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# AN INTRODUCTION TO THE UK XFEL CONCEPTUAL DESIGN AND OPTIONS ANALYSIS

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*Abstract*

In October 2022, the UK XFEL project entered a new phase to explore how best to deliver the advanced XFEL capabilities identified in the project's Science Case. This phase includes developing a conceptual design for a unique new machine to fulfil the required capabilities and more. It also examines the possibility of investment opportunities at existing XFELs to deliver the same aims, and a comparison of the various options will be made. The desired next-generation capabilities include transform-limited operation across the entire X-ray range with pulse durations ranging from 100 as to 100 fs; evenly spaced high rep. rate pulses for enhanced data acquisition rates; optimised multi-colour FEL pulse delivery and a full array of synchronised sources (XUV-THz sources, electron beams and high power/high energy lasers). The project also incorporates sustainability as a key criteria. This contribution gives an overview of progress to date and future plans.

## INTRODUCTION

In early 2019, the UK initiated a project to develop the science case for a UK XFEL, which was published in 2020 [1, 2]. Subsequent exercises demonstrated the support of the UK community and in June 2022, UK Research and Innovation announced funding for the next phase of the project: a 3-year conceptual design and options analysis (CDOA), which started in October 2022. This phase includes developing a conceptual design for a unique new UK machine, alongside examining investment opportunities at existing facilities e.g. [3–12], both with the aim of realising 'next-generation' XFEL capabilities (the features of which are discussed below). By the end of this phase of the project (October 2025) we will have:

- mapped out how best to deliver advanced XFEL capabilities identified in the Science Case;
- explored a conceptual design for a unique new machine that can fulfil all required capabilities;
- examined other investment options and collaborations in existing XFELs;
- updated the Science Case to feed into the process and inform future decisions;
- held multiple Townhall Meetings around the UK engaging with the user community;
- investigated the socioeconomic impact of a next generation XFEL.

Year 1 has so far focused on the project launch, surveying the science requirements, preliminary engagement with overseas XFEL facilities, planning the Townhall meetings and initial conceptual design and layout work. Informed by work this year, Year 2 will focus on R&D targeting gaps in key physics and technology areas, including collaborative work with overseas XFEL facilities, and the continuation of Townhall meetings and other workshops. In Year 3, R&D activities will continue and the final CDOA report will be written, detailing the preferred options, including socio-economic analysis, and an update to the Science Case. This paper gives an overview of progress to date.

## NEXT-GENERATION XFEL CAPABILITIES

Starting from our Science Case, our project clearly sets an emphasis on enhancing XFEL capabilities and on widening access to such capabilities, defined as follows:

- Transform-limited operation across the entire X-ray range (0.1 - 20 keV and 100 as - 100 fs).
- High efficiency facility, with a step change in the simultaneous operation of multiple end stations.
- Evenly spaced, high rep. rate pulses to match samples & detectors.
- Improved synchronisation/timing data with external lasers to < 1 fs.
- Widely separated multiple colour X-rays to at least one end station.
- Full array of synchronised sources: XUV-THz, e-beams, high power & high energy lasers at high rep. rate.

This list of features results from both the Science Case and work in this phase, including a detailed survey of our science team, results of which are shown in Fig. 1. We are presently focusing our preliminary activities on the capabilities listed above, particularly the first two, which we consider to be the most challenging and fundamental to the machine design (see sections below). Other requested capabilities, e.g. higher photon energies will be considered beyond the preliminary focus and are briefly summarised below.

The options will ultimately be assessed on a range of criteria including the above capabilities, technology readiness level, environmental sustainability and cost.

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## PROGRESS TOWARDS A CONCEPT FOR A NEXT-GENERATION FACILITY

We are presently in the early stages of defining our concept for a next-generation facility - the preliminary designs and ideas are presented here for discussion and to highlight potential collaboration opportunities.

### *Photon Energy, Repetition Rate and Pulse Energy*

Figure 1 shows the photon energy and repetition rate requirements identified in the Science Case (grey boxes) and survey (coloured points - pulse energy requirements are also indicated for these). For our preliminary activities, we have identified the core requirements as being photon energies from 0.1 to 20 keV (at the fundamental) and with 100 kHz delivered to each experiment. Meeting the repetition rate requirement implies that we must operate with superconducting RF technology. We are assuming a repetition rate of ~1 MHz to allow multiplexing to multiple experiments. The beam energy should be around 8 GeV to reach the highest photon energies with high pulse energy. This preliminary working point is indicated as the shaded region in Fig. 1. Options for higher photon energy and/or pulse energy are described in a later section.

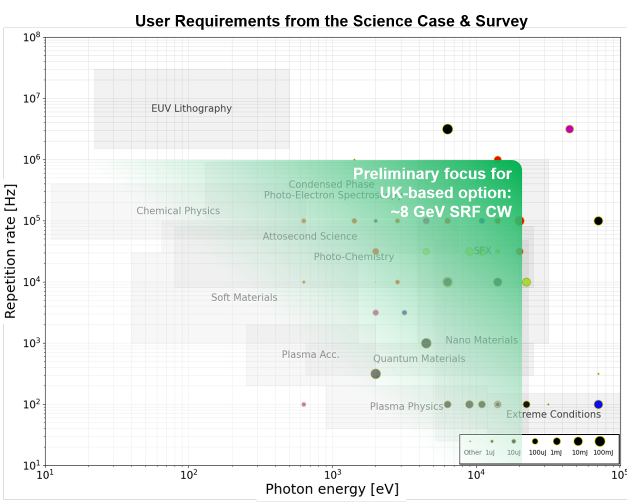


Figure 1: Photon energy, repetition rate and pulse energy requirements from the Science Case (grey boxes labelled by science area) and recent user survey (unlabelled points, colours represent different science areas), and approx. coverage provided by the proposed facility design parameters.

### *Transform-Limited Pulses*

A key focus of our preliminary activities is the requirement for transform-limited operation across the entire X-ray range, from 0.1 - 20 keV and 100 as - 100 fs. 'Laser like x-rays' for users across such a broad range is a challenging aim that could be a distinguishing feature of a next-generation facility and R&D will be valuable to the international XFEL community. Figure 2 shows the photon energy-pulse length parameter space, with the preliminary focus region of 0.1 to 20 keV and 100 as to 100 fs indicated. The corresponding relative FWHM bandwidth for a transform-limited pulse within this space is indicated by contours, and indicative positions of some of the leading FEL techniques to meet the requirements are shown.

It is evident that several FEL techniques are required to cover such a large parameter space. Many such schemes are well established at international XFELs, however there remains much opportunity for development, e.g. to utilise advances in conventional lasers to drive external seeding as used at e.g. FERMI [6] to much higher rep. rate (~100 kHz) and to higher photon energy (potentially ~1-2 keV). Techniques for attosecond (e.g. XLEAP [13]) and narrow bandwidth (e.g. self-seeding [14, 15]) pulses are well-established and so present opportunities to pursue high rep. rate operation, increased tunability and other advanced features [16]. Techniques such as HB-SASE [17] (with potentially TW peak power, few-fs pulses at any wavelength & rep. rate [18]) and XFELO [19] are under experimental development. Furthermore, the prospect of operating multiple such techniques simultaneously is a major challenge and potentially a distinguishing feature of a next-generation machine.

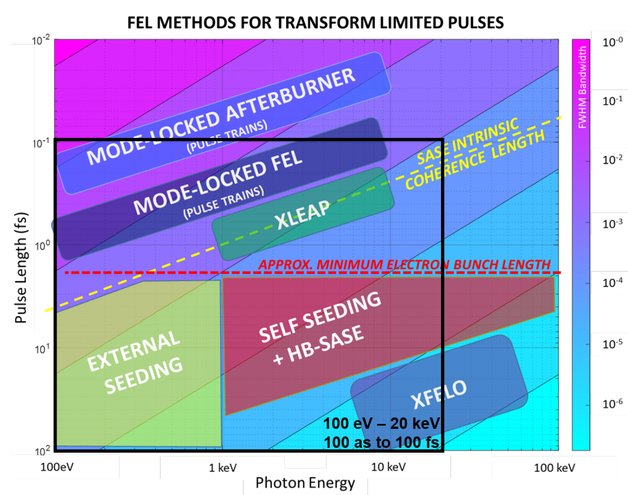


Figure 2: The project's aim for transform-limited pulses from 0.1 to 20 keV and 100 as to 100 fs is shown by the black box in the photon energy-pulse length parameter space. The contours show the relative bandwidth of a transform-limited pulse within the space and the estimated coverage of some relevant FEL techniques is shown.

### *Simultaneous Operation of Multiple FELs*

Another focus of our preliminary activities is to develop a concept for a high efficiency facility with a step change in the simultaneous operation of multiple end stations. Even given the pre-eminent capabilities of existing XFELs, it is widely recognised that it would be hugely beneficial to increase the scientific output from their investment. While challenging, this is a major opportunity to differentiate the next generation of XFELs from existing machines, and is already part of the thinking for upgrades to existing facilities.

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Our initial thinking is that this capability would be best achieved through operating with fixed accelerator settings up to full energy, and so multiplexing ~1 MHz bunches with fixed properties to several undulator lines, each operating at ~100 kHz, potentially using kicker magnets as shown in Fig. 3. The fixed bunch properties at the end of the linac would then be manipulated within each FEL line to deliver the varying bunch requirements of the various FEL techniques described in the previous section. Significantly more work is required on such an approach but truly independent operation of multiple high-performance FEL lines would be highly advantageous. Bunch-to-bunch variation upstream of the spreader could also be considered, e.g. by laser pulse shaping [20] in the photoinjector or laser heater.

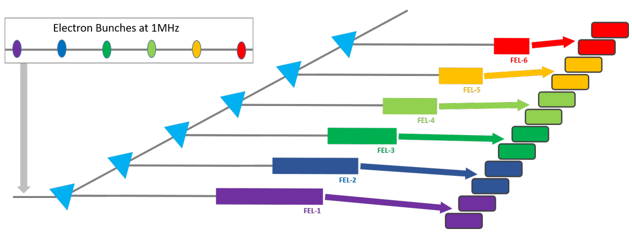


Figure 3: Initial FEL concept: electron bunches at ~1 MHz and constant energy are divided e.g. by kicker magnets (light blue triangles) to multiple independently tunable FEL lines at ~100 kHz, which each provide output to multiple end stations. The different colours of the bunches indicate which FEL line they pass through, with different wavelengths set by the undulators parameters.

Assuming the electron beam energy to all FELs to be fixed at 8 GeV, then to cover 0.1 to 20 keV while allowing for some overlap in tuning is best covered by at least ~6 FELs as shown in Fig. 3. Potential tuning ranges for these are shown in Table 1 though they are only indicative for discussion with our science team. Given the fixed electron beam energy, the relative width of the tuning range is narrower for the highest photon energy FEL to optimise performance, and can be successively broader for lower photon energies. The FEL lines would likely have some specialisms in terms of techniques, e.g. FELs 5 and 6 could feature high rep. rate seeding, while others could focus on e.g. attosecond or narrow-bandwidth schemes.

Table 1: Draft FEL Tuning Ranges

| **FEL** | **Photon Energy [keV]** | **Factor** |
|---|---|---|
| FEL-6 | 0.1 - 1 | ×10 |
| FEL-5 | 0.25 - 2 | ×8 |
| FEL-4 | 1 - 5 | ×5 |
| FEL-3 | 2.5 - 10 | ×4 |
| FEL-2 | 5 - 20 | ×4 |
| FEL-1 | 10 - 20 | ×2 |

Given the nominal repetition rates, there is potential for more FELs or other lines using the electron beam e.g. novel acceleration, and there is potential for staging over time. Figure 3 shows two end stations per line, which is again indicative and is the subject of discussion within our team and with existing facilities.

### *Combining FEL Lines*

A feature that we are considering from an early stage due to its potentially significant impact on the design is that of synchronously combining output from multiple FELs at a single end station. This isn't shown in Fig. 3 but essentially builds on our concept devised for the CompactLight project [21]: the bunch pattern from the injector is adjusted to bring two bunches into adjacent RF cycles, such that they both initially traverse the same FEL line, then a GHz subharmonic deflecting cavity is used to deflect one bunch onto an adjacent line. The FEL pulses are then combined in one end station, with time of flight matching and scanning achieved using electron delay chicanes.

### *Beyond the Preliminary Focus*

Beyond the preliminary focus, there are several other technical capabilities that will be considered in the course of this phase. Very high pulse energies of ≥100 mJ have been requested in some cases, e.g. for study of matter in extreme conditions. Very high photon energies are also of interest e.g. 50 - 100 keV. In both cases we will consider how these could be incorporated into a UK XFEL design, potentially with a booster to higher electron beam energy in one of the lines post-spreader. Synchronous sources have not been considered in great detail so far but will be a major part of our proposal. The present focus is on laser-based NIR-visible sources, which are most highly demanded, but we will also consider the best way to deliver terahertz radiation, which is the next most requested synchronous source. Calls for protons, ions and gamma sources have also been received and will be explored further with our science team.

## NEXT STEPS

Our present work is focused on developing the concept in more detail and analysing its implications for the main physics and technology areas. This includes identifying key R&D areas and taking steps to undertake the required work both within the project team and in collaboration with international partners. A series of Townhall meetings and other workshops will begin in June 2023 to extend the UK user community and to update the Science Case.

## ACKNOWLEDGEMENTS

While the authorship of this paper is limited to the facility design side of our project and our Science Lead, we would like to recognise the innovative contributions and advice of all our science team and international collaborators.

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