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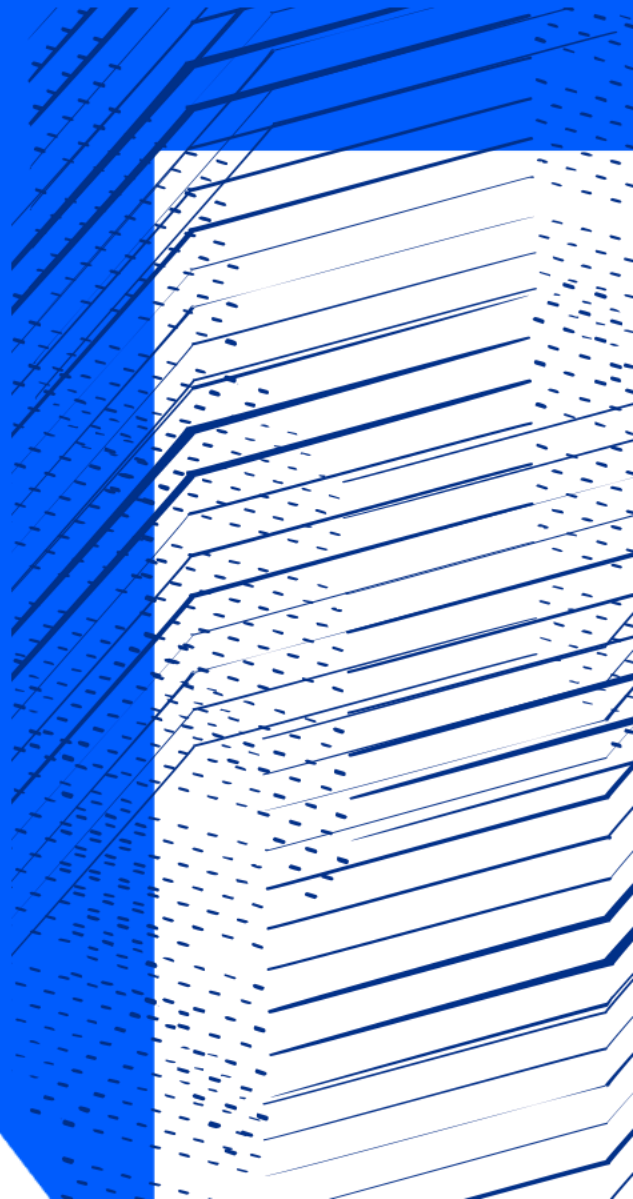
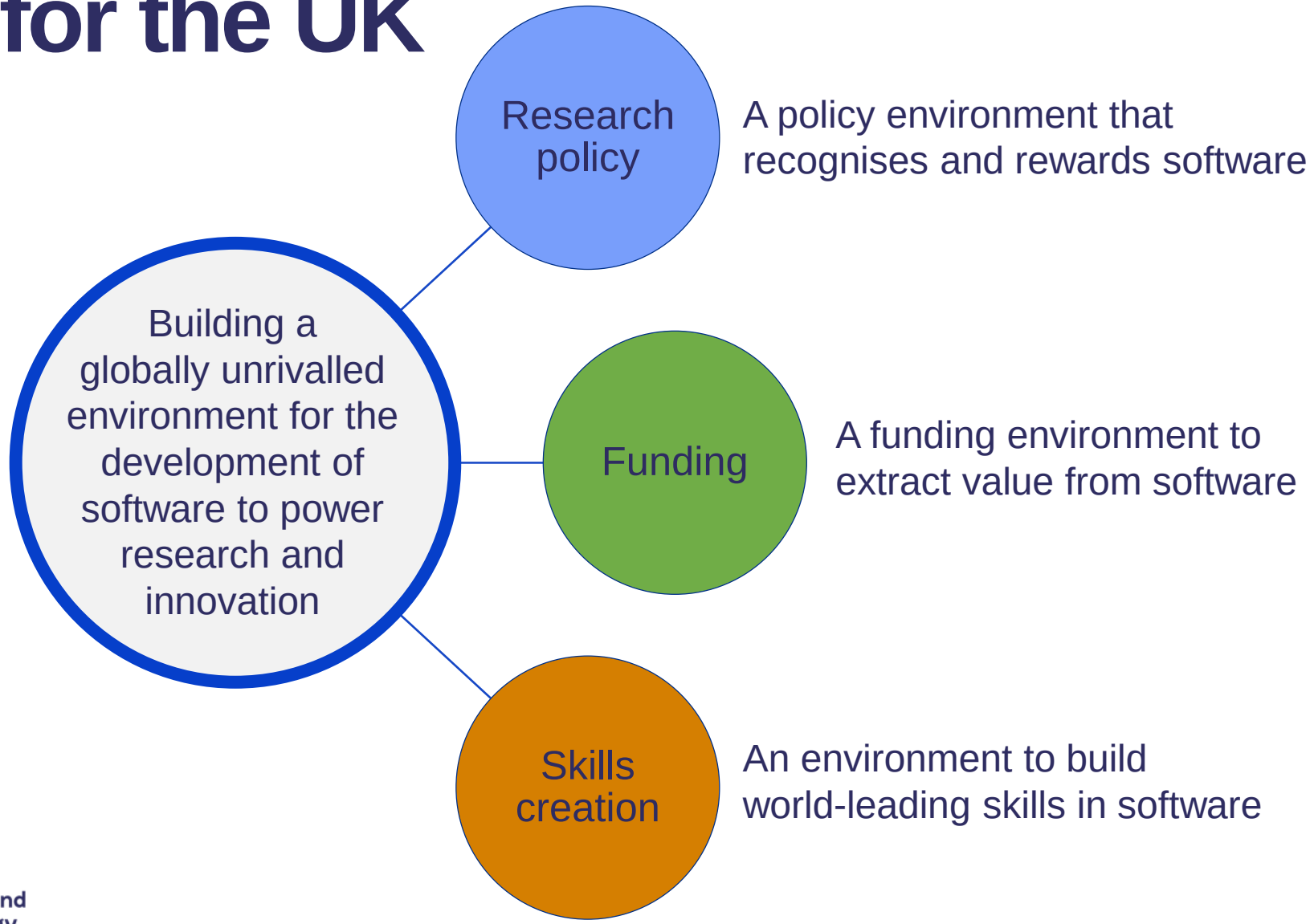
White paper on software, skills and training

Editors: Simon Hettrick, Alys Brett
Authors: Alys Brett, Neil Chue Hong, James Hetherington, Simon Hettrick, Barbara Montanari, Christopher Woods



Vision for the UK



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Total budget: £615M

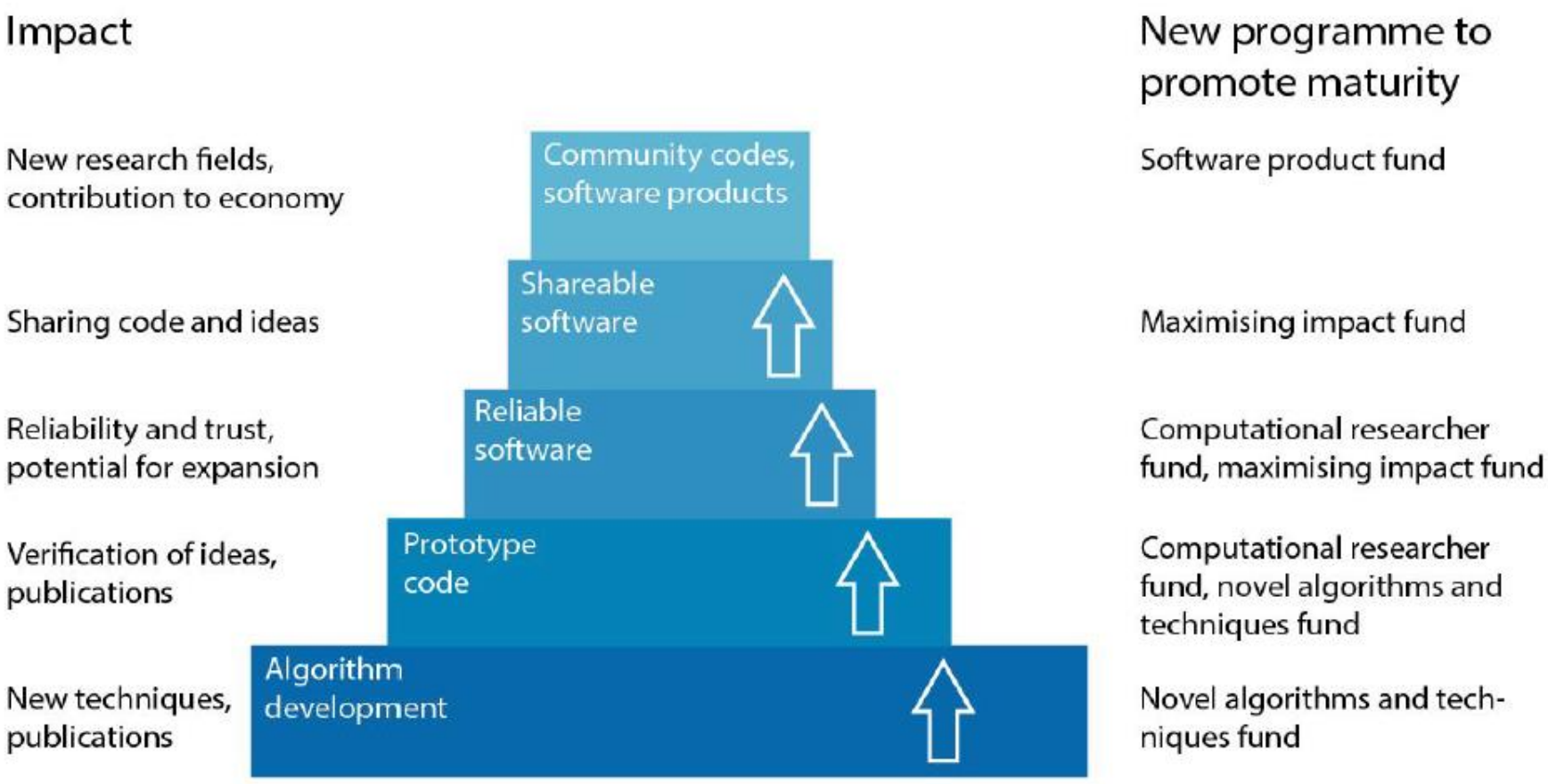
The Rationale for Software

- Hard to envisage any research that will not need software over current decade
- Research reproducibility relies on high-quality software
- Software encapsulates knowledge

Also:

- Software drives value extraction from investments such as hardware, instrumentation, researchers' time, …
- Embodiment of methods and algorithms, including AI, is software
- Data pipeline relies on software (from instrument control to publication)
- Even this presentation was done by software! (very "meta" of me…)

Software Lifecycle



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Challenges

- Software is highly diverse
- Current research evaluation practices do not recognise software adequately
- Software needs to be funded according to its infrastructure nature
- Software is intangible and its essential role often goes unnoticed
- Software needs an army of specialised and dedicated people, driven by research but focused on the software as an infrastructure, for development, maintenance, porting, user training and support, etc.
- The rapid pace of research and technology requires a constant updating of skill and expertise as well as the nourishment of close relationships among software engineers, methods and algorithm developers, researchers, hardware and data experts, etc.

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Recommendations

- **Change funding practices to reflect the importance of software**:
  - Fund software appropriately throughout its lifecycle
  - Provide long-term cross-UKRI support for software maintenance and development which spans CSRs
  - Provide researchers with greater access to expert RSEs through a nationally coordinated and funded service

- **Improve understanding of RoI in software**:
  - Increase evidence base used to direct future UKRI software funding strategy
  - Support the recognition of software as a research output

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Recommendations

- **Fully exploit investment in R&I by increasing access to software experts**:
  - Promote networking and sharing of expertise and resources in research
  - Support existing software communities
  - Attract and retain skilled software specialists
  - Provide broadly required services centrally
  - Investigate the usefulness of an audit/quality kite mark for software

- **Expand training to meet evolving requirement of research**:
  - Maintain UK leadership in research software
  - Improve training at all career stages
  - Support an analysis of software training

Goal-driven Interventions Logic: an example

Theme 1: a policy environment that recognises and rewards software			
Goal	**Objectives**	**Short-term interventions**	**Long-term interventions**
1. Recognise that software is an essential, valuable and impactful part of research	All research funding proposals include a review of their software needs and costs	UKRI provides guidance to all applicants, reviewers and other stakeholders, that the intended use or development of software must be adequately described in all funding proposals. To highlight software, the UKRI will conduct and publish an investigation of the software requirements as part of the development of new strategies or investments.	Implement Research Output Management Plans (replacing Data Management Plans), which explicitly cover software management, as part of all UKRI funding calls to encourage better management and re-use of all research outputs. UKRI updates guidance for reviewers to indicate that all applicants should be scored highly for planning well-designed, reliable, reproducible and re-usable software.
	Support the recognition of software as a research output	UKRI publishes a position statement that a wide range of research outputs, including software, are vital to research, that these outputs may equal or surpass the impact of a publication, and that a broader range of outputs should feature more heavily in the REF. UKRI conducts and publishes an annual analysis of Researchfish outcomes, including software outcomes, and provides guidance on whether the outcome distribution reflects its expectations.	UKRI supports new REF guidance to provide clear instruction on how to submit and assess software as a research output post-REF2021. Applicants who receive funding that includes software development should be mandated to register software outcomes, and these software outcomes should become part of their track record against which future proposals are judged.
	Make research software openly available	UKRI funds a campaign to showcase the benefits of open-licensed software to research and innovation.	UKRI provides mandates that UKRI-funded software outputs should by default be open licensed, unless a case is made for an exception.

Policy

Goals

- Recognise that software is an essential, valuable and impactful part of research
- Improve the effectiveness of funding invested into software use and development

Investments

- Recommendations rely on changes to UKRI policy and, as such, will be costed by UKRI

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Funding

Goals

- Design investment to meet current and future research challenges
- Extract full value from software throughout its lifetime

Investments

- Novel algorithms and techniques: £25M
- Software evidence: £2.5M
- Maximising impact: £200M
- Software product fund: £70M
- Challenge fund:£2.5M

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Skills

Goals

- Attract and develop talent
- Improve and expand training in software skills
- Improve access to specialist skills

Investments

- National facility of RSEs: £75M
- Specialist networks: £900k
- Computational research: £77M
- Training analysis: £1M
- Digital skills materials: £2.5M
- Software communities: £155M
- eCSE programme: see Supercomputing white paper

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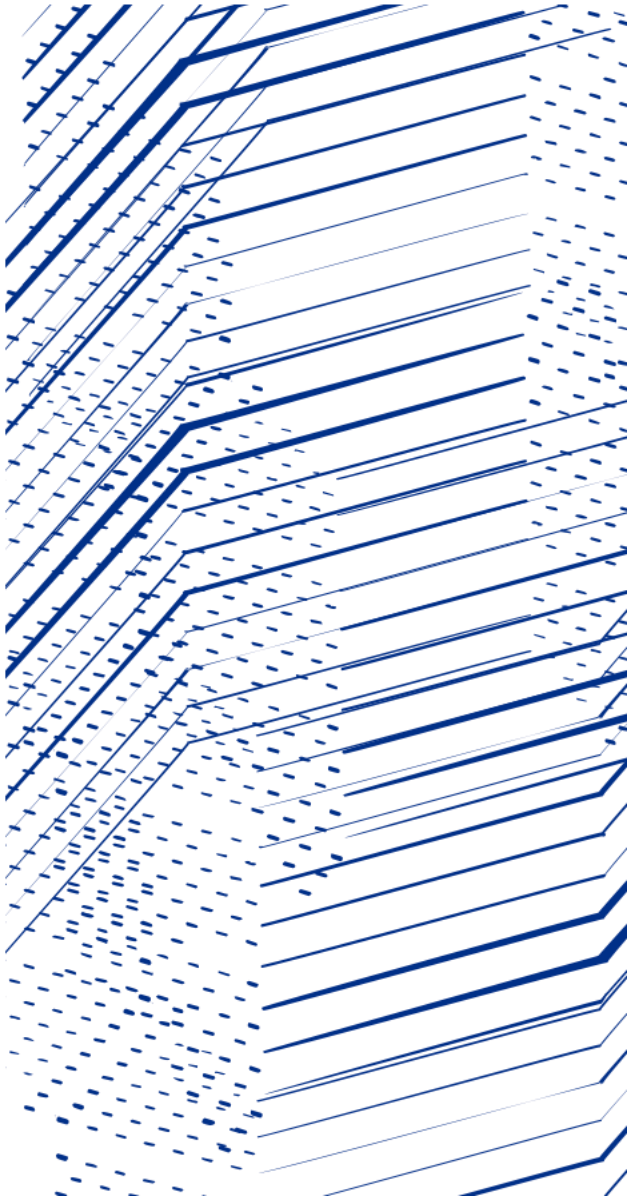
Software for STFC

Barbara Montanari
Head of the Computational Science and Engineering Division
Scientific Computing Department
STFC



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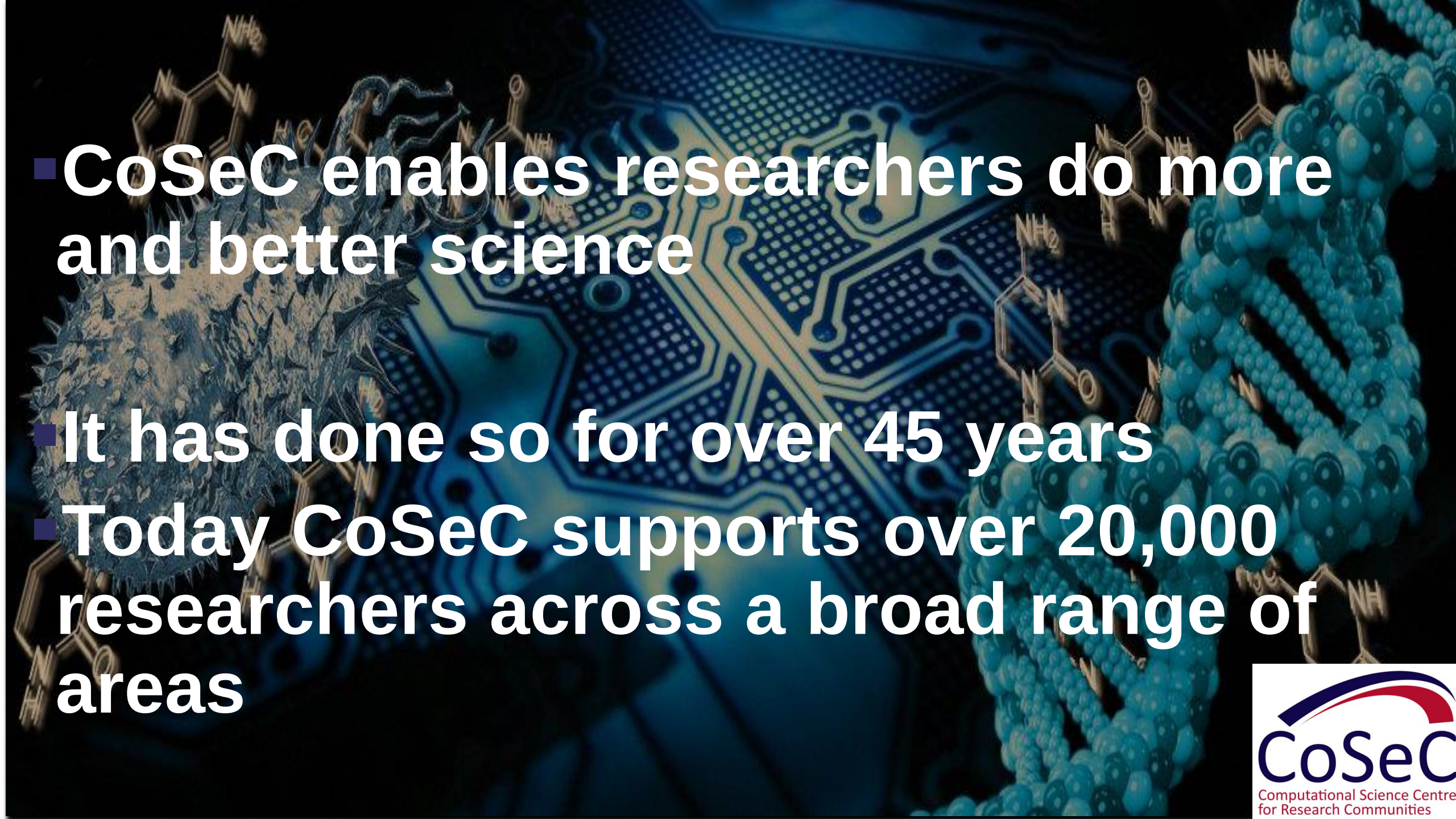
Split Remits in STFC Software Activities?

STFC Research and Innovation

- National experimental facilities
- Hartree Centre
- Scientific Computing Dept for STFC R&I
- Particle physics, nuclear physics and astronomy
- Etc.

Beyond STFC Research and Innovation

- CoSeC
  Computational Science Centre for Research Communities
- JASMIN
- Activities funded by external grants
- Etc.



- CoSeC enables researchers do more and better science
- It has done so for over 45 years
- Today CoSeC supports over 20,000 researchers across a broad range of areas

CoSeC
Computational Science Centre for Research Communities

1973: Collaborative Computational Projects

"Primary aim is to bring together scientists to:

- Provide for the rapid interchange of information on theory, algorithms, and computer codes
- Collect, maintain and develop relevant items of software
- Encourage basic research by providing facilities for rapid computer implementation of new methods and techniques
- Assess and advice on associated computational needs
- Disseminate information among scientists"

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Computer Physics Communications **114** (1998) xii-xvii

1973: Collaborative Computational Projects

"To assist the CCPs, the Science Research Council will provide support as follows:

- Support from staff from the Research Council's Laboratories
- Short term appointments of Senior Visiting Fellows
- Longer term Research Assistantships
- Funding for networking events"

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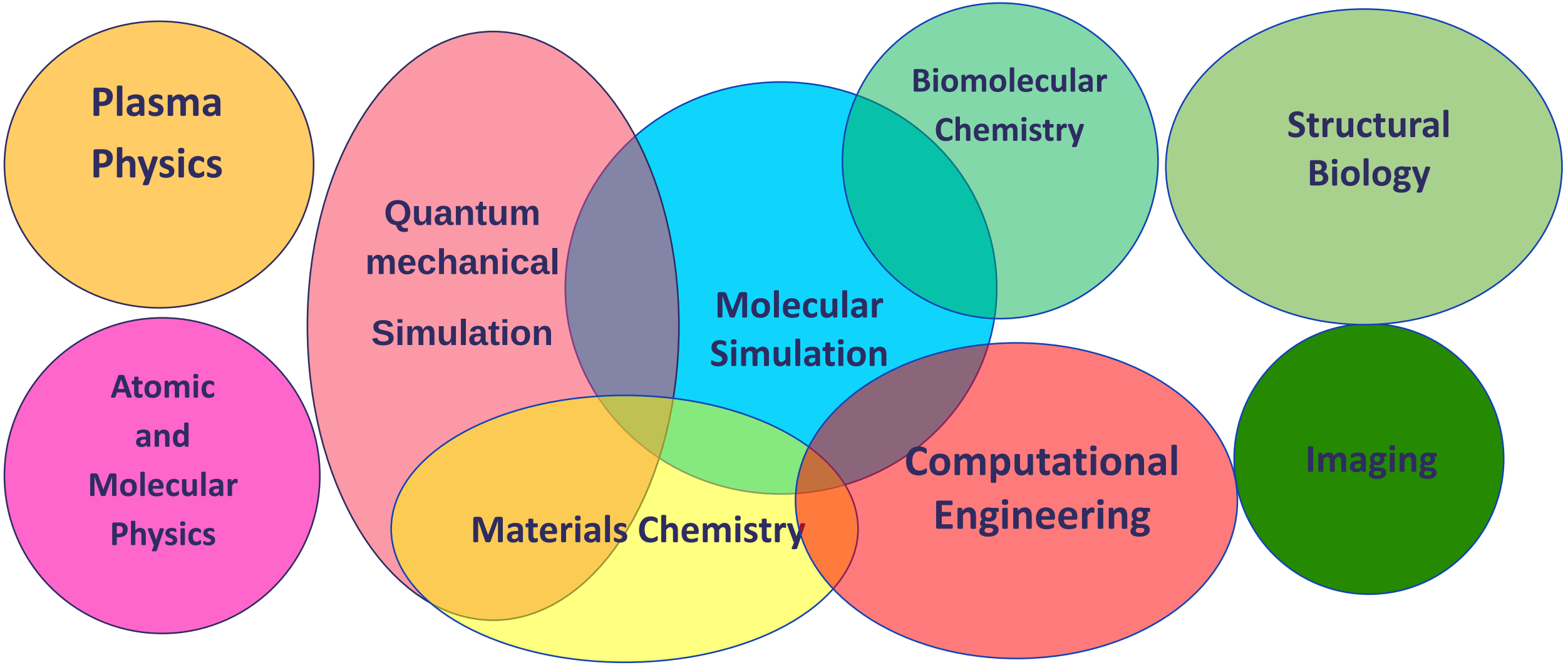
Computer Physics Communications **114** (1998) xii-xvii

Research Areas Currently Supported

CoSeC
Computational Science Centre
for Research Communities



CoSeC Infrastructure Ethos

CoSeC
Computational Science Centre for Research Communities

- CoSeC supports research communities to share knowledge and expertise rapidly and effectively, encapsulating it in **community software**, developed and maintained as a research *infrastructure* for the benefit of all researchers.

- CoSeC people are specialist RSEs, i.e., scientists who combine the science domain expertise with the software engineering expertise

- Skills pools built over decades and non-transferable

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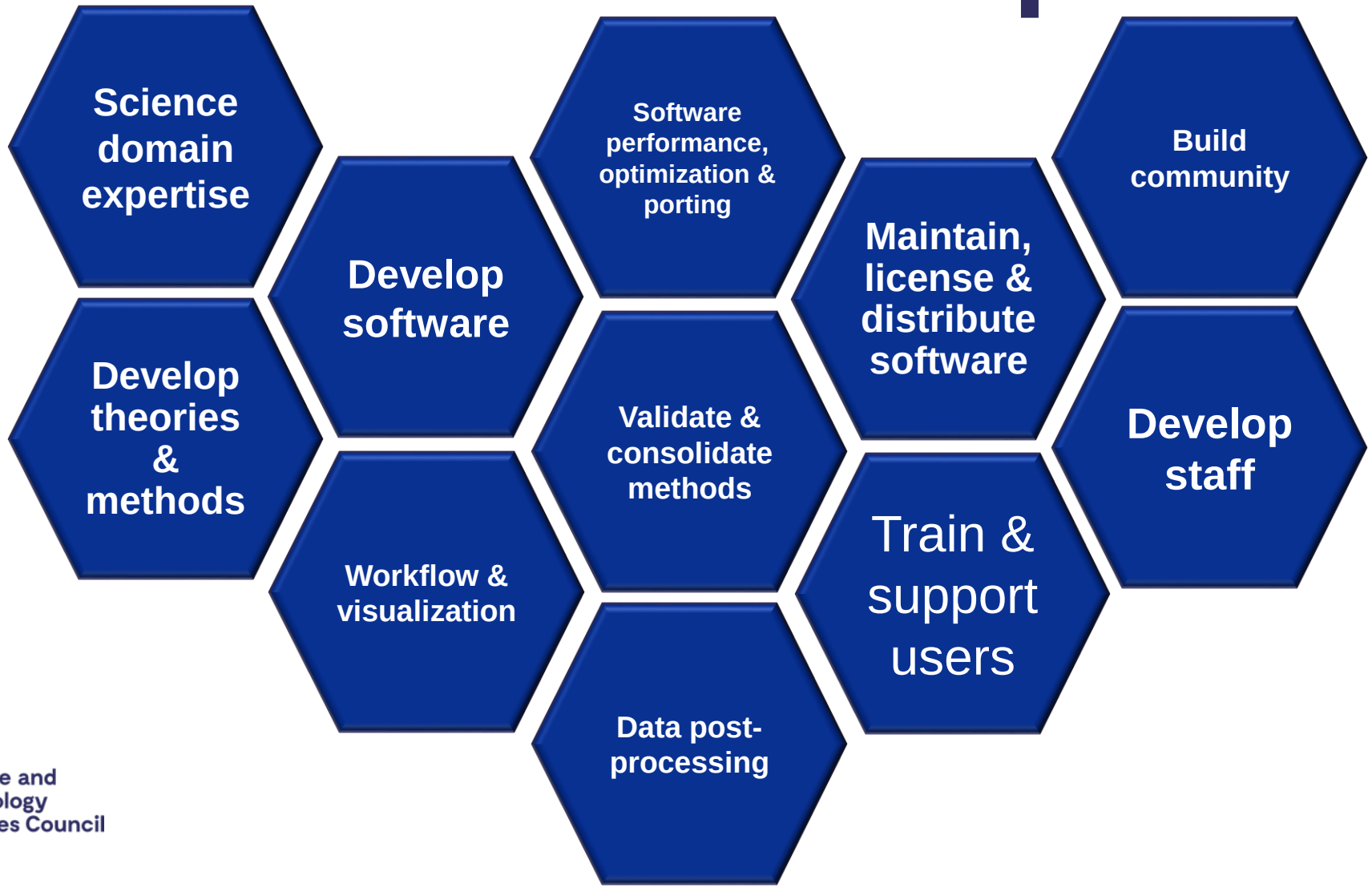
What CoSeC People Do



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2018 Chemistry Nobel Prize

"Directed Evolution of Enzymes and Binding Proteins"

Frances H Arnold, CALTECH, California, USA

CCP4

CoSeC
Computational Science Centre for Research Communities

BBSRC
bioscience for the future

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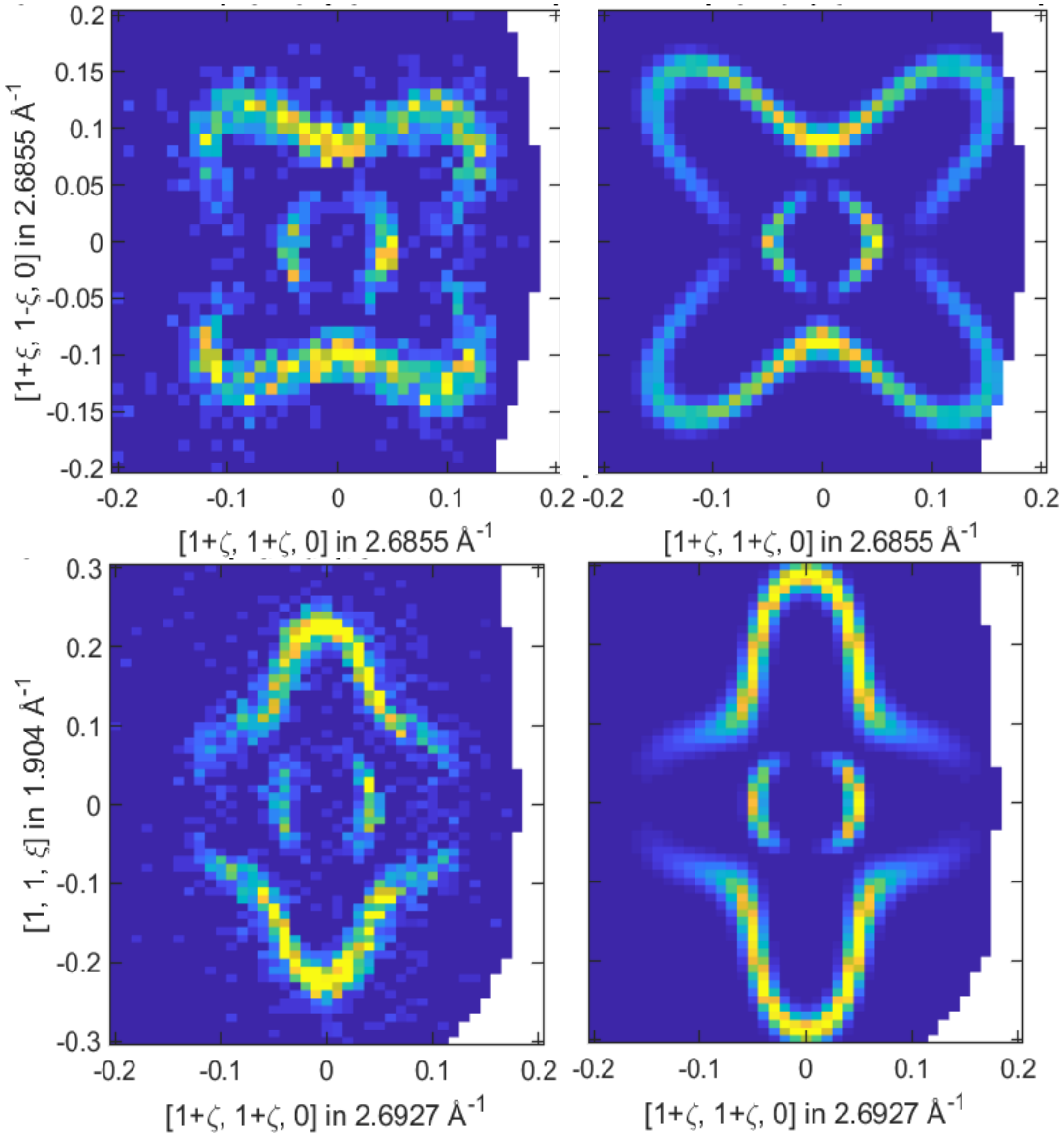

PACE Project

- SCD staff have developed a tool to directly compare simulated vibrational data with experiments conducted at ISIS.
- Benchmarking and validation against other tools has led to improvements that benefit ISIS, ORNL and PSI/ESRF.
- To quote one instrument scientist as ISIS – *"It has revolutionized my workflow." -DV*

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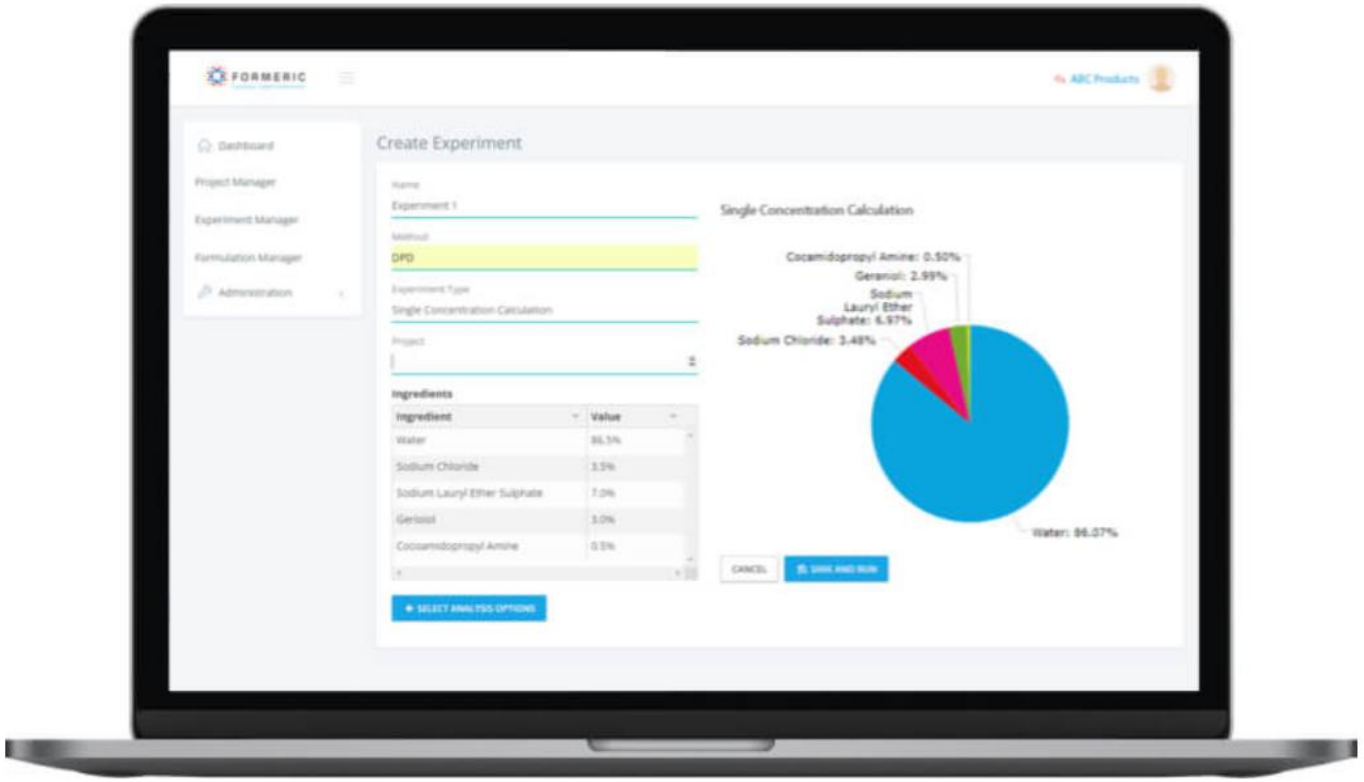
ISIS

CoSeC
Computational Science Centre for Research Communities

Software for Industry with Hartree Centre



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CoSeC
Computational Science Centre for Research Communities

Challenges/Opportunities

Technological

- Exascale
- Data deluge
- AI
- Quantum computing
- Etc.

Social

- Open research
- Strategic approach
- Community cohesion
- User expectations
- People pipeline
- Diversity and inclusion
- Etc.

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CoSeC Computational Science Centre for Research Communities

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Questions?

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Thank you

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