

# Introduction to Mantid

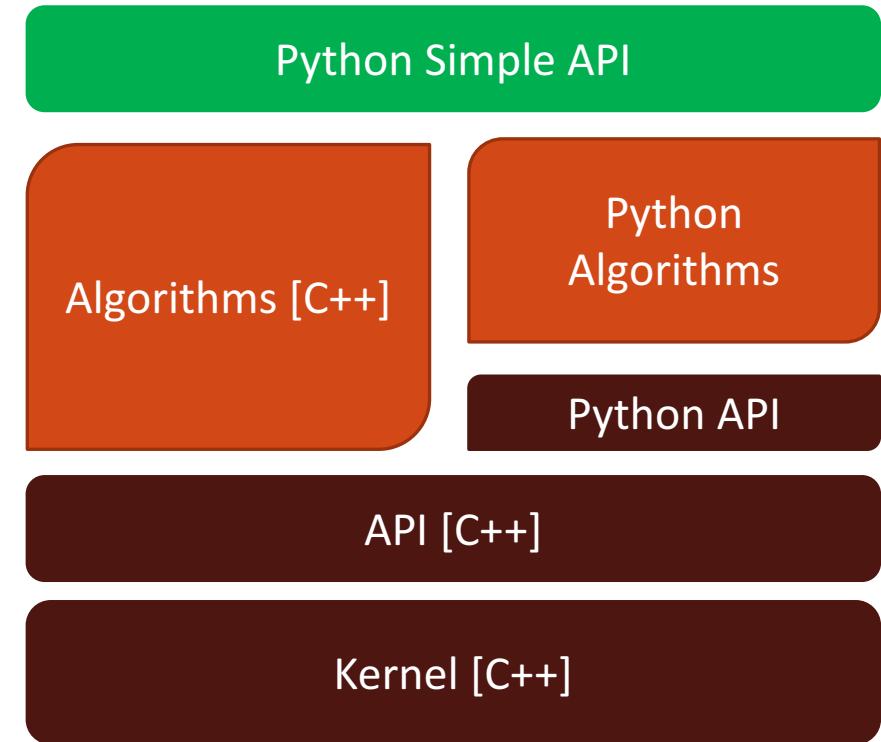
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31.03.17, ILL

# Mantid framework

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- High performance data treatment and visualisation solution tailored for neutron scattering experiments
- Core implemented in C++, API exposed to python
- Easily extendible due to plug-in architecture
  - Shipped with O(800) existing algorithms
  - New algorithms can be created and plugged in
  - Python algorithms plugged in at run time
- Open source, cross-platform (Linux, OS X, Windows)
- Main tool at ISIS, SNS, ESS and soon at ILL
- Data manipulation is performed using key concepts as **workspaces** and **algorithms**



# Workspaces

- Are the main data containers, analogue concept exists in LAMP
- Several types of workspaces exist; Matrix, Events, Peaks, Table, MD etc.
- Most common is the MatrixWorkspace which is a list of 1D histograms

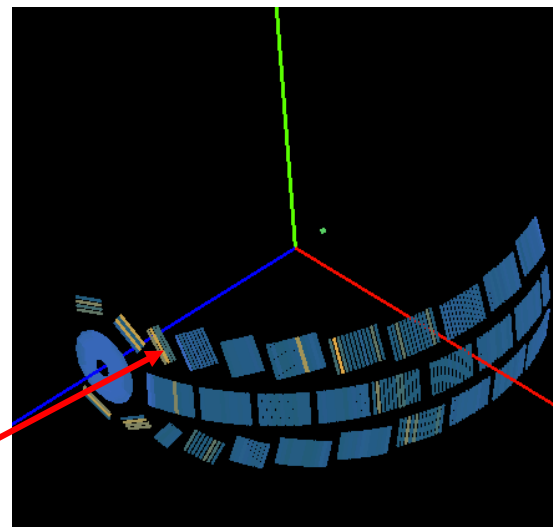
Detector data

	0 266.8K	1 258.654K	2 249.923K
0 sp-0	0,144177	0,151535	0,161796
1 sp-1	0,178321	0,187072	0,198562
2 sp-2	0,190916	0,200196	0,213337
3 sp-3	0,159553	0,16689	0,179411
4 sp-4	0,17331	0,180447	0,195429
5 sp-5	0,157991	0,16699	0,179352
6 sp-6	0,145446	0,152051	0,166156
7 sp-7	0,109014	0,114242	0,125274
8 sp-8	0,145847	0,154115	0,16687
9 sp-9	0,221201	0,236249	0,256957
10 sp-10	0,200287	0,213504	0,232027

Map between spectrum number to detector pixel

Index	Spectrum No	Detector ID(s)	R	Theta	Q
1	0	1	2,000000000...	15,92499999...	0,580251921...
2	1	2	2,000000000...	14,97499999...	0,545840788...
3	2	3	2,000000000...	14,02499999...	0,511392140...
4	3	4	2,000000000...	13,07499999...	0,476908344...
5	4	5	2,000000000...	13,07499999...	0,476908344...
6	5	6	2,000000000...	14,02499999...	0,511392140...
7	6	7	2,000000000...	14,97499999...	0,545840788...
8	7	8	2,000000000...	15,92499999...	0,580251921...
9	8	9	2,000000000...	19,07499999...	0,694053604...
10	9	10	2,000000000...	20,02499999...	0,728275737...
11	10	11	2,000000000...	0,762447816...	
12	11	12	2,000000000...	21,92499999...	0,796567493...
13	12	13	2,000000000...	24,97499999...	0,905727922...
14	13	14	2,000000000...	25,92499999...	0,939601280...
15	14	15	2,000000000...	26,87499999...	0,973440060...

Full 3D instrument geometry



Metadata

Name	Type
ReducedRunsList	string
run_number	numeric
run_title	string
sample.chemicalFormula	string
sample.constitance	string
sample.density	string
sample.field	numeric
sample.mass	string
sample.pressure	numeric
sample.regulation_temperature	numeric
sample.sampleId	string
sample.scatteringLengthDensity	string
sample.setpoint_field	numeric
sample.setpoint_pressure	numeric
sample.setpoint_temperature	numeric
sample.size	string
sample.surfaceArea	string
sample.temperature	numeric
sample.typeInstall	string
sample.unitCellType	string

History of algorithm execution

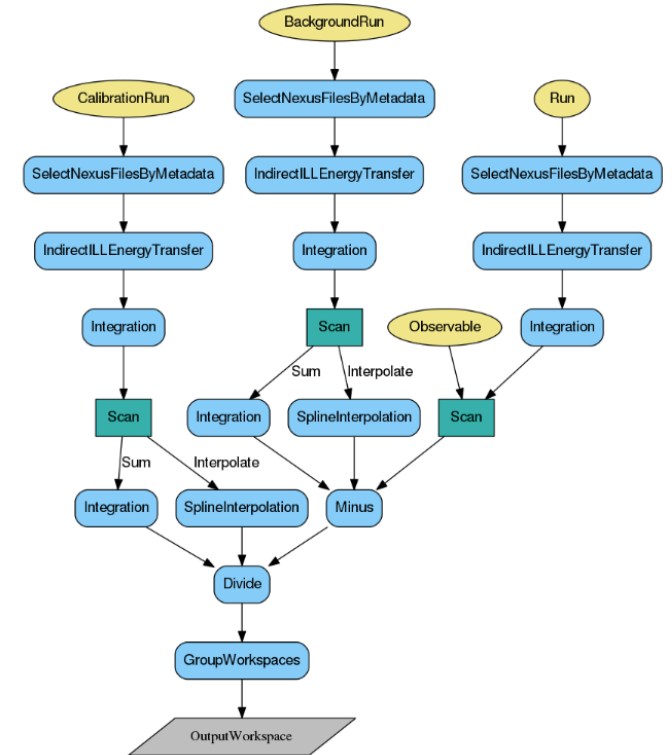
Algorithms	Name	Value	Default?	Direction
IndirectLLReductionFWS v.1	Run	/Volumes/u...	No	Input
	BackgroundRun	Yes	Yes	Input
	CalibrationRun	Yes	Yes	Input
	Observable	sample.tem...	Yes	Input
	SortXAxis	0	Yes	Input
	BackgroundScalingFactor	0.10000000...	No	Input
	BackgroundOption	Sum	Yes	Input
	CalibrationOption	Sum	Yes	Input
	MapFile	Yes	Yes	Input
	ManualPSIntegrationRange	1,128	Yes	Input
	Analyser	silicon	Yes	Input
	Reflection	111	Yes	Input
	OutputWorkspace	single_red	No	Output

In a typical raw TOF data, each row represents a time-of-flight spectrum of a single detector pixel.

# Algorithms

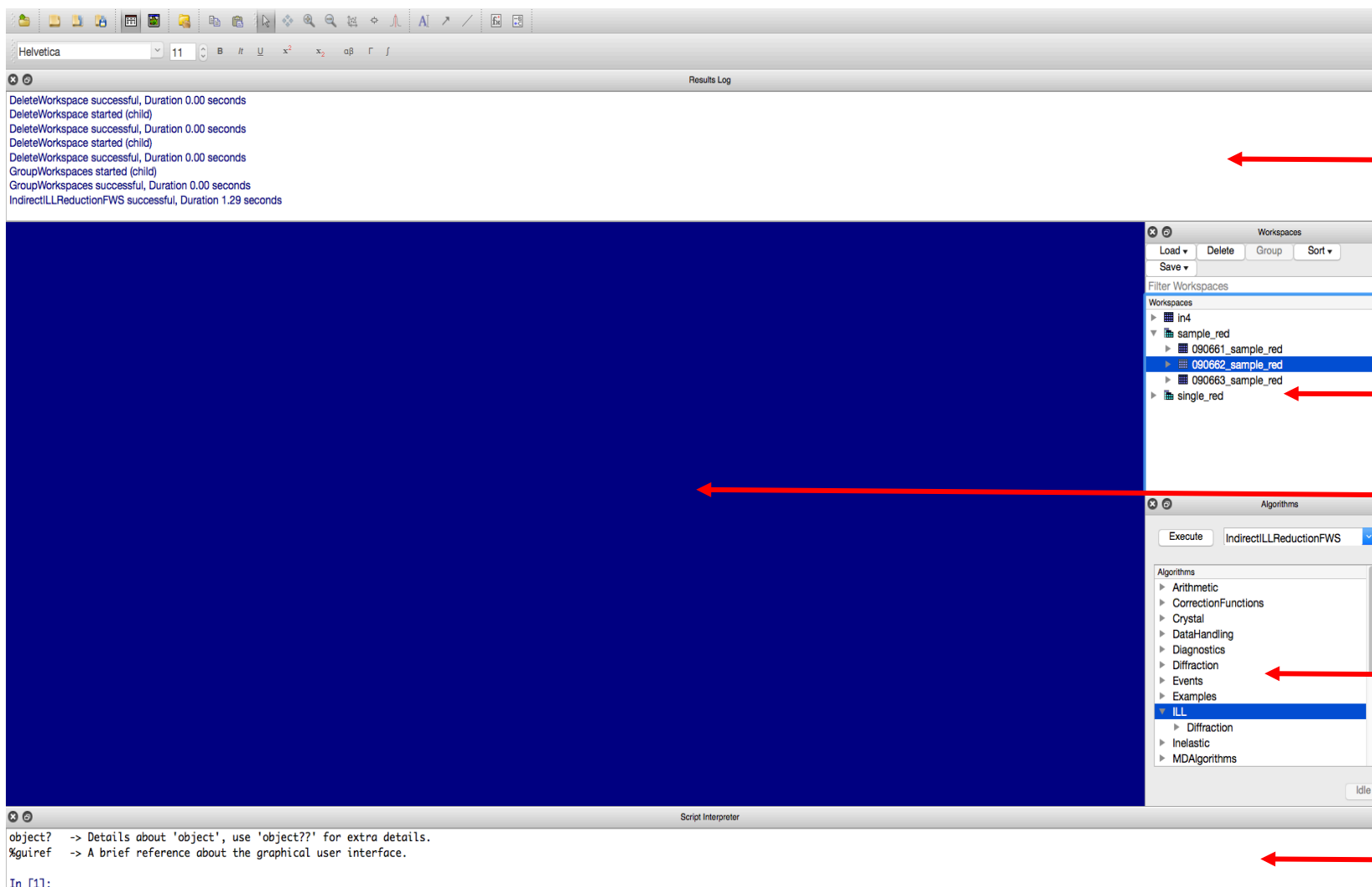
- Manipulate the data in workspaces or files
- Examples can be arithmetic operations, e.g. **Integrate**, **Sum**, **Transpose**, etc.
- New algorithms can be created and added both in C++ and python
- Reduction algorithms are written in python and represent workflow-type algorithms, which call many other algorithms in a sequence
- For each algorithm, a simple GUI dialog is automatically generated on-the-fly
- Python simple API provides function-like interface for invocation of the algorithms, no matter they are written in C++ or python

```
> result = SomeAlgorithm(InputWorkspace = inWS, Param="value")
```



A workflow algorithm flowchart.

# MantidPlot GUI



Log shell

Workspace browser

Main working area

Algorithm browser

IPython shell

# MantidPlot GUI

Workspace  
matrix view

Python  
script editor

Plotting  
window

Instrument  
view

Custom interface window

Auto-generated interface dialog

