



Science & Technology  
Facilities Council

# Puffin

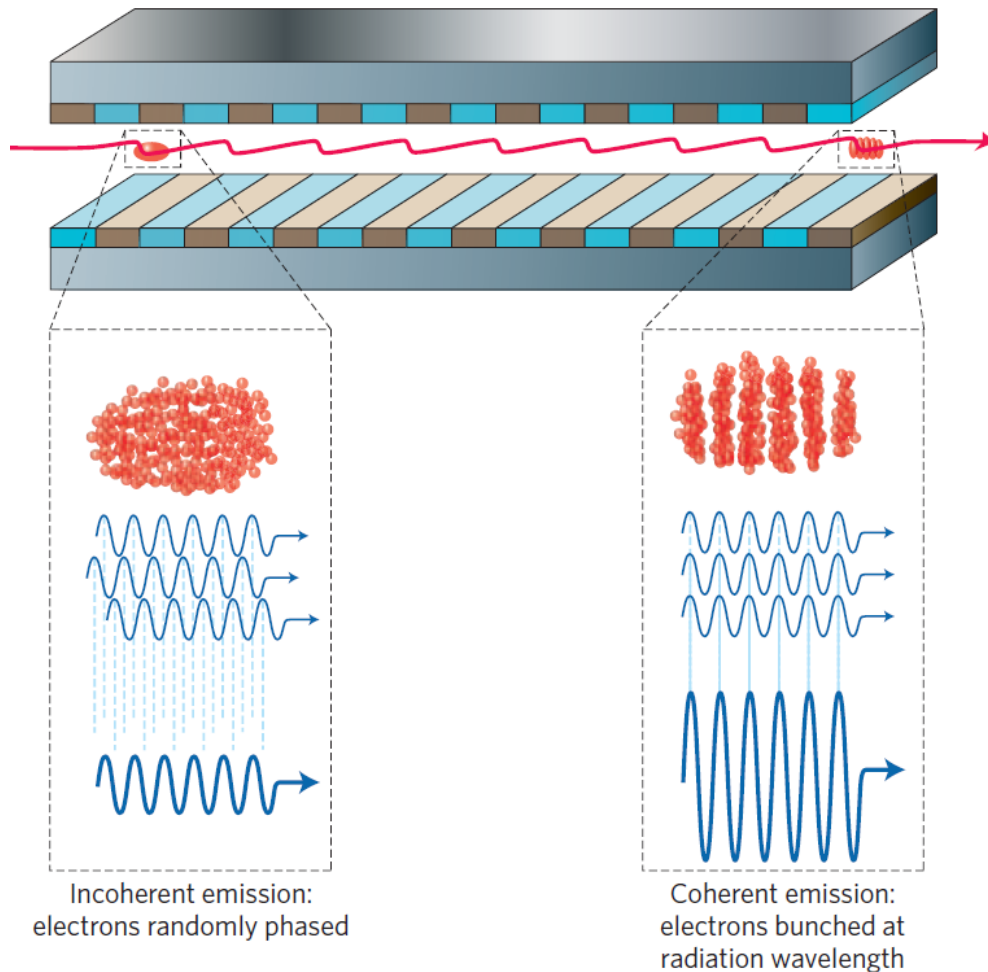
L.T. Campbell & B.W.J. McNeil  
University of Strathclyde



University of  
**Strathclyde**  
Glasgow

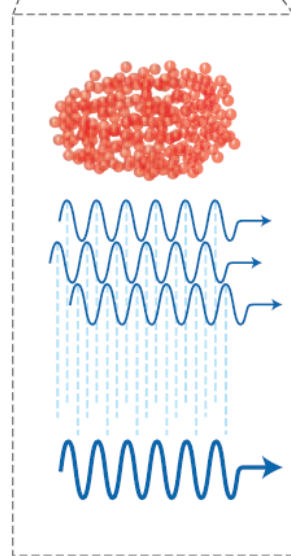
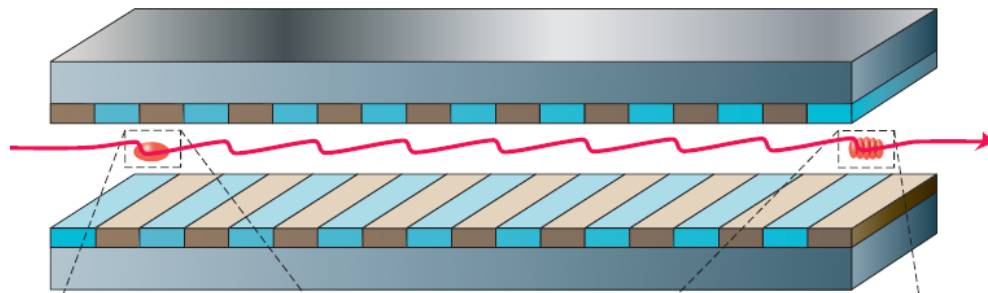


# What is an FEL?

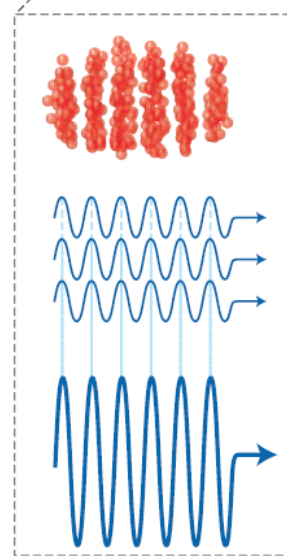


- In a Free Electron Laser (FEL), a beam of relativistic electrons and a radiation field co-propagate an undulator or wiggler
- An undulator or wiggler is a periodic array of alternating magnetic poles
- This forces the electrons to oscillate in the direction transverse to propagation
- This oscillating component of velocity allows an energy transfer between electrons and radiation field
- The interaction causes the electrons to bunch spatially, and they begin to coherently amplify the radiation field, giving an exponential growth in intensity

# What is an FEL?



Incoherent emission:  
electrons randomly phased

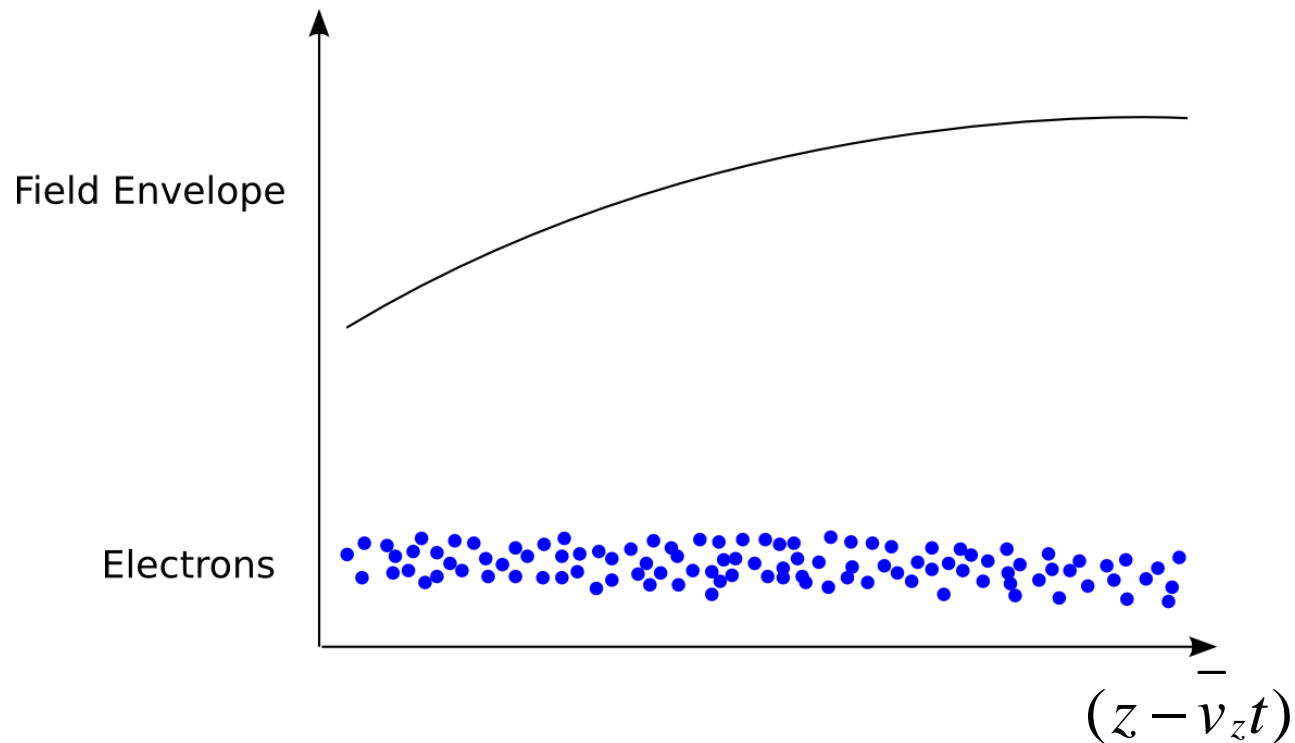


Coherent emission:  
electrons bunched at  
radiation wavelength

- Electrons amplify field at a certain resonant frequency
- “slow” amplification process (w.r.t. the FEL resonant wavelength)
- Use Slowly Varying Envelope Approximation (SVEA), and use averaged quantities to drive radiation field
- Call this ‘averaged model’

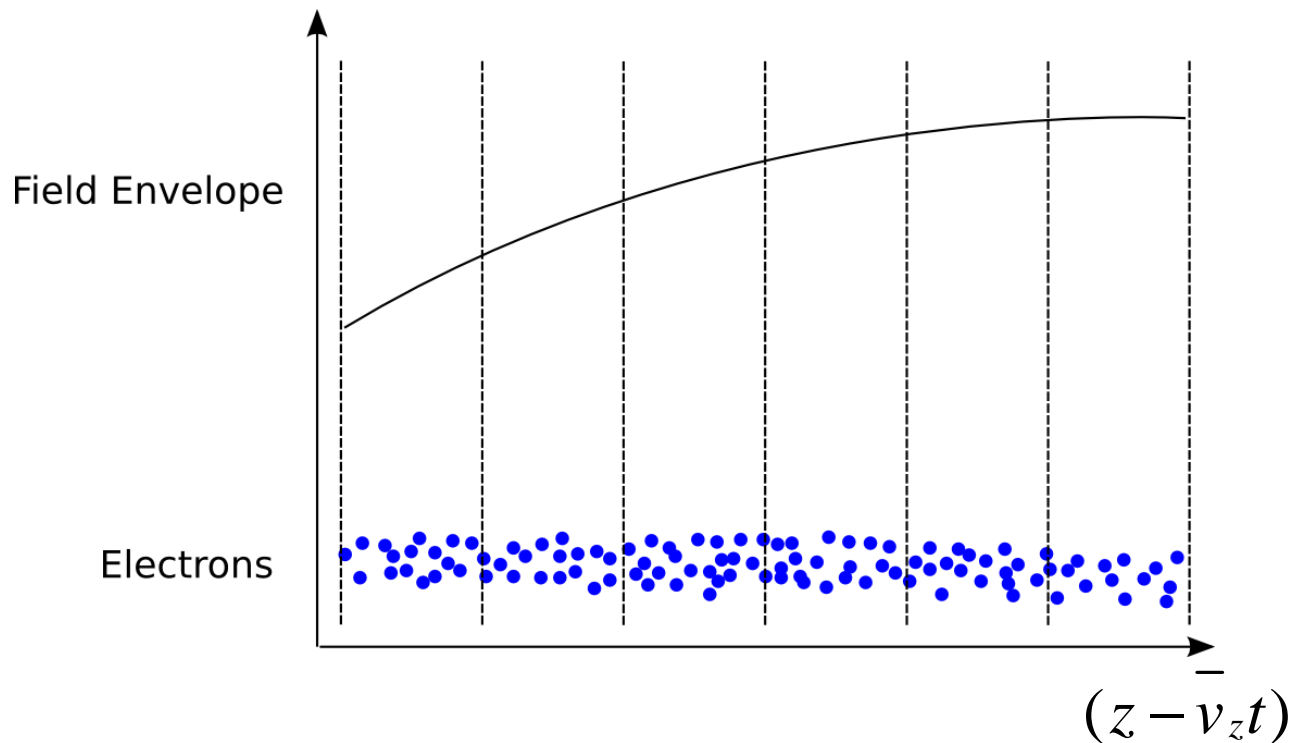
# FEL Averaged Code - Basic

- Radiation field and electrons co-propagate an undulator



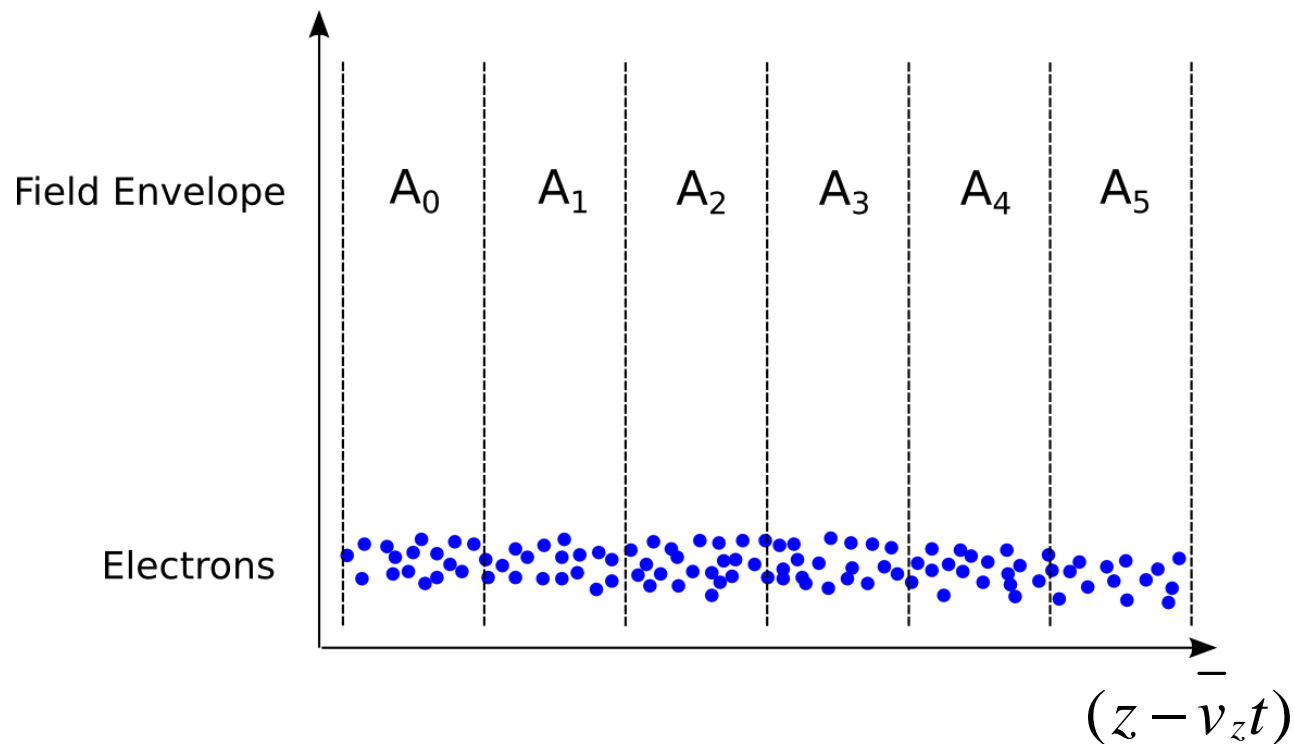
# FEL Averaged Code - Basic

- Use Slowly Varying Envelope Approximation (SVEA), and use averaged quantities to drive field



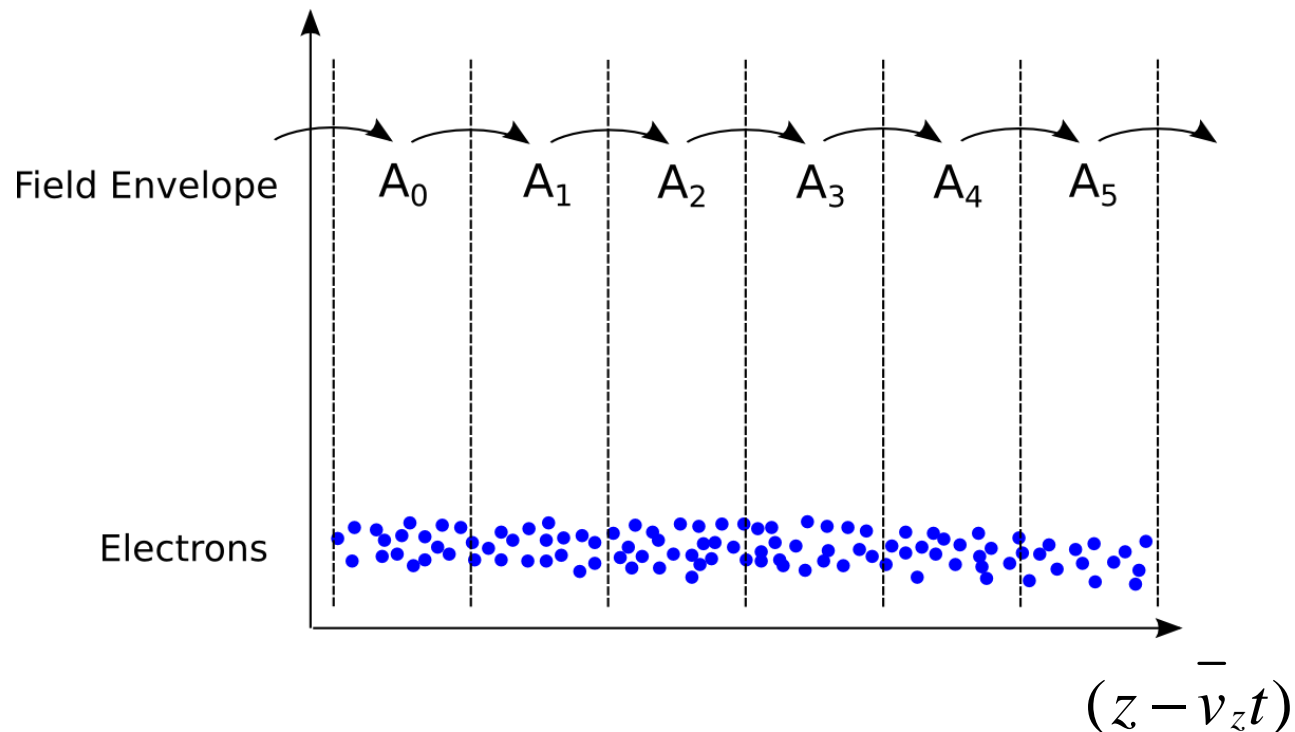
# FEL Averaged Code - Basic

- Use Slowly Varying Envelope Approximation (SVEA), and use averaged quantities to drive field



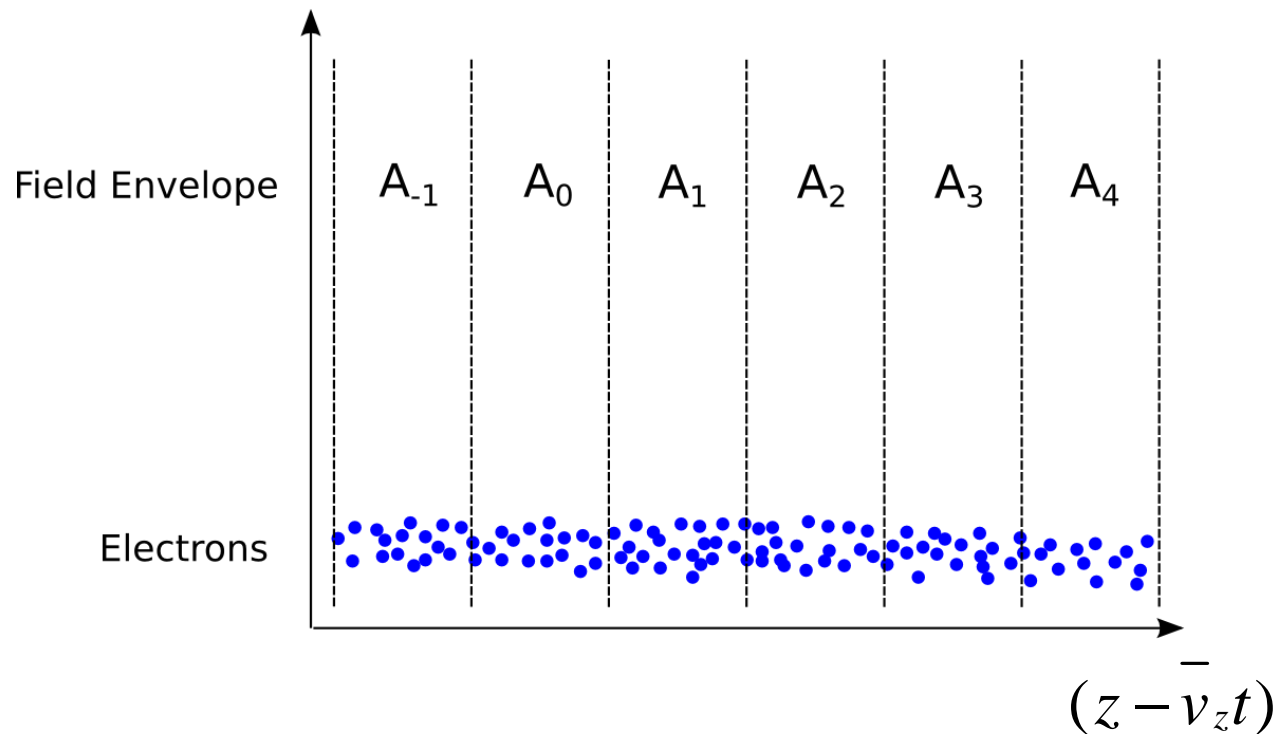
# FEL Averaged Code - Basic

- Electron velocity  $< c$
- To simulate relative electron-radiation 'slippage,' pass field on to next slice



# FEL Averaged Code - Basic

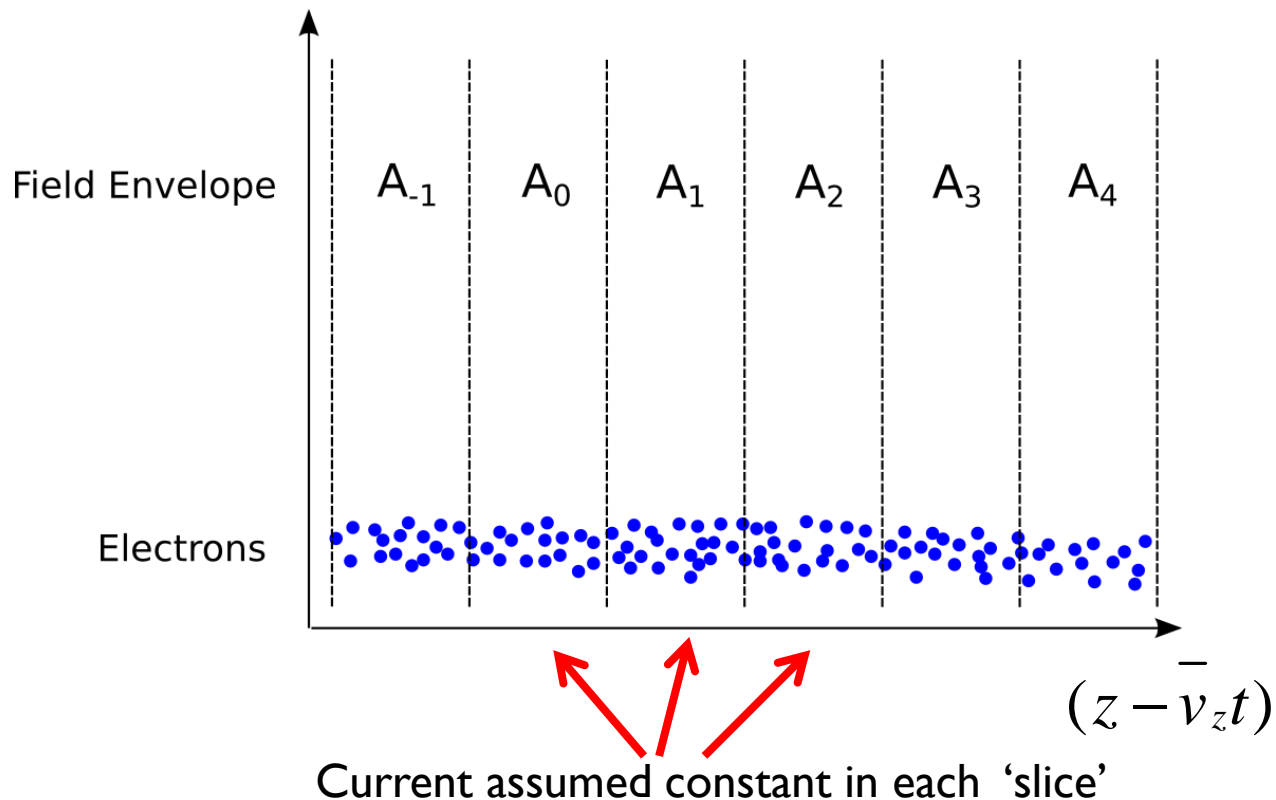
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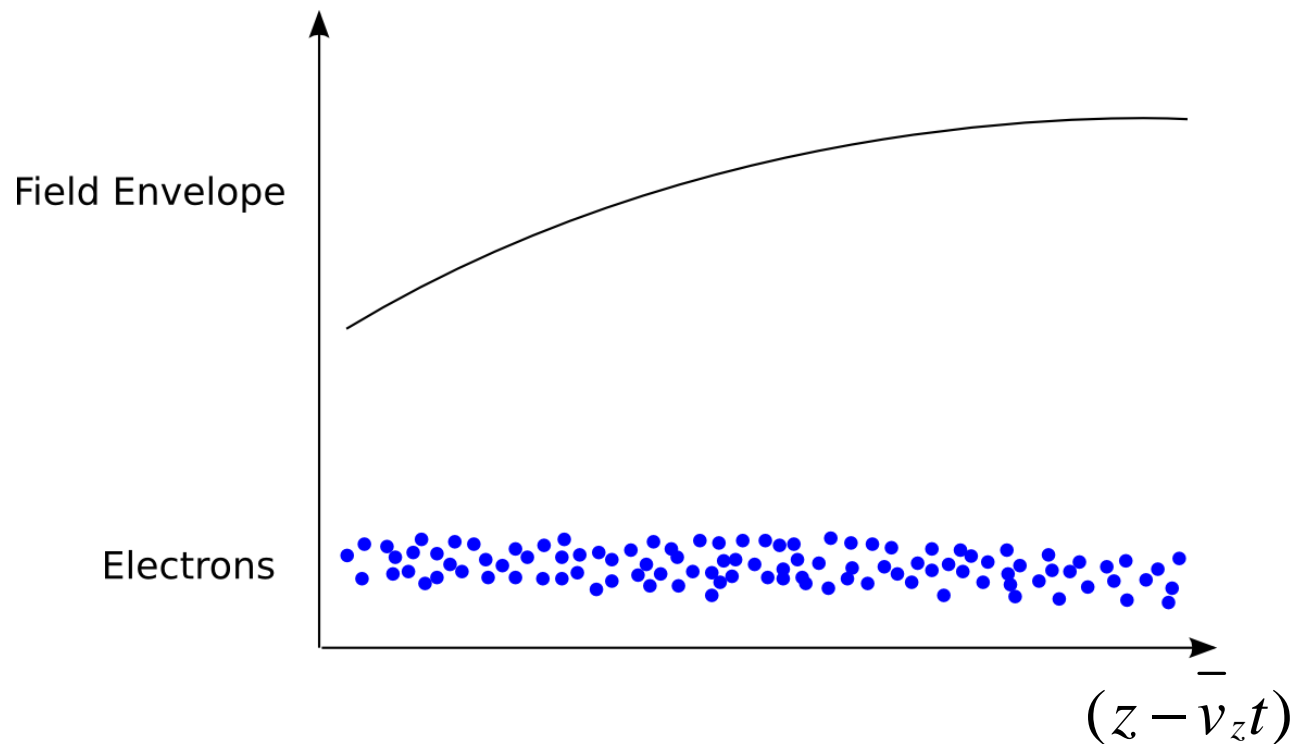
# FEL Averaged Code - Basic

- In this model, electrons are confined to each slice, within periodic BC's in phase space i.e. over a slice:



# FEL Unaveraged Code

- In an unaveraged code, we do not perform the SVEA or averaging process, and the radiation field is sampled on a much finer grid – a Particle In Cell (PIC) model



# Unaveraged FEL codes

- In an unaveraged code, the radiation field envelope can vary quickly, and so can model the full radiation spectrum self consistently (limited by the Nyquist frequency) – so can model coherent emission arising from current gradients in the beam
- Electrons are not confined to slices – can model current redistribution during propagation

# Motivation

- FEL's now operating in hard x-ray (around 1 Å) with pulse lengths of 10's of fs and peak powers of  $\sim 10^{10}W$ , to probe ultrafast, ultras-small phenomena. Evolves from noise – process known as SASE – and SVEA can model this
- Cannot model coherent spontaneous emission arising from current gradients in the beam
- Cannot model electron transport fully

# Motivation II

- Hard to model different frequencies with SVEA, can only model resonant frequency
- New techniques to improve temporal output and shot-to-shot stability may violate SVEA
- e.g. EEHG involves violent changes in electron position to prepare the beam
- Laser Plasma Accelerators produce short electron pulses which may exhibit a large degree of coherent emission, which averaged codes cannot model
- Such short electron pulses could involve large changes in relative electron positions – averaged codes cannot model this

# Puffin

- Parallel Unaveraged Fel Integrator
  - Unaveraged Free Electron Laser (FEL) code
- Puffin is first unaveraged FEL code in 3D
- Written in Fortran 90 using MPI
- Models a variably polarised undulator FEL
- Intended for probing new FEL schemes and ideas

PHYSICS OF PLASMAS **19**, 093119 (2012)

## **Puffin: A three dimensional, unaveraged free electron laser simulation code**

L. T. Campbell<sup>1,2,a)</sup> and B. W. J. McNeil<sup>1,b)</sup>

<sup>1</sup>*University of Strathclyde (SUPA), Glasgow G4 0NG, United Kingdom*

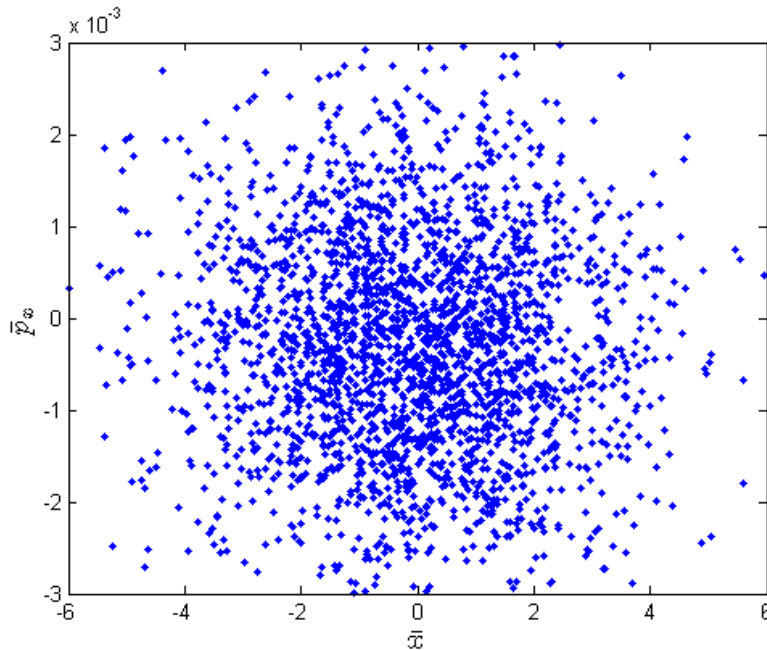
<sup>2</sup>*ASTeC, STFC Daresbury Laboratory and Cockcroft Institute, Warrington WA4 4AD, United Kingdom*

(Received 18 June 2012; accepted 29 August 2012; published online 26 September 2012)

An unaveraged 3D model of the free electron laser (FEL) is presented which is capable of modelling electron interactions with broad bandwidth radiation that includes electron beam shot-noise and coherent spontaneous emission effects. Non-localised electron transport throughout the beam is modelled self-consistently allowing better modelling of systems where a larger electron energy range is required. The FEL interaction can be modelled with undulator fields of variable polarisation. A modular undulator system allows insertion of other magnetic structures, such as chicanes. A set of working equations that describe the model are derived, the parallel numerical method that solves them described, and some example FEL interactions presented. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4752743>]

# Numerical Solution - Electrons

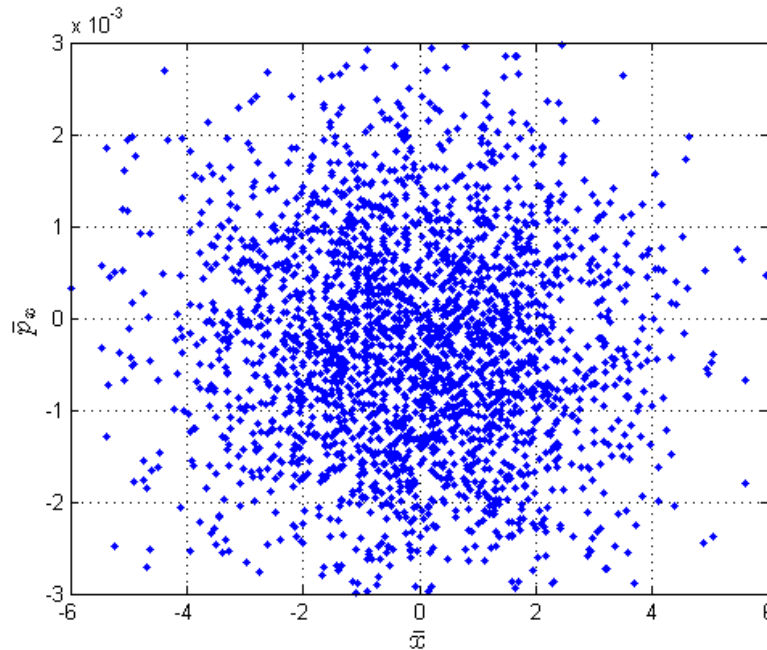
- Electron beam is discretised into electron macroparticles by method of [1]



- Sampling an electron beam with a gaussian current distribution

# Numerical Solution - Electrons

- Electron beam is discretised into electron macroparticles by method of [1]

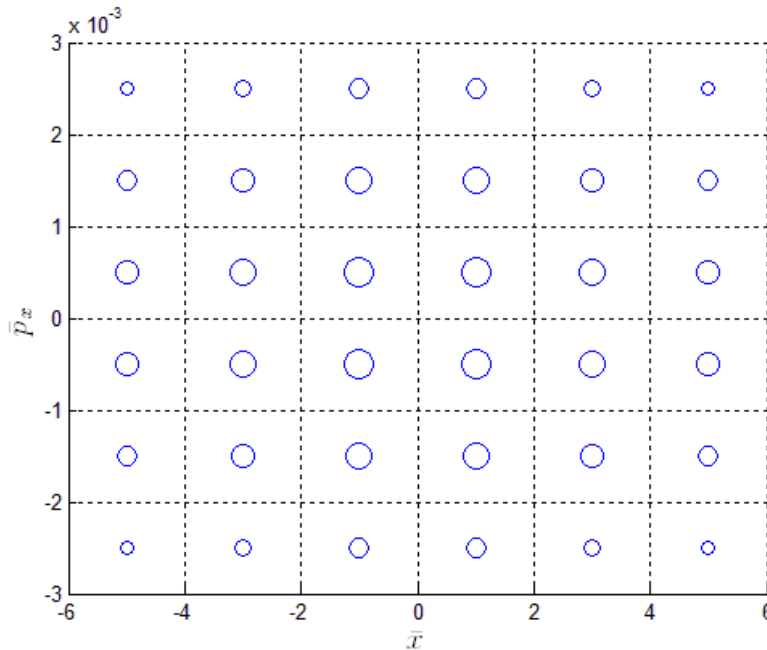


- Sampling an electron beam with a gaussian current distribution
- Create a grid...



# Numerical Solution - Electrons

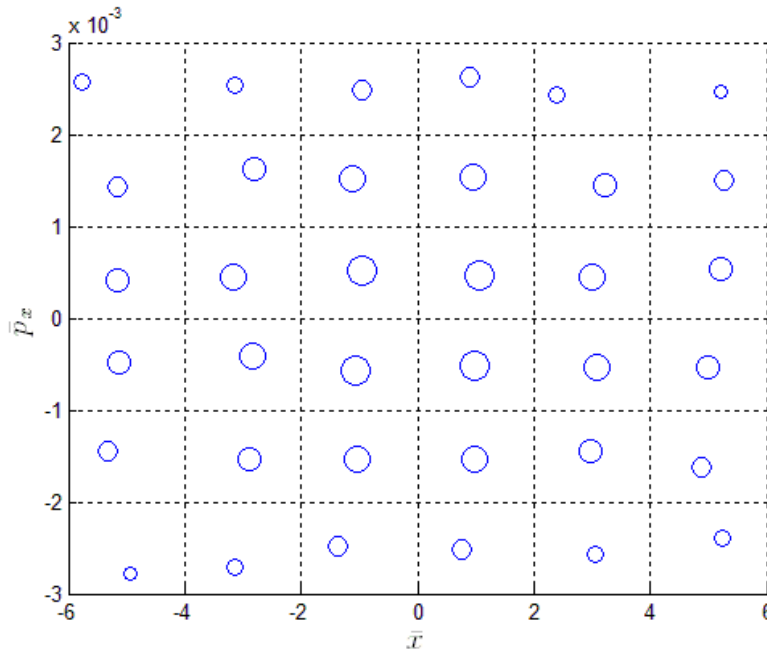
- Electron beam is discretised into electron macroparticles by method of [1]



- Sampling an electron beam with a gaussian current distribution
- Create a grid, and into each grid element we assign a macroparticle with charge weight determined by the current distribution

# Numerical Solution - Electrons

- Electron beam is discretised into electron macroparticles by method of [1]



- Sampling an electron beam with a gaussian current distribution
- Create a grid, and into each element we assign a macroparticle with charge weight determined by the current distribution

- To simulate noise assign random Poisson deviate to each macroparticle charge weight & position

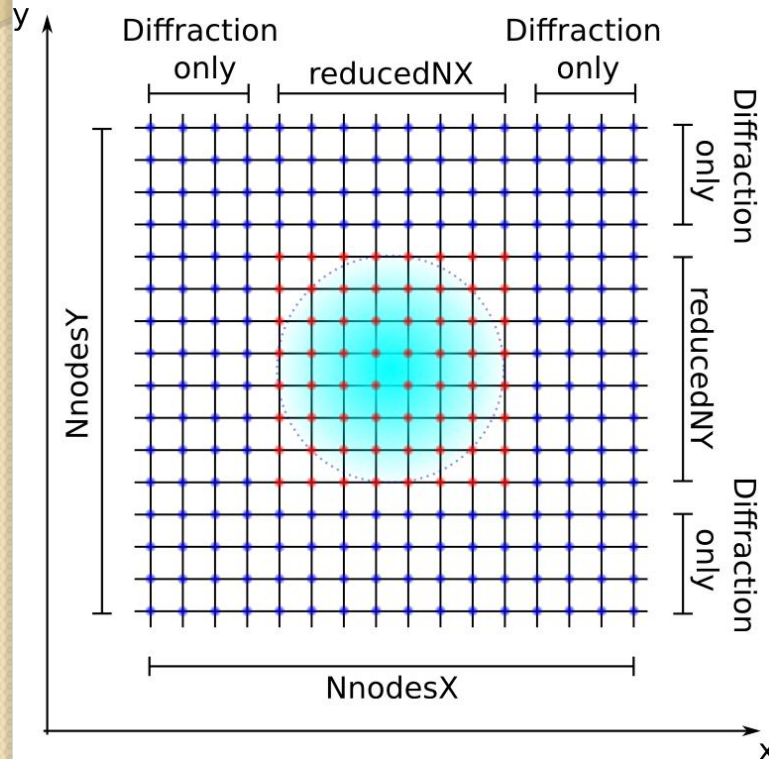
# Numerical Solution - Field

- Solve field with split step Fourier method [1]
  - 1<sup>st</sup> half step: Field diffraction solved with Fourier Transforms
  - 2<sup>nd</sup> half step: Field source (amplification and absorption by electron macroparticles) and electron propagation
- Field Source solved with Finite Element (Galerkin) Method [2]
- Involves solution of sparse linear system

[1] - R.H. Hardin and F.D. Tappert, SIAM Rev. **15**, 453 (1973)

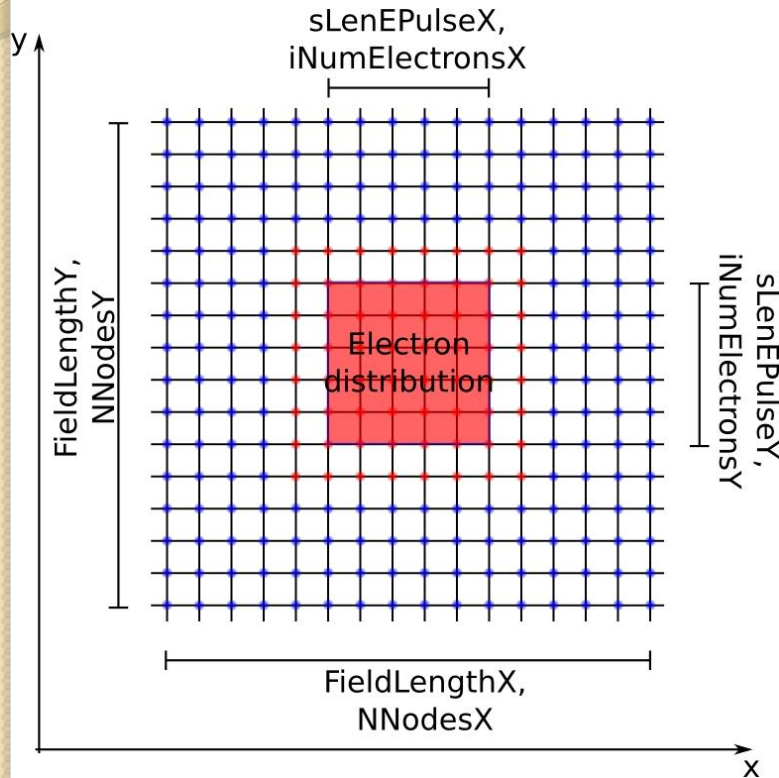
[2] - K.H. Huebner, E.A. Thornton and T.G. Byrom, *The Finite Element Method for Engineers*

# Matched Electron Beam



- Radiation field is modelled with a grid of nodes with linear interpolant, macroparticles move freely throughout field elements
- Electron beam is matched to undulator, meaning in transverse space it is focussed such that the beam has a constant radius

# Matched Electron Beam



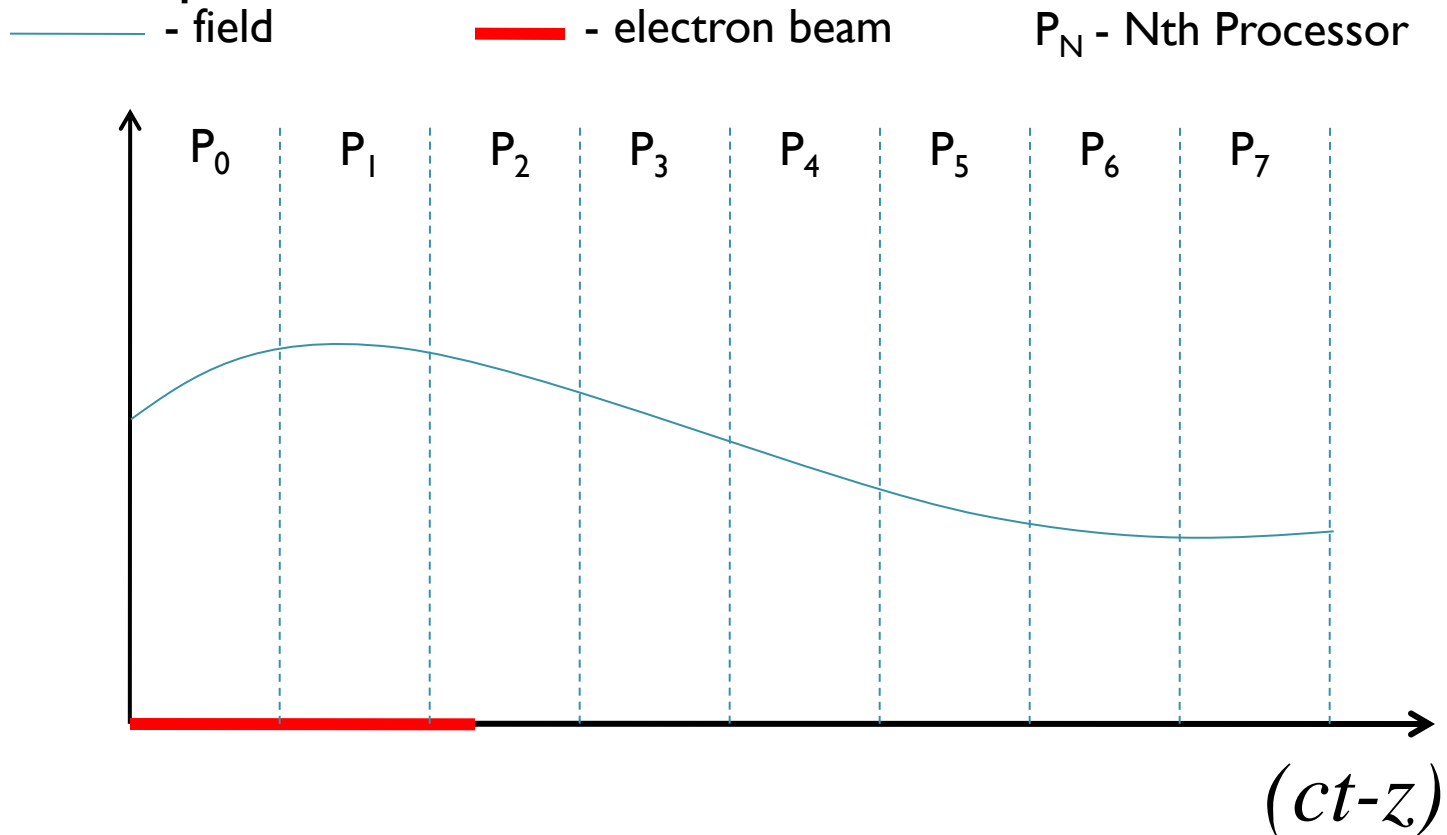
- Electrons will therefore remain confined to an inner set of nodes. Outer field nodes are then used only for diffraction
- Low frequency components diffract very quickly out the system. This causes an unphysical low frequency background signal to emerge which may interfere with the FEL interaction. Currently filter out low frequencies during propagation.

# Parallelism

- Large data sets
- Num of macroparticles  $\sim 10^9$  – would like to go orders of magnitude larger, need to distribute large electron arrays
- MPI
- Parallel Fourier Transforms
- Parallel Linear Solver for Sparse Systems
- We use:-
  - FFTW 2.1.5 for Fourier Transforms
  - MUMPS for Linear Solver - Possible change to Hiper for linear solver in future

# Memory Distribution

- Not immediately intuitive how to maintain a consistent memory distribution with minimum processor communication

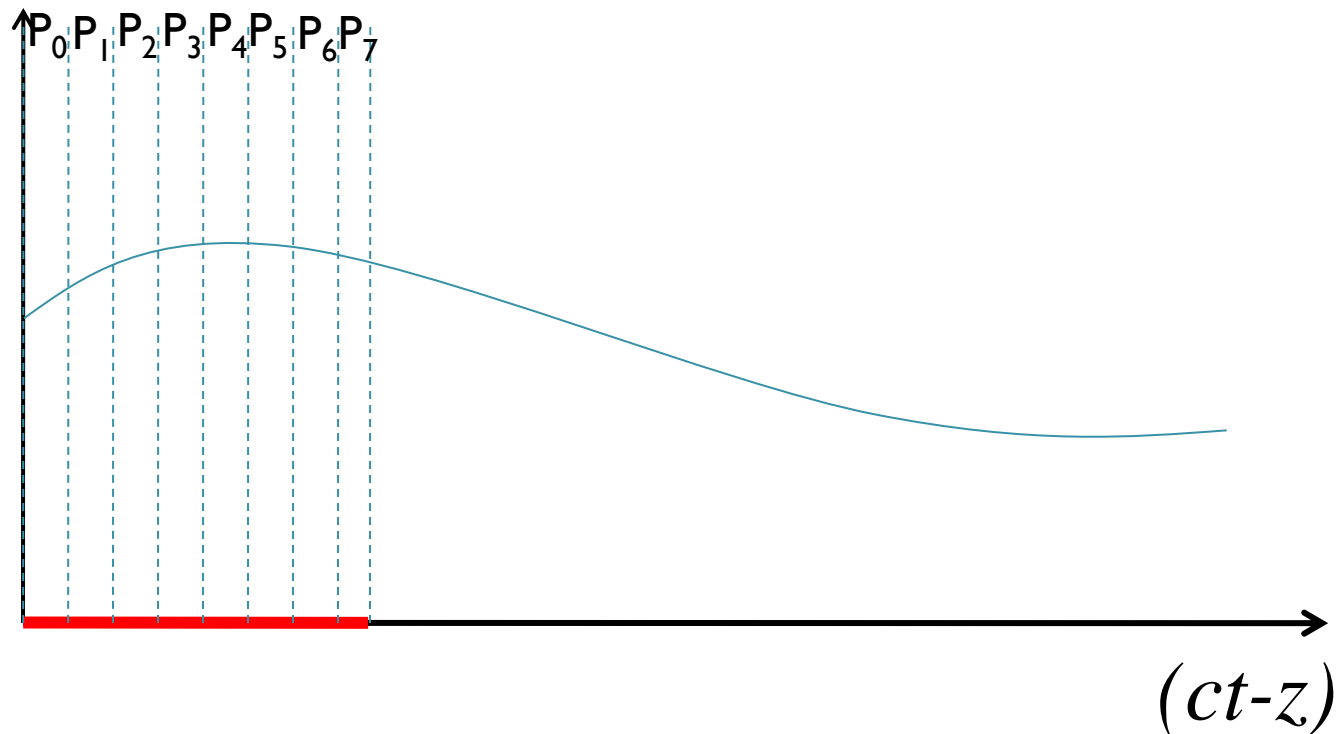


# Memory Distribution

- Not immediately intuitive how to maintain a consistent memory distribution with minimum processor communication

— - field

— - electron beam

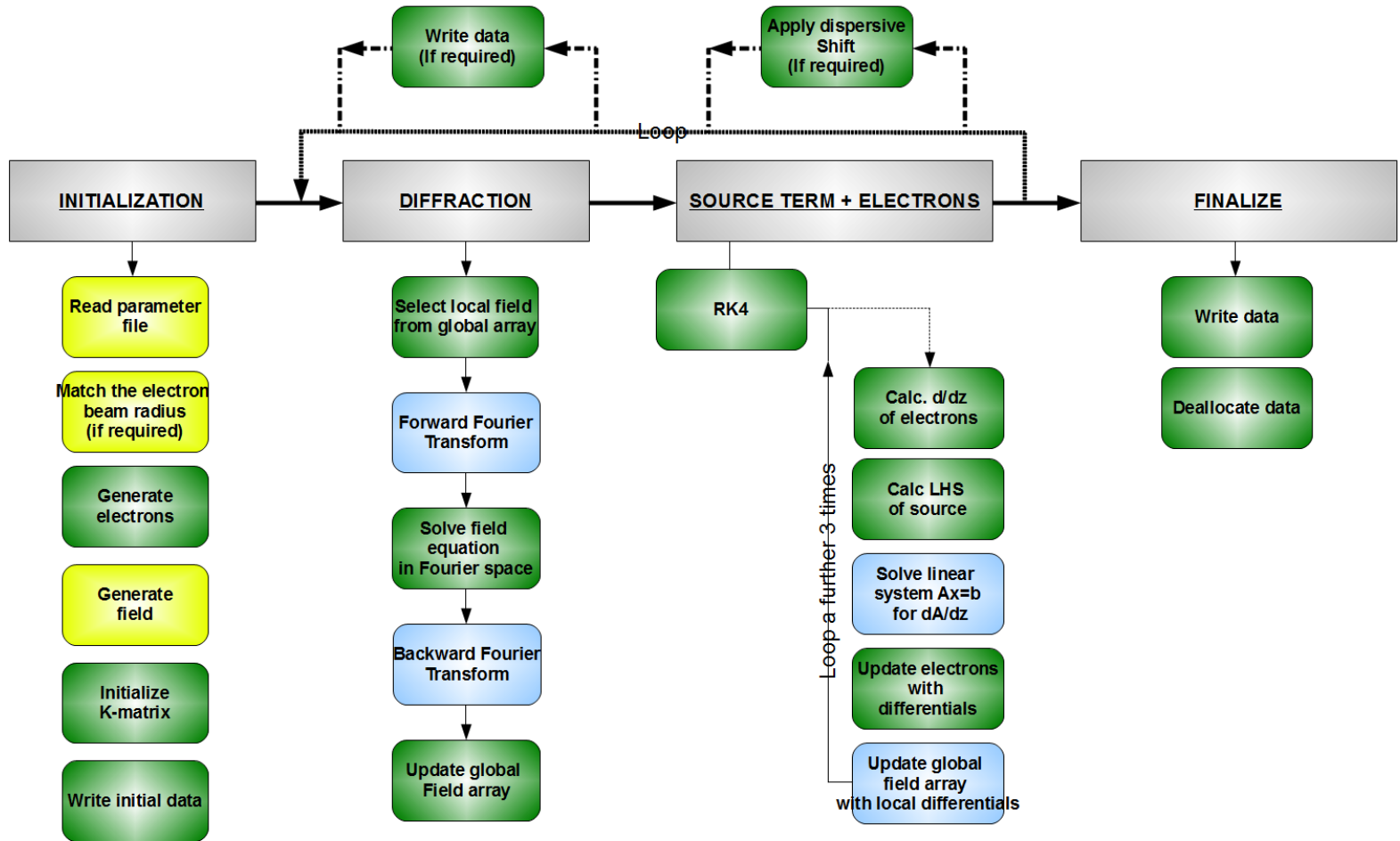




# Parallelism

- Electrons propagate freely through radiation field elements at  $v < c$
- Store full field array on each processor
- Electrons are distributed evenly amongst processors
- Since num macroparticles  $\gg$  num field nodes (6D beam vs 3D field)

# Code



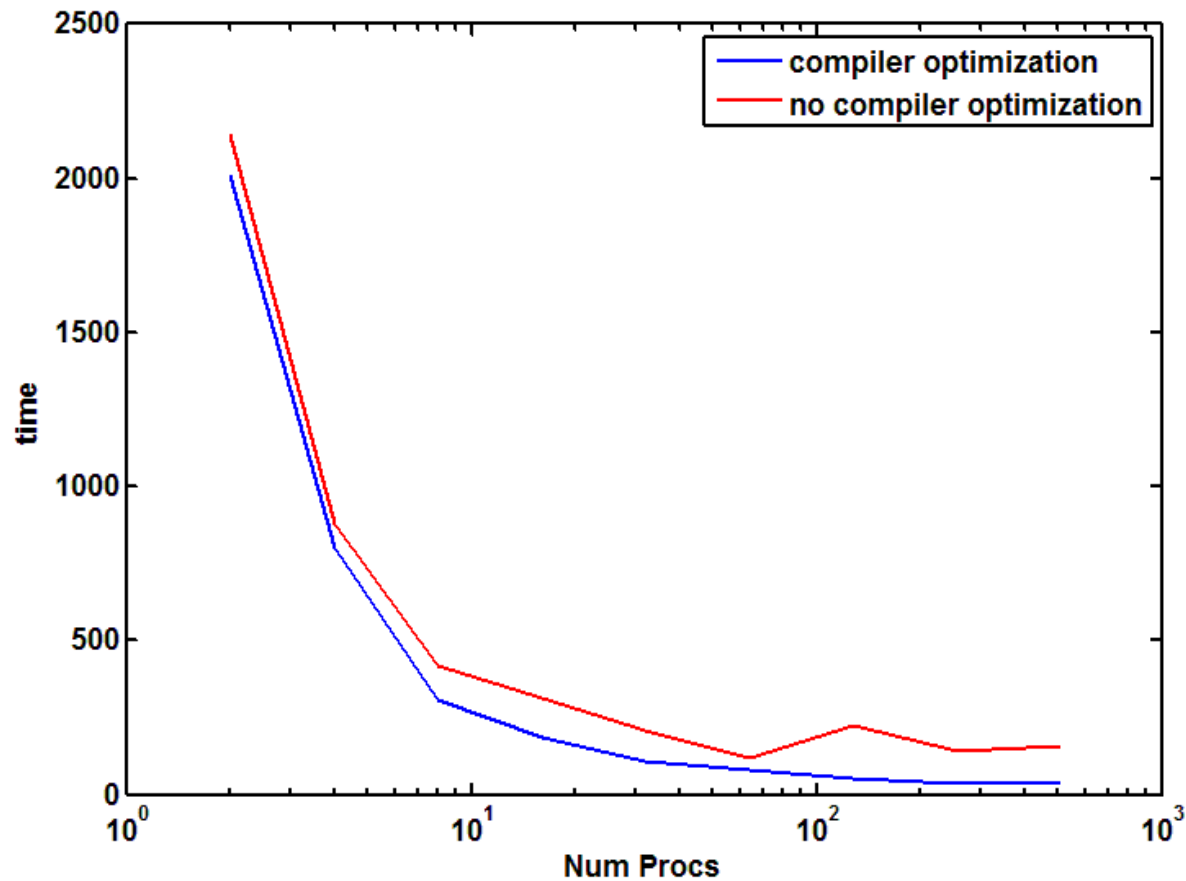
Key:- □ Parallel communication □ Parallel operation □ Independent

# Machines Used

- In house Sun x4600 server
  - 16 cores
- DL1 on NW grid at Daresbury
  - 30-40 cores
- ARCHIE at University of Strathclyde
  - 200-300 cores
- Hartree?
  - ???

# Current

- Benchmarking performed by Lucian Anton at Hartree



# Need for more processors/parallelism

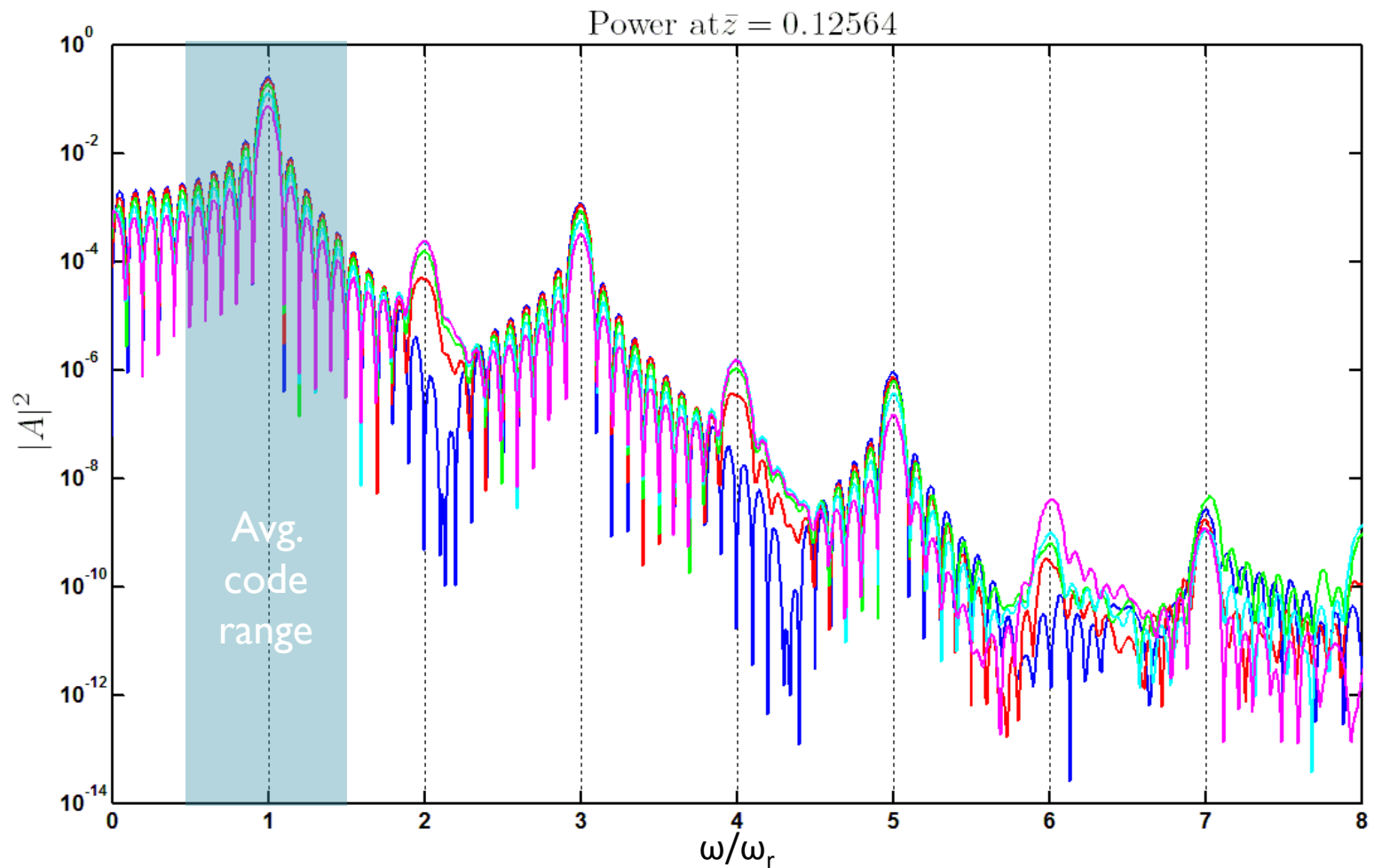
- Currently using around  $10^9$  macroparticles
- For larger systems would like to increase to at least  $10^{11} - 10^{12}$
- Linear solver can be replaced to be more efficient, currently it appears to take the most time in each integration step

# Ongoing Work

- Output and post-processing
  - Previously using custom Matlab interface
  - Now using scripts, need to link these into the Matlab GUI
  - Data files too large, inconvenient for storage and transport

# Broadband Field - variation with observation angle

— on-axis spectra, then in order of increasing arbitrary angle: — — — —



# Ongoing Work

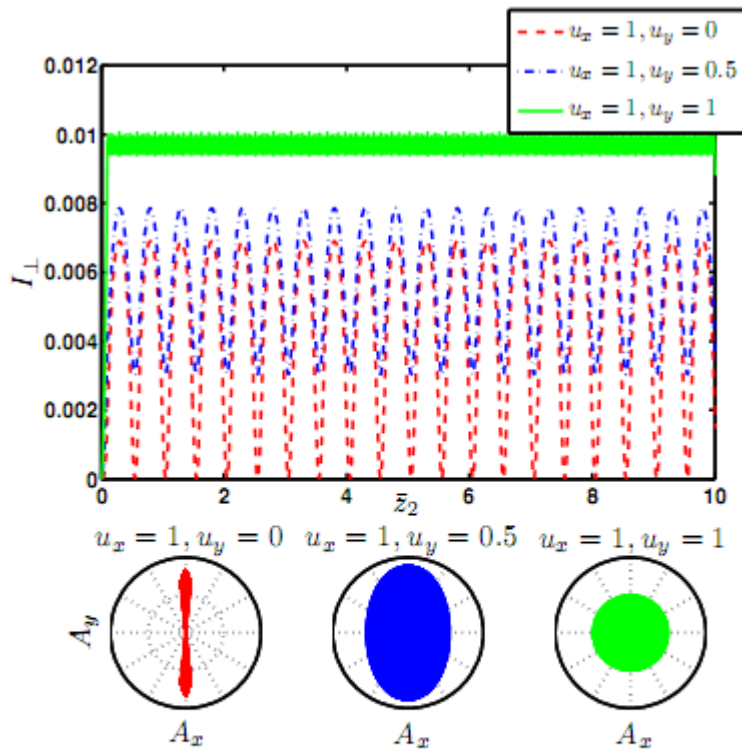
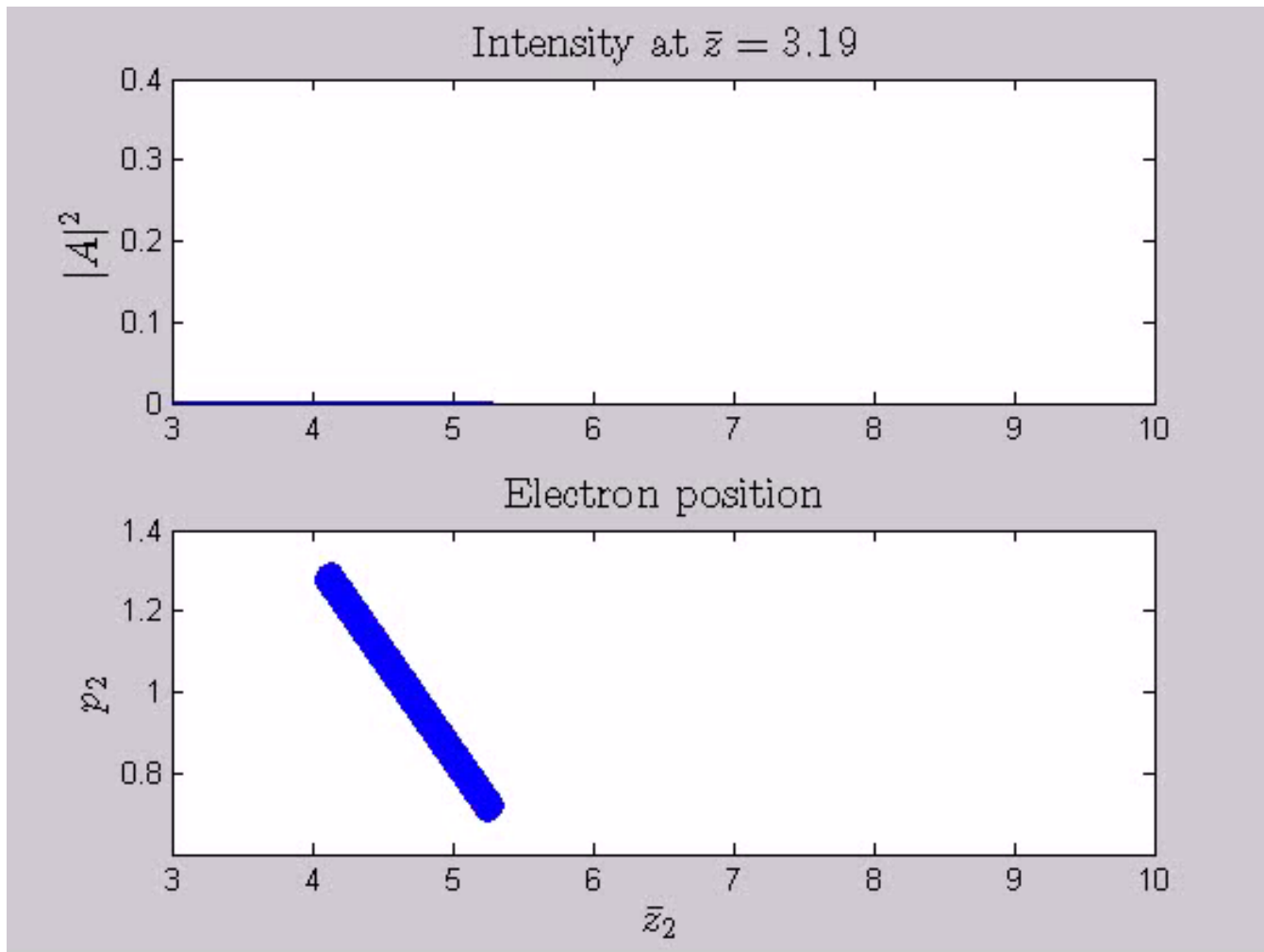


FIG. 1. Example of different field polarisations as driven by electrons in planar (red), elliptical (blue) and helical (green) undulators as specified by  $u_x$  and  $u_y$ . The radiation polarisation profiles are shown at the bottom, and the scaled powers on top.

- Models variably polarized undulator
- Radiation field polarization solved self-consistently – electrons only interact with correct polarization
- May be useful investigating FEL concepts with variable polarization and multifrequency model

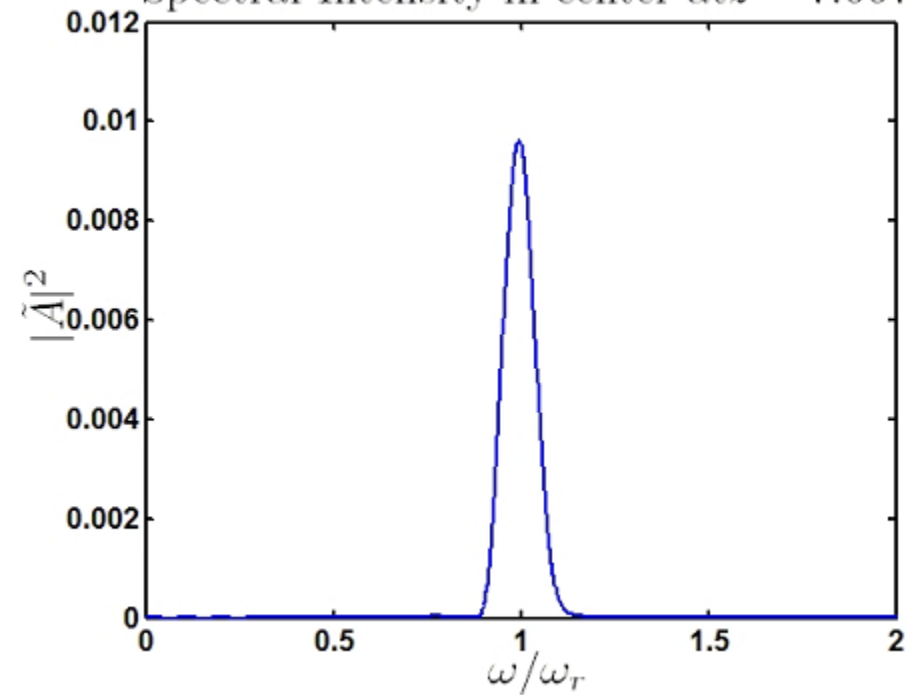


# Ongoing Work

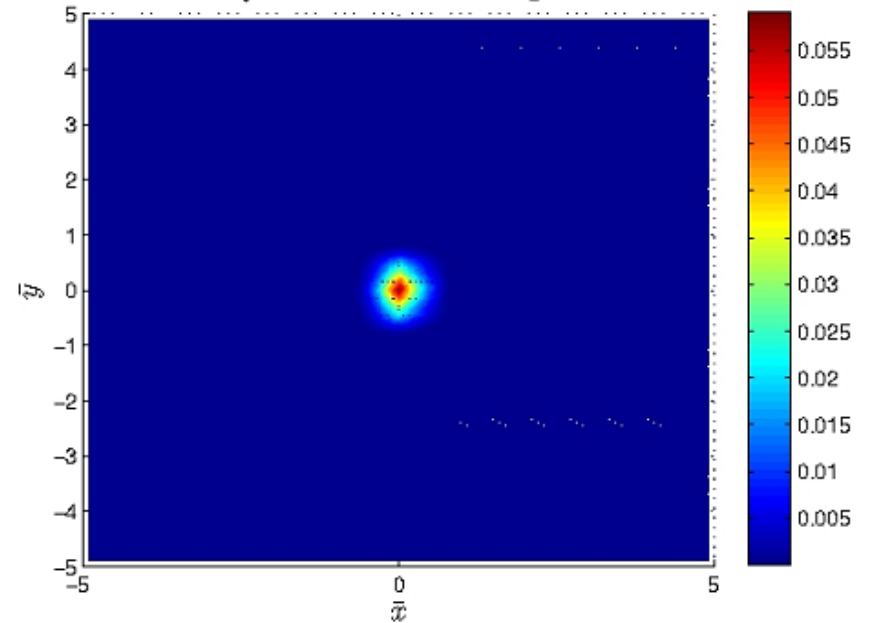


# Ongoing Work

Spectral Intensity in center at  $\bar{z} = 7.6676$



Intensity at  $\bar{z} = 7.6676$  and  $\bar{z}_2 = 7.0456$

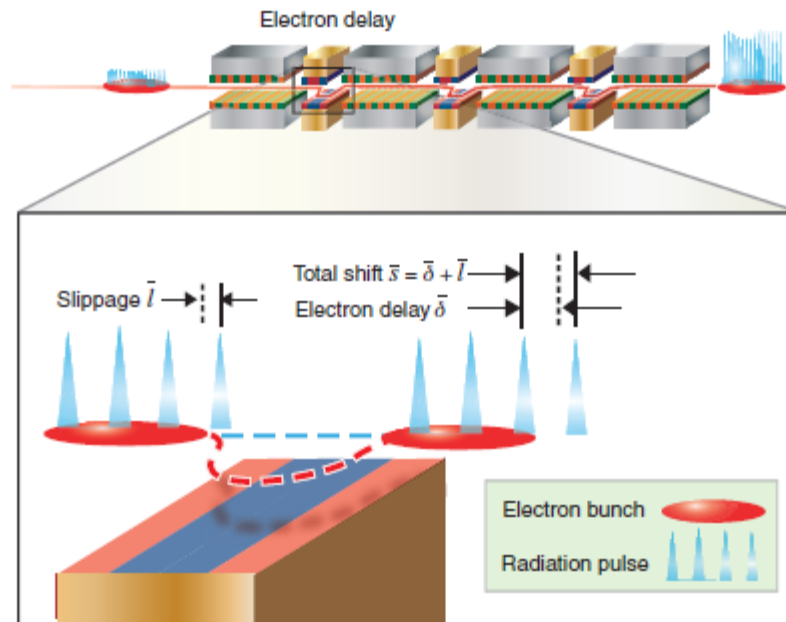


# Ongoing Work

- Mode locked FEL
- HHG seeding

J. Phys. B: At. Mol. Opt. Phys. 44 (2011) 065404

B W J McNeil *et al*



**Figure 1.** Schematic of the mode-coupled amplifier FEL interaction operating with an HH seed. The inset shows details of the electron delay.

# Ongoing Work

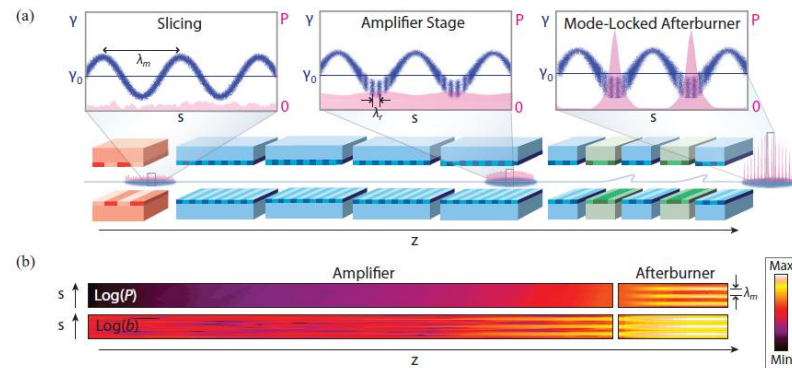


FIG. 1: (a) Schematic layout of the proposed technique and (b) Example simulation results. An electron beam is sliced (e.g. using an external laser and a short undulator to apply an energy modulation, as shown), such that a comb structure develops in the FEL-induced electron micro-bunching (b) in a long undulator (amplifier stage). Further amplification of the radiation intensity ( $P$ ) with periodic electron delays (mode-locked afterburner stage) generates a train of few-cycle radiation pulses.

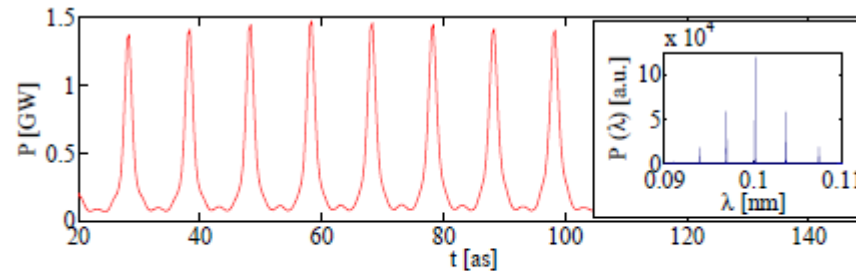


FIG. 4: Hard x-ray mode-locked afterburner simulation results: Radiation power profile and spectrum after 40 modules. The duration of an individual pulse is  $\sim 700$  zs rms.

[D.J. Dunning](#), [B.W.J. McNeil](#), [N.R. Thompson](#), [arXiv:1212.2047v1](#)



# End

- Thank you