

# Muon Galaxy – an open web platform for computational muon science

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# Outline

**1 Muon Spectroscopy Computational Project**

**2 Galaxy and Muon Galaxy**

**3 Demo**

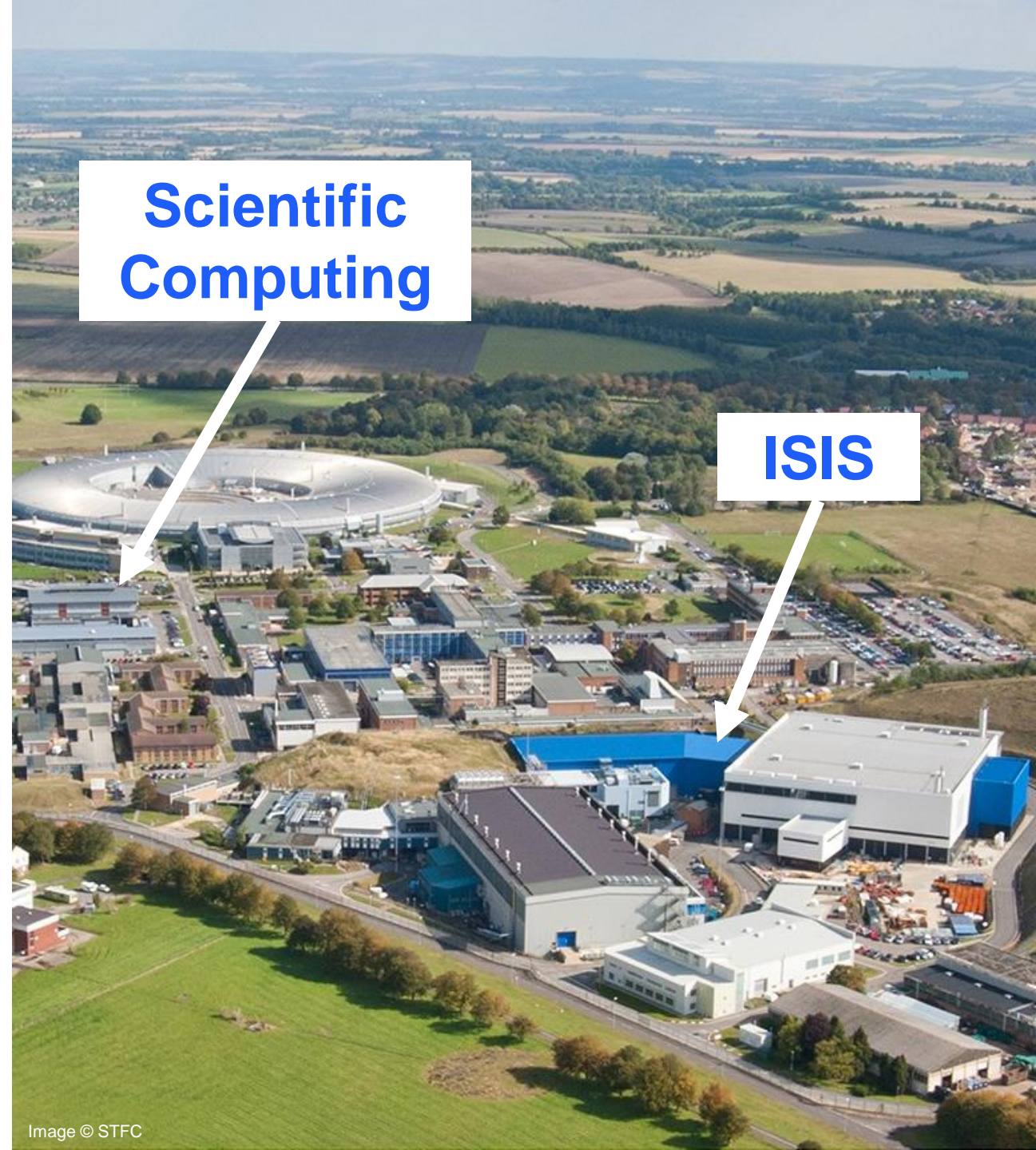
**4 Benefits of Galaxy**

**5 Upcoming Development**

# Muon Spectroscopy Computational Project (MSCP)

Collaboration between the Scientific Computing Department and the ISIS Muon Group at STFC RAL

Creating a sustainable, accessible, and open source ecosystem of tools for muon science



# MSCP Tools

- **pymuon-suite** – model muon stopping sites, phonons, and quantum effects
- **muspinsim** – model spin dynamics of systems containing a muon
- **mudirac** – muonic atom Dirac equation solver
  
- **Muon Galaxy** – GUI for the tools above (and more)

# Galaxy and Muon Galaxy



**Galaxy:** open source web platform for data intensive research

- Run complex workflows without programming experience
- Share and publish data, workflows, visualisations
- Well established in life sciences domain
- Works at scale: Galaxy Europe instance handles ~2m jobs/month

**Muon Galaxy:** extends Galaxy to include tools for muon science



# EuroScienceGateway



Horizon Europe project, WP5 focused on extending Galaxy to new domains, including materials science

**Muon Galaxy:** extends Galaxy to include tools for muon science

AND

**Materials Galaxy:** Galaxy Europe subdomain for materials science

# Muon Galaxy graphical interface to muon science tools

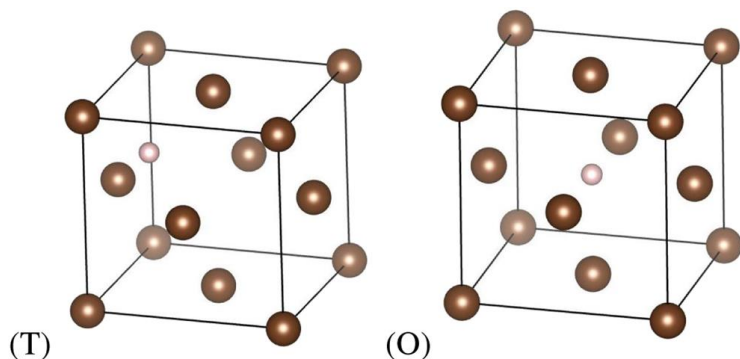
The screenshot displays the Galaxy muSR interface. At the top, the navigation bar includes 'Galaxy muSR', 'Workflow', 'Visualize', 'Shared Data', 'Admin', 'Help', 'User', and system icons. The main content area shows a workflow titled 'PyMuonSuite AIRSS UEP Optimise run UEP optimisation (Galaxy Version 0.2.1+galaxy1)'. The workflow steps are: 1: Si.castep (CASTEP log), 2: Si.cell (Muonated structures), 3: Si.den\_fmt (Charge density file), 4: Configuration for struct, 5: Muonated Si.cell using Configuration for struct, and 6: UEP results for Muonated Si.cell using Configuration for struct. A 'History' panel on the right lists these steps in reverse order. A 'Tools' panel on the left lists available tools like 'PyMuonSuite AIRSS Cluster', 'PyMuonSuite AIRSS DFTB+ Optimise', and 'PyMuonSuite AIRSS Generate'. A 'WORKFLOWS' section is also visible at the bottom left.

Tools connect to command-line programs

Workflows chain tools together

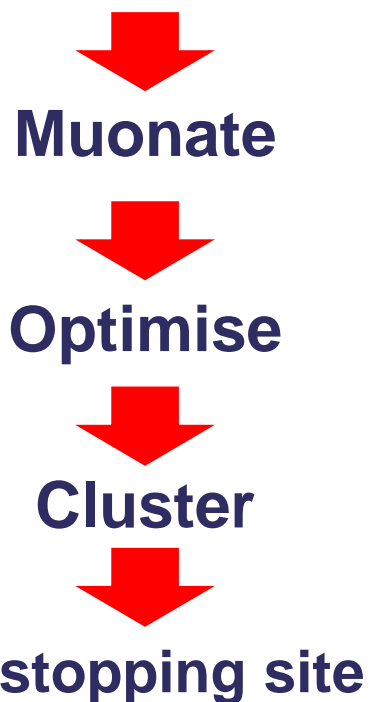
History stores data files – input and output

# A Muon Simulation Workflow



Example: crystalline metallic copper. Small pink dots are muon stopping sites

Structure file from DFT



Perform these stages with Muon Galaxy



# Demo

Recorded by Anish Mudaraddi

# Benefits of Galaxy

# Adding tools is easy


1. Write an XML file to configure the tool
2. Publish on the Galaxy 'Tool Shed' repository
3. Install on any Galaxy instance!

No need to write any web UI – Galaxy renders the tool form automatically according to the XML.

Support from tutorials, best practices, and Galaxy community 😊

# Reproducibility

- Tools and workflows are versioned

 PyMuonSuite AIRSS UEP Optimise run UEP optimisation (Galaxy Version 0.2.1+galaxy1)

- Tools run in pre-built containers with the relevant dependencies – jobs can be rerun with *exactly* the same environment
- Histories can be made public & importable by others via link
- Workflows can be published and given a DOI

# Interactive Tools

- e.g. Jupyter Notebooks with custom environments
- Run in containers on the server
  - Read and write to/from the Galaxy history
  - Can use multiple interactive tools at once
  - Closing the browser tab doesn't stop the tool – you can navigate back to it later
- Include in workflows just like any other tool

Tools ☆ ▼search tools ×⬆ Upload DataInteractive tools ▲**Interactive JupyterTool and notebook****GPU enabled Interactive Jupyter Notebook for Machine Learning****Interactive Climate Notebook****Interactive Pangeo Notebook****RStudio****Pylron Interactive Jupyter Notebook****HiGlass** an interactive Hi-C data visualizer.**OpenRefine** Working with messy data**Ubuntu XFCE Desktop****Panoply** interactive plotting tool for geo-referenced data**AskOmics** a visual SPARQL query builder**Interactive CellXgene Environment**

# Tutorials

- Galaxy has **excellent** tutorial infrastructure
- Slides & tutorials configurable as Markdown files
- Videos created alongside
- Community experience running training workshops
- Tutorials for developers and admins too!



# Further Galaxy features

- Dataset collections – run jobs on collections of many files
- Pull reference data from external databases
- Run multi-core jobs on a compute cluster or HPC
- Administration – automated configuration with Ansible
- Subcommunities / subdomains for climate, genomics, ecology... and materials!

# Other users of Galaxy for materials

- **Oak Ridge National Lab** – neutron scattering analysis using supercomputer resources
- **X-ray Imaging of Microstructures Gateway (XIMG)** – supporting users of Cornell High Energy Synchrotron Source (CHESS) with tools for X-ray scattering analysis



# Upcoming Development

- More tools & workflows – e.g. mudirac
- Tutorials for MSCP tools & workflows
- Improve crystvis-js visualiser
- Underlying Galaxy platform is always improving
  
- **Build the community around materials science in Galaxy**



# Thank you



**Muon Galaxy** – run by STFC

[muongalaxy.stfc.ac.uk](http://muongalaxy.stfc.ac.uk)

**Materials Galaxy** – run by Galaxy Europe:

[materials.usegalaxy.eu](http://materials.usegalaxy.eu)

Contact the team:

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Software  
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