PAUL SCHERRER INSTITUT

PSI

Sven Reiche :: SwissFEL - Beam Dynamcis Group :: Paul Scherrer Institute

Numerical Computation for X-Ray FELs

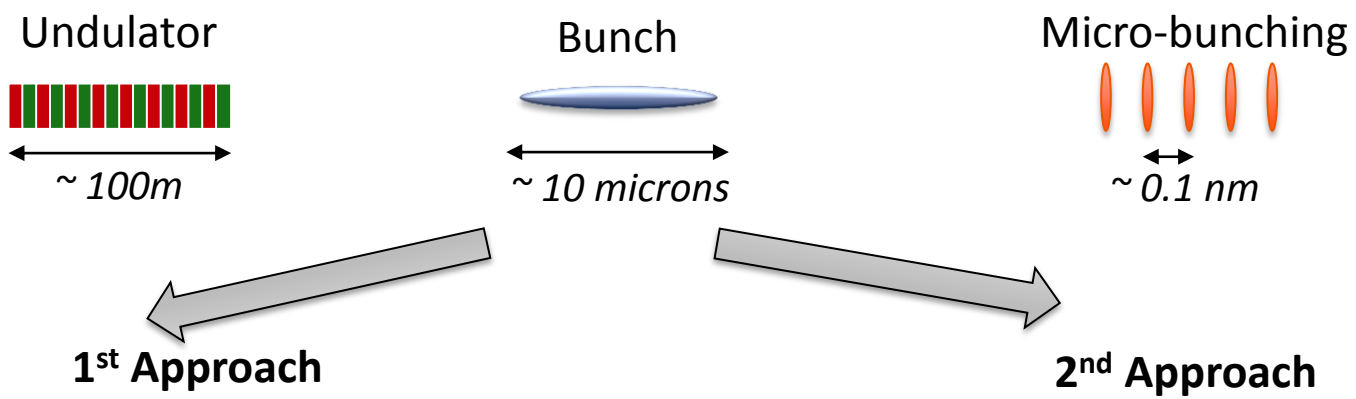
Beam Dynamics Workshop – IPAM/UCLA

PAUL SCHERRER INSTITUT

PSI

Basic Algorithms and Field/Beam Representation

Dealing with the FEL Length Scales



- Put grid over electron bunch in co-moving frame
- Adjust Maxwell equations for co-moving frame
- Treat undulator field as external, time-dependent field

About 100.000 longitudinal grid points

- Apply Lorenz transformation
  - Bunch is stretched
  - Undulator becomes EM wave with shorter wavelength
- Choose boost frame to obtain equal length for bunch and field
- Use a PIC solver for Inverse Compton Scattering (ICS)

About 200.000 longitudinal grid points

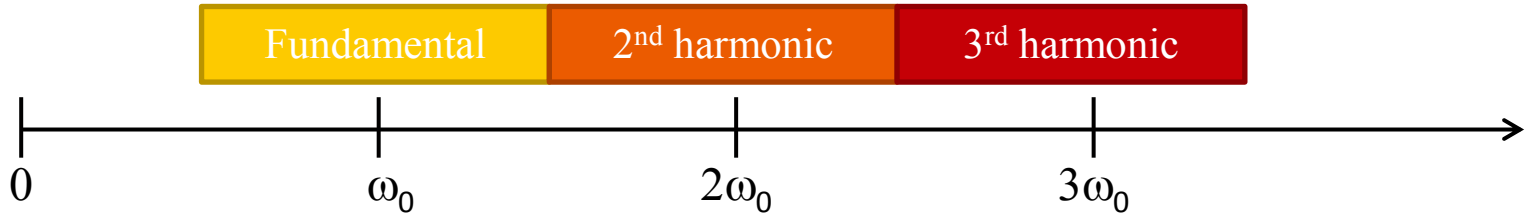
3rd Approach of transforming into electron rest frame is only beneficial if bunch has only one spike in SASE

Resonant Interaction

- Assuming resonant interaction (narrow bandwidth signal) and a slowly varying envelope (SVE) A_0 of the signal, Maxwell equation can be approximated:

$$\left[\vec{\nabla}^2 - \frac{\partial^2}{c^2\partial t^2}\right]\vec{A}_0 e^{ik_0(z-ct)} = \mu_0 \vec{J} \quad \Longrightarrow \quad \left[\vec{\nabla}_\perp^2 + 2ik_0\left(\frac{\partial}{\partial z} + \frac{\partial}{c\partial t}\right)\right]\vec{A}_0 = \mu_0 \vec{J}\cdot e^{-ik_0(z-ct)}$$

- By extracting the carrier frequency $\omega_0 = ck_0$, it is sufficient to sample field only once every wavelength (or even less)



- If harmonics are considered:
  - Each harmonic has its own SVEA Maxwell equation
  - Sampling with the fundamental wavelength to avoid overlap in frequency band, resulting in same grid sizes

Common Numerical Solver I: Finite Mode

- Make a projection onto a set of orthonormal functions (e.g. Gauss-Hermite modes of free space) to calculate evolution of mode amplitude

$$\left[\vec{\nabla}_{\perp}^{2} + 2ik_0 \frac{\partial}{\partial z}\right] A = \mu_0 \tilde{j} \quad \Longrightarrow \quad \left[\nu_{n,m} + 2ik_0 \frac{\partial}{\partial z}\right] a_{n,m} = \mu_0 \tilde{j}_{n,m}$$

Fourier coefficient of current density

Precalculated eigenvalue of eigen-function

- Solve each coefficient like an ordinary differential equation

Works very efficient for smooth undulators and continuous FEL amplification

- Common problem is to find the right set of orthonormal function to be efficient (fast convergence in total power with number of exited modes).

Field Discretization for Finite-Difference Methods

- Common solver for partial differential equations on parallel computers due to "local" calculation of the field.
- Example of 1D free space paraxial equation:

$$\left[\partial_{xx} + 2ik\partial_z\right]a = 0$$

- Field is sampled with a grid spacing Δx and an integration step Δz.
- The field points can be represented as a vector and the differential operation as a matrix operation
- Field solver advances from know solution a(z) to new solution a(z+Δz)
- **But, when is the transverse Laplace operator evaluated?**

Fully Explicit

$$\begin{pmatrix} -2 & 1 & 0 & \dots \\ 1 & -2 & 1 & \dots \\ 0 & 1 & -2 & \dots \\ \dots & \dots & \dots. & \dots \end{pmatrix} \vec{A}(z) + 2ik\Delta x^2 \frac{\left(\vec{A}(z+\Delta z) - \vec{A}(z)\right)}{\Delta z} = 0$$

Laplace Operator L

Fully Implicit

$$\begin{pmatrix} -2 & 1 & 0 & \dots \\ 1 & -2 & 1 & \dots \\ 0 & 1 & -2 & \dots \\ \dots & \dots & \dots. & \dots \end{pmatrix} \vec{A}(z+\Delta z) + 2ik\Delta x^2 \frac{\left(\vec{A}(z+\Delta z) - \vec{A}(z)\right)}{\Delta z} = 0$$

Or a linear combination of both equations

Common Numerical Solver II: Finite Difference

- Keep option for explicit/implicit methods open by using linear combination

$$\left[\vec{\nabla}_{\perp}^{2} + 2ik_0 \frac{\partial}{\partial z}\right] A = \mu_0 \tilde{j} \quad \Longrightarrow \quad \underline{L}\left(\alpha \vec{a}_j + (1-\alpha)\vec{a}_{j+1}\right) + 2ik_0 \frac{\vec{a}_{j+1} - \vec{a}_j}{\Delta t} = \mu_0 \vec{j}_{j+1/2}$$

Weighting factor, when Laplace operator is evaluated

Index j indicates time step

- Theoretical solution would be to find $\left[(1-\alpha)\underline{L} - \frac{2ik_0}{\Delta t}\underline{I}\right]^{-1}$ but requires square of number of grid points to store solution

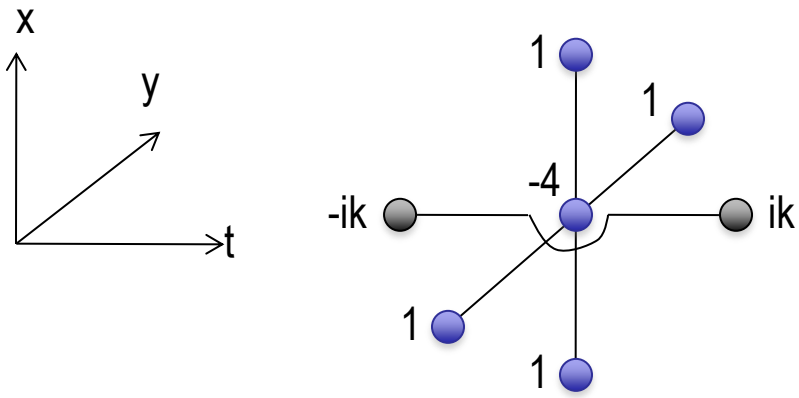
- Instead the solution is solved directly:
  - Method for tridiagonal matrix for 1D grid and $\alpha > 0.5$
  - Alternate direct implicit (ADI) method (2D or higher), splitting into sub steps with one fully implicit step ($\alpha = 1$) for each dimension

Rather robust against strong changes in source term

Advanced Algorithm III – Fully 3D Field solver

- Solving the A(x,y,t,z) on a true 3D grid with a single solver (instead of series of 2D grid solver in quasi-time-dependent solver).
- Example: Stanza of finite-difference approach

$$\left[\vec{\nabla}_{\perp}^{2} + 2ik_0\left(\frac{\partial}{\partial z} + \frac{\partial}{c\partial t}\right)\right]\vec{A}_0 = \mu_0\vec{J}\cdot e^{-ik_0(z-ct)}$$



- Solver must also consider topology of the computer cluster to avoid unnecessary exchange of information
- Most likely candidates:
  - Recursive solver, using adaptive multigrid solver
  - Frequency analysis in the “t”-direction

Averaged vs Non-Averaged Code

- In resonance approximation, wavenumber *k* is well-defined and FEL equations can be averaged over one period

$$e\mu_0 \sum_j \frac{K}{\gamma} \cos\left(k_u z\right) e^{-ik(z-ct)} \delta(z - z_j(t)) \quad \Rightarrow \quad e\mu_0 \sum_j \frac{K}{\gamma} f_c e^{i\theta_j}$$

Electron Trajectory

Ponderomotive Phase

Coupling Factor

Pros	Cons
• Does not need to resolve motion within undulator period • Faster calculation due to larger integration steps • Harmonics can be omitted	• Harmonics are treated as independent fields • Off-resonance frequencies are artificially damped • Excludes finite transverse oscillation in 3D

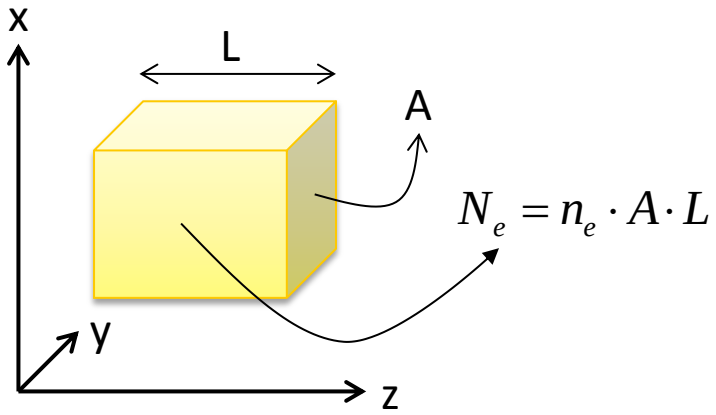
Shot Noise Statistic

- Assumption: On the scale of the resonant wavelength the electron positions are random (white noise)

- Emission is effectively the same for all electrons except for the emission phase. The collective phase and amplitude is equivalent to a random walk in complex plane.

- Bunching factor:

$$b = \frac{1}{N_e} \sum_j e^{i \frac{2\pi}{L} z_j}$$



- Statistic:

$\langle b \rangle = 0$ *Phase is fully random*

$\langle |b|^2 \rangle = \frac{1}{N_e}$ *Amplitude given by number of electrons*

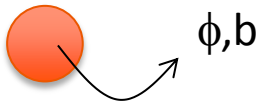
Modeling Statistic and Shot Noise

Problem:

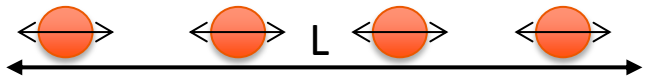
Number of simulation particles not necessarily same as electrons to be modelled.

Solutions:

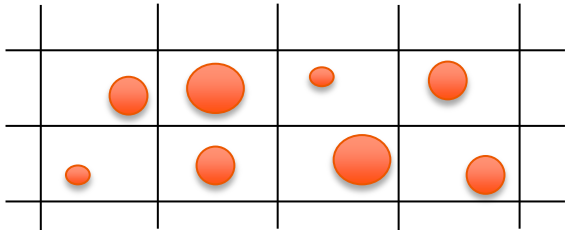
1. Assign internal degrees of freedom (phase + amplitude) to macro particles, representing a set of electrons [*Litvinienko*]



2. Place group of particles (beamlets) evenly of L to force bunching to zero (quiet start) and then apply noise in longitudinal position in a controlled way [*Penman*, *Fawley*]



3. Place particles in a grid and then add noise to position, energy, momenta and charge [*McNeil*]



4. Resolve each electron.

Solution 1+2 only works for discrete values of L, while solution 3+4 for continuous values

Solution 1+2 do not include shot noise in energy (secondary effect),

Solution 3 does not preserve statistics for long drifts

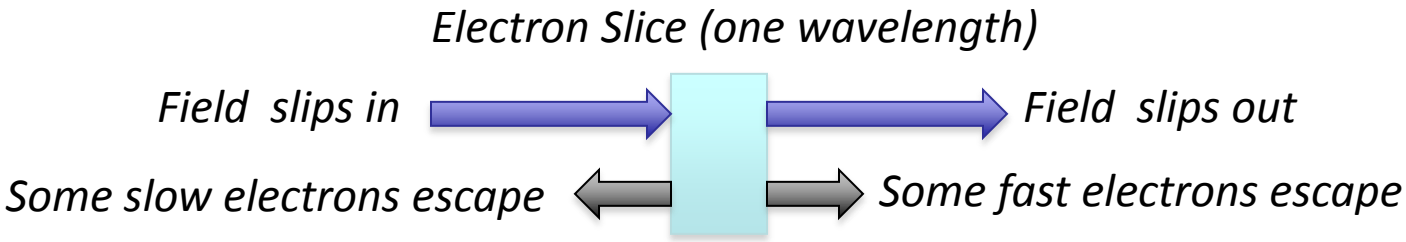
PAUL SCHERRER INSTITUT

PSI

Available Computer Resources and Complexity in FEL Simulations

Core Algorithm – Steady State Simulation

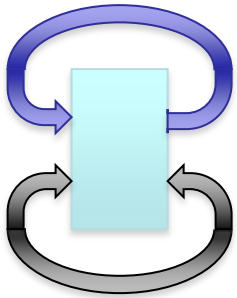
- Two step algorithm (Leap-frog Algorithm):
  - Advance radiation field (diffraction + emission by electrons)
  - Advance electrons (interaction with field and change in ponderomotive phase)



- In steady-state simulations:
  - Infinite long bunch with the same properties (no time-dependence)
  - Zero net flow of field and electrons of any slice

    → field and particles are fed back into the same slice

Tracking of only on radiation field and one electron slice



Self-fed Amplifier

Required Resources

- Steady-State Simulation
  - About 10.000 macro particles in slice (6 dimensions a 8 Byte)
  - Up to 10.000 transverse modes (16 Byte per mode)

  In Memory: about 600 kByte per harmonic

- Time-Dependent Simulation (LCLS like)
  - About 100.000 slices
  - Memory Requirement per slice as steady-state simulation

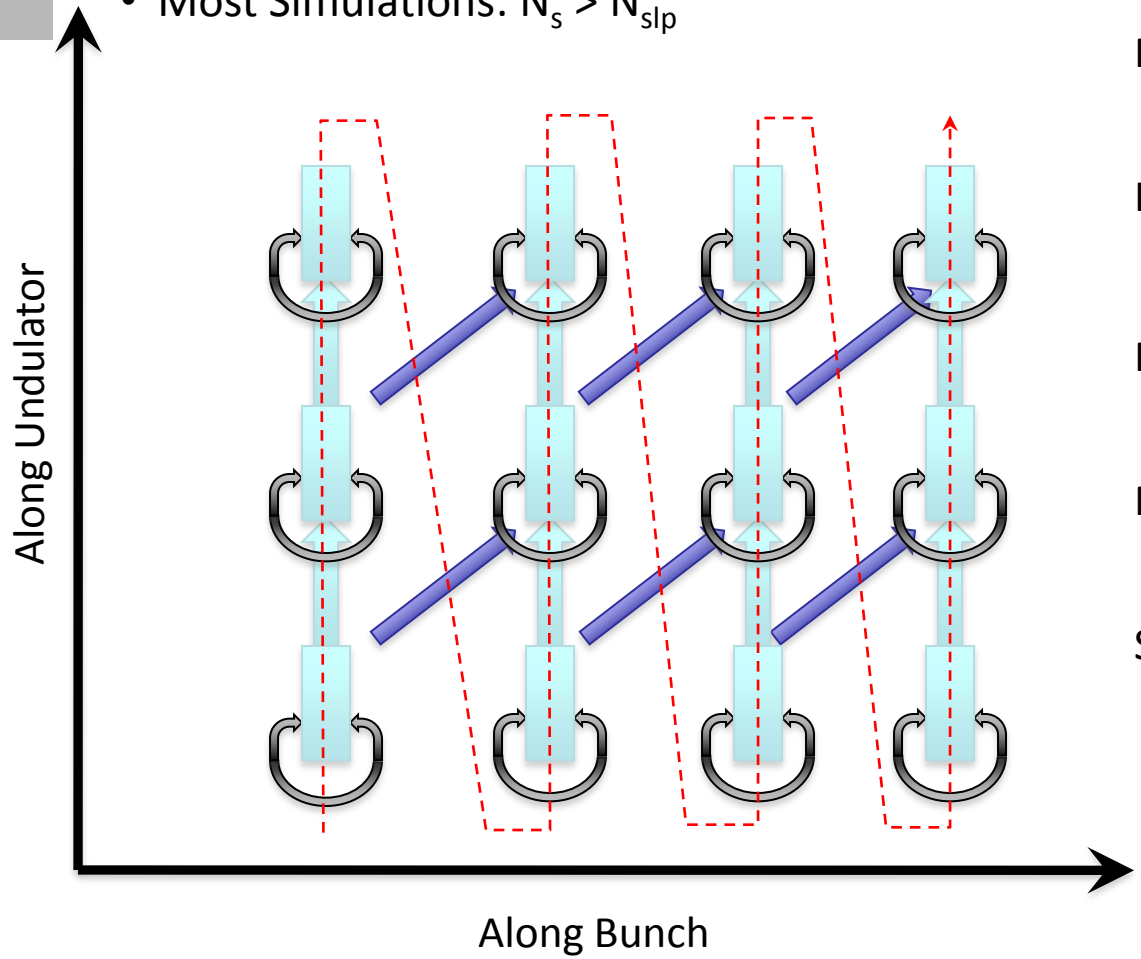
  In Memory: about 60 GByte per harmonic

- Connected Slices due to Slippage(LCLS like)
  - About 2.000 slices
  - Memory Requirement per slice as steady-state simulation

  In Memory: about 1.2 GByte per harmonic

Quasi-Time-Dependent Simulations

- Requirement: Tracking N_s slices over N_z steps along undulator.
- Minimum required slices: $N_{slp} = \lambda/\lambda_u N_z$ (Slippage)
- Most Simulations: $N_s > N_{slp}$



Propagate Field to Next Slice

Keep Slice in position

Feed electrons back into slice

Model of chained amplifiers

Simulation can crawl through bunch:

- Inner loop: undulator
- Outer loop: bunch

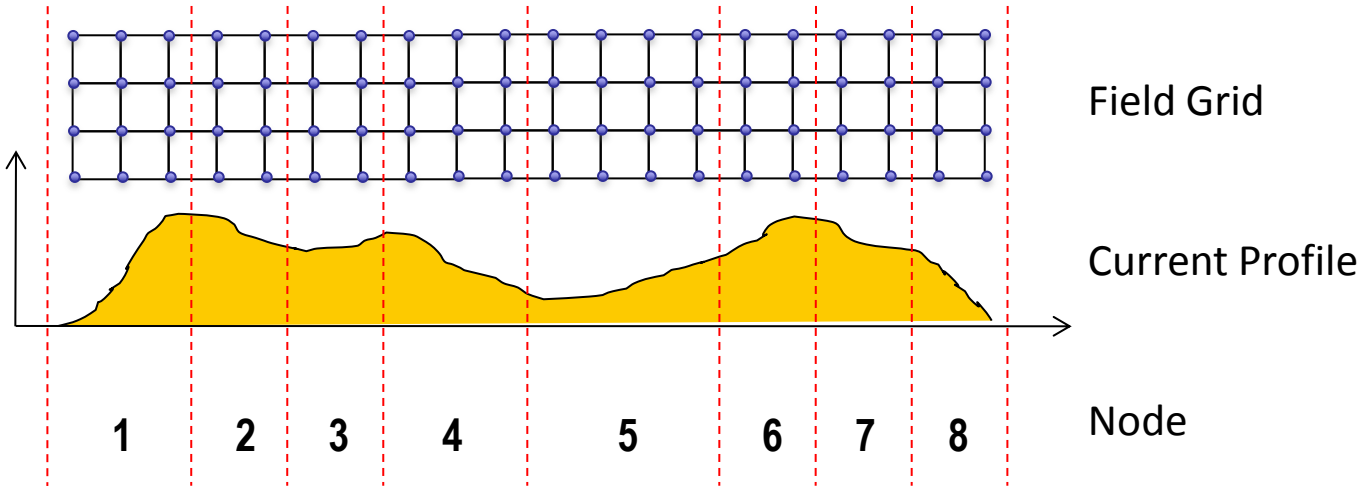
Pros & Cons of Quasi-Time-dependent Simulations

- **Pros:**
  - Very efficient memory demand (1 Electron Slice and N_{slp} Radiation Slices)
  - Easy implementation on parallel computers (N_{core} Electron Slices, N_{slp} Radiation Slices)
  - Fixed number of macro particles per slice (charge scaling) yields highly efficient performance on parallel computer

- **Cons:**
  - No exchange between electron slices (Rigid current profile)
  - Enhanced slippage (e.g. iSASE) blows up memory demand.
  - Pre-calculated collective effects (undulator wakefields) instead of self-consistent models
  - Crude approximation of longitudinal chirps (no chirp within a slice)
  - Calculation wasted in low current slices

Utilizing Clusters

- Even with mid-size cluster, entire radiation field and beam can kept in memory distributed over the nodes.



- The FEL dynamics with its well defined longitudinal order prefers a 1D topology
- Minimal exchange of data:
  - Pushing roughly one wavefront slice to preceeding node per step
  - Exchange of particles when sorting is enabled (preferable using fast bubble sort algorithm due to limited electron motion)
- New codes emerging

PAUL SCHERRER INSTITUT

Grand Challenges in FEL Simulations

Large Slippages (iSASE, HB-SASE, Mode-locking)

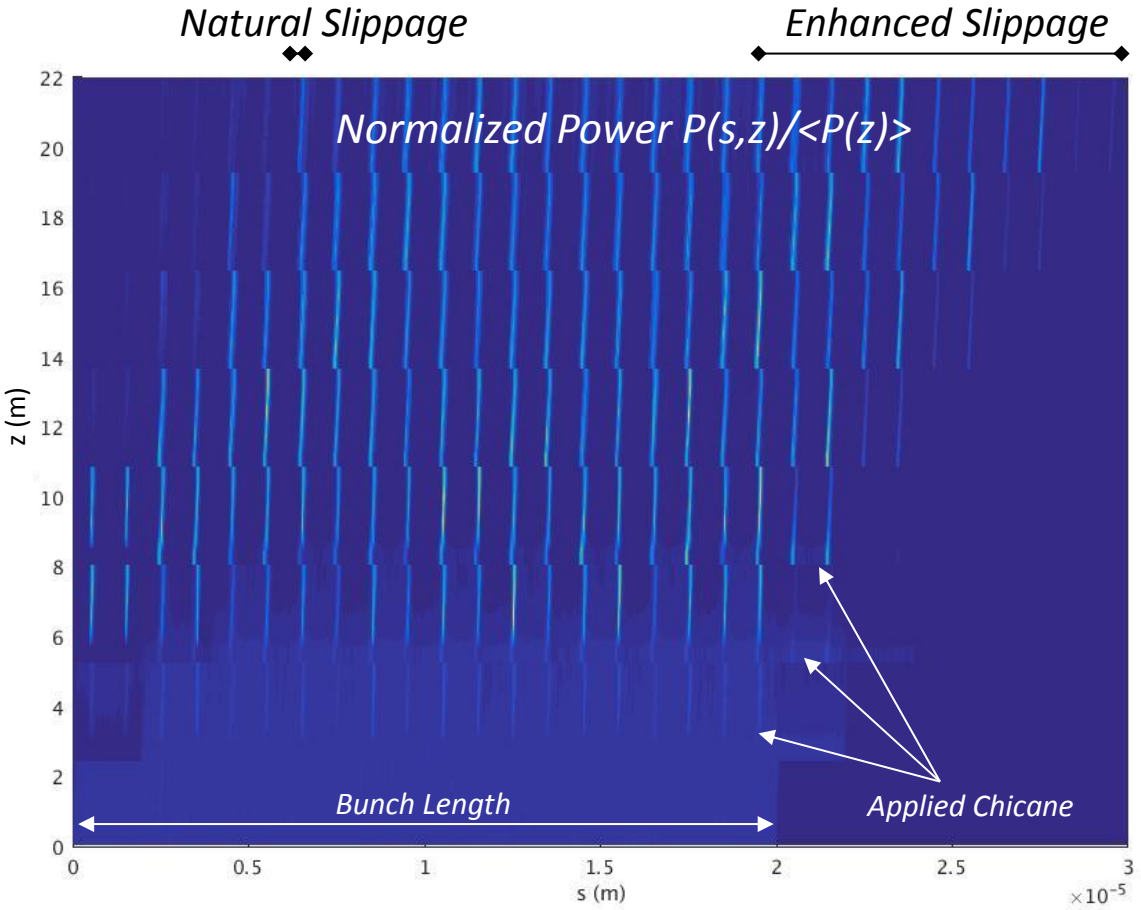
- Quasi time-dependent simulations suffer from enhance slippage, exceeding the memory on the master node.

Lots of phase dumps

About 500 Gbyte per Run

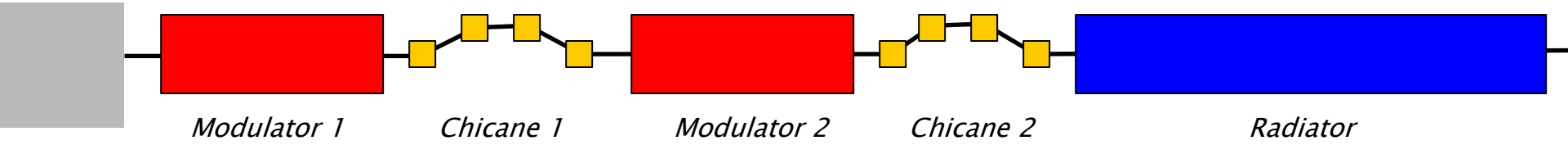
Model entire beam on cluster

Mode-locked Configuration for SwissFEL-Athos



Large Harmonic Conversions (EEHG/HGHG)

Example: EEHG

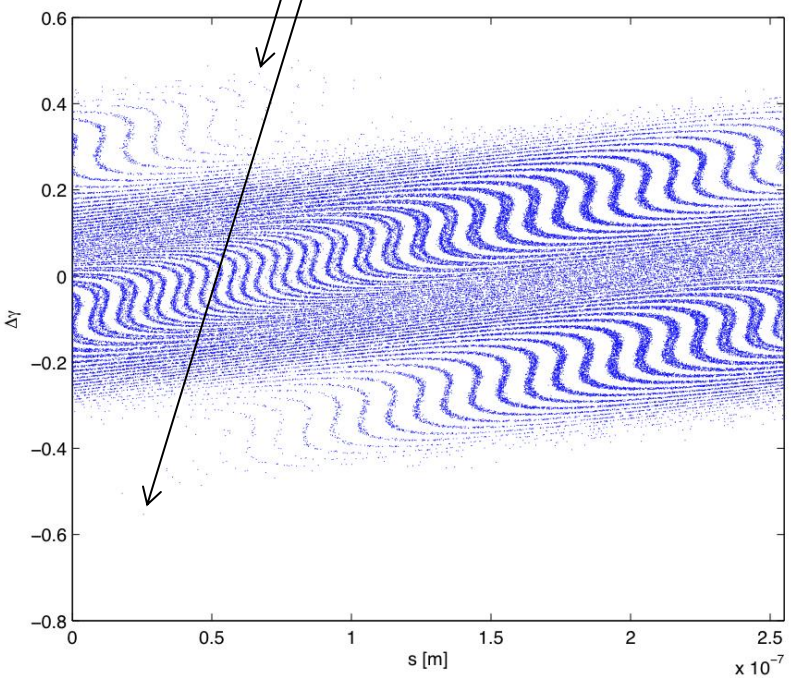


- Carrying high harmonics from the beginning is very unpractical
- Harmonic conversion is done by scaling the ponderomotiv phase $\theta \rightarrow n\theta$

Problems:

1. Numeric bandwidth +/-(50/n) % can be smaller than FEL bandwidth
2. Beamlets are strongly distorted but cannot be split.
3. Shotnoise not correct

Come from 50 wavelengths away



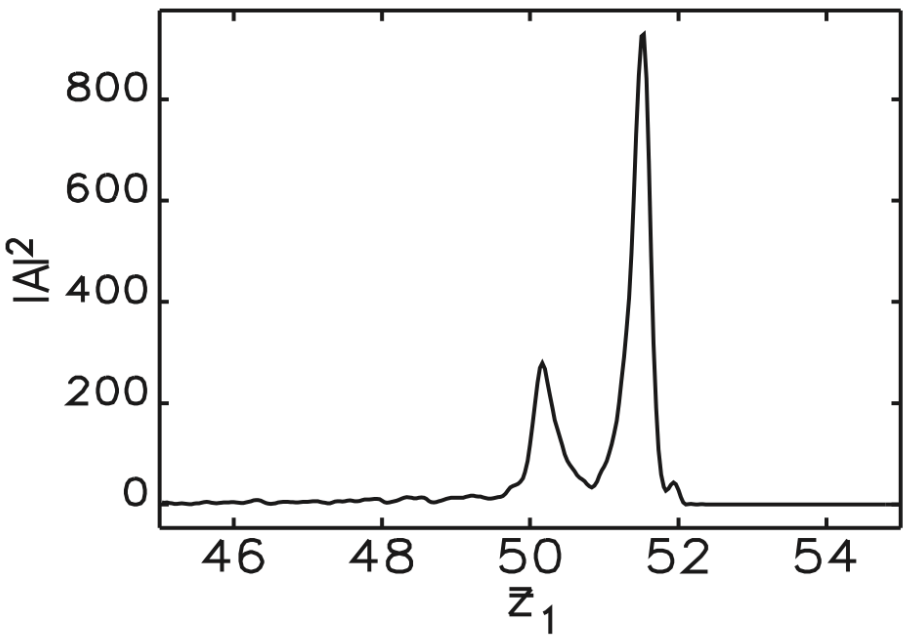
Resolve each electron, slice and sort

Superradiance

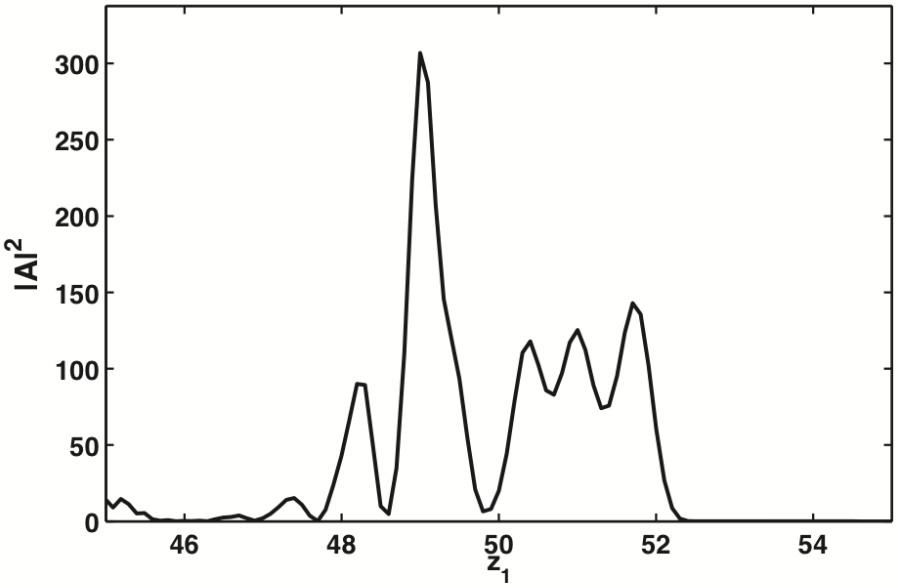
- Radiation spike above saturation power gets shorter with amplification
- Spectrum gets broader, violating resonance and slowly-varying amplitude in FEL model.

Use Non-average Code

Non-averaged Code



SVEA Code



Optimization of Time-Dependent Simulations

- Finding the optimized undulator profile (and phase shifter setting) for best performance is prone to have many local maxima
- Problem would be a good candidate for advanced algorithm (e.g. genetic algorithm)
- Example:
  - About 20 genes (undulator K-value and phase shifter settings)
  - Population about 100
  - Expected generations: 50
  - Time-dependent run on 128 core custer for one sample: 4h

→ Total time: about 2.3 years

Reduce genes (e.g. predefined taper)

Optimized for steady-state simulations

Use actual machine with 50 Hz rep rate ☺

Things, which are still unsatisfying

	Problem	Solution
Grid Boundaries/ Mode Numbers	Start-up excites many transverse modes, while in the high gain regime only a few have noticible amplitudes., resulting in calculation of non-important modes	Explore absorbing boundaries condition or adaptive multigrid methods.
Collective effects	Space charge and wakefields must/can be calculated in advance because the current profile is kept constant	Having entire beam in memory these effects can be modelled self-consistently, including transient regime and change in current profiles
Broken symmetry	Changing polarizations 8e.g. cross undulator) breaks the asumption of symmetry to model only one polarization plane	Could be treated as harmonics if needed
Emittance coupling to even harmonics	Various mechanism of harmonic coupling not included, in particular symmetry breaking coupling by emittance to even harmonics.	If «broken symmetry» is modelled then this can be included as well

Summary

- FEL simulations are numerically challenging but solutions (and codes) exist
- Algorithm rather “bread and butter”, not really advanced solver
- Modern cluster able to hold entire information, eliminating some approximation and book-keeping.
- New ideas are still pushing the capability of existing codes
-