SPUR: A NEW CODE FOR THE CALCULATION OF SYNCHROTRON RADIATION FROM VERY LONG UNDULATOR SYSTEMS

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Abstract

The accurate calculation of synchrotron radiation from an undulator is a common problem and numerous codes have been developed that describe the radiation from analytic and measured undulator fields. However, for very long undulator systems there is not a suitable code that can handle the amount of data in a convenient manner and which runs in a practically realisable time limit. The development of a new code, SPontaneous Undulator Radiation (SPUR) [1], is presented which computes the spontaneous radiation from electron beams passing through a system of undulators. The code supports parallel architecture, and uses the HDF5 [2] technology to efficiently handle the multi-dimensional data. The latest developments and benchmarking are presented.

INTRODUCTION

Many new undulator systems are very long, in excess of 100s of metres, and comprise of many shorter undulator modules. Examples include LCLS, X-FEL and the ILC positron source undulator [3, 4, 5]. The accurate calculation of the synchrotron radiation (SR) emitted by such systems can be time consuming or even impractical using current codes, such as SPECTRA [6], running on single processors.

SR calculations typically involve either calculating the brightness as a function of wavelength at a single observation point or the flux into an aperture. To calculate the flux into an aperture one calculates the brightness at a number of observation points within the aperture. The distance between the points is assumed to be small enough that the brightness in the small area surrounding each point is constant. Each point's flux is then the product of the point's brightness and the area assigned to it. The total aperture flux being given by the sum of all the observation points' fluxes.

Such calculations are time consuming, so the ability to reuse calculated data is favourable to recalculation. When calculating the spectrum into an aperture it is better to output each individual point's spectrum, rather than only the whole aperture's spectrum. Thus new apertures whose observation points are a subset of the original aperture's points require no further calculation.

Outputting many such spectra rather than one can result in very large amounts of data of complex types, and thus an efficient and flexible data format is required.

CODE DESCRIPTION

SPUR calculates the spectrum of radiation at either a single point, or into a rectangular aperture centred on the undulator axis and orthogonal to it. The aperture is defined by the user giving the longitudinal distance from the beginning of the undulator system to the aperture, its size in the two transverse directions and the number of points within the aperture to be calculated.

For each observation point the spectrum is calculated from the electric field in the retarded time domain given by

$$\vec{E} = \frac{e}{4\pi\varepsilon_0 c}\left(\frac{c(1-|\vec{\beta}|^2)(\vec{n}-\vec{\beta})}{|\vec{R}|^2 (1-\vec{n}\cdot\vec{\beta})^3} + \frac{\vec{n}\times[(\vec{n}-\vec{\beta})\times\dot{\vec{\beta}}]}{|\vec{R}|(1-\vec{n}\cdot\vec{\beta})^3}\right)_{\mathrm{ret}} \quad (1)$$

where $\vec{R}$ is the vector from the electron to the observation point, and $\vec{n}$ its unit vector. The electron's motion is calculated by modelling its trajectory in steps of equal distance along the undulator axis, either from an analytic formula or by modelling the motion through a user defined magnetic fieldmap. The electric field is then interpolated into equal time spacing before being Fast Fourier Transformed into the frequency domain.

Parallelisation

To make synchrotron radiation calculations within a practicable time SPUR takes advantage of parallel processing using the Message Passing Interface (MPI) method [7]. Since the electric field signals are calculated in retarded time, which is dependant on the observation point, the program is parallelised so that many observation points' spectra can be calculated simultaneously.

The main program runs on one processor, assigning the calculation of the radiation of separate points to run in parallel on other processors, which each write out their output to a different file. The main program then merges the output from each of the processors into a single output file.

Analytic Calculation

The analytic calculation can model a system of planar, helical or elliptical undulator modules. It calculates the vector **R** each period and calculates the spectrum using (1), describing the motion of the particle as sinusoidal

functions. To efficiently do so the sine and cosine functions are pre-calculated and stored in an array.

Since for the helical and planar cases some of the vector components of $\vec{\beta}$ and $\dot{\vec{\beta}}$ are zero, less terms from an expanded form of (1) need to be calculated, and thus these types of calculation require less running time.

Fieldmap Calculation

SPUR can also model a user defined fieldmap which gives the three dimensional magnetic field as a function of longitudinal distance from the beginning of the undulator system. To do this it models the electron's motion by calculating the Lorentz force due to the magnetic field present. It calculates **R** for each of a user defined number of steps down the undulator, interpolating the given magnetic field and calculating the motion for each step. It is assumed that the electron does not lose any energy due to emission of synchrotron radiation whilst travelling through the magnetic field.

Data Formatting

SPUR takes advantage of the Hierarchical Data Format (HDF5) [2], allowing the program to make custom data types of unlimited size that are fully portable. HDF also allows efficient file operations in both parallel and single processor environments. It is a suitable file format for calculations of radiation into an arbitrary number of observation points whilst taking advantage of parallel processing.

Calculation Options

SPUR allows some approximations to be optionally made in order to decrease the calculation time. Two farfield approximations can be made; either to calculate only the 1/**R** term in (1) or to assume that the distance to the observer is sufficiently large compared to the undulator length that the vector **R** is assumed to remain constant as the particle travels through the undulator.

Depending on the type of undulator the user may also want to take advantage of symmetry of the spectra for different observation points and can therefore choose to calculate the spectra at points in only one quadrant of the desired aperture.

BENCHMARKING

SPUR has been benchmarked against SPECTRA near field partial flux calculations for various undulator types. The results presented below use the ILC Reference Design Report (RDR) [8] undulator parameters with an ideal beam unless otherwise stated. Comparisons between the calculation times when run using SPUR and SPECTRA are given in Table 1.

Analytic Undulator Comparison

Calculations were made of the spectral flux from 2m and 100m long planar undulators. For the 2m undulator

the flux into rectangular apertures sized $2\times2\mu m$ at a distance of 10m from the end of the undulator was calculated. SPUR calculated the aperture as 121 observation points. SPECTRA calculated the spectrum from the 2m undulator using accuracy levels of 1 and 2. Comparisons of the 2m spectra are shown in Figure 1. The two programs show a good agreement between the calculated spectra other than a slight photon energy offset.
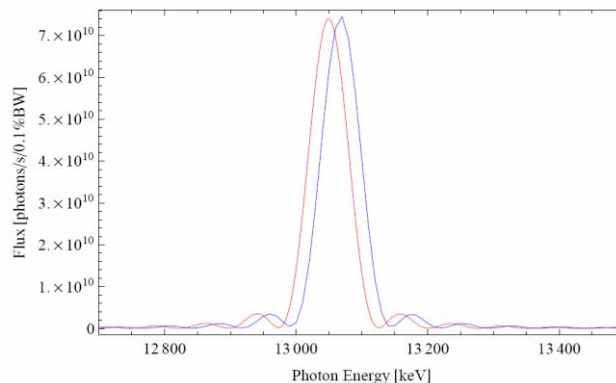

Figure 1. Comparison of SPECTRA accuracy level 2 (red) and SPUR (blue) spectra from a planar undulator into an aperture.

The 100m undulator's spectrum was calculated into an aperture of $20\times20\mu m$ at a position centred on axis 150m from the end of the undulator system. The SPUR calculation split the aperture into 81 observation points, the SPECTRA calculation was done with an accuracy level of 1. The SPECTRA calculation did not manage to complete within a practical time, having run for over a week with most of the calculation remaining unfinished.
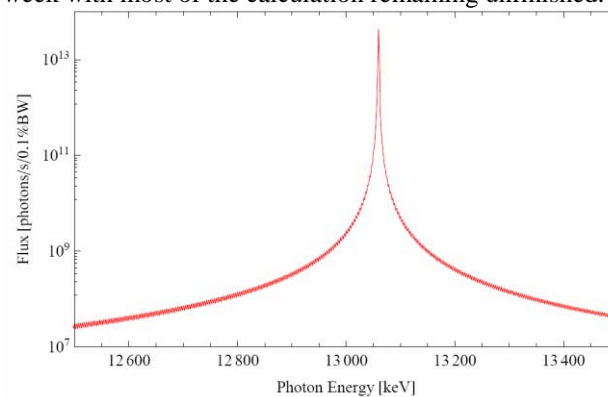

Figure 2. SPUR spectrum from a 100m planar undulator into an aperture.

2m User Defined Fieldmap Comparison

The spectrum from a 2m long user defined magnetic field was calculated. The magnetic fieldmap was made of 20000 magnetic field points along the undulator axis. Calculations were made of the spectral flux into a rectangular aperture of size $2\times2\mu m$ centred on the undulator axis 10m from the undulator. SPUR calculated the radiation at 1225 observation points while SPECTRA ran using an accuracy level of 1. The resulting spectra are

shown in Figure 3. There is generally a good agreement between the two programs' spectra.
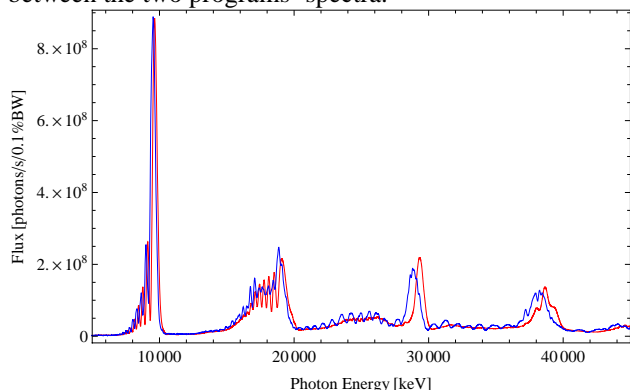

Figure 3. Comparison of SPECTRA (red) and SPUR (blue) spectra from a user defined fieldmap into an aperture.

Calculation Times

In the above comparisons SPUR completed its calculations in considerably less time than SPECTRA due to its parallelisation. The difference is of most importance as the undulators get long, where it can mean the difference between whether the calculation was possible in a practical time or not. For the fieldmap calculation this advantage is quite evident, with the calculation taking hours rather than days. As the accuracy level of SPECTRA is increased further the difference also becomes much more pronounced.

Table 1. SPUR and SPECTRA calculation times.

Calculation	SPUR		SPECTRA	
	Time	nodes	Accuracy level	Time
Fieldmap	4 hr	45	1	68 hr
2m Planar	10 min	30	1	2 hr
2m Planar Higher accuracy	45 min	30	2	49 hr
100m Planar	2 hr	30	1	>1 week

Calculation Output Files

SPECTRA outputs an ASCII file containing a single spectrum with a typical size of 4MB. SPUR outputs an HDF file containing a user defined number of spectra. Despite including much more data the HDF format allows for many spectra in files that are not so large as to be impractical. For the comparisons above with SPUR outputting between 81 and 1225 spectra the HDF files ranged from 11MB to 160MB

FURTHER WORK

SPUR is still in a development phase. Future development plans include the inclusion of non-ideal electron beams and also more options in defining the aperture or observation point.

Currently SPUR calculates the electron from a single electron's pass through the undulator system. More realistic output will require the modelling of electron bunches with user defined emittance and energy spread. It is expected that modelling bunches of electrons will also take advantage of parallelisation to minimise the adverse affect on calculation times.

Optional aperture definition by angle instead of with absolute coordinates is to be added, as is different aperture shapes including circular apertures and rings. The user will also be able to position the apertures so that they are centred off axis.

The polarisation of the radiation will also be optionally calculated and along with particle trajectories and electric field signals included in the output HDF file.

CONCLUSION

The synchrotron radiation code SPUR is in development. It takes advantage of parallel processing and HDF data format to calculate synchrotron radiation spectra from undulator systems defined either analytically or numerically in practicable time. The code is particularly designed for SR calculations for long undulator systems containing a number of undulator modules and parallelisation allows their calculation within a practicable time.

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