

Visualise

Subtask from the PSI meeting:

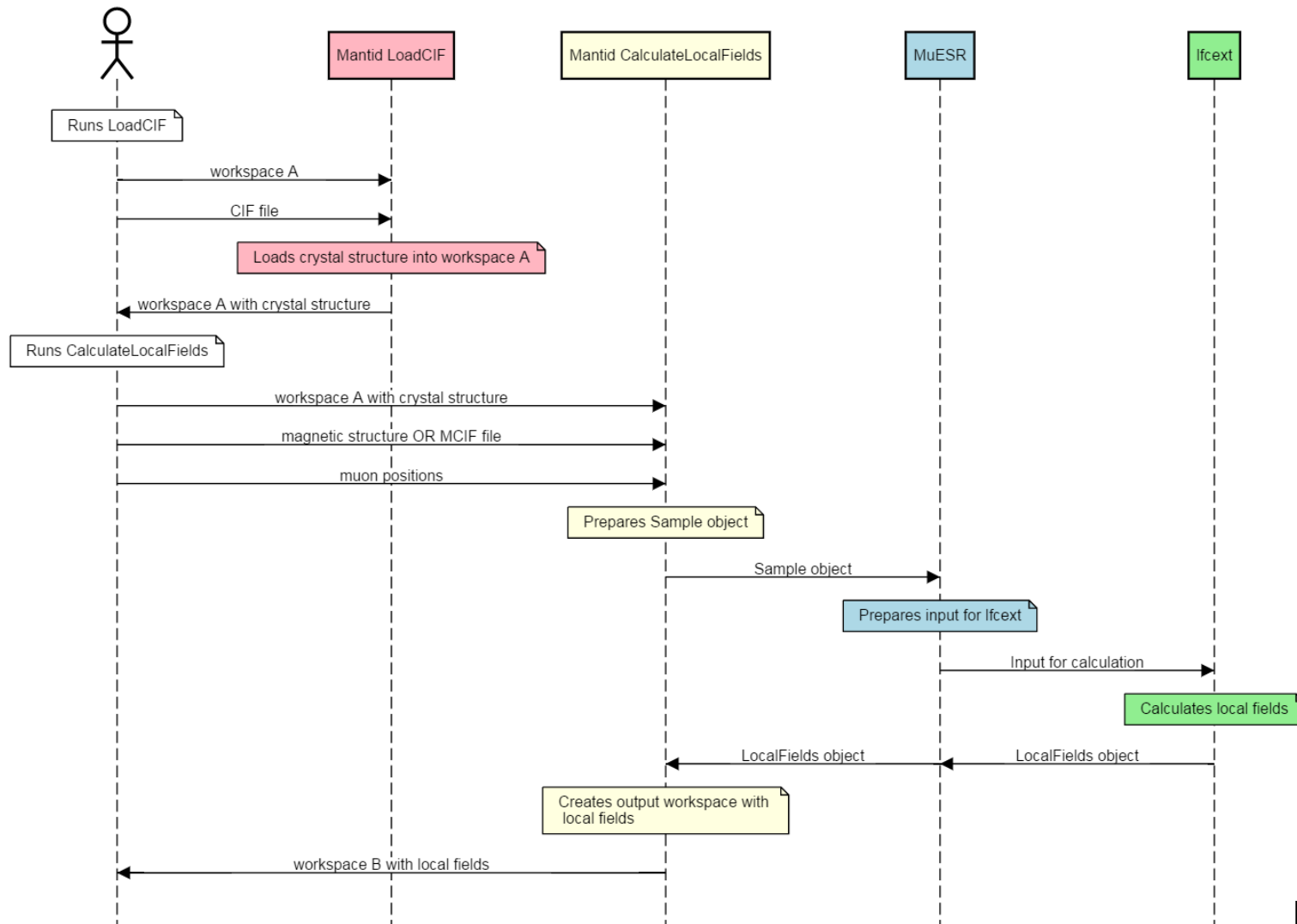
- Development of methods to visualise results.
 - visualisation in Mantid
 - external resources

Subtask from the PSI meeting:

- Developing DFT methods as a predictive tool for muon sites, contact hyperfine fields and evaluating stability of candidate sites.
 - Community requirements → Workshop
 - Implementation
 - Partial implementation in ASE/Mantid

Mantid Interface to MuESR

Usage Workflow



Picture courtesy of
Thomas Perkins

Mantid Interface to MuESR

Working proof of concept:

- Uses PyQT and threaded execution of heavy computation
- Exploits all available data from Mantid:
 - Sample definition in Workspace for Lattice structure description
 - Output provided in TableWorkspace

To be implemented:

Flexibility to exploit most of the MuESR functionalities

(example: average over field distribution in incommensurate orders, automatic addition of symmetry equivalent muon sites, ...)

Mantid Interface

The screenshot displays the Mantid software interface. At the top, there is a menu bar with options: File, Edit, View, Catalog, Interfaces, and Help. Below the menu bar is a toolbar with various icons for file operations and editing. The main window title is "MantidPlot - untitled".

The "Results Log" panel is visible, displaying the following text:

```
Welcome to Mantid 3.7.20160822.927
Please cite: http://dx.doi.org/10.1016/j.nima.2014.07.029 and this release: http://dx.doi.org/10.5286/Software/Mantid
Failed to load plugin /opt/Mantid/plugins/python/algorithms/LRAutoReduction.py. Error: Missing parentheses in call to 'exec' (scripter.py, line 615)
Failed to load plugin /opt/Mantid/plugins/python/algorithms/VesuvioTOFFit.py. Error: invalid syntax (backgrounds.py, line 77)
```

Workspaces

Load Delete Group

Sort Save

Filter Workspaces

Workspaces

Algorithms

Execute

- Arithmetic
- CorrectionFunctions
- Crystal
- DataHandling
- Diagnostics
- Diffraction
- Events
- Examples
- Inelastic
- MDAlgorithms
- Muon
- Optimization
- PythonAlgorithms
- Reflectometry
- SANS
- SINQ
- Sample
- Simulation
- Transforms

Details

Script Interpreter

```
help -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra details.

In [1]:
```

Mantid Interface

The screenshot displays the Mantid software interface. At the top, a menu bar includes 'File', 'Edit', 'View', 'Catalog', 'Interfaces', and 'Help'. Below the menu is a toolbar with various icons for file operations and editing. The main window title is 'MantidPlot - untitled'. The 'Results Log' panel at the top left shows the following text:

```
Welcome to Mantid 3.7.20160822.927
Please cite: http://dx.doi.org/10.1016/j.nima.2014.07.029 and this release: http://dx.doi.org/10.5286/Software/Mantid
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Failed to load plugin /opt/Mantid/plugins/python/algorithms/VesuvioTOFFit.py. Error: invalid syntax (backgrounds.py, line 77)
```

The 'Workspaces' panel on the right side of the interface shows a list of workspaces and buttons for 'Load', 'Delete', 'Group', 'Sort', and 'Save'. Below this is a 'Filter Workspaces' input field and a 'Workspaces' list area.

The 'Algorithms' panel on the right side of the interface shows a list of algorithm categories and a 'Details' button. The categories listed are:

- Arithmetic
- CorrectionFunctions
- Crystal
- DataHandling
- Diagnostics
- Diffraction
- Events
- Examples
- Inelastic
- MDAlgorithms
- Muon
- Optimization
- PythonAlgorithms
- Reflectometry
- SANS
- SINQ
- Sample
- Simulation
- Transforms

The 'Script Interpreter' panel at the bottom left shows the following text:

```
Script Interpreter
help      -> Python's own help system.
object?  -> Details about 'object', use 'object??' for extra details.

In [1]:
```

A 'Load Dialog' window is open in the center of the interface. It contains the following text and fields:

Attempts to load a given file by finding an appropriate Load algorithm.

File:

OutputWorkspace:

Wavelength:

WavelengthSpread:

Keep Open

Mantid Interface

The screenshot displays the Mantid software interface. At the top, the title bar reads "MantidPlot - untitled". Below it is a menu bar with "File", "Edit", "View", "Catalog", "Interfaces", and "Help". A toolbar with various icons is visible. The main workspace area is currently empty. A "Results Log" panel at the top left shows the following text: "All instrument definitions up to date", "Load started", and "Load successful, Duration 0.25 seconds".

In the center, a "LoadCIF input dialog" window is open. It contains the following text: "This algorithm loads a CIF file using the PyCifRW package and assigns a CrystalStructure to the sample of the workspace." Below this text are two input fields: "Workspace" with a dropdown menu set to "MuonData", and "InputFile" with the text "CrGe3/cif/4002001.cif" and a "Browse" button. There is also a checkbox for "LoadUBMatrix" which is currently unchecked. At the bottom of the dialog are buttons for "?", "Keep Open", "Run", and "Close".

On the right side, the "Workspaces" panel shows a list of workspaces with "MuonData" selected. Below it is the "Algorithms" panel, which has a dropdown menu set to "LoadCIF". A red arrow points to this dropdown menu. The "Algorithms" list includes categories like Arithmetic, CorrectionFunctions, Crystal, DataHandling, Diagnostics, Diffraction, Events, Examples, Inelastic, MDAgorithms, Muon, Optimization, PythonAlgorithms, Reflectometry, SANS, SINO, Sample, Simulation, and Transforms.

At the bottom, the "Script Interpreter" panel shows the following text: "help -> Python's own help system.", "object? -> Details about 'object', use 'object??' for extra details.", and "In [1]:".

Mantid Interface

The screenshot displays the Mantid software interface. At the top, the title bar reads "MantidPlot - untitled". Below it is a menu bar with "File", "Edit", "View", "Catalog", "Interfaces", and "Help". A toolbar contains various icons for file operations and data manipulation. The main window area is mostly grey, indicating a sample definition is available. On the right side, there are two panels: "Workspaces" and "Algorithms". The "Workspaces" panel shows a list of workspaces with "MuonData" selected. The "Algorithms" panel shows a list of algorithm categories, with "LoadCIF" selected in the "Execute" dropdown. At the bottom, a "Script Interpreter" window shows the following text:

```
help      -> Python's own help system.  
object?  -> Details about 'object', use 'object??' for extra details.  
  
In [1]: %run ~/TMP/scriptrepository-master/muon/MUESR/RunGUIScript.py
```

Annotations with arrows point to the "MuonData" workspace and the script execution line in the interpreter.

Sample definition
now available

Run as script

Mantid Interface

The screenshot displays the Mantid software interface. At the top, the menu bar includes File, Edit, View, Catalog, Interfaces, and Help. Below the menu bar is a toolbar with various icons. The main window shows the Results Log with the message: "ciao2 LoadCIF successful, Duration 0.17 seconds".

In the center, a dialog box titled "MantidPlot" is open. It contains several sections:

- Workspace:** A text field containing "MuonData" and an "Apply" button.
- CIF file:** A text field and an "Apply" button.
- K vec:** A text field.
- Mag Structure:** A dropdown menu set to "Cartesian". Below it is a table with columns: Re[S_X], Re[S_Y], Re[S_Z], Im[S_X], Im[S_Y], Im[S_Z].
- Muon positions:** A table with columns: X, Y, Z.
- Supercell:** A text field.
- Run Options:** A text field and a "Run" button.
- Buttons:** "Cancel", "Add", "Remove", and "OK".

A red arrow points to the "Apply" button next to the "Workspace" field. To the right of the dialog box, the text "Click to populate" is displayed. An arrow points from the text "Interactive Interface" on the left to the dialog box.

On the right side of the interface, there are panels for "Workspaces" and "Algorithms". The "Workspaces" panel shows a list of workspaces, including "MuonData". The "Algorithms" panel shows a list of algorithms, including "LoadCIF".

At the bottom, the Script Interpreter shows the following output:

```
Core init!  
Starting core  
Starting CORE loop
```

Mantid Interface

MantidPlot

Workspace

CIF file

K vec

Mag Structure

	Re[S_X]	Re[S_Y]	Re[S_Z]	Im[S_X]	
La (0.333 0.667 0.750)	0.0	0.0	0.0	0.0	0.0
La (0.667 0.333 0.250)	0.0	0.0	0.0	0.0	0.0
Cr (0.000 0.000 0.000)	0.0	0.0	0.0	0.0	0.0
Cr (0.000 0.000 0.500)	0.0	0.0	0.0	0.0	0.0

Muon positions

X	Y	Z
---	---	---

Supercell

Run Options

Mantid Interface

The screenshot shows the MantidPlot interface with the following settings:

- Workspace: MuonData
- CIF file: (empty)
- K vec: 0 0 0
- Coordinate system: Cartesian
- Mag Structure table:

	Re[S_X]	Re[S_Y]	Re[S_Z]	Im[S_X]	
La (0.333 0.667 0.750)	0.0	0.0	0.0	0.0	0.0
La (0.667 0.333 0.250)	0.0	0.0	0.0	0.0	0.0
Cr (0.000 0.000 0.000)	0.0	0.0	1	0.0	0.0
Cr (0.000 0.000 0.500)	0.0	0.0	1	0.0	0.0

Below the Mag Structure table is an "Apply" button.

The Muon positions table is shown below:

	X	Y	Z
1	0	0	0.45
2	0	0	0.4
3	0	0	0.35
4	0	0	0.3

Below the Muon positions table are "Add" and "Remove" buttons.

The Supercell is set to 100 100 100.

Run Options: Run

Buttons: Cancel, OK

A red arrow points from the text "Run asynchronously as many times as needed" to the "Run" button.

Mantid Interface

The screenshot displays the Mantid software interface. At the top, the menu bar includes File, Edit, View, Graph, Data, Format, Windows, Catalog, Interfaces, and Help. Below the menu bar is a toolbar with various icons for file operations and data manipulation. The main workspace is divided into several panels:

- Results Log:** Shows the execution of 'LoadCIF successful, Duration 0.17 seconds' and 'CreateEmptyTableWorkspace started'.
- Table-1 - MuESR_RUN_1:** A table with 9 columns: 'luon site[X]', 'orentz X[Y]', 'orentz Y[Y]', 'Lorentz Z[Y]', 'Dipolar X[Y]', 'Dipolar Y[Y]', and 'Dipolar Z[Y]'. The 'Dipolar Z[Y]' column is highlighted in blue.
- Workspaces:** A panel on the right showing a list of workspaces, including 'MuESR_RUN_1' and 'MuonData'.
- Algorithms:** A panel on the right showing a list of algorithms, including 'Arithmetic', 'CorrectionFunctions', 'Crystal', 'DataHandling', 'Diagnostics', 'Diffraction', 'Events', 'Examples', 'Inelastic', 'MDAlgorithms', 'Muon', 'Optimization', 'PythonAlgorithms', 'Reflectometry', 'SANS', 'SINQ', 'Sample', 'Simulation', and 'Transforms'.
- Graph1:** A plot titled 'MuESR_RUN_1' showing 'Dipolar Z' on the y-axis (ranging from 0 to 80) versus 'Muon site' on the x-axis (ranging from 1 to 9). The data points are connected by a line, showing a sharp increase at sites 1 and 9, and a minimum near site 4.
- Script Interpreter:** A panel at the bottom showing the execution of 'Dipolar field (Tesla): 0.0000 0.0000 77.5596' and 'Ending CORE loop'.

Results in TableWorkspace