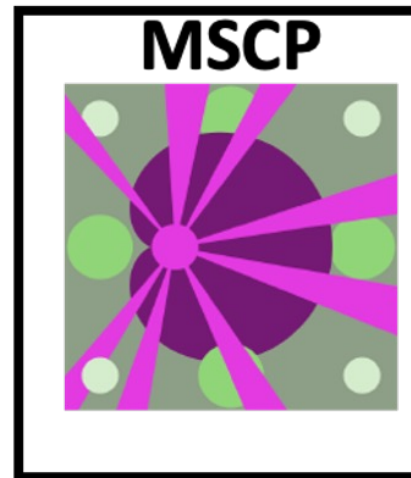


Muongalaxy – Tools, Workflows and More for Muons and Materials Science

Leandro Liborio¹, Patrick Austin², Alejandra González-Beltrán²,

¹Theoretical and Computational Physics Group, SCD, STFC

²Data and Software Engineering Group, SCD, STFC



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

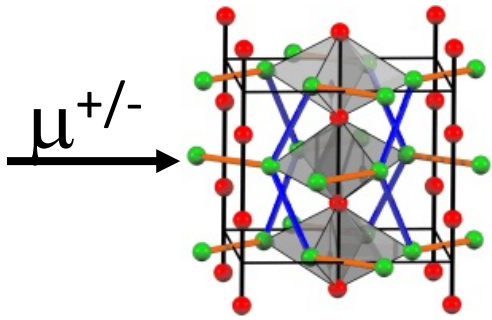


ISIS Neutron and
Muon Source



Software
Sustainability
Institute

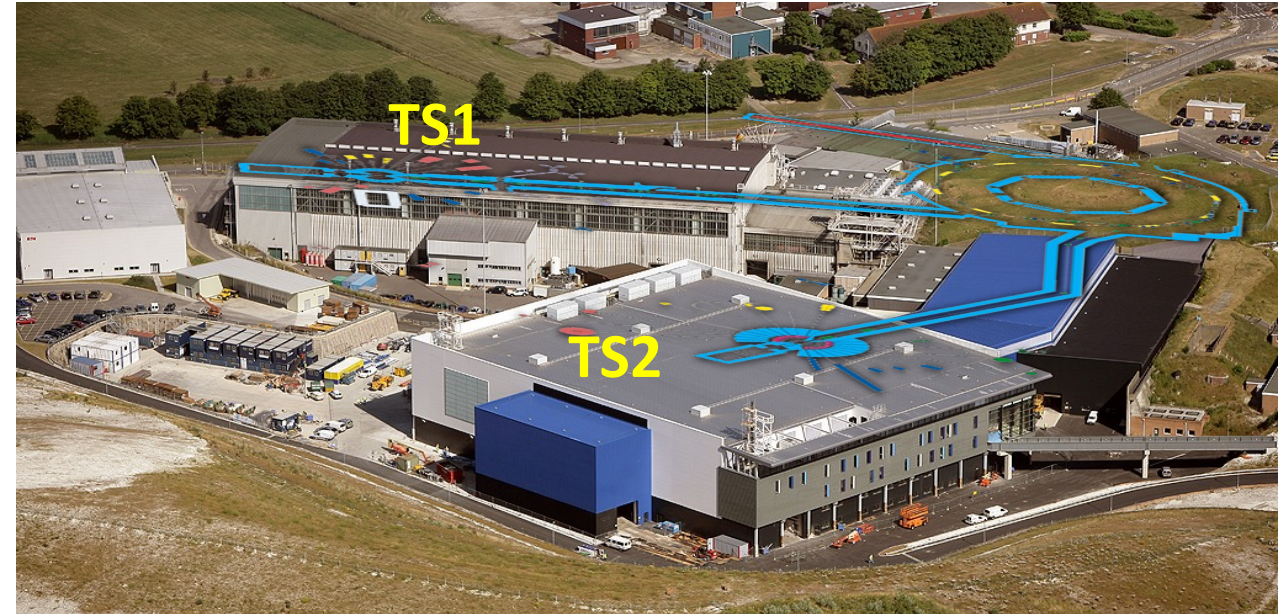
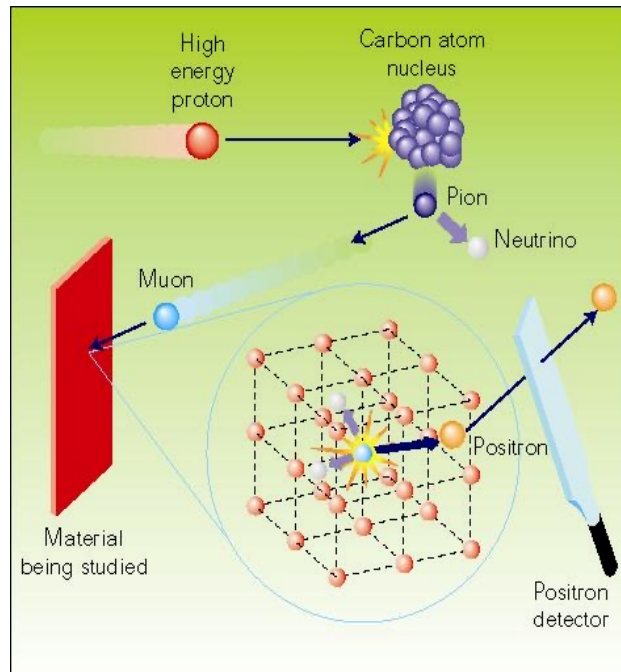
What are Muons?



Properties

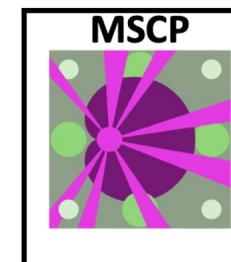
- Sub-atomic particles
- Heavy electron / Light proton
- Implanted into a sample
- Lifetime 2.2 ms
- μ SR experiments in TS1

Implantation site



Importance of Simulations

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



Muon Spectroscopy Computational Project

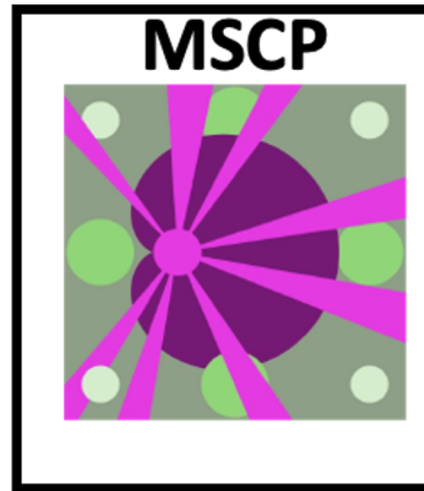
<https://muon-spectroscopy-computational-project.github.io>

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

MuDirac

treat muonic atoms

pymuon-suite
muon stopping sites



pm-nq

muon quantum effects

Muspinsim

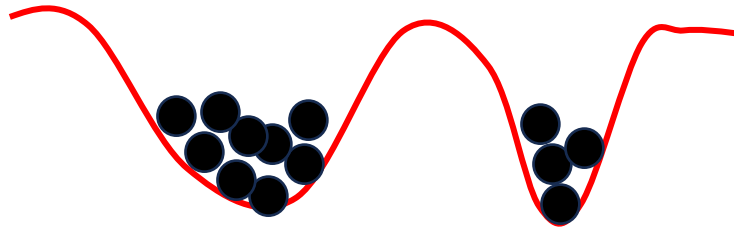
spin dynamics of systems of a muon
plus other spins

 **eOSC**

EuroScienceGateway

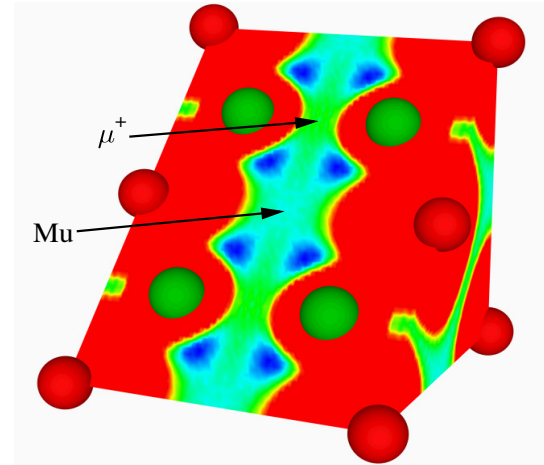
Muon Galaxy *Leandro Liborio-TCPG, Patrick Austin-DSEG, Eli Chadwick-TCPG, Alejandra G. Beltran-DSEG*

Theoretical Basis of our Variant of the UEP Method



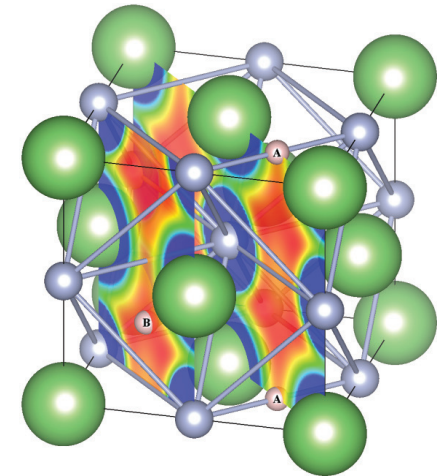
Schematic electrostatic potential landscape. Similar minima, different attractor.

μ^+ and μ^+e^- in CaF



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

μ^+ in YF₃



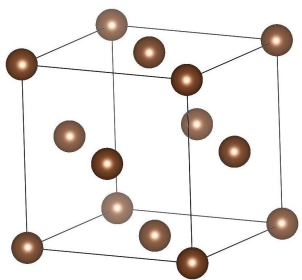
PRB **87**, 115148 (2013)

- **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 ONE DFT simulation of the unperturbed host material**
- **Tested in many systems and proven reliable. However, users must exercise scientific criteria when analyzing results from the method**

Workflow for Finding the μ^+ stopping site

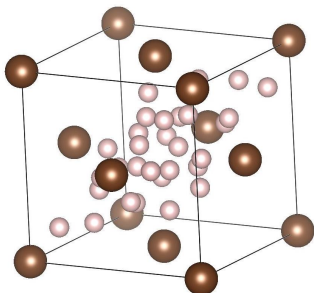
1

DFT pure host



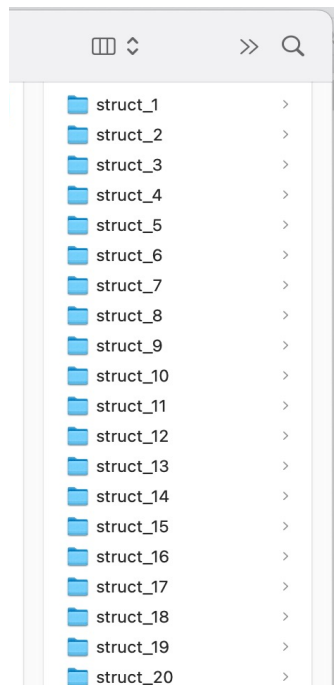
2

Create randomly populated muonated structures



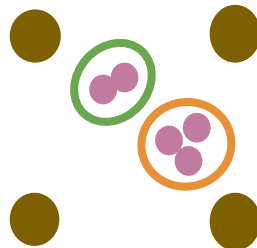
3

Relax electrostatic forces on muons



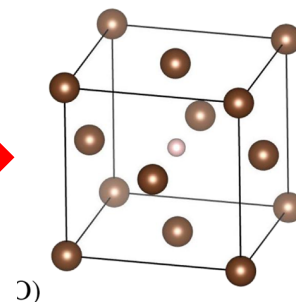
4

Cluster relaxed structures



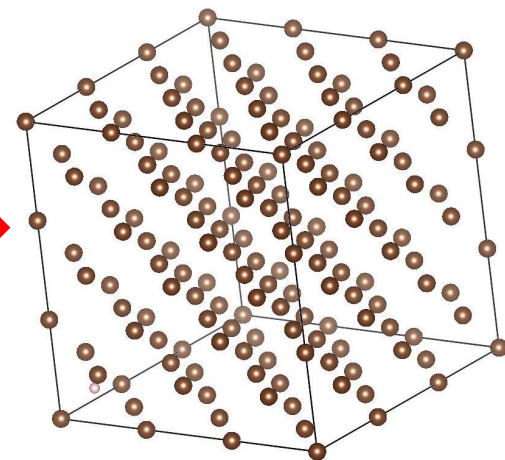
5

μ^+ stopping sites



6

DFT supercell muonated structures



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

1



2

`pm-muairss`



3

`pm-uep-opt`



4

`pm-muairss`

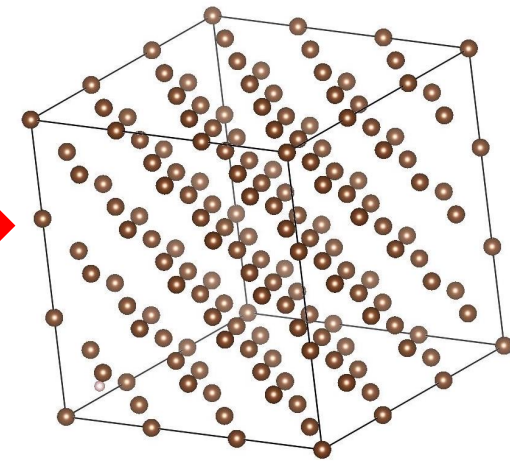
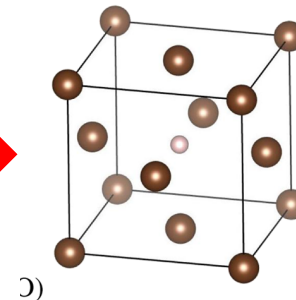
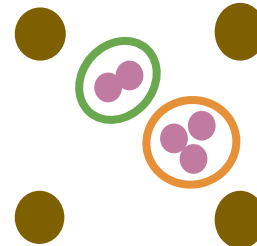
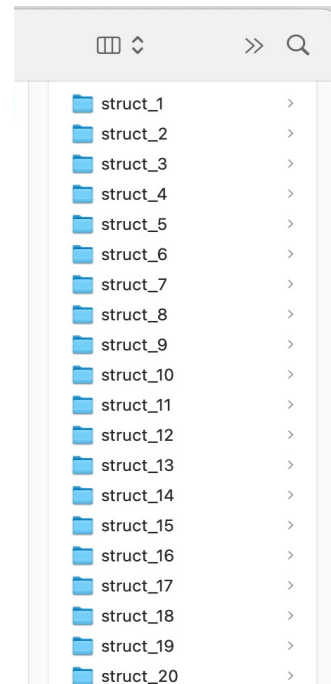
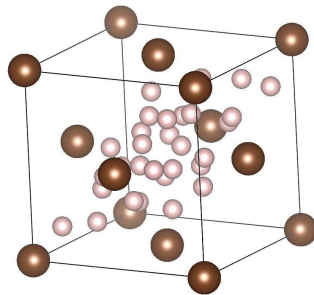
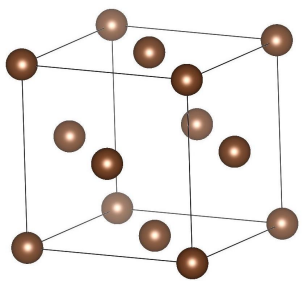


5

μ^+ stopping sites



6



Workflow for Finding the μ^+ stopping site in

1



2

PyMuonSuite AIRSS UEP Optimise
run UEP optimisation



3

PyMuonSuite AIRSS Cluster
run clustering for optimised
structures

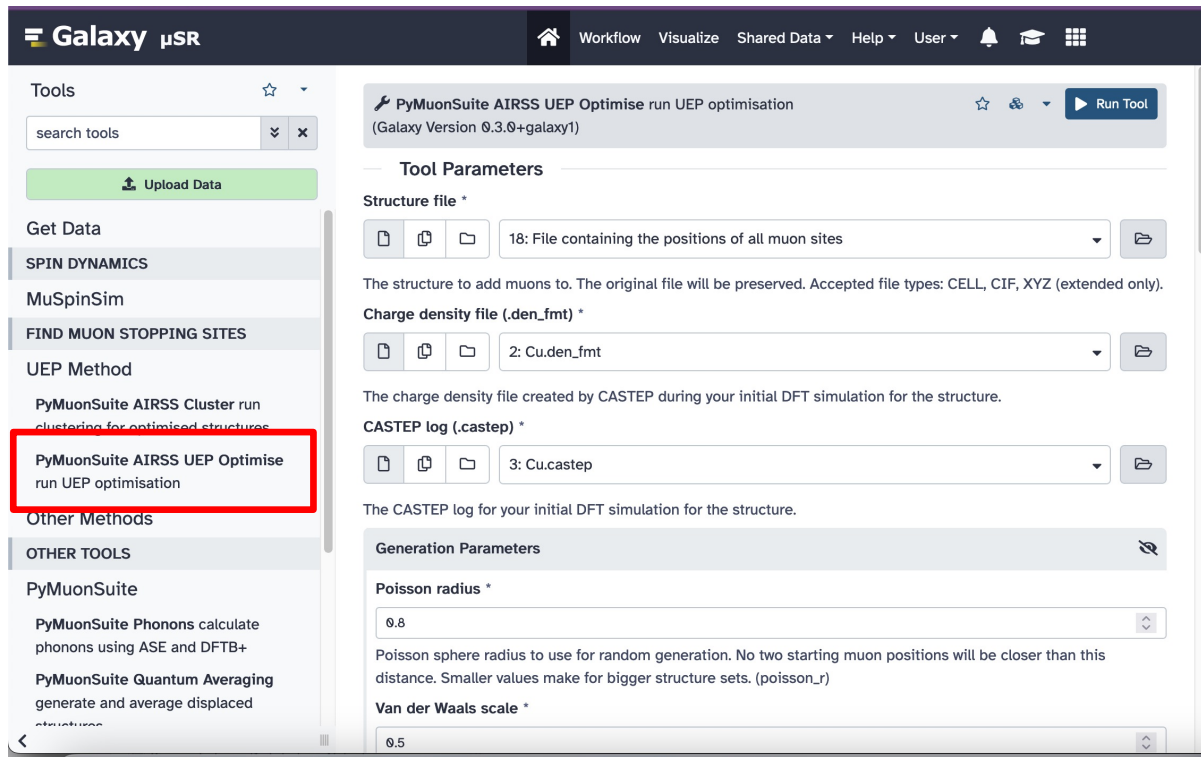


5

μ^+ stopping
sites



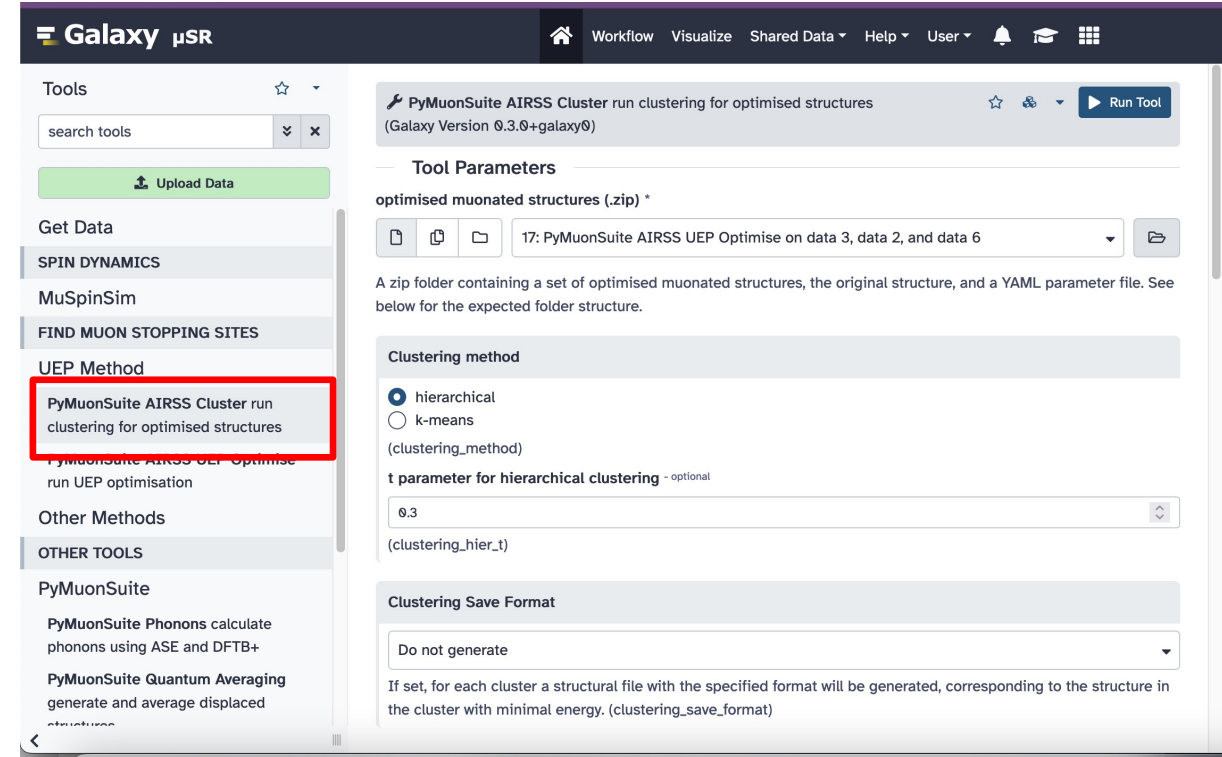
6



The screenshot shows the Galaxy interface for the tool "PyMuonSuite AIRSS UEP Optimise run UEP optimisation". The tool parameters are as follows:

- Structure file *: 18: File containing the positions of all muon sites
- Charge density file (.den_fmt) *: 2: Cu.den_fmt
- CASTEP log (.castep) *: 3: Cu.castep
- Generation Parameters:
 - Poisson radius *: 0.8
 - Van der Waals scale *: 0.5

PyMuonSuite AIRSS UEP Optimise
run UEP optimisation



The screenshot shows the Galaxy interface for the tool "PyMuonSuite AIRSS Cluster run clustering for optimised structures". The tool parameters are as follows:

- optimised muonated structures (.zip) *: 17: PyMuonSuite AIRSS UEP Optimise on data 3, data 2, and data 6
- Clustering method:
 - hierarchical
 - k-means
- t parameter for hierarchical clustering - optional: 0.3
- Clustering Save Format: Do not generate

PyMuonSuite AIRSS Cluster
run clustering for optimised structures

Workflow for Finding the μ^+ stopping site in



PyMuonSuite AIRSS UEP Optimise
run UEP optimisation



PyMuonSuite AIRSS Cluster
run clustering for optimised
structures



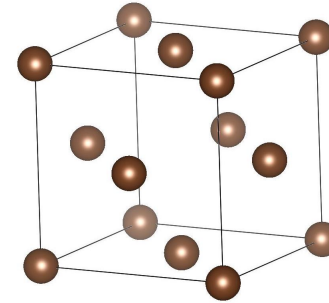
μ^+ stopping
sites



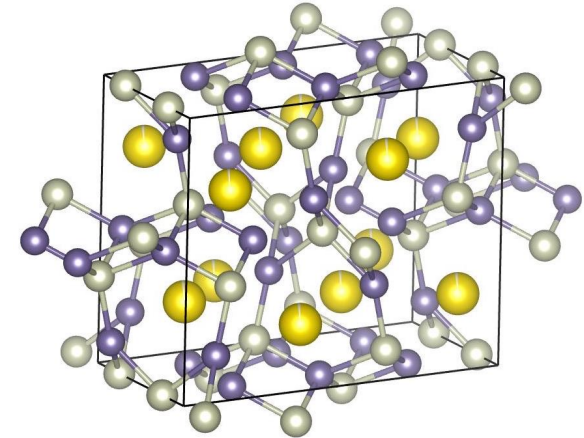
<https://muongalaxy.stfc.ac.uk/>

1

DFT Relaxation of Pure Host material with




Cu






Pr₂Rh₃Ge₅



- 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** μ SR Using 29.8 MB

[Home](#) [Workflow](#) [Visualize](#) [Shared Data](#) [Help](#) [User](#)   

Tools

search tools  

 Upload Data

Get Data

- SPIN DYNAMICS
- MuSpinSim
- FIND MUON STOPPING SITES
- UEP Method
- Other Methods

OTHER TOOLS

- PyMuonSuite
- File Conversion
- Deprecated
- Collection Operations

WORKFLOWS

- All workflows

Welcome to Muon Galaxy!

Muon Galaxy provides access to 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, with various experimental setups and couplings
- Fit a spin dynamics simulation to experimental data

Muon Galaxy is based on the Galaxy framework, which guarantees simple access, easy extension, flexible adaption to personal and security needs, and sophisticated analyses independent of command-line knowledge.

New to Muon Galaxy?



Take an interactive tour: [Galaxy UI](#) [History](#) [Scratchbook](#)


Or try these tutorials:




- [Galaxy 101 for everyone](#)
- [Finding muon stopping sites with PyMuonSuite \(coming soon\)](#)
- [Modelling spin dynamics with MuSpinSim \(coming soon\)](#)



Available Tools


History

search datasets  

Find muon site Cu - Oxford 

 0 B  0 

 This history is empty.
You can load your own data or get data from an external source.

PyMuonSuite AIRSS Cluster: Galaxy PROJECT

Tools

search tools

Upload Data

Get Data

SPIN DYNAMICS

MuSpinSim

FIND MUON STOPPING SITES

UEP Method

PyMuonSuite AIRSS Cluster run clustering for optimised structures

PyMuonSuite AIRSS UEP Optimise run UEP optimisation

Other Methods

OTHER TOOLS

PyMuonSuite

File Conversion

Deprecated

PyMuonSuite AIRSS UEP Optimise run UEP optimisation

(Galaxy Version 0.3.0+galaxy1)

Run Tool

Tool Parameters

Structure file *

5: File containing the positions of all muon sites

The structure to add muons to. The original file will be preserved. Accepted file types: CELL, CIF, XYZ (extended only).

Charge density file (.den_fmt) *

2: Cu.den_fmt

The charge density file created by CASTEP during your initial DFT simulation for the structure.

CASTEP log (.castep) *

3: Cu.castep

The CASTEP log for your initial DFT simulation for the structure.

Generation Parameters

Poisson radius *

0.8

Poisson sphere radius to use for random generation. No two starting muon positions will be closer than this distance. Smaller values make for bigger structure sets. (poisson_r)

History

search datasets

Find muon site Cu - Oxford

747 kB

5 6 4

- 5 : File containing the positions of all muon sites
- 4 : PyMuonSuite AIRSS UEP Optimise on data 3, data 2, and data 1
- 3 : Cu.castep
- 2 : Cu.den_fmt
- 1 : Cu-out.cell

Workflow creation:

Tools

search tools

Upload Data

Get Data

SPIN DYNAMICS

MuSpinSim

FIND MUON STOPPING SITES

UEP Method

PyMuonSuite AIRSS Cluster run clustering for optimised structures

PyMuonSuite AIRSS UEP Optimise run UEP optimisation

Other Methods

OTHER TOOLS

PyMuonSuite

File Conversion

Deprecated

PyMuonSuite AIRSS Cluster run clustering for optimised structures

(Galaxy Version 0.3.0+galaxy0)

Run Tool

Tool Parameters

optimised muonated structures (.zip) *

4: PyMuonSuite AIRSS UEP Optimise on data 3, data 2, and data 1

A zip folder containing a set of optimised muonated structures, the original structure, and a YAML parameter file. See below for the expected folder structure.

Clustering method

- hierarchical
- k-means

(clustering_method)

t parameter for hierarchical clustering - optional

0.3

(clustering_hier_t)

Clustering Save Format

Do not generate

If set, for each cluster a structural file with the specified format will be generated, corresponding to the structure in the cluster with minimal energy. (clustering_save_format)

History

search datasets

Find muon site Cu - Oxford

762 kB

8 6 6

+

18 : Cluster data for PyMuonSuite AIRSS UEP Optimise on data 3, data 2, and data 1

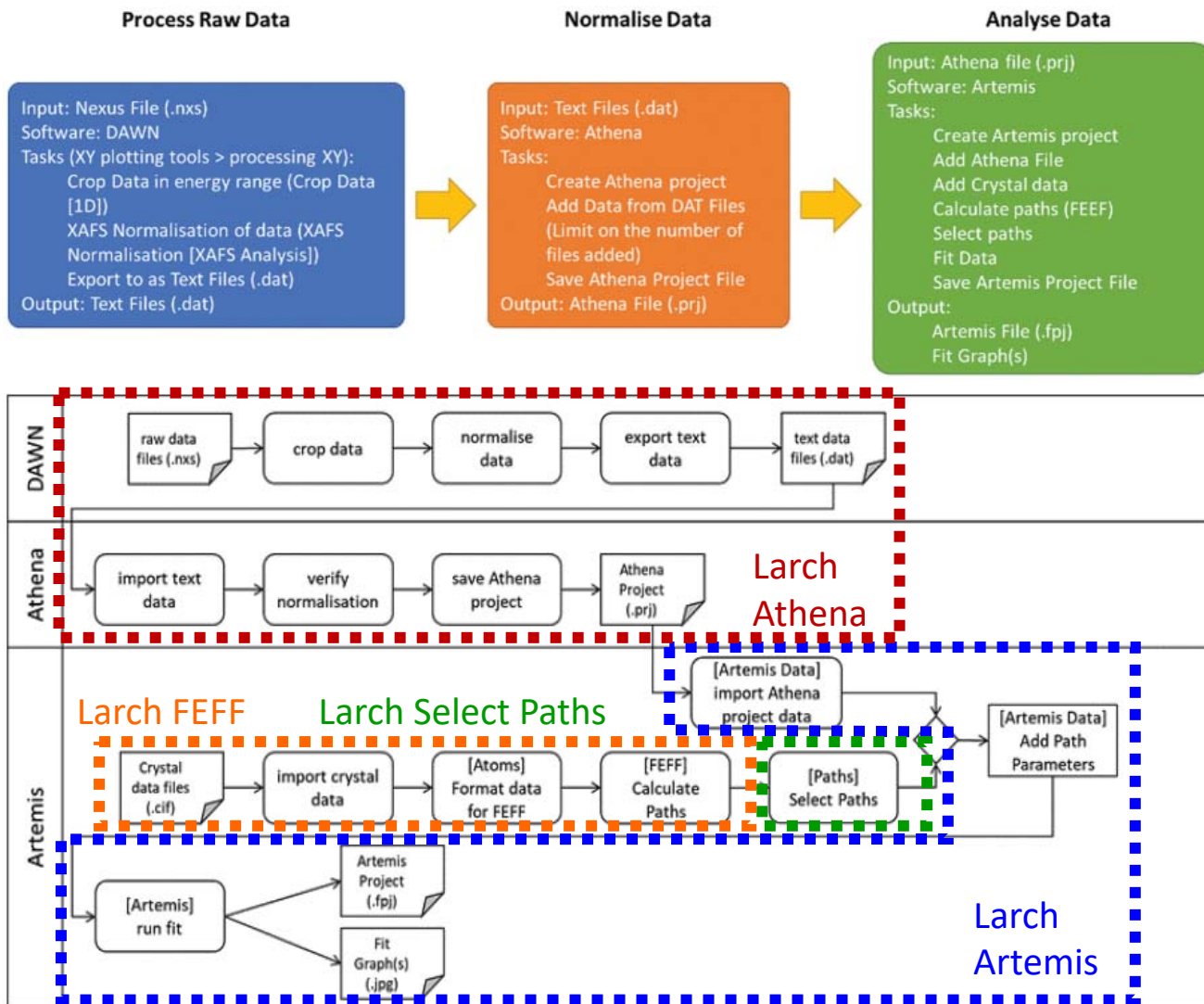
17 : Cluster report for PyMuonSuite AIRSS UEP Optimise on data 3, data 2, and data 1

16 : Minimal energy structures
a list with 2 datasets

5 : File containing the positions of all muon sites

4 : PyMuonSuite AIRSS UEP

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).



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



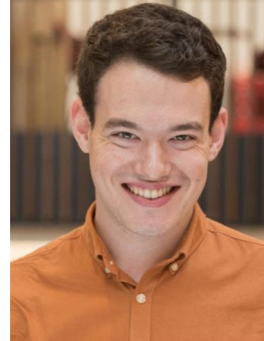
HILLIER



PRATT



COTTRELL

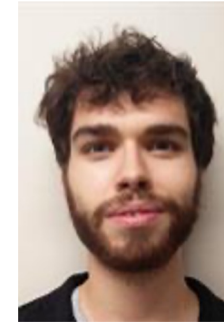


WILKINSON

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



ISIS Neutron and
Muon Source

