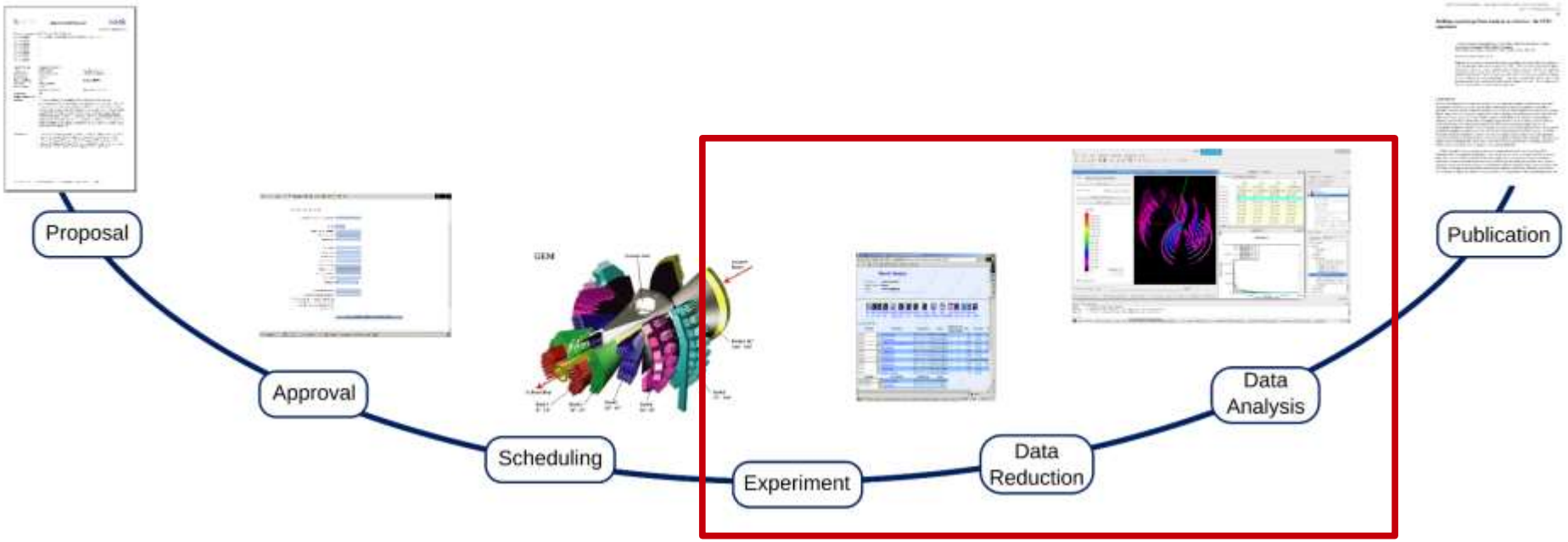
Science & Technology Facilities Council
10 Years of Impact and Inspiration

DAaaS
Data Analysis as a Service

Frazer Barnsley

Software Engineering Group, SCD

Experiment Life Cycle



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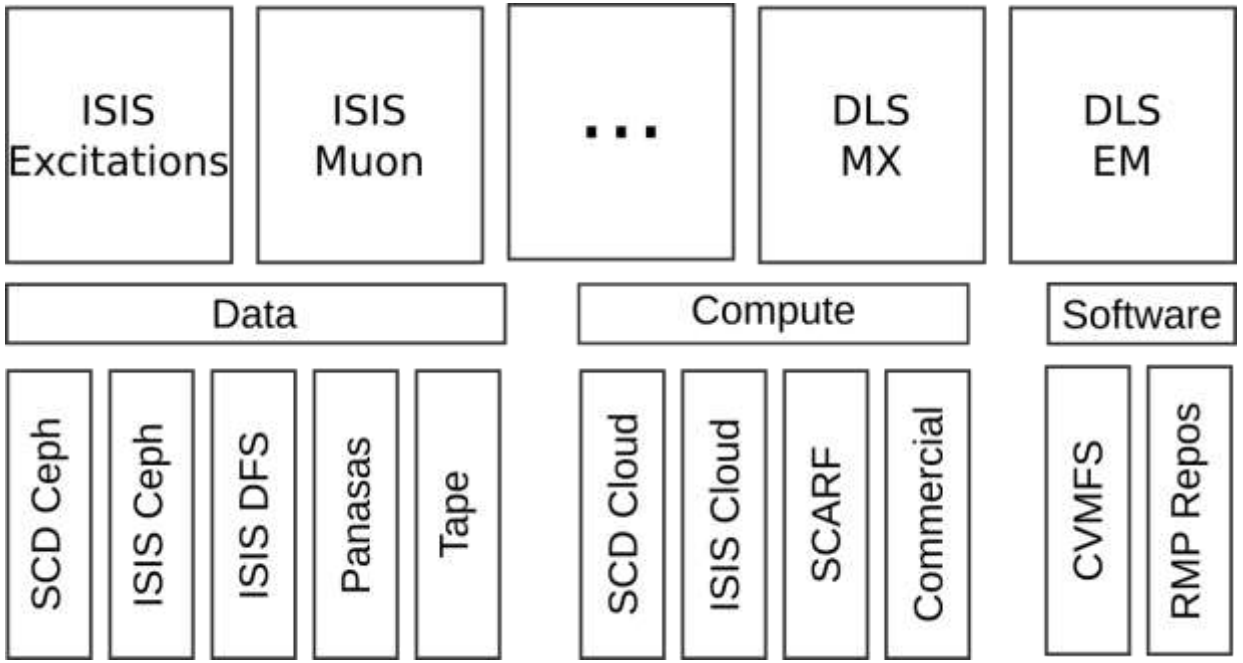
10 Years of Impact and Inspiration

Aims

- Improving the scientific output of the facilities
  - **Decrease** time to publication
  - **Increase** experiment to publication conversion rate
- **Simplify** the deployment of new workflows
- **Simplify** the development of new innovations
- **Simplify** data analysis process for users and developers

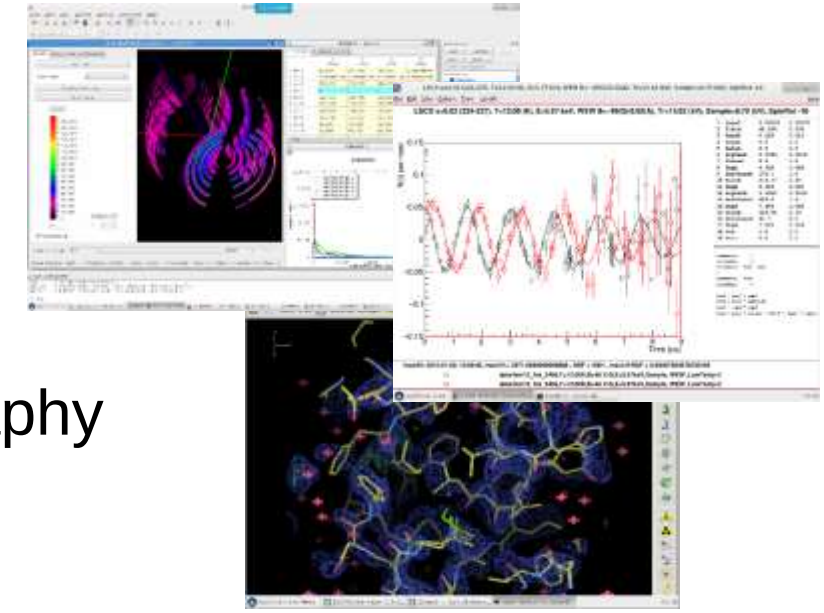
DAaaS

- Three main components
  - Software
  - Data
  - Compute
- Simplification and automation



Who

- ISIS
  - Excitations
  - Muon
- Diamond
  - Macromolecular Crystallography
  - Tomography
- Octopus

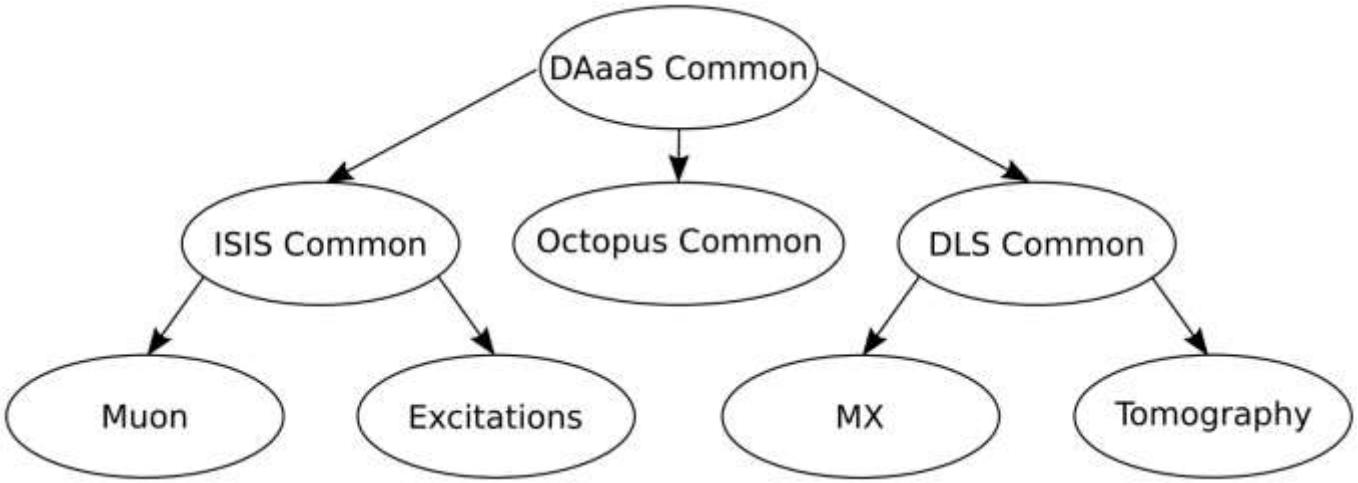


Configuration Management

- VM completed configured by Quattor

quattor

- Configuration Management
  - Installs software
  - Mounts network data sources
  - Sets up desktop



Configuration Management

- Crystallography
- Disordered Materials
- Excitations and Polarized Neutrons
- Large Scale Structures
- Molecular Spectroscopy
- Muons

- MX
- Surfaces and Interfaces
- Spectroscopy
- Engineering and Environment
- Materials
- Soft Condensed Matter

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Configuration Management

- Small Angle Scattering (SANS)
- Neutron Diffraction
- Reflectometry
- Neutron spectroscopy
- Muon spectroscopy
- Chip Irradiation
- Neutron Imaging

- Macromolecular Crystallography (MX)
- Fragment Screening
- X-ray Diffraction
- Residual Stress Strain Mapping
- X-ray Pair Distribution
- Small Molecule X-ray Crystallography
- Small Angle X-ray Scattering (SAXS)

- Protien SASX (BioSAXS)
- X-ray Absorption Spectroscopy (XAS)
- Scanning X-ray Microscopy (SXM)
- X-ray Potoelectric Spectroscopy (XPS)
- Infrared SPectroscopy
- UV and Visible Circular Dichroism
- X-ray Magentic Circular Dichroism
- ARPES
- Cryo Electron Microscopy (eBIC)
- X-ray Tomography
- X-ray Imaging
- High Resolution TEM (ePSIC)

Now

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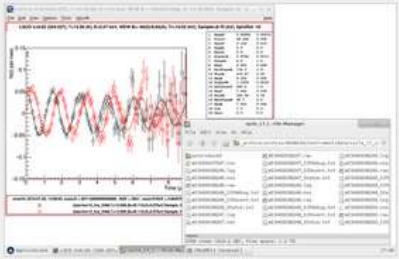
My Data | Analysis | Browse | Search

Analysis Environments

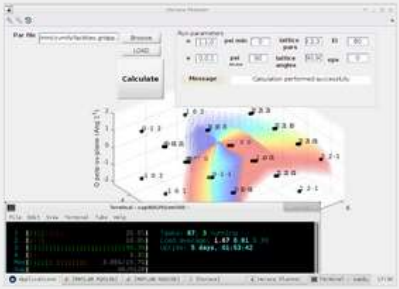
Create



Muon!

Host: vm560.nubes.stfc.ac.uk
Date created: 2017-08-22
Owner: Mr Frazer Barnsley

Share | Launch



Excitations

Host: vm568.nubes.stfc.ac.uk
Date created: 2017-10-13
Owner: Mr Frazer Barnsley

Share | Launch

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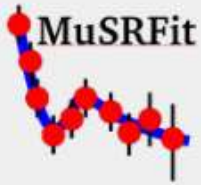
Create Analysis Environments

Excitations

This environment has been tailored for the analysis of in-elastic neutron scattering data from the ISIS Excitations Group. It comes complete with Mantid, Matlab, Horace and MSlice as well as access to the ISIS Experiment Archive.



Muon

This environment has be setup to test the MuSRFit software.

Create Close

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Home Contact Help Admin Downloads Logout ()

Create Analysis Environments

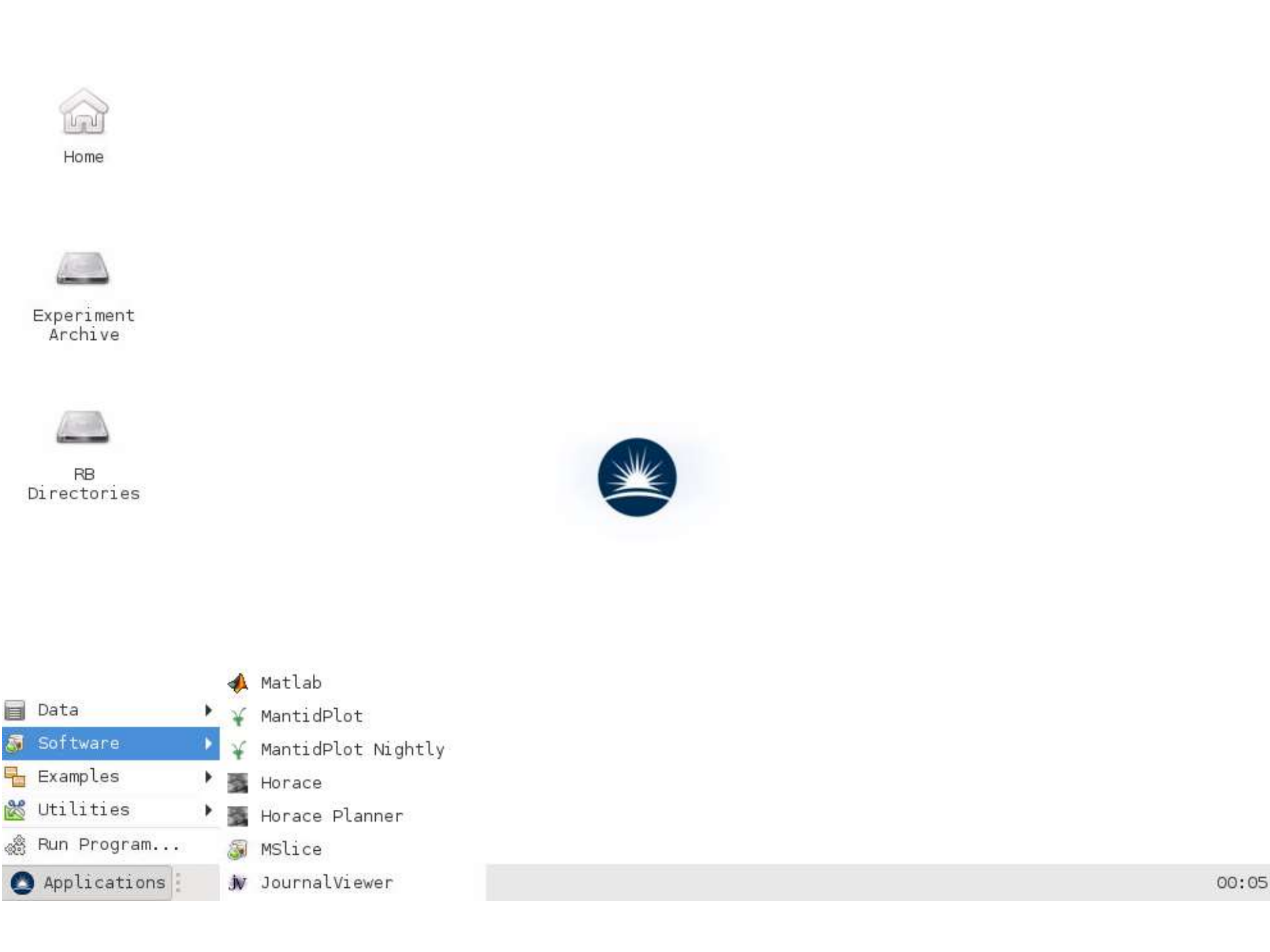
Tomography

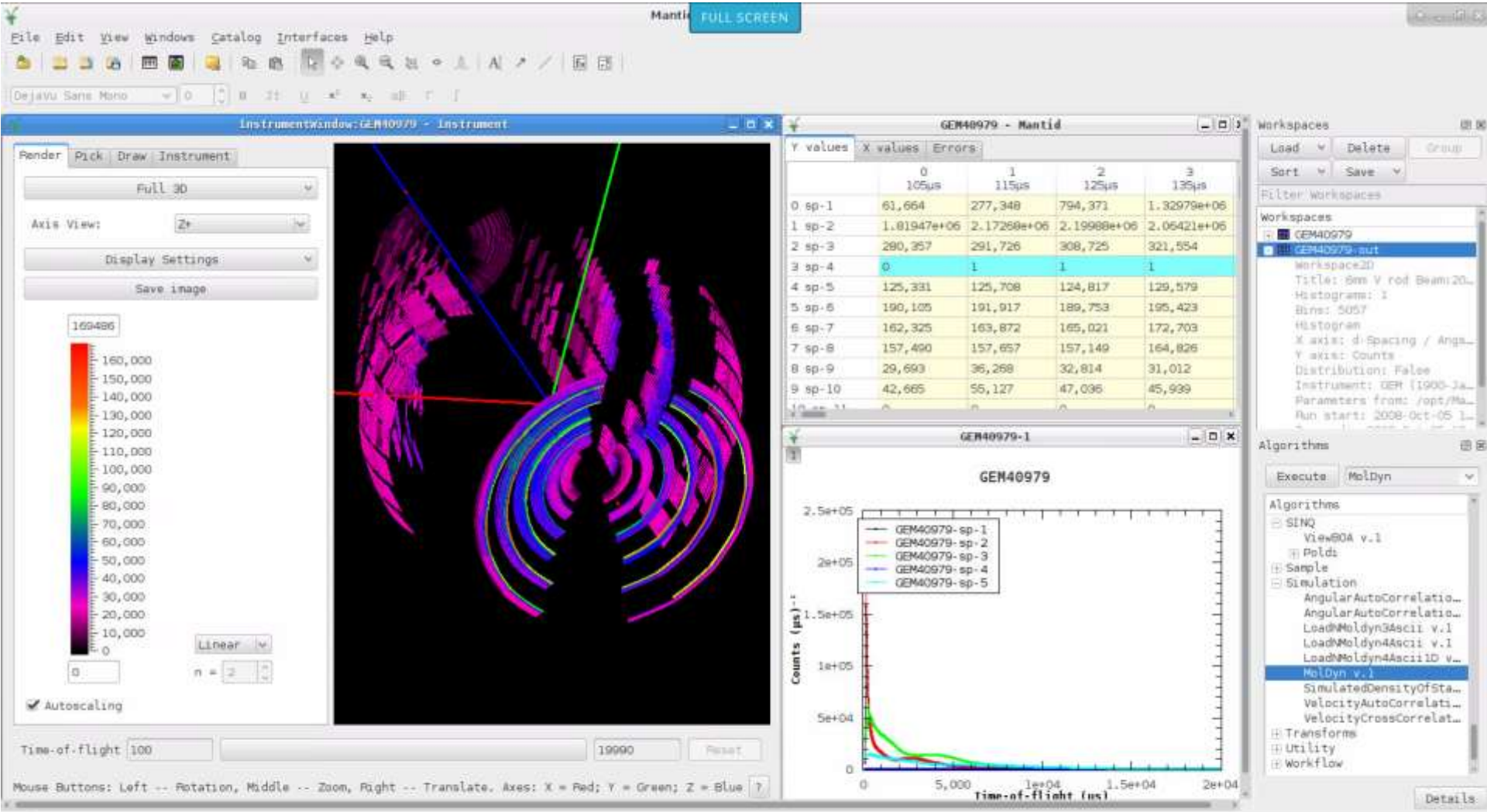
This analysis environment has been setup to allow tomographic reconstruction and visualisation using the SCARF cluster.

Macromolecular Crystallography

This analysis environment has been setup to allow macromolecular processing and visualisation using the SCARF cluster.

Create Close


Home
Experiment Archive
RB Directories
Data
Software
Examples
Utilities
Run Program...
Applications
Matlab
MantidPlot
MantidPlot Nightly
Horace
Horace Planner
MSlice
JournalViewer
00:05

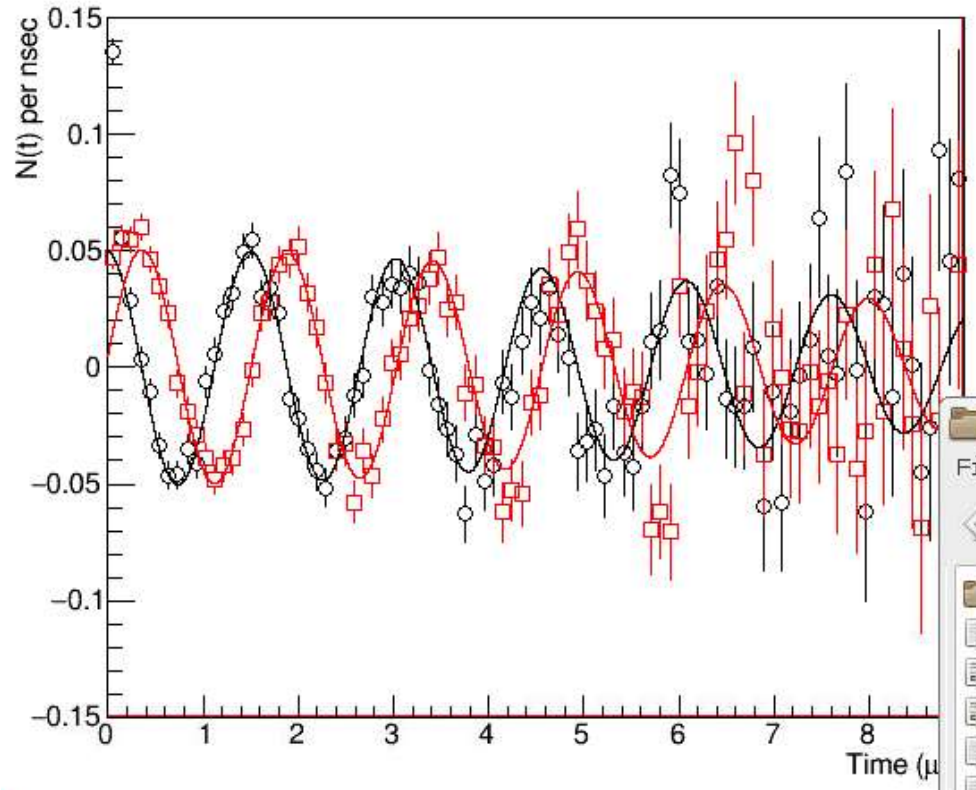

FULL SCREEN
File Edit View Windows Catalog Interfaces Help
InstrumentWindow:GEM40979 - Instrument
Render Pick Draw Instrument
Full 3D
Axis View: Z+
Display Settings
Save image
169486
160,000
150,000
140,000
130,000
120,000
110,000
100,000
90,000
80,000
70,000
60,000
50,000
40,000
30,000
20,000
10,000
0
Linear
n = 2
Autoscaling
Time-of-flight 100
19990
Reset
Mouse Buttons: Left -- Rotation, Middle -- Zoom, Right -- Translate. Axes: X = Red; Y = Green; Z = Blue
GEM40979 - Mantid
Y values X values Errors
0 105μs 1 115μs 2 125μs 3 135μs
0 sp-1 61,664 277,348 794,371 1.32979e+06
1 sp-2 1.81947e+06 2.17268e+06 2.19988e+06 2.06421e+06
2 sp-3 280,357 291,726 308,725 321,554
3 sp-4 0 1 1 1
4 sp-5 125,331 125,708 124,817 129,579
5 sp-6 190,105 191,917 189,753 195,423
6 sp-7 162,325 163,872 165,021 172,703
7 sp-8 157,490 157,657 157,149 164,826
8 sp-9 29,693 36,268 32,814 31,012
9 sp-10 42,665 55,127 47,036 45,939
GEM40979-1
GEM40979
GEM40979-sp-1
GEM40979-sp-2
GEM40979-sp-3
GEM40979-sp-4
GEM40979-sp-5
Counts (μs)⁻¹
2.5e+05
2e+05
1.5e+05
1e+05
5e+04
0
5,000
1e+04
1.5e+04
2e+04
Time-of-flight (μs)
Workspaces
Load Delete Group
Sort Save
Filter Workspaces
Workspaces
GEM40979
GEM40979-sut
Workspace2D
Title: 6mm V rod Beam:20...
Histograms: 1
Bins: 5057
Histogram
X axis: d-Spacing / Angs...
Y axis: Counts
Distribution: False
Instrument: GEM (1900-Ja...
Parameters from: /opt/Ma...
Run start: 2008-Oct-05 1...
Algorithms
Execute MolDyn
Algorithms
SINQ
ViewBOA v.1
Poldi
Sample
Simulation
AngularAutoCorrelatio...
AngularAutoCorrelatio...
LoadNMoldyn3Ascii v.1
LoadNMoldyn4Ascii v.1
LoadNMoldyn4Ascii1D v...
MolDyn v.1
SimulatedDensityOfSta...
VelocityAutoCorrelati...
VelocityCrossCorrelat...
Transforms
Utility
Workflow
Details
Script Interpreter
help -> Python's own help system.
object? -> Details about 'object', use 'object??' for extra details.
%guiref -> A brief reference about the graphical user interface.
In [1]:
Applications
[Analysis | DaaS Dem...
MantidPlot - untitled
sap86629 - File Mana...
[Terminal - sap86629...
[Terminal - sap86629...
[Terminal - root@vm4...
[Terminal - sap86629...
13:26

LSCO x=0.02 (224-227), T=12.00 (K), E=5.57 keV, WEW B=~49(G)/8.62(A), Tr=15.02 (kV), Sample=8.

File Edit View Options Tools Musrfit Help

LSCO x=0.02 (224-227), T=12.00 (K), E=5.57 keV, WEW B=~49(G)/8.62(A), Tr=15.02 (kV), Sample=8.70 (kV), SpinRot -10

1	AsymT	0.05052	0.00072
2	Field	48.298	0.095
3	RateT	0.129	0.010
4	AsymL	0.0	0.0
5	RateL	0.0	0.0
6	AlphaLR	0.9784	0.0013
7	PhaseL	6.6	1.6
8	BkgL	6.920	0.048
9	RelPhaseR	178.7	1.9
10	NormR	419.47	0.40
11	BkgR	8.393	0.050
12	AlphaTB	1.1025	0.0015
13	RelPhaseT	269.0	1.9
14	BkgT	7.466	0.049
15	NormB	393.08	0.39
16	RelPhaseB	90.7	2.0
17	BkgB	7.091	0.048
18	One	1.0	0.0
19	Zero	0.0	0.0



musrfit: 2015-01-05, 13:58:40, maxLH = 3971.6999999999998 , NDF = 4001 , maxLH/NDF = 0.99267

data/lem12_his_2466,T=12.00K,B=49.11G,E=5.57keV,Sample, V

data/lem12_his_2466,T=12.00K,B=49.11G,E=5.57keV,Sample, V

MuSRFit Terminal

lp

##########

MuSRFit

SRFit terminal to run MuSRFi

.mu.web.psi.ch/musrfit/user/

oc/musrfit/examples/test-his

##########

cycle_17_2 - File Manager

File Edit View Go Help

:_archive/archive/NDXMUSR/Instrument/data/cycle_

autoreduced	MUSR00064921.nxs_v2	MUSR000
MUSR00064920.log	MUSR00064921.RAW	MUSR000
MUSR00064920.nxs	MUSR00064921_ICPdebug.txt	MUSR000
MUSR00064920.nxs_v2	MUSR00064921_ICPevent.txt	MUSR000
MUSR00064920.RAW	MUSR00064921_Status.txt	MUSR000
MUSR00064920_ICPdebug.txt	MUSR00064922.log	MUSR000
MUSR00064920_ICPevent.txt	MUSR00064922.nxs	MUSR000
MUSR00064920_Status.txt	MUSR00064922.nxs_v2	MUSR000
MUSR00064921.log	MUSR00064922.RAW	MUSR000
MUSR00064921.nxs	MUSR00064922_ICPdebug.txt	MUSR000

7673 items (2.1 GB), Free space: 9.9 TB

Applications | LSCO x=0.02 (224-227... | cycle_17_2 - File Ma... | [MuSRFit Terminal] | MuSRFit Terminal | 17:38

Future

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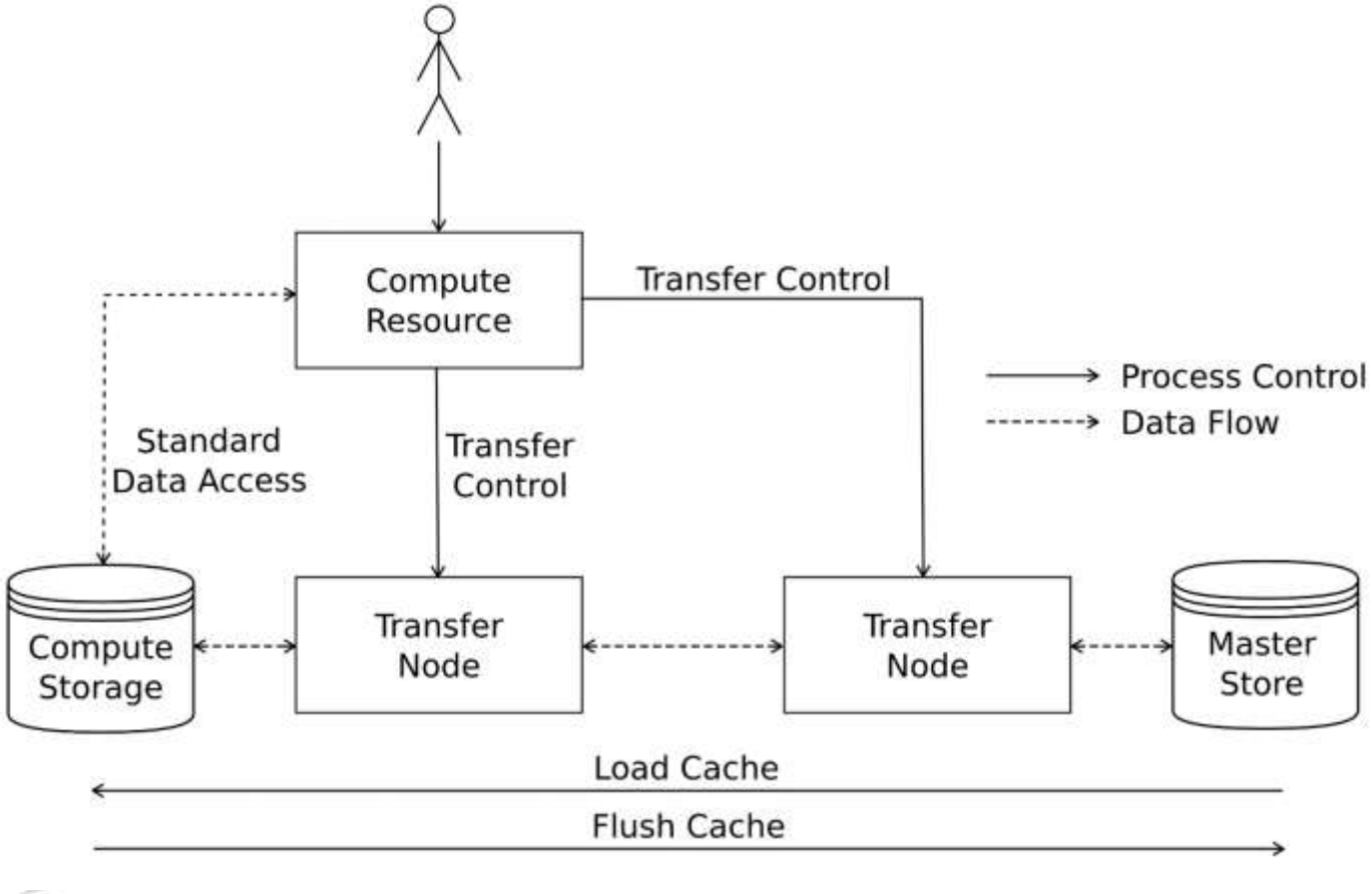
Data Management System

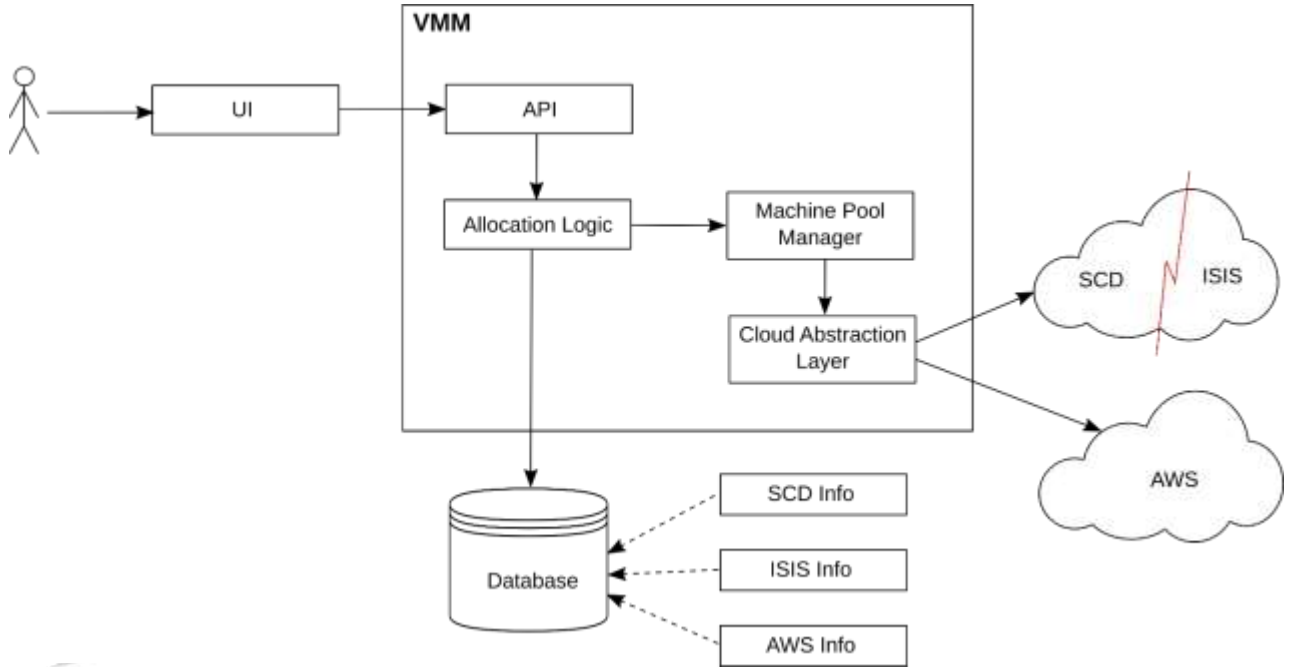
- Automatically move data to compute storage
- Compute storage acts as cache
- FUSE for control, GridFTP for transfer



Virtual Machine Manager

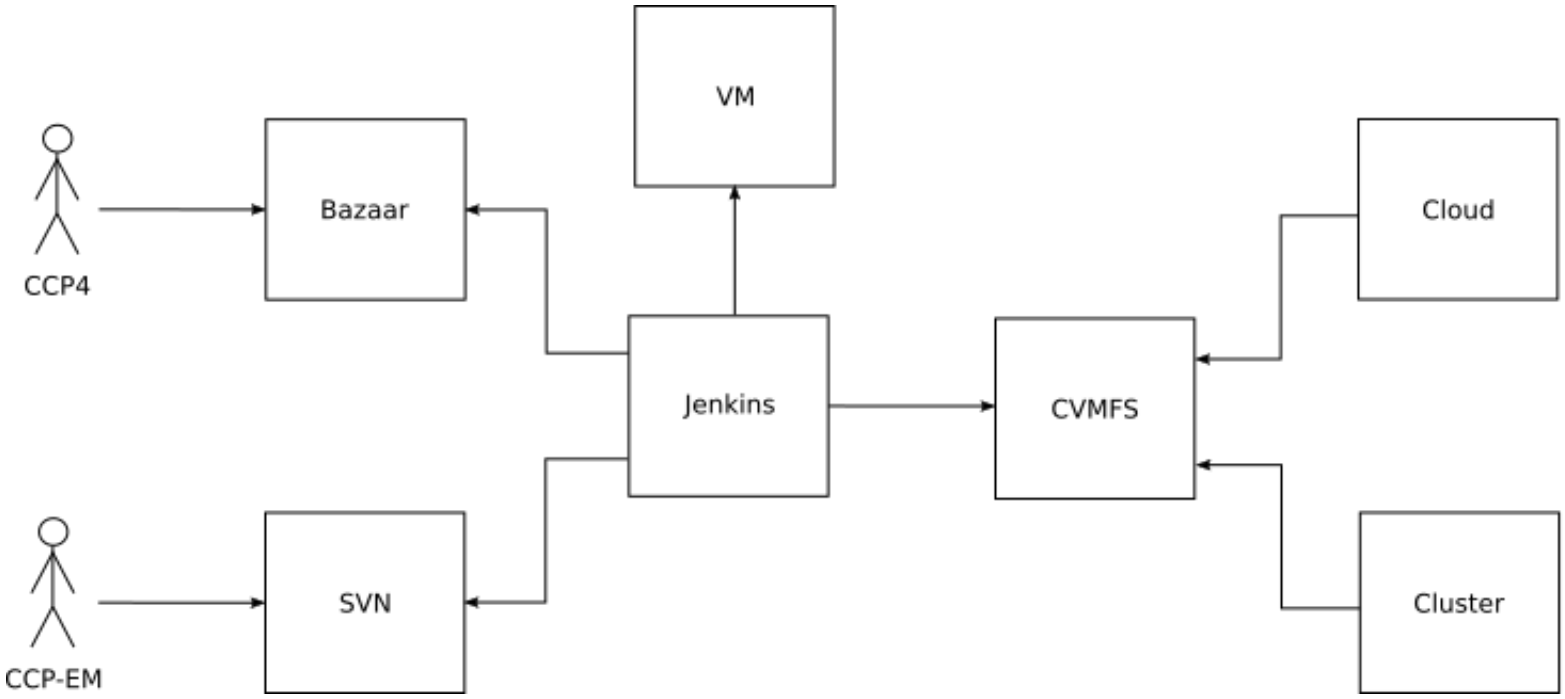
- GPU / CPUs / Memory
- Locations - ISIS, SCD, commercial

- Graphically intensive – move VM to user
- Large data volumes – move VM to data



Software Deployment Pipeline

- Automated deployment of software
- Quicker release of updates
- Improve software development process
- Software deployed to multiple systems



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