UK Research and Innovation

The UK e-Infrastructure Landscape

Dr Susan Morrell
Chair of UKRI e-Infrastructure Group





MRC Medical Research Council

BBSRC bioscience for the future

Arts & Humanities Research Council

E·S·R·C ECONOMIC & SOCIAL RESEARCH COUNCIL

EPSRC Pioneering research and skills

Science & Technology Facilities Council

NERC SCIENCE OF THE ENVIRONMENT

Jisc

Met Office

Image credits: Shutterstock, NERC, FreePik, Innovate UK, STFC

UK Research and Innovation

E-Infrastructure is a Research Tool (not an IT system)

- E-Infrastructure is essential for carrying out research
  - Ubiquitous
  - Underpins most industrial sectors
  - Better, more efficient research
- Optimisation, modelling, simulation
- Data from large experiments and observation: analysis
- Social, medical, health data: analysis
- Real-time data – smart devices
- New and emerging areas: interface between data and computing

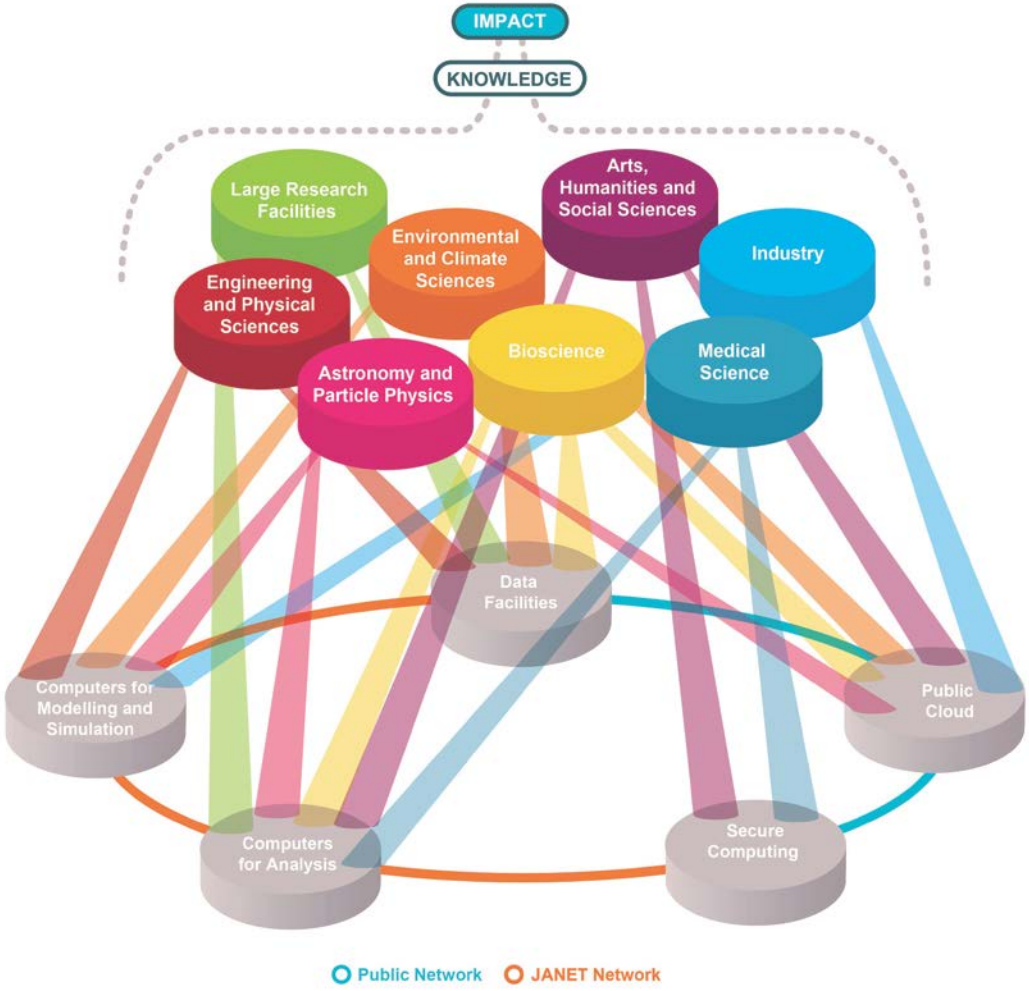
UK Research and Innovation

Diversity, Heterogeneity, Complexity

- Requirements:
  - Diverse workflows, each optimised for efficiency
  - Range of technologies
  - One size cannot fit all
- Types of user:
  - Expert users need access to competitive infrastructure to tackle increasingly complex problems: complex simulations and calculations, multi-scale modelling, data analysis
  - New fields now using computational techniques for the first time – large numbers of `non-experts`

UK Research and Innovation

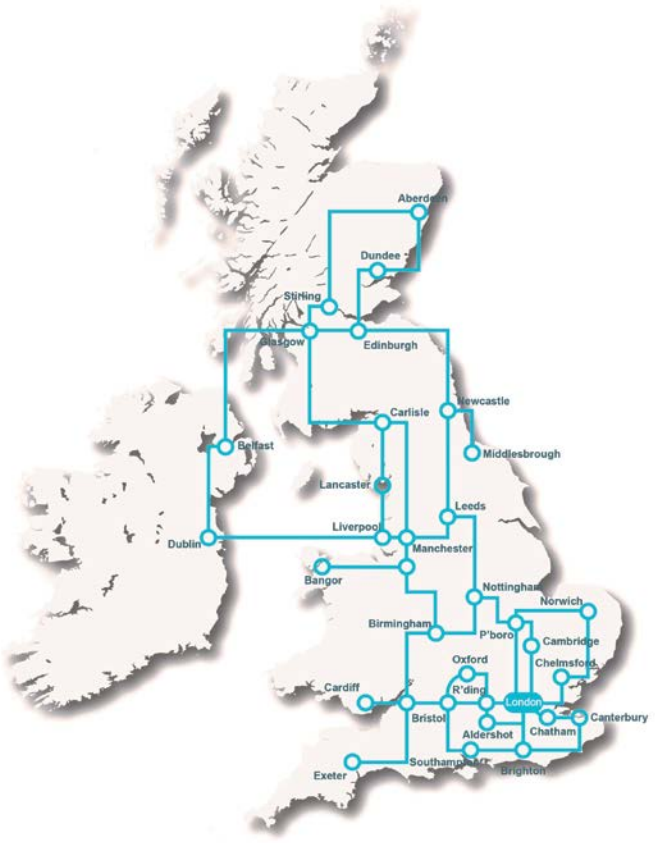
Diversity, Heterogeneity, Complexity



UK Research and Innovation

Diversity, Heterogeneity, Complexity

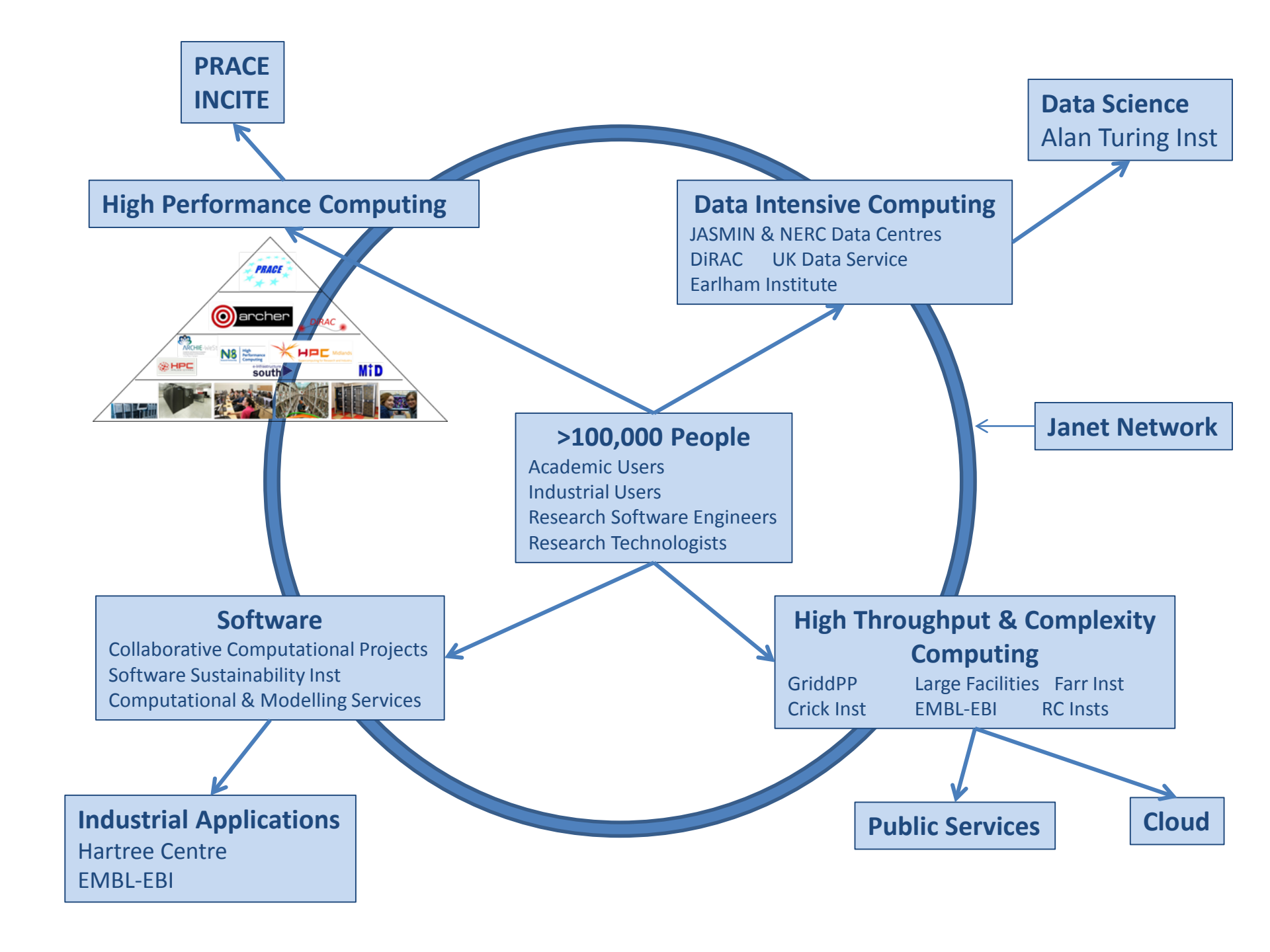
- Geographical diversity
- Physical network – Janet
- Virtual networks of practice
  - Communities
  - Collaborations
- International dimension



UK Research and Innovation

Types of Computing

Type	Characteristics
High Throughput Computing	• Computes huge numbers of the same simple workflow • Link with experimental equipment e.g. LHC, bioinformatics, images and spectra from medical scanners, telescopes, large facilities, cryo-EM etc. • Increasingly data intensive as the measurements are increasing in number and accuracy
Secure Computing	• Where there are strict requirements governing the access to and handling of the data • Medical and social science domains
Operational Computing	• Where things have to be done in a particular time window to a particular performance level e.g. weather forecasting
High Performance Computing	• This requires high performant CPU, Interconnect and file system performance. Job sizes run from 32 to 100,000 cores • Used to model weather, climate, materials properties, aerodynamics, chemical properties and kinetics, transport systems, environmental systems, structure of sub-atomic particles, planet formation
High Performance Data Analytics	• Use of High Performance Computing techniques applied to data analytics, data modelling and data fitting. • Characterised by the performance of multiple distinct activities • Examples: the fitting of weather/climate/engineering hydrodynamical/chemical models to measurements, the exploration of observed data to produce new data such as structures etc. which require the new generation of AI/machine learning techniques


PRACE
INCITE
Data Science
Alan Turing Inst
High Performance Computing
Data Intensive Computing
JASMIN & NERC Data Centres
DiRAC UK Data Service
Earlham Institute
Janet Network
>100,000 People
Academic Users
Industrial Users
Research Software Engineers
Research Technologists
Software
Collaborative Computational Projects
Software Sustainability Inst
Computational & Modelling Services
High Throughput & Complexity Computing
GriddPP Large Facilities Farr Inst
Crick Inst EMBL-EBI RC Insts
Industrial Applications
Hartree Centre
EMBL-EBI
Public Services
Cloud

UK Research and Innovation

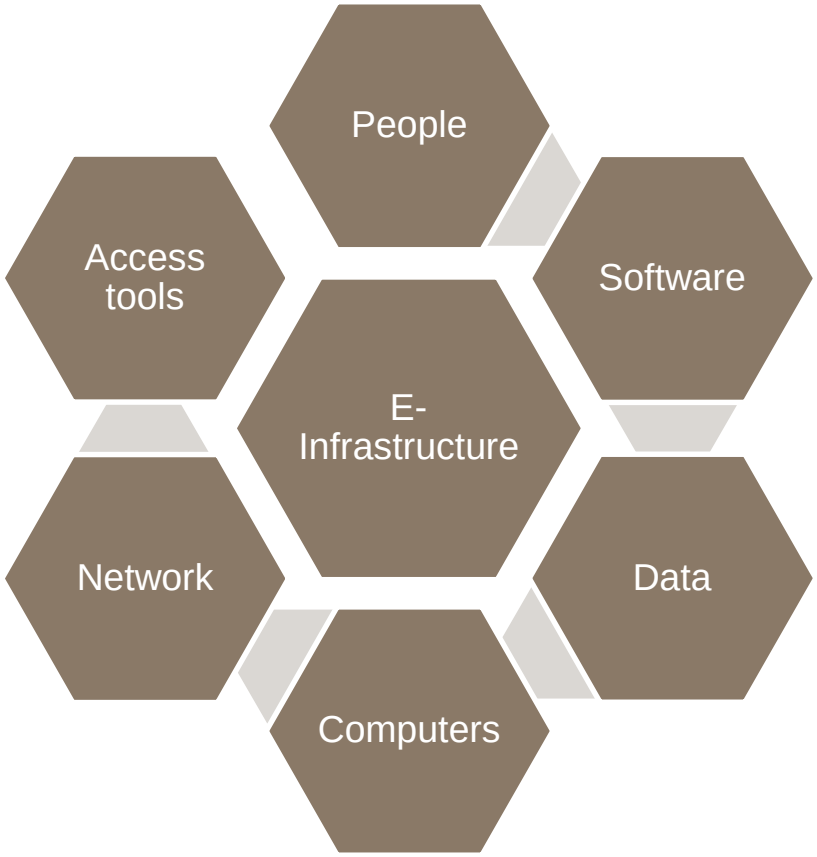
Tier 2 Centres

- Broadens access to researchers new to HPC;
- Provides access for industry;
- Encourages skills and expertise in software engineering;
- Is integrated with the HPC ecosystem across the UK, both vertically and horizontally: a truly national Tier 2 layer
- Provides a diversity of computing architectures

Centre	Type
Cirrus (Edinburgh)	Standard cluster
HPC Midlands Plus	Standard cluster
MMM	Standard cluster
Isambard (Bristol)	ARM
Peta-5 (Cambridge)	Knights Landing GPU
Jade (Oxford)	GPU

UK Research and Innovation

Not just computers



UK Research and Innovation

Better Software, Better Research

- Seven out of 10 UK researchers report that their work would be impossible without research software
- Attributes: sustainability, reproducibility, reusability, quality, trust…
- Recognition as a research output
- EPSRC Software as an Infrastructure Strategy
- Funding:
  - Software Sustainability Institute (EPSRC, BBSRC, ESRC)
  - Collaborative computational projects (EPSRC, BBSRC, MRC)
  - Computational Science Centre for Research Communities (CoSeC) (EPSRC)
  - Embedded CSE support for ARCHER users (EPSRC, NERC)
  - BBSRC Tools and Resources Development Fund
  - EPSRC Software for the Future calls

UK Research and Innovation

Research Software Engineers

- RSE Association:
  - Many hundreds of members
  - Annual conference
  - International impact
- EPSRC RSE Fellows:
  - Leadership and advocacy
- Research Software Groups in universities

UK Research and Innovation

Research Software Engineer Fellows

Name	Organisation	Title
Ian Bush	University of Oxford	Software Engineering - In Support of the Exascale
Christopher Woods	University of Bristol	Sustainable RSE Careers for Sustainable Software Development
Paul Richmond	University of Sheffield	Accelerating Scientific Discovery with Accelerated Computing
Louise Brown	University of Nottingham	Research Software Engineering Fellowship - Software for Textile Modelling and Simulation
Oliver Henrich	University of Edinburgh	EPSRC Research Software Engineer Fellowship
Christopher Richardson	University of Cambridge	Expressive Finite Element Modelling for HPC: enabling advanced techniques for scientists
Mike Croucher	University of Sheffield	Building Capability and Support in Research Software
Phil Hasnip	University of York	Transforming Research-Oriented Software Engineering
L Muresan	University of Cambridge	Computational microscopy in Cambridge Advanced Imaging Centre
Jo Leng	University of Leeds	Research Computing and Imaging
Jeremy Cohen	Imperial	A Research Software Engineering Hub for Computational Research

UK Research and Innovation

Skills and Training

- Software carpentry, data carpentry – SSI
- RSE teams
- Centres for Doctoral Training
- CCPs
- CoSeC
- Training provided by infrastructures and centres e.g. ARCHER, ELIXIR, EMBL-EBI etc.

UKRI Infrastructure Roadmap Objectives

Create a long-term (approximately 2030) research and innovation infrastructure roadmap based on a picture of existing UK infrastructure (including key international facilities in which the UK participates), future requirements (research, economic and social), and resulting investment priorities.

In addition

- Identify future research and innovation infrastructure capability priorities ;
- Identify opportunities for increasing inter-connectivity;
- Support development of UKRI's overall long-term investment plan;
- Promote the UK capabilities as a global leader in research and innovation;
- Set out the trajectory and major steps needed to reach the long term vision

What are R&I infrastructures?

Facilities, resources and services that are used by the research and innovation communities to conduct research and foster innovation in their fields. They include: major scientific equipment (or sets of instruments), knowledge-based resources such as collections, archives and scientific data, e-infrastructures, such as data and computing systems and communication networks and any other tools that are essential to achieve excellence in research and innovation.

Scope & definition of infrastructure

The programme will focus on infrastructures which receive significant public funding.

- **Purpose:** Research and Innovation infrastructures are facilities, resources and services used by the research and innovation community to conduct or facilitate excellent research and innovation.
- **Accessibility:** Pooling effort can enhance excellence in highly-demanding fields where economic and research drivers require a collaborative approach. An infrastructure must provide access, resources or related services to the wider, UK research and innovation community outside the infrastructure institution itself.
- **Scale and longevity:** An infrastructure must have some degree of international/ national importance and existing or planned long term sustainability

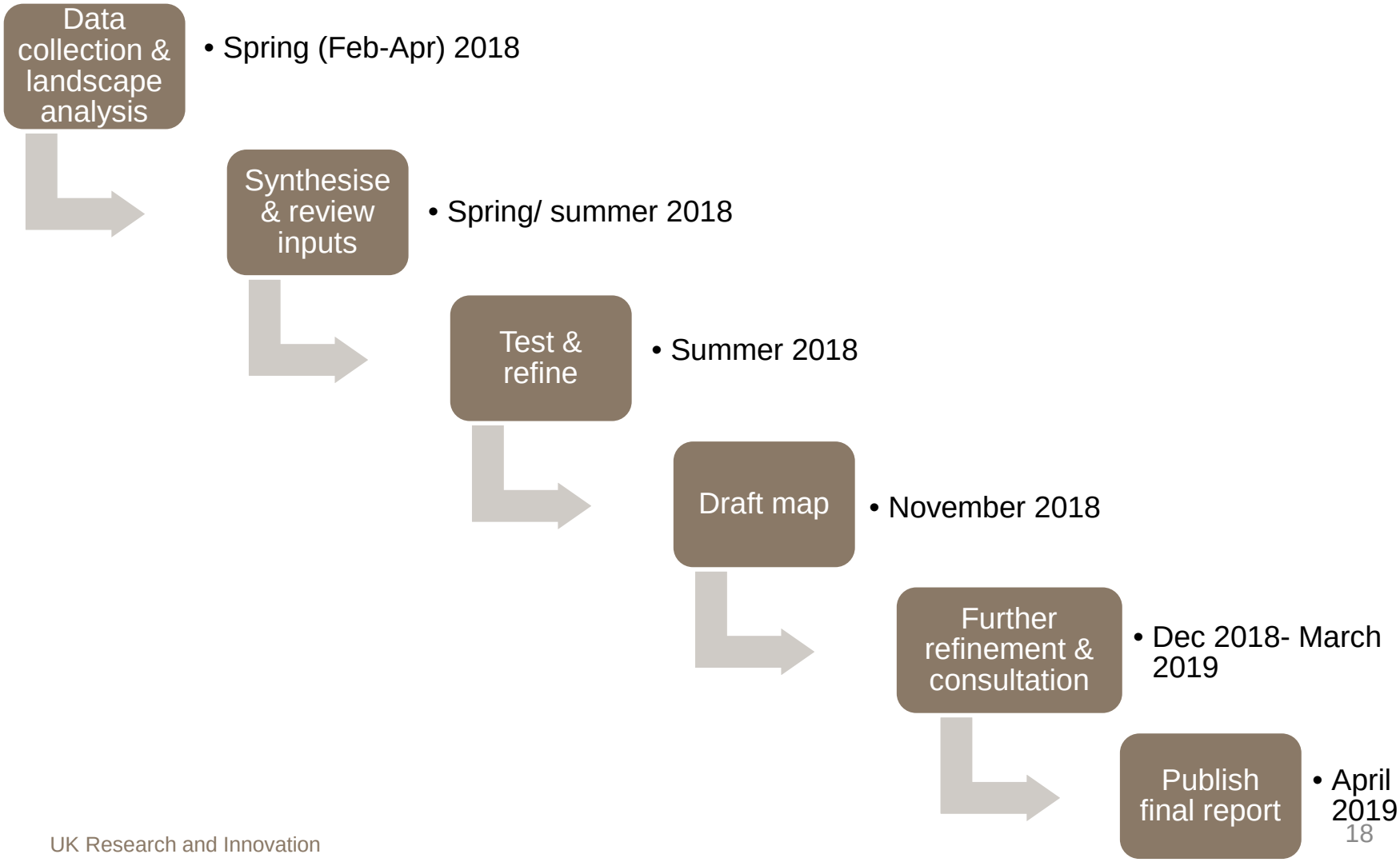
Scope & definition of infrastructure

Following the approach taken by ESFRI the roadmap will be structured in the following sectors:

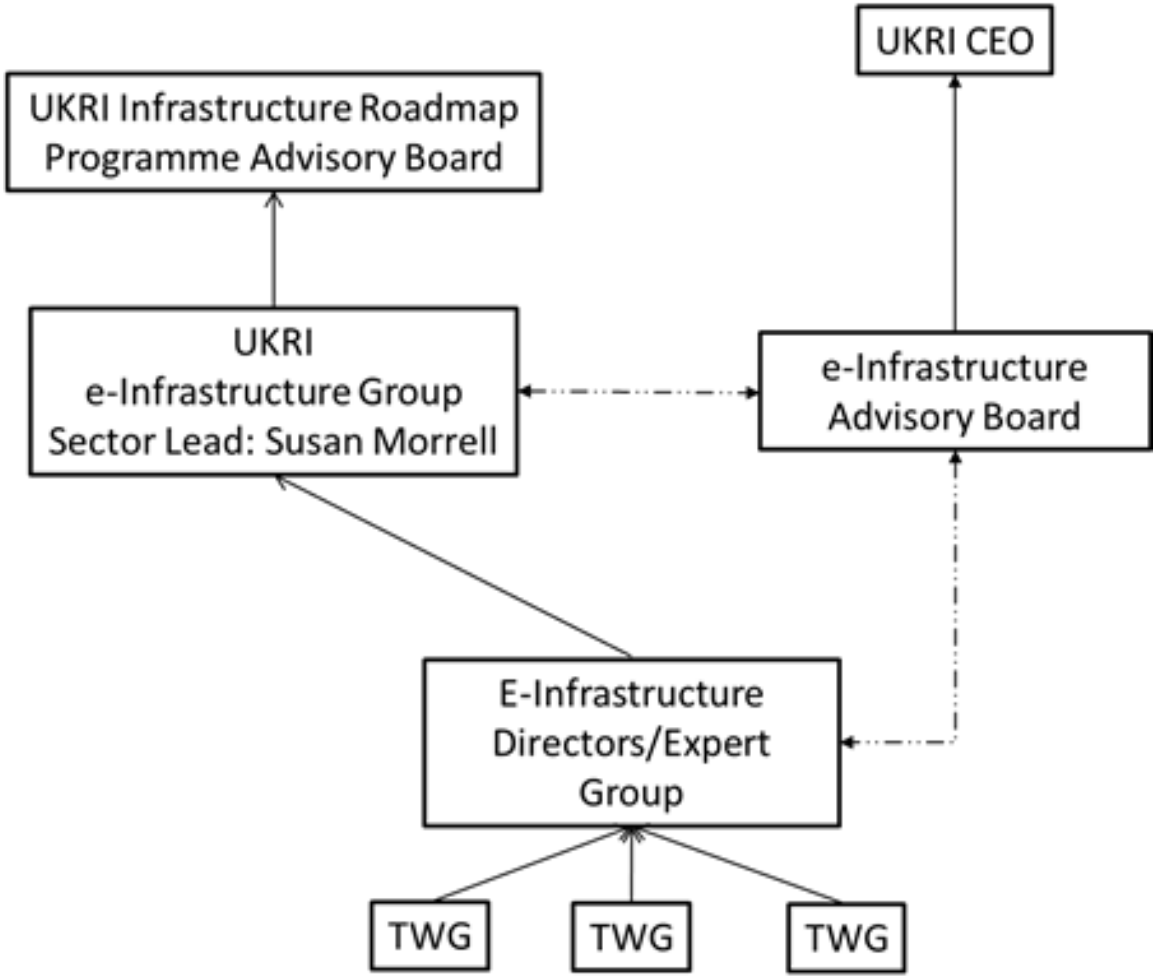
- Biological Sciences, health and food
- Environment
- Energy
- Physical sciences & engineering
- Social sciences, arts and humanities
- Computational & e-infrastructures

Recognise we will also need to capture cross cutting themes and many infrastructures will contribute to more than one sector

Timeline


Data collection & landscape analysis
• Spring (Feb-Apr) 2018
Synthesise & review inputs
• Spring/ summer 2018
Test & refine
• Summer 2018
Draft map
• November 2018
Further refinement & consultation
• Dec 2018- March 2019
Publish final report
• April 2019

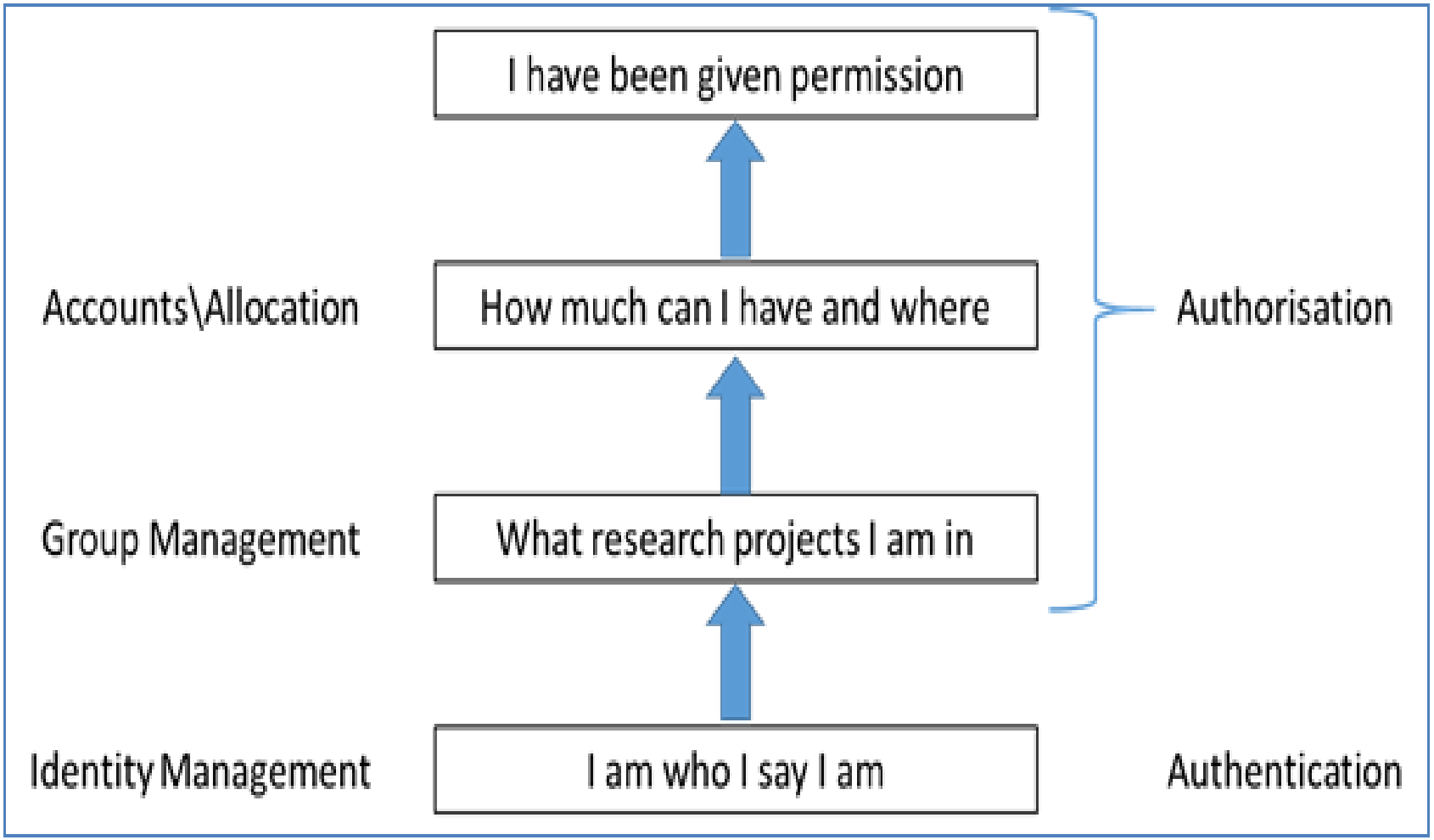
Governance


UKRI CEO
UKRI Infrastructure Roadmap Programme Advisory Board
UKRI e-Infrastructure Group Sector Lead: Susan Morrell
e-Infrastructure Advisory Board
E-Infrastructure Directors/Expert Group
TWG
TWG
TWG

Cloud strategy

- Across many research domains, use of cloud technologies is part of normal business
- Strategies developed in various domains:
  - In response to in-depth understanding of user requirements and technology developments
- Agenda well-understood and being actively managed
  - Providing the e-infrastructure the researchers require with the technical capabilities needed at the right time and right cost
- Now need to bring this knowledge together and create an integrated strategy ready for UKRI via eAB
- Aiming for May

AAAI in a nutshell



Benefits

- Opens door to integration across e-infrastructures
  - Single Sign on: Removes a major barrier to access for users
  - Enables hardware to be shared across domains
  - From a service provider perspective this encourages aggregation and pooling of resources
  - Allows cloud and data services to work effectively, efficiency and appropriately
    - You know who I am, what I can do, how I'll be measured, and where I live…..
  - Could form an element in the roadmap?

UK Research and Innovation

Personal observations

- Funding: comes in clumps, seemingly randomly, rather than consistently and in a sustained way
- Silos: much work done over the last five years to break these down. Much stronger collaboration between RCs, and between e-infrastructure directors. UKRI gives an opportunity to build on this.
- User industry: challenging to engage Innovate UK.
- Data: huge agenda, no one owner.
- AI/machine learning: what to do?

UK Research and Innovation

What can we do for you?

- Provide ideas and input for agenda items
- Provide strategy documents, think pieces for discussion
- Provide a single point of access to the main e-infrastructures

UK Research and Innovation

What can you do for us?

- Provide constructive input on the developing outputs from the roadmap, acting as sounding board/challenge panel
- Endorse strategies, recommendations coming from expert group via UKRI group
- Act as advocates with UKRI, government on importance of e-infrastructure in research and innovation
- Help us make the case for funding and investment