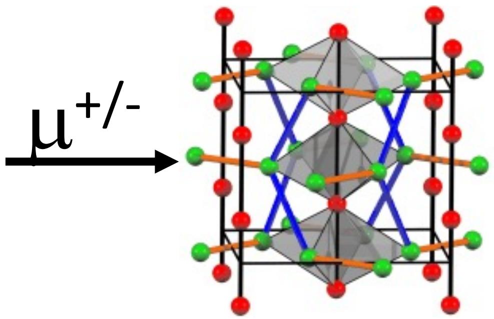
Muongalaxy – Tools, Workflows and More for Muons and Materials Science

Leandro Liborio[1], Patrick Austin[2], Alejandra González-Beltrán[2] ,
[1]Theoretical and Computational Physics Group, SCD, STFC
[2]Data and Software Engineering Group, SCD, STFC

European Galaxy Days 2023, 4th, 5th and 6th October, Freiburg, Germany

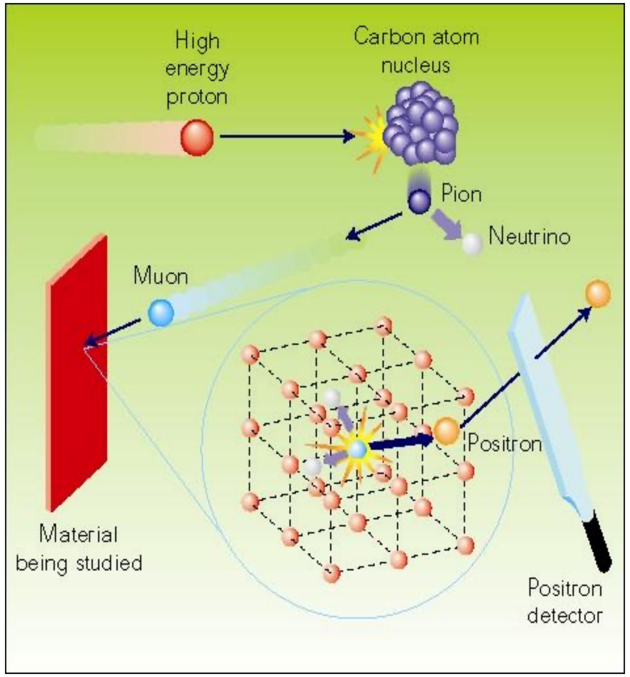
What are Muons?



Properties

- Sub-atomic particles
- Heavy electron / Light proton
- Implanted into a sample
- Lifetime 2.2 ms
- μSR experiments in TS1

Implantation site



Importance of Simulations

- **Started approx. 10 years ago**
- Important for interpreting experiments
- Muon Spectroscopy Computational Project is part of this approach

MSCP

Muon Spectroscopy Computational Project

https://muon-spectroscopy-computational-project.github.io

Sustainable, User-friendly and Reproducible Software Tools for Interpreting Muon Experiments

MuDirac
treat muonic atoms

pymuon-suite
muon stopping sites

MSCP

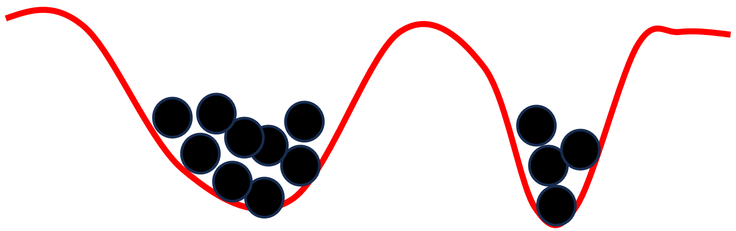
pm-nq
muon quantum effects

Muspinsim
spin dynamics of systems of a muon plus other spins

eosc | EuroScienceGateway

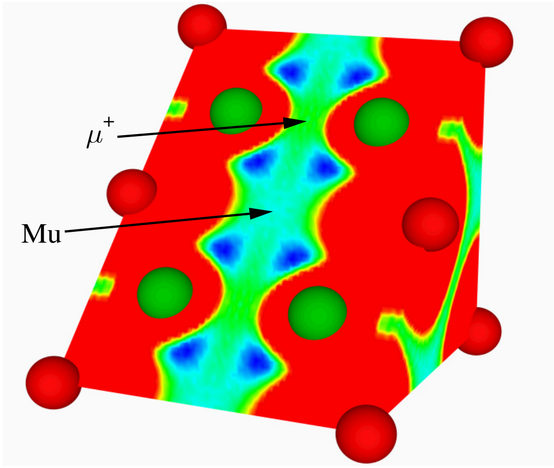
Muon Galaxy *Leandro Liborio-TCPG, Patrick Austin-DSEG, Eli Chadwick-TCPG, Alejandra G. Beltran-DSEG*

Theoretical Basis of our Variant of the UEP Method



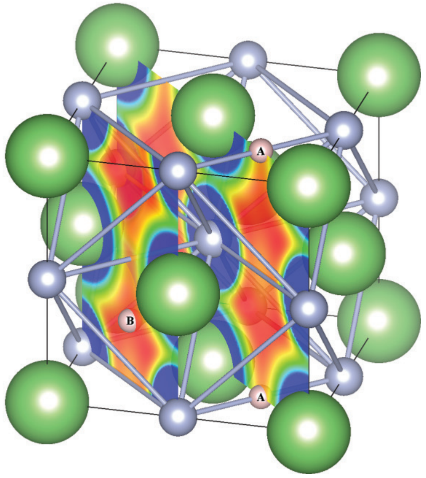
Schematic electrostatic potential landscape. Similar minima, different attractor.

μ^+ and μ^+e^- in CaF



PRB **87**, 121108(R) (2013)

μ^+ in YF_3



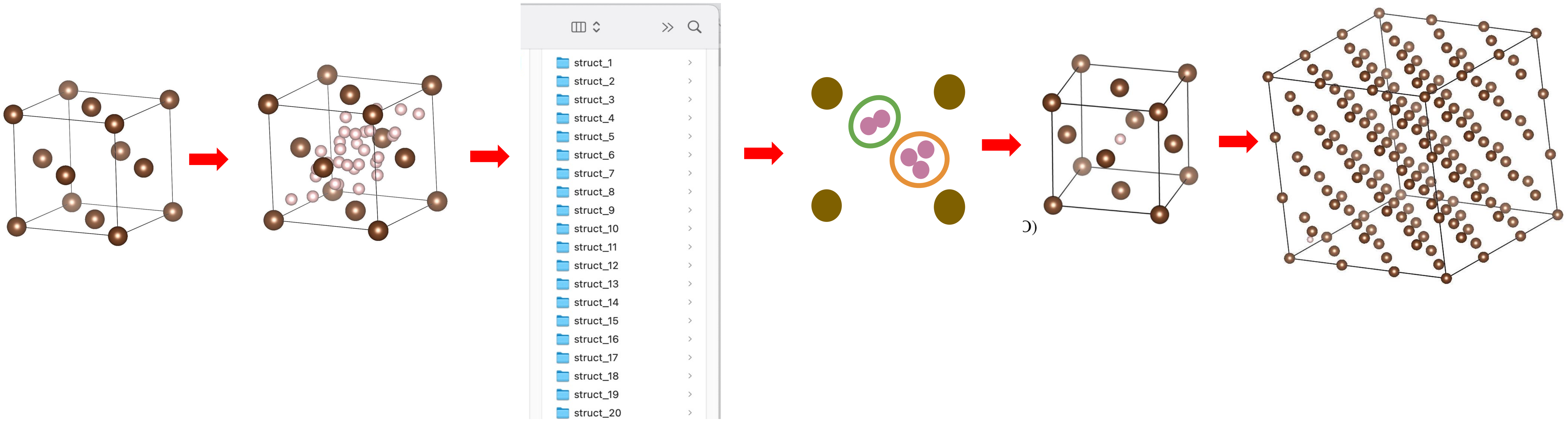
PRB **87**, 115148 (2013)

- **Efficient method to scan 3D electrostatic potential of samples**
- **Uses clusters to determine the 'attractor size' and value of electrostatic potential's minima**
- **Relies on only <u>ONE</u> DFT simulation of the unperturbed host material**
- **Tested in many systems and proven reliable. However, users must exercise scientific criteria when analyzing results form the method**

S. Sturniolo and L. Liborio, The Journal of Chemical Physics, 153, 044111 (2020)

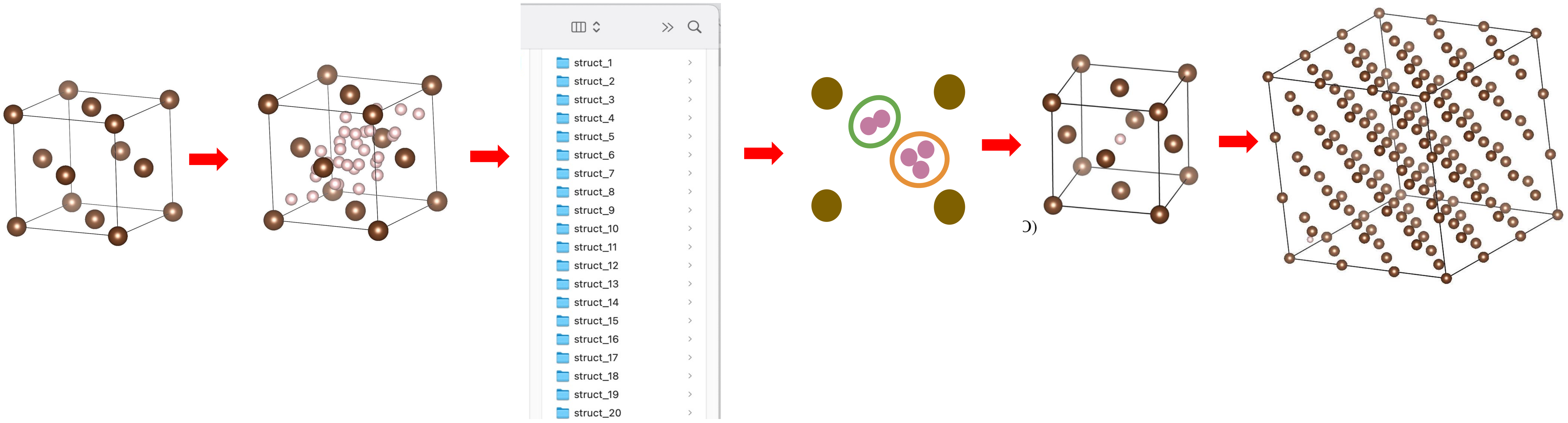
Workflow for Finding the μ^+ stopping site

1. DFT pure host
2. Create randomly populated muonated structures
3. Relax electrostatic forces on muons
4. Cluster relaxed structures
5. μ^+ stopping sites
6. DFT supercell muonated structures



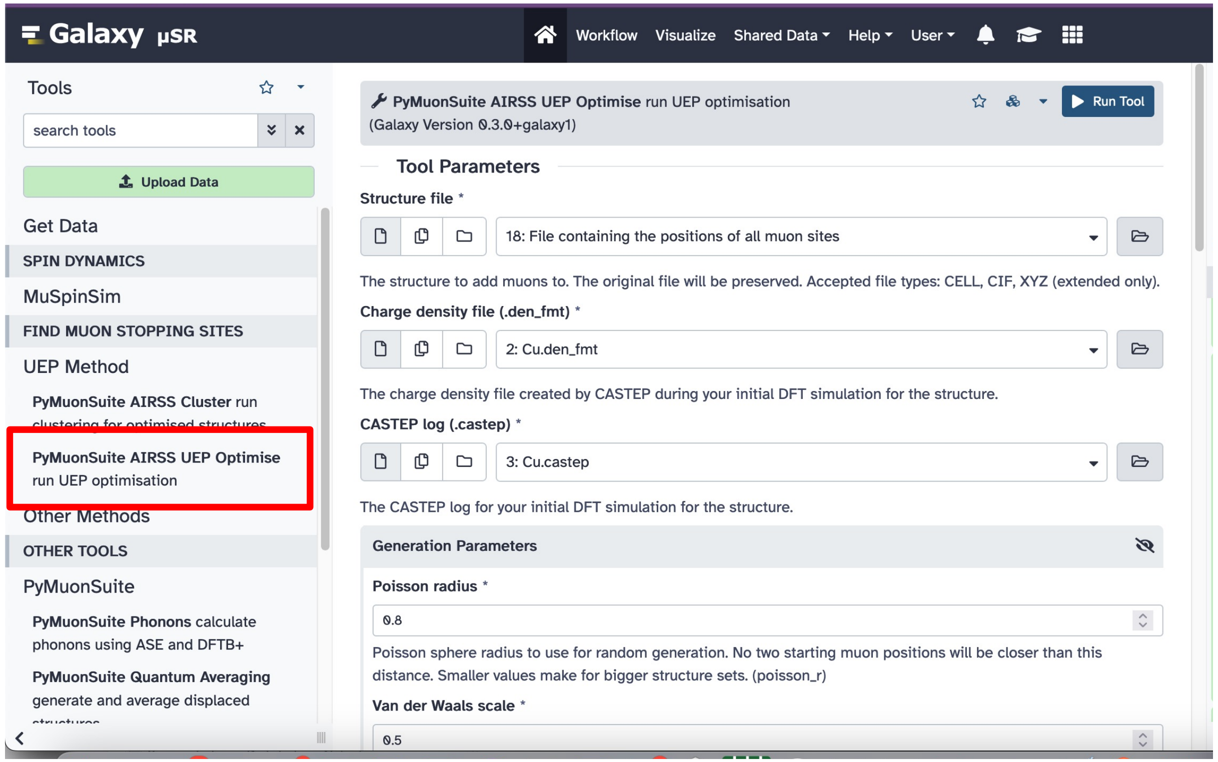
Workflow for Finding the μ^+ stopping site: `command line tools`

1 CASTEP → 2 `pm-muairss` → 3 `pm-uep-opt` → 4 `pm-muairss` → 5 μ^+ stopping sites → 6 CASTEP

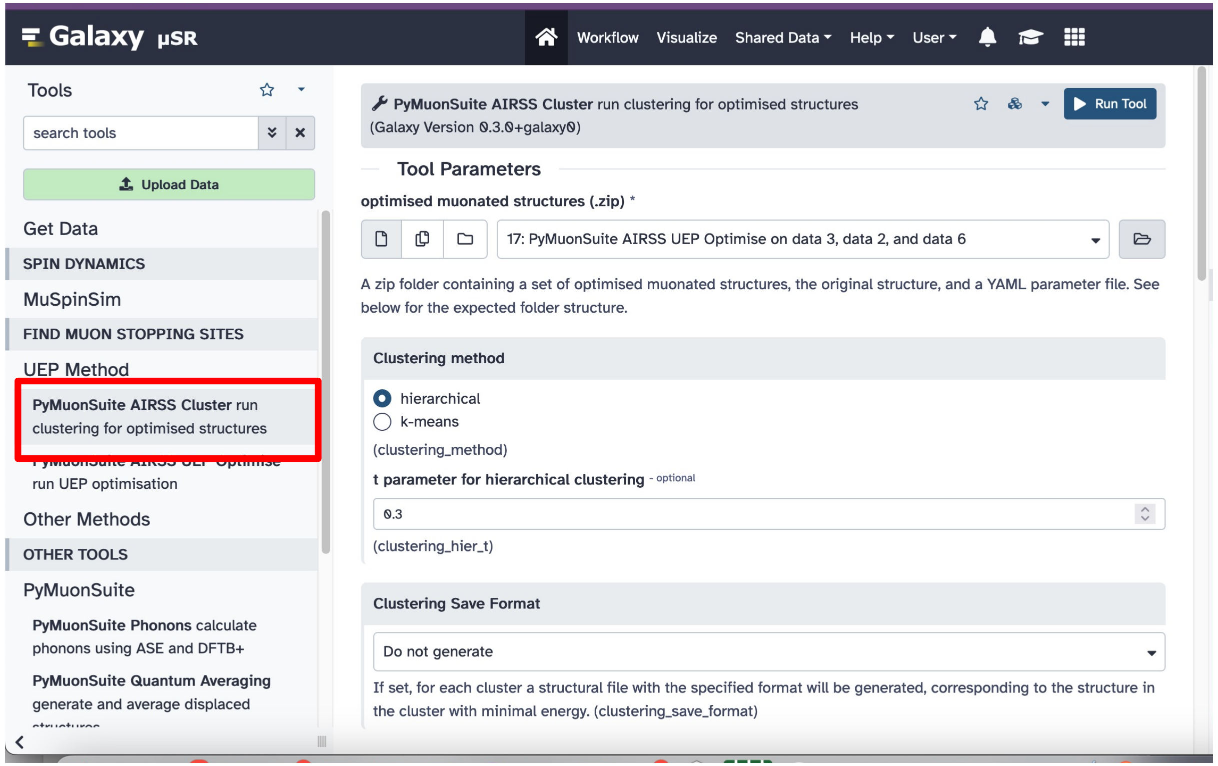


Workflow for Finding the μ^+ stopping site in Galaxy PROJECT

1 CASTEP → 2 3 **PyMuonSuite AIRSS UEP Optimise** run UEP optimisation → 4 **PyMuonSuite AIRSS Cluster** run clustering for optimised structures → 5 μ^+ stopping sites → 6 CASTEP



PyMuonSuite AIRSS UEP Optimise
run UEP optimisation



PyMuonSuite AIRSS Cluster
run clustering for optimised structures

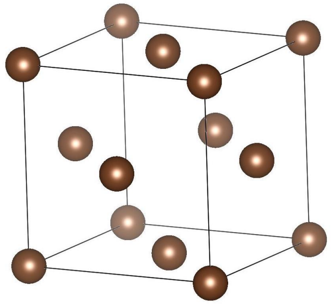
Workflow for Finding the μ^+ stopping site in Galaxy PROJECT

CASTEP → **PyMuonSuite AIRSS UEP Optimise** run UEP optimisation → **PyMuonSuite AIRSS Cluster** run clustering for optimised structures → μ^+ stopping sites → CASTEP

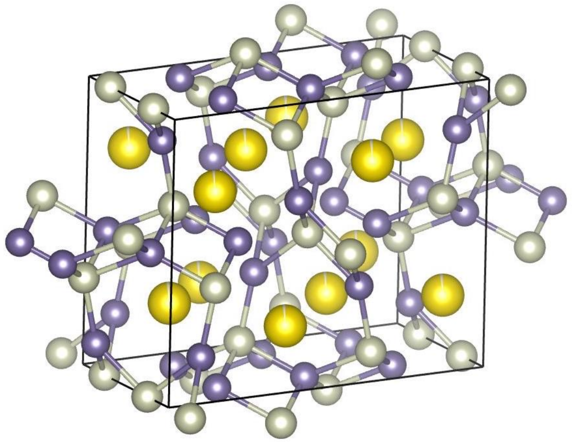
https://muongalaxy.stfc.ac.uk/

1

DFT Relaxation of Pure Host material with CASTEP



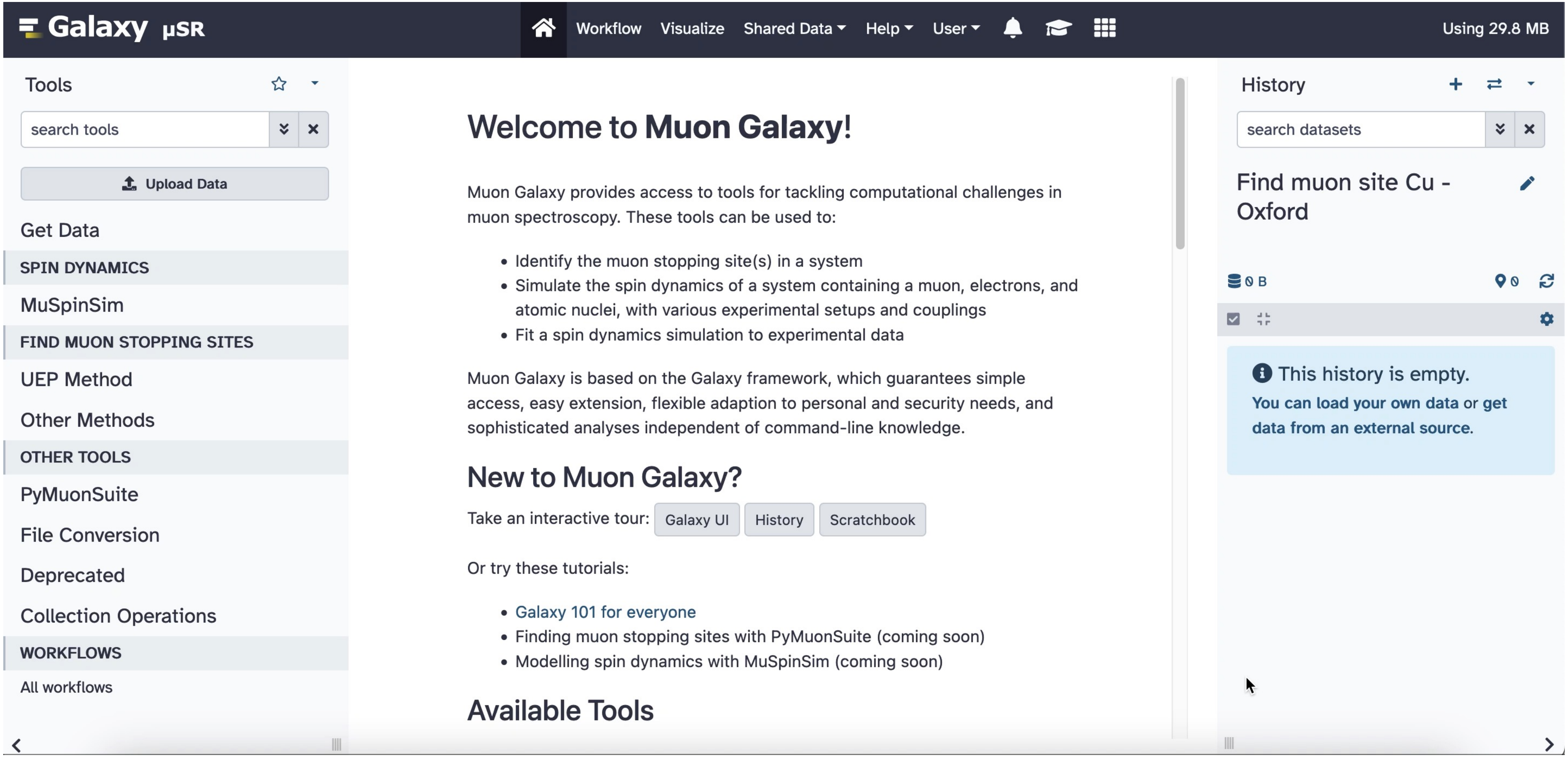
Cu



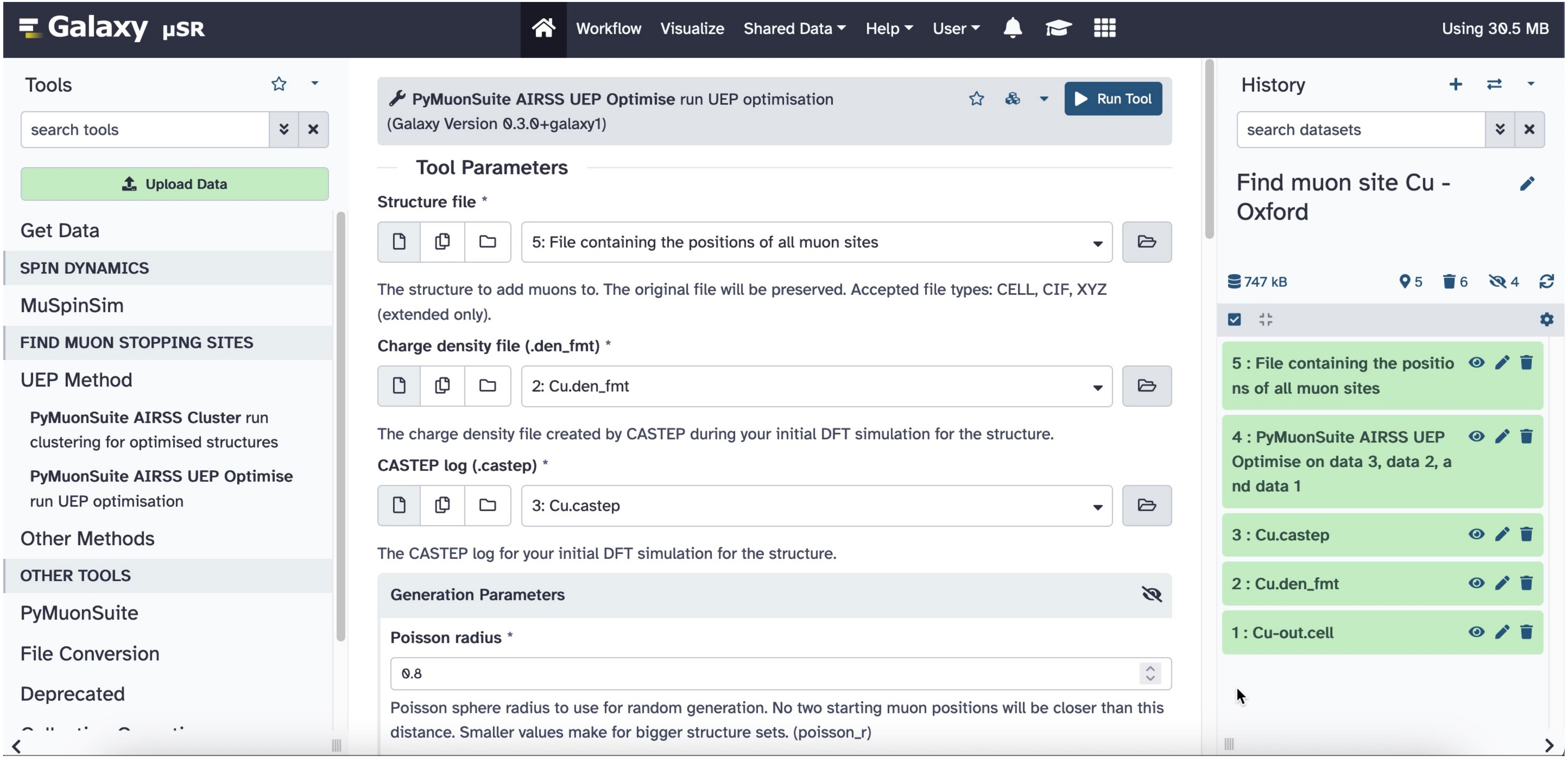
$Pr_2Rh_3Ge_5$

- Can provide access to Scarf cluster
- Can provide **basic** support for CASTEP simulations
- Need 3 files:
  - **Cu.castep** (main CASTEP output file)
  - **Cu.den_fmt** (CASTEP charge density file)
  - **Cu-out.cell** (CASTEP structural file for the relaxed host material)

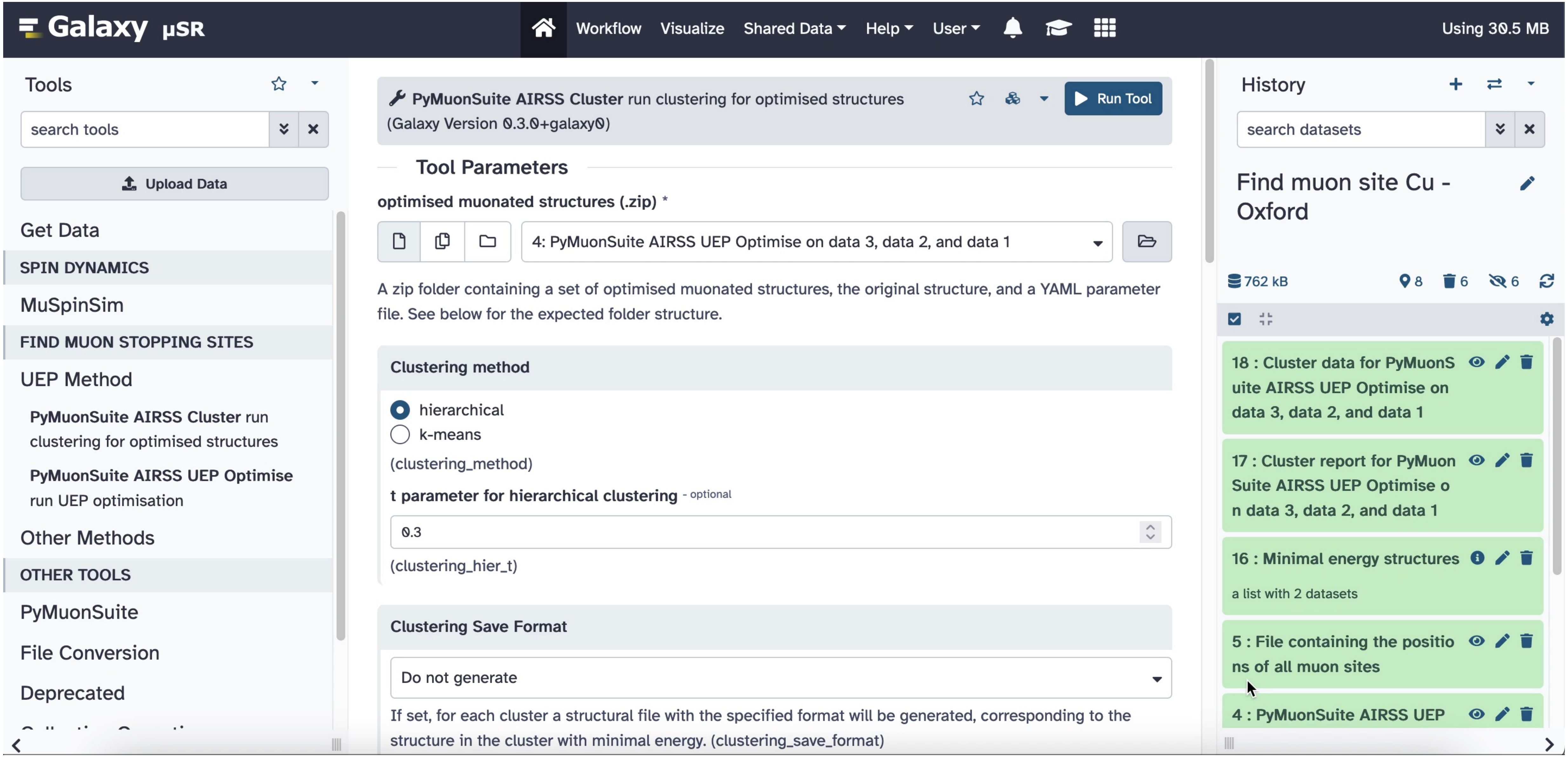
PyMuonSuite AIRSS UEP Optimise: Galaxy PROJECT



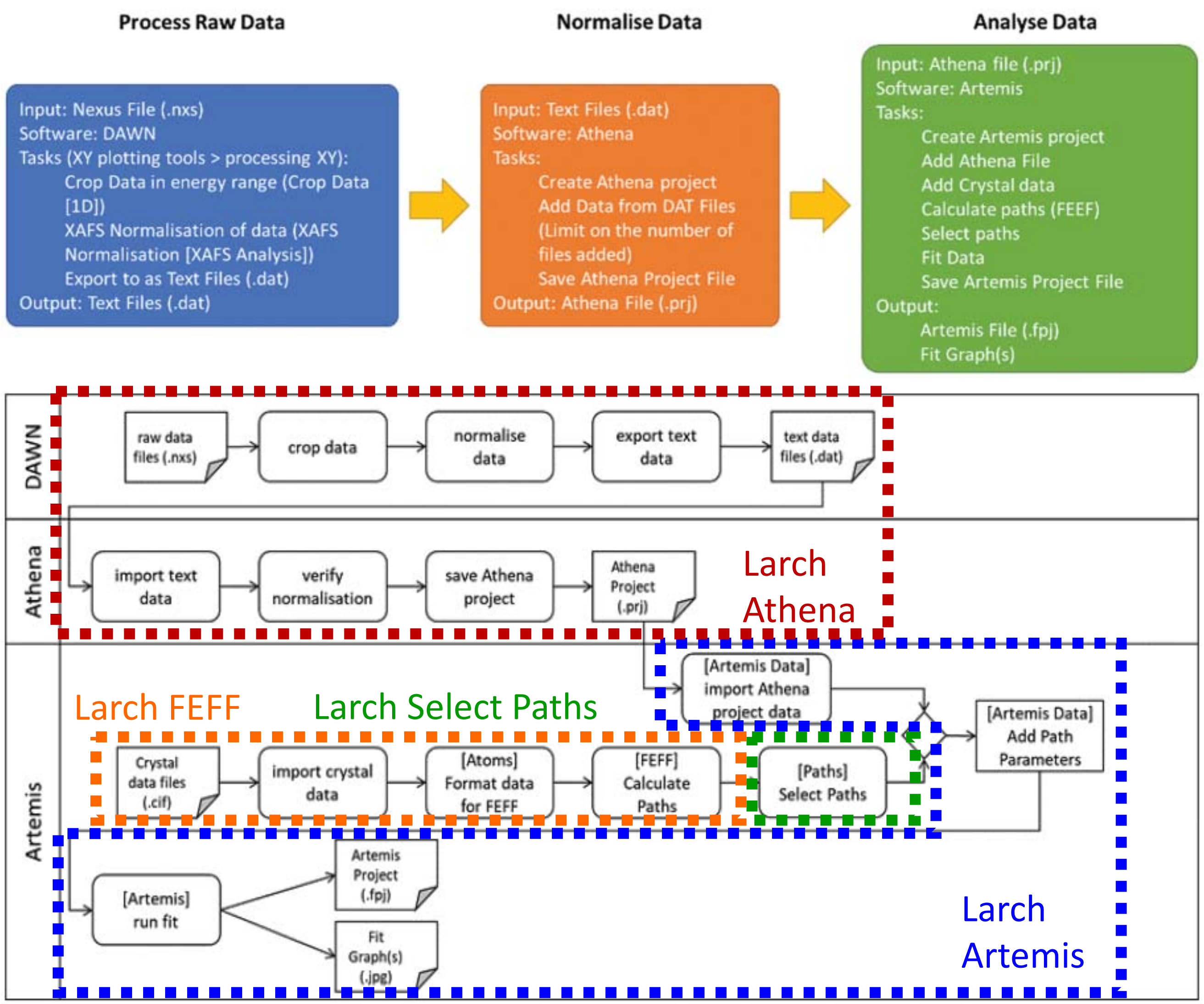
PyMuonSuite AIRSS Cluster:



Workflow creation:



Galaxy Tools for XAS Data Processing



Portions of the existing workflow are covered by different "tools" in Galaxy. Each tool executes a Python script which uses the Larch library:

- Larch Athena:
  - Processing and Normalization of raw data
  - Cropping energy range of data
  - Outputs Athena project file and plots
- Larch FEFF:
  - Load from cif and converts to FEFF input file (or loads FEFF input directly)
  - Outputs zipped directory of FEFF paths
- Larch Select Paths:
  - Selects which paths from Larch FEFF to use
  - Defines GDS parameters for these paths
- Larch Artemis:
  - Performs fitting on FEFF paths
  - Outputs report on fitting and plots

Have also implemented a 5th tool for combining and plotting results from multiple files (not shown on diagram).

PSDI PHYSICAL SCIENCES DATA INFRASTRUCTURE

CatalysisHub

Conclusions and Future Work

- Our version of the UEP method can be efficiently used to predict muon stopping sites.
- It can be run as a command-line tool or in muongalaxy.
- The method requires **properly converged CASTEP DFT simulations**.
- We will officially release this method at 2024 Muon Intn'l Workshop @ STFC.
- Working on expanding Galaxy to XAS catalysis experiments -> Materials Galaxy

Muon Spectroscopy Computational Project

https://muon-spectroscopy-computational-project.github.io/

Theoretical and Computational Physics Group - SCD

LIBORIO

STURNIOLO

Now @ comind™

CHADWICK

Now @ The Carpentries

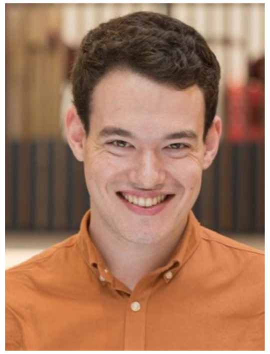
PLUMMER

Muon Group - ISIS

HILLIER

PRATT

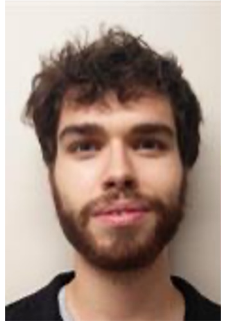
COTTRELL



WILKINSON

Data & Software Engineering Group SCD

GONZALEZ-BELTRAN



AUSTIN

SCD Graduates:

Joel Davies
Anish Muddaradi
Jyothish Thomas
Samuel Jackson
Adam Laverack
Thomas Dack
Josh Owen
Laura Murgatroyd
Sarah Byrne

UKRI Science and Technology Facilities Council

ISIS Neutron and Muon Source

Galaxy PROJECT

ada lovelace centre

MSCP