A Parallel Multi-Physics Beam Dynamics Simulation Package: IMPACT

Ji Qiang

JLEIC Collaboration Meeting, Oct. 5-7, 2016, JLab

BERKELEY LAB
U.S. DEPARTMENT OF ENERGY | Office of Science
ACCELERATOR TECHNOLOGY & APPLIED PHYSICS DIVISION ATAP

Berkeley Lab Accelerator Simulation Toolkit

http://blast.lbl.gov

Detailed modeling of:

- beams, plasmas, laser-plasma inter., linacs, rings, injectors, plasma accelerators, traps, ...

Using state-of-the-art codes:

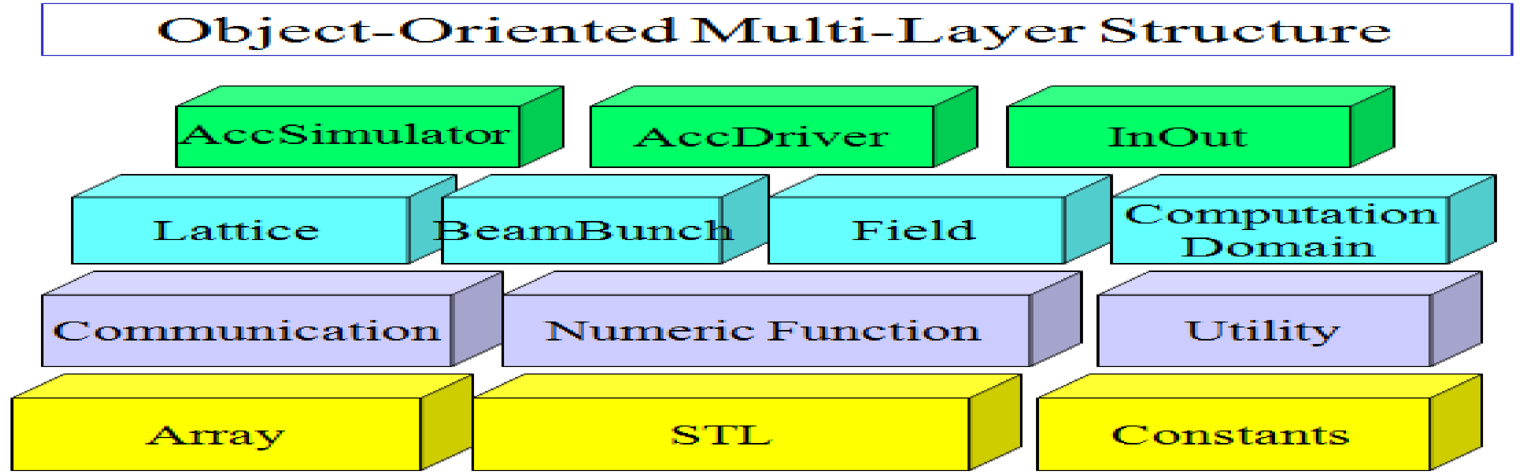
- BEAMBEAM3D, IMPACT, INF&RNO, POSINST, WARP.

With original advanced algorithms:

- boosted frame, IGF, laser envelope, SEY, AMR, relativ. particle pusher, EM spectral Circ, ...

IMPACT: Integrated Map and Particle Tracking Code

- The IMPACT(-Z depend.) started around middle of 90s (R. Ryne) including:
  - Drift, Quadrupole, RF linear transfer map
  - one 3D space-charge solver with open BCs
  - a few thousand lines of High Performance Fortran (HPF) code
- Redesign of the IMPACT code around the end of 90s (J. Qiang):
  - object-oriented design and implementation using F90
  - domain decomposition parallelization using MPI
  - multiple 3D space-charge solvers with open BCs, periodic BCs, conducting pipes



IMPACT: Recent Advances

- Current Features (with >100,000 lines of code) include:
  - Z dependent and T dependent tracking
  - Detailed 3D RF accelerating and focusing model, dipole, solenoid, multipole, ...
  - Multiple charge states, multiple bunches
  - 3D shifted-integrated Green's function space-solver
  - 3D spectral finite difference multigrid space-solver
  - Structure + resistive wall wakefields
  - CSR/ISR
  - Gas ionization
  - Photo-electron emssion
  - Machine errors and steering
- Can be used to model beam dynamics in:
  - Photoinjectors
  - Ion beam formation and extraction
  - RF linacs
  - Rings

Governing Equations in the IMPACT Code

$$\frac{\partial f(\vec{r},\vec{p},t)}{\partial t}+\dot{\vec{r}}\frac{\partial f(\vec{r},\vec{p},t)}{\partial \vec{r}}+\dot{\vec{p}}\frac{\partial f(\vec{r},\vec{p},t)}{\partial \vec{p}}=0$$

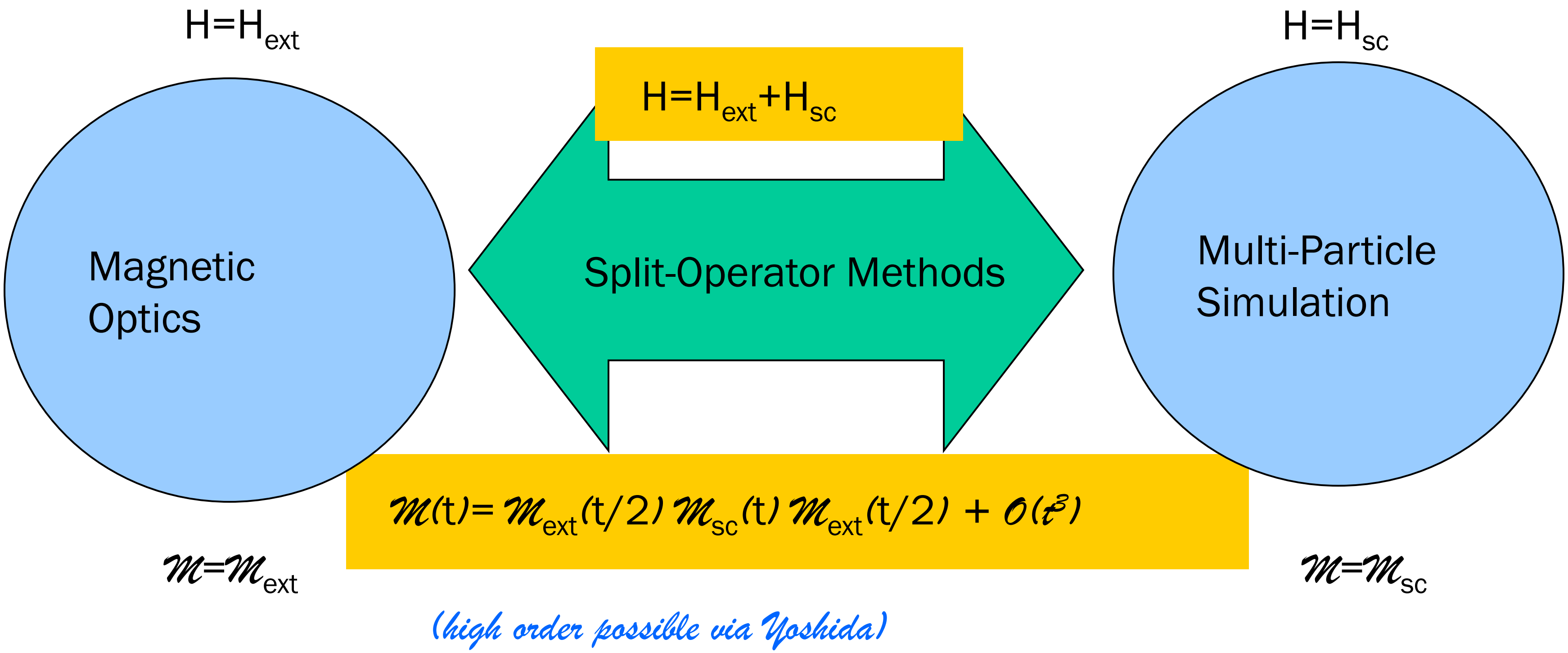
$$\dot{\vec{r}}=\frac{\partial H}{\partial \vec{p}}$$

$$\dot{\vec{p}}=-\frac{\partial H}{\partial \vec{r}}$$

$$H \doteq H_{ext}+H_{sc}$$

$$\nabla^2\phi=-\rho/\varepsilon \qquad \rho=\iiint f(r,p,t)d^3p$$

Split-Operator Method for Particle Advance



- Rapidly varying s-dependence of external fields is decoupled from slowly varying space charge fields
- Leads to very efficient particle advance:
  - Do not take tiny steps to push millions - billions of particles
  - Do take tiny steps to compute maps; then push particles w/ maps

Different Boundary/Beam Conditions Need Different Efficient Numerical Algorithms O(Nlog(N)) or O(N)

FFT based Green function method:

- Standard Green function: low aspect ratio beam
- Shifted Green function: separated particle and field domain
- Integrated Green function: large aspect ratio beam
- Non-uniform grid Green function: 2D radial non-uniform beam

Fully open boundary conditions

Spectral-finite difference method:

2D open boundary
Transverse regular pipe with longitudinal open

Multigrid spectral-finite difference method:

Transverse irregular pipe

J. Qiang, S. Paret, "Poisson solvers for self-consistent multiparticle simulations," ICFA Mini-Workshop on Beam-Beam Effects in Hadron Colliders, March 18-22, 2013.

Green Function Solution of Poisson's Equation (I) (open boundary conditions)

$$\phi(r) = \int G(r, r')\rho(r')dr' \qquad ; \; r = (x, y, z)$$

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

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

Direct summation of the convolution scales as N^2 !!!!
N – total number of grid points

FFT based Hockney's Algorithm /zero padding:- *scales as (2N)log(2N)*

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

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

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

Integrated Green Function Method (II)

(large aspect ratio beam with open boundary conditions)

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

$$\boxed{G_i(r,r') = \int G_s(r,r')\,dr'}$$

integrated Green function

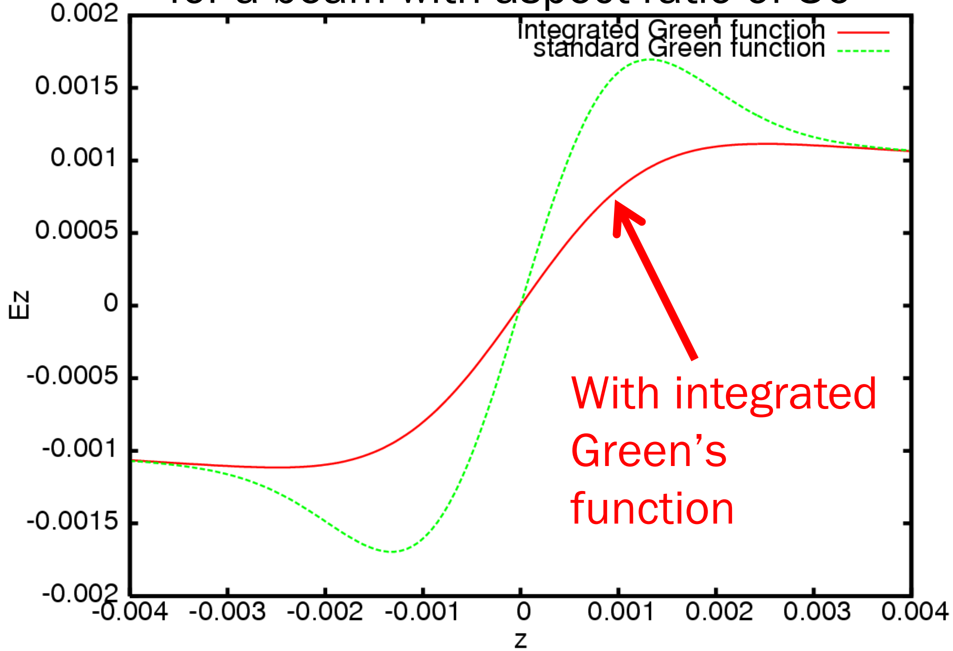
$$\boxed{G_s(x,y,z) = 1/\sqrt{(x^2+y^2+z^2)}}$$

standard Green function

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

(O(N log N))

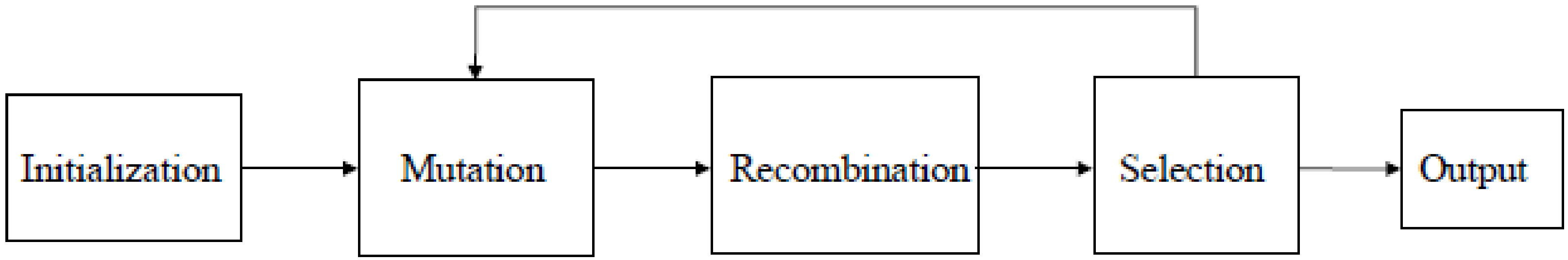
Comparison between the IG and SG for a beam with aspect ratio of 30



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).

Evolutionary Algorithm for Global Optimization



Differential Evolution Algorithm

- A population of control parameter vectors are randomly generated from the control parameter space.
- A new perturbed vector $\vec{v}_i$ is generated for each parent $\vec{x}_i$ using one of several mutation strategies.
- A trial control parameter vector is generated by:

$$\vec{U}_i = (u_{i1}, u_{i2}, \cdots, u_{iD}) \qquad \text{rand}_j \in [0,1]$$

$$u_{ij} = \begin{cases} v_{ij}, & \text{if} \quad \text{rand}_j \le CR \quad \text{or} \quad j = \text{mbr}_i \\ x_{ij}, & \text{otherwise} \end{cases} \qquad \text{mbr}_i \in \{1, 2, \ldots, D\}$$

- If the trial vector produces a better objective function value than $\vec{x}_i$, it will be put into the next generation. Otherwise, the original parent vector is kept in the next generation.

R. Storn and K. Price, Journal of Global Optimization 1a1:341-359, (1997).

An Adaptive Unified Differential Evolution Algorithm

Some standard DE mutation strategies:

DE/rand/1: $\vec{v}_i = \vec{x}_{r1} + F_{xc}(\vec{x}_{r2} - \vec{x}_{r3})$

DE/rand/2: $\vec{v}_i = \vec{x}_{r1} + F_{xc}(\vec{x}_{r2} - \vec{x}_{r3}) + F_{xc}(\vec{x}_{r4} - \vec{x}_{r5})$

DE/current-to-best/1: $\vec{v}_i = \vec{x}_i + F_{cr}(\vec{x}_b - \vec{x}_i) + F_{xc}(\vec{x}_{r1} - \vec{x}_{r2})$

DE/current-to-rand/1: $\vec{v}_i = \vec{x}_i + F_{cr}(\vec{x}_{r1} - \vec{x}_i) + F_{xc}(\vec{x}_{r2} - \vec{x}_{r3})$

DE/rand-to-best/1: $\vec{v}_i = \vec{x}_i + F_{cr}(\vec{x}_b - \vec{x}_i) + F_{xc}(\vec{x}_{r2} - \vec{x}_{r3})$

. . .

randomly chosen solutions

current solution

best solution

Unified DE mutation strategy (uDE):

$$\vec{v}_i = \vec{x}_i + F_1(\vec{x}_b - \vec{x}_i) + F_2(\vec{x}_{r1} - \vec{x}_i) + F_3(\vec{x}_{r2} - \vec{x}_{r3}) + F_4(\vec{x}_{r4} - \vec{x}_{r5})$$

Encompasses standard DE mutation strategies as special cases. Four control parameters + CR.

J. Qiang and C. Mitchell, in OO digest, 2015.

Integration of Self-Consistent Beam Dynamics Simulation with Design Parameter Optimization

A new parallel adaptive unified variable population external storage parallel multi-objective differential evolution (VPES-PMDE) algorithm for multi-objective optimization.

1. Define the minimum size, *NPmin* and the maximum size, *NPmax* of the parent population. Define the maximum size of external storage, *NPext*.

2. Generate an initial population of *NPini* parameter vectors randomly to uniformly cover the entire solution space.

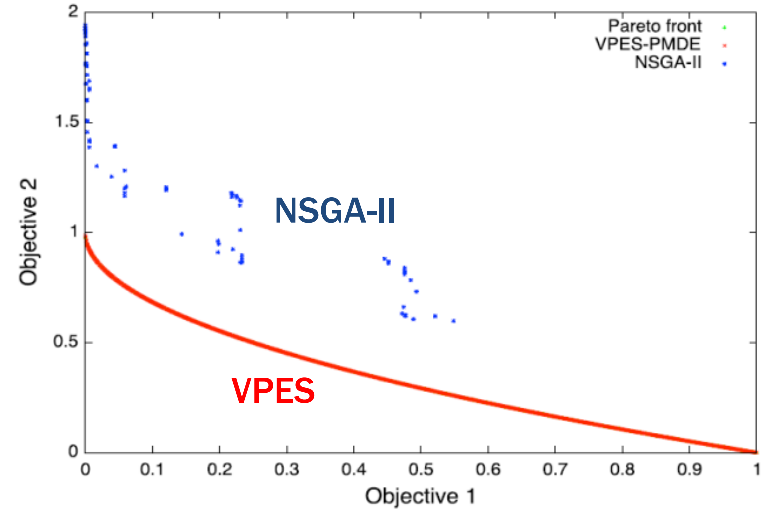
3. Generate an offspring population using the differential evolutionary algorithm.

4. Check the new population against boundary conditions and constraints.

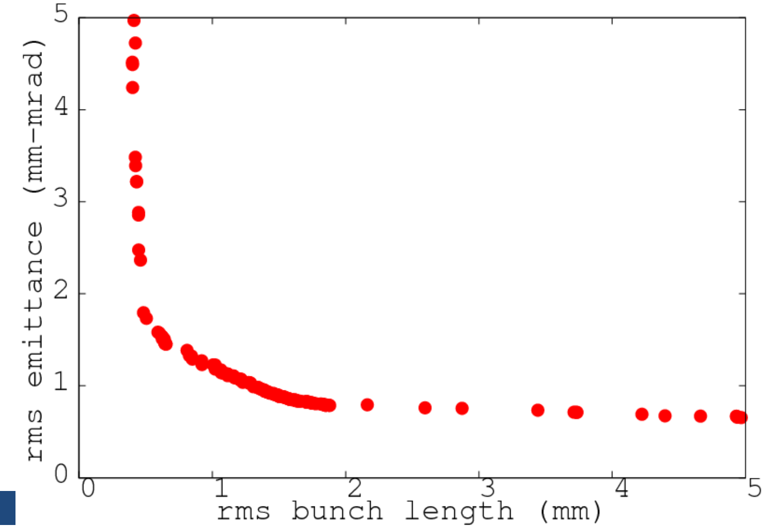
5. - Combine the new population with the existing parent population from external storage and determine the non-dominated solutions (*Ndom*).
   - Move *min(Ndom, NPext)* solutions back into external storage. Pruning is used if *Ndom>NPext*.
   - Select *NP* parent solutions from this group of solutions for next generation production.

6. If *NPmin* <= *Ndom*<=*NPmax*, *NP* = *Ndom*.
   Otherwise, *NP*=*NPmin* if *Ndom*<*NPmin* and *NP*=*NPmax* if *Ndom* > *NPmax*.

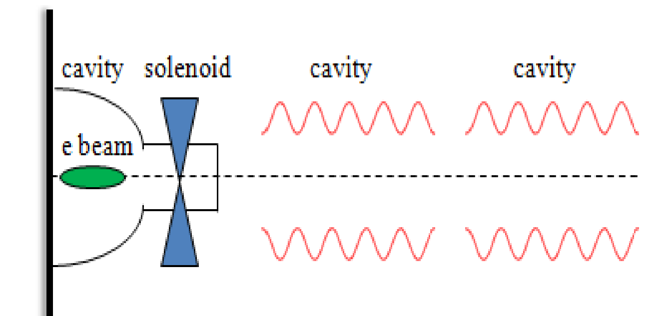
7. If the stopping condition is met, stop. Otherwise, return to Step 3.



A comparison of the optimal test solutions from VPES-PMDE and the popular code NSGA-II



optimal final bunch length and emittance solutions



J. Qiang, C. Mitchell, in the Proc. FEL2014, THP020.

A Fully Symplectic Multi-Particle Tracking Model with Space-Charge Effects

multi-particle Hamiltonian $H(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{p}_1, \mathbf{p}_2, \cdots, s)$

$$H = \sum_i \mathbf{p}_i^2/2 + \frac{1}{2}\sum_i \sum_j q\phi(\mathbf{r}_i, \mathbf{r}_j) + \sum_i q\psi(\mathbf{r}_i)$$

space-charge Coulomb potential

external focusing/acceleration

$$\frac{d\mathbf{r}_i}{ds} = \frac{\partial H}{\partial \mathbf{p}_i}$$

$$\frac{d\mathbf{p}_i}{ds} = -\frac{\partial H}{\partial \mathbf{r}_i}$$

$$\frac{d\zeta}{ds} = -[H, \zeta]$$

A formal single step solution

$$\zeta(\tau) = \exp(-\tau(:H:))\zeta(0)$$

$$\boxed{H = H_1 + H_2}$$

$$\begin{aligned}\zeta(\tau) &= \exp(-\tau(:H_1: + :H_2:))\zeta(0) \\ &= \exp(-\frac{1}{2}\tau :H_1:)\exp(-\tau :H_2:)\exp(-\frac{1}{2}\tau :H_1:)\zeta(0) + O(\tau^3)\end{aligned}$$

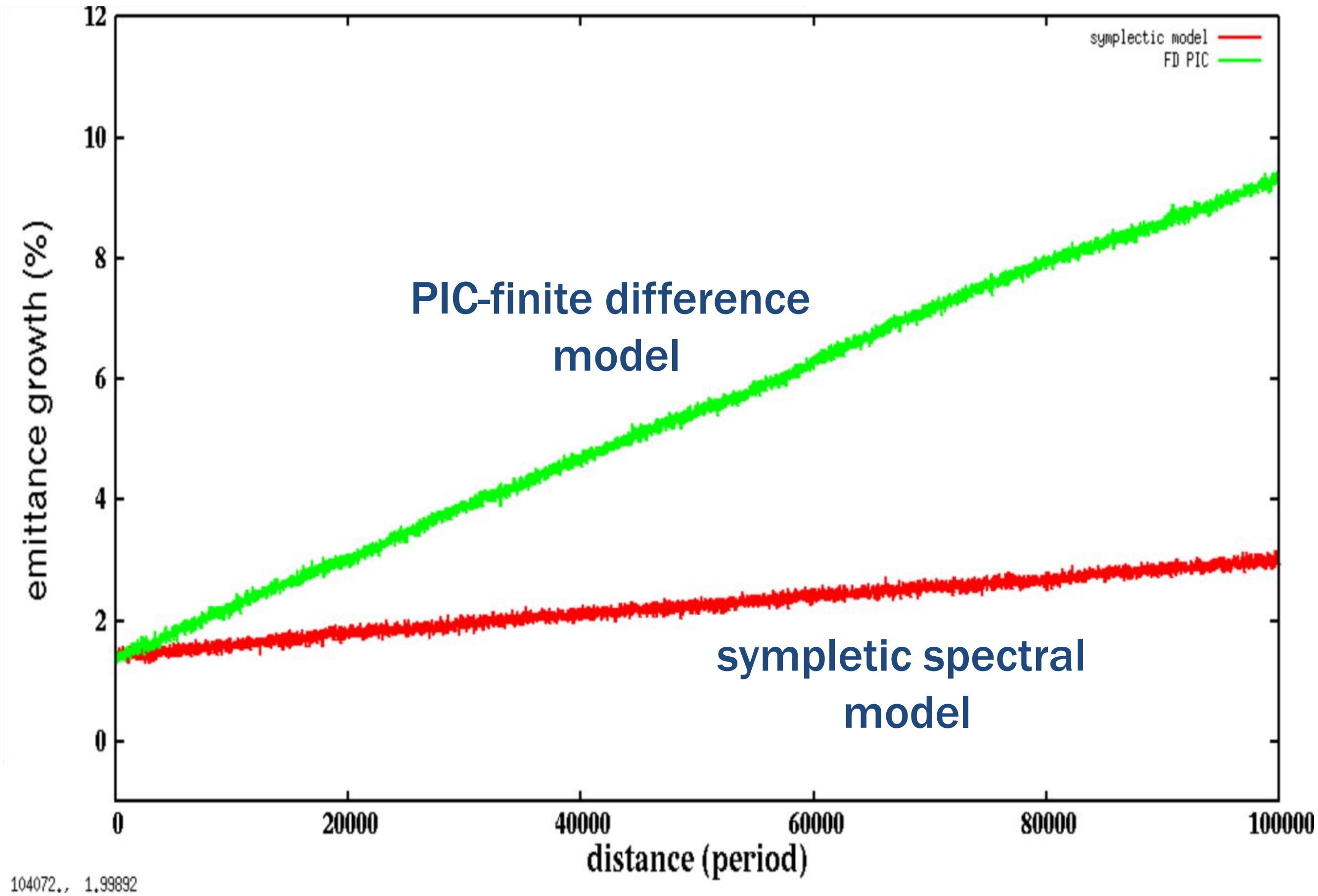
$$\boxed{\begin{aligned}\zeta(\tau) &= \mathcal{M}(\tau)\zeta(0) \\ &= \mathcal{M}_1(\tau/2)\mathcal{M}_2(\tau)\mathcal{M}_1(\tau/2)\zeta(0)\end{aligned}}$$

Single Step Symplectic Map for H_2

$$H_2 = \frac{1}{2\epsilon_0}\frac{8}{abc}w\sum_i\sum_j\sum_l\sum_m\sum_n\frac{1}{\gamma_{lmn}^2}\sin(\alpha_l x_j)\sin(\beta_m y_j)\sin(\gamma_n z_j)\sin(\alpha_l x_i)\sin(\beta_m y_i)\sin(\gamma_n z_i)$$

$$\begin{aligned}
p_{xi}(\tau) &= p_{xi}(0) - \tau\frac{1}{\epsilon_0}\frac{8}{abc}w\sum_j\sum_l\sum_m\sum_n\frac{\alpha_l}{\Gamma_{lmn}^2} \\
&\quad \sin(\alpha_l x_j)\sin(\beta_m y_j)\sin(\gamma_n z_j)\cos(\alpha_l x_i)\sin(\beta_m y_i)\sin(\gamma_n z_i) \\
p_{yi}(\tau) &= p_{yi}(0) - \tau\frac{1}{\epsilon_0}\frac{8}{abc}w\sum_j\sum_l\sum_m\sum_n\frac{\beta_m}{\Gamma_{lmn}^2} \\
&\quad \sin(\alpha_l x_j)\sin(\beta_m y_j)\sin(\gamma_n z_j)\sin(\alpha_l x_i)\cos(\beta_m y_i)\sin(\gamma_n z_i) \\
p_{zi}(\tau) &= p_{zi}(0) - \tau\frac{1}{\epsilon_0}\frac{8}{abc}w\sum_j\sum_l\sum_m\sum_n\frac{\gamma_n}{\Gamma_{lmn}^2} \\
&\quad \sin(\alpha_l x_j)\sin(\beta_m y_j)\sin(\gamma_n z_j)\sin(\alpha_l x_i)\sin(\beta_m y_i)\cos(\gamma_n z_i)
\end{aligned}$$

Much Less Numerical Emittance Growth Using the Symplectic Spectral Model

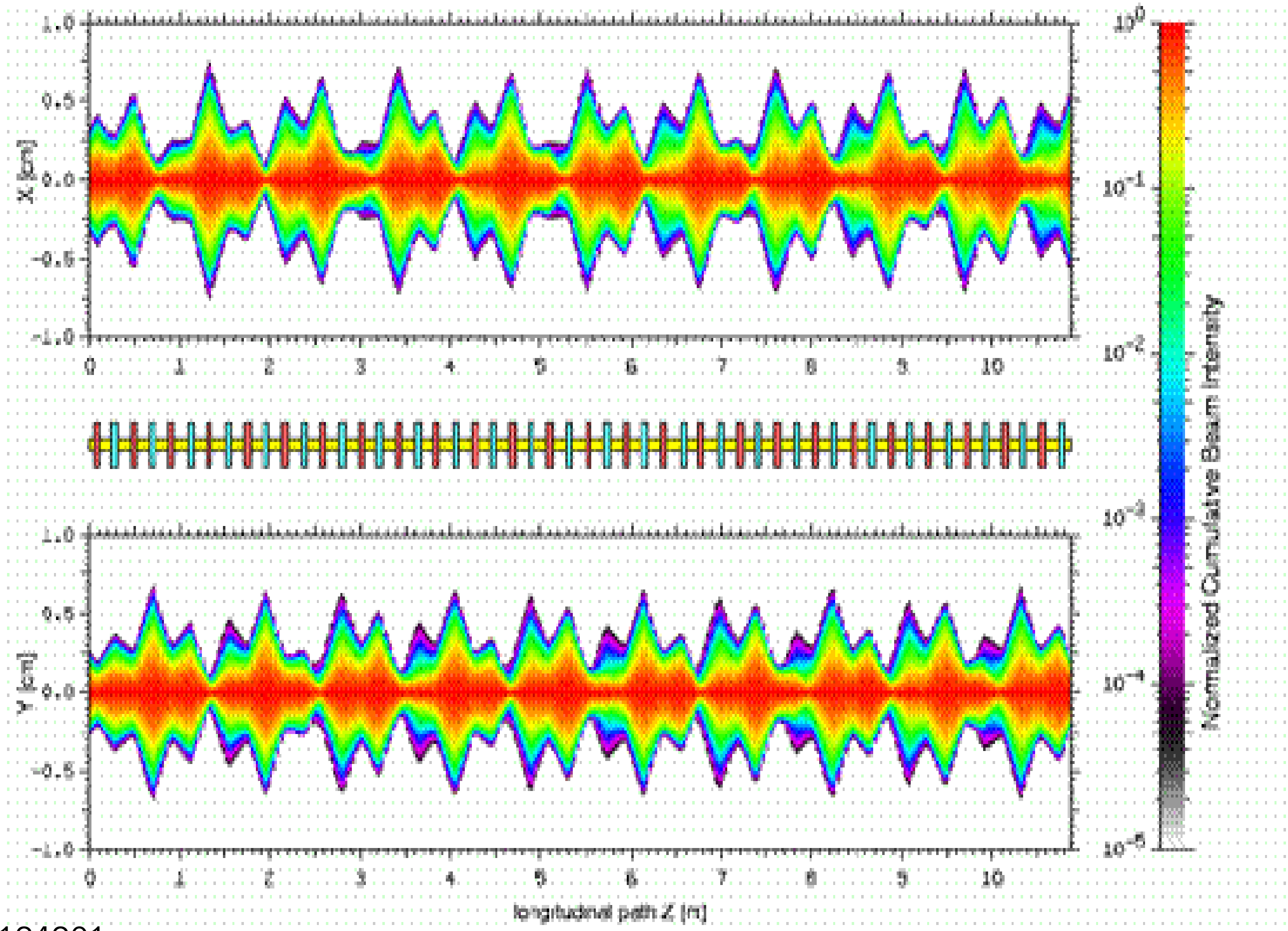


Some Application Examples of the IMPACT Code

- Simulation of a high intensity proton beam halo experiment
- Simulation of space-charge driven coupling resonance in PS
- Simulation of space-charge effects in next generation light sources

Macroparticle Simulation of a Proton Beam Halo Experiment

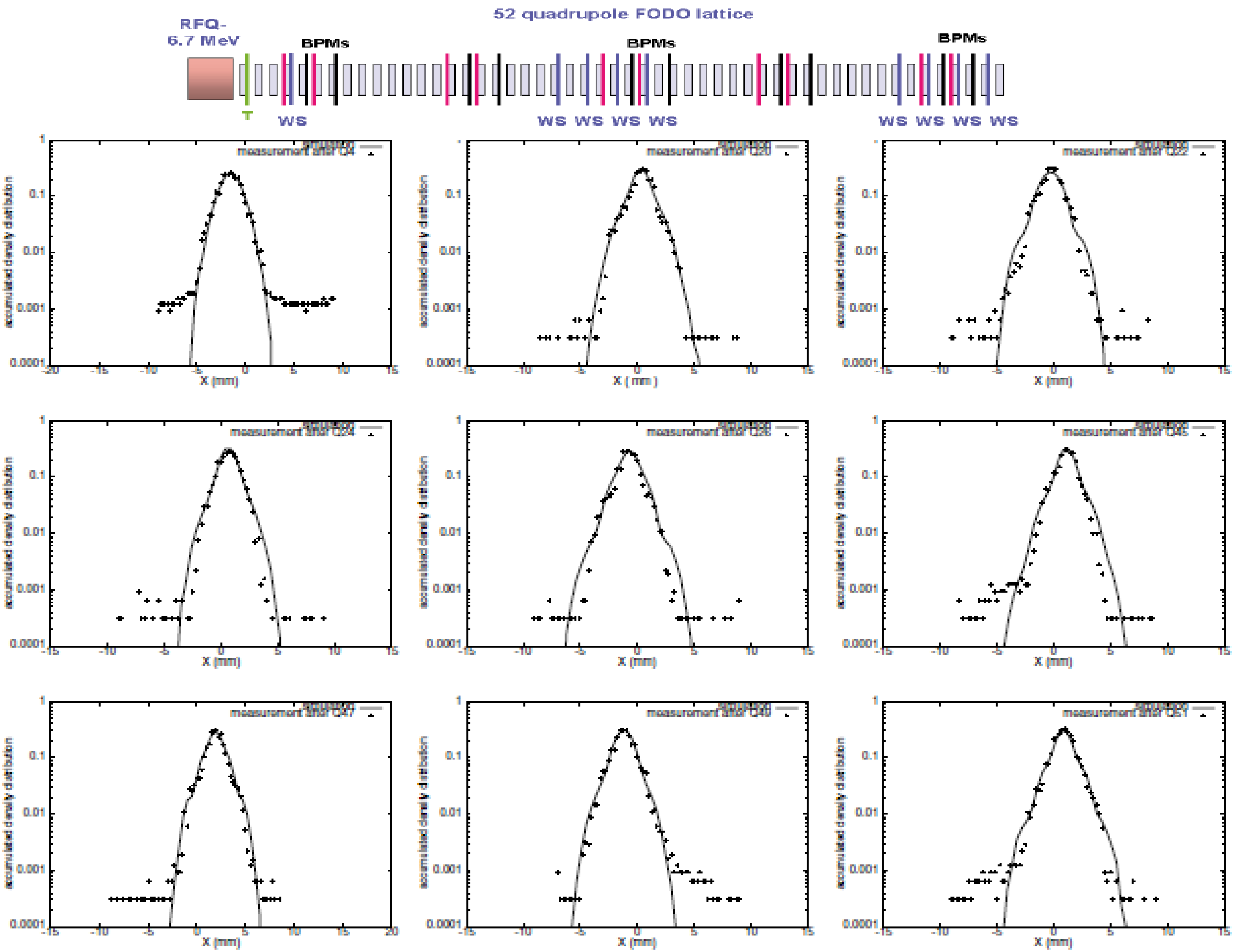
Evolution of the Normalized Cumulative Beam intensity



J. Qiang et. al, PRST-AB 5, 124201.

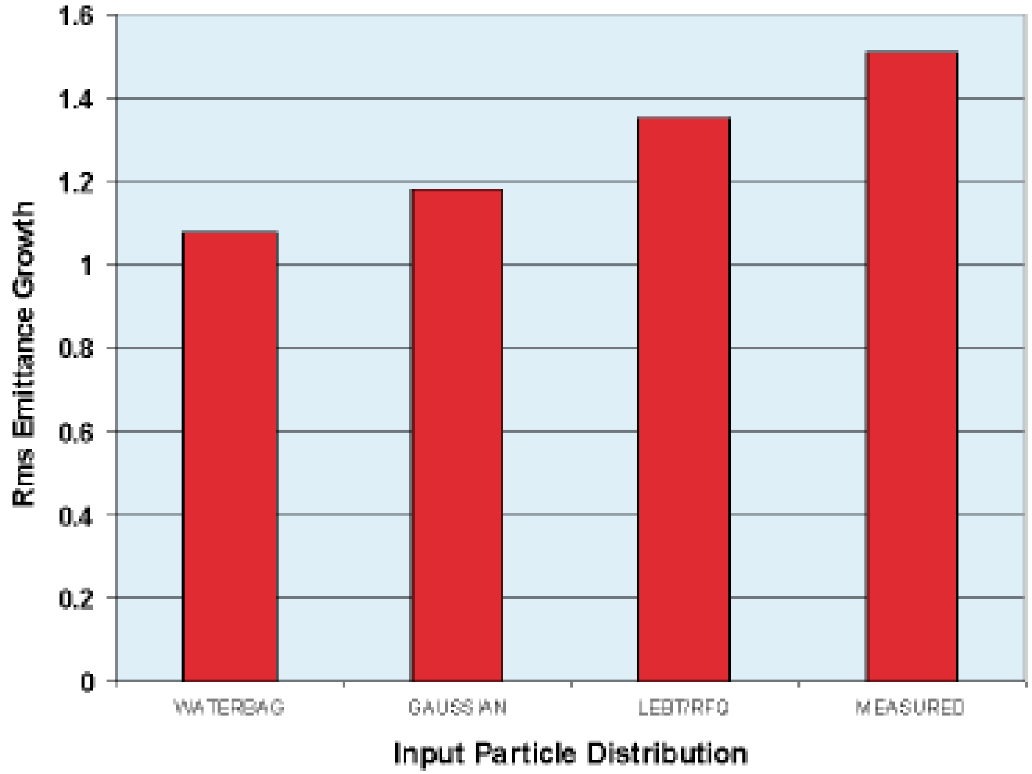
Horizontal Beam Profiles at 9 Wire Scanners

(matched case)



Final Emittance Growth with Different Initial Distributions

(same RMS sizes and emittances)

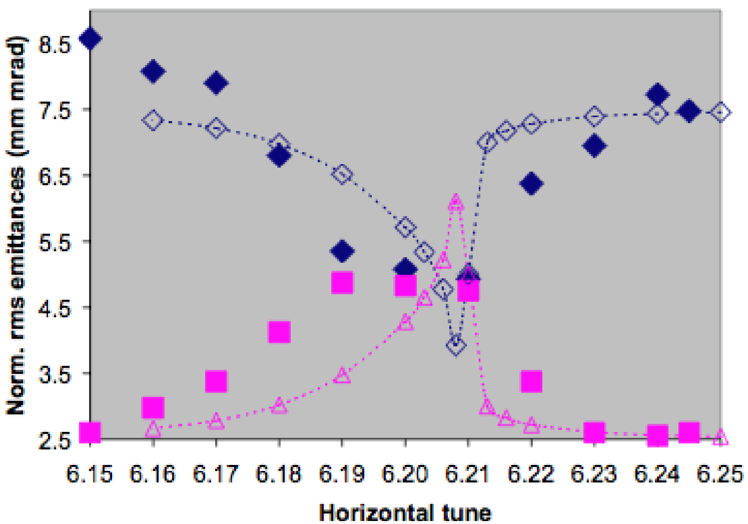


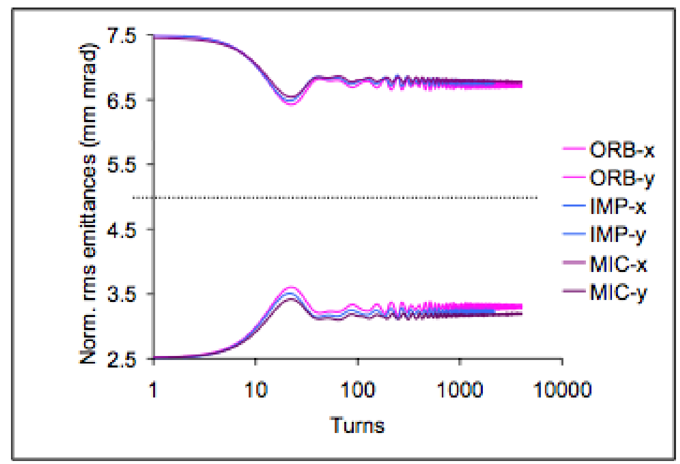
The detail of the initial distribution matters!

Space-Charge Driven Coupling Resonance at PS

"For this purpose increasing levels of complexity have been planned with simulations, first in 2D approximation and up to 2000 turns:
- step (1) in constant focusing approximation;
- step (2) using a linearized version of the AG lattice;
- step (3) using the fully nonlinear lattice of the PS [7]);
- step (4) the 21/2 D or 3D bunched beam simulation including all lattice effects;
- step (5) extension up to the full 13,000 turns of the measurements provided that necessary CPU times – pre- sumably of the order of months – are not prohibitive.

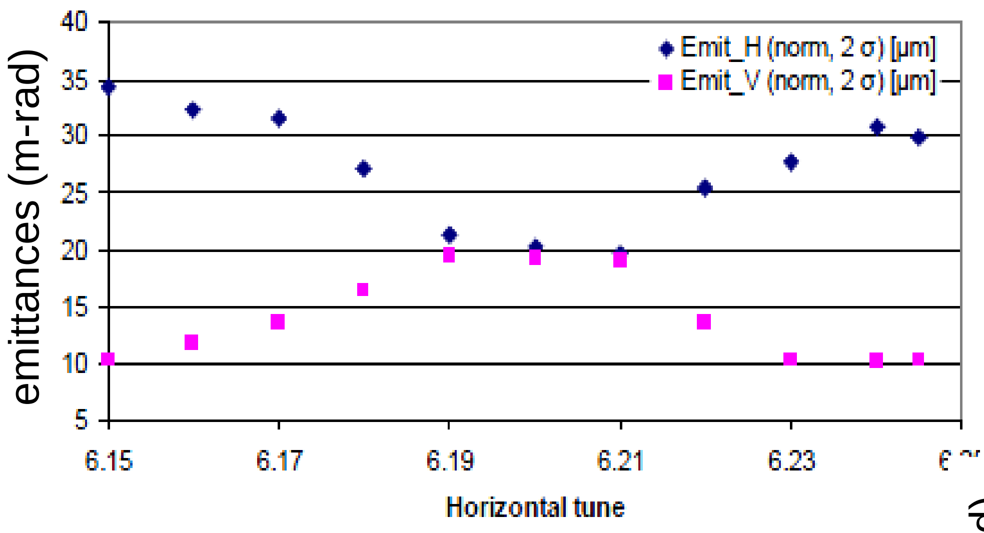
At a later point, after suitable code optimization, the even more ambitious dynamical crossing may be addressed, preferably after new measurements are carried out over less than the demanding 44.000 turns of the 2003 experiment." - I. Hofmann et al., Proceedings of 2005 PAC



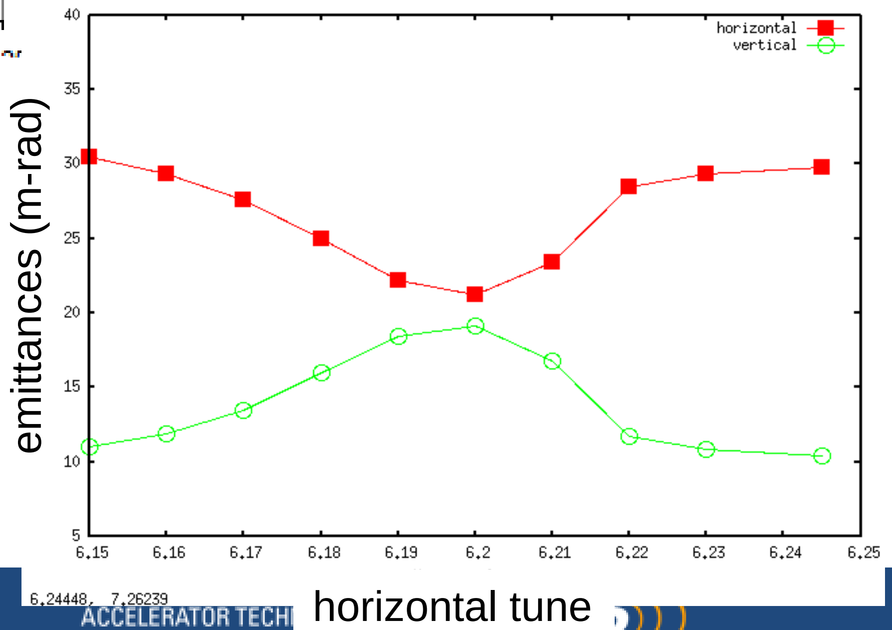


Static Montague Resonance Crossing at PS

measurements



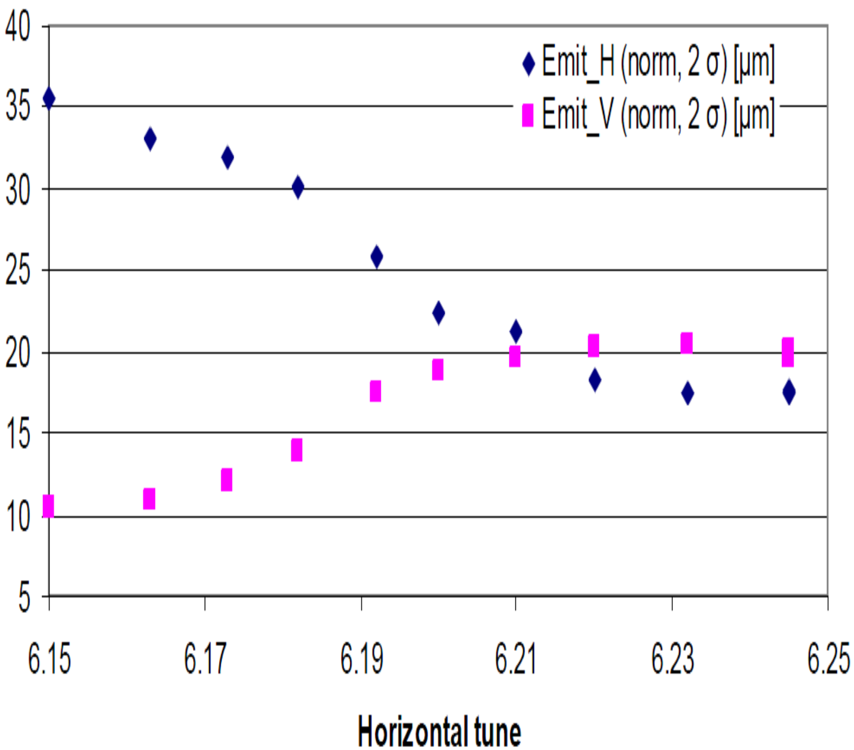
IMPACT simulation



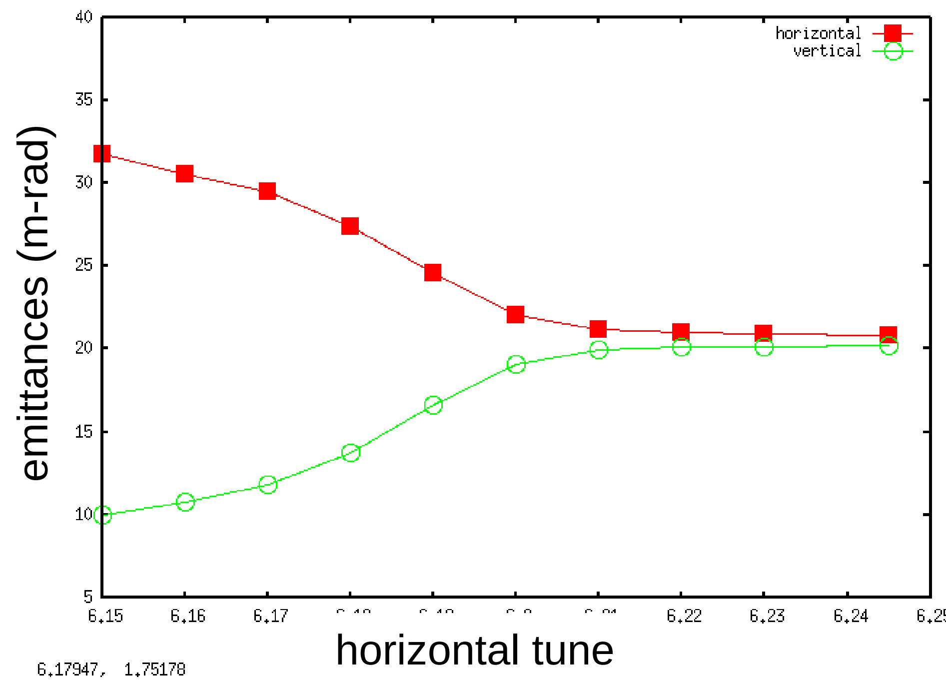
Dynamics Montague Resonance Crossing at PS

100 ms dynamic Crossing

measurements



IMPACT simulation:
fully 3D+nonlinear lattice

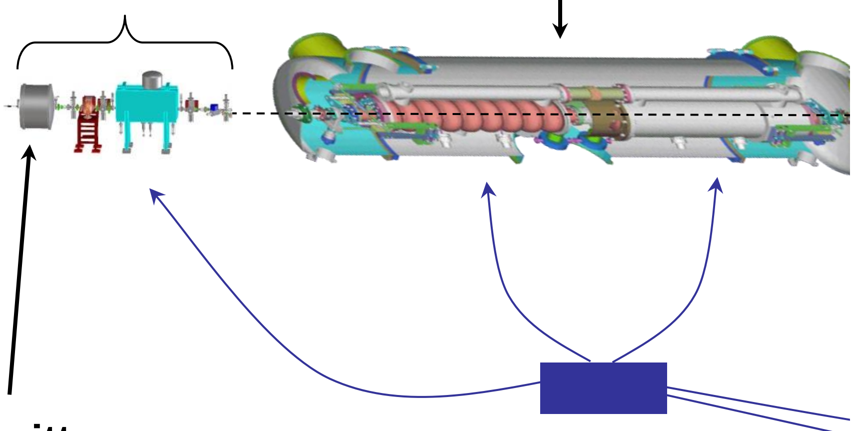


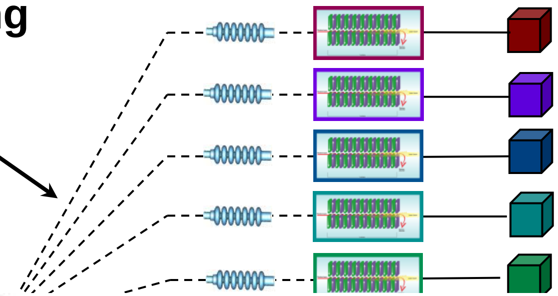
IMPACT Application in Electron Linac for Next Generation Light Sources

Beam manipulation and conditioning

Beam distribution and individual beamline tuning

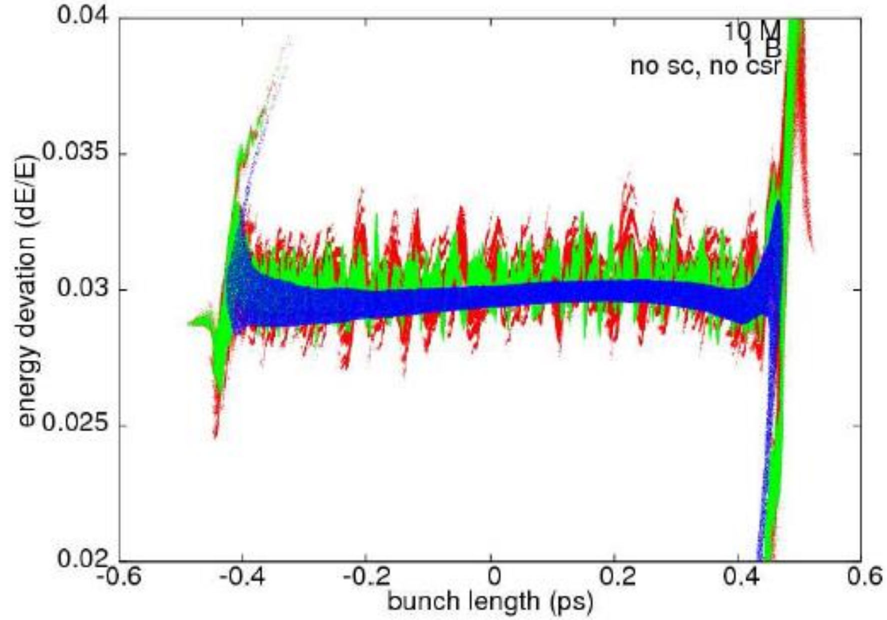
~2 GeV CW superconducting linac





Low-emittance, high rep-rate electron gun

Laser systems, timing & synchronization

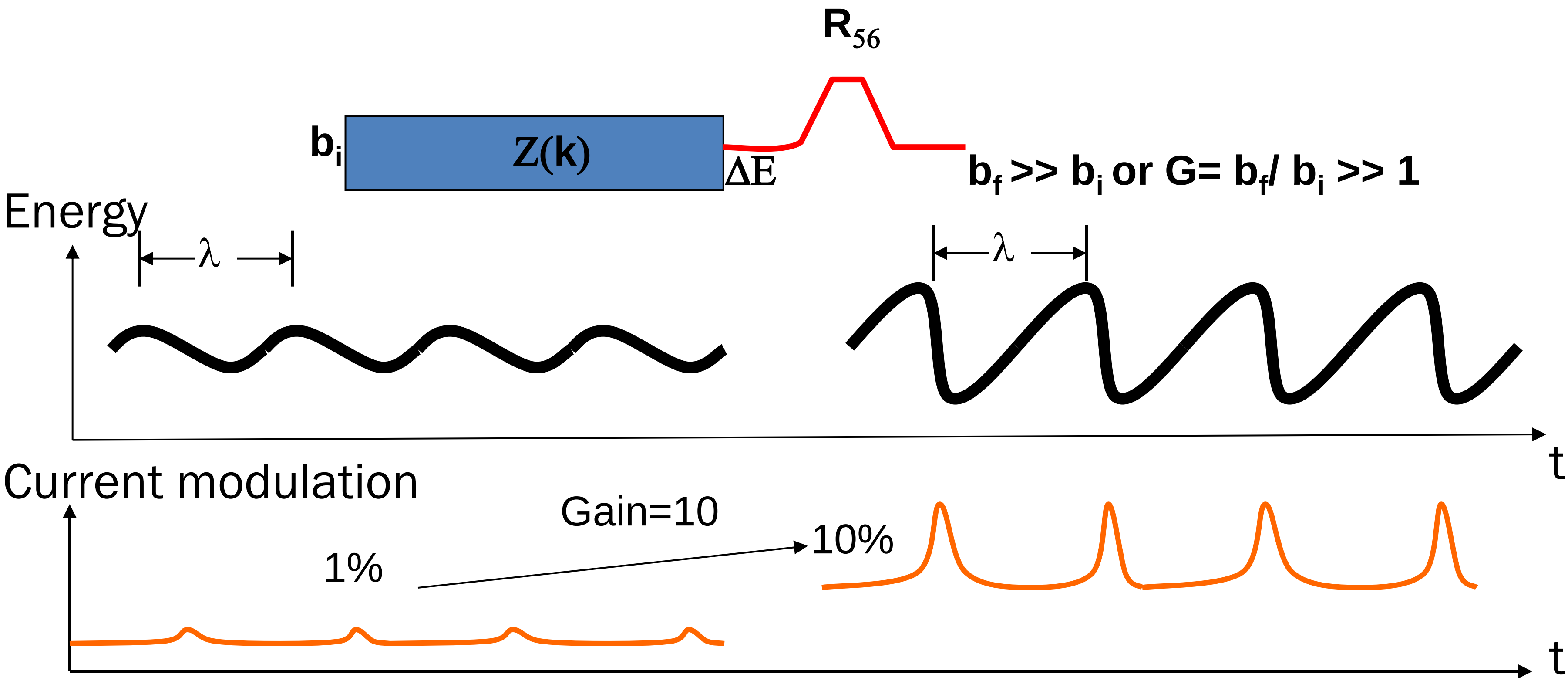


The longitudinal phase space of a beam at the exit of a linac

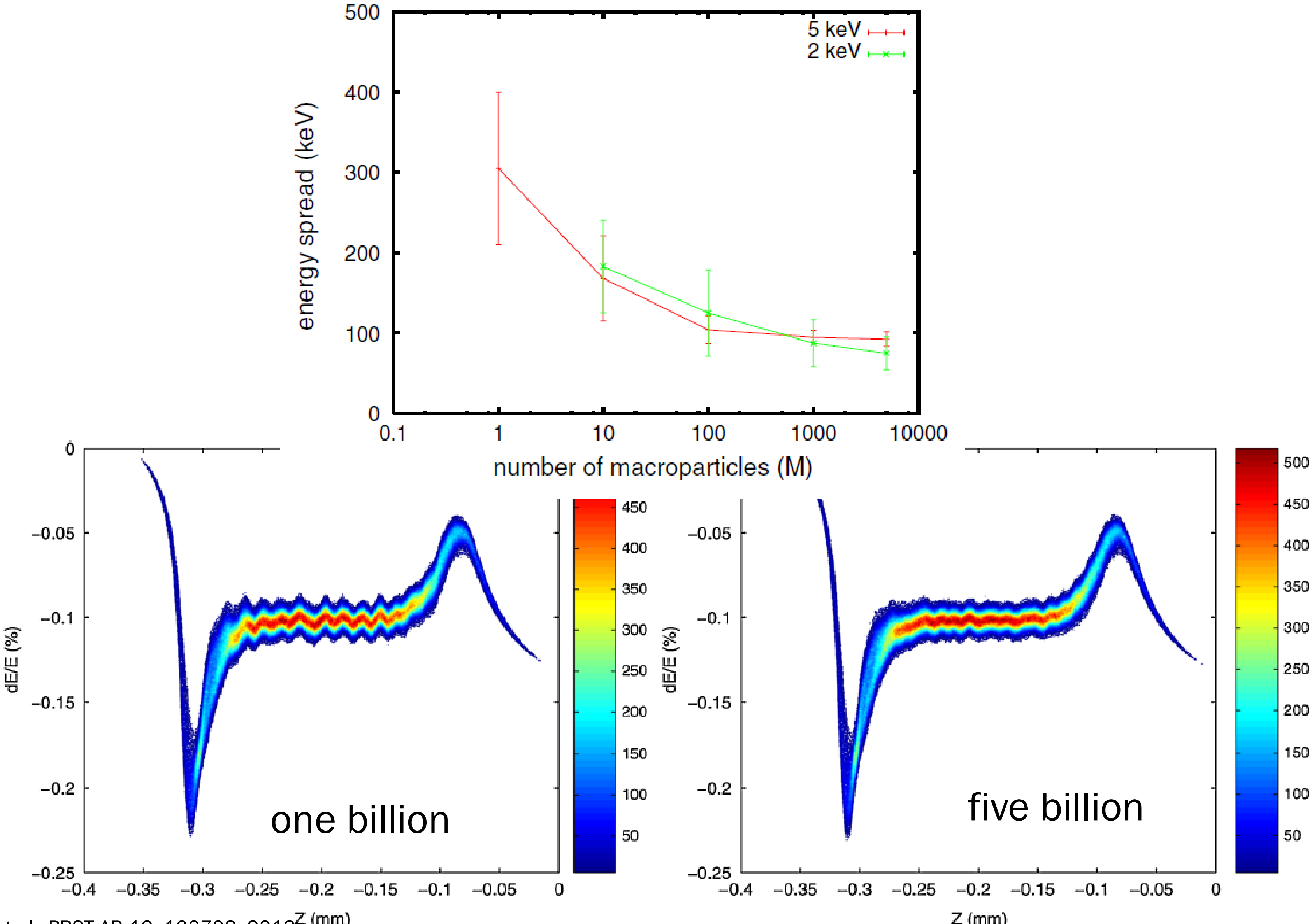
FEL Power/ undulator length $\sim f\left(I_{peak}, \frac{\varepsilon_n}{\gamma}, \sigma_E\right)$

Longitudinal Space-Charge Effects: 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!

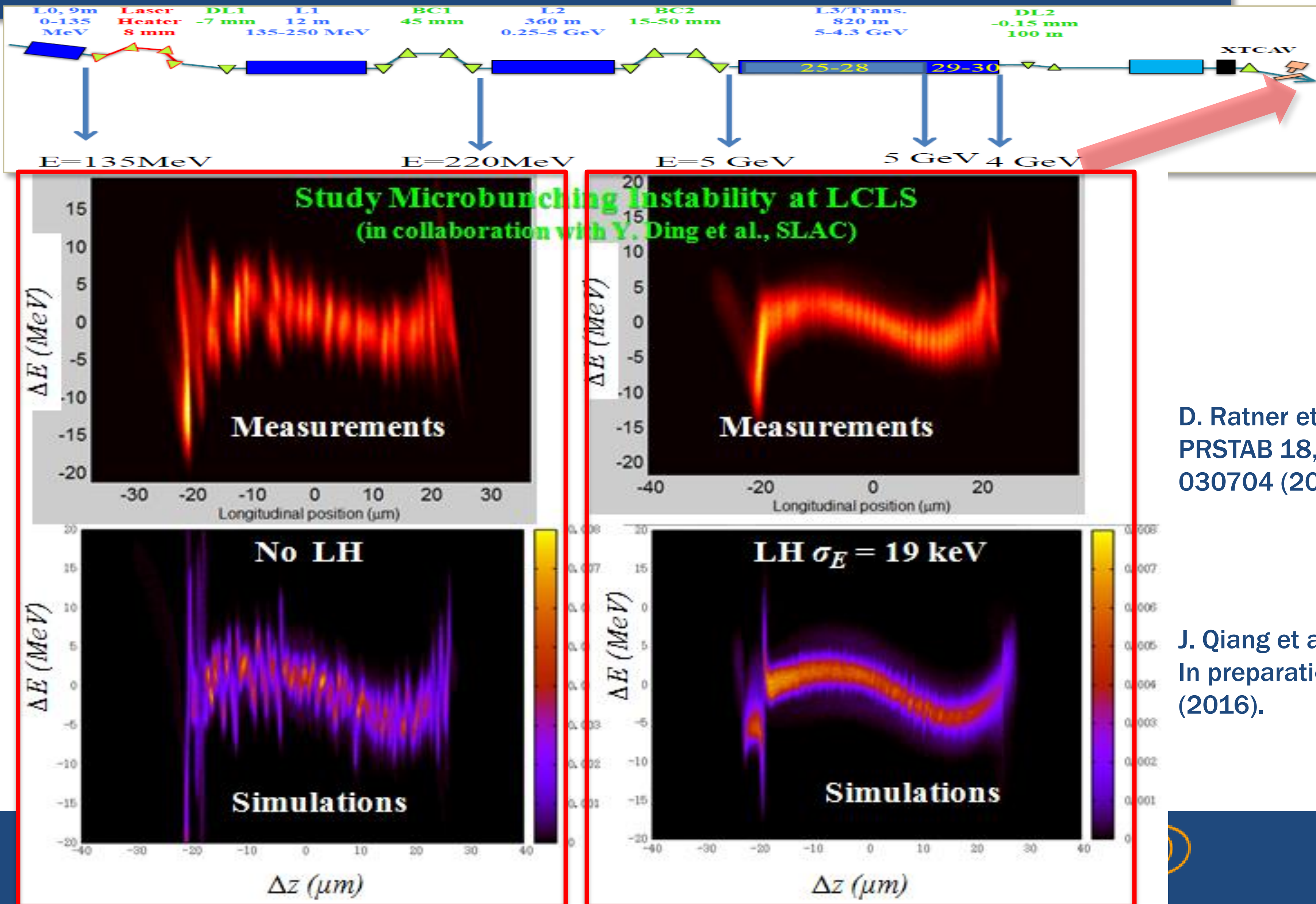


Final Longitudinal Phase Space and RMS Slice Energy Spread



J. Qiang et al., PRST-AB 12, 100702, 2012.

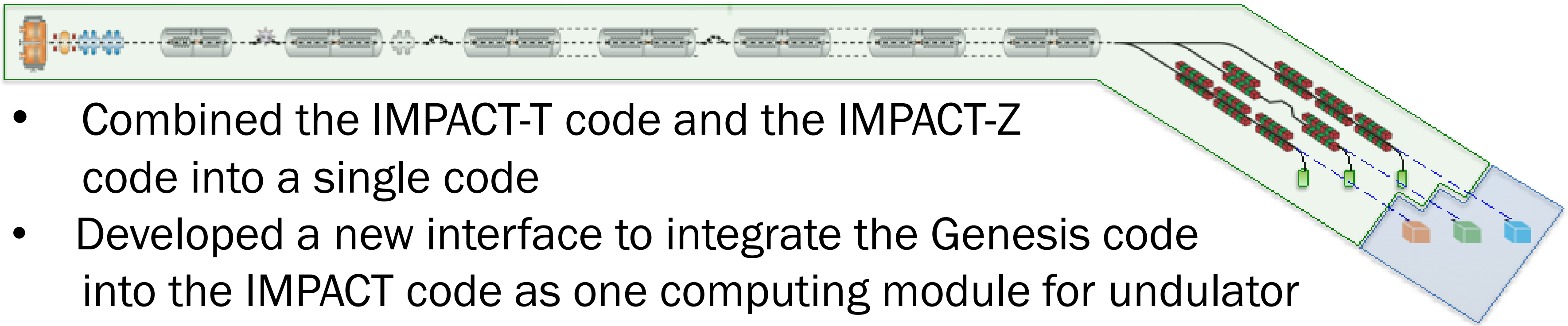
Experimental Observation of uBI: Benchmark IMPACT Simulations against LCLS Measurements



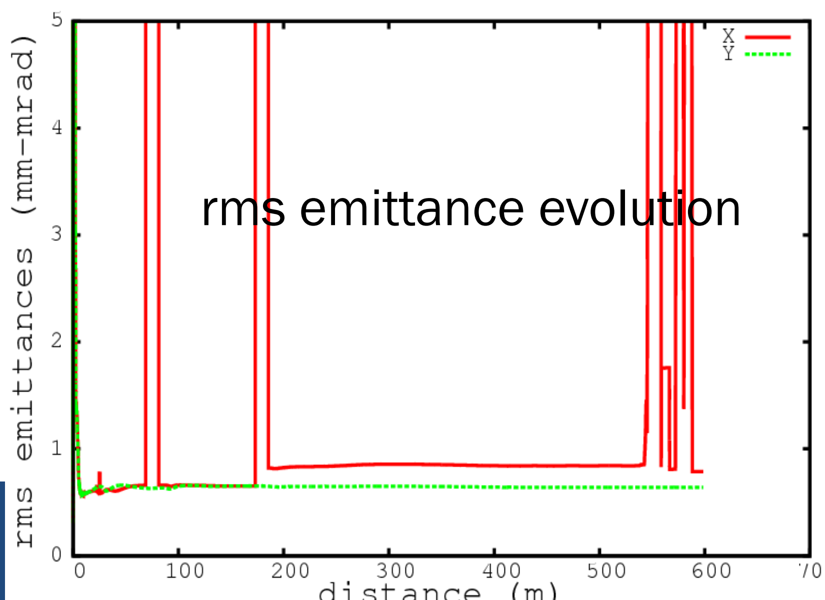
D. Ratner et al., PRSTAB 18, 030704 (2015).

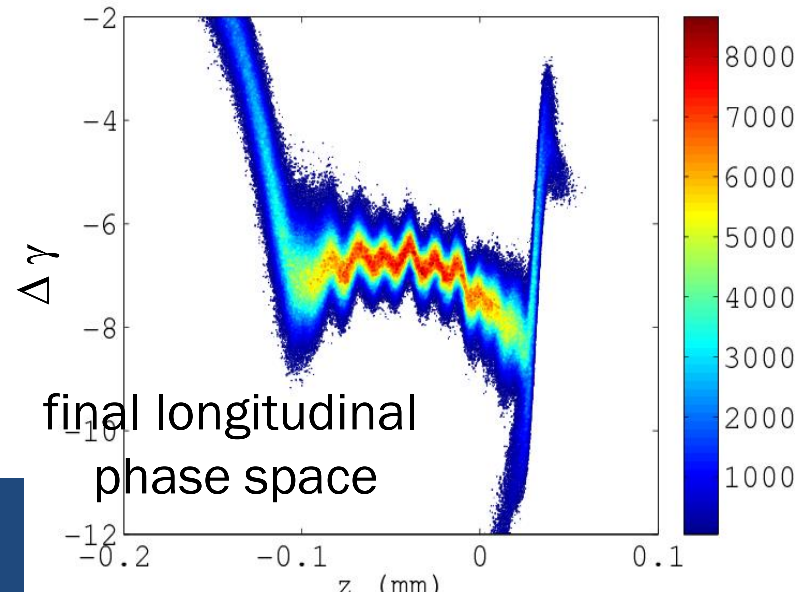
J. Qiang et al., In preparation (2016).

First-Time Start-to-End Simulation of FEL X-Ray Radiation **Using Real Number of Electrons**



- Combined the IMPACT-T code and the IMPACT-Z code into a single code
- Developed a new interface to integrate the Genesis code into the IMPACT code as one computing module for undulator
- The start-to-end multi-physics simulation includes:
  - self-consistent 3D space-charge effects,
  - 1D CSR effects, ISR effects, structure wakefields,
  - self-consistent 3D electron and x-ray radiation interaction

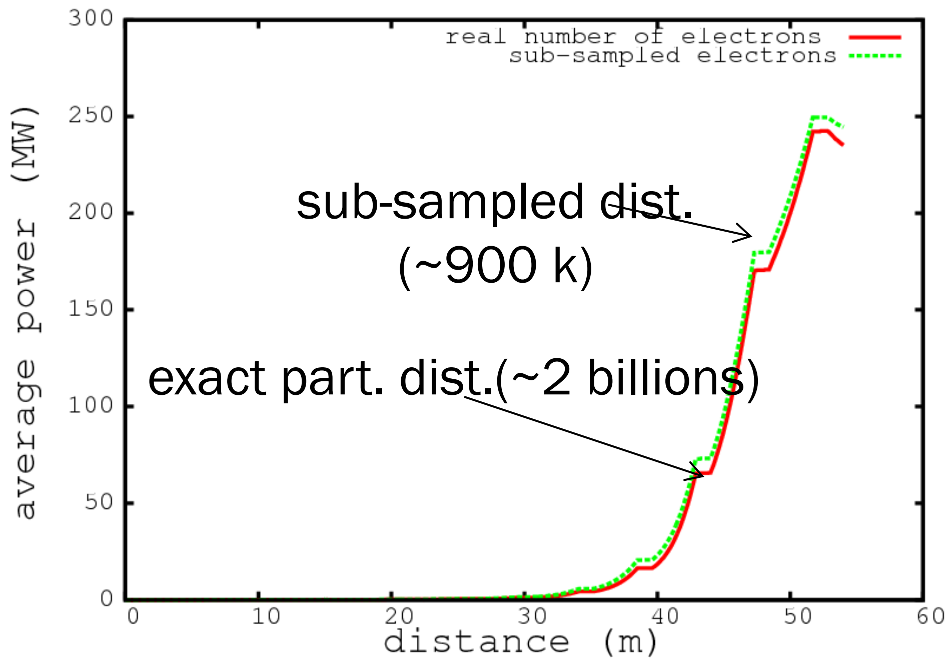




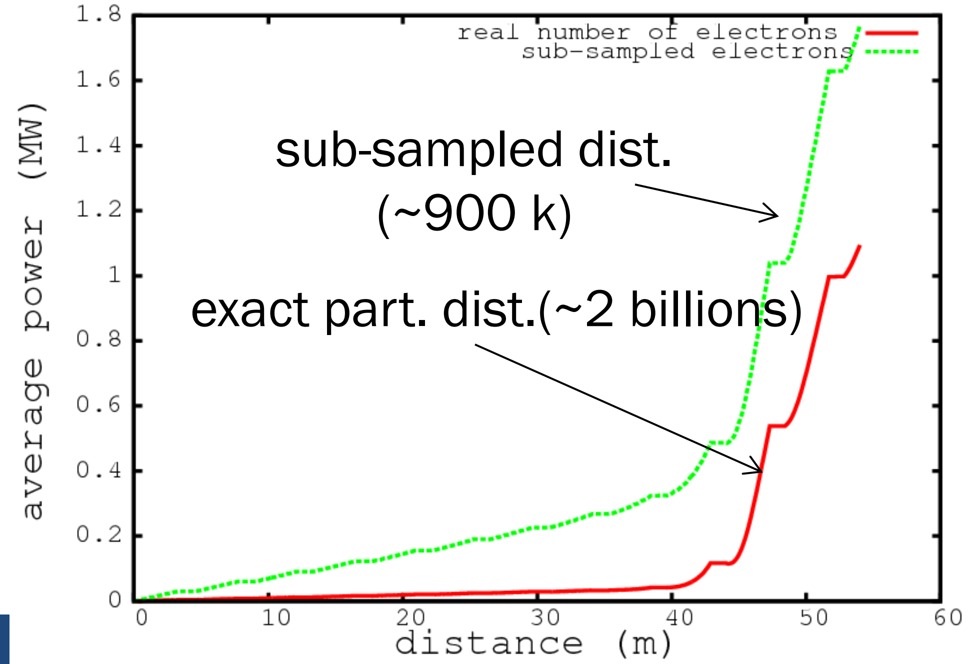
Real Number of Electron Matters : No Need for Shot Noise Model

Evolution of X-Ray FEL Radiation Power

fundamental 1 nm average power evolution (MW)



3rd harmonic 0.333 nm average power evolution (MW)



J. Qiang et al., Phys. Rev. ST Accel. Beams, vol. 17, 030701 (2014).

Thank You!