HPC SIMULATION SUITE FOR FUTURE FELS

R.J. Allan[1], L.T. Campbell[2,3], A.J.T. Colin[4], D. Dunning[3], B.W.J. M^{c}Neil[2], B. Muratori[3], J.D.A. Smith[5], N.R. Thompson[3], P. Traczykowski[2], P. Williams[3]
[1]The Hartree Centre, STFC Daresbury Laboratory, Warrington, UK
[2]SUPA, Department of Physics, University of Strathclyde, Glasgow, UK
[3]ASTeC, STFC Daresbury Laboratory and Cockcroft Institute, Warrington, UK
[4]SUPA, Department of Physics and Astronomy, University of Glasgow, Glasgow, UK
[5]Tech-X UK Ltd, Sci-Tech Daresbury, Warrington, UK

Abstract

A new HPC simulation suite, intended to aid in both the investigation of novel FEL physics and the design of new FEL facilities, is described. The integrated start-to-end suite, currently under development, incorporates both plasma (VSim) and linac (ELEGANT, ASTRA, VSim) accelerator codes, and will include the 3D unaveraged FEL code Puffin to explore novel FEL methods.

INTRODUCTION

Free Electron Lasers are now operating successfully in SASE mode at X-ray wavelengths [1, 2] with others planned or under development [3]. Like the first conventional lasers developed in the early 1960s, X-ray FELs are in their infancy and have the potential for further significant development, particularly with respect to their temporal coherence, pulse durations, potential to deliver synchronised, multi-colour output, and the possibility of being driven by new electron beam sources. Research is now focussing on these future possibilities. Experimental facilities such as [4] and [5] are designed with the dedicated purpose of testing out new techniques for such improved output. At the same time, plasma accelerators have emerged as a promising potential driver of future FELs, with the potential to reduce the size and cost of the facilities.

FEL simulation codes are fundamental tools in the investigation of FEL theory, novel methods and the design of facilities. The most commonly used codes perform approximations including the Slowly Varying Envelope Approximation (SVEA) on the radiation field [6], averaging the electron motion over an undulator period, and discretisation of the electron beam and radiation field into ‘slices’ (of minimum width equal to the radiation wavelength) over which periodic boundary conditions are applied [7].

As a consequence of these approximations, the averaged SVEA codes are unable to model processes occurring at a sub-resonant wavelength scale (equivalently radiation outside a narrow bandwidth centred on the resonant frequency) [8], or significant changes in the electron beam phase space such as current redistribution during the FEL interaction [9, 10]. While these effects are not important for the basic operation of the FEL, some advanced methods currently proposed to improve the temporal output in the next generation of FELs rely on just such processes [11, 12]. SVEA codes are also unable to model the Coherent Spontaneous Emission (CSE) arising from current gradients in the electron pulse; this can act as a strong seed for the FEL interaction [13]. For these reasons it is necessary to use unaveraged, non-SVEA codes to model FELs driven by Laser Plasma Accelerators (LPAs), which typically produce short, broadband electron beams.

The FEL simulation code PUFFIN (Parallel Unaveraged Fel INtegrator) was developed [14] to be free of the averaging and SVEA approximations which limit other commonly used codes. The primary aim of PUFFIN was to provide a flexible research resource that can be adapted to test new ideas and methods for future FEL development. It was therefore not focused on FEL facility design and leaves it lacking in some features desirable to those designing real experiments. It also lacks simulation paths to and from other accelerator codes, and a good visual on-site interface for outputs.

In the following, we describe a start-to-end (s2e) simulation suite currently under development. It is anticipated that it will aid in the design of the UK CLARA FEL test facility [5] and in interpreting the results of experiments to be performed there. As part of the project, Puffin will undergo development, both to optimize algorithms for new HPC architectures and to implement useful physical features required for proper facility simulation. The suite will include a common visual interface throughout the simulator which will use ASTRA [15], elegant [16, 17] and VSim [18] for the accelerator simulators in conjunction with Puffin for

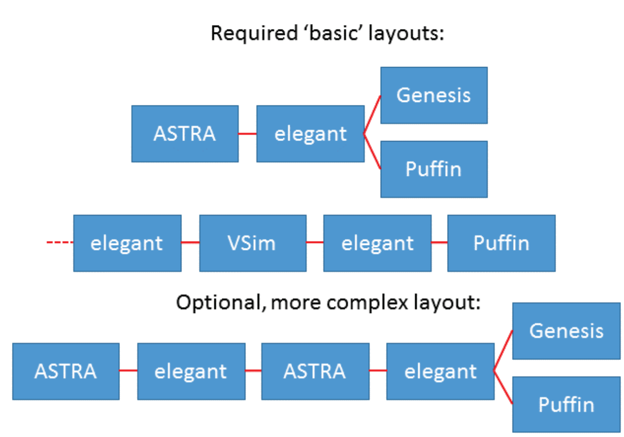

Figure 1: Various simulation layouts afforded by the suite.

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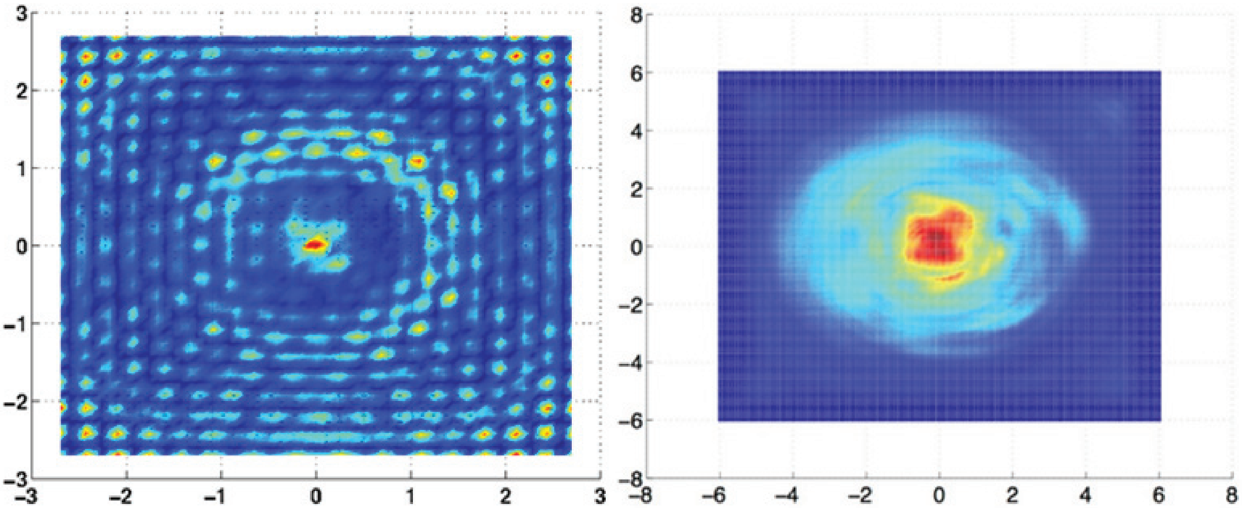

Figure 2: Diffraction before (left) and after (right) the implementation of the absorbing boundary conditions, for identical parameters.

the FEL. Genesis [19] will probably also be included for situations where the extra computational resolution of Puffin is not required. This will result in a s2e suite able to model both plasma accelerator and linac driven FELs that may implement novel accelerator and FEL methods.

SOFTWARE AND LICENCING

The existing codes which will be used in the main simulation chain (elegant, ASTRA, VSim, Puffin) will require simulation 'handshakes' to be written which will pass the electron beam between codes. Further extensions to this

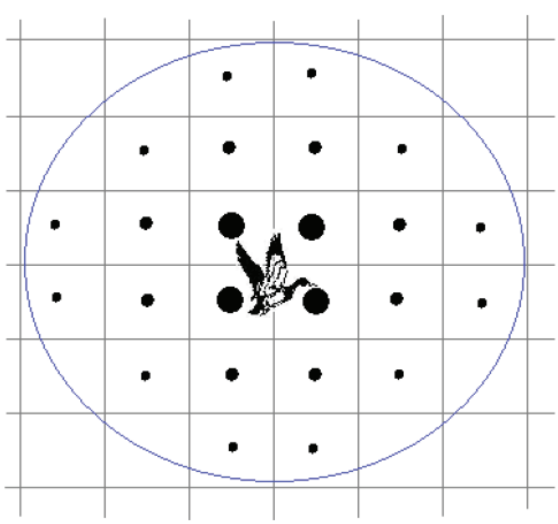

Figure 3: The 'shotgun' model of particle spreading. The heavier macroparticle from the coarse accelerator distribution is the shotgun cartridge and the finer shot (of varying size) are the microparticle. The pellets from the shotgun cartridge spread out over the blast radius according to a spreading factor.

model are probable, e.g. it would be useful to include Genesis for benchmarking results with Puffin. These software packages should provide a good platform to perform s2e simulations of the most crucial parts of a facilty. The 2 most basic setups, see Figure 1, allows s2e simulation of a simple RF-linac or plasma accelerator driven FEL. However, more complex scenarios will also be developed and supported.

The deployment of the s2e suite onto HPC facilities will be simplified through use of the bilder [21] package management system and the scimake [20] extensions to cmake for finding scientific simulation software packages. Puffin, with the new software and documentation will be released under a BSD or other non-restrictive licence, while extensions to bilder and scimake will be available under their existing open source licenses. As the entire s2e suite supports both closed and open software, hooks will be provided for detection of the presence of other codes (VSim, ASTRA) that have been licensed on the system and addition of the appropriate 'handshakes' for passing data between them. As the configuration software is open source, other software tools may be added in future.

In Puffin, the required resolution of simulation particles is at the sub-resonant wavelength scale. However, in accelerator codes such as elegant, the electrons are usually not required to be so finely sampled. A general code written in C for converting a coarse distribution of few macro-particles into a finer distribution consisting of a greater number of micro-particles is therefore being developed which converts the coursely sampled electron beam from the output of the accelerator codes for input into Puffin. The code takes the coarse macroparticle distribution and breaks it up to distribute them in phase space to a finer distribution consisting of many more microparticles, with the correct Poissonian shot-noise statistics of [22]. An analogy is made in Figure 3 as the spread of pellets (microparticles) from a shotgun car-

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tridge (macroparticle)[1]. A number of spreading profiles of the microparticles are available, the simplest of which are gaussian and top-hat. User-defined spreading profiles may also be used.

IMPROVEMENTS TO PUFFIN

Improvements to Puffin over that as described in [14] include the implementation of transverse boundary conditions to absorb radiation diffracting out the numerical grid. The algorithm involves the use of a transverse 'mask', similar to that described in [23], to absorb a broadbandwidth of frequencies. Previously, periodic boundary conditions, present as a consequence of solving the field diffraction in Fourier space, caused artificial transverse interference when in highly diffractive regimes. See Figure 2 for an example of this, and the subsequent clean-up observed with the absorbing boundaries.

The current 3D undulator field models were described previously in [24], and in the future may utilize field maps to try to correctly simulate *e.g* APPLE II type undulators. The addition of quadrupoles and phase shifters is also a priority for this project to allow e.g. FODO focussing. Current work involving 'ramping' up the undulator field at the start and end of each module indicates that auto phase-matching between undulator modules of the radiation field to a bunched electron beam is a non-trivial task if one has a broadband and/or multi-peaked-spectra beam, and such issues require further work.

The undulator field tapering can be performed by utilizing the model initially developed to produce 2-colour output, (see [10] for an example of the use of tapering in Puffin).

Puffin currently utilizes MPI for parallelism, but there is a requirement to also implement OpenMP to properly utilize resources on the largest HPC machines. A rudimentary hybrid MPI/OpenMP version of Puffin has now been developed, and exhibits a modest scaling with the number of OpenMP threads (depending on the number of macroparticles).

After performance benchmarking and optimization, development to test Puffin on new architectures will also be performed; further development will involve porting to the Intel Xeon Phi architecture, and the appropriateness of using GPU's with Puffin has yet to be evaluated. While Puffin currently implements parallelism with the electron beam, it may be necessary to also develop a parallel field algorithm as larger field grid sizes begin to be used for e.g. high harmonic simulations.

Puffin has not yet been benchmarked against experiment. However, it has been benchmarked against analytic expressions for the broadband spontaneous output, and also the M. Xie fitting formulae [25], and gives excellent agreement in both cases. As part of this project, there will be direct benchmarking against Genesis results and experiments in a variety of cases. This will help to identify the regimes where unaveraged codes are necessary.

[1] No ducks were harmed in the writing of this article.

VISUALISATION

Throughout the the full s2e chain, a suggested or idealized workflow is that the output data will be processed by SDDS [26], then converted to HDF5 [27] formatting with VizSchema compliance for visualization using VisIt [28] (see Figure 4). The SDDS package has extensive, well-tested post-processing scripting routines for extracting relevant, commonly used measurements for accelerator physicists, and the use of VisIt will provide a convenient common interface for all stages of the design process for users.

However, it is expected that pragmatic considerations may alter this visualization chain in some specific cases. For example, VSim already uses VisIt for plotting, meaning it is convenient to utilize those routines which are already in place.

CONCLUSIONS

The HPC suite currently under development and described here will enable the exploration of new FEL methods and allow designs to test them to be developed at facilities such as CLARA and the NLCTA. The suite will also assist in research towards plasma accelerator driven FELs. It is hoped that the portability afforded by the build system will lower the technical barrier of installing and linking these codes together at HPC facilities. The build system produced will also be useful for building Puffin more easily for running on smaller local machines, e.g. in 1D mode on personal laptops.

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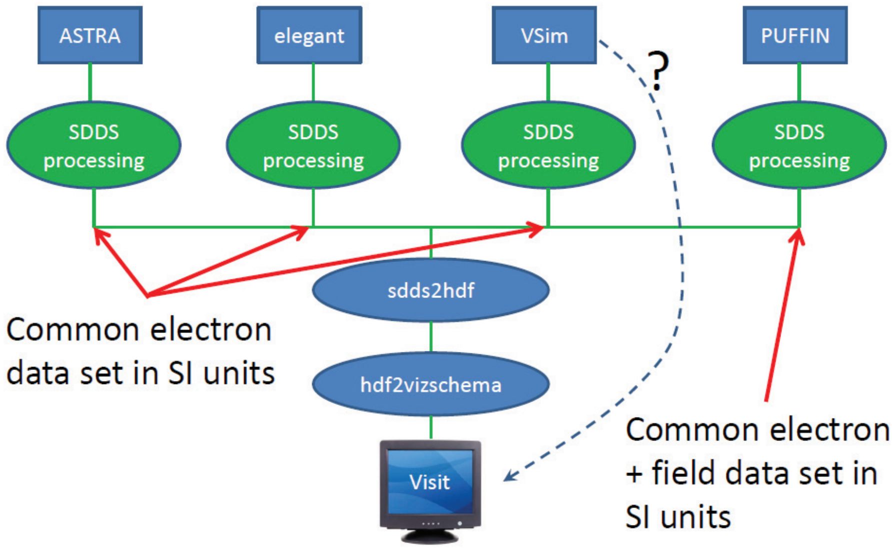

Figure 4: Schematic of the proposed, idealised visualization chain for the simulation suite. SDDS is used for post-processing and VisIt is used for viewing the results after conversion to HDF5 format. Note that VisIt can already directly visualize VSim data, so it may be be more convenient to utilize this functionality within this project.

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