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RCS RESEARCH COMPUTING SERVICE
Gateway to Discovery

Research Computing Services Advisory Board

6th December 2021

Dr Andrew Richards

Head of Research Computing Service

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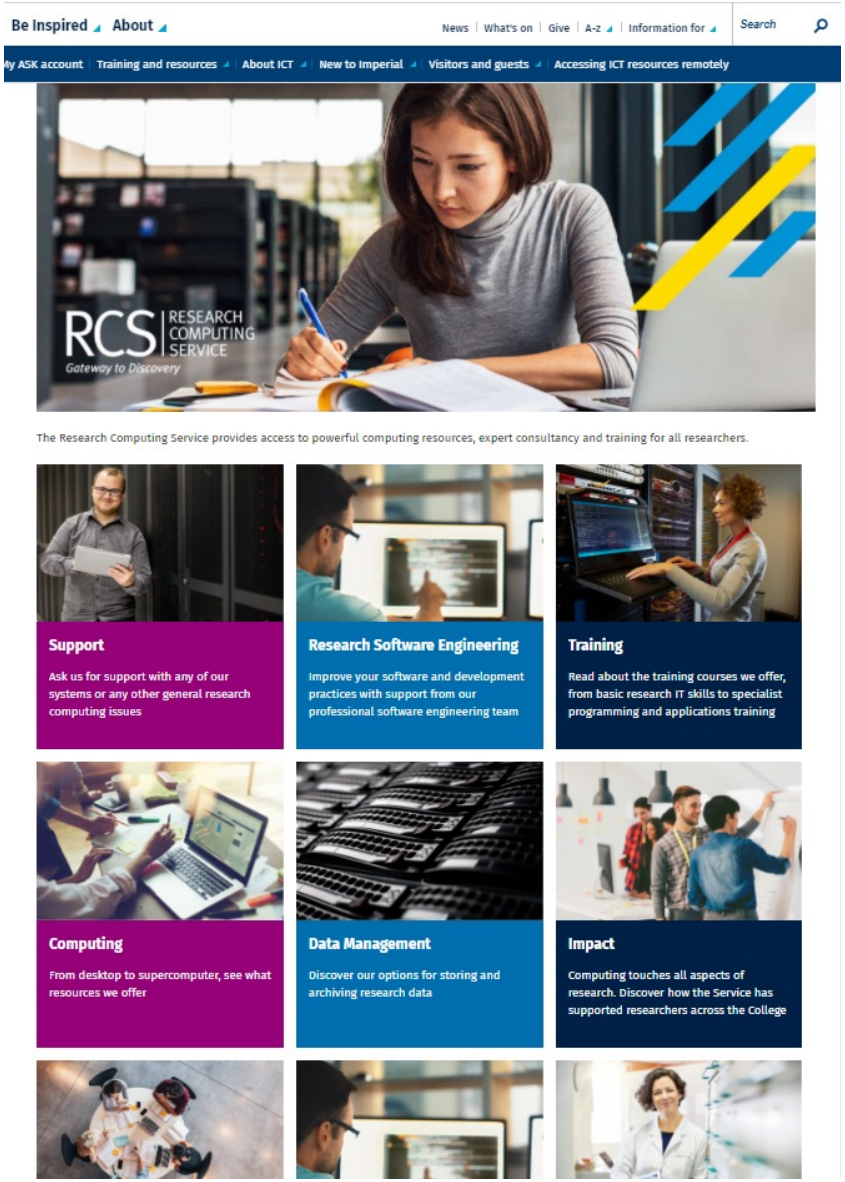
What is RCS Today ?

- Central computing and data services focussed on High Performance Computing
- Research Software Engineers
- *Some* Support for Research Data Management
- User support & *Training*
- *Strategy for what RCS is to be reviewed.*



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ICT Strategy

In partnership with the college drive digital maturity and deliver transformative work in 6 Priority areas:

1. The student journey
2. Education
3. **Research**
4. Service and support
5. Cyber security
6. ICT workforce.

Vision for Research IT

- Imperial is a world leading, Research led university and the ICT / Research computing provided to support that should be fit for purpose, production quality, easy to use, act as an enabling platform for research

  such that

- Research Computing Services should underpin the research lifecycle

  in order

- To provide services/products that enable research, manage research outputs (data), and support the research process

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Supporting the Research Lifecycle

. Research Data Lifecycle (Longwood Medical Area Research Data Management Working Group (LMA RDMWG)

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Aims

1. To provide world-class research computing resources to support research across Imperial.

2. To utilise appropriate hybrid computing environments to support the range of high-performance computing and interactive, near real-time, computing requirements.

3. To provide free at the point of use services for all research domains

4. To provide an enhanced service access route for grant funded projects

5. To support college activities through Research Software Engineers

6. To support a college wide research data policy through the provision of appropriate storage, archive and data sharing services

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Research Computing Strategy

4 Themes of activity:

1. Hybrid research computing platforms
   - On-premise, cloud, interactive, responsive
2. FAIR Research Data platforms
   - Store, process, share, archive, curate data
3. Research Software Engineering Centre of Excellence
   - Develop, advise, define standards, accelerate research
4. Underpinning research support applications
   - Support end to end research lifecycle applications

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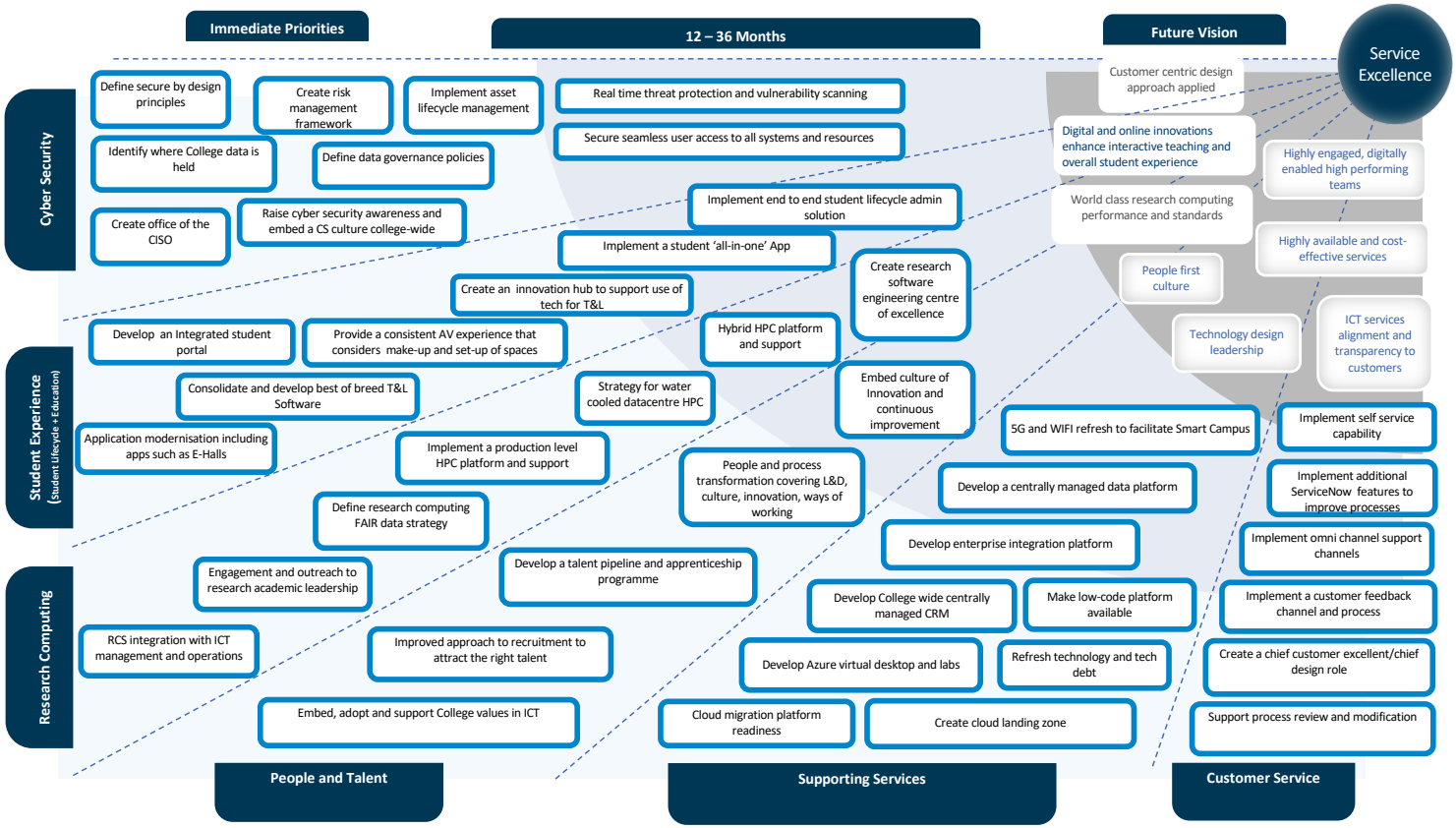
5 Year Roadmap: Our Transformation Journey

Today - Current State
Preparation for digital journey: creating a shared understanding of requirements, priorities & dependencies of stakeholders.

12-18 Months - Interim State
Transition & technical debt focus: Preparing the infrastructure to enable the 'new world'; updating and modernising the estate.

18-60 Months- Target State
Transformation: Focus is on the future of transforming the student and staff experience to realise the College's ambitions.



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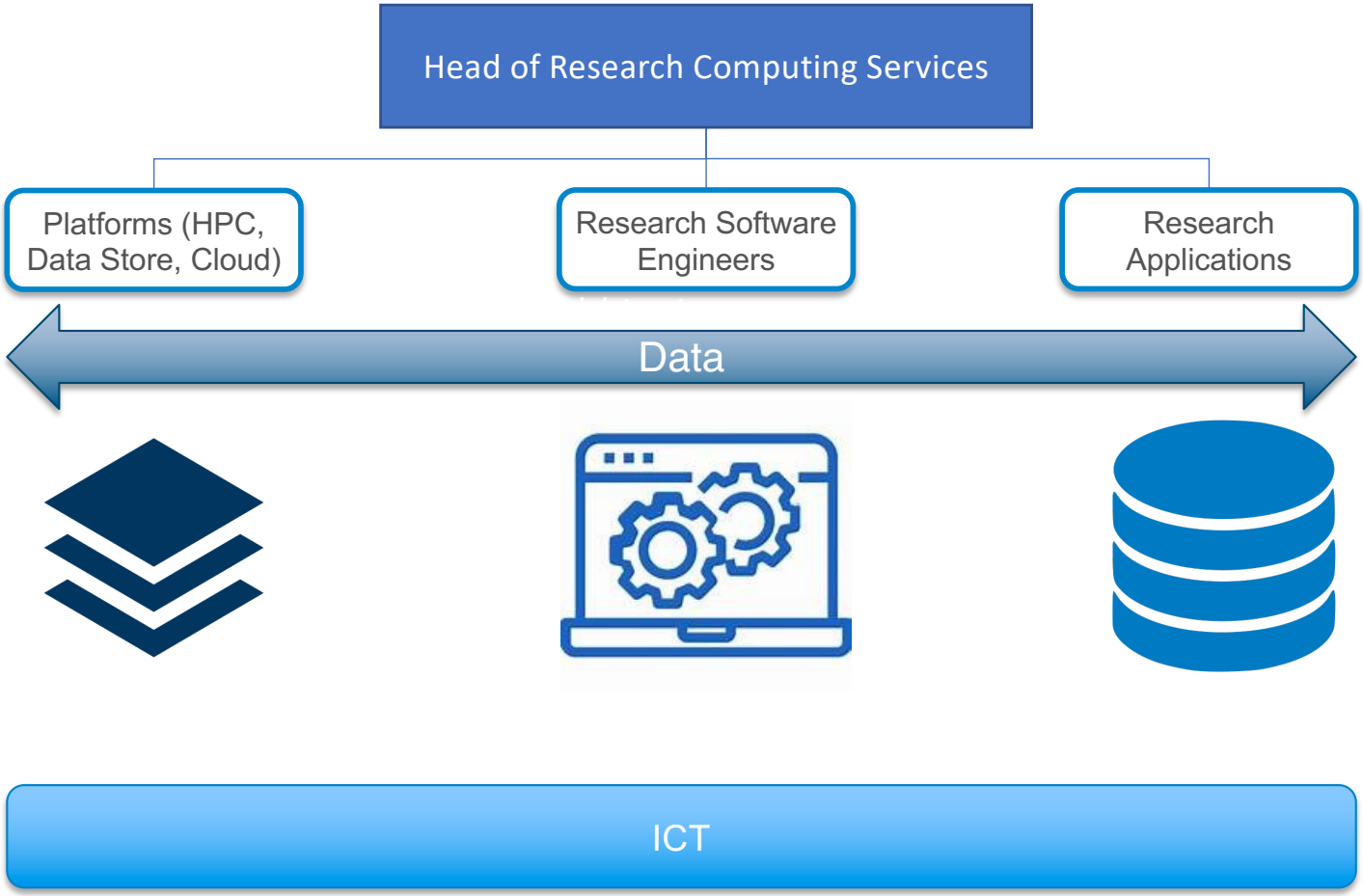
Research Computing Roadmap

- **Immediate Priorities**
  - RCS integration with ICT management and operations
  - Engagement and outreach to research academic leadership
  - Define research computing FAIR data strategy (Findability, Accessibility, Interoperability, and Reusability data)
  - Implement a production level High Performance Computing (HPC) platform refresh and support

- **12-26 Months**
  - Strategy for water cooled datacentre HPC
  - Hybrid High Performing Computer platform and support
  - Create research software engineering centre of excellence

- **5 year vision (2026)**
  - World class hybrid HPC platforms supporting research across Imperial
  - Part of UK national Research Computing infrastructure
  - Integrated compute, data, software service to college


Head of Research Computing Services
Platforms (HPC, Data Store, Cloud)
Research Software Engineers
Research Applications
Data
ICT

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College wide engagement : Academic Leadership Team

Ensure a broad buy in from the academic community and to set priorities for RCS

- Director or Research Computing: *Spencer Sherwin (FoE)*
- Director of Data Strategy*: Dave Colling (FoNS), Paul Aylin (FoM)*
- Director of User Engagement: *Mike Bearpark (FoNS)*
- Director of RSE Strategy: *Jeremy Cohen (FoE)*

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Recent updates

- RCS group structure update
- FY 2020/21 Hardware refresh of £2.5M completed
- New login nodes, service stability (improving), work to remove single points of failure
- **Secure Research Data Environment**
  - Project board created in September
  - Progress to develop Information Governance and Technical implementation in Azure
- ICT 5 year strategy and business case
  - What is in-scope and out of scope for RCS in ICT?
- TRAC Charges reviewed for RCS, simplified charging model
- RedHat Linux Site agreement in place
  - 5 year commitment, provides college wide support

RCS Platforms: Refresh/Expansion 2021

- **HPC**
  - **Increase from 69K cores to 87K cores**
    - Replace 13.3K CPUs with 30.7K cores
      - 210 x AMD 64 core nodes (512GB Memory)
      - *Same as ARCHER-2 but with more memory per node*
  - **12 New 'very' large memory (4TB) nodes**
    - Replaces AX4 SMP system
  - **Increase GPU to ~200 in total Refresh added 80 x Nvidia RTX6000**
- **RDS**
  - **Storage expansion from 11PB to 14PB**

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Proposed Infrastructure Capital Plan FY 21/22 and FY 22/23

- Budget of £2.93M per year after Director costs removed

- Combine two years funding for large refresh and transformation project
- Project 1:
  - £300K on pilot 'Hybrid Cloud' deployment + Object store
  - Develop capability in cloud for research computing

- Project 2:
  - Combine remaining budget ~£5.5M for HPC refresh:
  - Replace remaining CX1 and entire CX2 HPC system
  - Determine architecture of system from community consultation
    - Aim to support HPC (MPI) and GPU workloads with NDR IB and Fast object storage to support AI/ML initial community (pump prime activity with view to bid for an Imperial-X Tier 2 system later)
  - Release tender March/April 2022
  - Install date target end 2022, early 2023 depending on supply chain

System Refresh questions

- Primarily replacing CX2 (SGI) what does the system need to support?

- **HPC platform**
  - MPI workloads up to <size> ?:
  - GPU workloads using 4 way or 8 way NVIDIA A100 cards
  - HTC workloads as backfill
  - Express Access that provides priority access to replace private queue model (and updated TRAC costs)

- **Hybrid Cloud platform**
  - Interactive workloads
  - Virtual private queue investments (on demand) ?
  - Custom research environments
  - IaaS – Infrastructure as a Service for Research groups

Future Questions / Challenges

- What services should we support, and how?
- Supporting the research data lifecycle?
- How to connect / integrate with other college computing / data / support services?
- How best does the RSE team support projects across the College
- How to prioritise different and competing academic needs?
  - Academic governance - partnership understanding with ICT, representation for service users and non-users'

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TRAC Charging Update: Revision from 2022

Proposed charges:

RSE day rate: £400 (based on a revised 220 days model)

CX – compute £0.01 (1p per core hour)

CX - GPU £0.13 (13p per GPU hour)

RDS TB/month -single copy - £1.50
RDS TB/month -dual copy - £3.00

New COLD Storage???? Charge ???

RDS-Archive - £ 100 /TB/decade (one off charge)

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HPC Service Levels Proposal

- **SLA1: General Access**
  - Free at the point of use
  - Limits on wall time and number of concurrent jobs
- **SLA2: Express Access**
  - Charged access
  - Ring-fenced resource for express access users
  - Credit based approach to ‘bank’ money from grants / small capital investments
  - No limits on walltime, fairshare number of concurrent jobs
  - *Maximum wait time before job start ?*
- **SLA3: Partnership**
  - Co-investment model for significant capital projects
  - Case by case, defined hosted service with additional staff effort and opex costs
  - *Combined with general service and a credit based approach to priority access*

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Data Storage Proposal

- **Active Data**
  - Active projects
  - Free (2TB) level for all or only project funded?
  - Backup/DR copy for all data?
- **Cold Data**
  - Post project (cheaper / free) storage of data for X time(years)?
- **Archive Data**
  - Formalised process to archive data for long term retention(some metadata) [owner access only]
  - Links to institutional repository for publishing data (DOI) +rich metadata [open data]