STFC

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Science and Technology Facilities Council

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Overview

- STFC – ISIS facility
- Team @ STFC
- The Portal Architecture test experience
- Facility needs
- ISIS DAaaS
- COVID and the impact on the team's roadmap
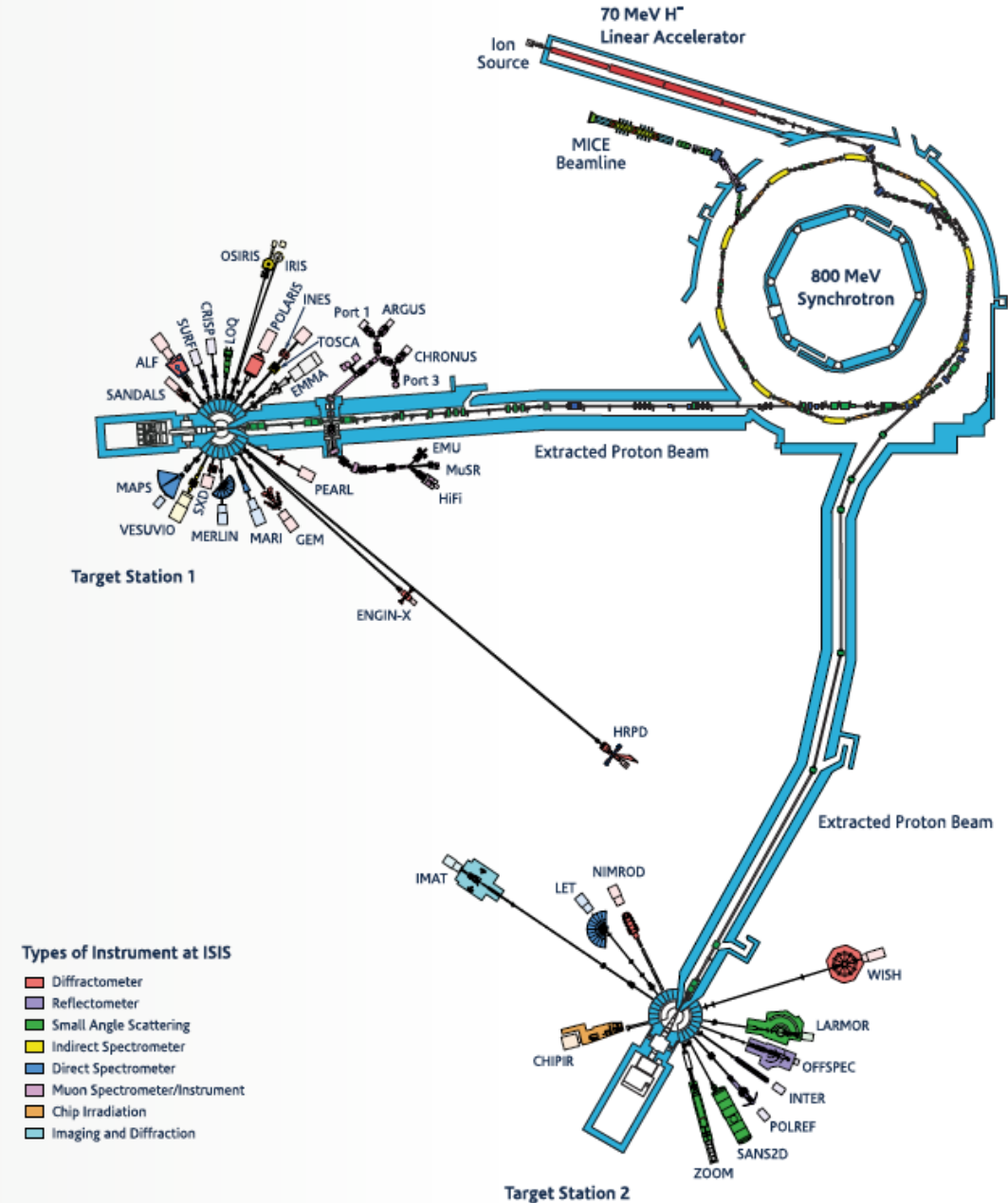
Facility

Name: ISIS Neutron and Muon Source,
Part of: STFC (Science and Technology Facilities Council)
Includes: ISIS and Scientific Computing Department
Location: UK
beamlines: 29 neutron beamlines, 5 muon beamlines in 2019

unique research visitors 1771

1505 proposals received from 32 countries

3478 user visits

Types of Instrument at ISIS
- Diffractometer
- Reflectometer
- Small Angle Scattering
- Indirect Spectrometer
- Direct Spectrometer
- Muon Spectrometer/Instrument
- Chip Irradiation
- Imaging and Diffraction

Team

Lamar Moore
Scientific Software Group Leader – ISIS
Expertise: data reduction (neutrons)
ExPaNDS: WP4

Brian Matthews
Data Science and Technology Group Leader – SCD
Expertise: FAIR data management
ExPaNDS: WP2 (lead), also WP3/WP5/Wp6

Stuart Pullinger
Software Developer – Software Engineering group (SCD)
Expertise: ICAT Metadata Catalogue
ExPaNDS: WP3

Abigail McBirnie
Senior Research Officer in Open Science – SCD
Expertise: library and information, knowledge, and data management
ExPaNDS: WP2

Anders Markvardsen
Analysis, Analytics and Infrastructure Section Leader – ISIS
Expertise: data policy, AAI, ML, data reduction (neutrons)
ExPaNDS: WP4

Alejandra Gonzales Beltran
Software Engineering Group Leader – SCD
Expertise: FAIR data management, data standards, software engineering
ExPaNDS: WP2/WP3

Franz Lang
Scientific Software Engineer – ISIS
Expertise: ISIS DAaaS, μ⁺SR, DFT
ExPaNDS: WP4

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The Portal Architecture test experience

- ## What went (reasonably) well?
  - installing on personal Windows 10 machine with Docker

- ## What could go better?
  - documentation: more discoverable and detailed, less technical
  - ability to test user experience without technical hurdles

- ## What is the gap between what's in your facility and what the Portal needs?
  - recent cloud update: Magnum for Kubernetes as a Service (KaaS)
  - liaising with cloud team as the first user/tester of Magnum
  - Kubernetes knowledge: workshop for staff

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Facility needs for the Portal

Must have:

- access to Ceph cluster
- NeXus/hdf5 file support
- GUI-based workflows (Mantid, Matlab, …)
- GPU compatibility
- staff/user feedback and input

ISIS DAaaS compatibility?

Nice to have:

- shared storage areas
- Slurm module (for use with ISIS SCARF)
- Singularity/docker compatibility
- technical support

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ISIS DAaaS

- supporting 28/34 instruments at ISIS

- 109 maximum concurrent VMs

- >60 scientific packages supported (many GUI-based)
  - ➢ via rpm repos, pypi , dockerhub, conda, local…

- customised environments (11 currently)
  - ➢ hardware via OpenStack + VMM
  - ➢ software via Ansible
  - ➢ permissions via ldap
  - ➢ remote connection via noVNC or RDP
  - ➢ resources recycled after 72h inactivity
  - ➢ sharing of VMs

- 4.5k CPUs, 21.6TB RAM, ~90 GPUs

- fortnightly user meetings, ticketing system

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COVID-19 and the impact on your team

- installation of new cloud resources was delayed

- remote working

- knock-on effects from more difficult recruitment at partner facilities

- remote experiments: ISIS DAaaS top priority

- filled/advertised positions:
  - Abigail McBirnie for WP2
  - summer student for WP4