Billion Particle Linac Simulations for Next Generation Light Sources

Ji Qiang

Lawrence Berkeley National Laboratory

LINAC08, Sep. 29 – Oct. 3, Victoria, Canada, 2008

In Collaboration With

—R. D. Ryne

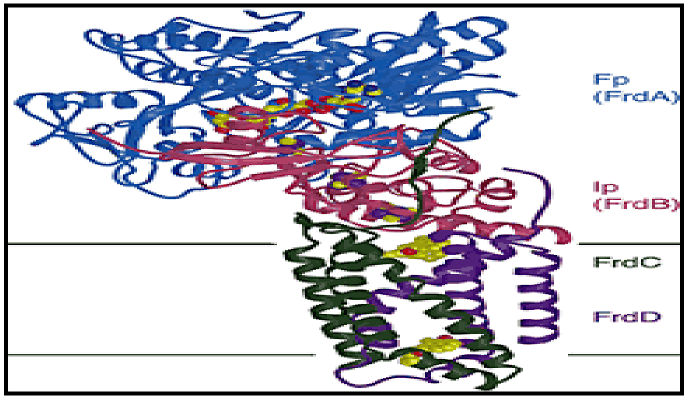
—M. Venturini

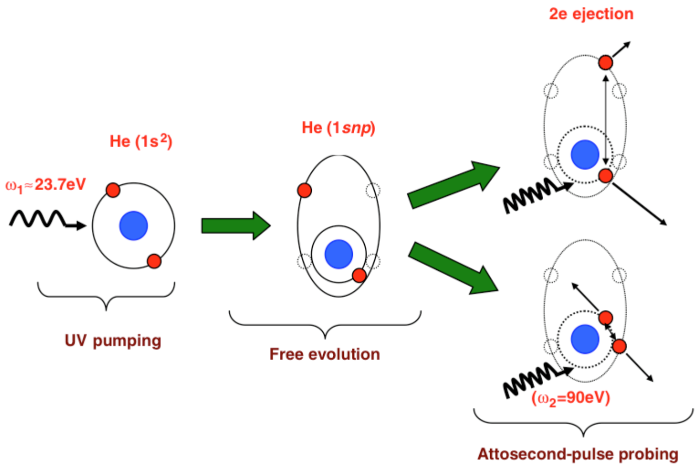
—A. A. Zholents

Work supported by the Office of Science, U. S. Department of Energy, under Contract No. DE-AC02-05CH11231 using computing resources **National Energy Research Scientific Computing Center**

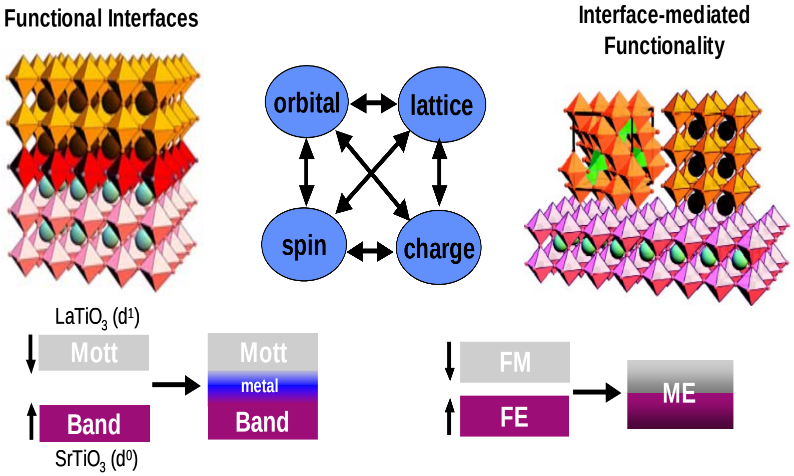
Next Generation Light Sources Present Great Opportunities for Scientific Discovery

- —Biology
- —Material science
- —Condense matter physics
- —Chemistry





Attosecond capabilities allow direct probing of atomic electron correlation (Hu and Collins, Phys. Rev. Lett. ***96****, 073004 (2006))*



Ultrafast x-ray spectroscopy offers new insight by providing elemental and interfacial sensitivity, quantification of electronics structure and bonding, dichroism to separate spin and orbital components of magnetic moments, atomic structural dynamics, and a capability for separating correlated phenomena directly in the time domain (figure courtesy R. Ramesh, LBNL-MSD).

Fundamental Parameters Driving FEL Cost and Performance

- **Electron beam emittance ε**
  - **High brightness gun, minimize emittance growth in accelerator**
  - **High gradient accelerator *as low energy as possible***
  - **Manipulate and condition beam for the FEL process**

$$\frac{\varepsilon_n}{\gamma} \approx \frac{\lambda_{x-ray}}{4\pi}$$

- **Peak current I_{peak}**
  - **Bunch compression, minimize distortion from longitudinal wakefields**

- **Energy spread σ_E**
  - **High brightness gun, minimize distortion from longitudinal wakefield and microbunching instability**

Power/ undulator length $\sim f\left(I_{peak}, \frac{\varepsilon_n}{\gamma}, \sigma_E\right)$

- **Electron beam energy γ**
  - **High gradient accelerator**
  - **Short period undulators**

$$\lambda_{x-ray} = \frac{\lambda_{undulator}}{2\gamma^2}\left(1+\frac{K^2}{2}\right)$$

Courtesy of A. Zholents

Challenges for Electron Beam Delivery System

—Generation of low emittance, low energy spread, high peak current, i.e. high brightness electron beam

—Acceleration, transport, and compression of high brightness electron beam

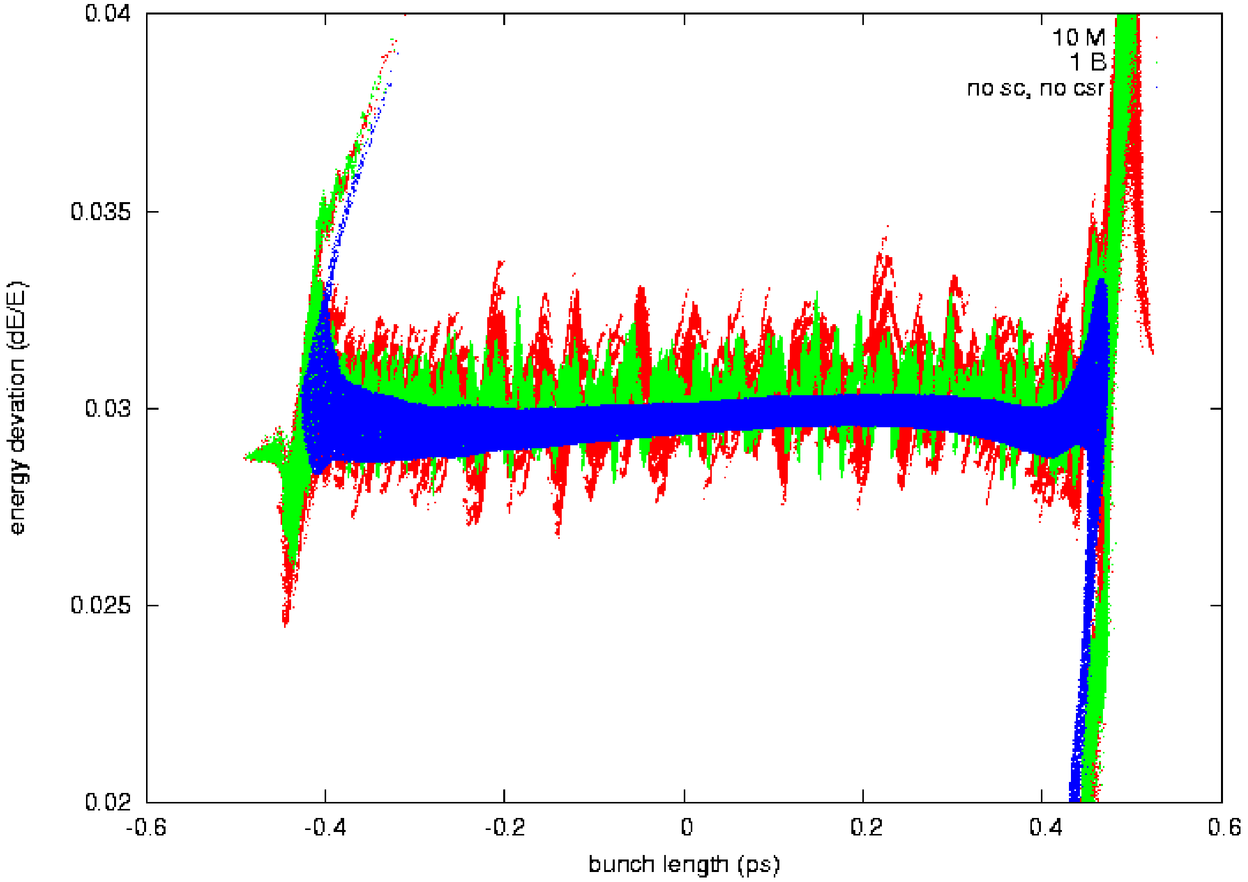
—Preservation of beam quality in the presence space-charge effects, wake fields, and coherent synchrotron radiation

—Lower machine cost

Need for Large Scale Simulations

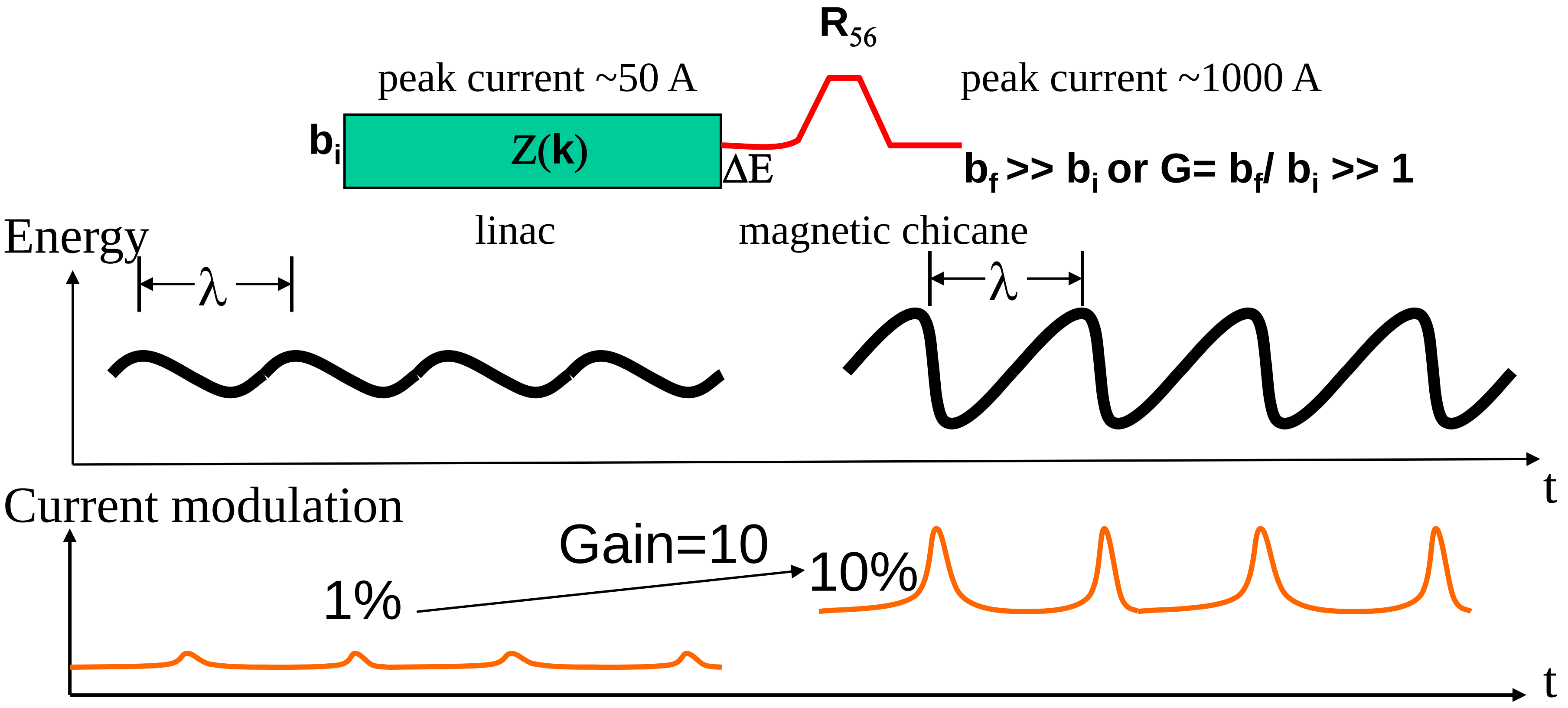
Final Longitudinal Phase Space Distribution w/o SC and CSR

(Using **10M** and **1B** particles)



Microbunching Instability

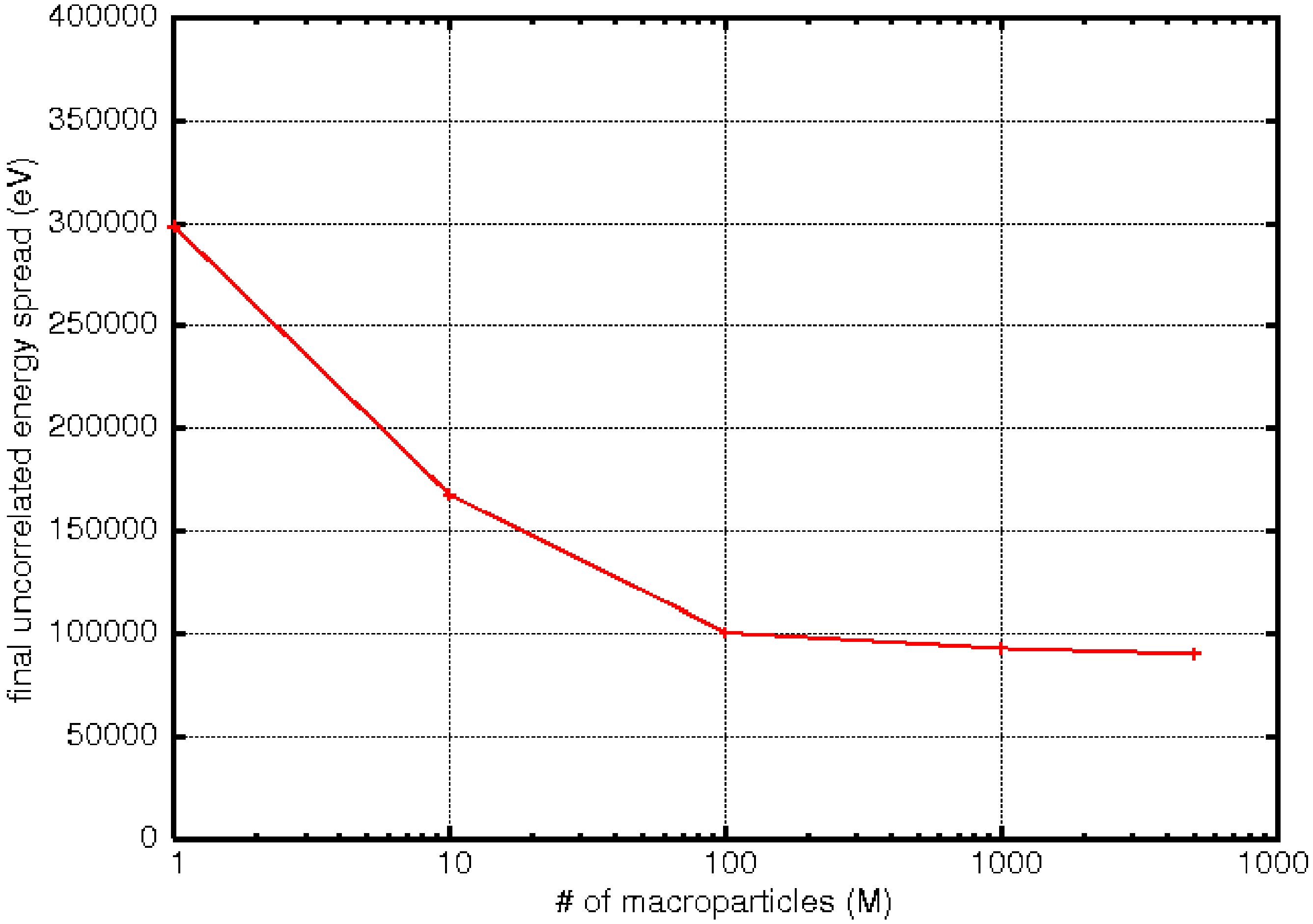
- Initial density modulation induces energy modulation through long. impedance Z(k), converted to more density modulation by a chicane ➔ growth of slice energy spread / emittance!



Courtesy of Z. Huang, SLAC

Predicting Uncorrelated Energy Spread in Future Light Sources: Convergence Studies up to 5 Billion Particles

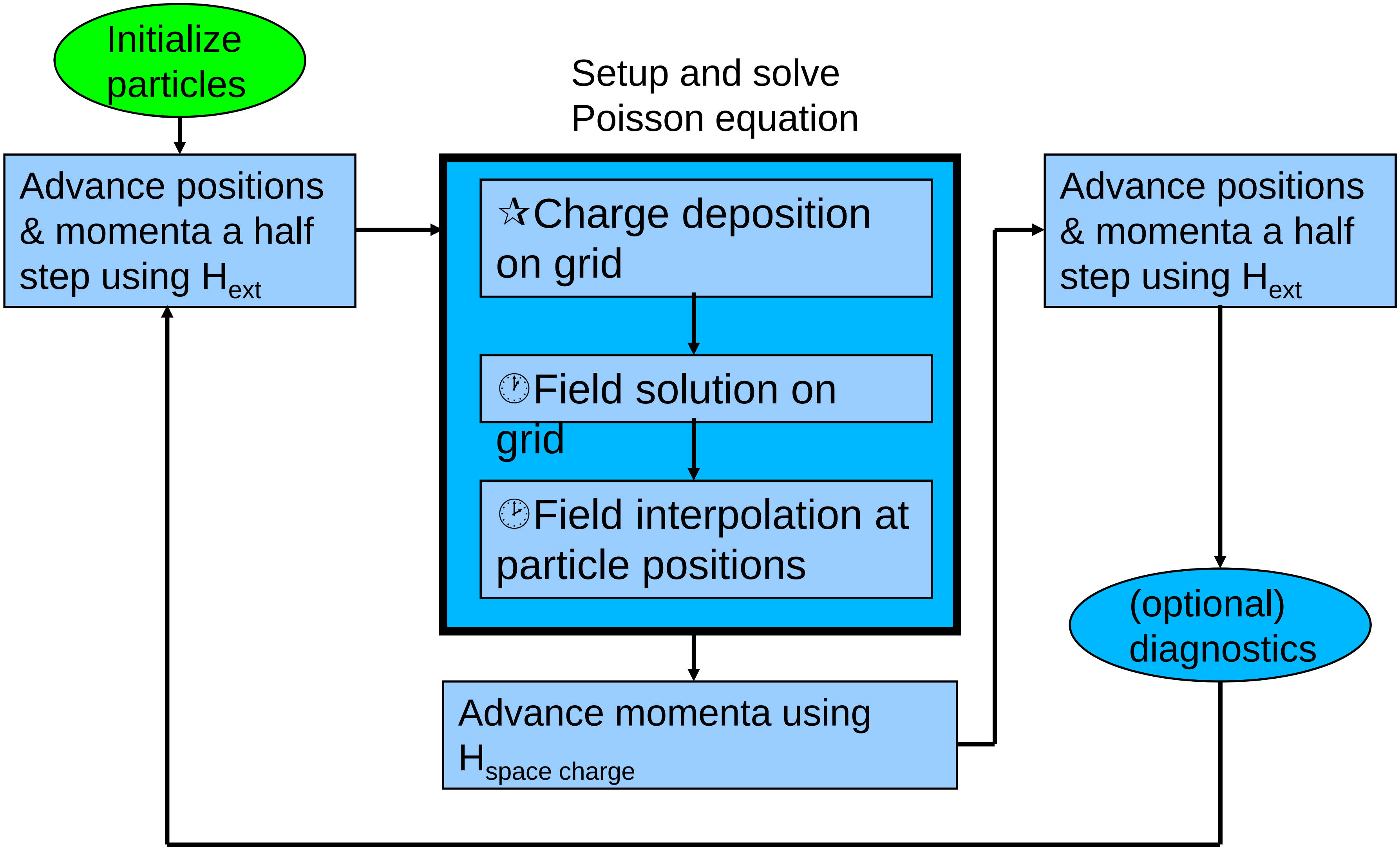
IMPACT-Z Uncorrelated Energy Spread versus # of Macroparticles: 10M, 100M, 1B, 5B



Current Features of the IMPACT Code

- External Beam Line Elements:
  - Quadrupole, Dipole, Solenoid + RF gap, 3D constant focusing channel, Sextupole, Octupole, Decapole
  - DTL, CCDTL, CCL, SC, User-defined element
- Two Numerical Integraors:
  - Linear Map
  - Nonlinear Lorentz Force Integrator
- 3D Space Charge with 6 Types of Boundary Conditions
- Transverse, longitudinal short range wakefields and CSR wakefields
- Multiple Charge States
- Two types of parallel implementations:
  - Domain decomposition with dynamic load balance
  - Particle-field decomposition
- Pre and post-processing codes

Particle-In-Cell Simulation with Split-Operator Method



Initialize particles

Advance positions & momenta a half step using H_{ext}

Setup and solve Poisson equation

☆Charge deposition on grid

🕐Field solution on grid

🕐Field interpolation at particle positions

Advance momenta using $H_{space\ charge}$

Advance positions & momenta a half step using H_{ext}

(optional) diagnostics

Courtesy of R. Ryne

Green Function Solution of Poisson's Equation (with 3D Open Boundary Conditions)

$$\phi(r) = \int G(r, r')\rho(r')dr'$$

$$\phi(r_i) = h\sum_{i'=1}^{N} G(r_i - r_{i'})\rho(r_{i'})$$

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

Direct summation of the convolution scales as N^6 !!!!
N – grid number in each dimension

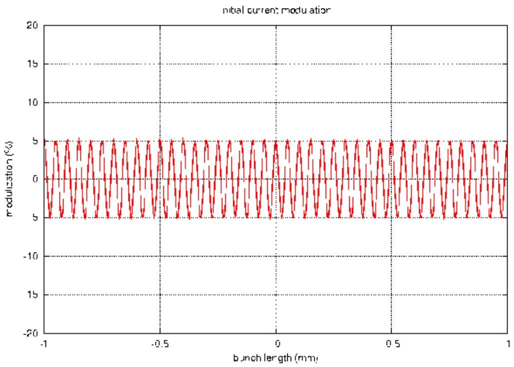
Hockney's Algorithm:- scales as $(2N)^3\log(2N)$

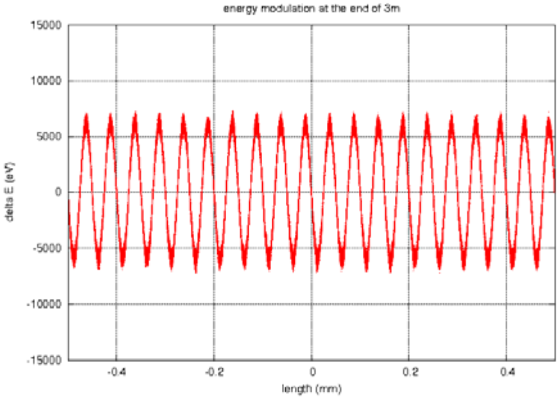
- Ref: Hockney and Easwood, ***Computer Simulation using Particles***, McGraw-Hill Book Company, New York, 1985.

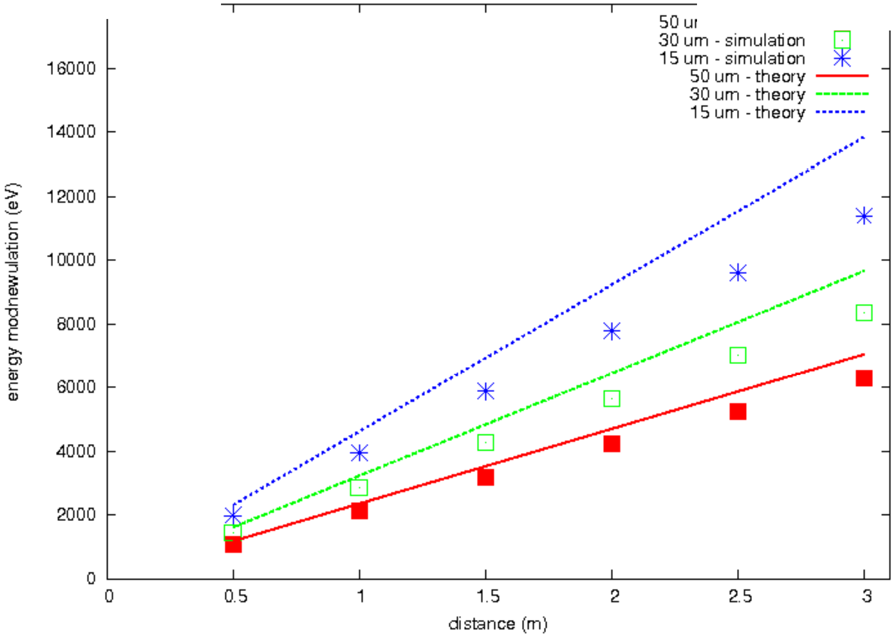
$$\phi_c(r_i) = h\sum_{i'=1}^{2N} G_c(r_i - r_{i'})\rho_c(r_{i'})$$

$$\phi(r_i) = \phi_c(r_i) \quad \text{for i} = 1, \text{N}$$

Space-Charge Driven Energy Modulation vs. Distance in a Drift Space







Calculation Longitudinal and Transverse Wakefield Using FFT

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

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

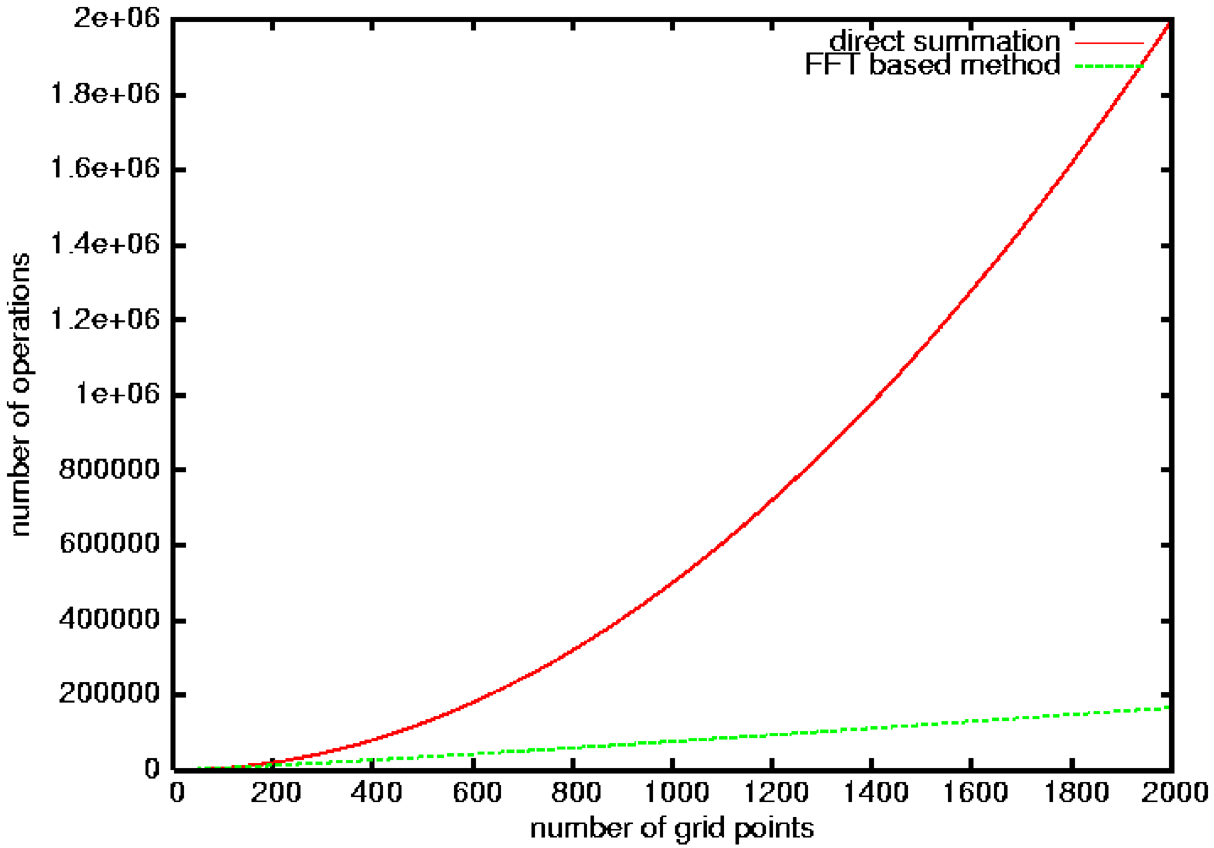
$$F(s) = \int_{-\infty}^{+\infty} G(s-s')\rho(s')ds'$$

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

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

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

Computing Operation Comparison between the Direct Summation and the FFT Based Method



1D CSR Wake Field Including Transient Effects

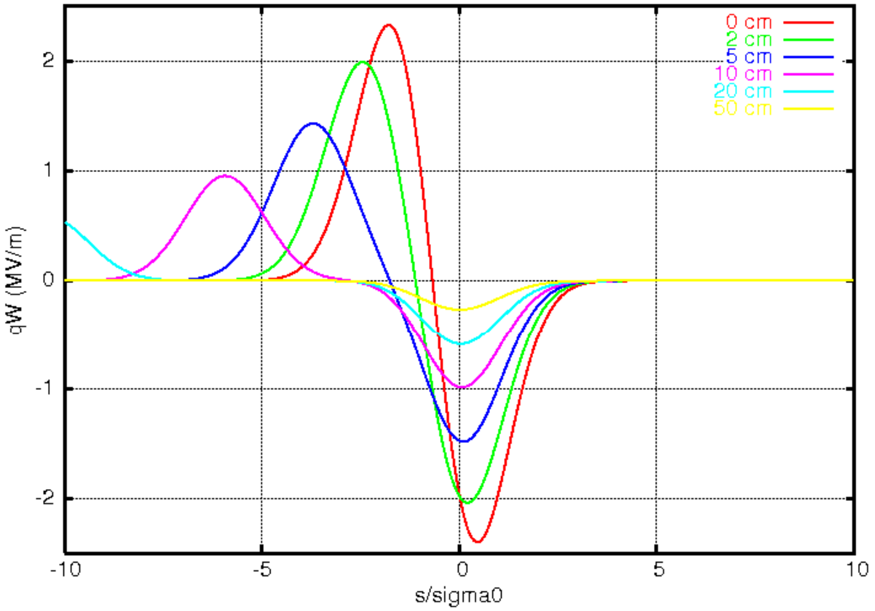
$$\frac{dE(s,\phi)}{cdt} = -\frac{2e^2}{4\pi\epsilon_0 3^{1/3} R^{2/3}}\left(\int_{s-s_L}^{s} \frac{1}{(s-s')^{1/3}}\frac{\partial\lambda(s')}{\partial s'}ds' + \frac{\lambda(s-s_L)-\lambda(s-4s_L)}{s_L^{1/3}}\right)$$

$$W(s) = \begin{cases} -\frac{4}{R}\frac{1}{(\phi_m+2x)}\lambda(s-\frac{R}{6}\phi_m^2(\phi_m+3x)) & for\ source\ in\ front\ of\ the\ bend \\ \frac{4}{R}\left(\frac{\lambda(s-\Delta s_{max})}{(\phi_m+2x)} + \int_{s-\Delta s_{max}}^{s}\frac{1}{\psi+2x}\frac{\partial\lambda}{\partial s'}ds'\right) & for\ source\ inside\ the\ bend \end{cases}$$

$$s - s' = \frac{R\psi^3}{24}\frac{\psi+4x}{\psi+x}$$

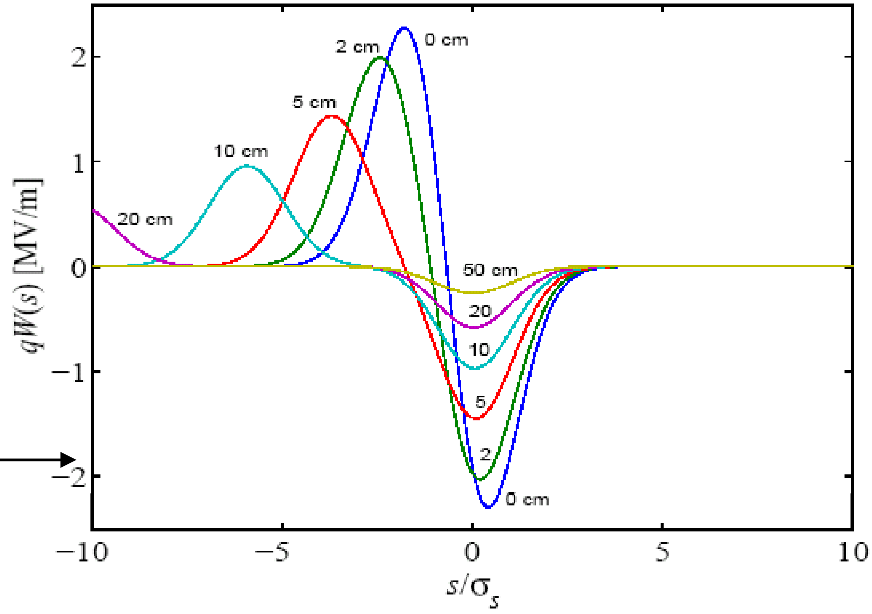
Ref: 1) E. L. Saldin, E. A. Schneidmiller, and M. V. Yurkov,
Nucl. Instrum. Methods Phys. Res., Sect. A398, 373 (1997).
2) M. Borland, Phys. Rev. Sepecial Topics - Accel. Beams 4, 070701 (2001).
3) G. Stupakov and P. Emma, ``CSR Wake for a Short Magnet in Ultrarelativistic Limit,"
SLAC-PUB-9242, 2002.

Test of the CSR Wake Implementation for a Short Bend



R = 1.5 m, Arc=10 cm

From G. Stupakov and P. Emma



Up Sampling of Initial Particle Distribution

—Maintain global properties of the original distribution

- emittances
- current profile,
- energy-position correlation

—Reduce shot noise of the original particle distribution by using more macroparticles

—A 6D box centered at the original is used to generate new macroparticles

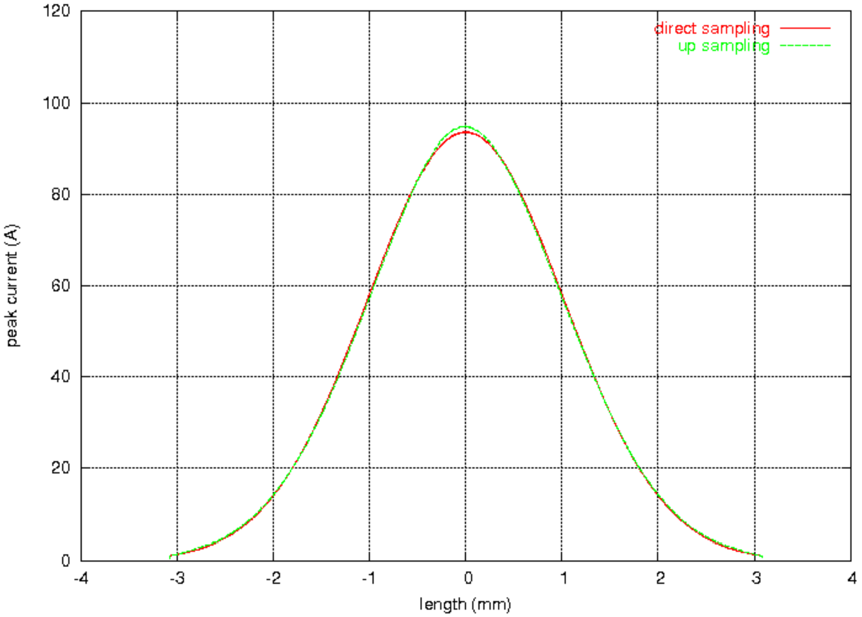
—Uniform sampling in transverse 4D

—Linear sampling in longitudinal position following original current profile

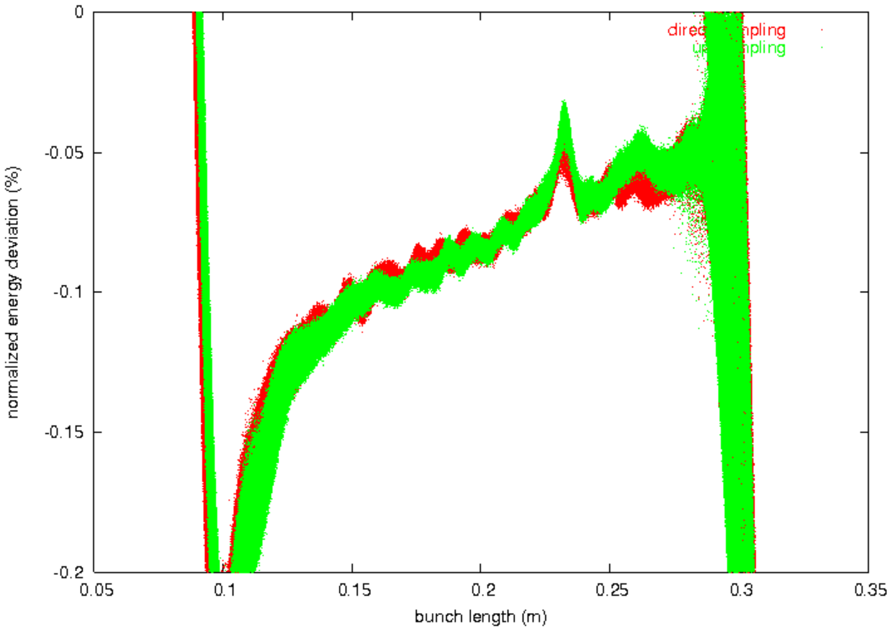
—Cubic spline to obtain the energy-position correlation

A Comparison of Direct Sampling and Up Sampling

Initial current profile from direct sampling and up sampling



Final longitudinal phase space from direct sampling and up sampling

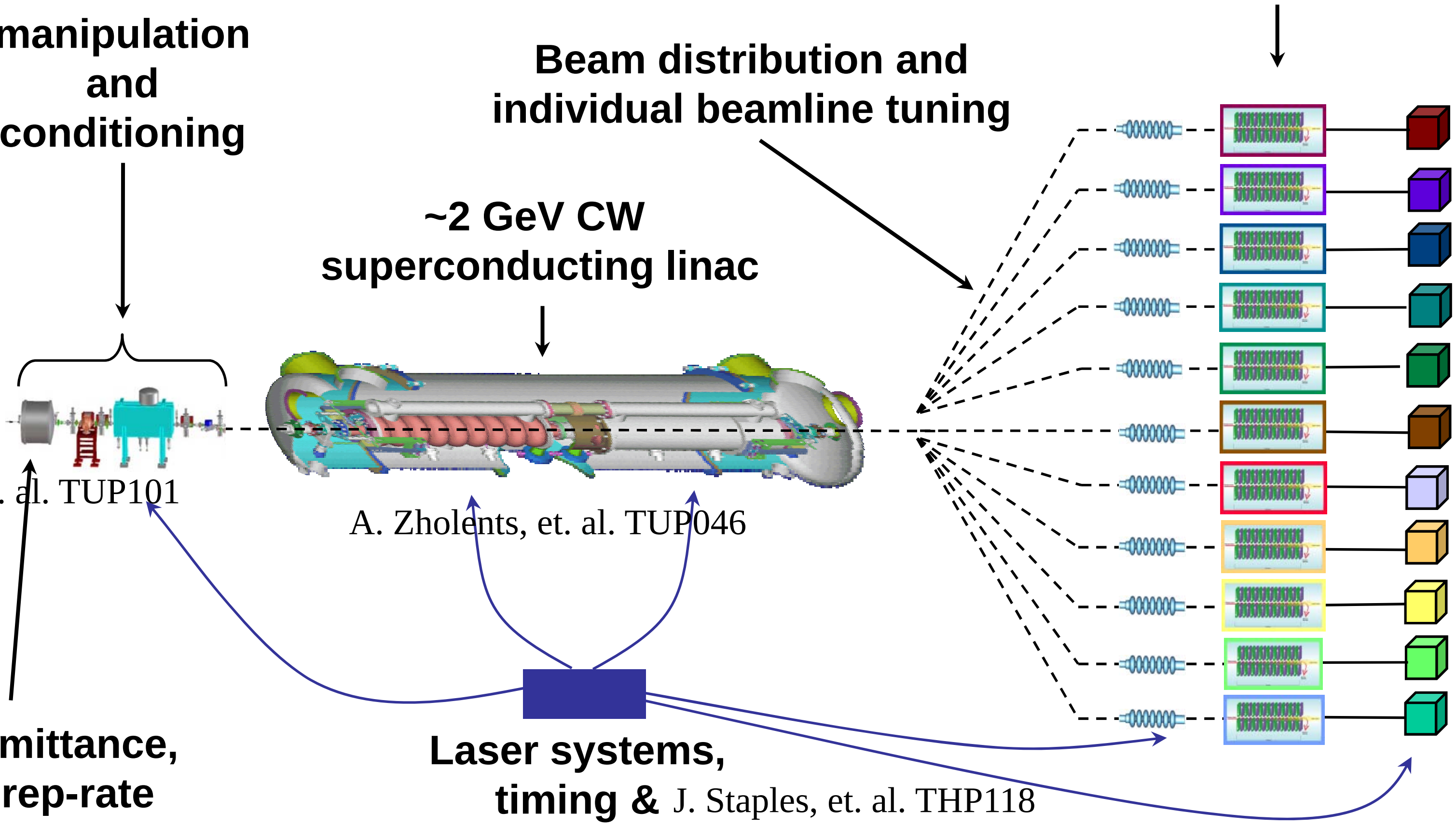


Vision for a Future Light Source Facility at LBNL

A HIGH REP-RATE, SEEDED, VUV — SOFT X-RAY FEL ARRAY

Courtesy of J. Corlett, LBL

Array of configurable FELs
Independent control of wavelength, pulse duration, polarization
Configured with an optical manipulation technique; seeded, attosecond, ESASE



Beam manipulation and conditioning

Beam distribution and individual beamline tuning

~2 GeV CW superconducting linac

W. Wan, et. al. TUP101

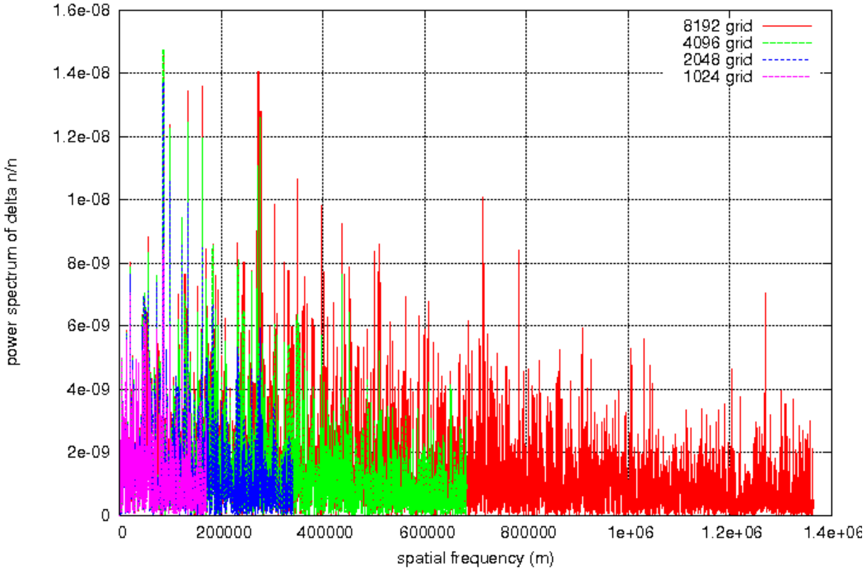
A. Zholents, et. al. TUP046

Low-emittance, high rep-rate electron gun

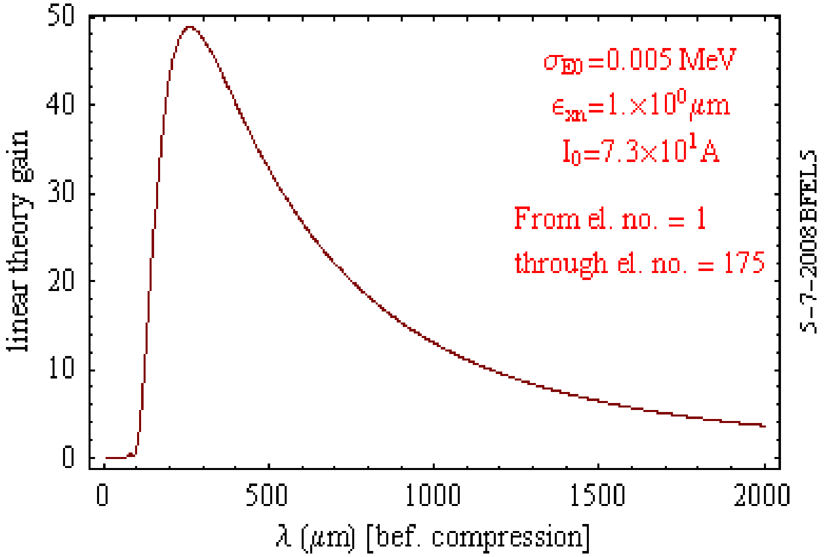
Laser systems, timing & synchronization J. Staples, et. al. THP118

Choice of Numerical Grid Point

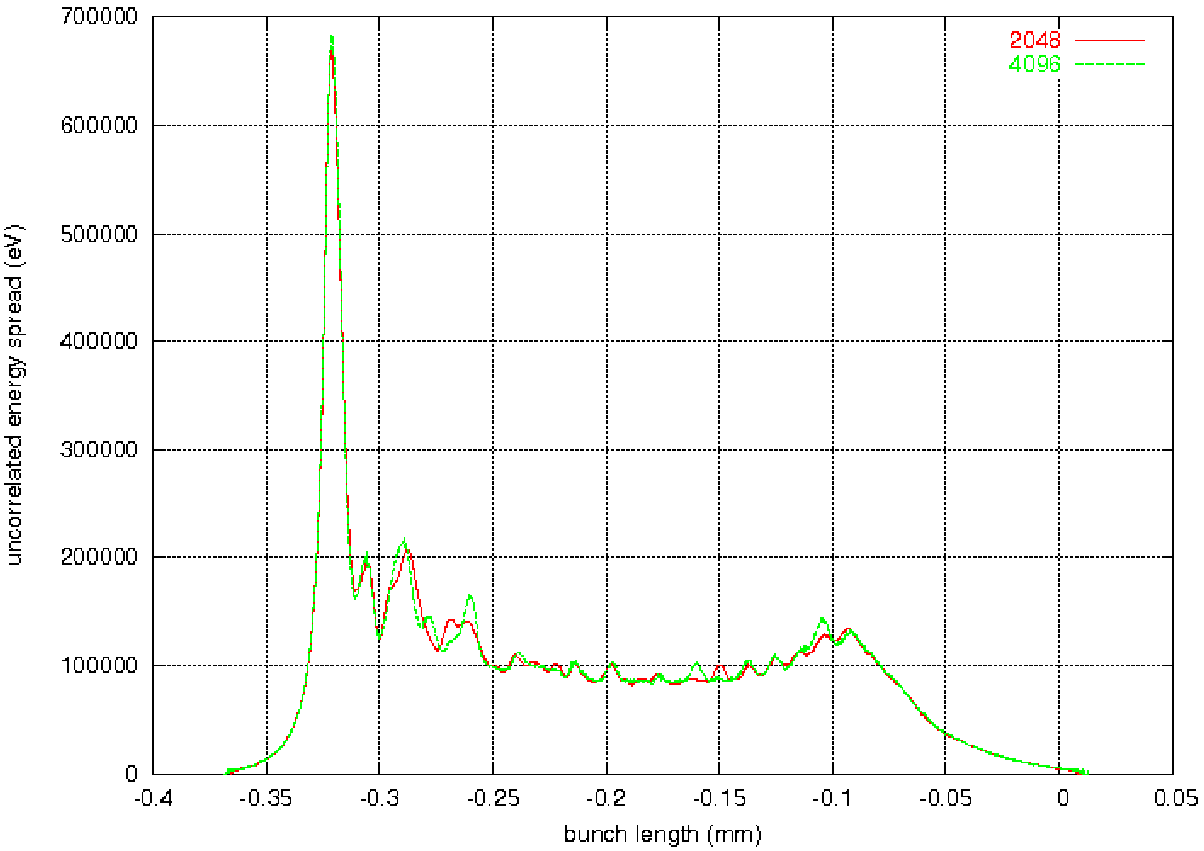
power spectrum of density fluctuation with different grid points



linear uBI gain function vs. wave length

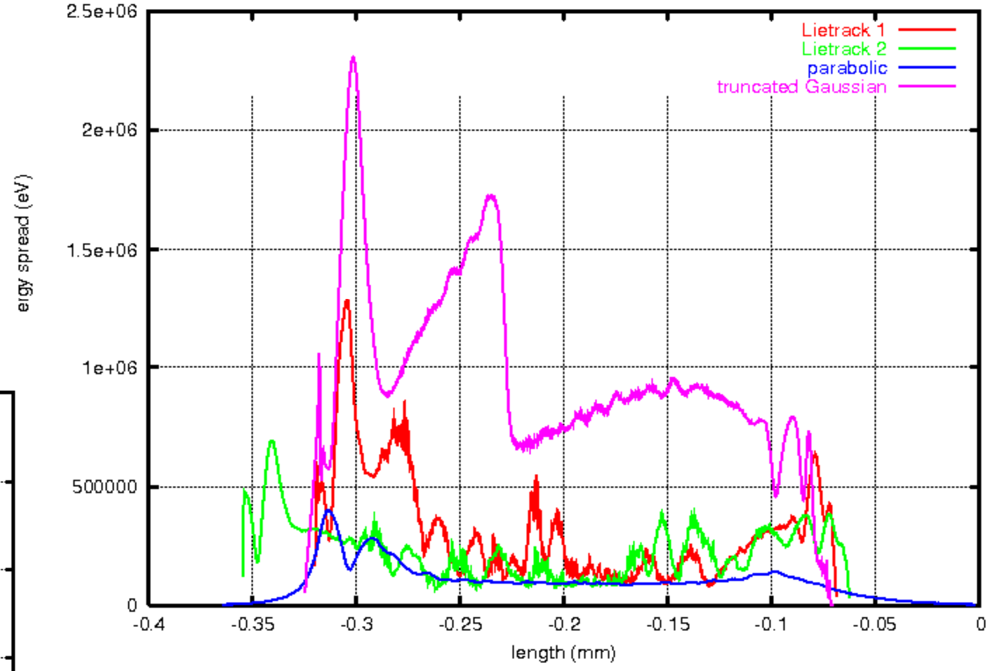


Final Uncorrelated Energy Spread with Different Number of Grid

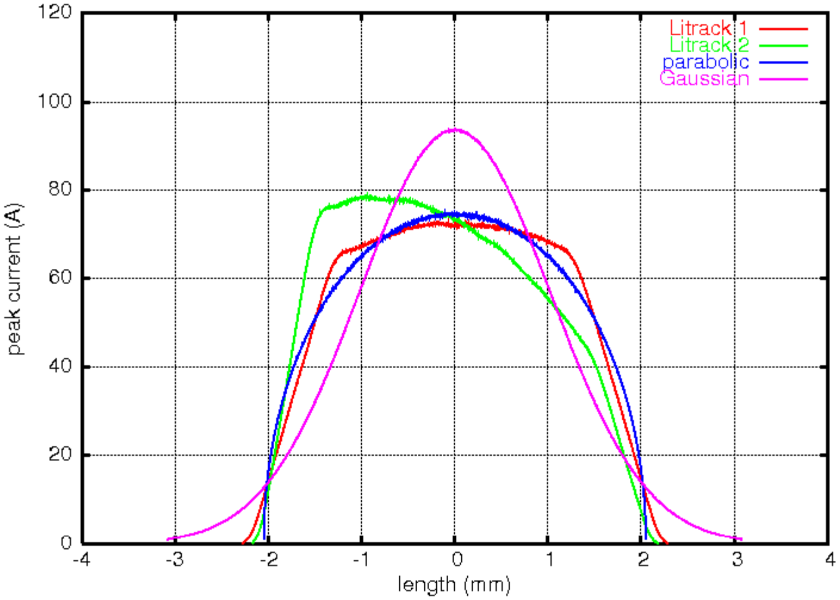


Effects of Initial Current Profiles

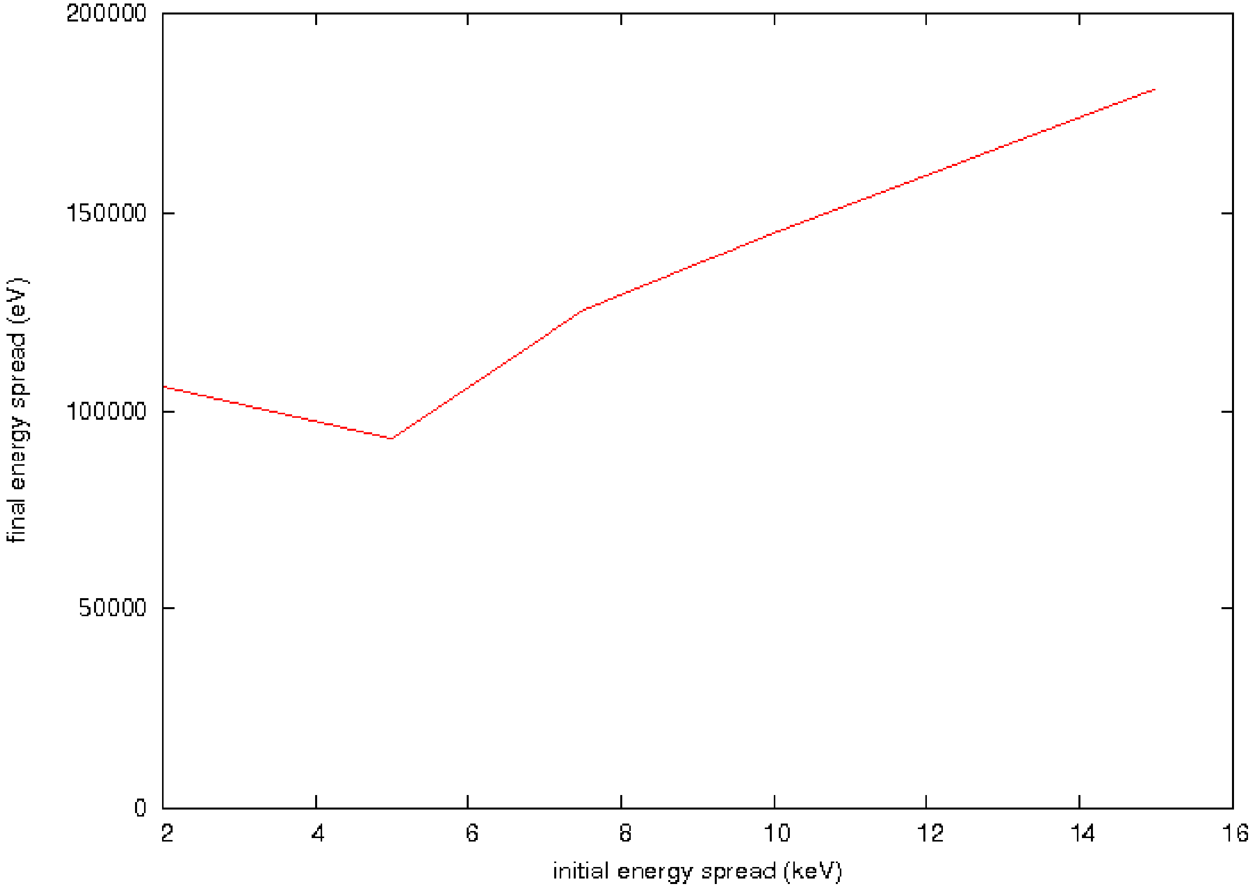
final energy spread with different initial current profiles



four types of initial current profiles

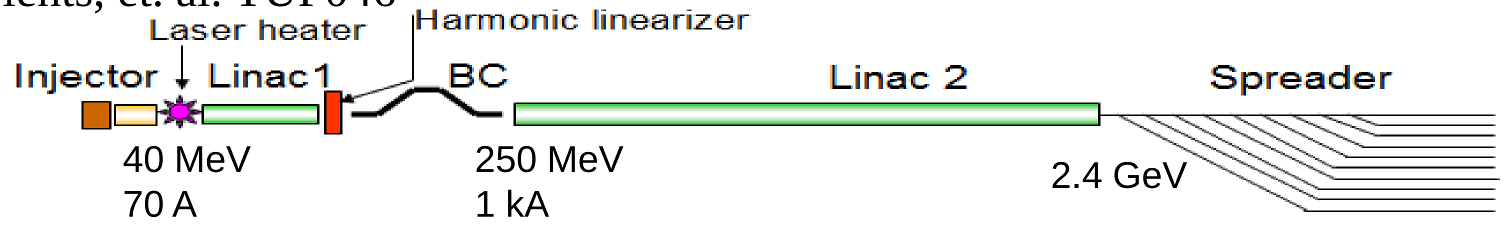


Final Energy Spread vs. Initial Uncorrelated Energy Spread



Final Longitudinal Phase Space Distribution
(5 billion Particle Simulation)

A. Zholents, et. al. TUP046



Laser heater

Harmonic linearizer

Injector

Linac1

BC

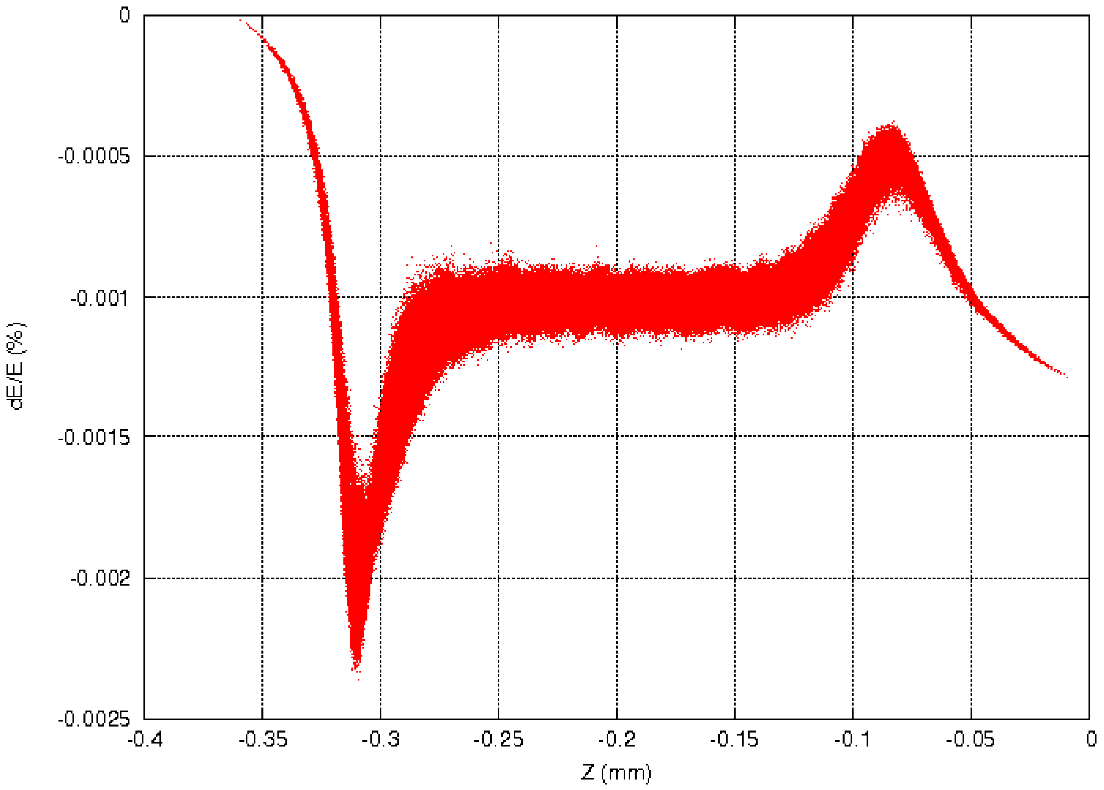
Linac 2

Spreader

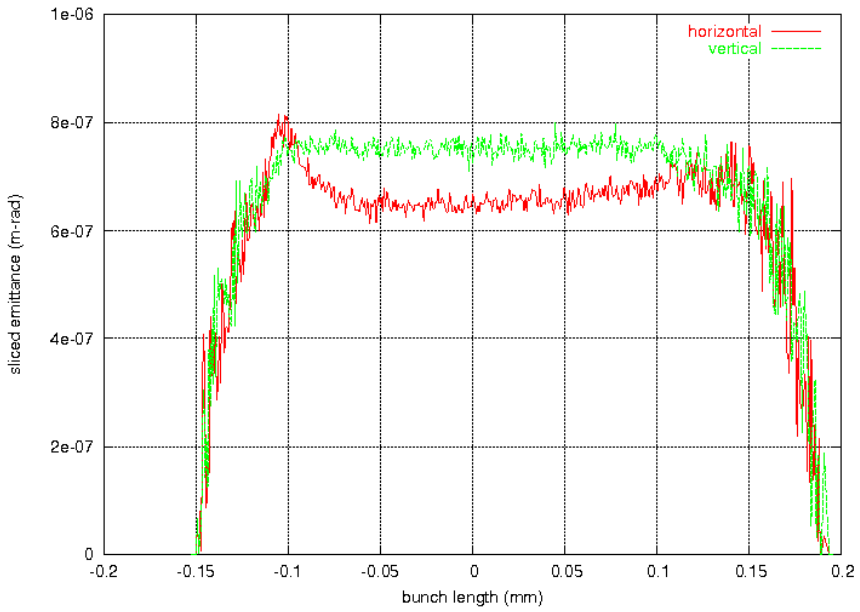
40 MeV
70 A

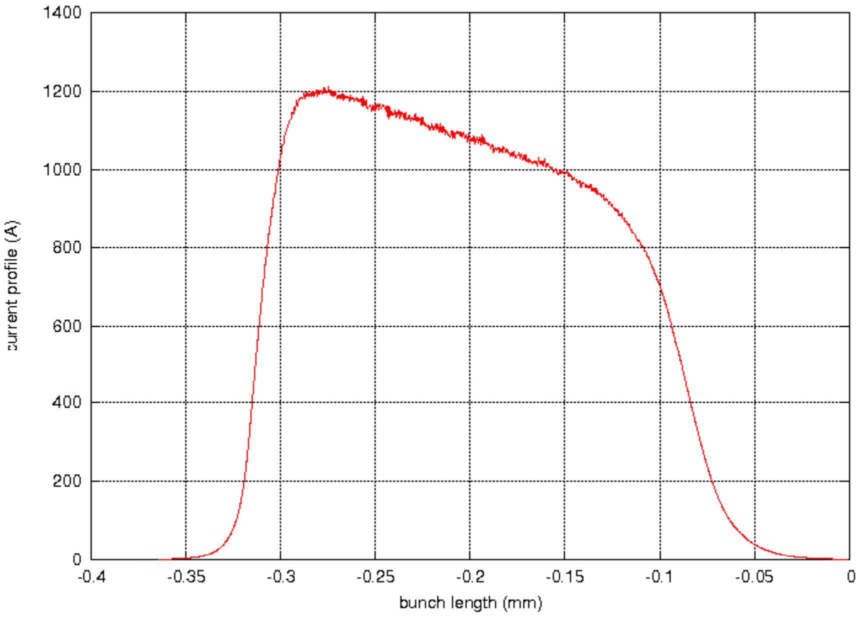
250 MeV
1 kA

2.4 GeV



Final Transverse Slice Emittance and Peak Current Profile





Summary and Future Plans

—Large number of macroparticles are needed for accurately simulation of electron beam transport through linac subject to microbunching instability

—Current linac design satisfy the performance requirements for an array of soft X-ray FELs.

—Integration of large scale linac simulation together injector simulation

—Benchmark simulations with experimental measurements