Scientific Computing

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STFC Facilities

Ada Lovelace Centre

Harwell and Daresbury Campus
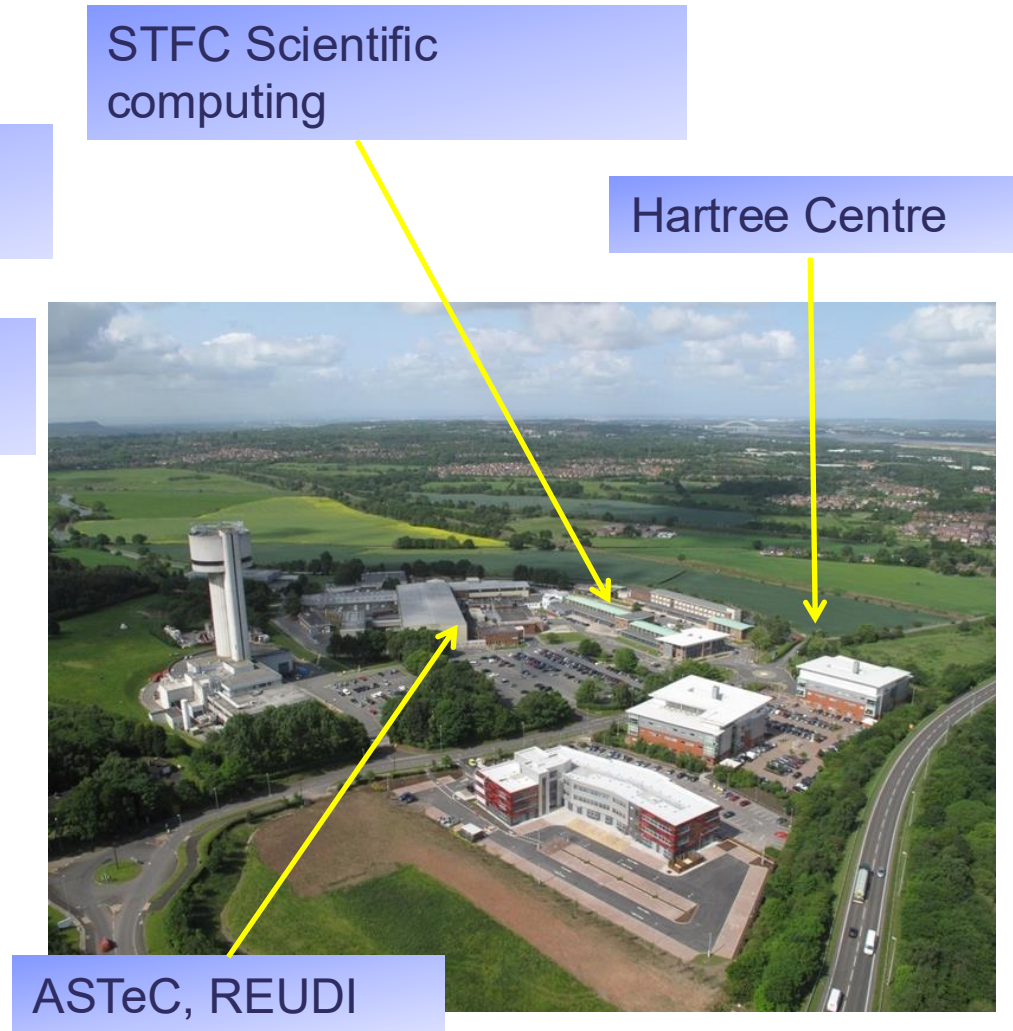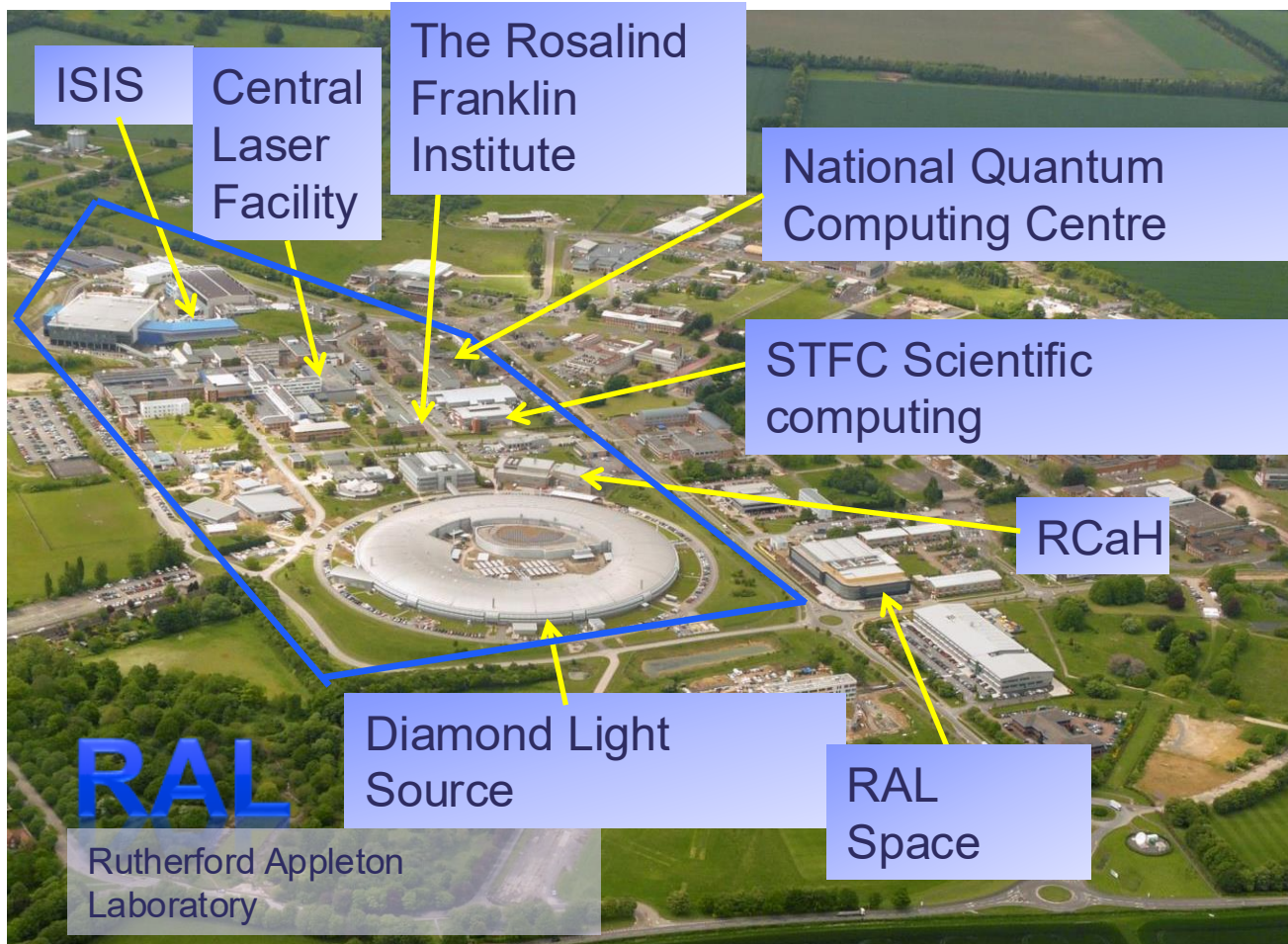
- 5 laser labs, each with an array of instruments
- 35 X-ray instruments, 10 electron microscopes
- Over 30 neutron and muon instruments
- Each focused on a different science areas
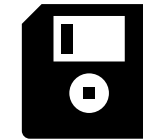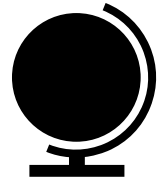- Each having different analysis needs

Annual Throughput

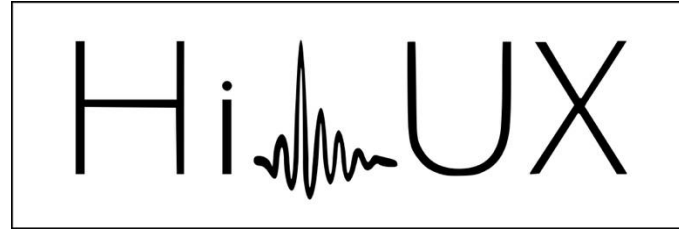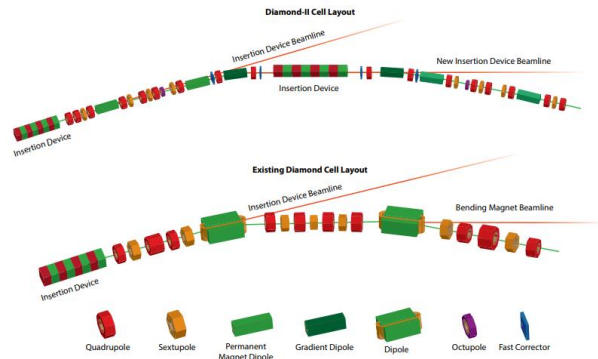| 2500 experiments | 8000 researchers | 1500 Publications | 18 Pb stored | 30 Countries |

New Facilities and Upgrades

UK XFEL

CLF HiLUX upgrades to Ultra and Artemis

CLF-EPAC
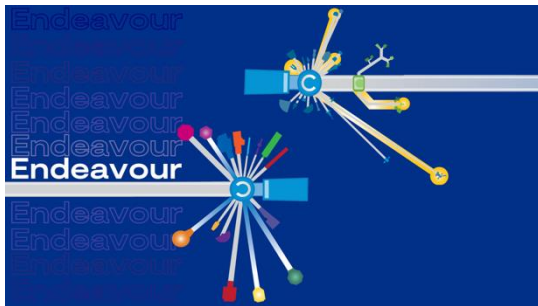

PetaWatt laser and X-ray source

Diamond-II - - Diamond Light Source

- x10-100 fold increases in power, flux, brightness
- Diamond "dark period" 2028 – 18 months
- Faster Timescales
- New instruments/techniques

ISIS The Endeavour Programme (stfc.ac.uk)

Relatvistic Ultrafast Electron Diffraction & Imaging

Experiment Life
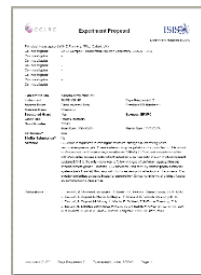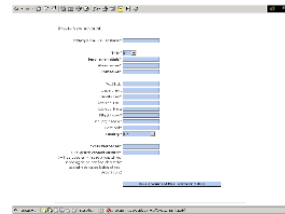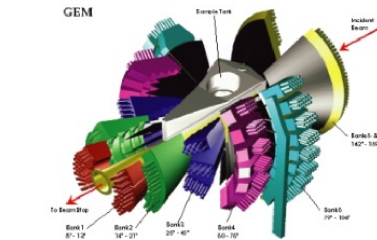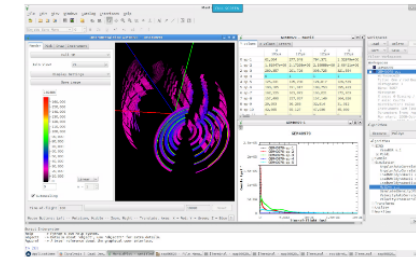
Activity Streams

Facilities adapting IRIS to their user needs

Supporting researcher projects

Ada Lovelace Centre

To expand use of advanced tools

Increase impact

Science and
Technology
Facilities Council

Ada Lovelace Centre

Highlight – IRIS supporting discovery

XChem

Fragalysis platform

Fragment screening for drug discovery
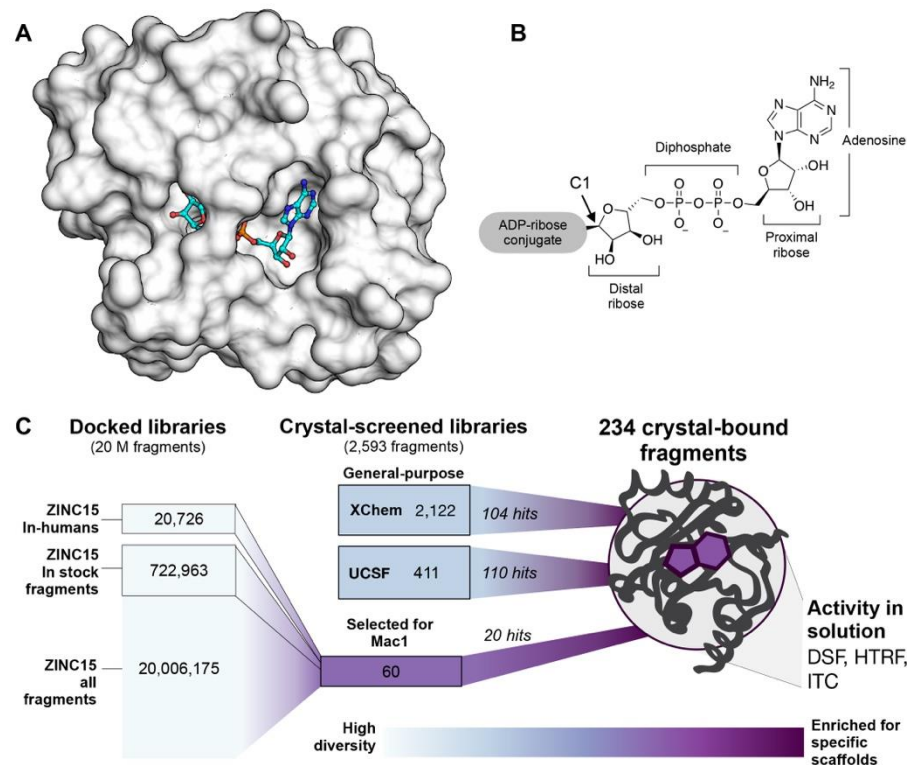
2025 - Openbind

Sovereign AI flagship
Professor Charlotte Deane of the University of Oxford said:
OpenBind realises a major gear-shift for AI in drug discovery by investing in the data that powers it.

Moonshot Project

Covid Moonshot was a global open-science project started in 2020 with the aim to develop a safe, globally accessible and affordable antiviral pill for Covid-19

UK RI Science and Technology Facilities Council

Ada Lovelace Centre

Science Advances DOI:10.1126/sciadv.abf8711

Outlook

- **A lot of exciting impact**

- Refine the platform offering – an integrated discovery platform (moving data, workflow standards, Slurm, VM's , AI tools, notebooks)

- "Next year we need 10x more" – IRIS flexibility is a big plus
  - Models of how we use data/compute changing
  - New tools and user communities
  - Varying role of AI

- Positioning, Redundancy and Service level
  - Experiments are short and access is limited
  - Drive for automation and *in-experiment decisions*

Questions

- What IRIS enabled you to achieve?

- In the next 2-3 years, which capabilities should IRIS prioritise to unlock the biggest step-change for you?

- How can we better capture impact of IRIS on your community?

Questions

- How do you balance diverse projects with competing priorities, and what allocation/charging/accounting approach best reflects real value?

- Which capabilities should be standardised across projects (identity, data management, workflow orchestration, observability), and where is bespoke unavoidable?

- How are you measuring and reducing energy/carbon impact without reducing scientific output?