Scientific Computing

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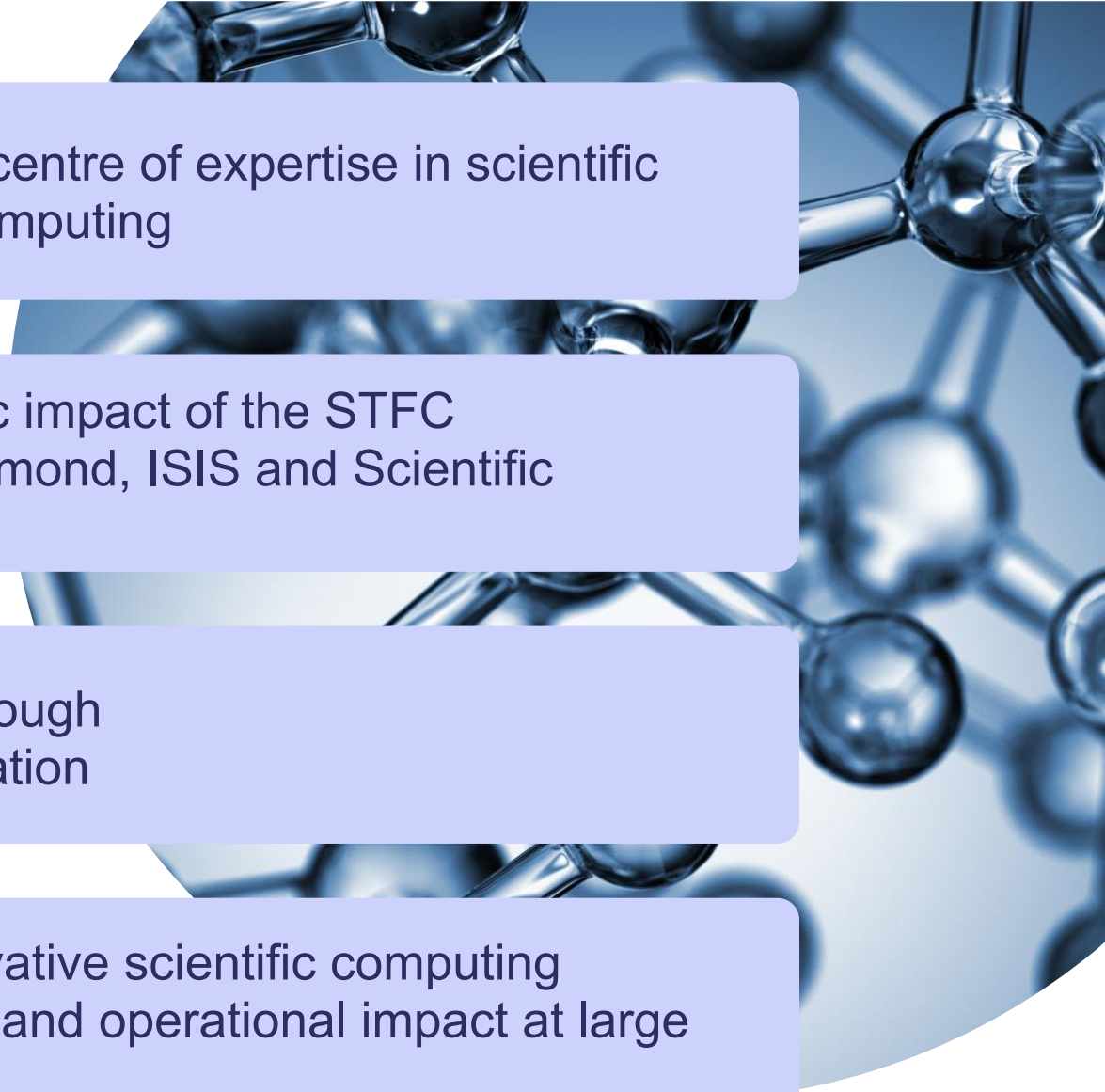
ALC overlap with IRIS

Scientific Computing



Ada Lovelace Centre

A centre of expertise in scientific computing

Purpose

To maximise the scientific impact of the STFC large facilities – CLF, Diamond, ISIS and Scientific computing

Vision

Transformative impact through challenge-driven collaboration

Mission

To create and deliver innovative scientific computing solutions to drive scientific and operational impact at large facilities.

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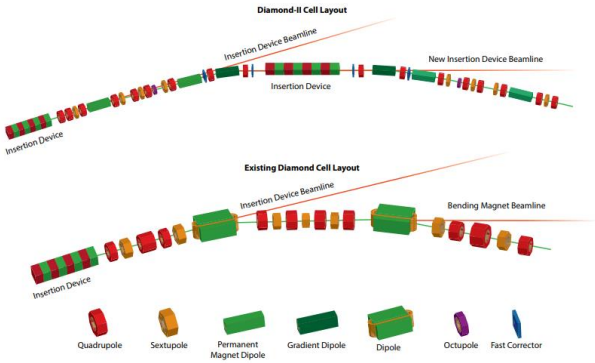
New Facilities and Upgrades

UK XFEL

CLF HiLUX upgrades to Ultra and Artemis

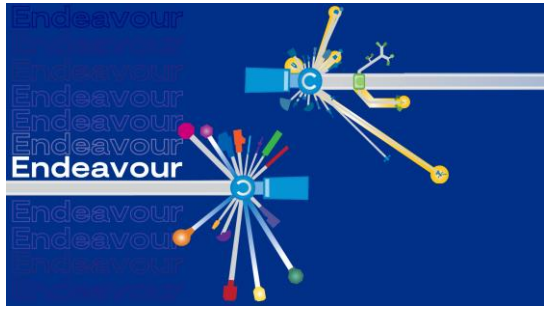
CLF-EPAC

PetaWatt laser and X-ray source



Diamond-II - - Diamond Light Source

- x10-100 fold increases in power, flux, brightness
- Faster Timescales
- New instruments/techniques



ISIS The Endeavour Programme (stfc.ac.uk)

RUEDI

UK Research and Innovation

Relativistic Ultrafast Electron Diffraction & Imaging

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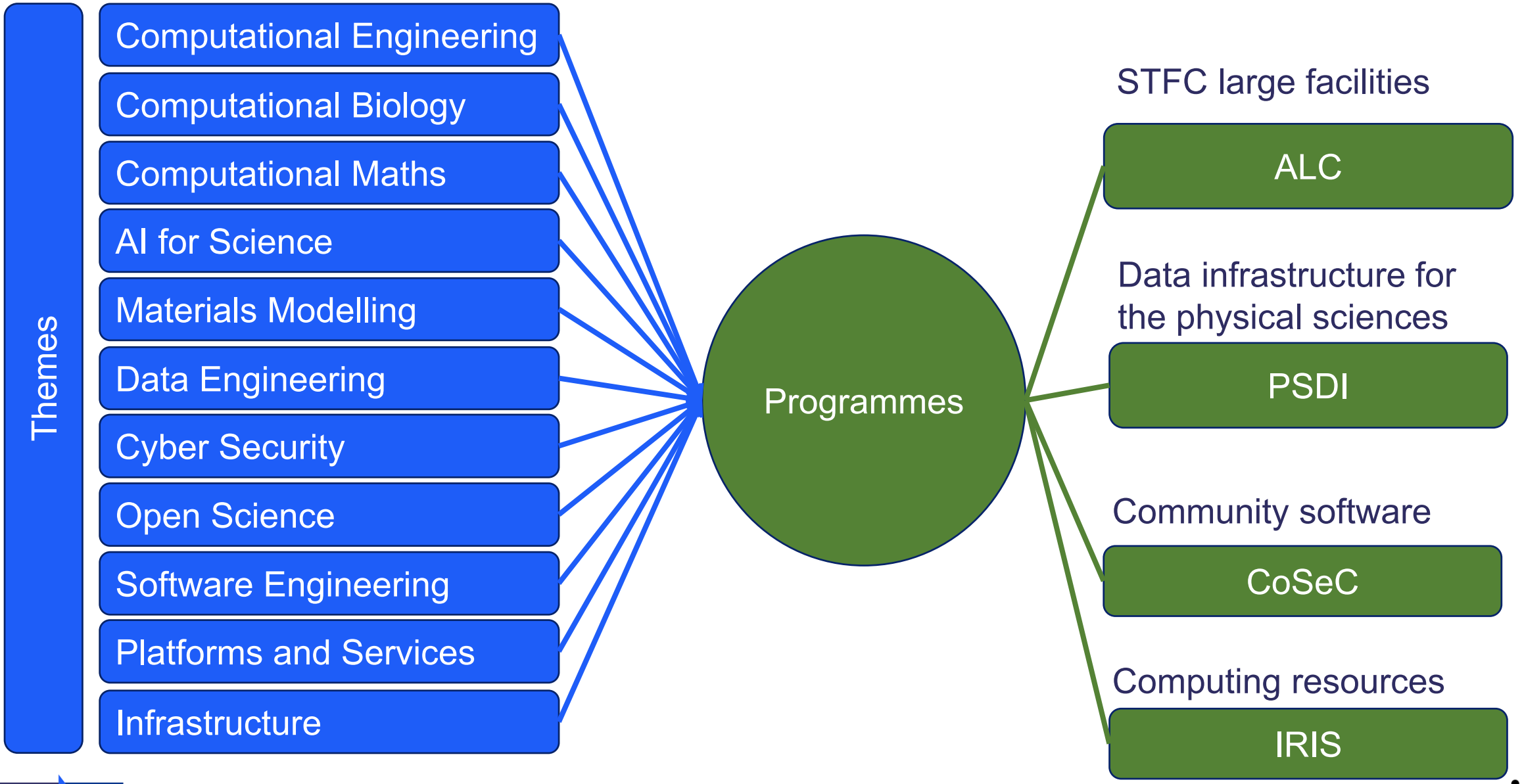

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ALC Themes\Strengths

Strengths of ALC/ STFC Scientific Computing and the facilities

- Advanced Imaging
- Computational biology
- Combination of facilities and overlaps in activities

Strengths of ALC/ STFC Scientific Computing

- Theory and Simulation
- Mathematics and AI for science and technology
- Big Data - Platforms and services for the facilities data lifecycle

What scale is ALC currently ?

Theme / Area	FTE
Modelling & Simulation	10
Imaging	5
Computational Maths	7.5
AI	10
Computational Engineering	3
Computational Biology	9
Data & Software Engineering	6
RSE Team	4
Data Analysis as a service	10
ALC Management & Governance	3.1

From an initial 20 FTE in 2022
Support 10 Joint PhD projects per year
Pilot, Responsive and Programmes modes
Training under development

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From Responsive Projects to Programmes

- Seeking to develop challenge led programmes
  - Engaging with facilities
  - Bringing multiple disciplines to bear on a challenge

- Bridge across activities on site
  - Ptychography (ISIS, RFI, CLF,DLS), Tomography (ISIS,DLS,CLF)
  - Data management infrastructure
  - Materials modelling

- Set directions
  - We can’t simply be responsive or wait for facilities to decide to do something

ALC – transitioning to a programme

- Deliver an AI and maths driven transformation
- Enhance science and operations with simulation
- Challenge led imaging
- Cross-cutting computational biology
- Platforms and services for scientific computing delivery

Example – Integration of simulation

- **Identified key CLF user groups and problems**
- **Projects – Artemis/ULTRA scientists and users**
  - Ultrafast dynamics of polarons in TiO_2
  - Ultrafast electron-ion dynamics for 2D materials
  - Ground state simulations of molecules and solvent after photoexcitation (vibrationally hot)
  - DFT for electrochemical interface

- We had no previous activity with CLF in this area
  - We need to prototype the tools
  - Train the users and scientists
  - Deploy a user-friendly interface
  - Transition to facility

ALC and IRIS

- IRIS provides the computing foundations for ALC

- Over 50 facilities projects with expanding needs for compute and storage
  - Greater use of materials modelling and engineering simulation
  - Expanding use of AI (more training)
  - Resolving bottlenecks – (automation and workflows)
  - Prototyping and Research and Development (pre-cursor steps for above)
  - Delivery platforms

- ALC expertise as a service
  - Help user groups who can't analyze their data or have a problem
  - Training user community in the new tools, workflows developed by ALC

ALC and IRIS

- What challenges do the projects face ?
  - Moving/Restoring data to the compute resource
  - Shared data or a workspace
  - Shared access
  - Collaborative computing

- Example – for a Diamond project it takes about the first 2 months to sort out access, data and compute environment.
- If we had project configurations- (space, VM with software, and resource etc.) it would potentially make collaboration much more effective - > IRIS
- Our services need to be more integrated (DAaaS, Data Gateway)

Questions

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