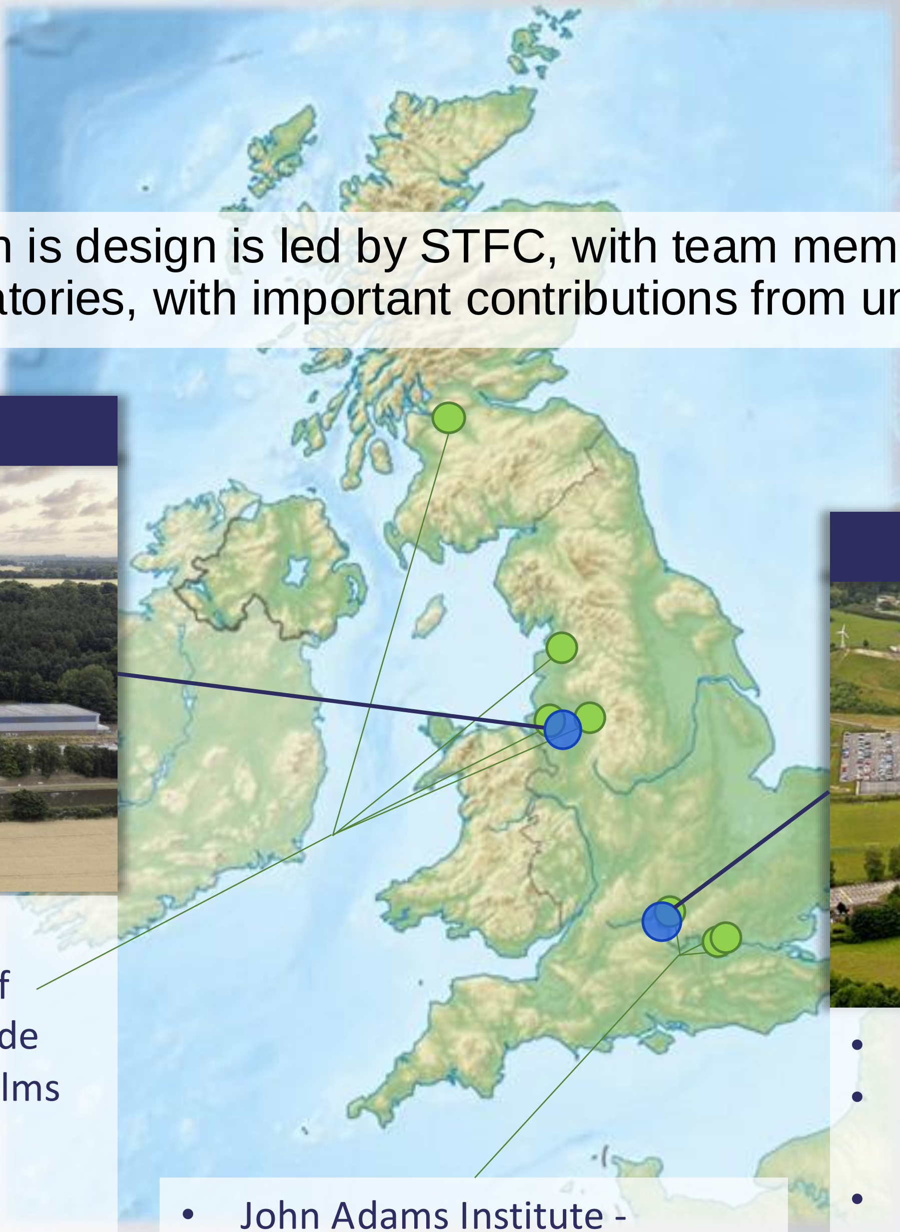
Science and Technology Facilities Council

The UK XFEL Project

Paul Aden and Dave Dunning,
STFC Daresbury Laboratory
22nd November 2024

Introduction

- The UK XFEL facility design is design is led by STFC, with team members at both Daresbury and Rutherford Appleton Laboratories, with important contributions from universities



Daresbury Lab/Campus

- CLARA – 250 MeV accelerator test facility
- Cockcroft Institute – ASTeC + Universities of Liverpool, Manchester, Lancaster, Strathclyde
- SRF capabilities – ESS, PIP-II, HL-LHC, thin films
- RUEDI ultrafast electron diffraction facility £124m recently funded
- High performance computing, technology department etc.

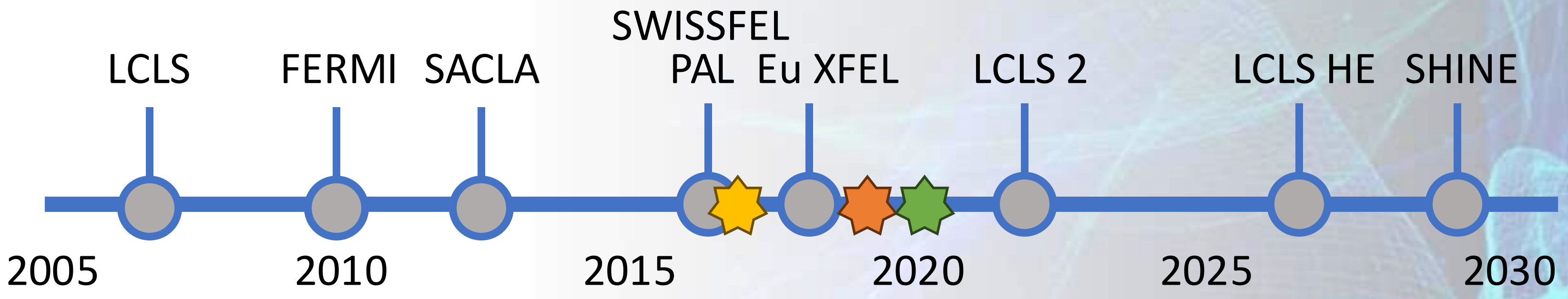
- John Adams Institute - University of Oxford, Royal Holloway, Imperial College

Rutherford Appleton Lab/Harwell Campus

- Central Laser Facility – e.g. DiPOLE laser
- Diamond Light Source, Rosalind Franklin Institute
- XFEL Life and Physical Science Hubs
- ISIS Neutron and Muon Source
- National Quantum Computing Centre
- Technology department, detector development etc.

A Conceptual Design Report and Options Analysis (CDOA)

on delivering Next Generation XFEL Access



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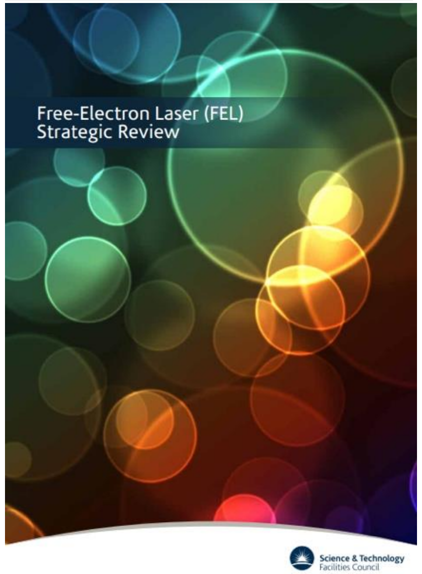

FEL Strategic Review

Highlighted a SwissFEL-like option + increased international engagement

2018

European XFEL

Eu-XFEL + UK

UK becomes a member of Eu-XFEL

2020

UK XFEL

Science Case

Soft x-rays &
Hard x-rays upto 1 MHz

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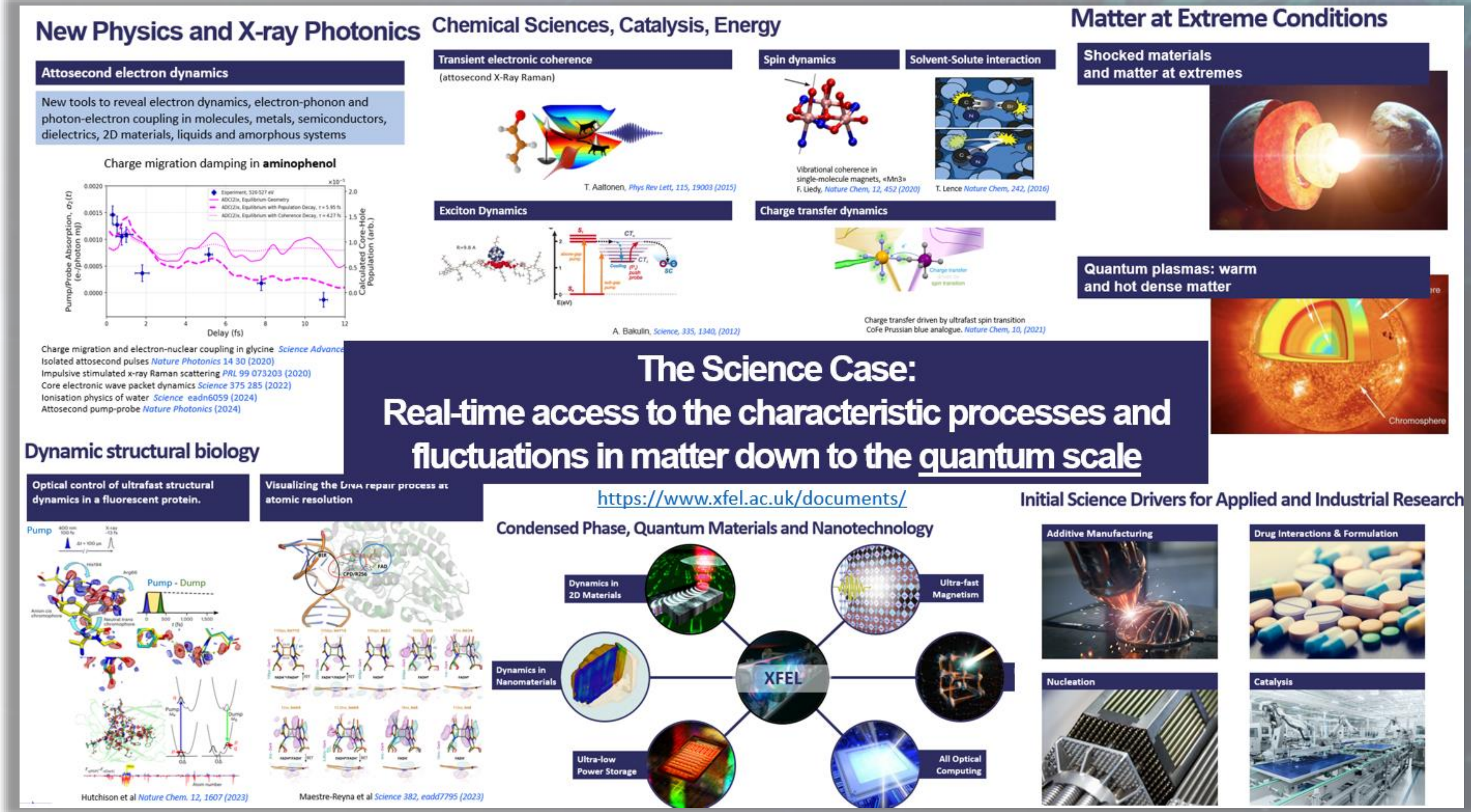
Science Case Published in 2020 – available online at xfel.ac.uk

UK XFEL Overview

The **UK XFEL Science Case** (2019–2020) demonstrated the scientific need for next-generation XFEL capability:



xfel.ac.uk

UK XFEL Overview

The **UK XFEL Science Case** (2019–2020) demonstrated the scientific need for next-generation XFEL capability:

The Science Team

Physical sciences

Jon Marangos (IC), Amelle Zair (KCL), Adam Kirrander (Edinburgh), Jason Greenwood (QUB), Elaine Seddon (Cockcroft)

Chemical sciences

Julia Weinstein (Sheffield), Russell Minns (Soton), Sofia Diaz-Moreno (Diamond), Alex Baidak (Manchester), Andrew Burnett (Leeds), Tom Penfold (Newcastle), Rebecca Ingle (UCL), Mark Brouard, Claire Vallance (Oxford)

Matter in extreme conditions

Andy Higginbotham (York), Andy Comley (AWE), Emma McBride (QUB), Sam Vinko (Oxford), Marco Borghesi (QUB), Malcolm McMahon (Edinburgh), Justin Wark (Oxford)

Life sciences

Allen Orville (Diamond), Jasper van Thor (IC), Xiaodong Zhang (IC), Shakil Awan (Plymouth), Adrian Mancuso (Diamond), Tian Geng (Heptares)

Nano/Quantum materials

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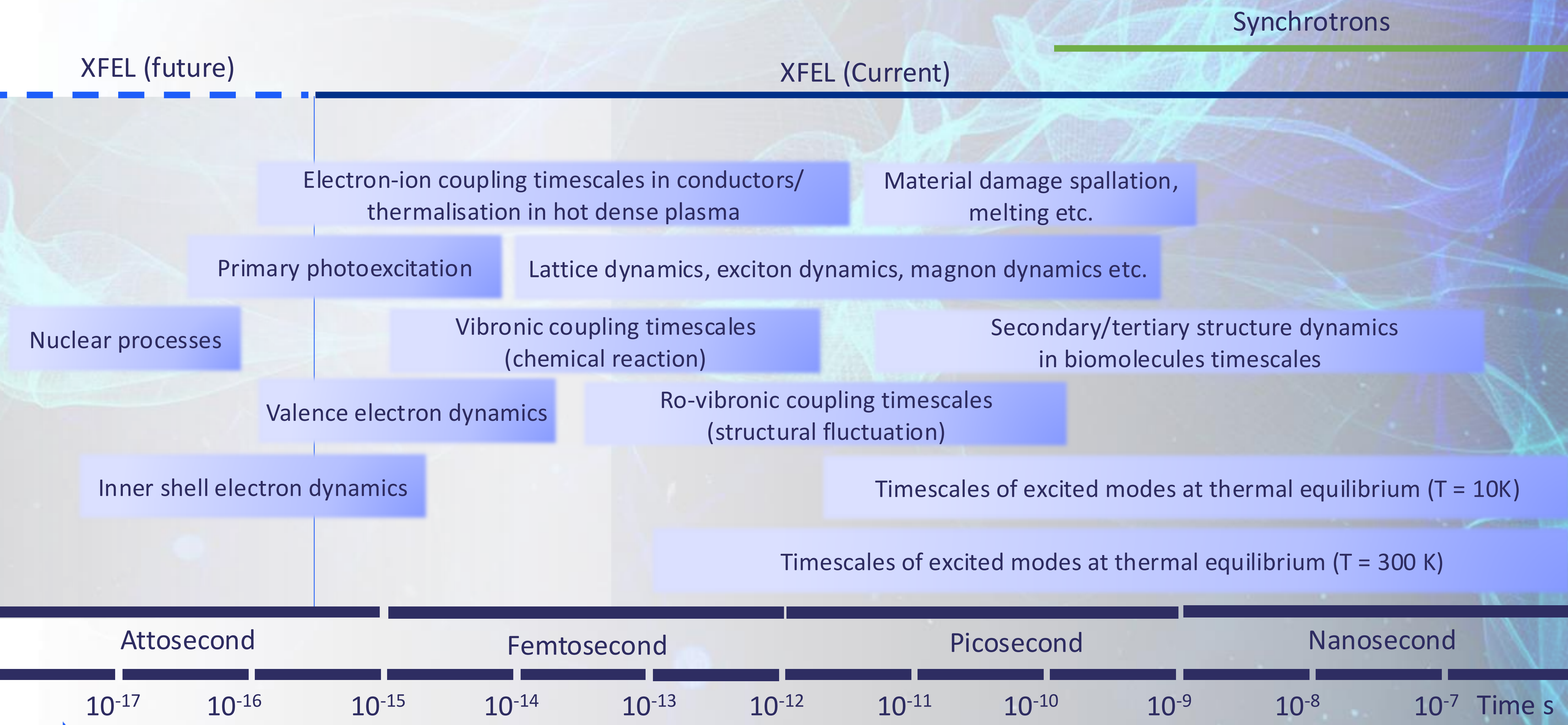
Engineering/Materials/ Applications

David Rugg (RR), Sven Schroeder (Leeds), David Dye (IC) Dan Eakins (Oxford), Mike Fitzpatrick (Coventry)

Real-time access to structural and electronic dynamics



Future Opportunities Unlocked With:

Transform limited operation across entire X-ray range

Fully resolving dynamics at the combined limits of temporal and energy resolution from uncovering the fastest electron dynamics to subtle excitations in quantum materials

High efficiency facility with a step-change in the simultaneous operation of multiple end stations

Expanding access to researchers by providing scope for many hundreds of unique experiments every year to ensure science and technology reaps the full benefits of XFELs

Evenly spaced, high-rep rate pulses to match lasers, samples & detectors

Enabling the most advanced measurement methodologies whilst supporting high throughput measurements with standard capabilities using the most suitable combinations of lasers, sample delivery and detectors for time resolved studies and nano-scale imaging

Improved synchronisation/timing data with external lasers to < 1 fs

Realising the full temporal resolution of x-rays and lasers to see dynamics unfold across multiple timescales down to ~ 1 fs or better

Multiple colour X-rays at one end-station and full array of synchronised sources:

To interrogate multiple electronic, vibronic, excitonic etc. modes to completely uncover the complex dynamical pathways and couplings in matter and to access extreme states of matter

Conceptual Design and Options Analysis (CDOA) phase

How best to deliver access to a Next Generation XFEL?

Evaluate five different options

including their feasibility, costs, benefits, risks, socio economic impact sustainability.

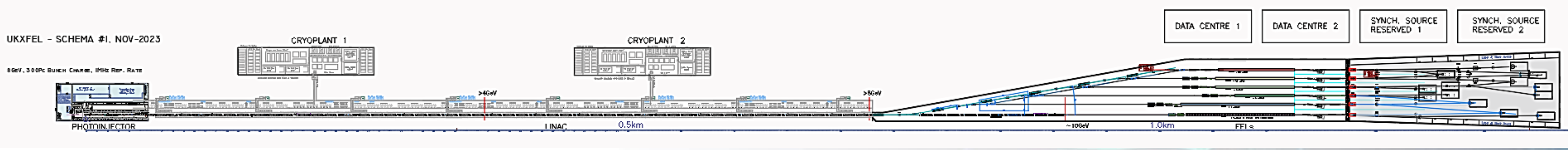
1. UK Facility in the UK
2. UK Facility in the UK with International partnerships
3. Invest in an International facility within Europe
4. Invest in an International facility internationally
5. No further investment

The **science case will also undergo a refresh** during this period along with research and development into new technologies required to deliver a **sustainable** next generation XFEL.

£3.2 million over three years, Project timescale **Oct 2022 to Oct 2025.**

Design Philosophy

1. UK Facility in the UK
2. UK Facility in the UK with International partnerships
3. Invest in an International facility within Europe
4. Invest in an International facility internationally
5. ~~No further investment~~



To develop a next-generation XFEL concept, we initially assume a new-build facility at an international scale, without constraints from location or from upgrading an existing machine.

Aspects of this design will later be mapped onto and compared against the different options (i.e UK-based/international investments).

Timeline

Year 1

- Project launch event January 2023
- Initial conceptual design and layout
- Preliminary engagement with overseas XFEL facilities
- Survey of the science team, workshops and town halls meetings begin

Year 2

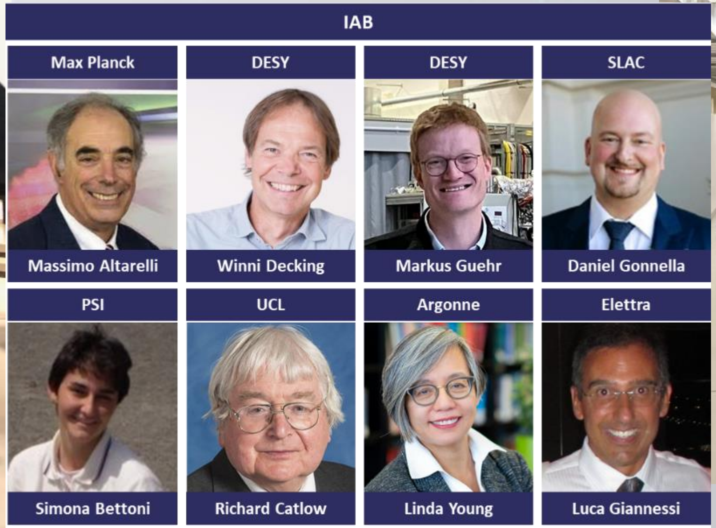
- Developing the concepts
- R&D targeting gaps in key physics and technology areas
- Collaborative activities and working groups with overseas XFEL facilities
- Workshops and town hall meetings continue

Year 3

- Summary of R&D activities
- Preferred options identified, socio-economic analysis
- Revision to science case published
- CDOA phase completed September 2025

International collaboration

- Our project has already benefitted hugely from the kind help of the international FEL community – in hosting visits, participating in our events, advising us through our advisory board and more

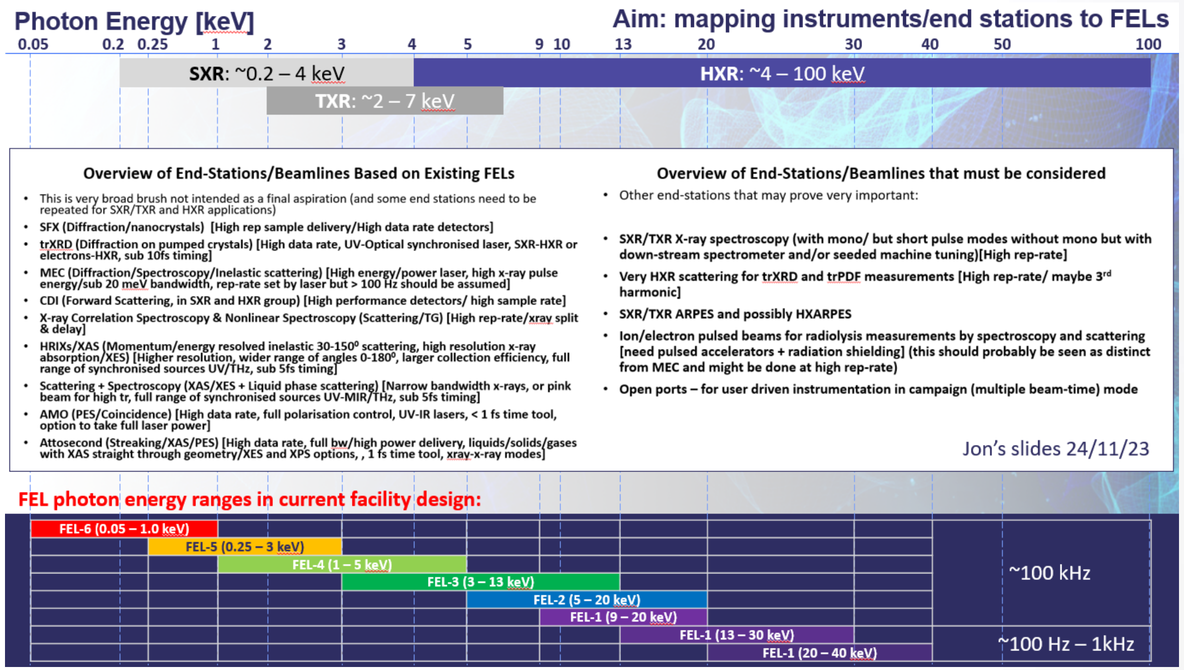


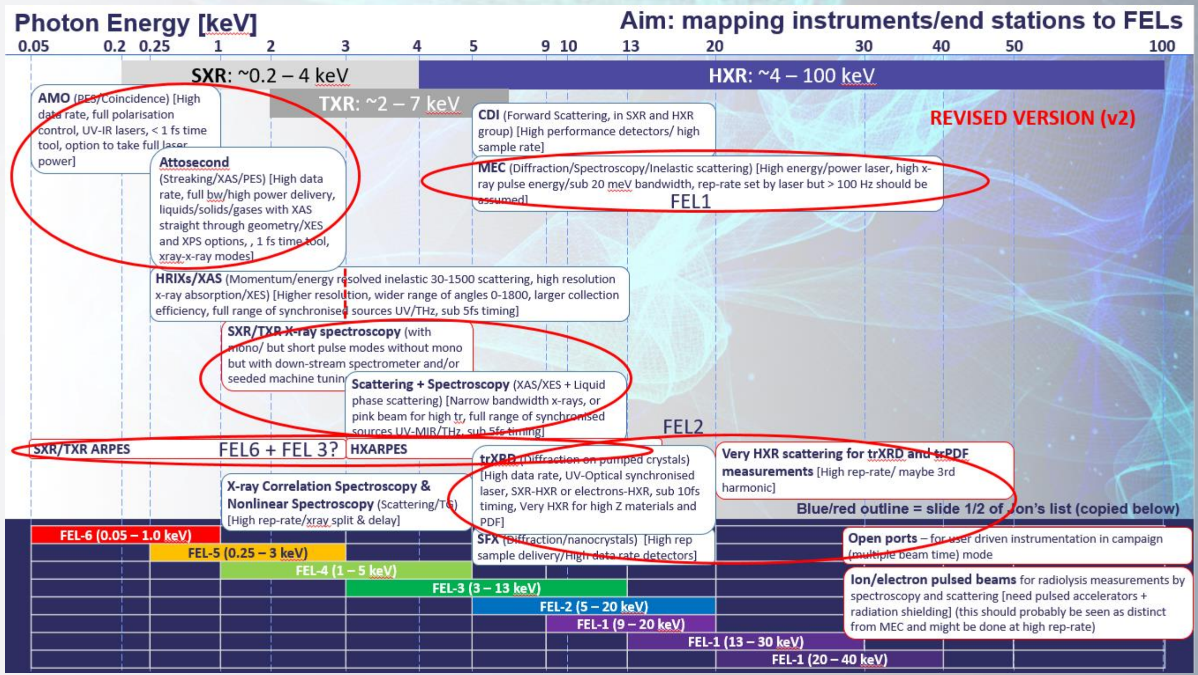
User Engagement

Over 500 participants

Defining the Specification

- Identified key end stations and relevant team members.
- Associated end stations with specific FELs and completed specification spreadsheet for each





UK XFEL Next Generation Definition

- **Evenly spaced, high repetition rate pulses to match samples, lasers, and detectors**
  - ~100 kHz per FEL, with flexibility of repetition rate
- **High efficiency facility, with a step-change in the simultaneous operation of multiple end stations**
  - Minimum of six FELs with capacity for 10, and upwards of ten end stations to be simultaneously operated
- **Near transform-limited operation across the x-ray range**
  - Photon energies from ~0.05-20 keV
  - Pulse durations from ~100 as to 100 fs
  - Non-transform-limited operation at ~20-50 keV
- **Widely separated, multiple colour x-rays to at least one end station**
- **Full array of synchronized sources**
  - XUV-THz, e-beams, ion beams, high power & high energy lasers at high repetition rate
- **Improved synchronization/timing data with external lasers to <1 fs**
- **Data and computing systems matched to the demands of high repetition rate acquisition**
- **Minimal carbon footprint with minimal energy consumption for both operation and build**

Facility design

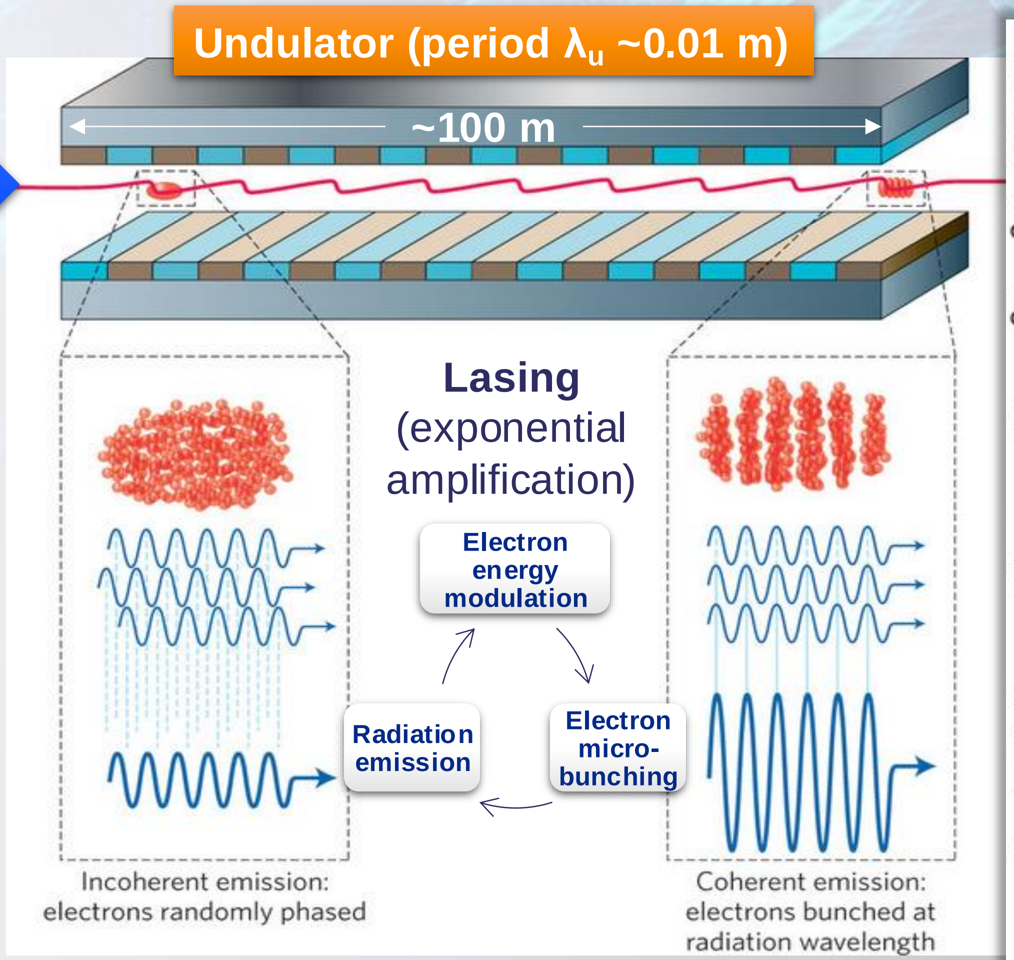
Introduction to XFELs

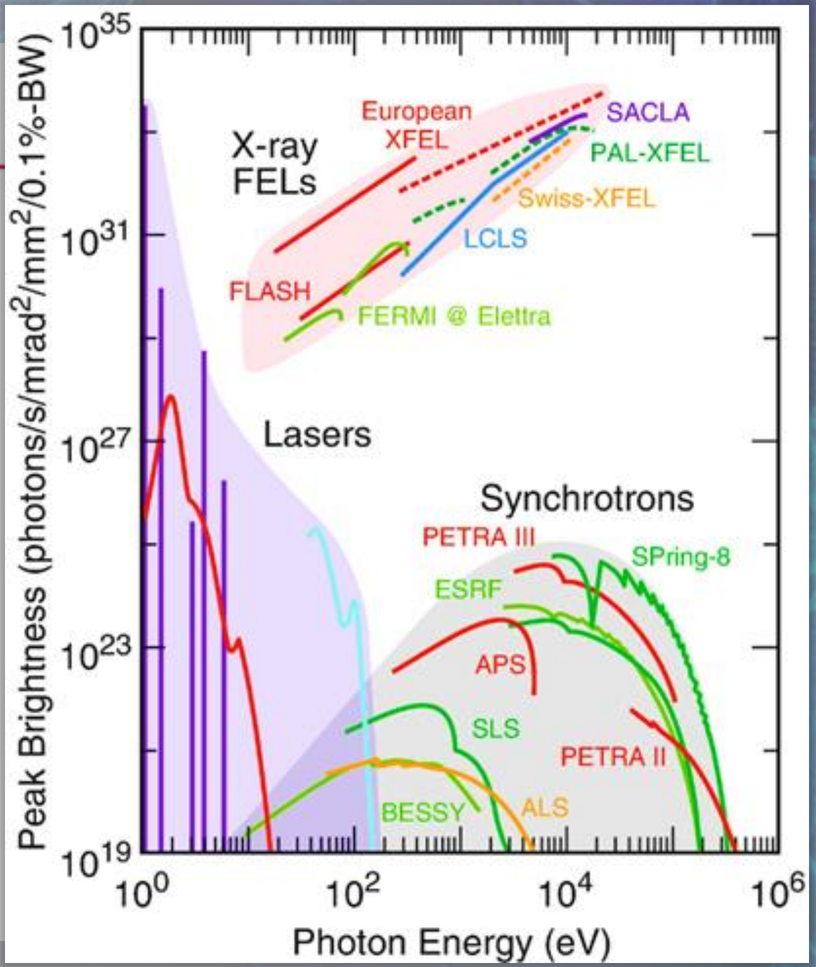
- XFEL = X-ray Free-Electron Laser
- ‘free-electron’ means the electrons are not bound in atoms but ‘freely’ propagating in a particle accelerator

Electron source

~ 0.5-1 km of linear accelerator

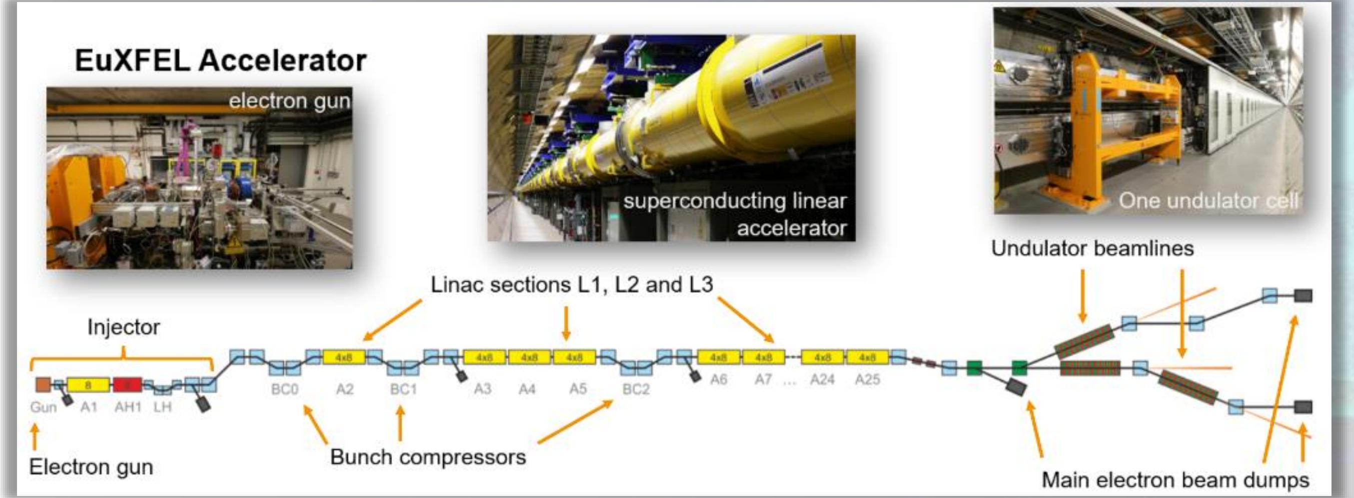
~ 4 – 15 GeV, Lorentz factor ϒ ~ several thousand





XFEL challenges and opportunities

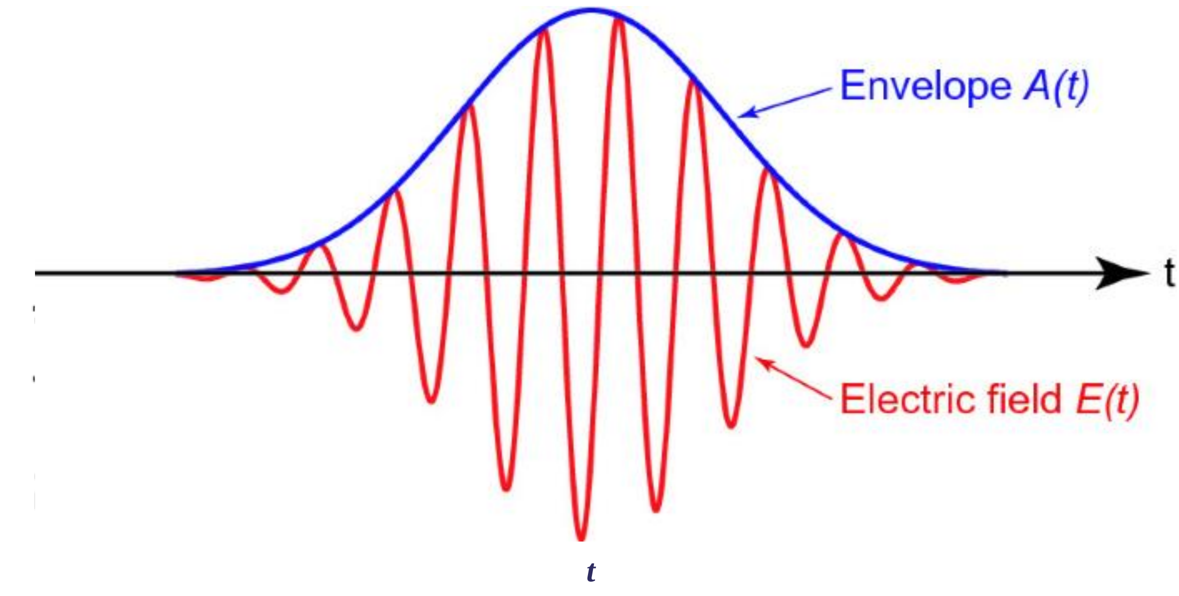
- XFEL lasing spoils the electron bunch quality (bunches can’t be re-used). So XFELs are based on *linear* accelerators: **less straightforward to serve many simultaneous experiments**



But bunch repetition rates are increasing by a factor of 10,000 compared to first-gen XFELs (~100 Hz -> ~1 MHz)

Multiplexing to **more simultaneous experiments**, with **much higher average flux** and **much higher data rates**

- **The X-ray pulses are naturally far from transform limited (amplified noise).** In the default SASE mode, there is an intrinsic coherence length of ~hundreds of wavelengths (hundreds of attoseconds at X-ray)

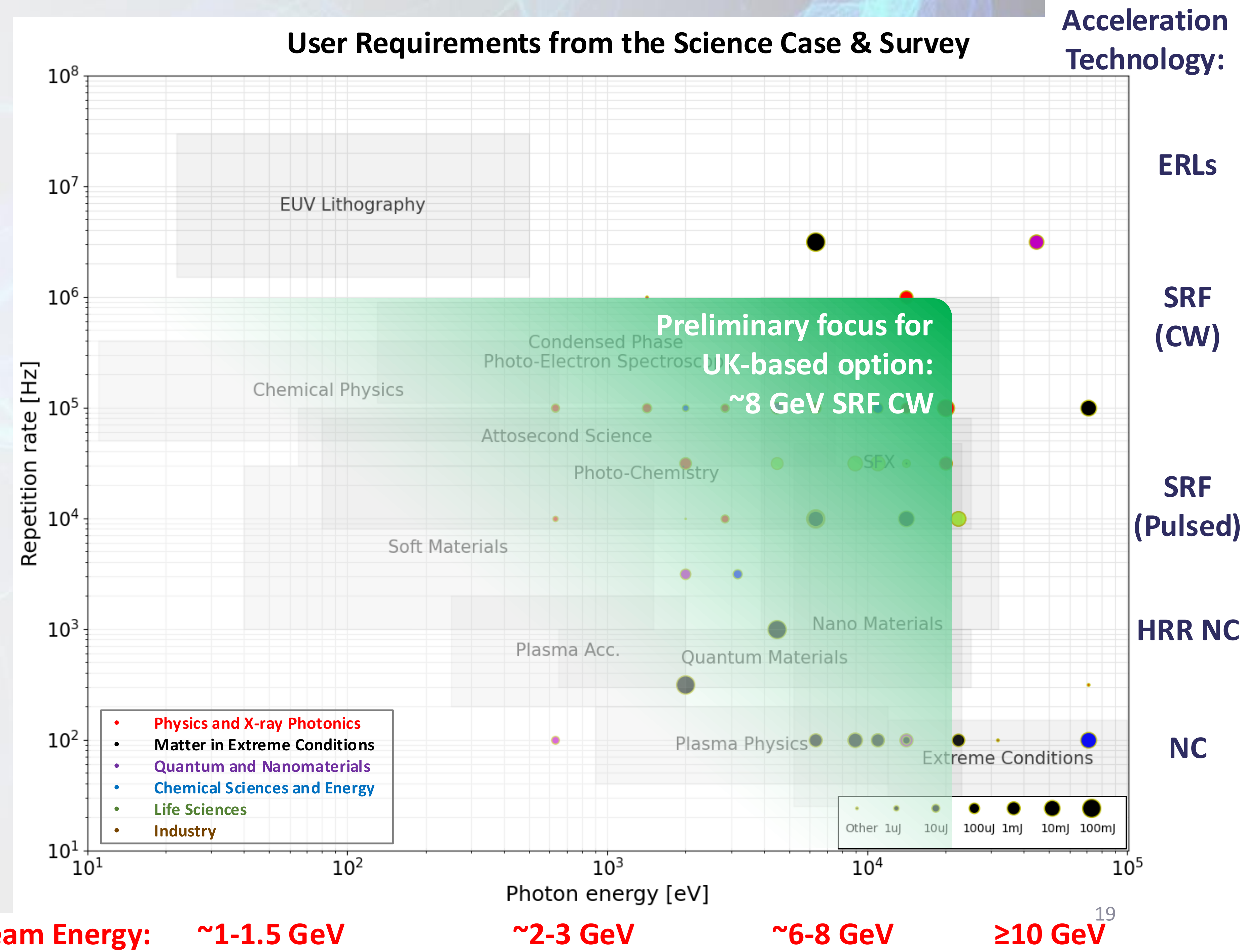


There are many demonstrated or emerging techniques for **near-transform limited pulses (i.e. high quality pulses across a range of pulse durations)**

Increasing capacity and capability go hand in hand

Top-level facility design choices

- Max. **photon energy** strongly influences the required **electron beam energy**
- **Repetition rate** largely dictates the **type of acceleration technology**
- Requirements suggest ~8 GeV superconducting RF linac



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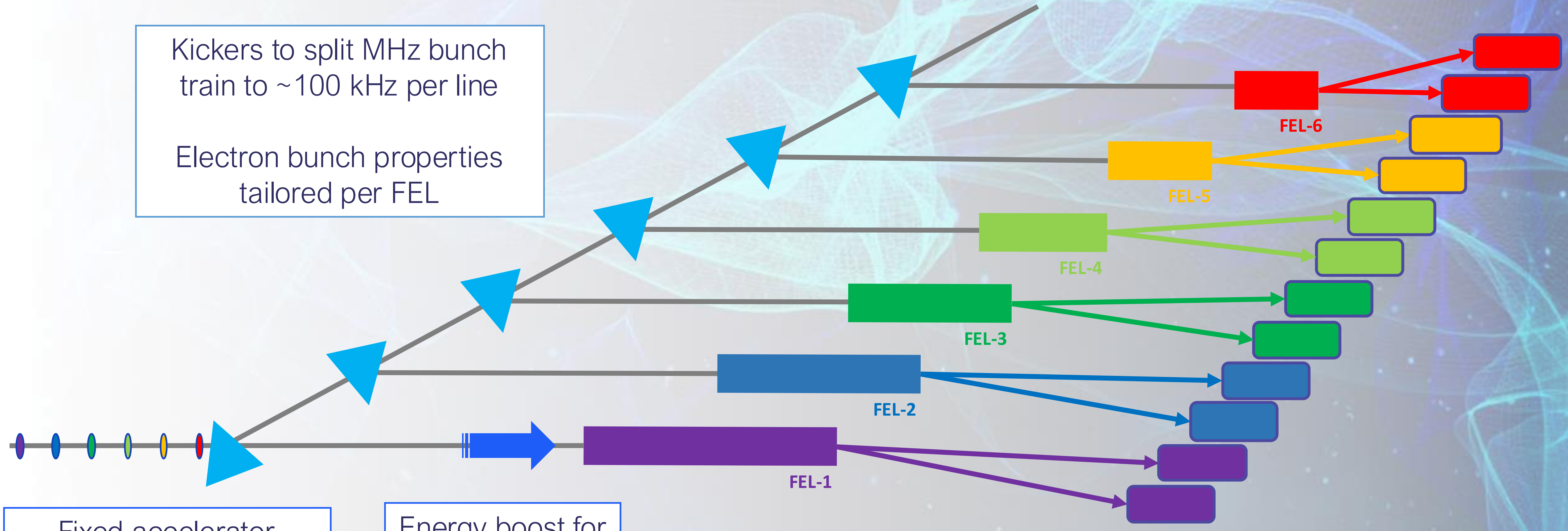
Facility concept: a step change in the simultaneous operation of multiple end stations

~6-10 FELs independently tuneable in terms of photon energy, pulse duration etc.
+ potential direct uses of electron beam

Kickers to split MHz bunch train to ~100 kHz per line

Electron bunch properties tailored per FEL



Fixed accelerator energy ~8 GeV, electron bunches at ~1 MHz

Energy boost for higher pulse energy/high photon energy

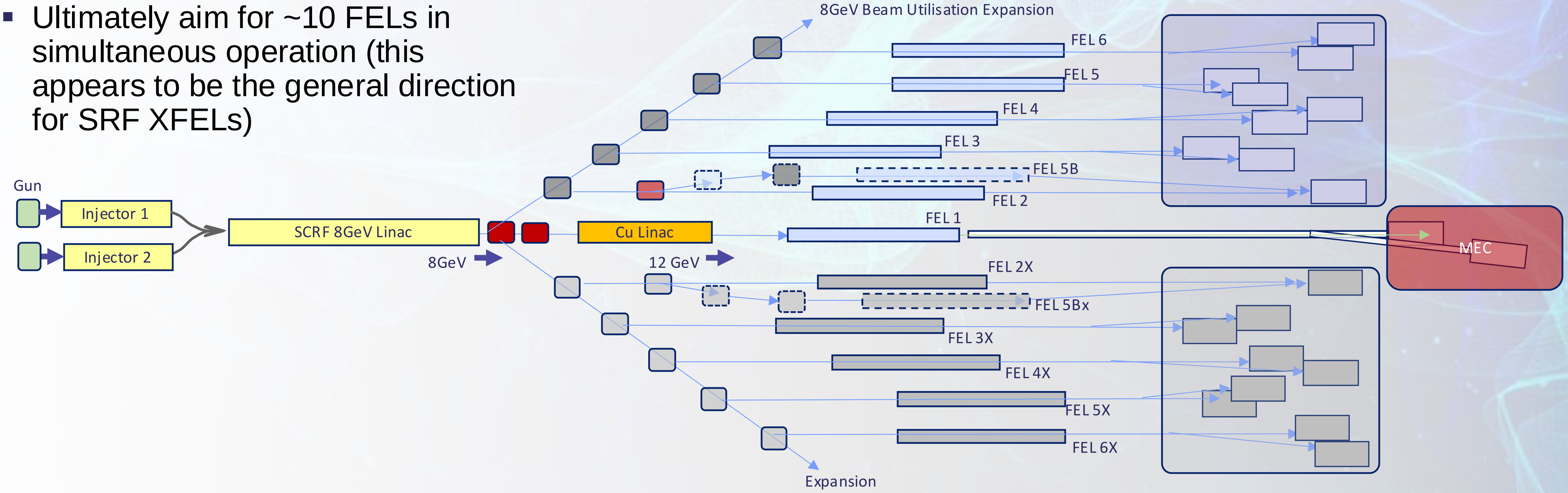
100 kHz Kicker

A more detailed schematic

Injector | Linac | Spreader | FELs | Photon Transports | Experimental Halls

"Day 1 +"

- Ultimately aim for ~10 FELs in simultaneous operation (this appears to be the general direction for SRF XFELs)



Development of end station specifications

Photon Energy [keV]

0.05 0.2 0.25 1 2 3 4 5 9 10 13 20 30 40 50 100

SXR: ~0.2 – 4 keV

HXR: ~4 – 100 keV

TXR: ~2 – 7 keV

REVISED VERSION (v2) still under development

AMO (PES/Coincidence) [High data rate, full polarisation control, UV-IR lasers, < 1 fs time tool, option to take full laser power]

Attosecond (Streaking/XAS/PES) [High data rate, full bw/high power delivery, liquids/solids/gases with XAS straight through geometry/XES and XPS options, , 1 fs time tool, xray-x-ray modes]

CDI (Forward Scattering, in SXR and HXR group) [High performance detectors/ high sample rate]

MEC (Diffraction/Spectroscopy/Inelastic scattering) [High energy/power laser, high x-ray pulse energy/sub 20 meV bandwidth, rep-rate set by laser but > 100 Hz should be assumed]

HRIXs/XAS (Momentum/energy resolved inelastic 30-1500 scattering, high resolution x-ray absorption/XES) [Higher resolution, wider range of angles 0-1800, larger collection efficiency, full range of synchronised sources UV/THz, sub 5fs timing]

SXR/TXR X-ray spectroscopy (with mono/ but short pulse modes without mono but with down-stream spectrometer and/or seeded machine tunin

Scattering + Spectroscopy (XAS/XES + Liquid phase scattering) [Narrow bandwidth x-rays, or pink beam for high tr, full range of synchronised sources UV-MIR/THz, sub 5fs timing]

SXR/TXR ARPES

HXARPES

trXRD (Diffraction on pumped crystals) [High data rate, UV-Optical synchronised laser, SXR-HXR or electrons-HXR, sub 10fs timing, Very HXR for high Z materials and PDF]

Very HXR scattering for trXRD and trPDF measurements [High rep-rate/ maybe 3rd harmonic]

FELs sequentially dis

X-ray Correlation Spectroscopy & Nonlinear Spectroscopy (Scattering/TG) [High rep-rate/xray split & delay]

SFX (Diffraction/nanocrystals) [High rep sample delivery/High data rate detectors]

Open ports – for user driven instrumentation in campaign (multiple beam time) mode

Ion/electron pulsed beams for radiolysis measurements by spectroscopy and scattering [need pulsed accelerators + radiation shielding] (this should probably be seen as distinct from MEC and might be done at high rep-rate)

FEL-6 (0.05 – 1.0 keV)

FEL-5 (0.25 – 3 keV)

FEL-4 (1 – 5 keV)

FEL-3 (3 – 13 keV)

FEL-2 (5 – 20 keV)

FEL-1 (9 – 20 keV)

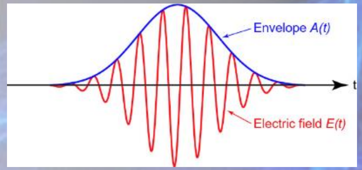
FEL-1 (13 – 30 keV)

FEL-1 (20 – 40 keV)

~100 Hz

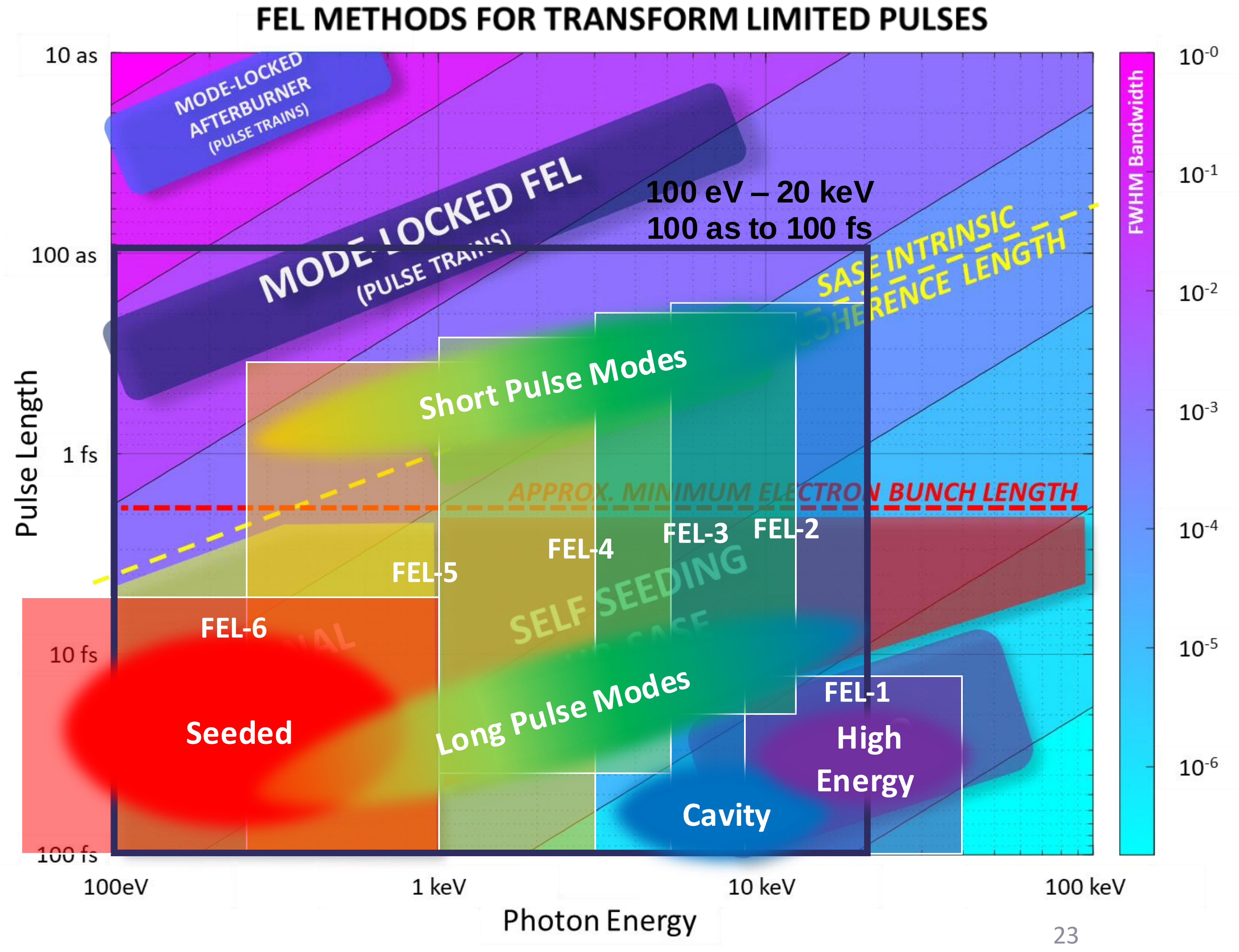
Near transform-limited pulses

Each FEL has 1-3 primary operating modes, covering both short-pulse and long-pulse options



FEL	Tuning	Mode	Technique	Transform Limited Pulse Duration
FEL-6	0.05 – 1.0 keV	Seeded	EEHG	5 – 100 fs
FEL-5	0.25 – 3.0 keV	Long pulse	EEHG/HB	100 fs – 20 fs
		Short Pulse	XLEAP	2 fs – 350 as
FEL-4	1.0 – 5.0 keV	Long Pulse	HB-SASE	40 fs – 15 fs
		Short Pulse	XLEAP	800 as – 275 as
FEL-3	3.0 – 13.0 keV	Long Pulse	HB-SASE	20 fs – 10 fs
		Short Pulse	XLEAP	400 as – 200 as
FEL-2	5.0 – 20.0 keV	Long Pulse	HB-SASE	16 fs - 12 fs
		Short Pulse	XLEAP	300 as – 200 as
		Cavity	XFELO	~ 100 fs
FEL-1	9 – 20 keV	High Power	SASE	~ 30 fs (not TL)
	13 – 30keV*	High Energy		
	20 – 40keV*	High Energy		

*via booster, possibly at lower rep. rate



Pulse durations estimated from simulations/scaling, intermediates between short and long pulse modes also accessible.

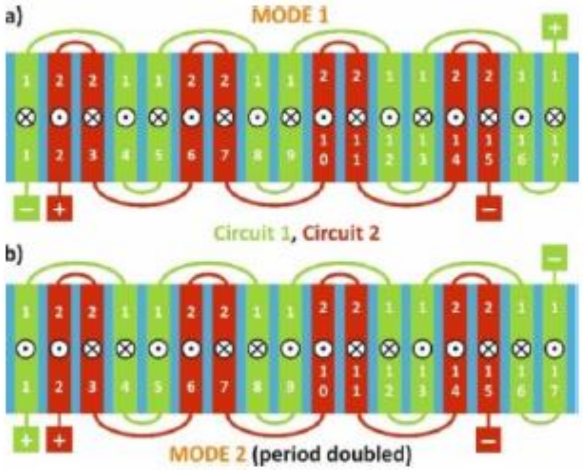
Other key capabilities

FEL for matter in extreme conditions

- Demand for 10’s mJ pulse energy at 5-10 keV, and to reach 40 keV
- NCRF booster to ~12 GeV
- Potential to use dual-period undulators

Superconducting undulator coils with period length doubling

To cite this article: S Casalbuoni *et al* 2019 *J. Phys.: Conf. Ser.* **1350** 012024



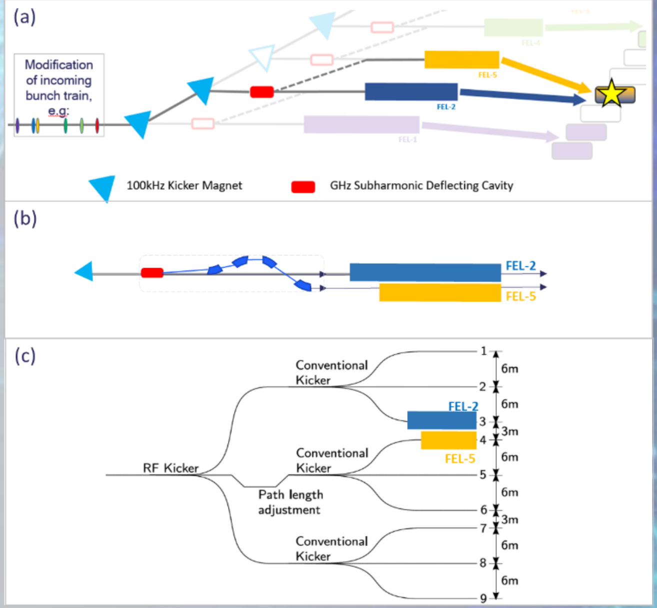
Next-gen XFELs are expected to be some of the biggest data machines on the planet

Unprecedented requirements in data rates (towards TB/s) and scale (PB per data set). AI and exascale computing potential, e.g. for real-time experiment steering

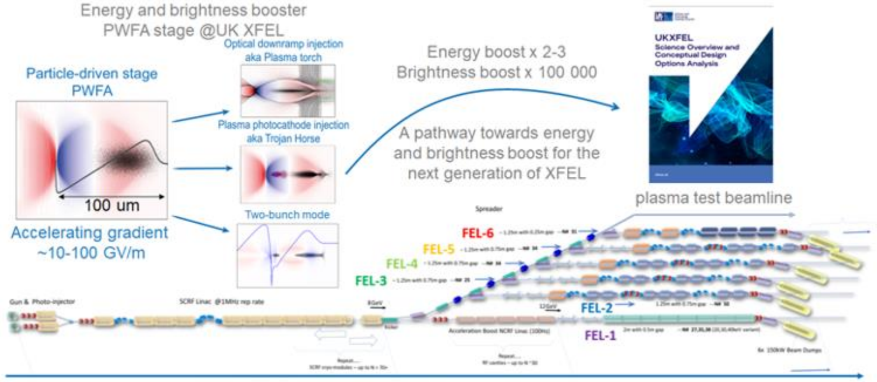
A laser facility as well as an accelerator facility

High rep. rate lasers over a wide range of spectral/temporal regimes using Yb-based technology + high pulse energy laser for MEC, e.g. DiPOLE. Laser or accelerator-based THz

Widely-separated two-colour capability could be a key feature of a next-generation XFEL



Direct uses of the e-beam, e.g. PWFA test area and potential output enhancements

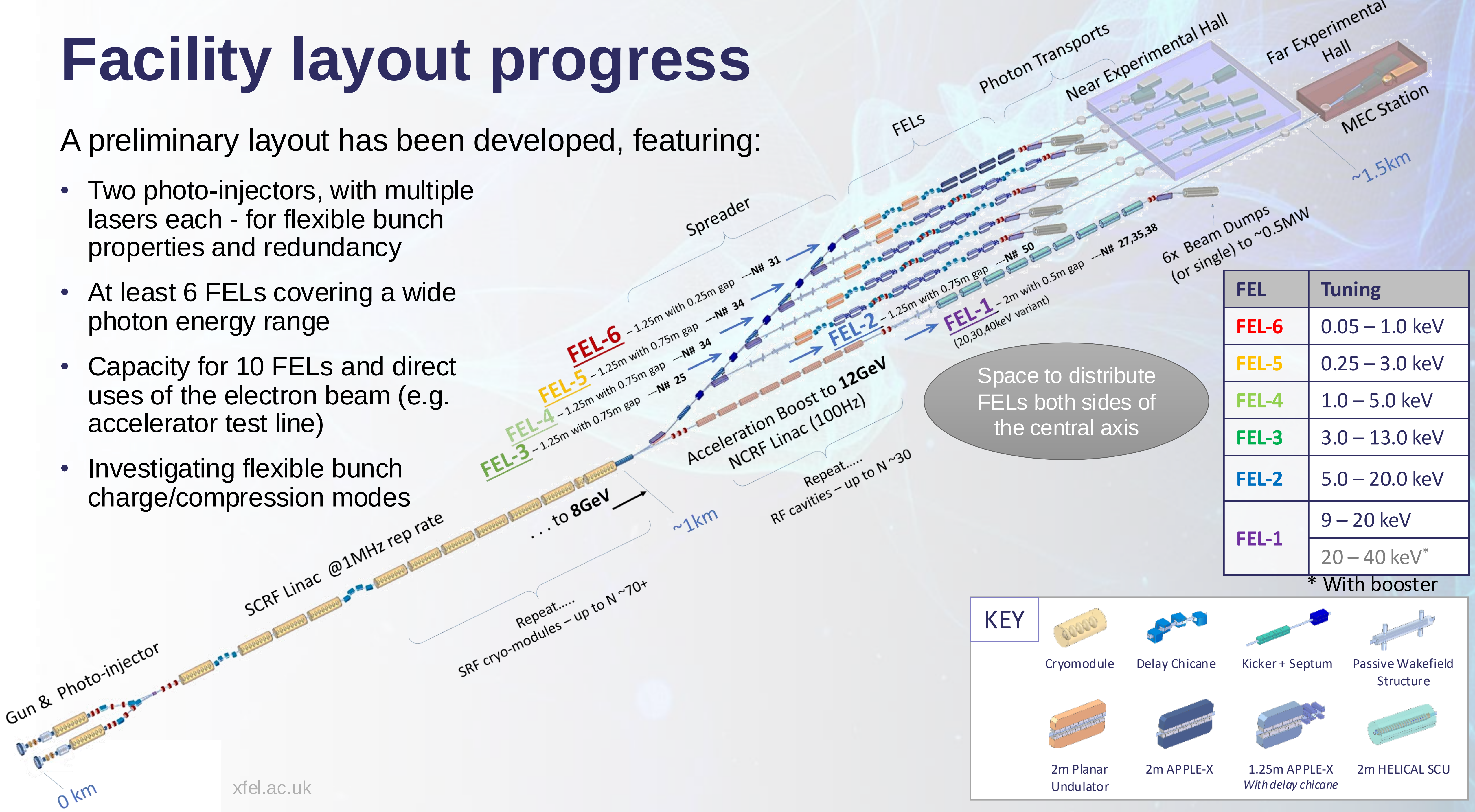


A preliminary UK XFEL layout options

Facility layout progress

A preliminary layout has been developed, featuring:

- Two photo-injectors, with multiple lasers each - for flexible bunch properties and redundancy
- At least 6 FELs covering a wide photon energy range
- Capacity for 10 FELs and direct uses of the electron beam (e.g. accelerator test line)
- Investigating flexible bunch charge/compression modes



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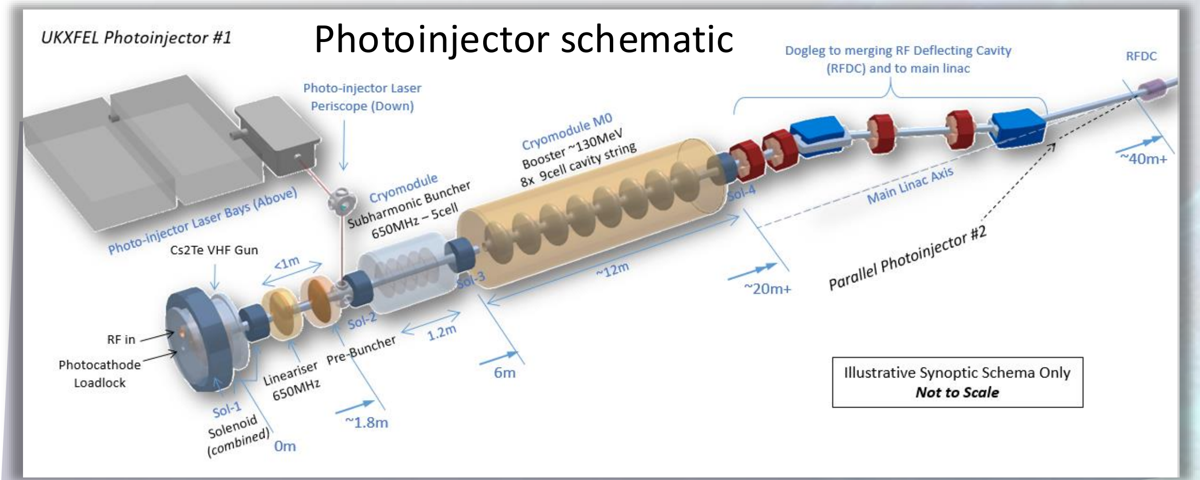
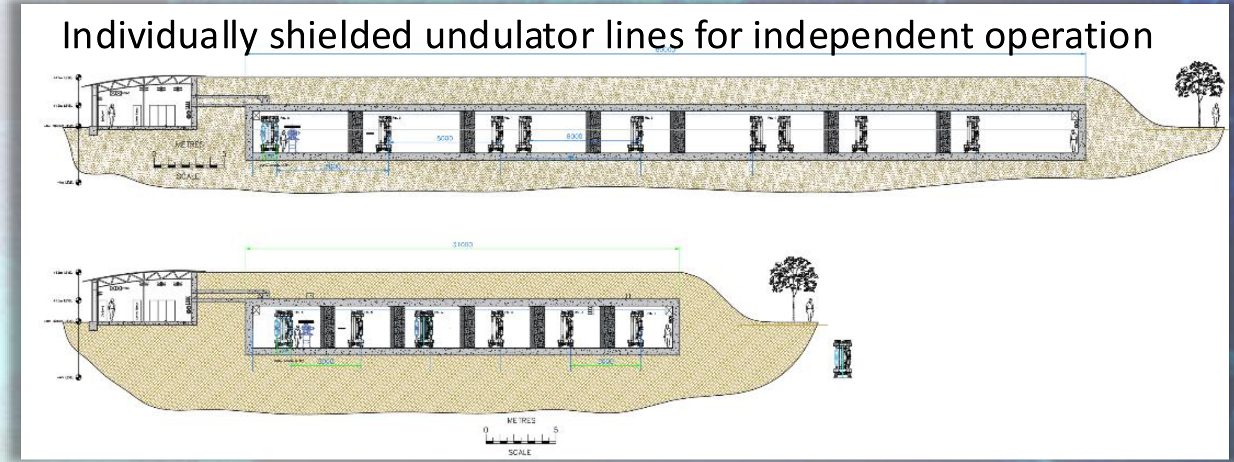
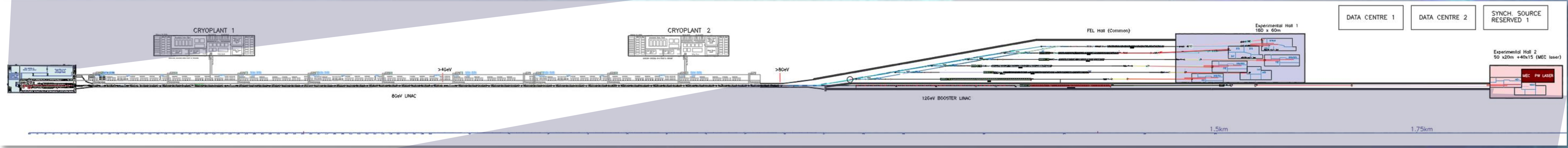
FEL-1	9 – 20 keV
	20 – 40 keV*

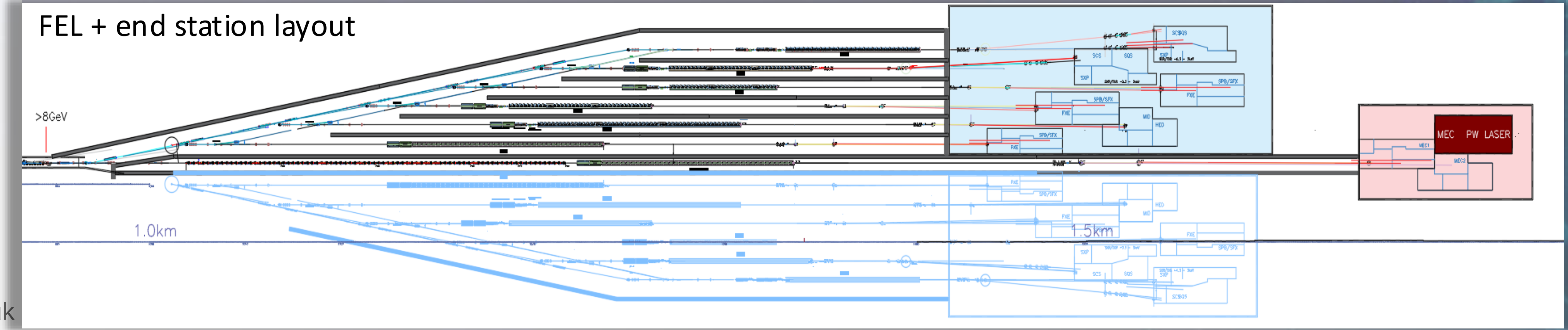
* With booster

Facility layout progress









Summary and next steps

- XFELs are a revolutionary technology with further orders of magnitude enhancements still to be realised: they are well positioned to be leading scientific facilities for decades
- UK users and accelerator community are highly enthusiastic about next-generation XFEL capabilities, enabled by SRF acceleration, other high-rep. rate sources, advances in data + AI/exascale, etc.
- There is clear demand for more regular access and reducing the barriers to entry

- Clearly these are major investments; our next steps are:
  - to compare socioeconomic benefits of UK vs international investment options
  - identify key R&D areas, including those to improve sustainability, reduce cost
  - this phase finishes October 2025: plan for Technical Design phase

Contact: ukxfel@stfc.ac.uk

Acknowledgements

Science and Technology Facilities Council

Science Team

Imperial College London
Brookhaven National Laboratory
Newcastle University
University of Plymouth
The University of Edinburgh
University of Oxford
King's College London
University of Southampton
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University of Leeds
AWE
The Cockcroft Institute of Accelerator Science and Technology
UCL
diamond
University of York
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University of Strathclyde Glasgow
Queen's University Belfast
University of Sheffield

UK Research Councils & Government

UK Research and Innovation
Biotechnology and Biological Sciences Research Council
Economic and Social Research Council
Research England
Engineering and Physical Sciences Research Council
Natural Environment Research Council
Innovate UK
Medical Research Council
Arts and Humanities Research Council
Department for Science, Innovation & Technology

Other XFELs

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LCLS
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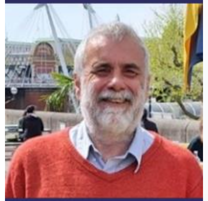
SACLA

Acknowledgements

Science Team

Science Lead



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Life sciences:

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Chemical sciences:

Julia Weinstein (Sheffield), Russell Minns (Soton), Sofia Diaz-Moreno (Diamond), Alex Baidak (Manchester), Andrew Burnett (Leeds), Tom Penfold (Newcastle), Rebecca Ingle (UCL), Mark Brouard, Claire Vallance (Oxford)

Physical sciences:

Amelle Zair (KCL), Adam Kirrander (Edinburgh), Jason Greenwood (QUB), Jon Marangos (IC), Elaine Seddon (Cockcroft)

+ around 100 additional experts from around the world contributing to Science Case

Facility design and support

Öznur Apsimon, Can Davut, Ben Hounsell, Suzanna Percival, Julian McKenzie, Lee Jones, Louise Cowie, Hywel Owen, Andy Wolski, Andrew Potter, Adam Dixon, Frank Jackson, Joe Crone, Ian Bailey, Peter McIntosh, Alan Wheelhouse Anthony Gilfellon, Aaron Farricker, Anisullah Baig, Fahim Habib, Lily Berman, Alan Mak, Alex Hinton, Brian McNeil, Katie Morrow, Amelia Pollard, Matt King, Alex Aiken, Patrick Sterling, Chris Armstrong, Matthew Veale, Sion Richards, Ben Shepherd, Andrew Vick, James Bourne, Emily Baker, Sonja Scott-Jones, Lynn Caddick, Lauren Hamblett

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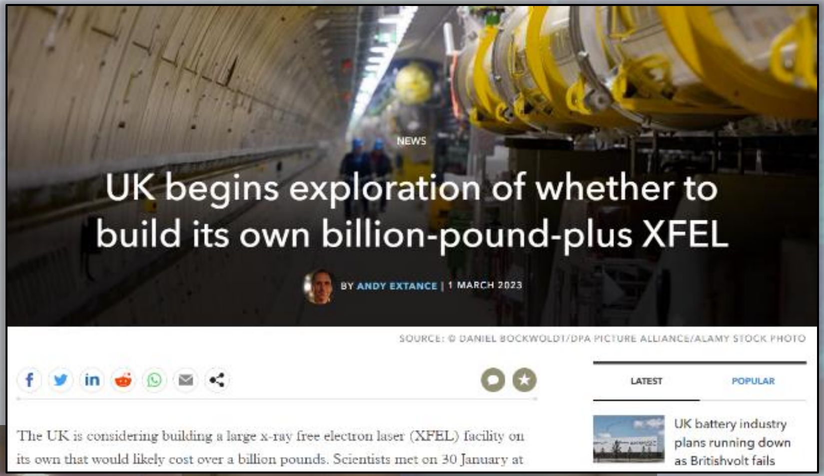
Thank You

Contact: ukxfel@stfc.ac.uk

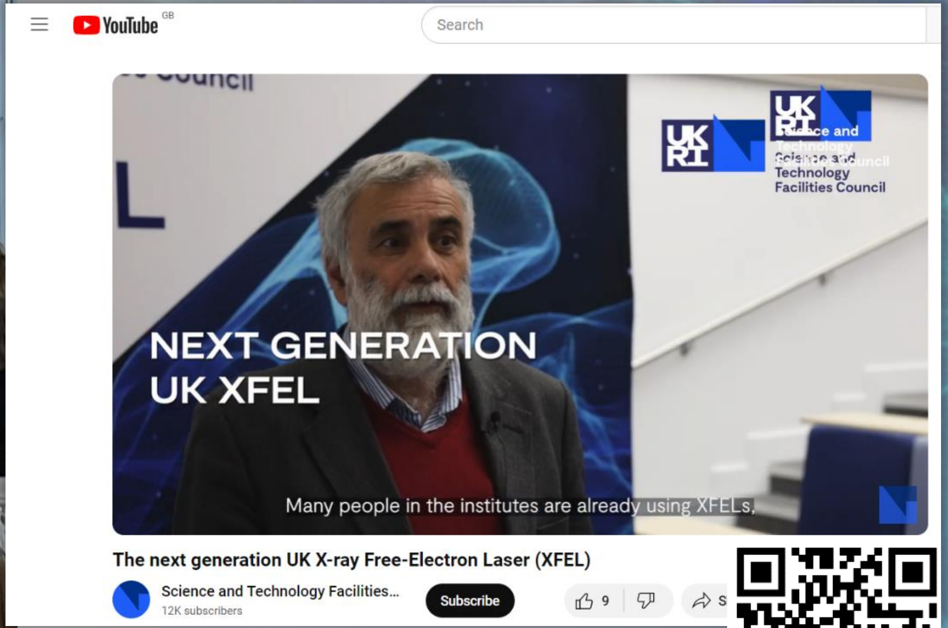
Project Launch

- Over 150 in-person attendees, with another 150 attending virtually
- Ongoing project comms activities to reach new communities

[Chemistry World]



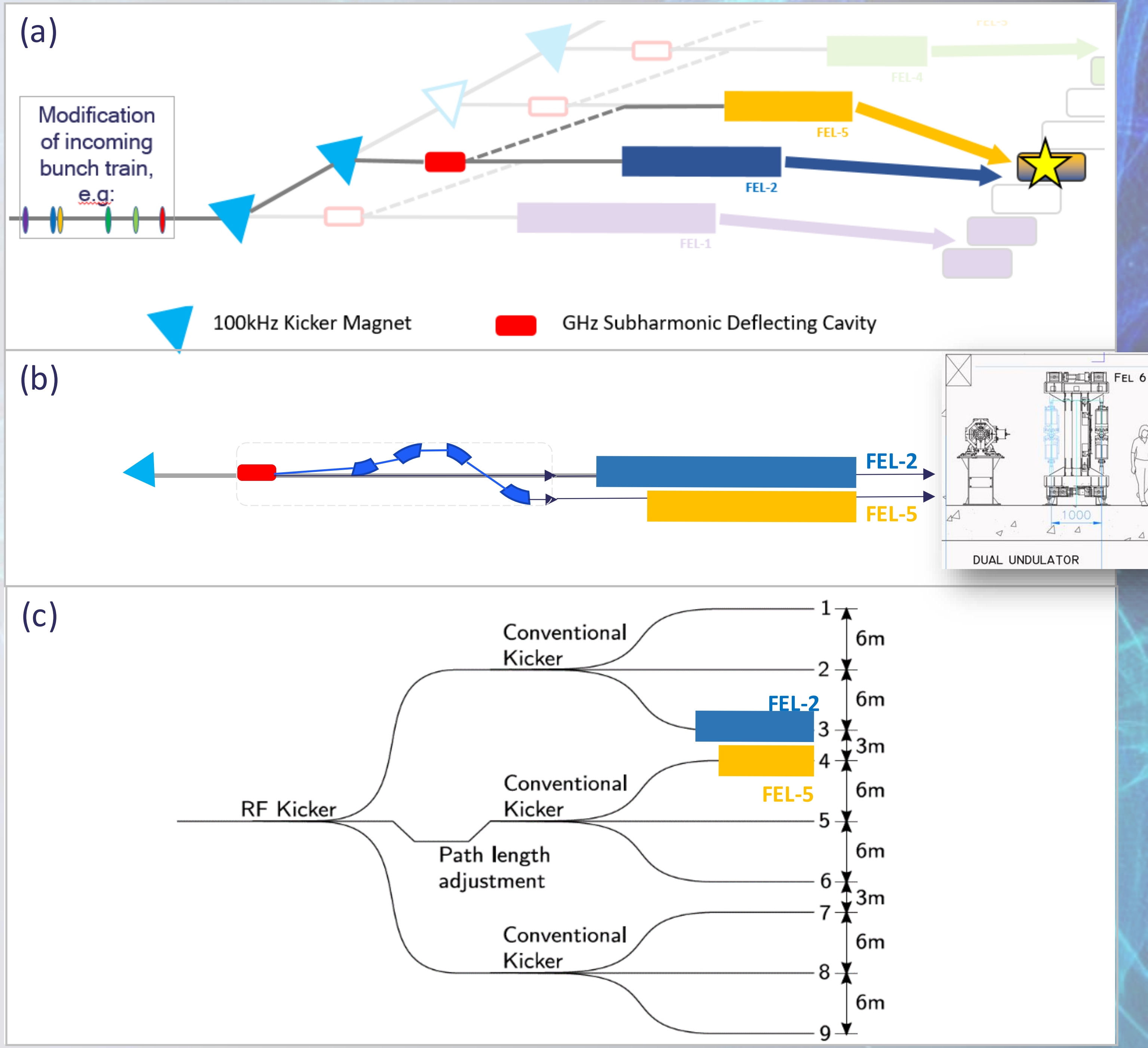
[Physics World]



[https://www.youtube.com/watch?v=z3DSFWprWC4&t=1s]

Concepts for two-colour

- *Widely-separated two-colour capability could be a key feature of a next-generation XFEL – but how and to what extent is it best to implement it?*
- End station away day activities were very useful for this topic: a specific combination has been identified for detailed studies ("FEL-5b" + FEL-2)
- Concepts developed with similar key features:
  - bunch pattern from the injector is adjusted to bring two bunches into adjacent RF cycles (Δt = 0.77 ns)
  - a GHz subharmonic deflecting cavity used to deflect one bunch onto an adjacent FEL
  - path length difference compensates the temporal separation



FEL for matter in extreme conditions

- Requirement for 10’s of mJ at 5-10keV, **and** as many mJ as possible at up to 40keV
- To approach 10’s mJ pulse energy, and to reach 40keV, we need a beam energy considerably greater than 8 GeV – assume booster to ~12 GeV
- But we also need a wide photon energy range….
- Suggestion is to use an undulator with dual periods.
- EuXFEL are developing a planar SCU which incorporates **period doubling**:

- **At maximum current of 450A:**
  - SCU17: Period 17mm, B = 1.26T, K = 2
  - SCU34: Period 34mm, B = 2.6T, K = 8.54
- **At 12 GeV:**
  - SCU17: Tunes 26keV (K = 2) to 53keV (K = 1)
  - SCU34: Tunes 1keV (K = 8.54) to 26keV (K = 1)

Superconducting undulator coils with period length doubling

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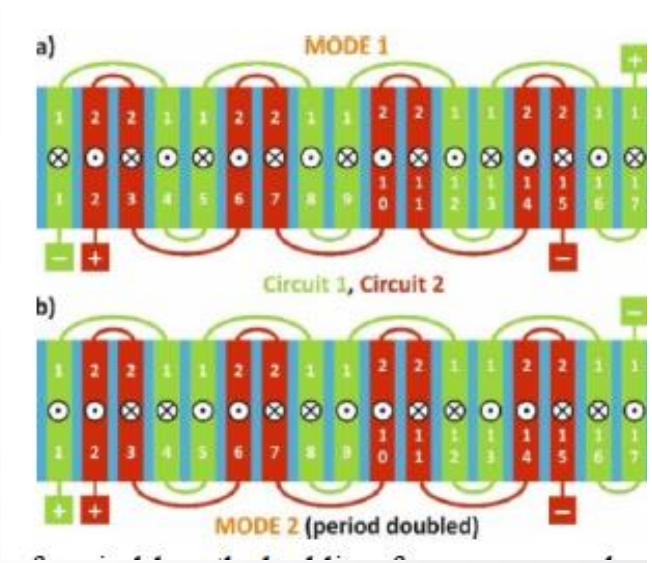
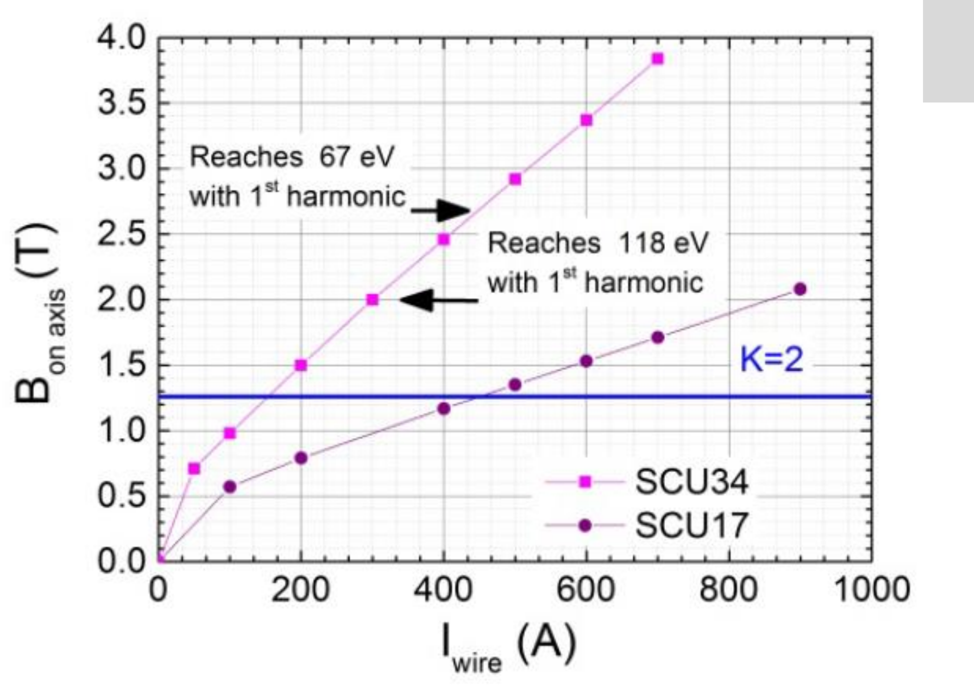
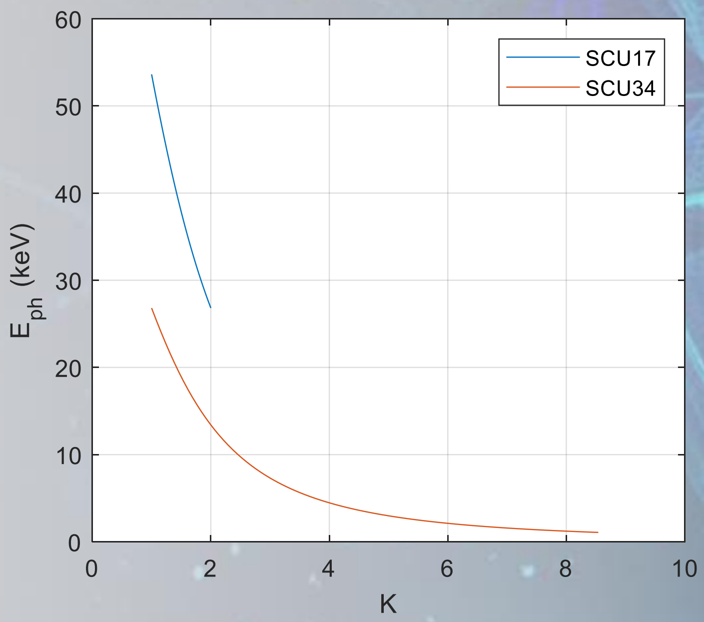
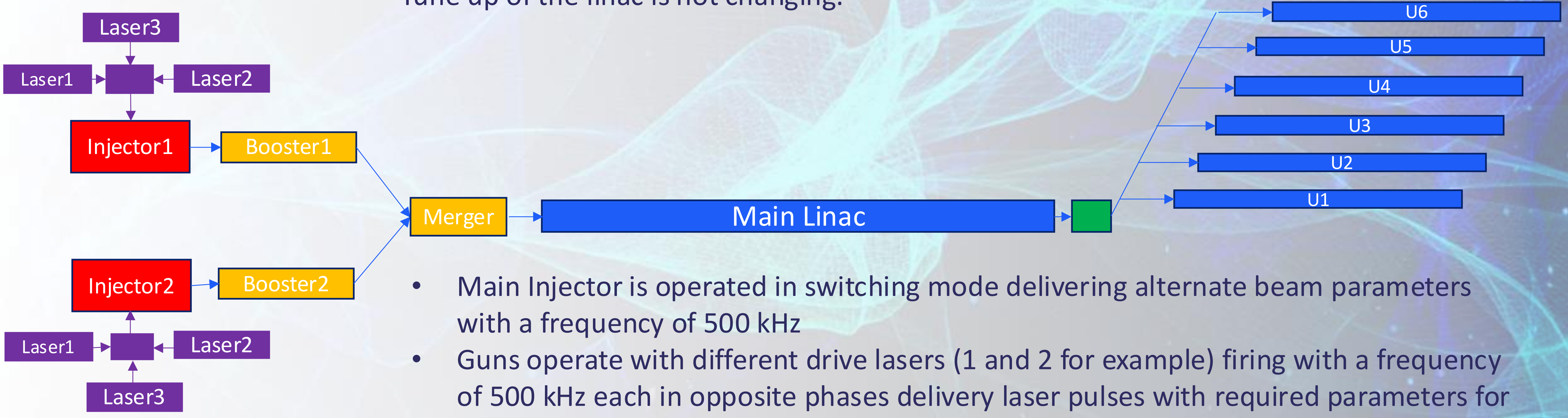






UKXFEL Low Energy Beamline. Multi-FEL Operation

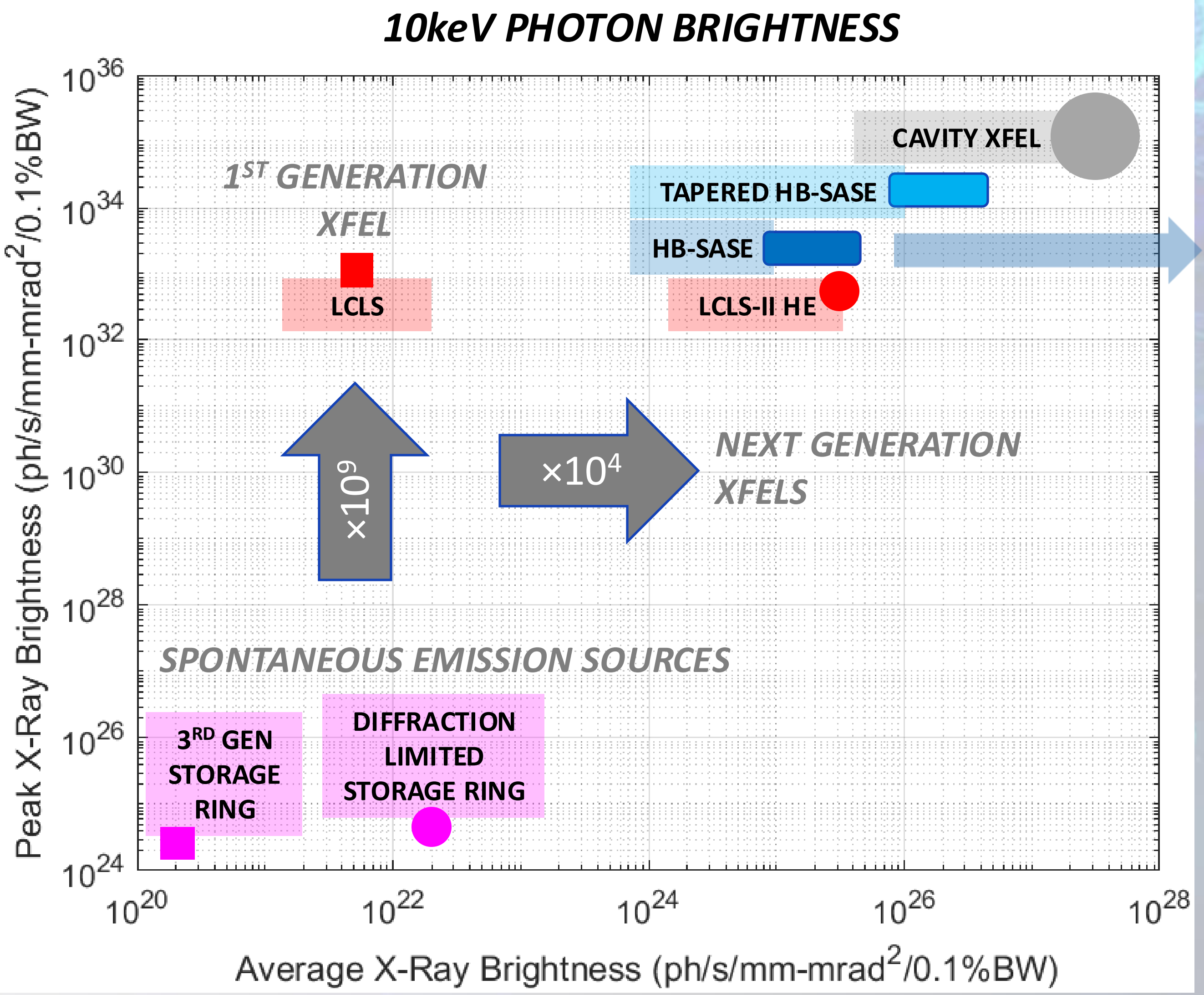
- Switch between undulators is provided at the exit of the linac.
- Tune up of the linac is not changing.

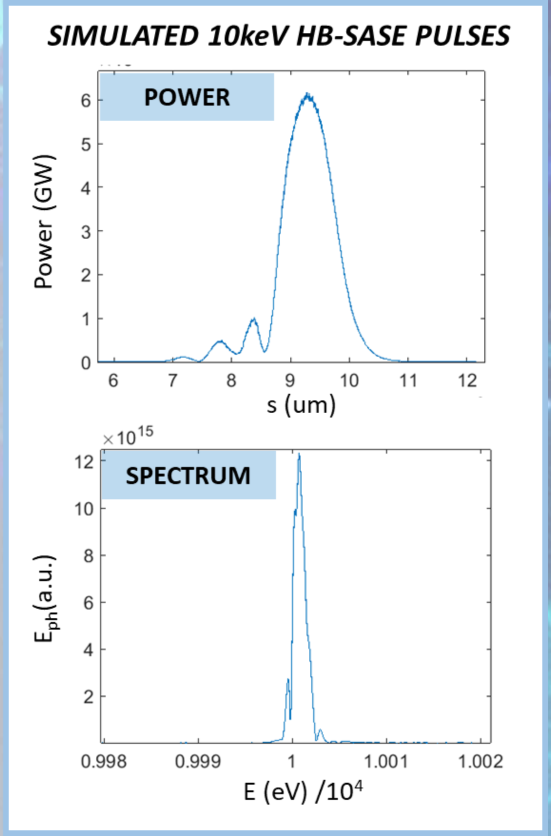


- Main Injector is operated in switching mode delivering alternate beam parameters with a frequency of 500 kHz
- Guns operate with different drive lasers (1 and 2 for example) firing with a frequency of 500 kHz each in opposite phases delivery laser pulses with required parameters for every beam mode in two separate beamlines
- For two FEL operation regime injectors are driven by two different lasers alternately with required frequency in opposite phases delivering pulses with necessary parameters for every FEL mode in two separate beamlines
- For pump-probe experiment the probe injector delivers beam with delay of ~0.77 ns (RF period of L-band) relative to the injector driving pump FEL or vice versa.

Evolution of peak and average brightness

- Superconducting accelerator technology enables a significant increase in *average* brightness, as well as peak brightness
- Advanced FEL modes provide further advantages





Adapted from LCLS figure: Mike Dunne, SLAC, Future Developments at LCLS, UK XFEL Launch Event 2023 https://youtu.be/sxipwNyXMhg

Expected timelines

Evaluate

2019 to 2020 Science Case – Completed

Design

Currently here → Oct 2022 to Oct 2025 Conceptual Design and Options Analysis

Funding bid ongoing Oct 2025 to ~2030 Technical Design Review

Construction

~2032 onwards Civil Construction work

~2033 onwards Accelerator Construction work

Funding Bids would need to be approved before the start dates suggested.