

MODELLING TWO-COLOUR FEL WITH WIDE WAVELENGTH SEPARATION AND INDIVIDUAL POLARISATION TUNING

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Abstract

Free-electron lasers (FELs) are currently enabling cutting edge research in chemistry, biology and physics. We use simulations to assess a new FEL capability that would add to the impressive repertoire of experiments made possible by the technology: a two-colour independent polarisation mode, which allows for light pulses with variable temporal separation, individually tuneable polarisation, and widely separated wavelength. Simulations are carried out using the broad bandwidth FEL code Puffin, the results of which are used to discuss the radiation properties of the output. This scheme is applicable to existing and proposed facilities which feature undulators with variable ellipticity and gap.

INTRODUCTION

Temporally separated pulses with individually tunable colour and polarisation allow for exotic spectroscopic methods, such as two-colour polarisation spectroscopy [1] and various two dimensional spectroscopies at wavelengths and energies that are out of reach of conventional laser systems. This is of interest for fields in pure chemistry, such as transition metals to biological molecules [2]. At LCLS a two-colour mode with variable polarisation on the second pulse has been achieved [3,4] while Dattoli et al. [5] have modelled a scheme with two colours at orthogonal polarisations.

The focus of this work was therefore to demonstrate the capability to model a FEL operating mode generating two light pulses with individually tuneable polarisation and with two widely separated, non-harmonically related wavelengths. Such a scheme is modelled using the parameters of the CLARA FEL test facility [6], which is presently under construction at Daresbury Laboratory.

FEL SCHEME

A relatively simple FEL scheme was considered, as shown in Fig. 1. The layout is essentially that of a standard SASE FEL except that shortly before saturation occurs a change is made in both undulator parameter, a_u (with α the relative undulator parameter $\alpha = a_u/a_{u0}$) and ellipticity (specified by degree of ellipticity ε and angle θ) such that a second SASE process starts up with different resonant wavelength, λ_r , and polarisation state to the first. A chicane is included

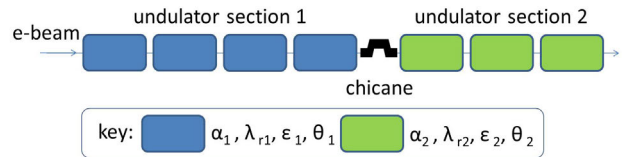


Figure 1: Schematic layout of the two-colour two-polarisation FEL scheme, with arbitrary number of modules.

between sections in order to provide a variable longitudinal offset between the two light pulses. Unlike methods which use two electron bunches (or regions of the same bunch) at different energies to generate two-colour output, an electron bunch at a single energy is used, similar to [5] and [7].

SIMULATION AND ANALYSIS METHODS

Many FEL simulation codes make the slowly-varying envelope approximation (SVEA) and so slice the radiation field at a minimum duration of λ_r . This limits the range of frequencies satisfied by the Nyquist condition to $\omega_r/2 < \omega < 3\omega_r/2$ (with ω_r the resonant frequency) and to a similarly narrow window around harmonics of the fundamental. This simulation approach is therefore suitable for only a subset of FEL operating modes. In this work we use the FEL simulation code Puffin [8] (version 1.8), which does not make the SVEA and so can model much broader bandwidth.

This capability has already been used to investigate two-colour FEL operation with wide frequency separation [7]. In addition to this we take advantage of the capability of Puffin to model undulators of different ellipticity within a single run and to have different polarisation states at different positions in the field. Most FEL codes require the same ellipticity within a single run (even where it can be changed between runs) and work with a single polarisation state at every point in the field. The Puffin code was used in both 1D and 3D modes, as part of the FXFEL simulation suite [9] utilising the high performance computing facilities of the Hartree Centre. Python plotting and post processing scripts have been used to visualize the data for this paper.

MODEL PARAMETERS

The scheme is modelled using parameters similar to those specified for CLARA. For 1D Puffin simulations the key parameters were the FEL parameter, $\rho = 5 \times 10^{-3}$ and the

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RMS relative energy spread (0.1% - set an order of magnitude higher than the nominal machine value to approximate diffraction and transverse emittance effects). A flat-top current profile with scaled length $50l_c$ was assumed, with $l_c = \lambda_r/4\pi\rho$ the FEL co-operation length. These settings are representative of machine parameters of 233 MeV electron beam energy, 100 pC charge, 265 fs bunch duration with 400 A flat-top current and 1 mm-mrad normalised emittance.

The CLARA FEL will have 17 planar undulator modules of 0.75 m length with 0.5 m intersections and an option is under consideration to make the undulators rotatable around the beam axis to provide an additional degree of freedom for implementing FEL schemes. Simulations used baseline values of $a_u = 0.716$ to give $\lambda_r=99.8$ nm with undulator period $\lambda_u = 2.75$ cm (although $\lambda_u=2.5$ cm has since been specified for CLARA). Care was taken to ensure optimum phase matching in intersections, taking into account the undulator fields being realistically tapered to zero. Three cases were considered in simulations: a baseline case with no change in undulator parameters, a case where only the polarisation state was changed, and a case where both the polarisation state and undulator parameter were changed.

The pulse energy growth for the baseline case can be seen in Fig. 2 alongside the two other modes, the results of which are described in more detail in the following sections.

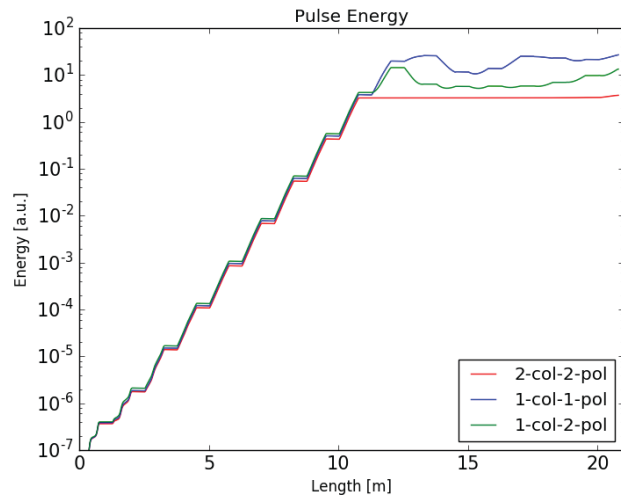


Figure 2: Pulse energy growth of the different schemes, with wavelength filtering applied to a bandwidth covering the two colours of interest.

1-COLOUR 2-POLARISATION

To achieve this mode the first nine undulators were set at baseline, after which the magnetic field was made orthogonal to alter the polarisation of emitted light. This would be achievable by rotating the undulator by 90° about the beam pipe and is expected to have the effect of shifting the polarisation state by the same degree. For ease of analysis a longitudinal shift of 330 fs was applied to offset the radiation emission from the two undulator stages. Since this value is somewhat arbitrary a dispersionless chicane was assumed

however the impact of dispersion could be considered in future work.

The total pulse energy growth is shown in Fig. 2. Upon changing polarisation the FEL growth continues, as is to be expected given that micro-bunching remains at the resonant wavelength. However growth is at a slower rate and ultimately saturates with pulse energy approximately 40% lower than the baseline case. The relative pulse energies may be controlled by altering the switchover point. If this is done before the saturation point each pulse will have a fraction of the saturation energy. Figure 3 shows resulting radiation field extracted at the point of saturation (12 m). The two pulses are well separated, have well defined linear polarisation orthogonal to each other, and feature similar longitudinal profiles as expected from micro-bunching in the first stage dictating emission in the second stage.

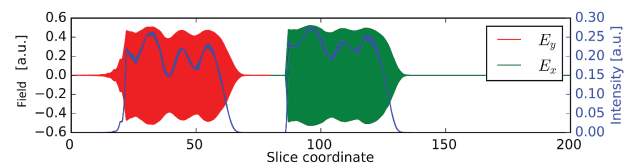


Figure 3: Radiation field at saturation showing the well separated horizontal (green) and vertical (red) electrical components and total intensity (blue).

2-COLOUR 2-POLARISATION

A natural progression from the successful simulation of pulses of individual polarisation is to also include a change in wavelength. This was done by altering the relative undulator parameter to 1.946 to simulate altering the undulator gap, which corresponds to altering the frequency by an inharmonic factor of 0.5144. As can be seen in Fig. 2 this has the effect of halting the FEL process at the original wavelength, and as seen on Fig. 4, restarting it at the second resonant wavelength. The growth profile is not purely exponential; this implies that there could be further phenomena to explore.

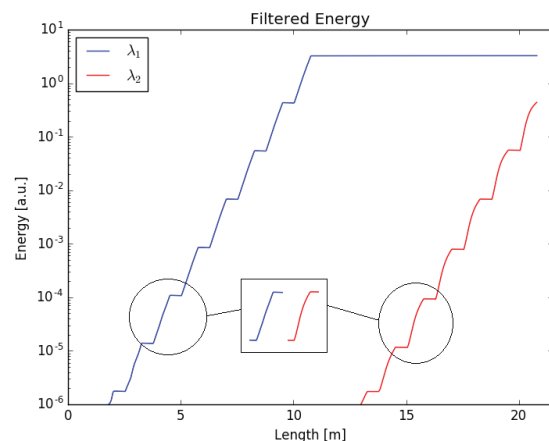


Figure 4: Energy growth of the two wavelengths

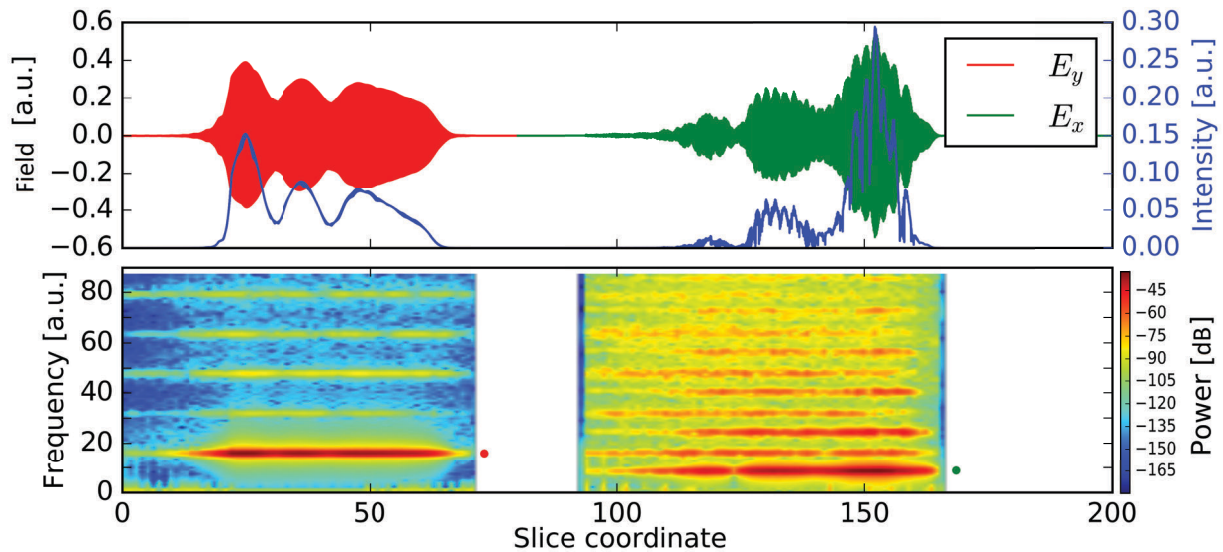


Figure 5: Two-colour two-polarisation mode 1D output at the undulator exit. Field and intensity (top) and time-frequency plots (bottom) are shown. The circles highlight the fundamental frequencies.

In addition to this, Fig. 5 shows that there is a high frequency modulation of the second pulse (in green) compared to the slower envelope that is found in both pulses. Although the second pulse does indeed have most of its intensity concentrated in its resonant wavelength, there is also a significant contribution from the third harmonic. Emission at other harmonics is also increased compared to running the second colour in isolation, though they remain at a low level: the color scale of the time-frequency plot in Fig. 5 is set to be logarithmic to show this content. This has been studied in [7] and is a result of bunching from the first wavelength and further bunching that develops in the second section. This includes the sum and difference frequencies and their respective harmonics.

Like in the previous case, the polarisation of the two pulses remains well defined but the almost inverse longitudinal profiles hint that the strong lasing in the head of the first pulse inhibited it from lasing in the second colour and the opposite effect is seen in the tails of the pulses.

3D RESULTS

3D simulations are more comprehensive but computationally intensive. It was not yet possible to separate the pulses due to memory limitations. Nevertheless similar effects such as the fast modulation and weak emission in the harmonics and original frequencies are found. In 3D diffraction is simulated and is found to be a significant consideration for the scheme, particularly at the relatively long wavelength of CLARA compared to X-ray FELs. As such, it should be expected that the radiation in the first section will be lost to the beam pipe at the wavelengths tested unless they are extracted.

The 3D radiation fields hold a full description and polarisation can be extracted at every recorded coordinate. For example Fig. 6 shows the polarisation angle of the trans-

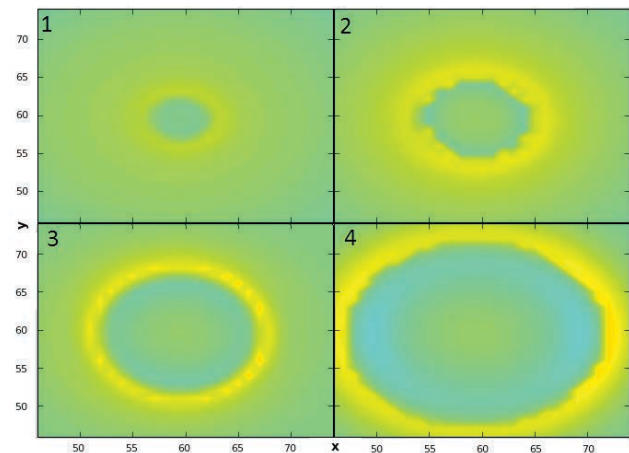


Figure 6: 3D simulation showing the polarisation angle at each coordinate per slice, green= 0° , red/blue = $\pm 90^\circ$

verse radiation field over four sequential slices along the longitudinal axis where some light with orthogonal polarisation is diffracting. The polarisations are averages over a longitudinal field length of $40\lambda_{r1}$. It shows that the two orthogonal radiation components combine to give variation in polarisation both longitudinally and transversely if there isn't a large enough separation between pulses.

CONCLUSION

Broadband two-polarisation single-colour and two-colour schemes were successfully simulated in 1D and 3D. Scripts to extract, analyse and visualize data from the simulations have been developed for both 1D and 3D Puffin outputs. This tool allows for exotic schemes, such as crossed undulators to generate light of arbitrary polarisation [4] and could be adapted to allow two pulses of circularly polarized light of opposite chirality to be simulated consistently.

REFERENCES

- [1] M. L. Costen and K. G. McKendrick, "Orientation and alignment moments in two-color polarization spectroscopy," *The Journal of Chemical Physics*, vol. 122, p. 164309, apr 2005.
- [2] L. X. Chen, X. Zhang, and M. L. Shelby, "Recent advances on ultrafast X-ray spectroscopy in the chemical sciences," *Chem. Sci.*, vol. 5, pp. 4136–4152, jun 2014.
- [3] A. A. Lutman, T. J. Maxwell, J. P. Macarthur, M. W. Guetg, N. Berrah, *et al.*, "Fresh-slice multicolour X-ray free-electron lasers," *Nature Photonics*, vol. 10, no. 11, pp. 745–750, 2016.
- [4] A. A. Lutman, J. P. MacArthur, M. Ilchen, A. O. Lindahl, J. Buck, R. N. Coffee, *et al.*, "Polarization control in an X-ray free-electron laser," *Nature Photonics*, no. 10, p. 468–472, 2016.
- [5] G. Dattoli, N. S. Mirian, E. Divalma, and V. Petrillo, "Two-color free-electron laser with two orthogonal undulators," *Physical Review Special Topics - Accelerators and Beams*, vol. 17, no. 5, 2014.
- [6] J. A. Clarke, D. Angal-Kalinin, N. Bliss, R. Buckley, S. Buckley, R. Cash, *et al.*, "CLARA conceptual design report," *Journal of Instrumentation*, vol. 9, no. 05, p. T05001, 2014.
- [7] L. T. Campbell, B. W. J. McNeil, and S. Reiche, "Two-colour free electron laser with wide frequency separation using a single monoenergetic electron beam," *New Journal of Physics*, vol. 16, no. 10, p. 103019, 2014.
- [8] L. T. Campbell and B. W. J. McNeil, "Puffin: A three dimensional, unaveraged free electron laser simulation code," *Physics of Plasmas*, vol. 19, no. 9, 2012.
- [9] R. J. Allan *et al.*, "HPC simulation suite for future FELs," in *Proc. of FEL2015*, pp. 384–3878, 2015. <http://accelconf.web.cern.ch/AccelConf/FEL2015/papers/tup017.pdf>.