Introducing RUEDI

A Proposed Relativistic Ultrafast Electron Diffraction & Imaging Facility for the UK

Julian McKenzie

(on behalf of the RUEDI team)

IOP PABG Annual Conference

26th July 2022, Liverpool

Science and Technology Facilities Council

University of Liverpool

The Rosalind Franklin Institute

Swansea University Prifysgol Abertawe

University of Leeds

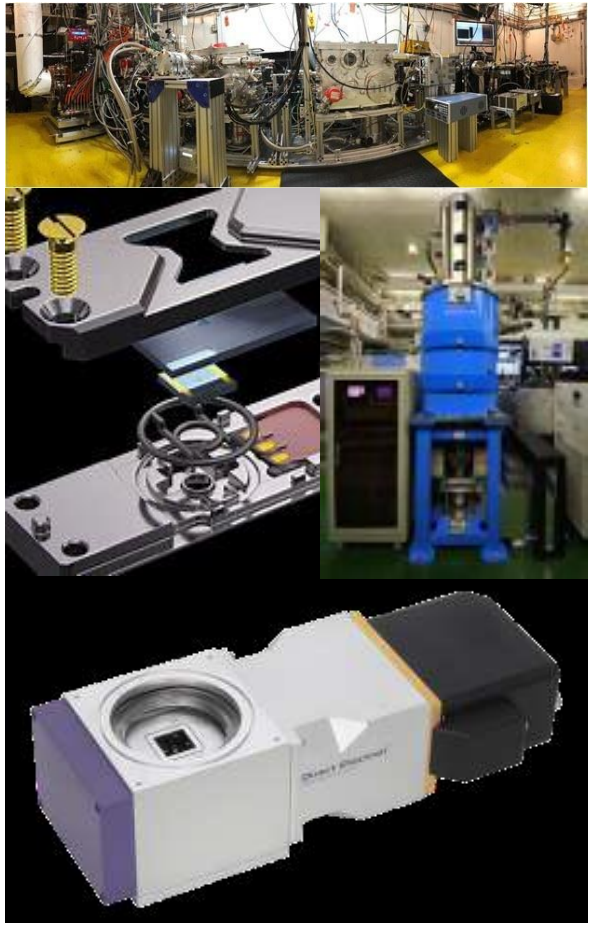
Engineering and
Physical Sciences
Research Council

What is RUEDI?

A national user facility using MeV electrons for imaging and diffraction on ultrafast timescales

Transformative Science Themes Accelerating UK Technologies

- Dynamics of Chemical Change
- Materials in Extremes
- Quantum Materials & Processes
- Energy Generation, Storage and Conversion
- In Vivo Biosciences



World leading advances in accelerator, lens, operando stages and detector designs coupled to advances in artificial intelligence

RUEDI

Electron Diffraction + Microscopy

- **Relativistic Ultra-fast Electron Diffraction & Imaging**
- **Facility for Structural Dynamics on the Femtosecond Timescale**
- *RUEDI allows the evolution of structural changes in materials to be observed through time-resolved pump-probe experiments*
- EPSRC “mid-range” national facility sited at Daresbury Laboratory

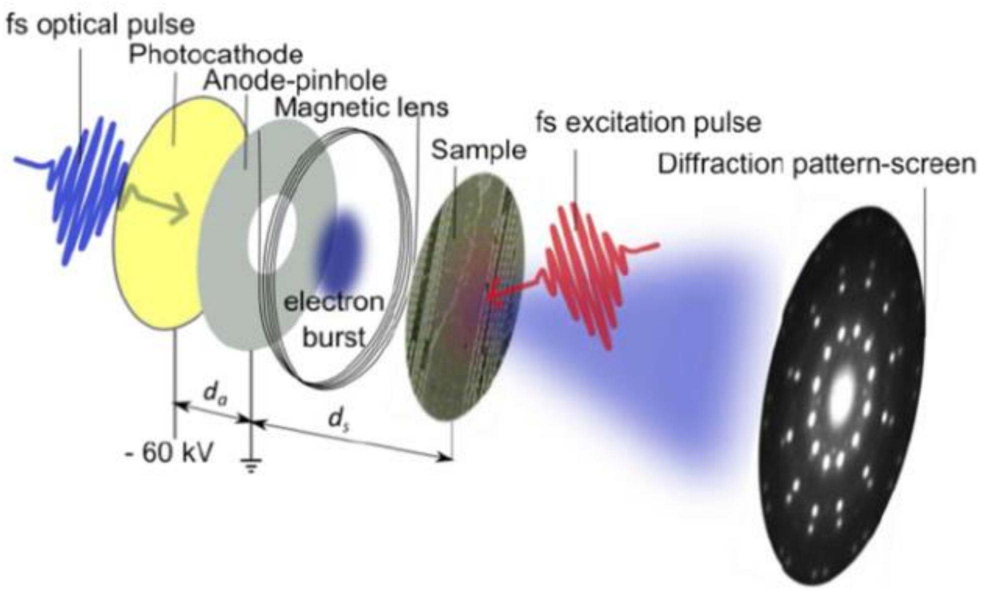
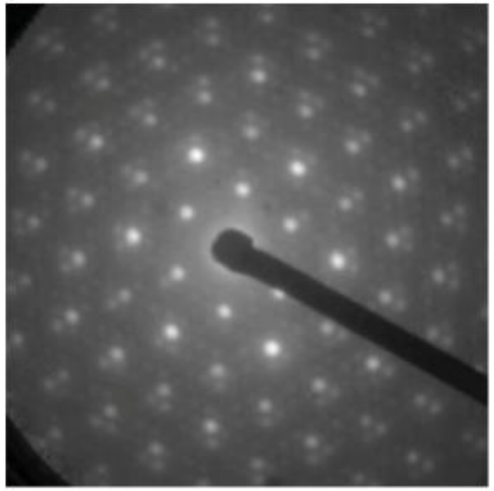


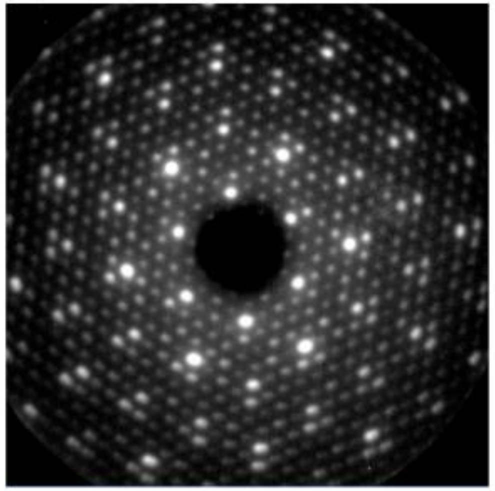
Image from Rep. Prog. Phys.74(2011) 096101

Going from keV to MeV

- Greater penetration depth (thicker samples)
- No velocity mismatch as $\beta \approx 1$
- Electron wavelength below atomic level → direct observation of movement of atoms
- Less multiple scattering and “real” flat Ewald-sphere
- Much reduced space-charge effects ($1/(\beta^2\gamma^3)$) leads to greater spatial-temporal resolution, more electrons per pulse



60 keV UED

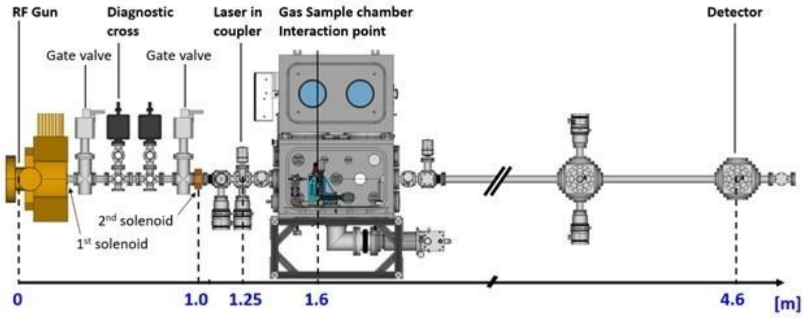


3 MeV UED

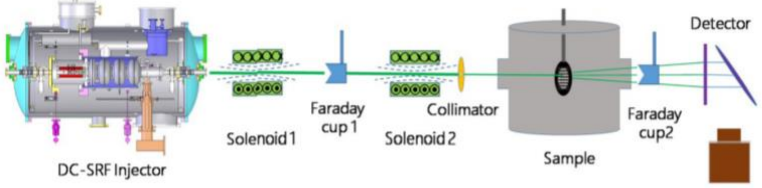
Images from BNL

Existing MeV-UED Facilities Worldwide:

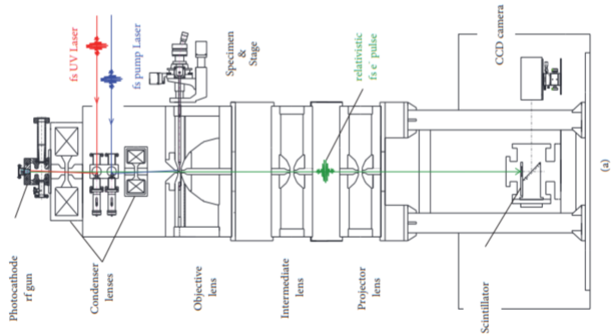
SLAC



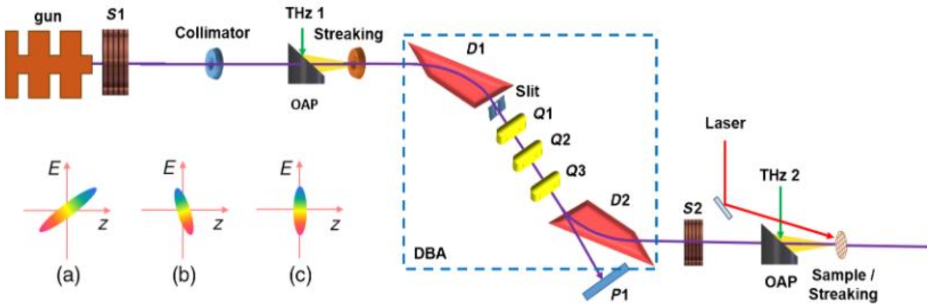
Peking University



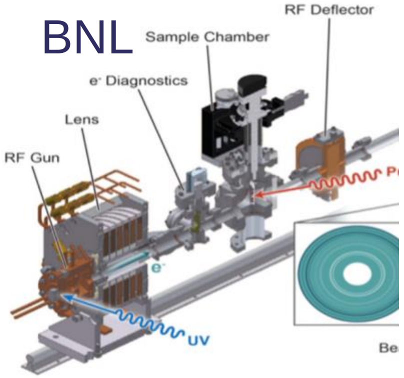
Osaka University



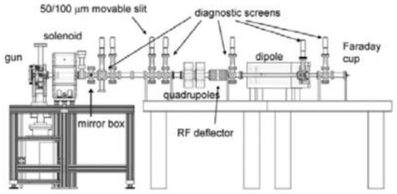
Shanghai



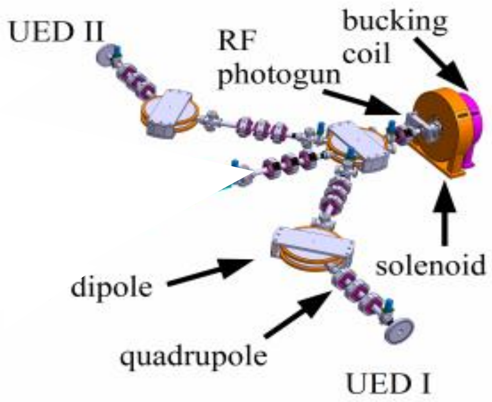
BNL



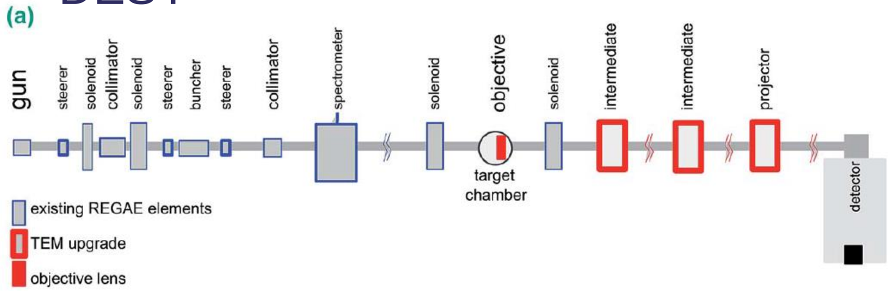
UCLA



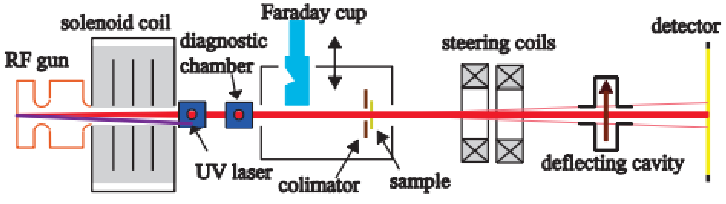
KAERI



DESY



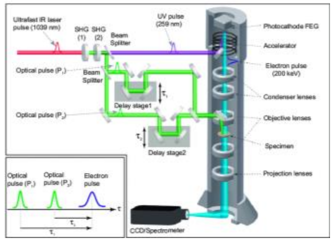
Tsinghua



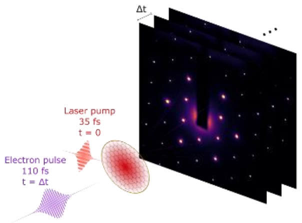
RUEDI

What Will Make RUEDI Unique?

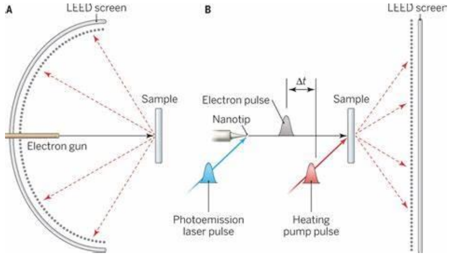
- **Combining MeV-UED with MeV UEM**
- Imaging dynamics with single electron precision
- Operando temp, pressure, liquid, mechanical, optical, full rotation
- Integrated AI for Low-signal image analytics
- **RUEDI Ecosystem (Hub and Spoke)**
- RUEDI Ecosystem combining main MeV instrument with smaller facilities at partner institutions around the country



keV-UEM

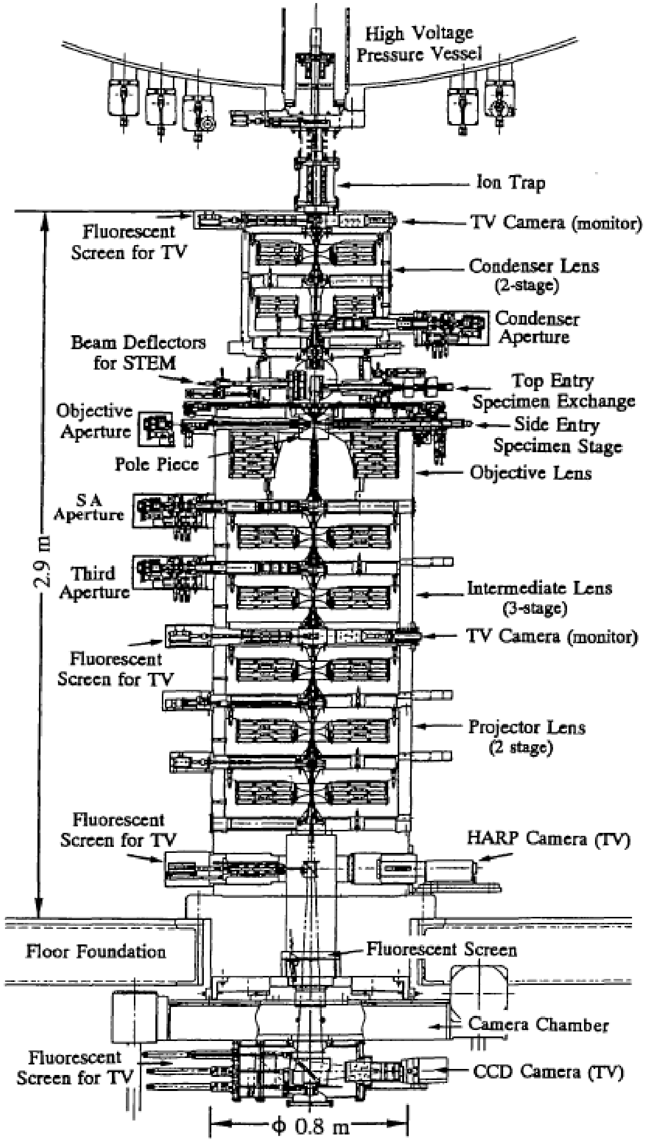


keV-UED



ULEED/ULEEM

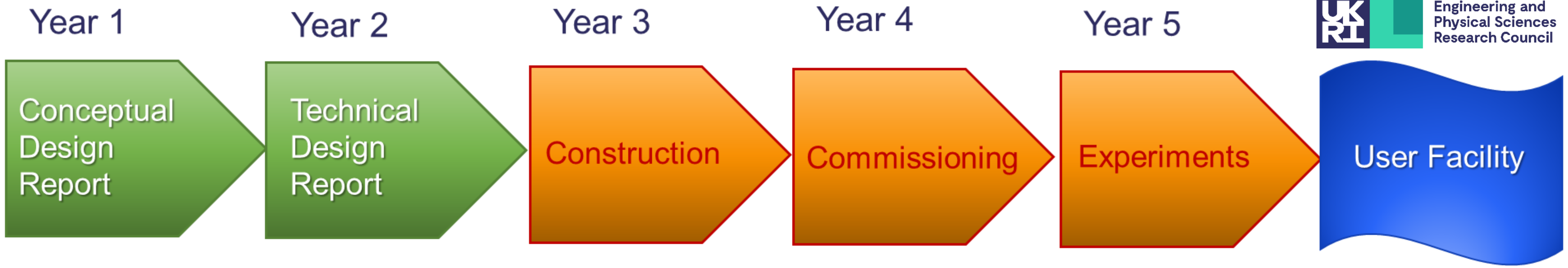
- Leveraging partners expertise in instrumentation, imaging, ultrafast methods, lasers, materials science, structural biology



MeV-TEM Osaka

Funding + Timescales

- UKRI Infrastructure Fund preliminary activity approved
- EPSRC National Facility
- Conceptual Design Report due end 2022
- Technical Design Report due end 2023



Engineering and Physical Sciences Research Council

- ~£40M, 3 year construction project starting in 2024
  - Awaiting next stage Infrastructure Funding

RUEDI

Leveraging UK Research Infrastructures

-the core team developing the facility

UNIVERSITY OF LIVERPOOL

The Rosalind Franklin Institute

UKRI Science and Technology Facilities Council
Daresbury Laboratory

The Materials Innovation Factory

Harwell Campus Hub

Cockcroft Institute

Negotiations underway to link access modes and research areas with national institutes and facilities

UKRI Engineering and Physical Sciences Research Council

RUEDI

RUEDI Organisation

RUEDI

Science Theme Meetings

- "Town Hall" meetings being arranged for each of the science themes
- More info and slides from past events on: http://www.ruedi.uk/events
- Scientific Summary Report on Energy Generation, Conversion and Storage to be uploaded soon
- Sign up to mailing list on website for updates on future events

Past events

2022-07-21 09:00 am

MATERIALS IN EXTREMES SCIENTIFIC THEME TOWN HALL EVENT

Materials in Extremes

Venue: **Cockcroft Institute, Daresbury, Cheshire**

2022-06-13

ENERGY SYSTEMS SCIENTIFIC THEME TOWN HALL EVENT

Ultrafast Energy Materials & Energy Storage

Venue: **Hope Street Hotel, Liverpool**

Coming up

In-vivo Biosciences, 26th September
Quantum Materials, September TBA
Chemical Change, September TBA

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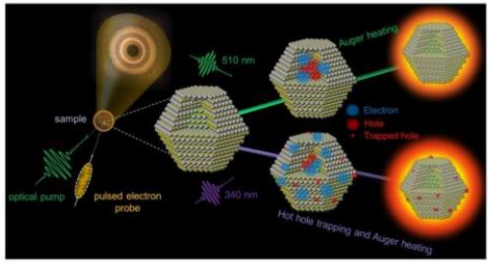
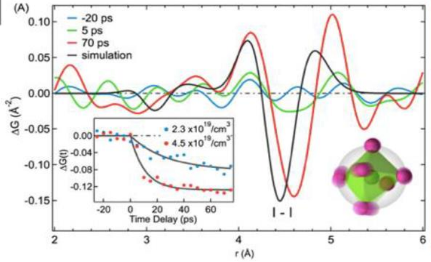
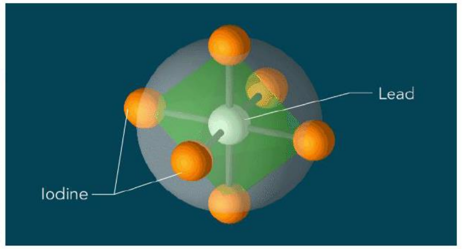
Projects from the Energy Town Hall

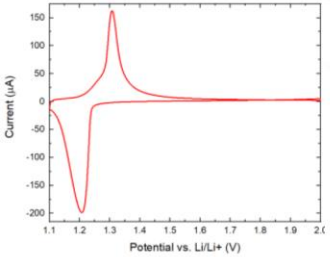
4 demonstration projects with wide-ranging applicability

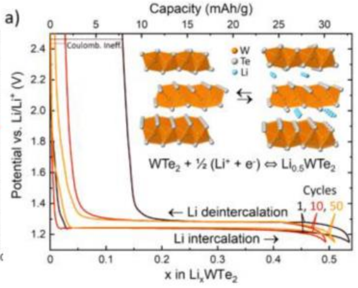
- Photocatalysis
  - Conversion efficiency across full reaction
- Hybrid Solar Cells
  - Optical absorption and defect formation
- Batteries
  - Degradation linked to transport at solid-liquid interface
- Glass Systems (nuclear)
  - Stability of structures under applied conditions

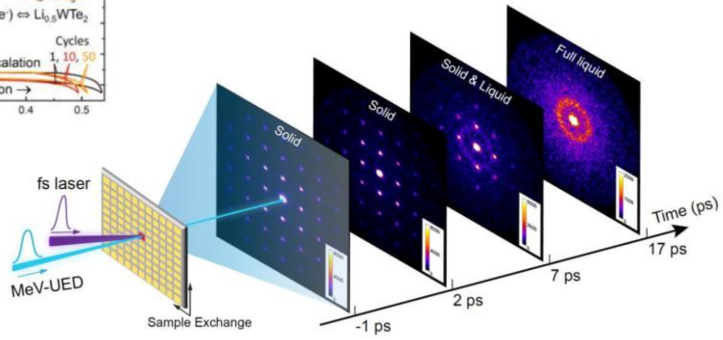






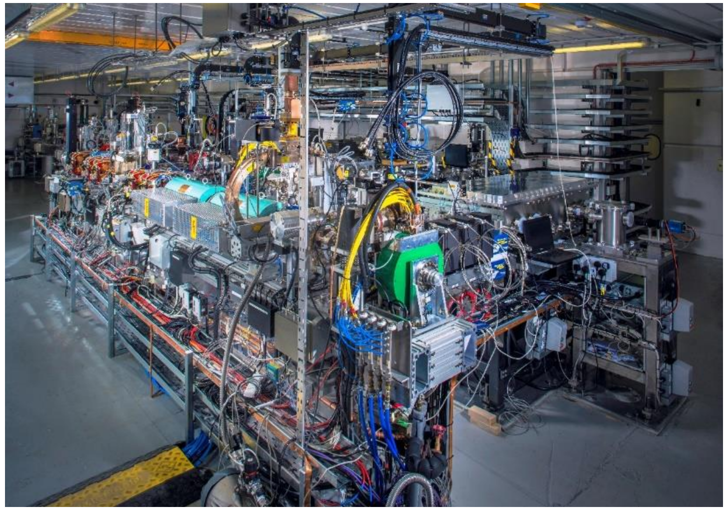


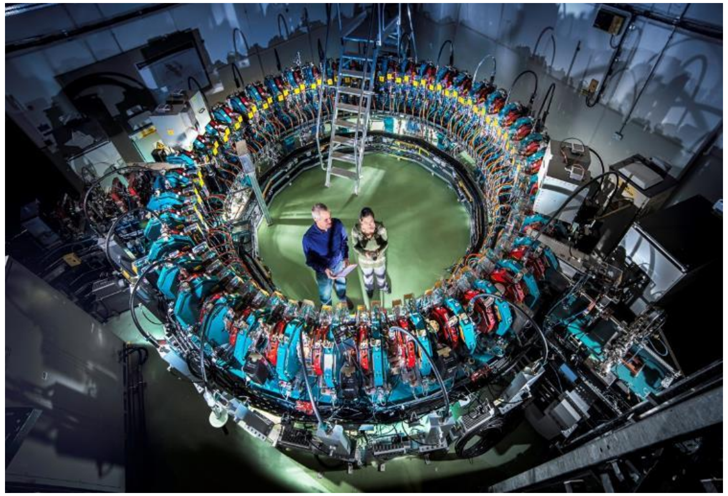




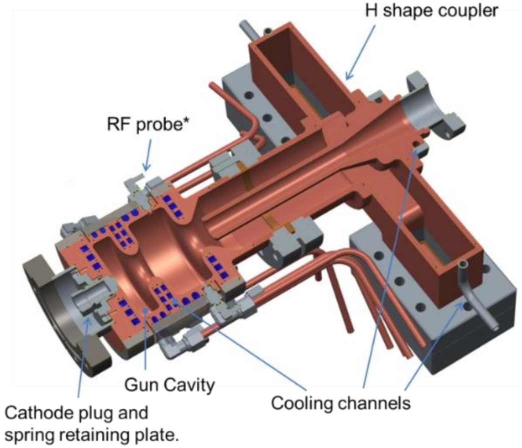
Leveraging STFC Daresbury Expertise

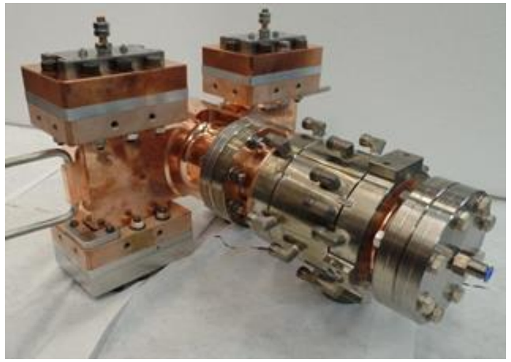
Design, build, and operation of particle accelerator facilities



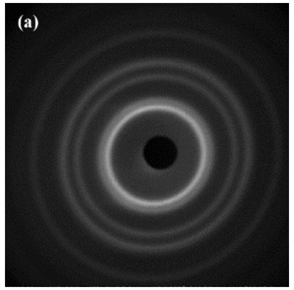


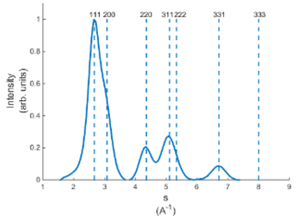
Femtosecond photoinjector development



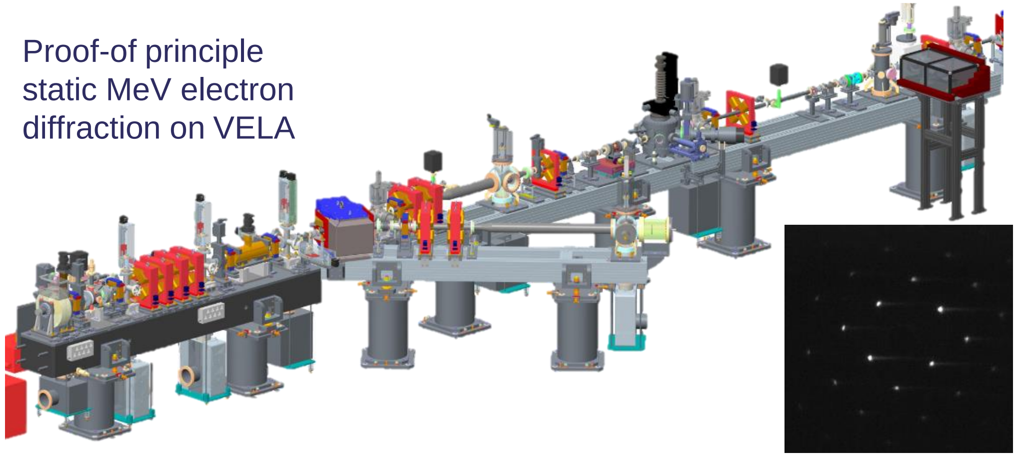


MeV ED experience





Proof-of principle static MeV electron diffraction on VELA



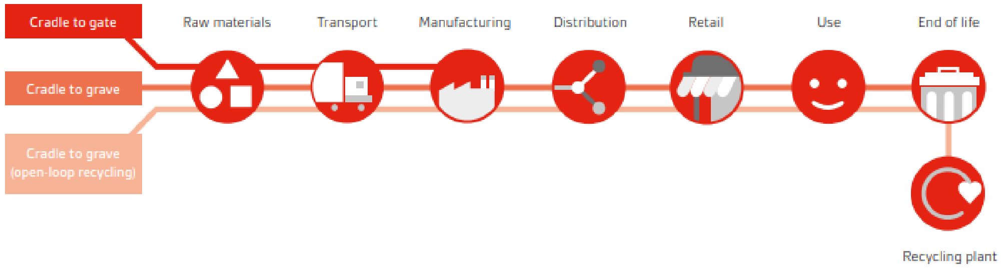
Instrument Design Principles

- RUEDI must be a reliable and robust user facility
- RUEDI should be a state-of-the-art facility as far as possible without compromising reliability
- RUEDI should measure key parameters shot-by-shot and make them available to users as far as reasonably practical
- The RUEDI design should leave scope for upgradability
- RUEDI should strive to be an environmentally sustainable facility

Sustainability: Accelerator Impact Review – Lifecycle analysis

ASTeC Sustainable Accelerators Task Force

- Detailed review of the climate impact of accelerator activities
- Where are the Big Sources of emissions?
  - Manufacturing? Steel / Copper / Aluminium / Concrete
  - Operations? Running RF and magnet systems. Cooling & AC
  - Disposal? End of life of components
- How could we reduce these for the biggest impact?
  - Using different materials
  - Smart powering schemes
- RUEDI is our ‘model facility’ for this exercise
- Consider wider applicability for other accelerators too
- Figure of merit should be $kgCO_2e$ per “delivered unit”
  - So at the end, we should have a database listing carbon emissions for components in every area
- Look at the big picture; **not** every gram of CO_2 - not a bean-counting exercise!



Modes of Operation

#	Purpose	Electron beam energy	Electrons per bunch	Temporal resolution	Spatial resolution	Spot size
1	**Imaging** *(higher resolution)*	2 MeV	10^6	Few ps	<1nm	
2	**Imaging** *(ultra-fast)*	2 MeV	10^6	<800 fs	~10nm	
3	**Diffraction**	4 MeV	10^6	100 fs		100um
4	**Diffraction** *(low-charge)*	4 MeV	10^4	10 fs		10um
5	**Diffraction** *(Streaking*)*	4 MeV	10^7	10 fs		100um

**streaking mode is single-shot, time-resolved, where the time information implanted onto transverse plane via a deflector/streaker*

Range of pump laser wavelength/durations/intensities

All modes limited to 100Hz repetition rate *(with potential future upgrade to 1kHz)*

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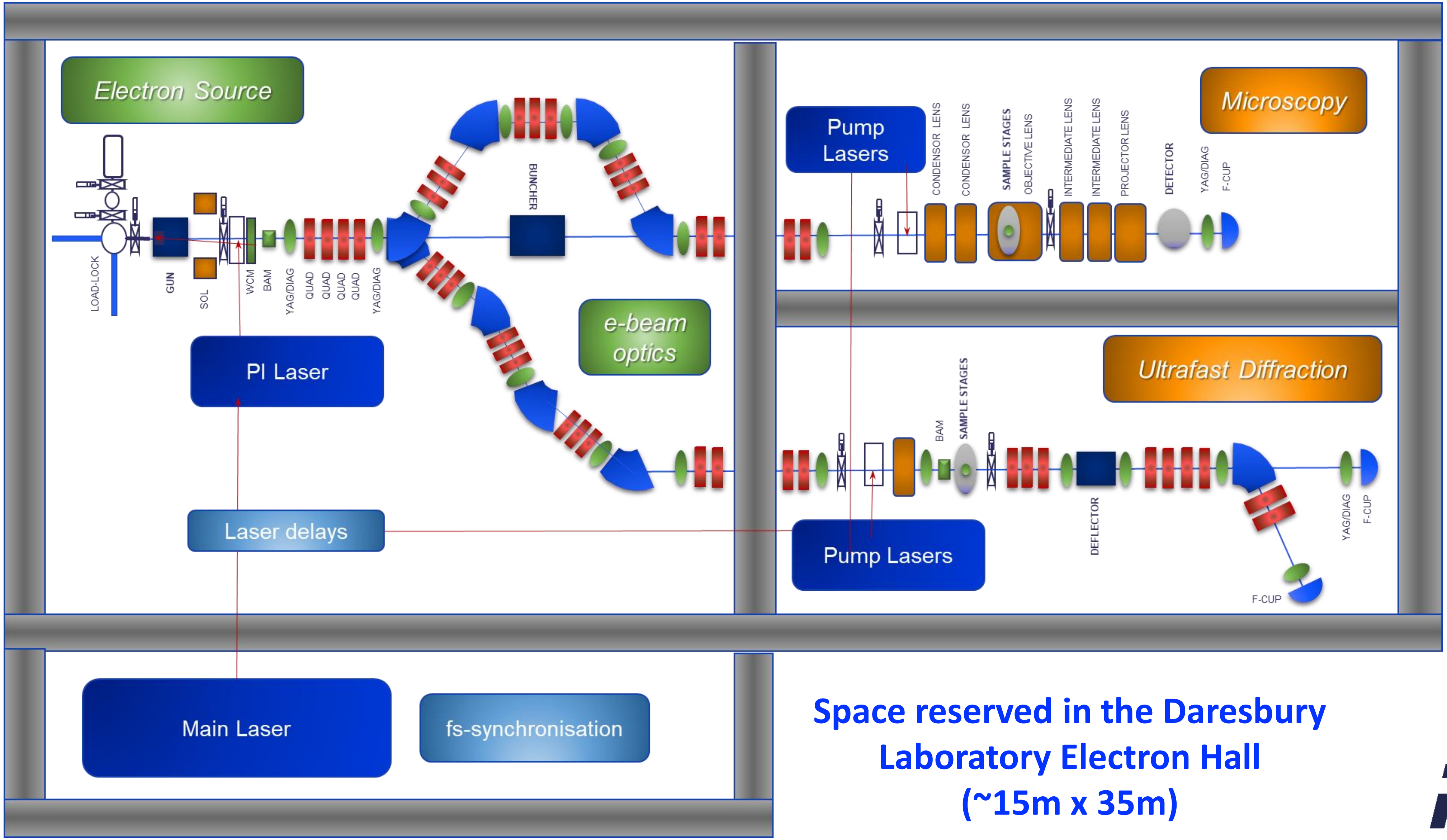
RUEDI Schematic v2.0



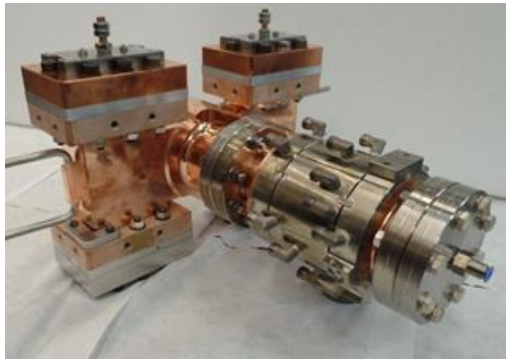
Design options to be studied and presented in CDR

Space reserved in the Daresbury Laboratory Electron Hall (~15m x 35m)

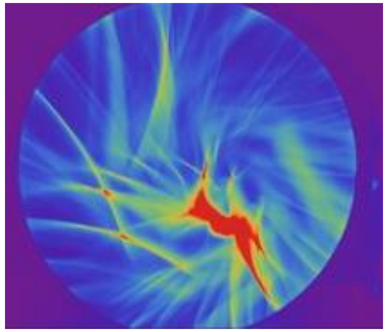
RUEDI

Electron Gun

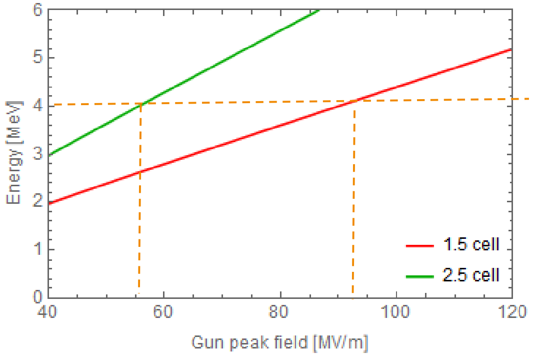
- S-band normal conducting RF gun
- Experience from CLARA design
- Dark current the main issue
  - Potentially larger charge than photoemitted beam!
  - Can swamp, interfere and distort images
- Design changes to lower dark current
  - Increase from 1.5 to 2.5 cell gun, lower field for same beam energy
  - No cathode interchange to reduce high field areas which produce more DC
  - Overcoupling for shorter RF pulse



CLARA gun



Dark current



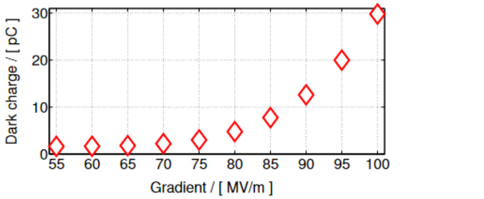
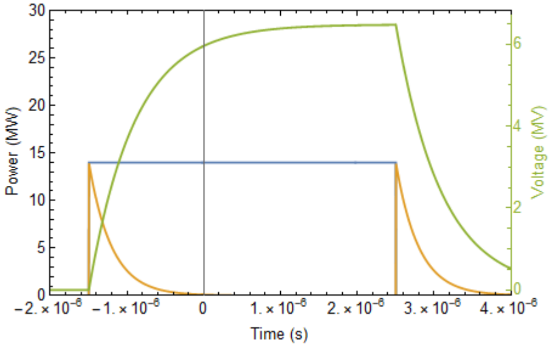


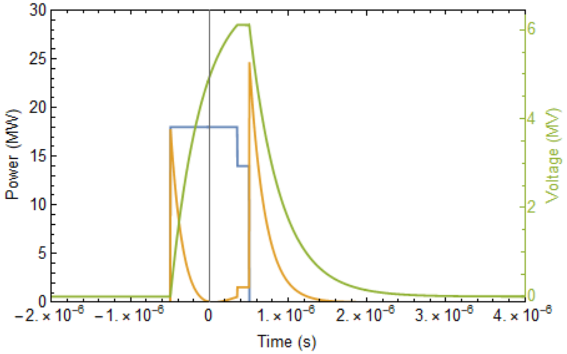
Figure 1: Measured dark charge vs. gradient for a 4.8μs long rf pulse at REGAE.

Normal coupling



Steady state after ~2.9 µs

Over-coupling



Steady state after ~ 0.8 µs

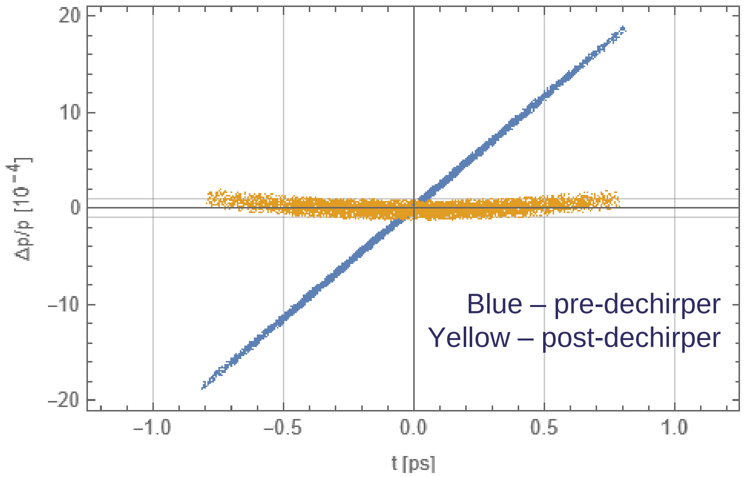
Electron Beam Transport - Microscopy

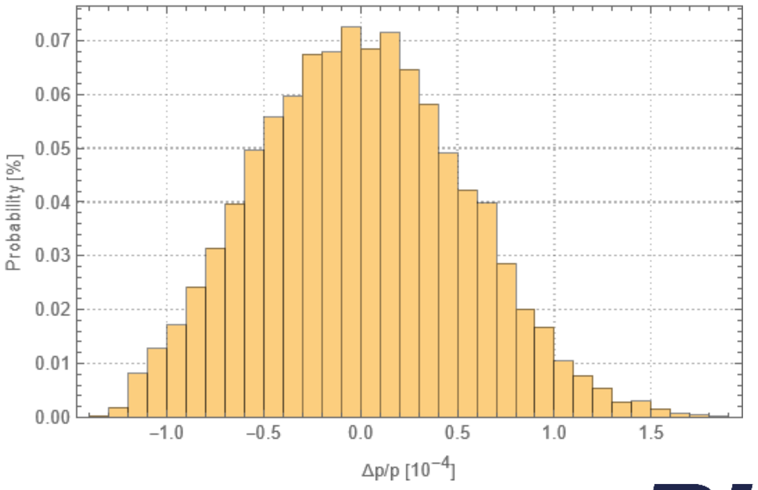
- Resolution limits:

$$d = \sqrt{(\lambda/\beta)^2 + (C_s\beta^3)^2 + (C_c\beta\delta\gamma/\gamma)^2}, \qquad (1)$$

where β is the objective aperture collection semiangle and $\delta\gamma/\gamma$ is the relative beam energy spread.

β ~ 1mrad
Cs ~ 10mm, spherical aberration coefficient
Cc ~ 10mm, chromatic aberration coefficient
For 1nm resolution, need <10^{-4} relative energy spread

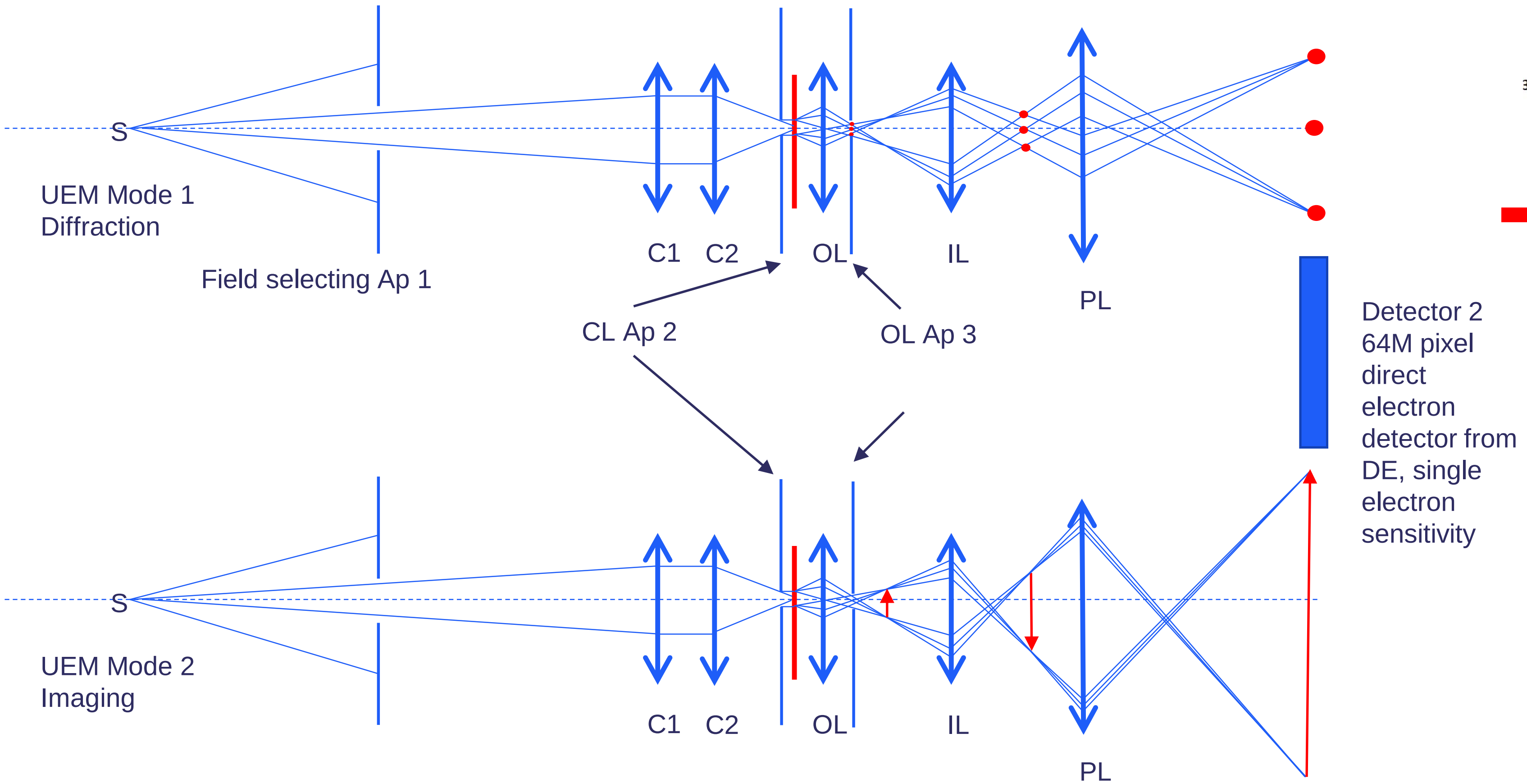




- Possible energy filter in chicane/alpha/omega magnet
- RF dechirper cavity
  - Also used to decelerate from 4 to 2 MeV

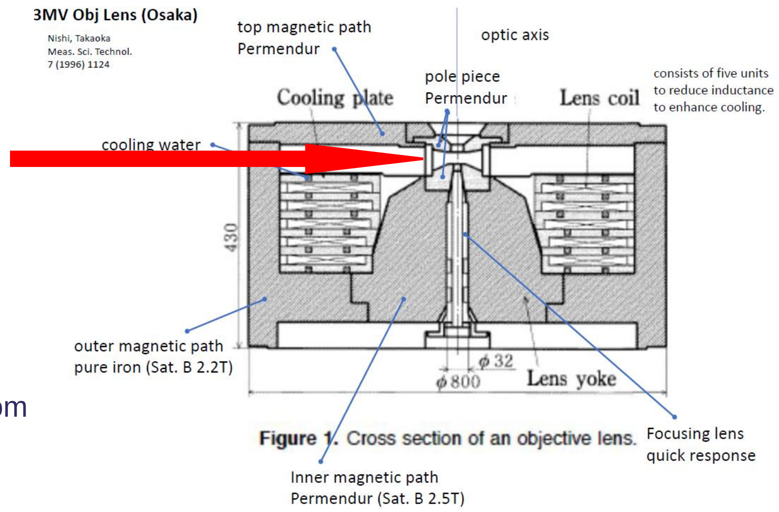
(1) Li & Musumeci, Phys. Rev. Applied, **2**, 024003 (2014)

Imaging Lens Design



Round lenses/quadrupoles/deflectors – emittance, astigmatism, aberrations, pulse broadening

Objective lens is the key to whole system



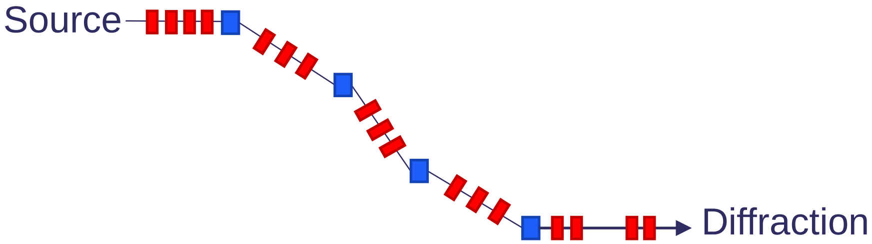
Samples inserted into middle of magnet (red arrow)

Consultation with leading EM producer – round lens saturates at ~ 2 MeV

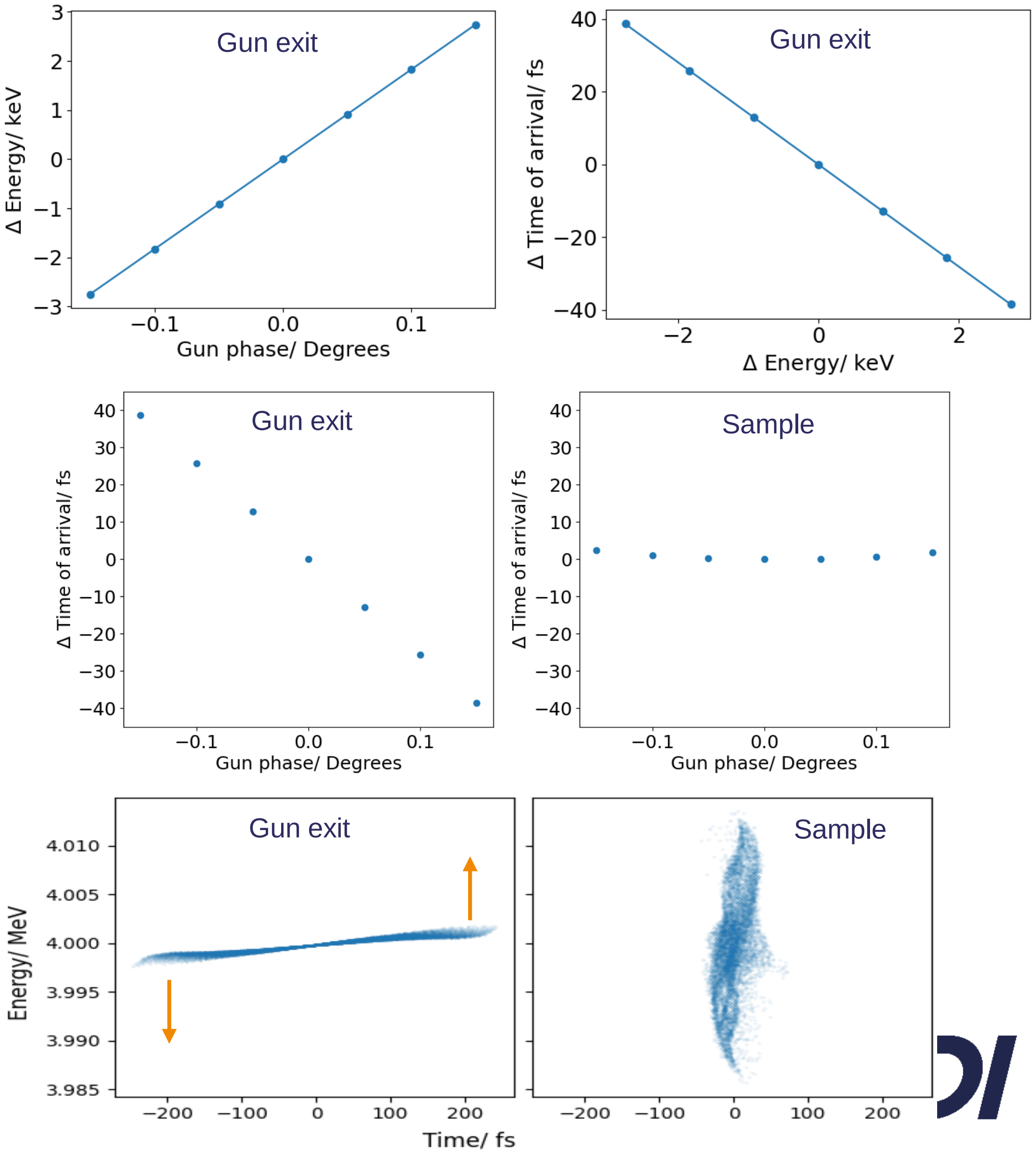
RUEDI

Beam Transport - Diffraction

- Aim to provide ultrashort bunches with small time of arrival jitter

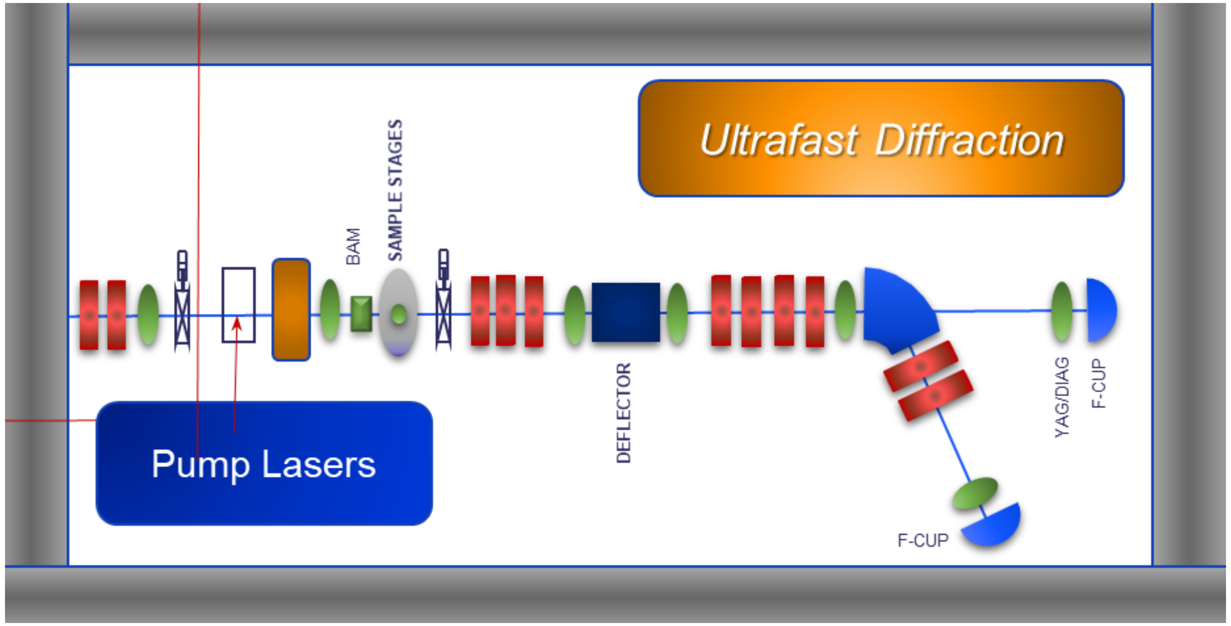


- Laser to RF timing jitter leads to time of arrival jitter at the exit of the gun
- We can tune the R56 of the magnetic transport line to cancel this initial timing jitter at the position of the sample
- The space charge forces will change particles energy along the bunch, allowing them to be compressed with the same R56

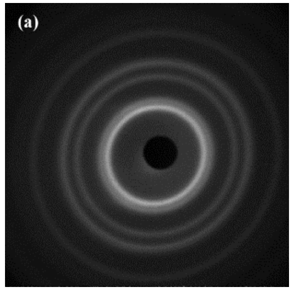


Ultrafast Diffraction Beamline

- More general purpose sample chamber to take same sample stages as imaging beamline, full goniometry, solid, liquid, gases, cryogenics
- Cavity based Beam Arrival Monitors
- Bunch length monitoring via RF Transverse Deflecting Cavity + THz

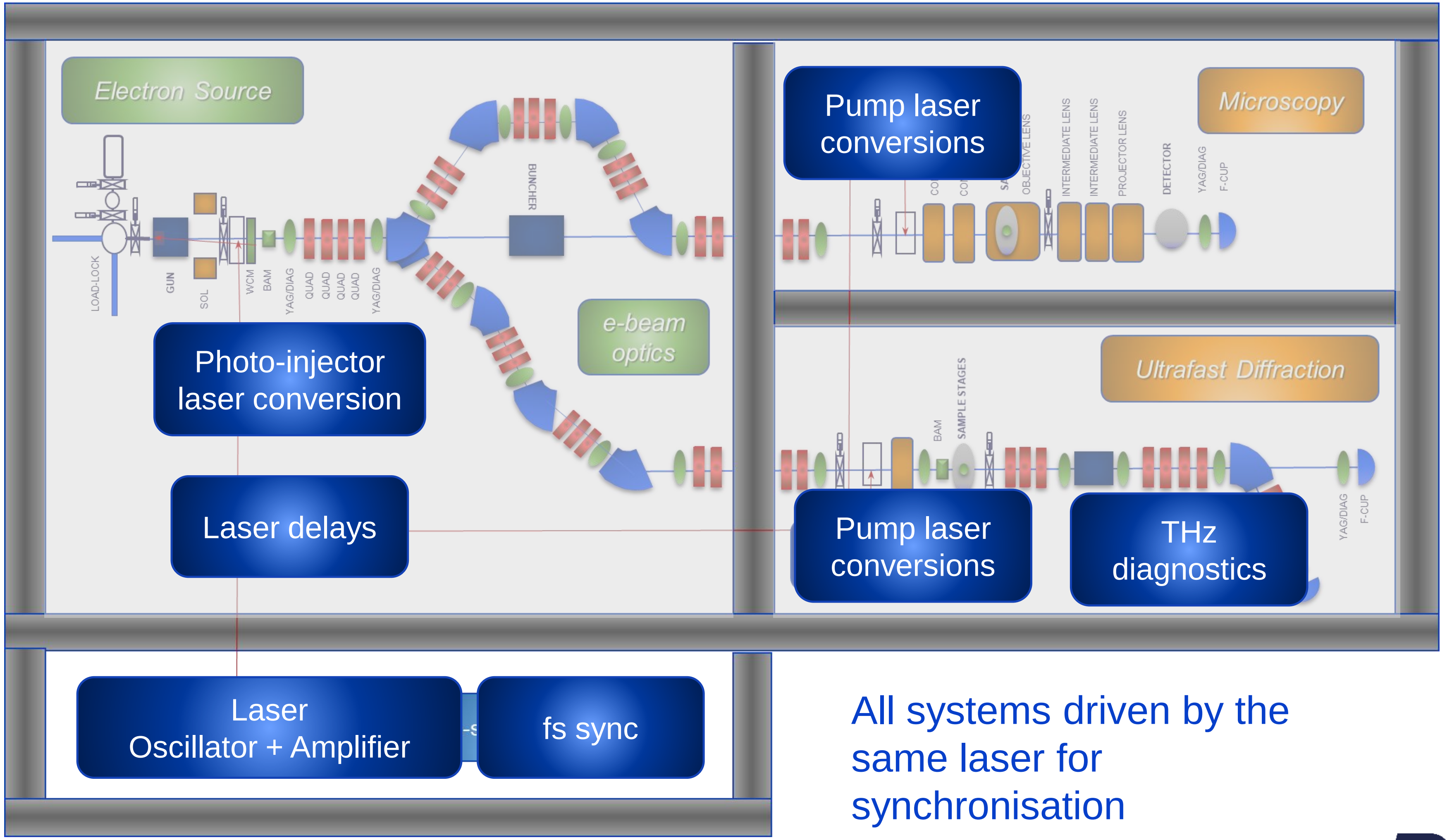


- Option for detector with hole to allow shot by shot measurements on non-diffracted beam



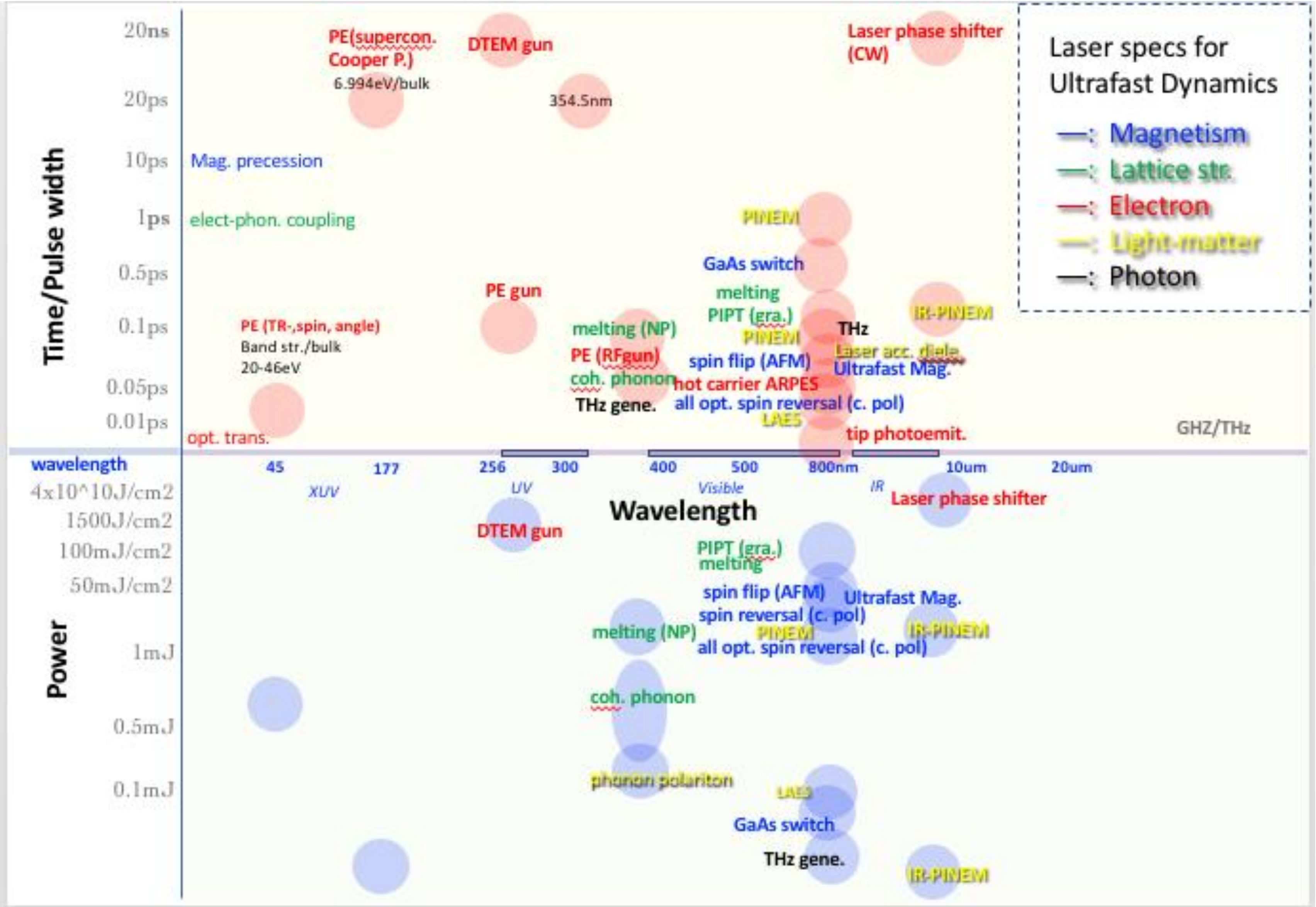
RUEDI

Laser system outline



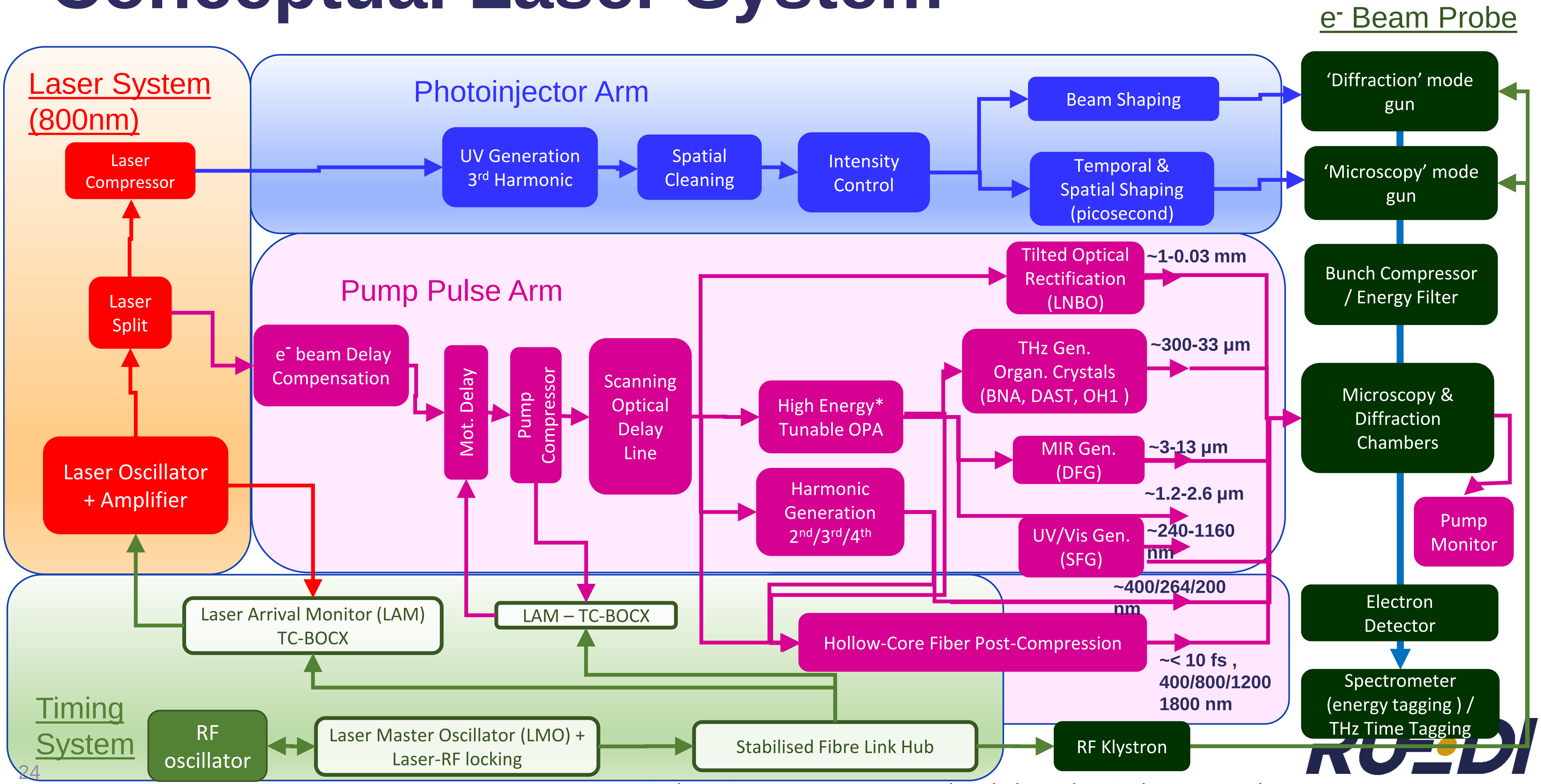
All systems driven by the same laser for synchronisation

Ultrafast dynamics vs Pump laser parameters



Some examples, doesn't cover all applications!

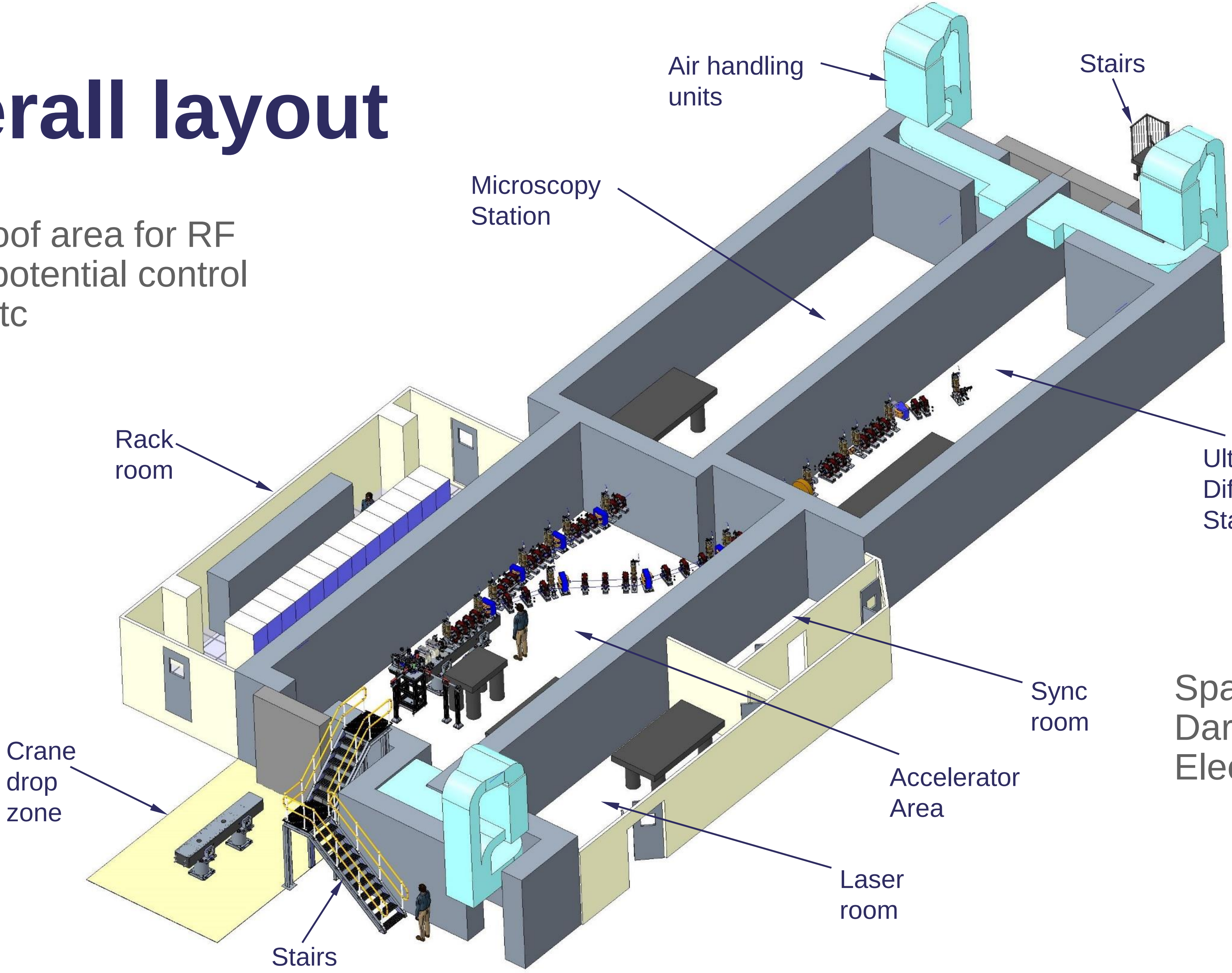
Conceptual Laser System



LAM: Laser Arrival Monitor, TC-BOCX: Two-Colour balanced optical cross-correlator

Overall layout

Utilise roof area for RF rooms, potential control rooms etc



Space reserved in Daresbury Laboratory Electron Hall

RUEDI

Summary

- 2-year design process underway
  Funding by UKRI Infrastructure Fund
- CDR to be published at end of this year
- 5 Science Themes cases progressing:
  - Dynamics of Chemical Change
  - Materials in Extremes
  - Quantum Materials & Processes
  - Energy Generation, Storage and Conversion
  - In Vivo Biosciences
- Visit www.ruedi.uk for more info

RUEDI

Acknowledgements

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- Will Bryan
- Simon Maskell
- B. Layla Mehdi
- Sven Schroeder
- Carsten Welsch
- Oznur Apsimon
- Gwyndaf Evans
- Dwayne Miller

- Ian Robinson
- Jasper Van Thor
- Lee Kelsall
- Alberto Acuto
- and more…

- Tim Noakes
- Mike Ellis
- Jim Clarke
- Boris Militsyn
- Alan Wheelhouse
- Mark Roper
- Nirav Joshi
- Yuri Saveliev
- Clive Hill
- Graham Cox
- Rachael Buckley
- Ben Hounsell
- Joe Crone
- Hywel Owen

- James Jones
- Bruno Muratori
- Omair Ghafur
- Storm Mathisen
- Tom Pacey
- Louise Cowie
- Russell McLean
- Anthony Gilfellon
- Andy Moss
- Conor Jenkins
- Ed Snedden
- Ben Shepherd
- Frank Jackson
- Tom Jones

- Mitchell Kane
- and more…

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Thank you for your attention!

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