Science and Technology Facilities Council

Scientific Computing

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Muon Galaxy – an open web platform for computational muon science

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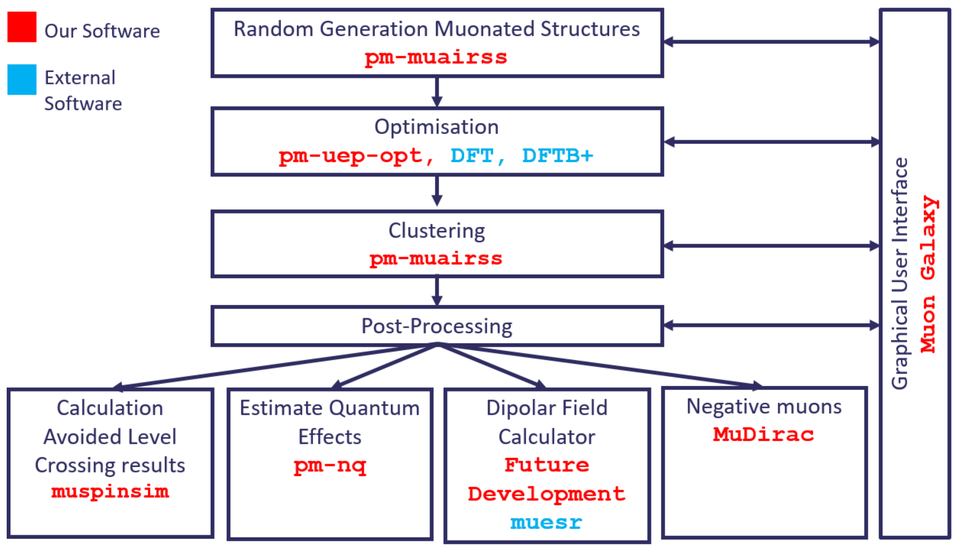
Muon Spectroscopy Computational Project

The Muon Spectroscopy Computational Project (MSCP) develops a collection of tools for tackling computational challenges in muon spectroscopy. These tools can be used to:

- Identify the **muon stopping site(s)** in a system
- Simulate the **spin dynamics** of a system containing a muon, electrons, and atomic nuclei, under different experimental setups
- Fit a spin dynamics simulation to experimental data
- Estimate **quantum effects** involving the muon, and their impact on stopping site stability
- Model **muonic atoms**

These tools can be chained together to form an analysis pipeline, as seen in the figure opposite.

We release some of our tools as Python packages: **pymuonsuite** and **muspinsim,** which can be installed using pip or conda. **mudirac** is a C++ package that can be installed from GitHub.

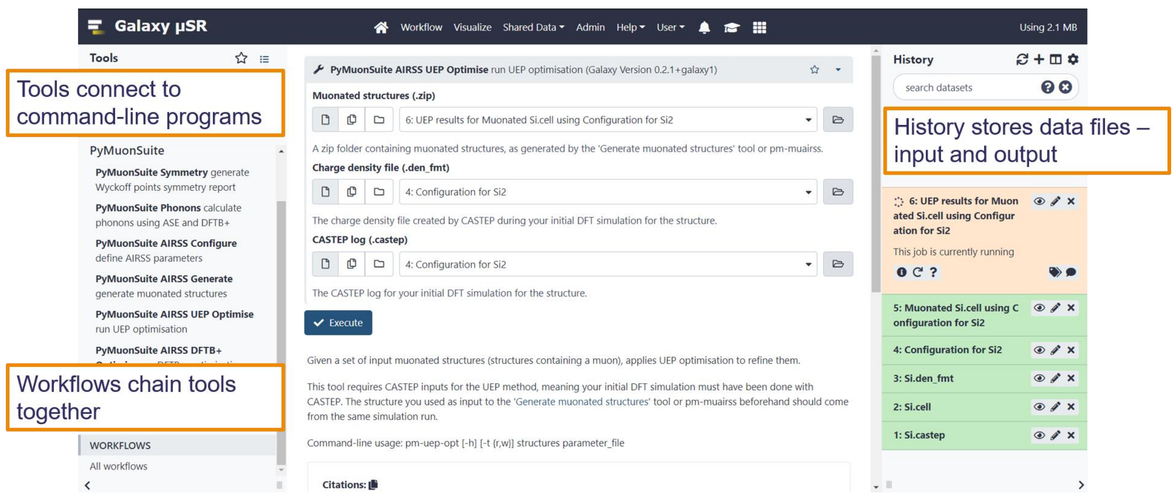


Muon Galaxy

Galaxy is an open-source web platform for data intensive research. It allows users to **run complex workflows** involving tools and visualisations without any programming experience. Analysis in Galaxy is **easily reproducible**, as a consistent computational environment is used for every job, and all data files are stored in a 'history'. Data and workflows can be **easily shared** with other researchers and / or made public; publishing a workflow alongside a paper is a great way to ensure reproducibility.

Galaxy is well established in the life sciences community, and we are extending it for muon and materials science through **Muon Galaxy** (run by STFC), and **Materials Galaxy** (run by Galaxy Europe). We are making all MSCP tools available in both instances, along with tutorials, example workflows, and visualisations.

muongalaxy.stfc.ac.uk **materials.usegalaxy.eu**



Why use Galaxy?

Modularity of Tools

Configure with XML
Publish to Tool Shed
Install in any instance

Galaxy Tool Shed

8681 valid tools on Apr 04, 2022

Reproducibility

Pre-built containers ensure environment consistency
Workflows publishable and given DOIs

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

- Version of underlying tool
- Version of Galaxy tool wrapper

Community

Benefit from global collaboration, alongside domain specific communities – we are looking to grow the **Galaxy for Materials Science Community**

Galaxy µSR

As a fork of the main Galaxy platform, we inherit its features

Galaxy

Interactive Tools

- Jupyter Notebooks
- Rstudio
- Visualisations

Usable in workflows alongside other tools

Interactive JupyTool and notebook

GPU enabled Interactive Jupyter Notebook for Machine Learning

Interactive Climate Notebook

Tutorials

- Topics cover use, development, administration of Galaxy
- Interactive tutorials, slides and video content
- Configurable via Markdown

Galaxy Training Network

HPC

Run multi-core jobs on compute clusters or HPC

Reference data

Pull data from external databases

Administration

Automated configuration management with Ansible

Data sharing

Can share data with groups of users, or make it public

MSCP

Software Sustainability Institute

ada lovelace centre

Science and Technology Facilities Council
ISIS Neutron and Muon Source

Galaxy PROJECT

eosc | EuroScienceGateway