START-TO-END SIMULATIONS OF THE CLARA FEL TEST FACILITY

D. J. Dunning∗1,4, D. Angal-Kalinin1,4, A. D. Brynes1,4, L. T. Campbell2,4, H. M. Castaneda Cortes1,4, J. K. Jones1,4, B. S. Kyle3,4, J. W. McKenzie1,4, B. W. J. McNeil2,4, J. D. A. Smith3, N. R. Thompson1,4, P. Traczykowski2,4, P. H. Williams1,4,
1STFC Daresbury Laboratory, Daresbury, 2University of Strathclyde, Glasgow, UK
3University of Manchester, Manchester, UK, 4The Cockcroft Institute, Daresbury, UK
5Tech-X UK Ltd, Sci-Tech Daresbury, Daresbury, UK

Abstract

CLARA is a new FEL test facility being developed at STFC Daresbury Laboratory in the UK, aiming to deliver advanced FEL capabilities including few-cycle pulse generation and Fourier transform limited output. Commissioning is underway on the front-end (photo-injector and first linac) while the later stages are being procured and assembled. Start-to-end (S2E) simulations of the full facility are presented, including optimisation of the accelerator setup to deliver the required properties of one of the electron beam modes specified for FEL operation. FEL simulations are performed using the Genesis 1.3 and Puffin codes and the results are compared.

INTRODUCTION

The UK is constructing a new FEL test facility called CLARA [1], which will be a dedicated accelerator R&D facility focused around demonstrating FEL schemes that can be applied to enhance the capabilities of X-ray FELs - including a potential UK XFEL [2]. It will operate with 250-MeV maximum energy and \( \lambda \approx 100–400 \) nm fundamental FEL wavelength. The front end (up to 50 MeV) is being commissioned [3,4] and the second phase (full energy accelerator) is being assembled while technical design and procurement of the later stages continues - aiming for FEL lasing in 2022.

The conceptual design of the FEL section was finalised in September 2017 and is summarised in [5]. Briefly, the aim is to demonstrate novel FEL capabilities that can be applied at X-ray FEL facilities including high-brightness SASE [6], mode-locking [7], mode-locked afterburner [8], optically slicing an isolated pulse [9] and others. It is a flexible design to accommodate new ideas and future changes.

As shown in Table 1, a number of electron beam operating modes have been defined [10], with short-bunch and long-bunch modes both specified as 250-pC Gaussian bunches with target 0.5 mm-mrad normalised emittance and 25 keV energy spread but with different compression (peak currents of 400 A and 125 A respectively). ‘Ultra-short’ and ‘flat’ modes are also specified, with the latter (not shown in Table 1) being similar to the short mode with the additional constraint of a 250-fs region with flat current and emittance. The design of the accelerator layout to deliver the required beams is now finalised [11] and is shown in Fig. 1.

Table 1: CLARA FEL Electron Beam Modes

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Long</th>
<th>Short</th>
<th>Ultra-short</th>
</tr>
</thead>
<tbody>
<tr>
<td>Energy [MeV]</td>
<td>150-240</td>
<td>150-240</td>
<td>240</td>
</tr>
<tr>
<td>( \Delta \text{FWHM} [\text{fs}] )</td>
<td>1875</td>
<td>585</td>
<td>50/40/35</td>
</tr>
<tr>
<td>Charge [pC]</td>
<td>250</td>
<td>250</td>
<td>25/40/50</td>
</tr>
<tr>
<td>( I_{\text{peak}} [\text{A}] )</td>
<td>125</td>
<td>400</td>
<td>~500/1000/1500</td>
</tr>
<tr>
<td>( \epsilon_{\text{norm}} [\text{mm-mrad}] )</td>
<td>0.5-0.8</td>
<td>0.5-1.0</td>
<td>1.0-1.5</td>
</tr>
<tr>
<td>( \sigma_{E} [\text{keV}] )</td>
<td>25-75</td>
<td>25-120</td>
<td>100-150</td>
</tr>
<tr>
<td>Chirp [MeV/ps]</td>
<td>&lt;1</td>
<td>&lt;1</td>
<td>-</td>
</tr>
</tbody>
</table>

S2E simulations of the finalised layout are underway for different electron beam modes and different FEL schemes. In this paper we report the results of S2E modelling for the FEL mode of self-amplified spontaneous emission (SASE), using the short-bunch electron beam mode at 240 MeV (‘short-240’ mode). SASE is the default operating mode for an amplifier FEL so this case serves as the baseline from which more advanced schemes can be compared. Details of the modelling and optimisation procedures are described.

ACCELERATOR OPTIMISATION

Simulations of the CLARA accelerator (up to the FEL) have been performed using a Python-based framework [12] for interacting with standard tracking codes, performing non-linear multi-variate optimisation and data analysis and plotting. The CLARA standard code is ASTRA [13] due to the strong longitudinal and transverse space-charge effects in a low-energy machine. ASTRA, however, does not include the effects of coherent synchrotron radiation in the variable bunch compressor, so CSRTrack [14] is used for this section. For benchmarking purposes the framework also tracks in Elegant [15]. The lattice is defined using a bespoke format and encoded in YAML [16], which is both well integrated into Python and is human-readable. Tracking I/O is interfaced through HDF5 [17] intermediary files, allowing an arbitrary choice of simulation code for each section of the lattice. Further benchmarking is performed in the GPT [18] code, which is currently being integrated into the framework. For optimisation we use the DEAP [19] package.

Results from the optimisation of the short-240 mode of CLARA (see Fig. 2) show acceptable bunch properties matching all of the desired FEL parameters with the exception of a residual longitudinal energy chirp of ~4–6 MeV/ps.
Slice properties of the bunch show normalised-emittance below 0.5 mm-mrad and acceptable slice energy spreads at peak-currents close to 400 A. This improvement in beam properties over previous studies is primarily driven by a standardisation of the RF gun peak field to 120 MV/m and photoinjector laser pulse profile to a 3-ps flat-top [20].

Attempts to reduce the residual energy chirp have so far resulted in significant reduction in the bunch quality. The implementation of improved wakefield models is expected to help to some extent. Separate studies on dielectric wakefield de-chirping [21] are on-going. Integration of the de-chirper dynamics into the simulation framework is a current high-priority topic. The effect of energy chirp on FEL performance is discussed in the following section.

**FEL MODELLING**

The FEL section was simulated in both Genesis 1.3 [22] (version 2) and Puffin [23–25] using the short-240 mode S2E bunch from the previous section, with additional parameters given in Table 2.

**Genesis Method**

Simulations in ASTRA and CSRtrack were carried out with a total of 262k particles, which was determined to be optimal in numerical convergence tests. The ASTRA output distribution was pre-processed to include matching of the initial distribution to the undulator FODO lattice and converting the electron distribution into a dist file to be read as input by Genesis. The pre-processing stages were carried out using the OCELOT framework [26]. OCELOT integrates Genesis with pre-processing and post-processing methods in order to automate the simulation runs and is implemented in Python. At the end of the simulation, plots of the most relevant FEL properties are obtained from the Genesis output files.

**Puffin Method**

Before use in Puffin, the ASTRA data was processed using the FXFEL [27] package, which pre-conditions the beam for the FEL simulation. This pre-conditioning involves upsampling the beam distribution to a number of particles that adequately samples each FEL wavelength, whilst adhering to fundamental shot-noise statistics [28]. The upsampling

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Undulator type</td>
<td>Planar</td>
</tr>
<tr>
<td>Field Orientation</td>
<td>Horizontal</td>
</tr>
<tr>
<td>Period, $\lambda_u$</td>
<td>25 mm</td>
</tr>
<tr>
<td>Module Length (total)</td>
<td>0.75 m</td>
</tr>
<tr>
<td>Inter-module gap length</td>
<td>0.5 m</td>
</tr>
<tr>
<td>Number of full periods</td>
<td>27</td>
</tr>
<tr>
<td>Active module length</td>
<td>0.675 m</td>
</tr>
<tr>
<td>Undulator parameter, $a_u$</td>
<td>0.8667</td>
</tr>
<tr>
<td>Resonant wavelength, $\lambda_r$</td>
<td>$\sim$100 nm</td>
</tr>
<tr>
<td>Electron beam transverse size, $\bar{\sigma}_{x,y}$</td>
<td>50 $\mu$m</td>
</tr>
</tbody>
</table>
is performed by utilising cumulative distribution functions of the initial particle density. The FXFEL package handles conversion from CSRTrack/ASTRA format to Puffin format via the intermediary Standard Units (SU) format [27, 29], where sliced analysis using the Xie parameterisation [30] is used to check the beam’s suitability for FEL amplification. The package matches the beam to the undulator FODO lattice, if desired. The entire pre-and-post processing chain in Puffin is implemented using these custom Python modules.

Results Comparison

Figure 3 shows FEL simulation results for the S2E bunch, simulated in Genesis and Puffin. The pulse energy vs distance through the undulator is shown together with the temporal and spectral profiles at saturation. For Genesis, multiple shot-noise realisations are shown. In general there is reasonable agreement between the two codes. The pulse energy grows slightly faster in Puffin (outside the range of the Genesis shot-noise realisations) and shows a clearer saturation point. The drops in pulse energy in break sections are expected to be due to radiation being absorbed by the transverse boundaries of the field mesh due to high diffraction in the system, though imperfect phase-matching between modules could also contribute - further study is underway. Due to the random shot-to-shot fluctuations inherent in SASE there is not close agreement between the temporal and spectral profiles but there is reasonable qualitative agreement.

Energy Chirp

The impact of energy chirp on SASE pulse energy and bandwidth has been assessed in Genesis simulations. It was found that the pulse energy decreased by ~10% and the bandwidth increased by ~5% per 1 MeV/ps of chirp (for chirps with lower energy at the head: chirps in the opposite sense increased pulse energy analogous to undulator tapering). While the pulse energy reduction can be compensated by undulator tapering, the bandwidth increase cannot. The S2E bunch was artificially dechirped and simulated in Genesis and the performance was found to meet that of an ideal Gaussian beam with the specified parameters. The maximum energy chirp for the short-bunch mode has been specified as 1 MeV/ps. Tolerance studies of more advanced FEL schemes could yet impose more stringent limits.

CONCLUSION AND OUTLOOK

CLARA SASE FEL S2E simulations have been carried out. The accelerator has been optimised such that the electron beam meets all specifications except energy chirp. Reasonable agreement has been found between Genesis and Puffin for FEL modelling, though further investigation of discrepancies is required. The next steps are to include dechirper modelling in the accelerator simulation, and to study advanced FEL schemes where the difference between FEL codes is expected to be more significant. S2E is one component of a larger framework for CLARA including a virtual accelerator [31] and accelerator control systems [3].

Figure 3: FEL simulation results. Top and second from top: FEL pulse energy with distance through the undulator on linear and log scales. Below: temporal profiles and spectra at saturation (15 m). For each plot there are multiple shot noise realisations shown for the Genesis results (grey), with one typical case highlighted (red) and the average also shown (black). One shot noise realisation is shown for Puffin (blue).
REFERENCES


[27] [Online]. Available: https://github.com/UKFELs/FXFEL


