

# Simple, Secure and Fast Access to Digital Research Infrastructure

Dr Fan Yang-Turner

**Group Leader, Data Analysis as a Service (DAaaS)**

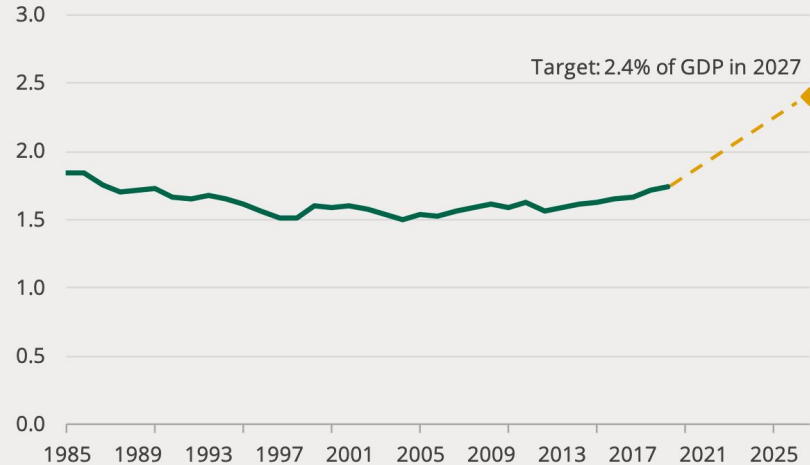
Scientific Computing, STFC, UKRI

12 January 2023 @ IRIS Collaboration Meeting

# UK ambition: become a science superpower

## Gross expenditure on research and development

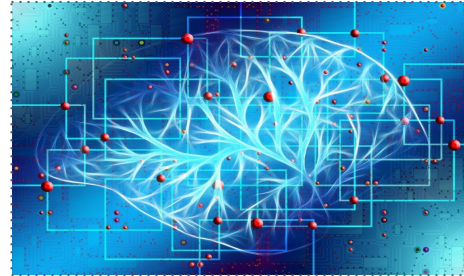
UK, as a % of GDP



Source: ONS series [GLBH](#), and Commons Library calculations.



R&D Workforce  
260,000+  
(2019-2027) <sup>1</sup>



R&D UKRI  
Infrastructure  
£481 million  
(2022-2025) <sup>2</sup>

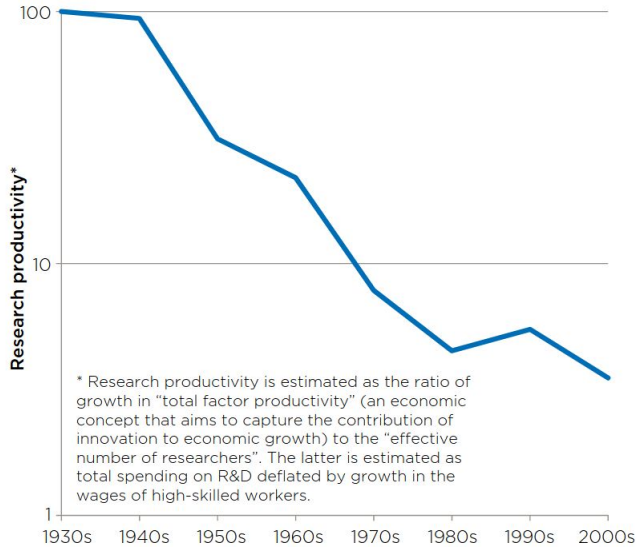
1. Kingman, K., [‘The 2.4% challenge: where will our researchers come from?’ speech at the Research culture: Changing expectations conference. The Royal Society, 30 October 2018](#)

2. UKRI Infrastructure Fund Projects: <https://www.ukri.org/what-we-offer/creating-world-class-research-and-innovation-infrastructure/funded-infrastructure-projects/>

# Research Productivity

Fig. 4: Long term trend of research productivity in the US

Index (1930 = 100), logarithmic scale



\* Research productivity is estimated as the ratio of growth in "total factor productivity" (an economic concept that aims to capture the contribution of innovation to economic growth) to the "effective number of researchers". The latter is estimated as total spending on R&D deflated by growth in the wages of high-skilled workers.

Source: Bloom et al (2019)

**3500**

world leading researchers interviewed\*

**85%**

say carrying out research is increasingly complex

*"we expect **digital transformation** to have an increasingly large impact on **scientific productivity** in years to come."*

\* Oxford Economics, 2021, The State of Scientific Research Productivity

<https://www.emdgroup.com/content/dam/web/corporate/non-images/scientific-research-productivity/us/Scientific-Research-Productivity-White-Paper-NA.pdf>

# What do scientists say?

Have all the software up-to-date out of the box.

No need to move data from one place to another

Can do analysis on single machine or a cluster

Can visualise my result from my HPC result.

Can have one place run all my workflow

Share and work with others in real time

# Digital Research Infrastructure

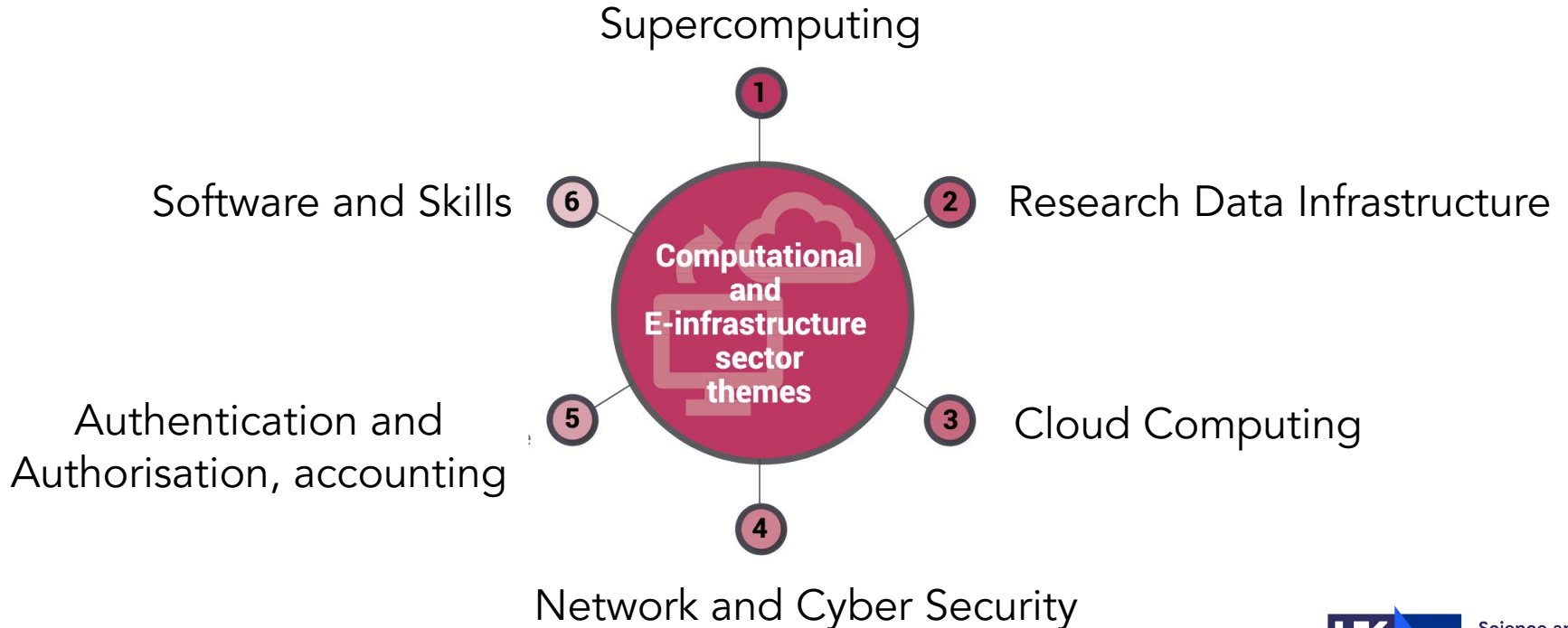


Figure 18. Computational and e-infrastructure themes overview.

# Simple, secure and fast access to DRI



Scientists

Data Analysis as a Service

Simple, secure  
and fast access

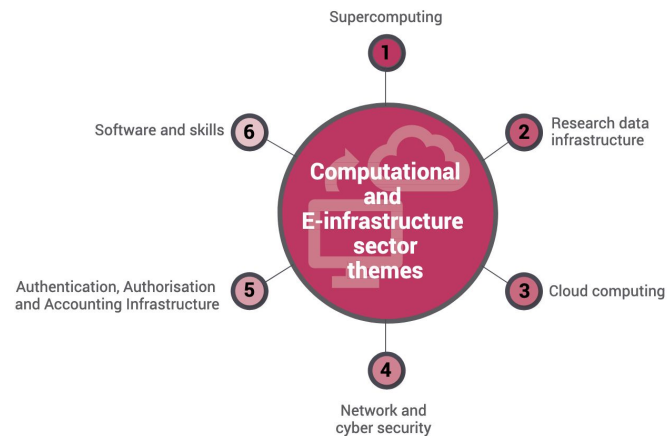


Figure 18. Computational and e-infrastructure themes overview.

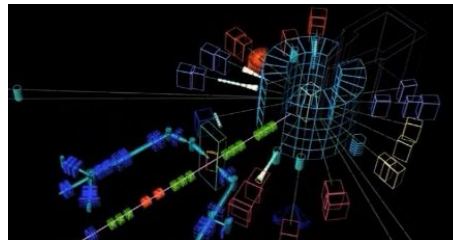
Digital Research Infrastructure

2020

ISIS Data Analysis  
as a Service



ISIS Neutron and  
Muon Source



**All 34 Instruments**  
**250+ concurrent users**  
**70+ software**

2021

CLF Data Analysis  
as a Service



Central Laser Facility



**4 of 5 research groups**

2022

Data Analysis as a  
Service - Training



Scientific Computing



**8 courses, 300+ users**



Scientific Computing

# Platform: Simple

Everything for scientist:

- Compute
  - Single VM, Cluster
- Data
  - Persisted
  - Backup
  - Policy
- Software
  - Container
  - Update
  - License

Workspaces

ISIS Data Analysis as a Service

Workspaces

Data

Experiments

Maintenance

Help

ARGUS > TEST-Muon

This Workspace has been configured for TEST-Muon experiments on the ARGUS instrument.

Resources

- 2 CPUs
- 8 GB RAM

Software

- ▶ ANTS2 - 4.36-singularity
- ▶ ATASAS - 3.0.1
- ▶ Anaconda3 - 2020.11
- ▶ Aten - 2.1.9
- ▶ DAVE - 2020.03.05
- ▶ DAVE - 2021.11.15
- ▶ EPSR - 26
- ▶ GROMACS - 2021.5

CREATE WORKSPACE

Select your type ...

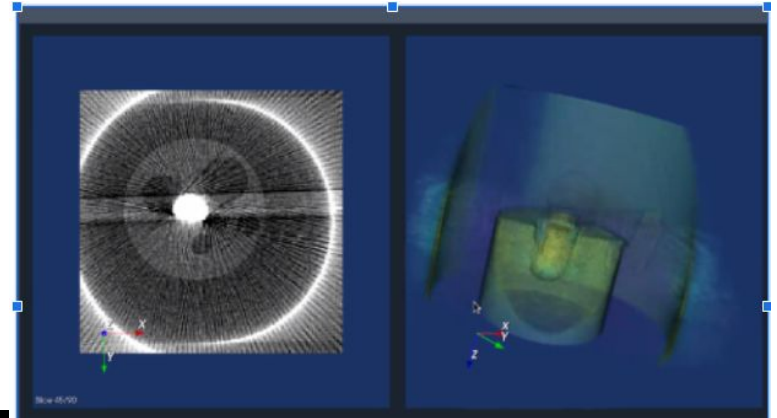
- TOMOGRAPHY RECOMMENDED
- TOMOGRAPHY ADVANCED LARGE
- ENGINE-X
- TOMOGRAPHY ADVANCED



# Platform: Perform

Just like local, but more powerful

- GPU applications
- Virtual Cluster
- Access to HPC



ShawL

## SLURM Dashboard

**Settings**

SLURM login node hostname:  
v11.scarf.rl.ac.uk

SLURM username:  
gek25866

SLURM password:  
.....

Local run path:  
/home/dv/stuff/code/shawL5/demo\_inputs

Remote run path:  
/work4/scd/scarf1123/shawL5run

**Actions**

These are in order.

Sync local to remote

Run job

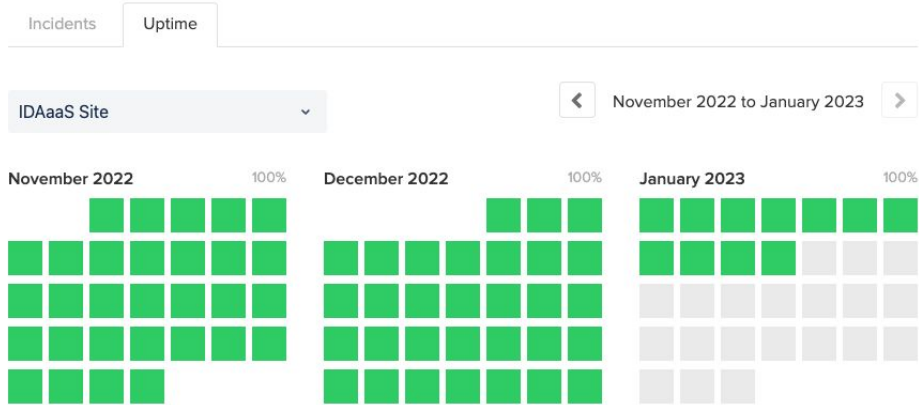
Watch queue

Open remote shell

Sync remote to local

Open file browser

# Platform: Reliable



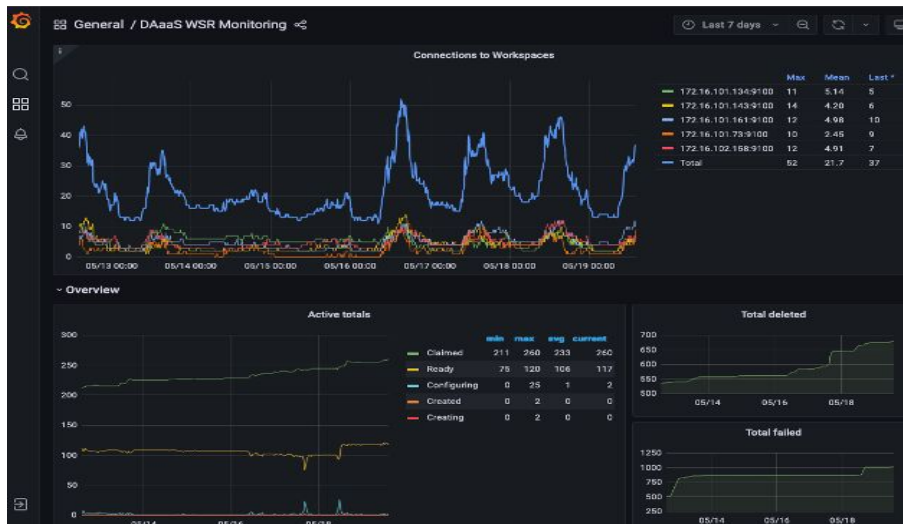
User Office Login	pass	Workspace Register	pass
> login	pass	> state hanging	pass
		> workspace pools	pass
		> aggregated health checks	pass: 0% bad

### Platform Components

Hosts	Services
> Avizo License Server Proxy :	> websockify :
> Websockify Proxy 2 :	> Websockify Proxy 2_health :
> LDAP :	> slapd :
> DAaaS Repo :	> httpd :
> Admin Panel :	> DAaaS Repo_health :
> ISIS Directory Manager :	> admin-panel :
> CLF Ansible Controller :	> platform-healthchecks :
> ISIS WFE Alias :	> slack-notifications :
> Last Activity :	> httpd :
> Workspace Register 1 :	> Admin Panel_health :
> Websockify Proxy 5 :	> isisdirectorymanager :
> ISIS Ansible Controller 1 :	> ansiblecontroller :
> ISIS Ansible Controller 2 :	> daas-wfe :
> CLF Group and Account Managers :	> httpd :
> Websockify Proxy 3 :	> ISIS WFE Alias_health :
> ISIS Ansible Controller 3 :	> lastactivity :
> ISIS Pool Manager :	> httpd :
> Websockify Proxy 1 :	> websockify :
> CLF Pool Manager :	> Websockify Proxy 5_health :
> CLF Samba :	> ansiblecontroller :
> ISIS WFE 2 :	> ansiblecontroller :
> CLF WFE :	> uo-account-manager :
> Monitoring :	> clfgroupmanager :
> Cache Updater TS2 :	> websockify :
> CLF Data Management :	> Websockify Proxy 3_health :
> ISIS WFE 1 :	> ansiblecontroller :
> Websockify Proxy 4 :	> rbmanager :

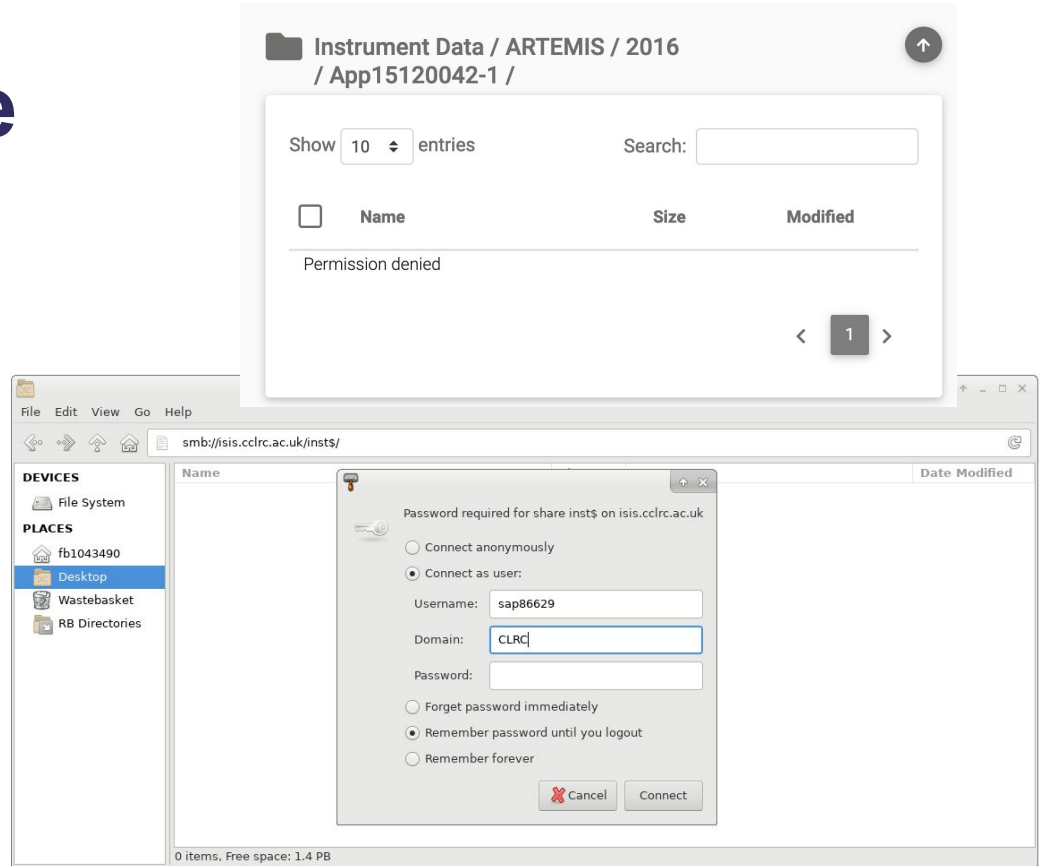
# Platform: Scale

- Research groups/scientists
- Resources (compute, data)
- Scientific Software
- Digital Research Infrastructure



# Platform: Secure

- OS Kernel Updates
- Software updates
- Data permission control
- Web security



"It was super convenient, to have the web based access to the cluster and it worked out really very nice."

"It was amazing to have everything in one place and you have it immediately from a browser."

"The platform is a life saver for us to continue our research during pandemic without any interruption."

"The platform removes all the complexity of computing, it just works out of box"

"We cannot work without the platform, it is our mission-critical application. We are so lucky to have it."

"It is such a great platform, I wish we have it in our institution."

# 2023 forward

Scientific  
Software  
Self-service

Training  
Platform

Partnerships

# We are hiring!



# Acknowledgements



Scientific Computing



ISIS Neutron and Muon Source



STFC Cloud Group

SC Data Service Group

SC Research Infrastructure Group



Central Laser Facility



Scientific Computing