accel. Beams, vol 9, 044204 (2006).

Efficient Shifted Green Function Method to Calculate Image Space-Charge Effects



Computational domain contains only the original beam



O(N log N)
vs
$O(N^2)$

J. Qiang, M. Furman, and R. Ryne, J. Comp. Phys. vol. 198, 278 (2004).

Efficient FFT Method to Calculate Longitudinal and Transverse Wakefields

$$F_x(s) = q\int_s^{+\infty} W_T(s-s')x(s')\lambda(s')ds'$$

$$F_z(s) = \int_s^{+\infty} W_L(s-s')\lambda(s')ds'$$

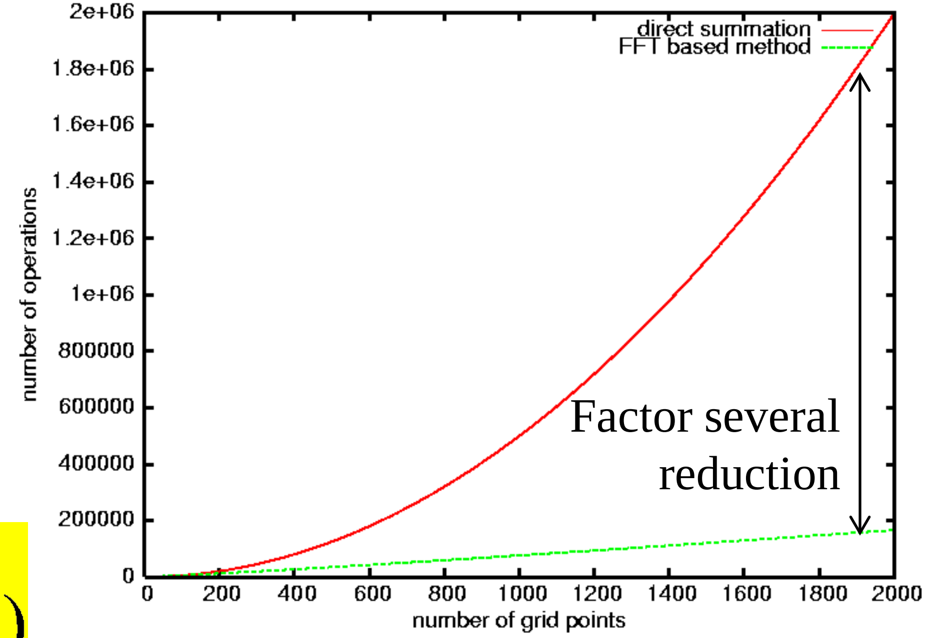
$$F(s) = \int_{-\infty}^{+\infty} G(s-s')\rho(s')ds'$$

$$G(s) = \begin{cases} W(s) & for\ s \geq 0 \\ 0 & for\ s < 0 \end{cases}$$

$$F_c(s_i) = h\sum_{i'=1}^{2N} G_c(s_i - s_{i'})\rho_c(s_{i'})$$

$$F(s_i) = F_c(s_i) \quad for\ i = 1,\ldots N$$

Operations comparison using the direct summation and the FFT based method

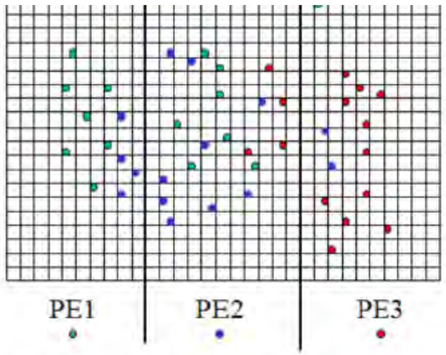


O(N log N) vs O(N^2)

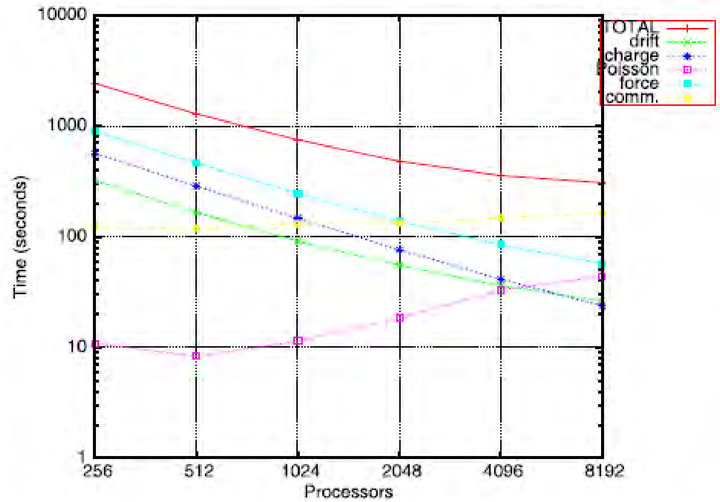
J. Qiang, R. D. Ryne, M. Venturini, A. A. Zholents, I. V. Pogorelov, Phys. Rev. ST Accel. Beams, 12, 100702 (2009).

Parallel Implementation Matters: Particle-Field Decomposition vs. Domain Decomposition

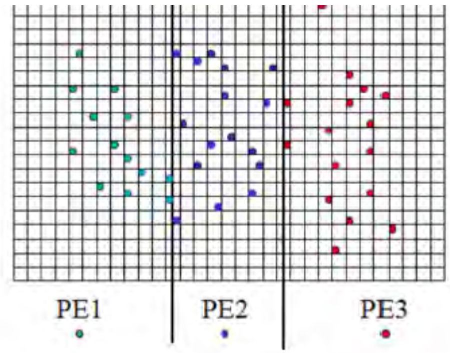
Balance particle distributions and fields between processors



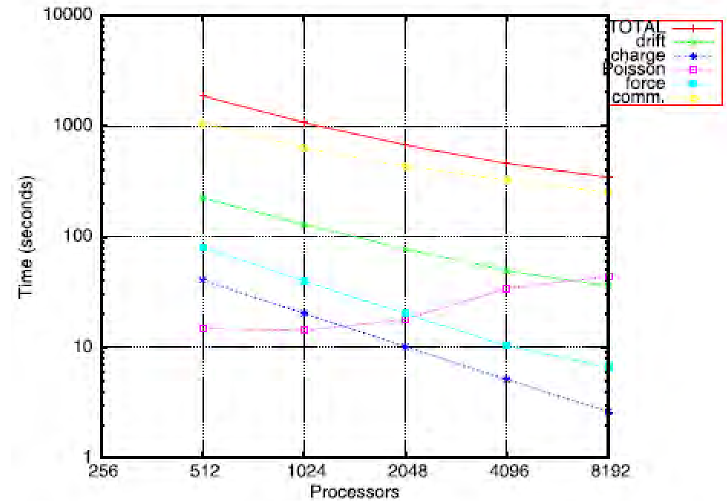
A schematic plot of the particle-field decomposition method in particle-in-cell simulation.



Balance only particle distributions between processors



A schematic plot of the domain decomposition method in particle-in-cell simulation.

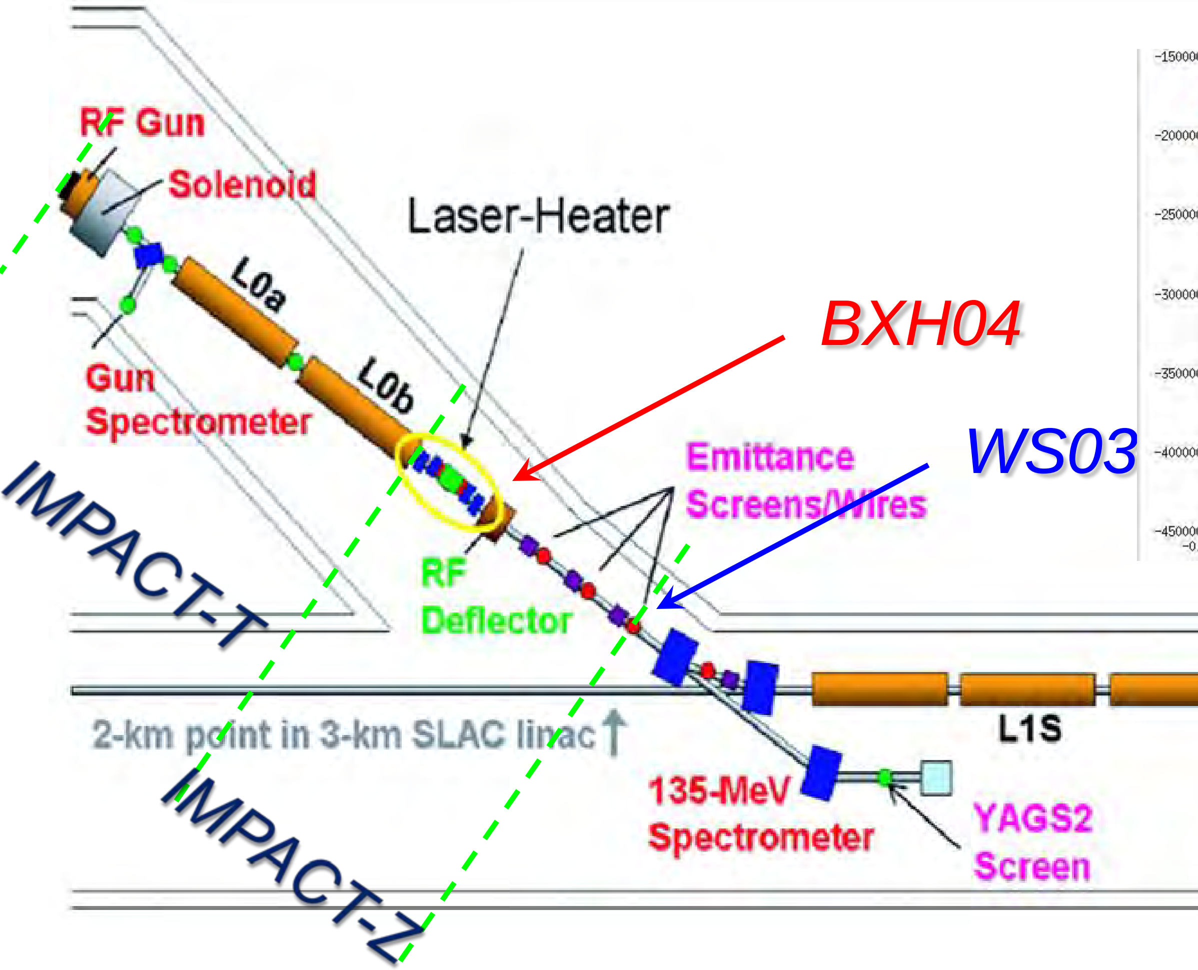


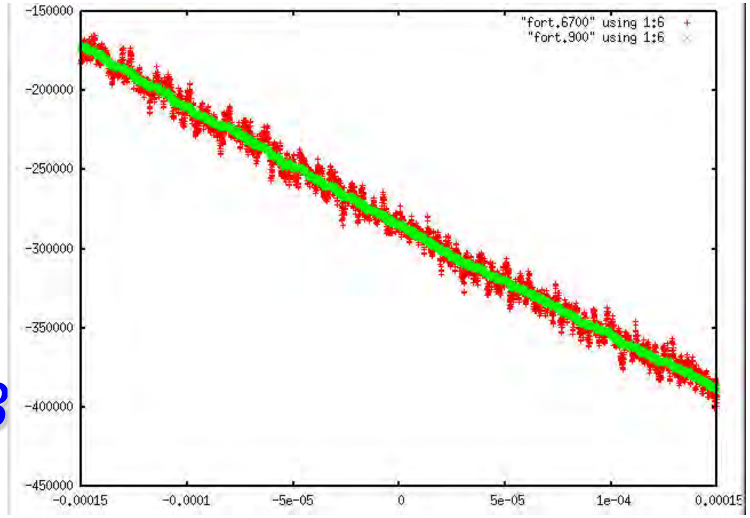
Particle-field decomposition out-performs the conventional domain decomposition

J. Qiang and X. Li, Comput. Phys. Comm., 181, 2024, (2010).

Some Application Examples

Application of the IMPACT Code to the **LCLS**



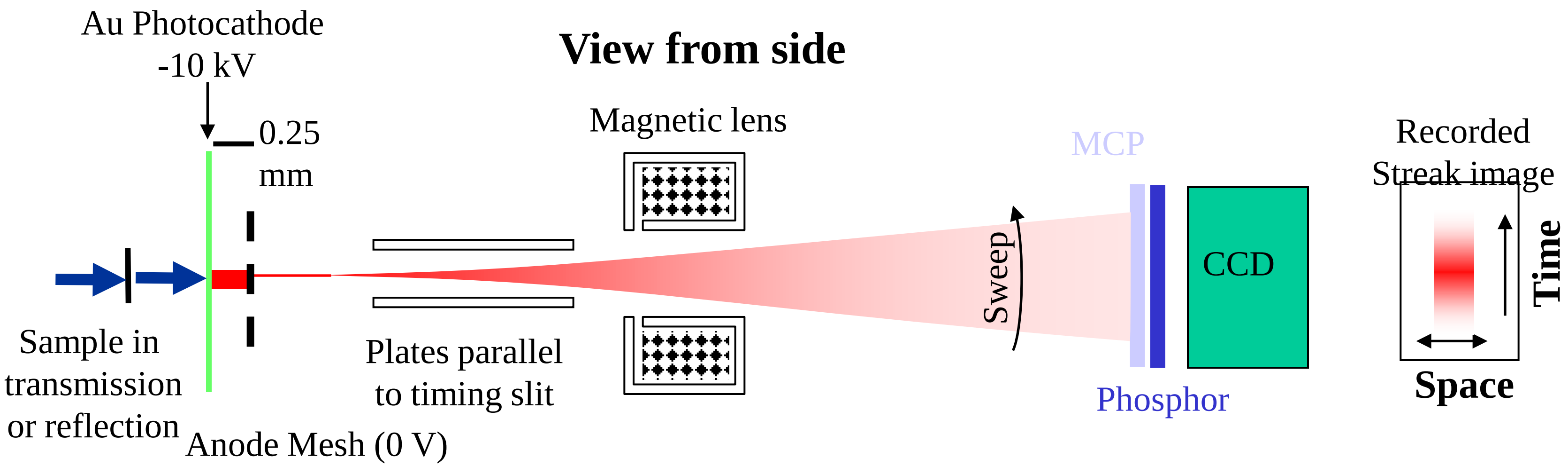


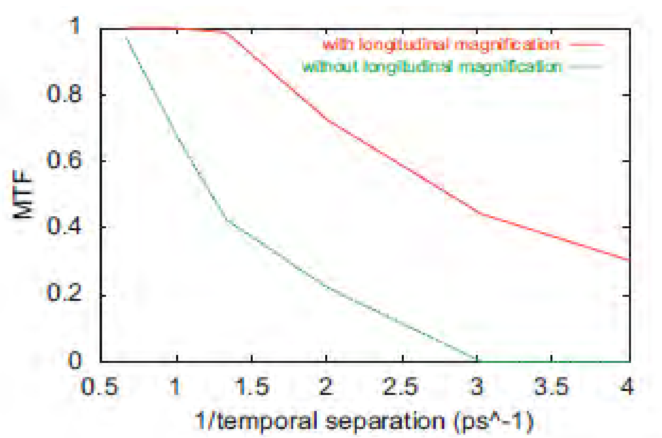
– *The red (at WS03) shows more microbunching than green (after BXH04), which indicates space charge amplified energy modulation*

R. Akre et al., PRST-AB, 11, 030703
K. Bane et a l., PRST-AB, 12, 030704

Courtesy of J. Wu

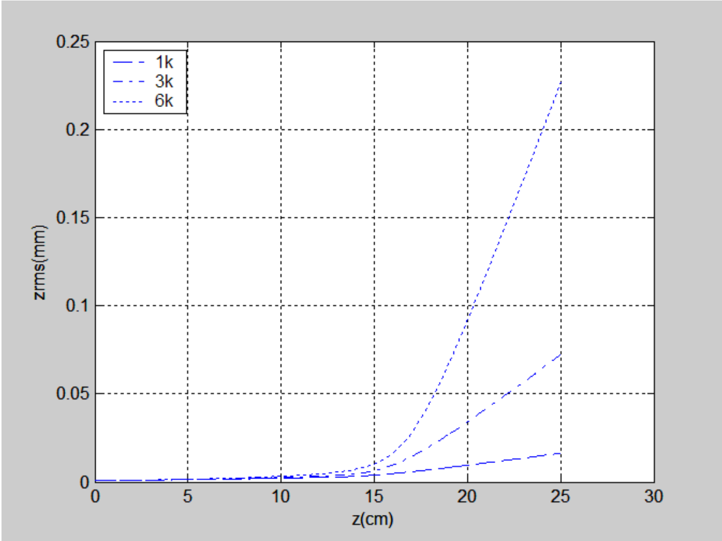
Modeling of the **ALS** Streak Camera Using IMPACT – with Space Charge Effects





X-ray streak camera temporal reslution improvement
using a longitudinal time-dependent field

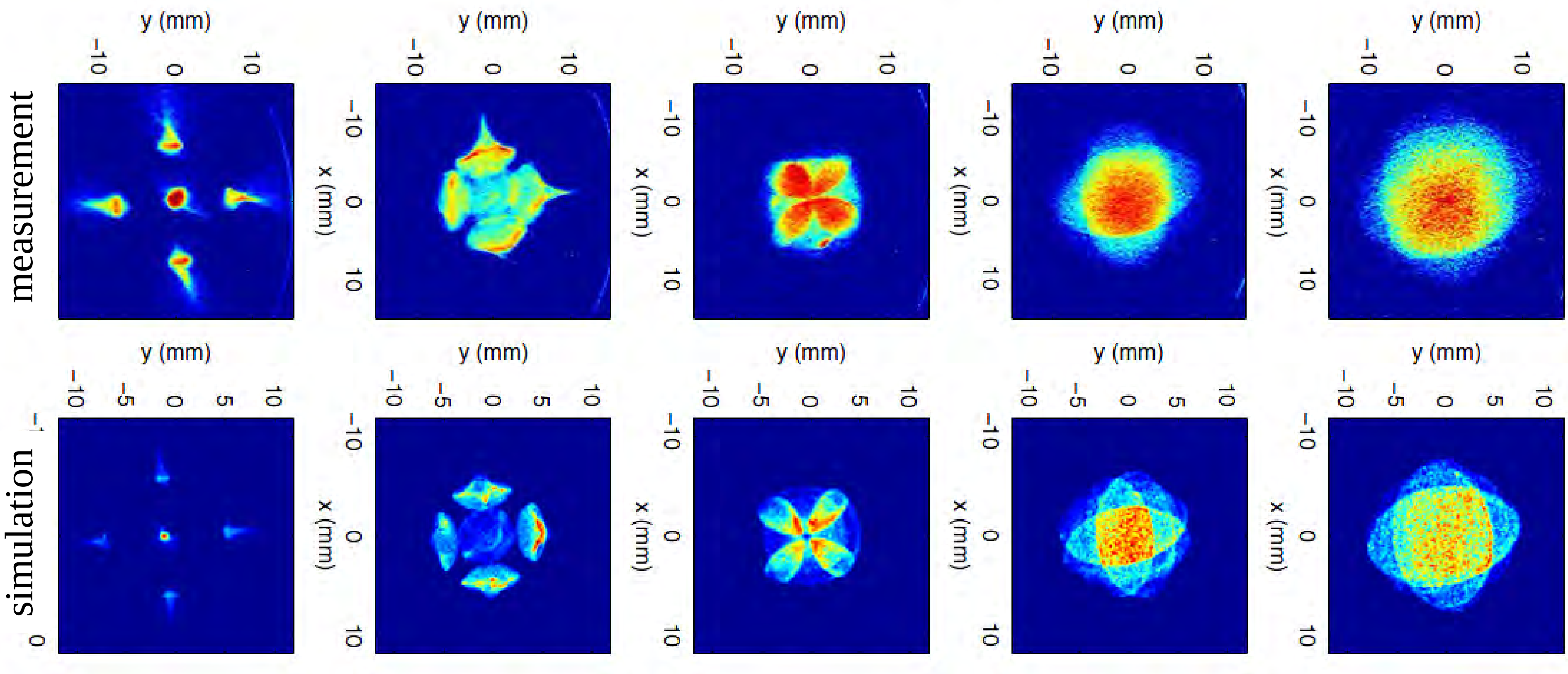
Space-Charge Effects in Streak Camera



J. Qiang, J. M. Byrd, J. Feng, G. Huang, Nuclear Instruments & Methods in Physics Research A 598,

J. Feng, et. al, Proceedings of SPIE, Vol.5920, 592009 (2005).

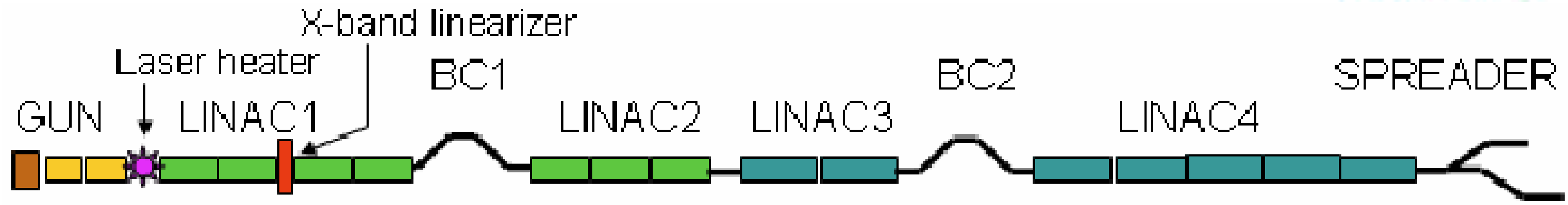
Application to the **ANL** Phase Space Manipulation (AWA measurement vs. IMPACT simulation)



increasing B field

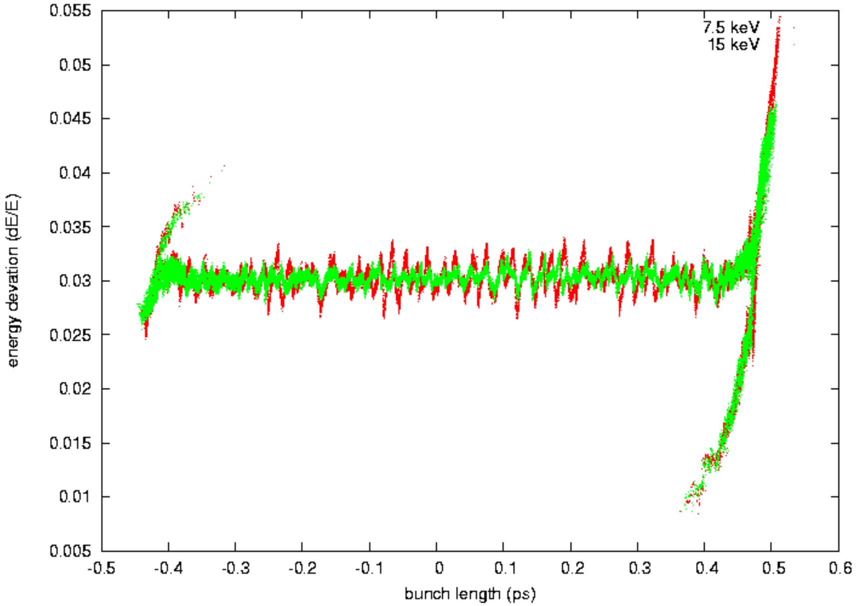
Courtesy of M. Rihaoui, PRST-AB 12, 124201 (2009).

High Resolution Modeling of the **FERMI@Elettra** FEL Linac with IMPACT

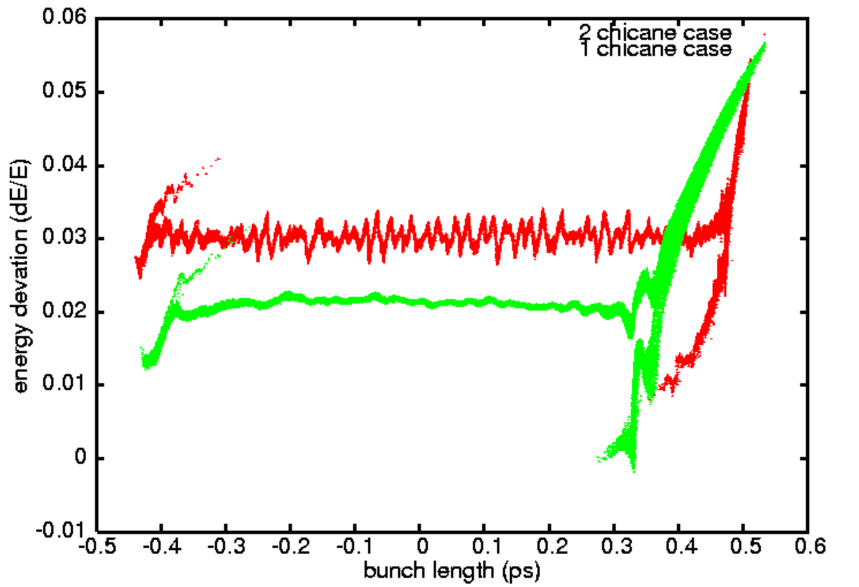


- Beam energy at the entrance of laser heater ~100 MeV (peak current ~70A), at the exit of Linac 4 E ~ 1.2 GeV (peak current 500A or 800A depending on configuration)

Final longitudinal phase space distribution
With 7.5 keV and 15 keV initial energy spread

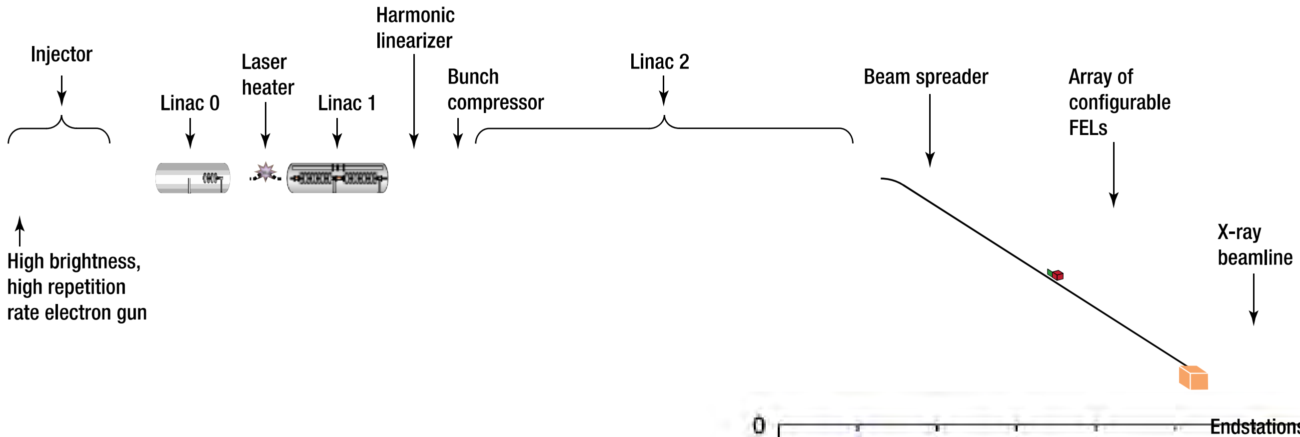


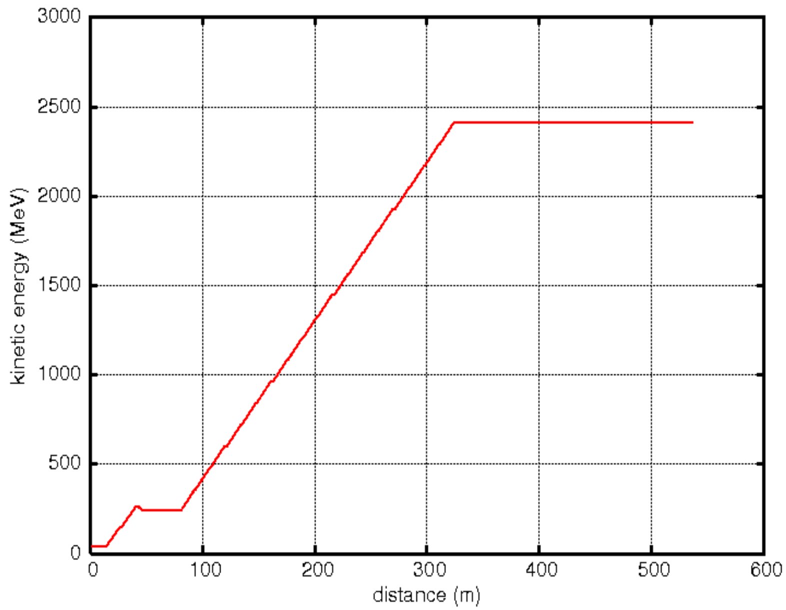
Final longitudinal phase space distribution
With 2 BC lattice and 1 BC lattice (initial ~7 kev)

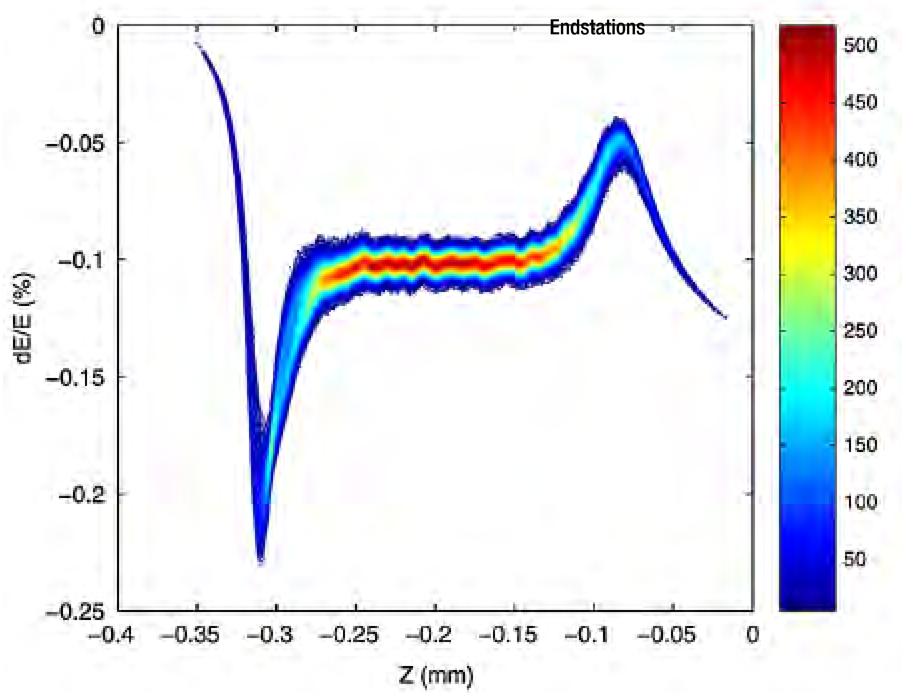


Billion-Particle Simulation of a FEL Linac Concept

(5 Billion macroparticles, ~5 hour computing time on 1024 processors)



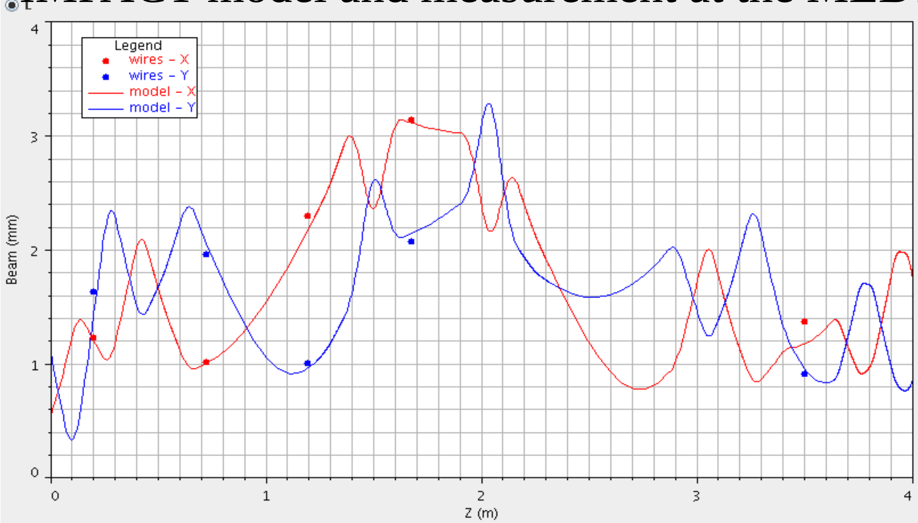




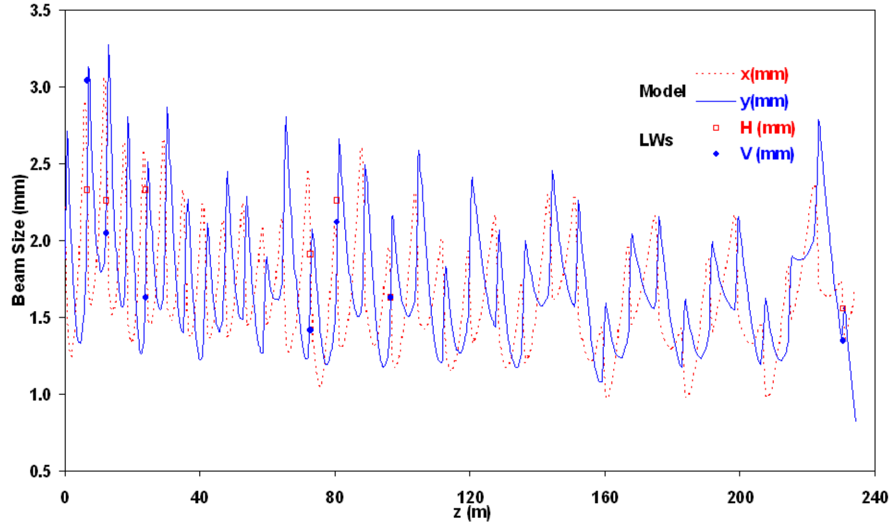
J. Qiang, R. D. Ryne, M. Venturini, A. A. Zholents, I. V. Pogorelov, Phys. Rev. ST Accel. Beams, 12, 100702 (2009).

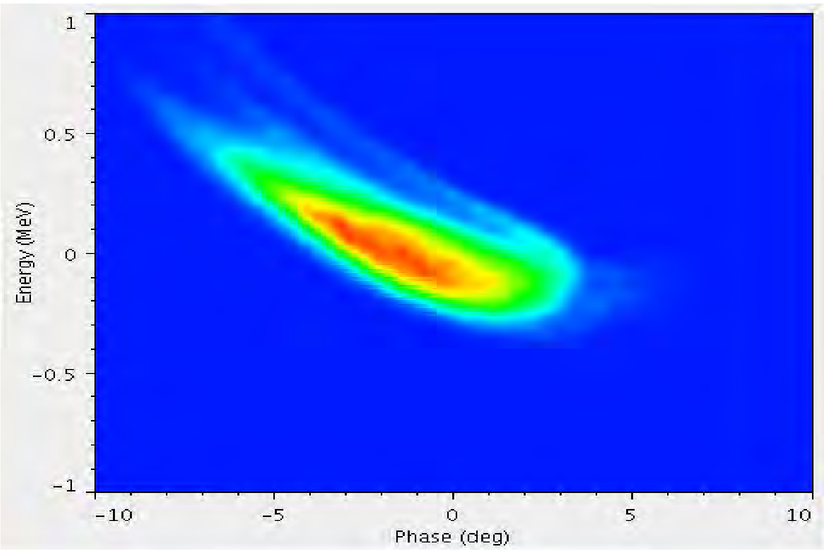
SNS Beam Dynamics Studies: Space-Charge and RF Nonlinearities Required for Accurate Model

IMPACT model and measurement at the MEBT

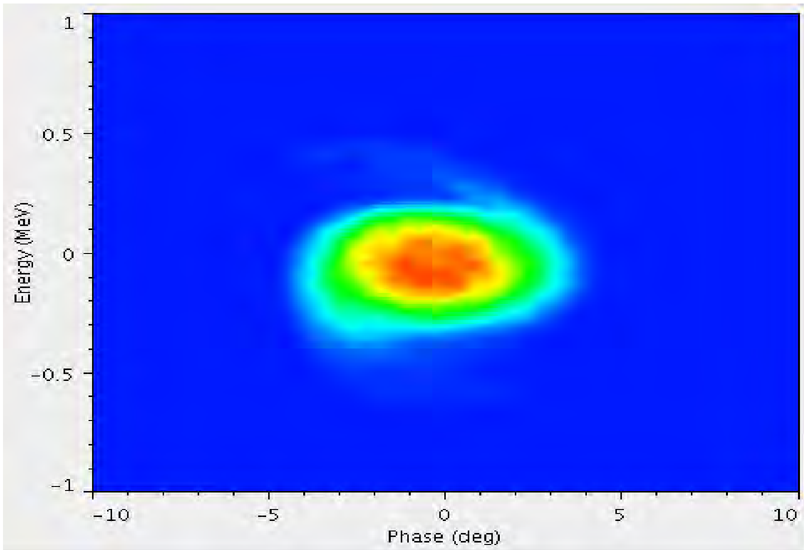


IMPACT model and the LWs measurements in SC linac





IMPACT model of DTL6 phase shifted by 6°.



IMPACT predicted profiles at the SCL entrance

Y. Zhang and J. Qiang, PAC09, p. 2653.

Future Work

- Year 1: Develop algorithms
  - CSR wakefield model including shielding effects
  - 3-step photoemission
  - 3-D S2E – merge [IMPACT-t/IMPACT-z/GENESIS]

- Year 2: Develop multi-scale capability
  - Develop a multi-scale Poisson solver based on the FFT method for open boundary conditions.
  - Implement the multi-scale Poisson solver into the IMPACT code suite.
  - Add the direct particle-particle Coulomb interaction to account for collisional effects

- Year 3: Simulation-based parallel parameter optimization
  - Parallel single objective function optimization based on a trust-region algorithm
  - Parallel multi-objective function optimization based on an evolutionary algorithm