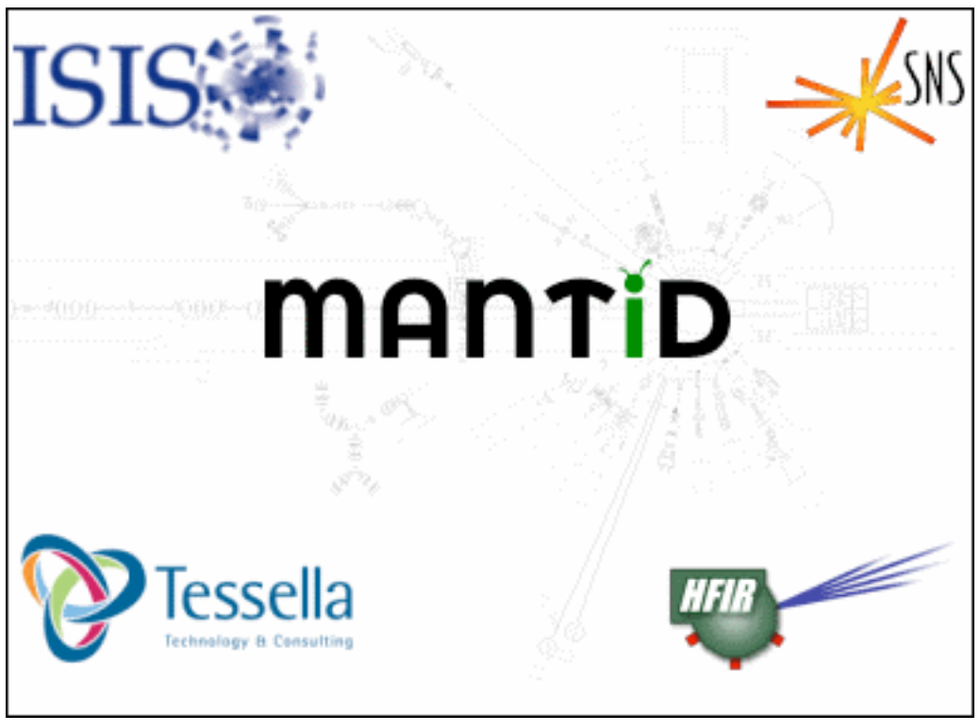
Maximising the scientific impact of large scale facilities: software development scientific computing

Jon Taylor
Jon.Taylor@stfc.ac.uk



Project WIKI (Binary downloads + help)
http://www.mantidproject.org
Source Code
https://github.com/mantidproject

U.S. DEPARTMENT OF ENERGY
Office of Science

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Acknowledgements

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Maximising the scientific impact of large scale facilities: software development scientific computing

The large scale facility science programme

Challenges to maximising the impact

Solutions

Software development: The mantid project

Programme access to scientific computing
Scientific computing @ Harwell Oxford

MANTID

Science & Technology Facilities Council
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Harwell Oxford

ISIS spallation neutron source 27 instruments

Diamond Light source 27 beam lines

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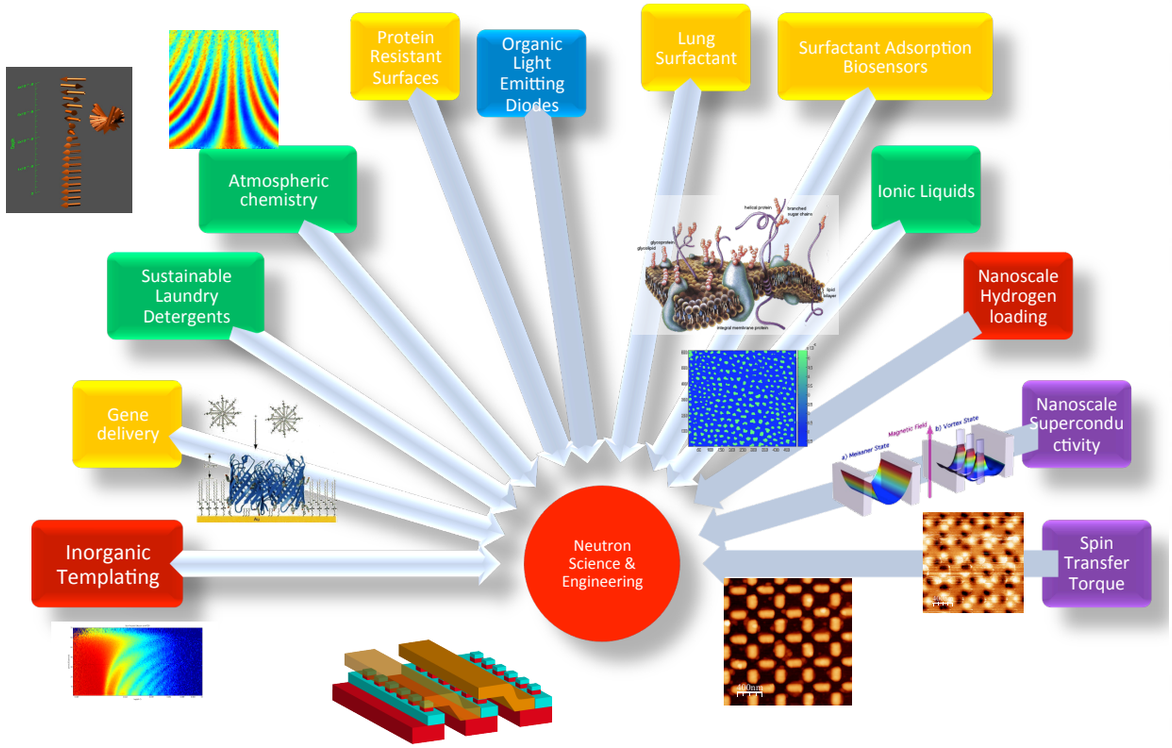
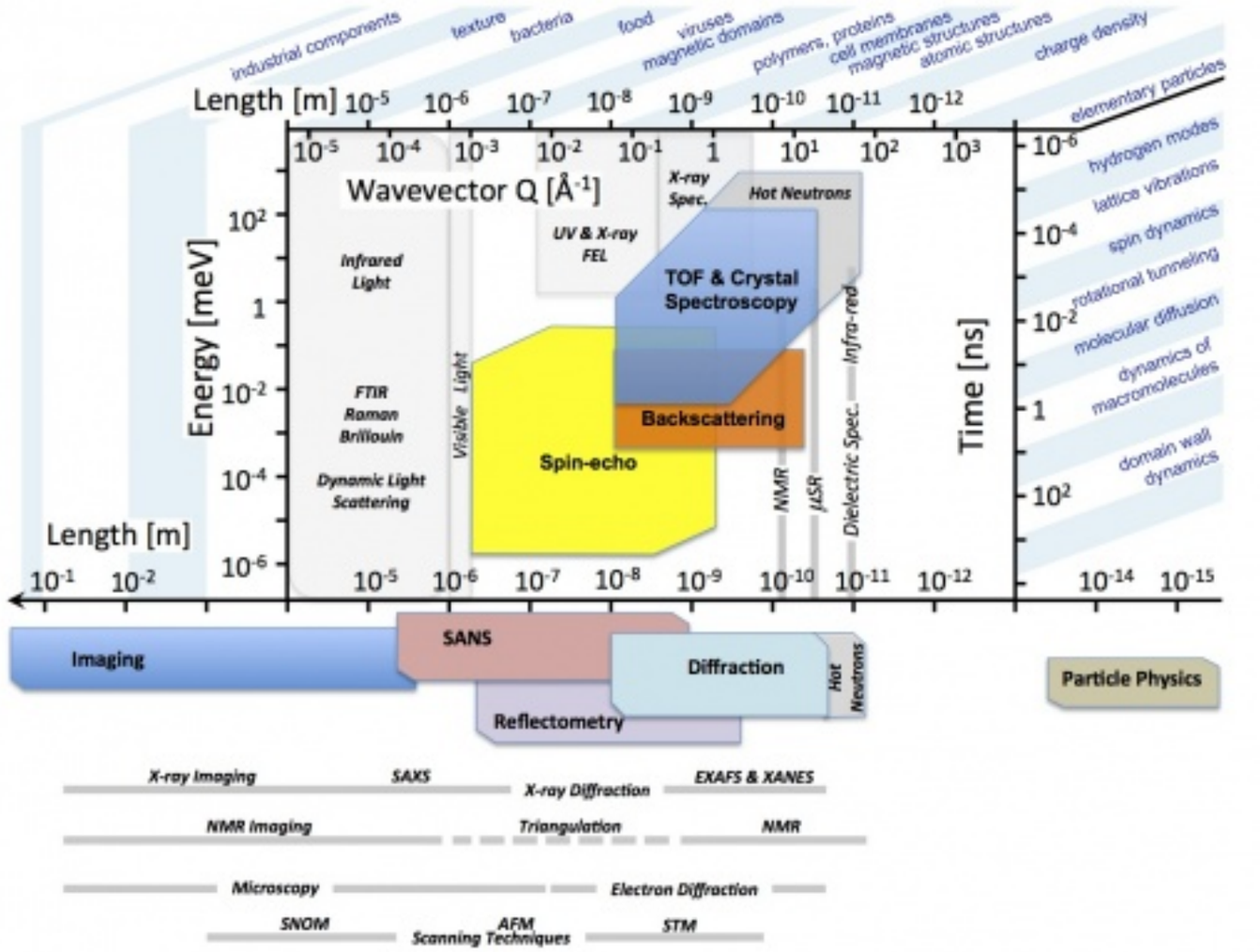
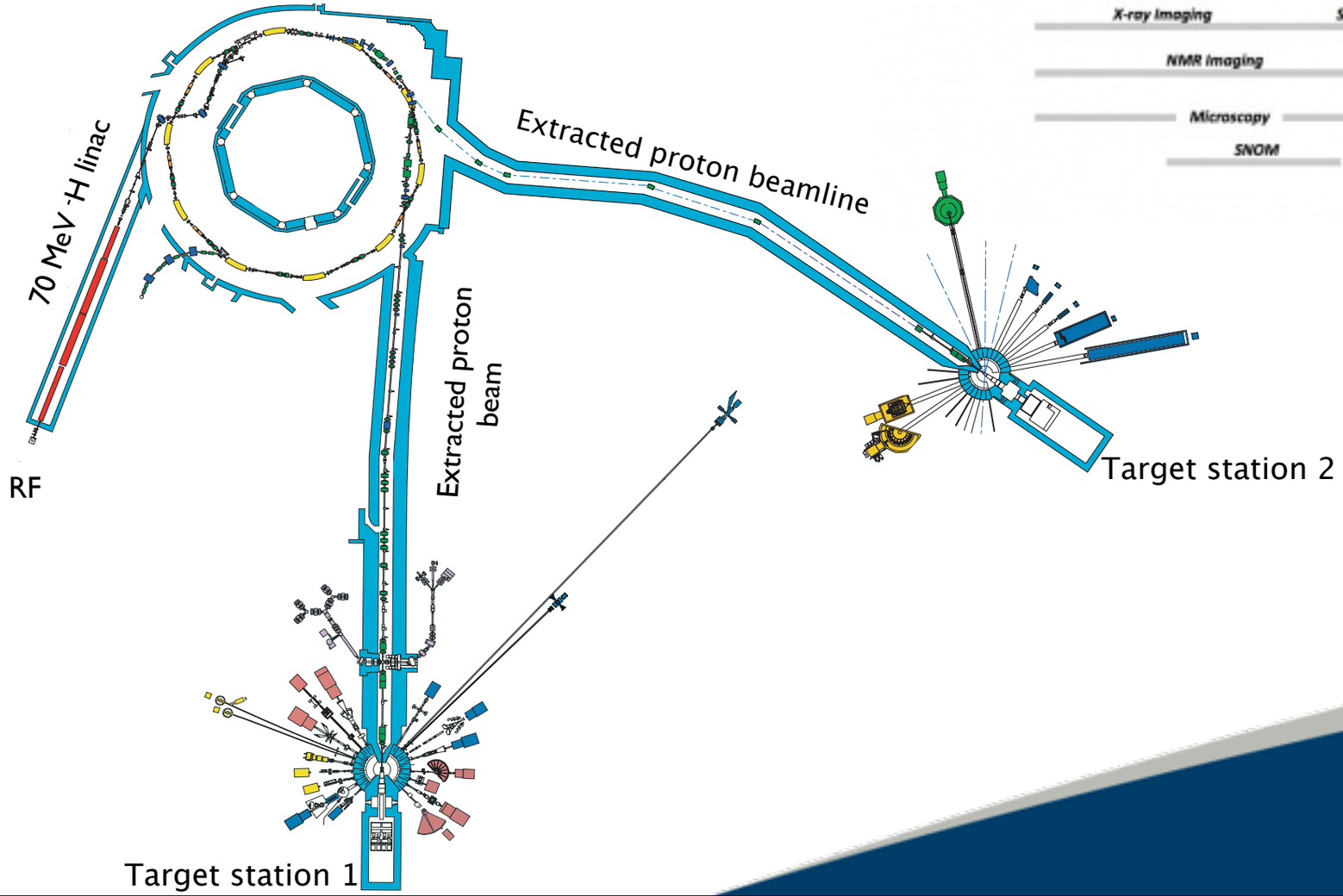
Fundamentally driven, *technologically relevant*







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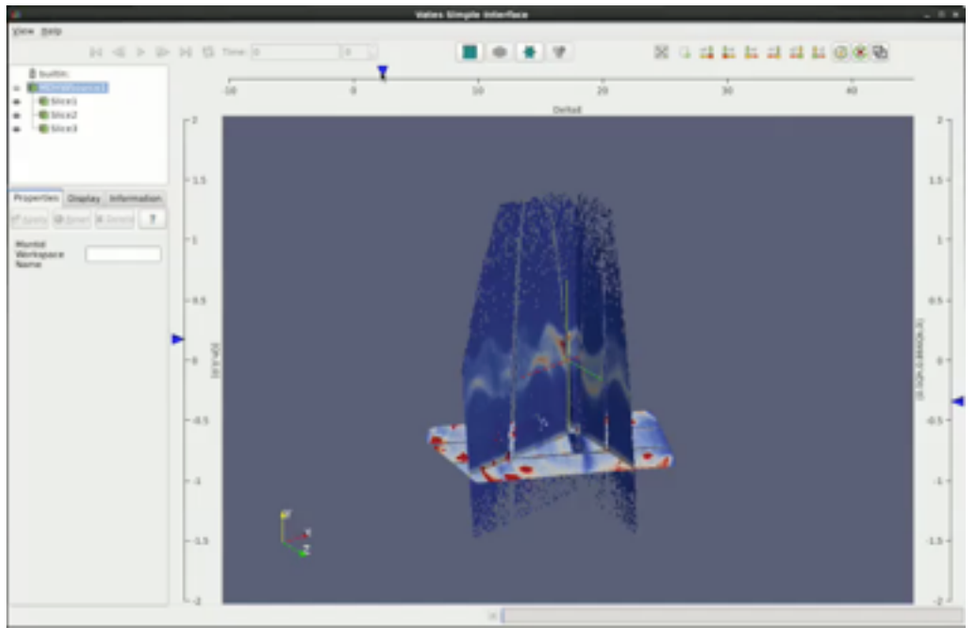
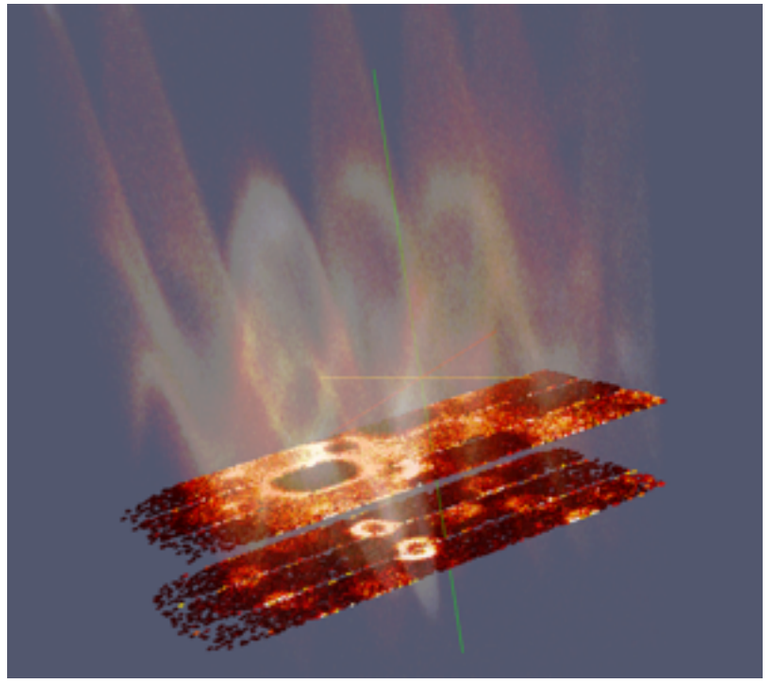
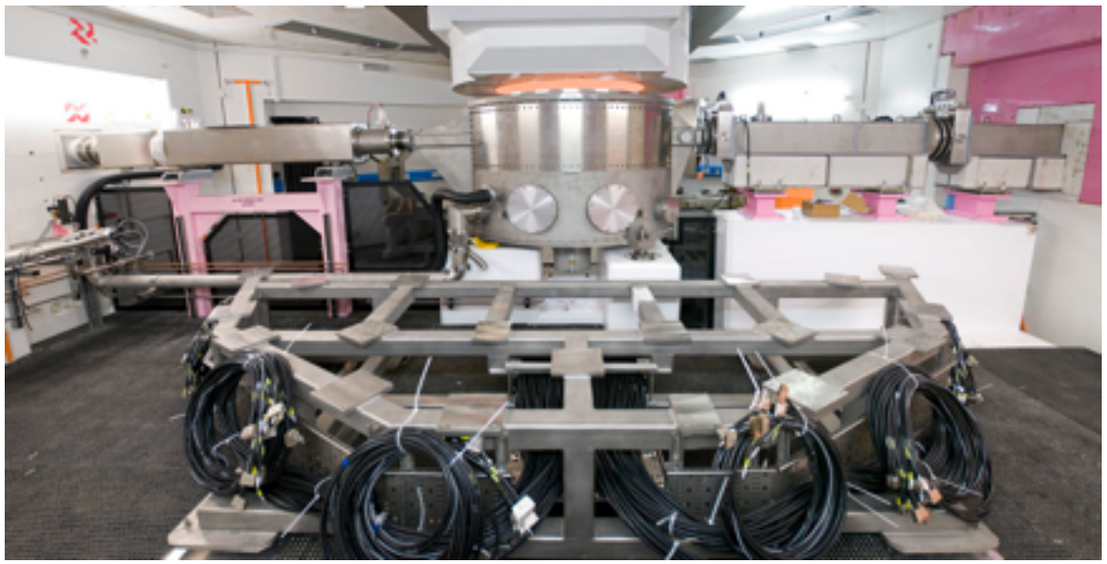




Big data



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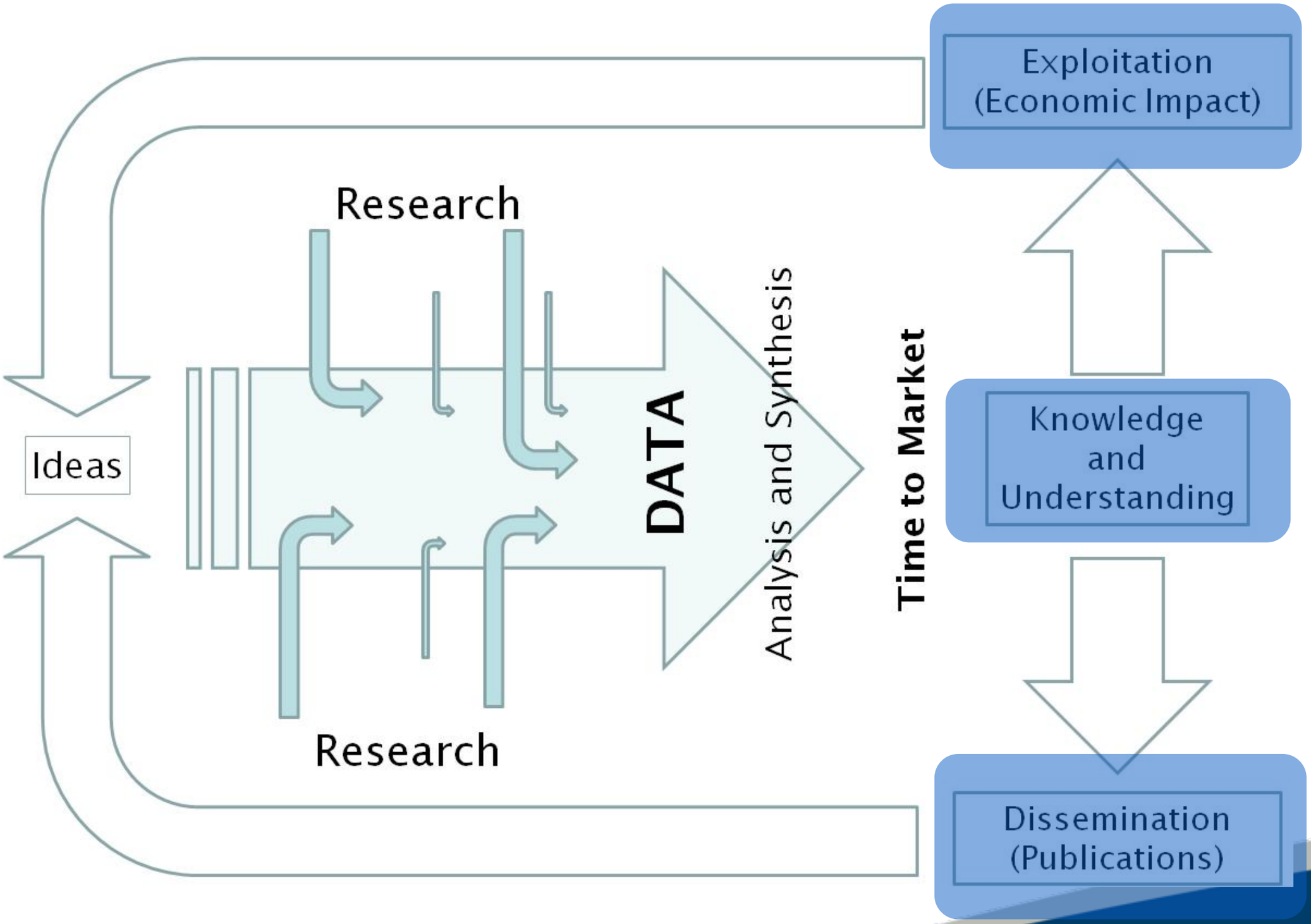

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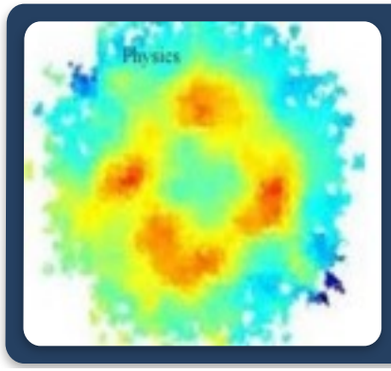
PHYSICS



ANGSTROMS AND PICOSECONDS

- electronic and magnetic structure
- strongly correlated electron systems

CHEMISTRY

SOFT MATTER & BIOLOGY

ENGINEERING & MATERIALS SCIENCE

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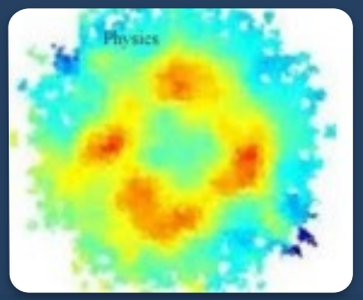


ANGSTROMS AND PICOSECONDS

- electronic and magnetic structure
- strongly correlated electron systems

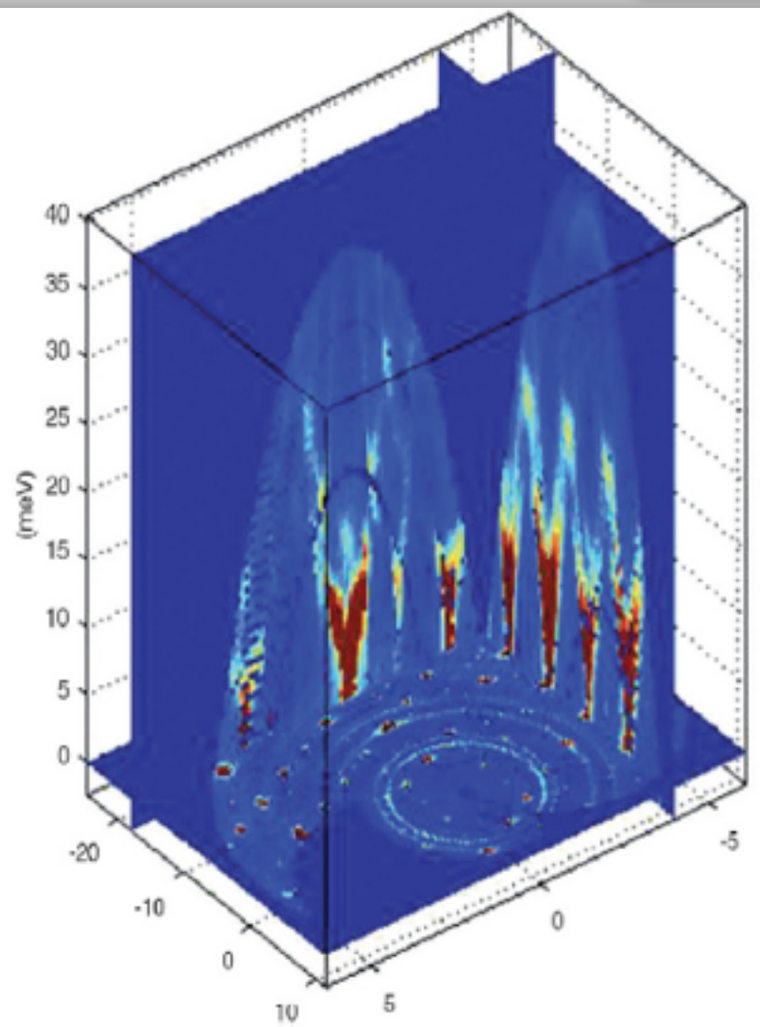
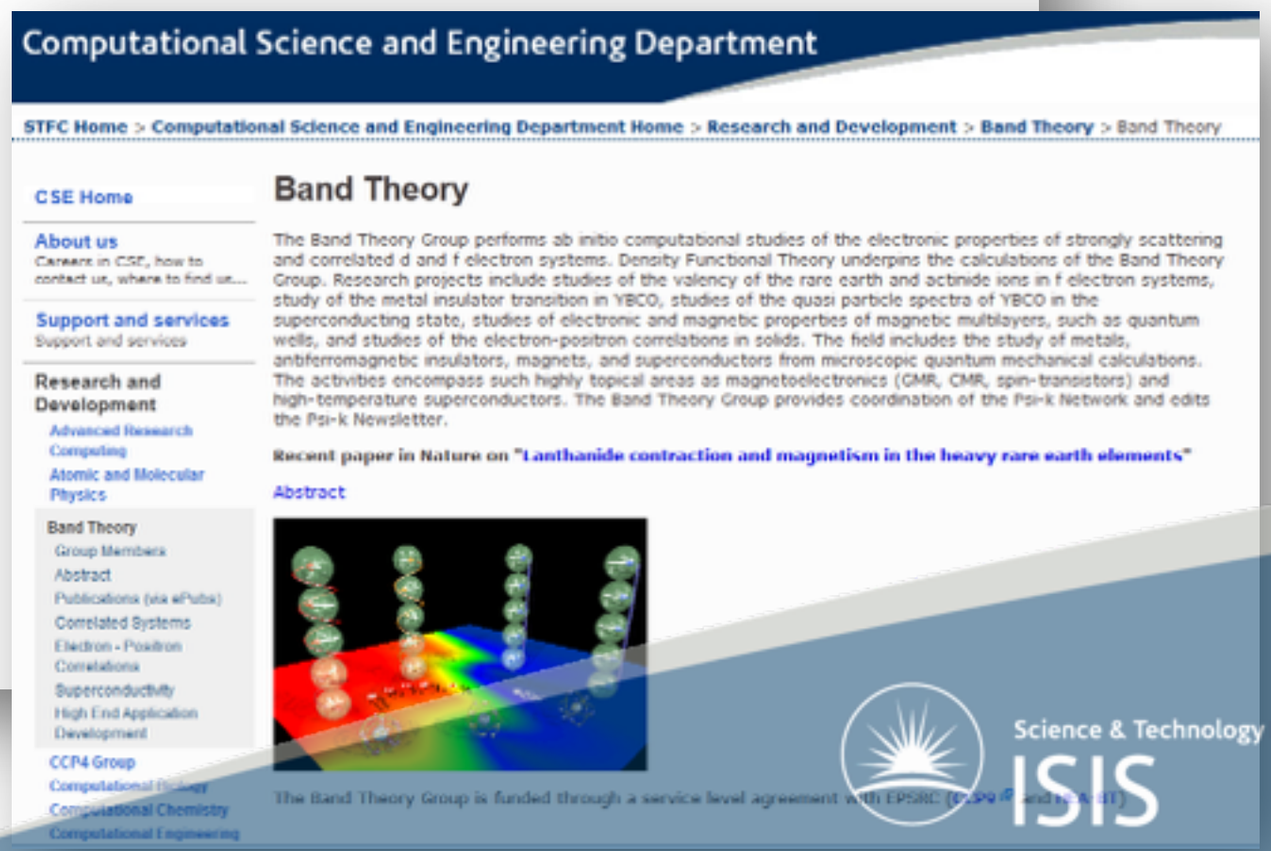


Fig. 5 A three-dimensional subset of the four-dimensional map of lattice vibrations in calcite($CaCO_3$). The fluctuations are shown as a function of energy for wavevectors of the form Q_1, 0, Q_2, where the three directions refer to the sides of the unit cell of the atomic structure.

Conclusion

These advances have been made possible not just by developments in detector technology, which give the latest spectrometers detectors areas of up to 40 m^2 divided into 300,000 elements, but also the IT and software infrastructure to enable the vast quantities of data they collect to be visualised and analysed. Indeed, the opportunities afforded by these advances are in their own right an area of scientific investigation.

For the non-specialist, unprecedented insight into the atomic motions of materials is now a routine option. Individual expertise in data-handling and software engineering can take a back seat allowing the scientific problem to remain the focus of the experimental activity. mt



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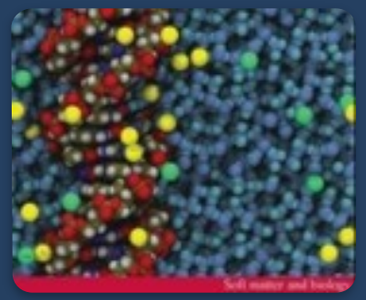
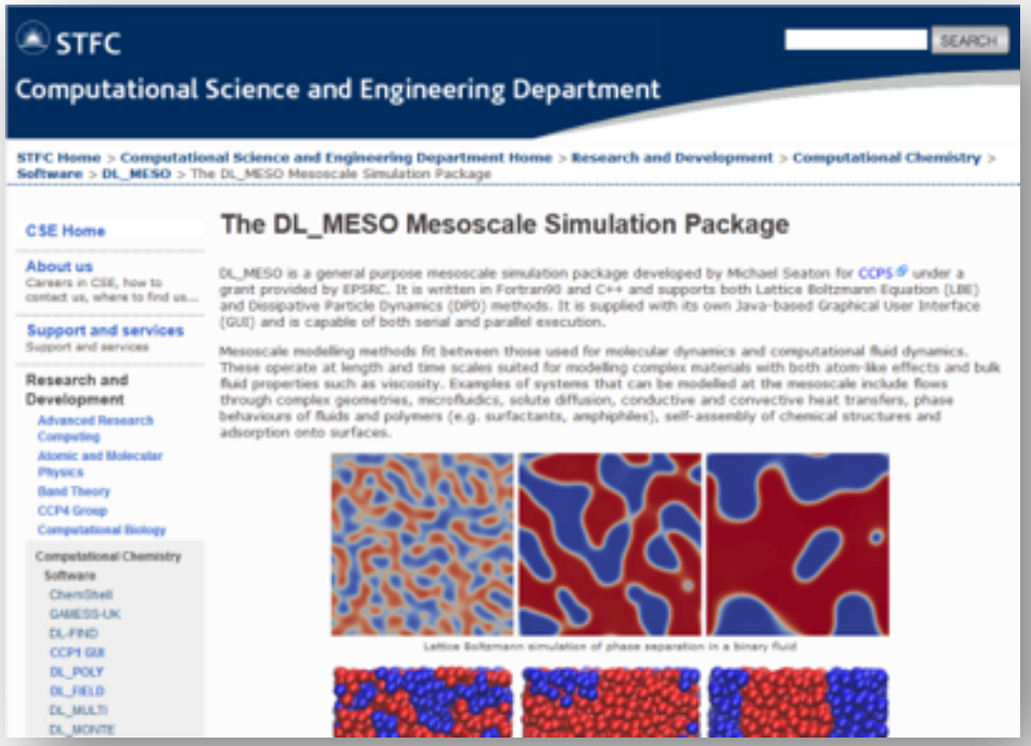


MICRONS AND MICROSECONDS

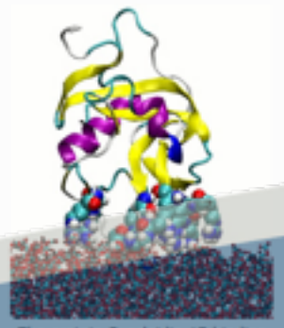
- ••interfaces, micelles, etc.
- ••protein structure and dynamics



The DL_POLY_4 code design is based on the principles of portability, maintenance, transparency and user verification. The code architecture adopts the Fortran90 modularisation in a C/C++ header style manner, where concepts and functionality are separated in a functional way by modules. The code routines relate to features/actions by their file names, which often relate to module names.

The DL_POLY_4 vanilla source is in fully self-contained, free-formatted Fortran90+MPI2 code (specifically Fortran90 + TR15581 + MPI1 + MPI-I/O only). The vanilla distribution complies with the NAGWare and FORCHECK Fortran90 standards with exception of the Fortran2003 feature known as TR15581, which is very rarely unavailable in the current Fortran95 compilers.

Extensions such as the netCDF I/O functionality and the CUDA port break this self-containment as they each add an additional dependence.



The protein Ovocleidin-17 binding to an amorphous calcium carbonate surface. The particular amino acid residues that bind to the surface are highlighted with a space-filling model.

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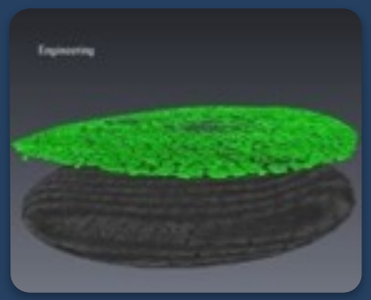


METRES AND MONTHS

- engineering measurements, archeometry
- tomography, residual stress, etc.

STFC

Computational Science and Engineering Department

SEARCH

STFC Home > Computational Science and Engineering Department Home > Research and Development > Computational Engineering > Computational Engineering

CSE Home

About us
Careers in CSE, how to contact us, where to find us...

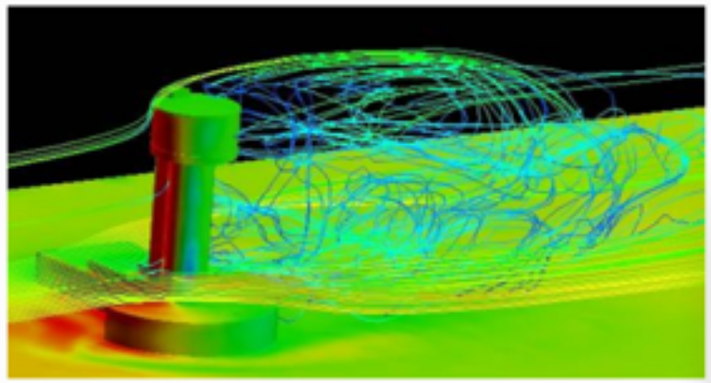
Support and services
Support and services

Research and Development
- Advanced Research Computing
- Atomic and Molecular Physics
- Band Theory
- CCP4 Group
- Computational Biology
- Computational Chemistry

Computational Engineering
- Collaborative Computational Project 12 (CCP12)
- Centre for Microfluidics and Microsystems Modelling (C3M)
- Research activities
- Industrial projects
- Publications

Computational Engineering

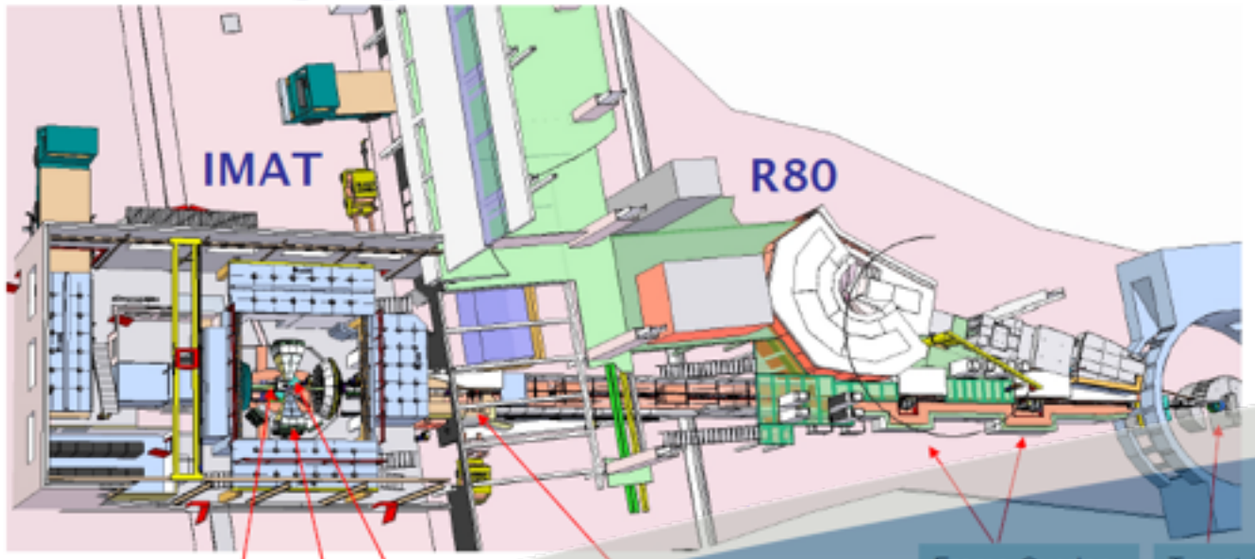
The Computational Engineering Group combines leading-edge expertise in fluid flow modelling with the latest high-performance computing solutions to help solve complex fluid dynamic problems. The group has been collaborating on groundbreaking projects with academia and industry for many years and specialises in high performance parallel computing, turbulence and combustion modelling, and microfluidics.



The image shows the computed air flow around the Daresbury Tower.
The calculations were performed on a 64 processor SGI Altix 3700.

The group is one of the world's leading players in the modelling and design of microfluidic and nanofl
This exciting new field offers many modelling challenges because, at such small scales, the fluid may
the same as that experienced in the macroscopic world.

IMAT: Imaging and Materials



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NANOMETRES AND NANOSECONDS

- chemical structure and dynamics
- structure/property relationships

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nature chemistry

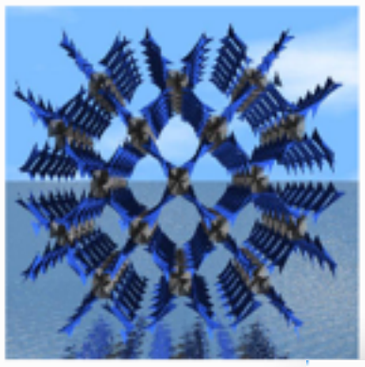
Selectivity and direct visualization of carbon dioxide and sulfur dioxide in a decorated porous host

Sihai Yang, Junliang Sun, Anibal J. Ramirez-Cuesta, Samantha K. Callear, William I. F. David, Daniel P. Anderson, Ruth Newby, Alexander J. Blake, Julia E. Parker, Chiu C. Tang & Martin Schröder

Affiliations | Contributions | Corresponding authors

Nature Chemistry **4**, 887–894 (2012) | doi:10.1038/nchem.1457
Received 19 March 2012 | Accepted 10 August 2012 | Published online 23 September 2012

Scientific discovery offers 'green' solution in fight against greenhouse gases



The crystal structure of NOTT-300

UK researchers have created a low cost, new material that can capture harmful gases, offering an exciting breakthrough in combating atmospheric pollution.

The porous material, dubbed NOTT-300, has the potential to reduce fossil fuel emissions through the cheaper and more efficient capture of polluting gases such as carbon dioxide (CO_2) and sulphur dioxide (SO_2).

The research, published in the scientific journal Nature Chemistry, demonstrates how the exciting properties of NOTT-300 could provide a greener alternative to existing solutions to adsorb CO, which are expensive and use large amounts of energy.

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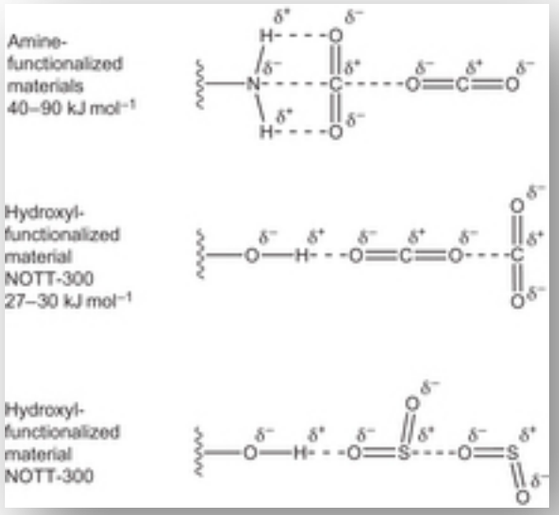
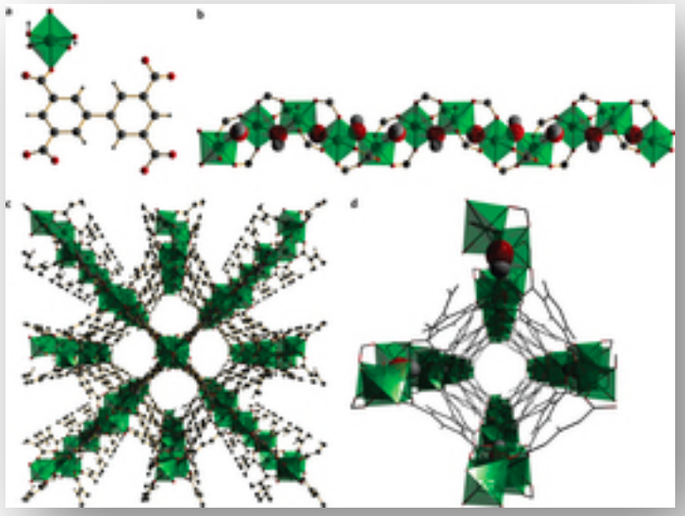
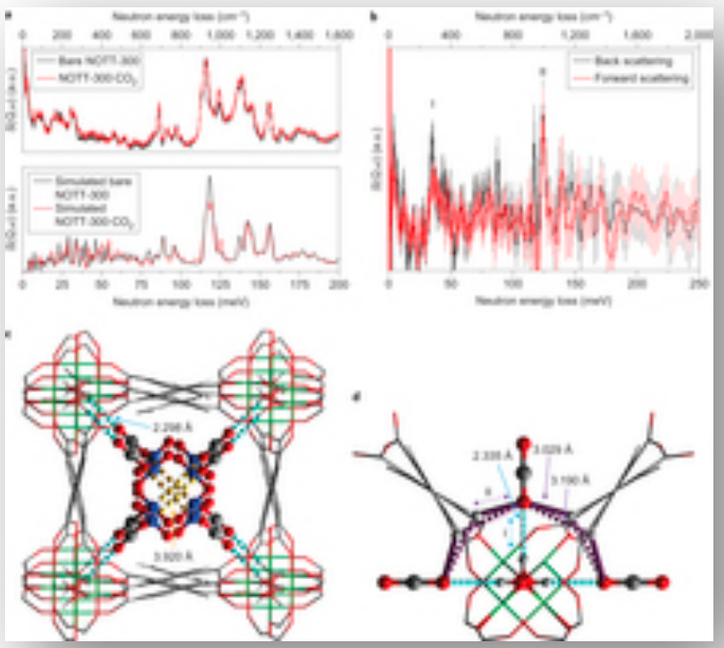


X-ray powder diffraction (I11, Diamond)



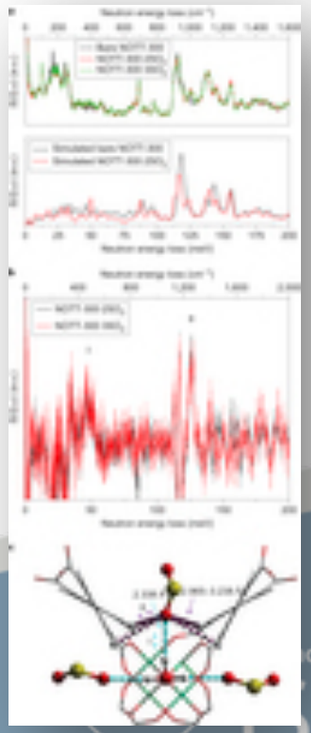
In-situ neutron powder diffraction (WISH)

Synthesis (Notts)



DFT modelling (aCLIMAX)

Inelastic neutron scattering (TOSCA)



12-16 Months

nature
Nature homepage
International weekly journal of science

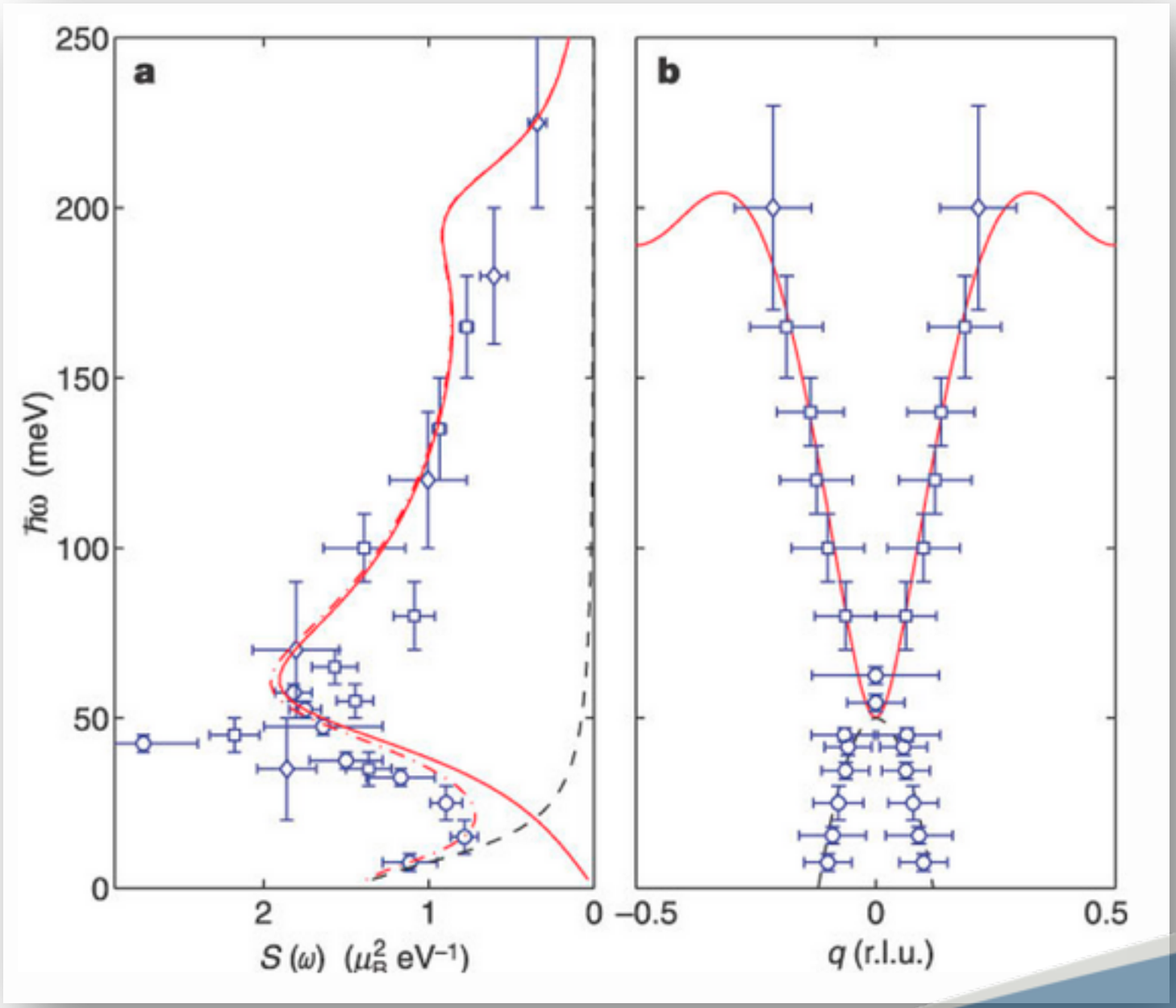
Nature **429**, 534-538 (3 June 2004) | doi:10.1038/nature02574; Received 26 January 2004; Accepted 16 April 2004

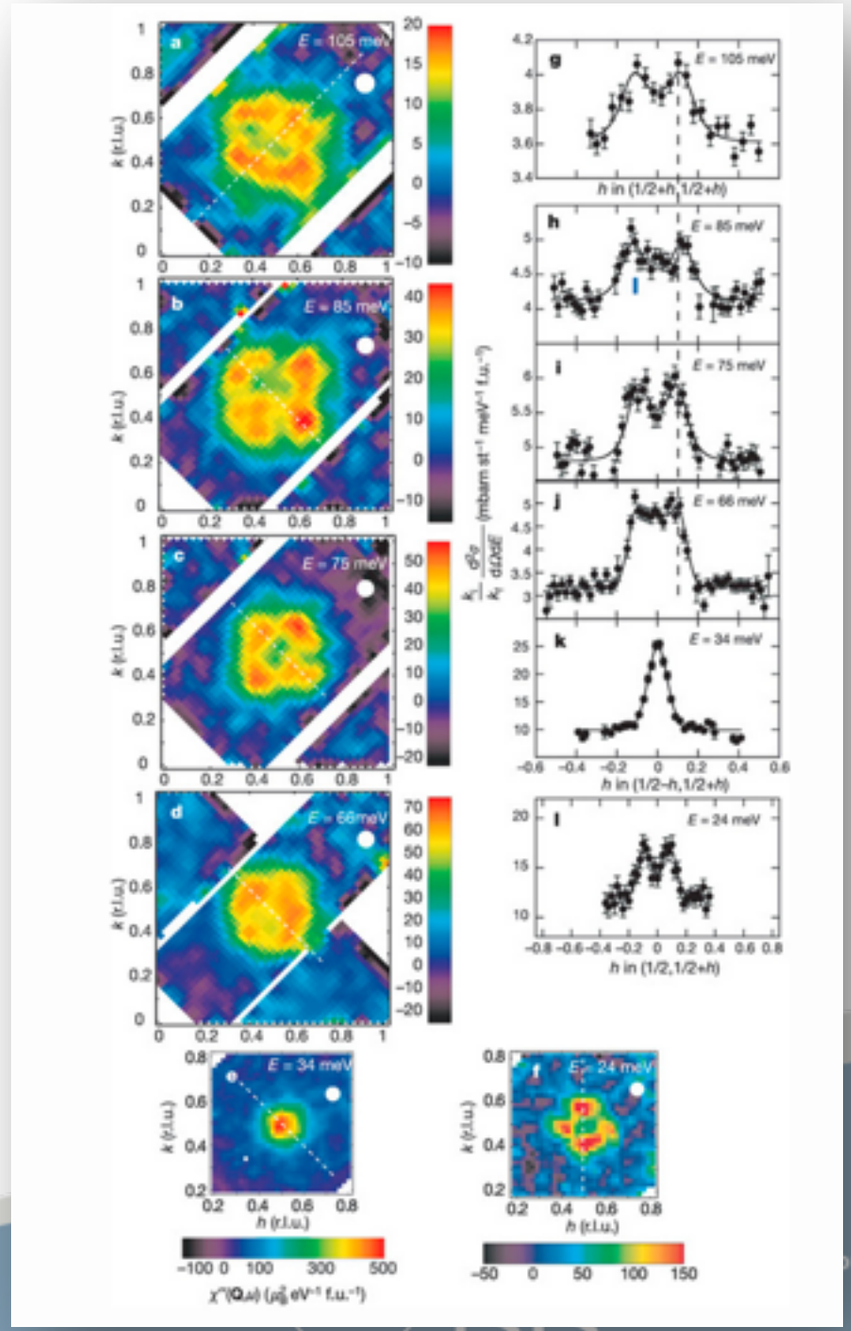
Quantum magnetic excitations from stripes in copper oxide superconductors

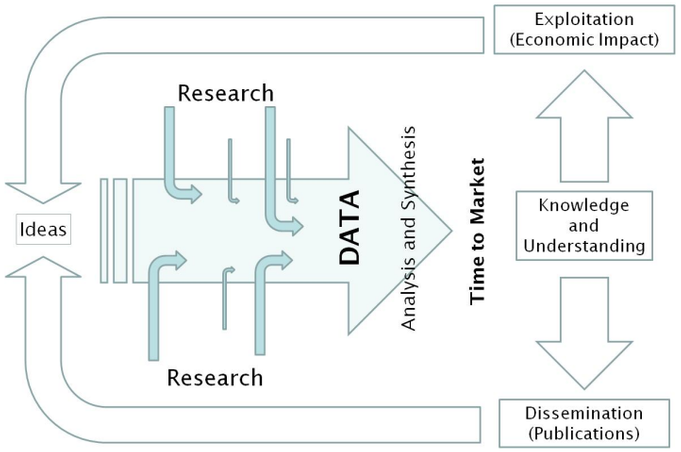
J. M. Tranquada[1], H. Woo[1,2], T. G. Perring[2], H. Goka[3], G. D. Gu[1], G. Xu[1], M. Fujita[3] & K. Yamada[3]

$$S(\mathbf{Q},\omega) \approx (\hbar\omega_{q_\parallel})^{-1}[\sin^2(q_\parallel a/2) + \sin^2(q_\perp a/2)]$$

$$\times[\delta(\omega - \omega_{q_\parallel}) - \delta(\omega + \omega_{q_\parallel})]$$







1. Experiment Planning → 2. Data collection → 3. Data reduction → 4. Data visulisation → 5. interpretation of results → 6. Publication

Pre Beamtime	Beamtime			Post Beamtime
Proposal	Experiment Planning	Data Collection	Data Reduction	Data Visualisation	Simulation Modelling Interpretation

Virtual experiment aided planning

Live data view
Data driven collection

Common data backplane
Simplified remote data access cloud technology
Common experiment and simulation data

Data collection needs to be Flexible

Data reduction needs to be Flexible

Analysis and interpretation are a barrier to publication

Data collection needs to be "informed"

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Understanding data is a barrier to publication

data with a meaningful model or analysis generates more citations

ISIS beamtime cost ~£15K per day

ISIS spends £1.2M pa on software development

ISIS has ~60 scientists to deliver the user programme for the community

Data analysis, modelling and simulation

Relies heavily on the goodwill of scientists

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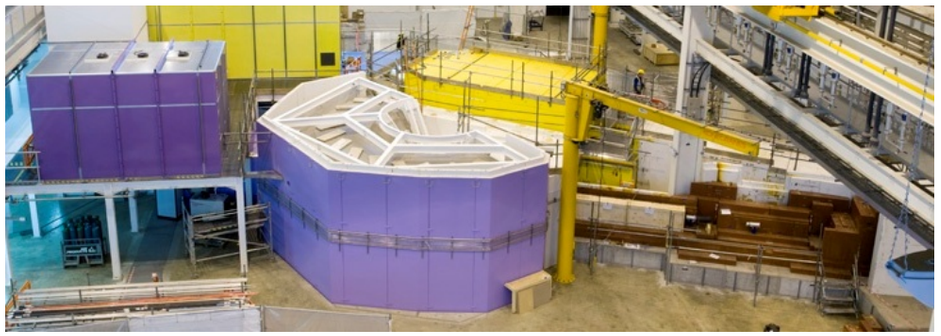
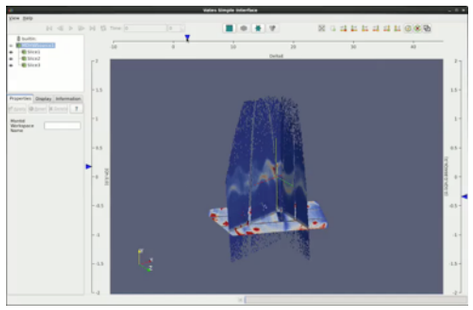
Analysis and interpretation is a barrier to publication

Analysis and interpretation is the tertiary spectrometer





Importance

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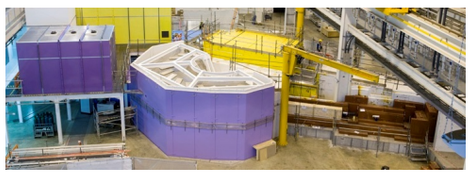

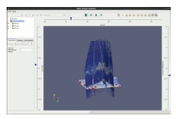

Resource level

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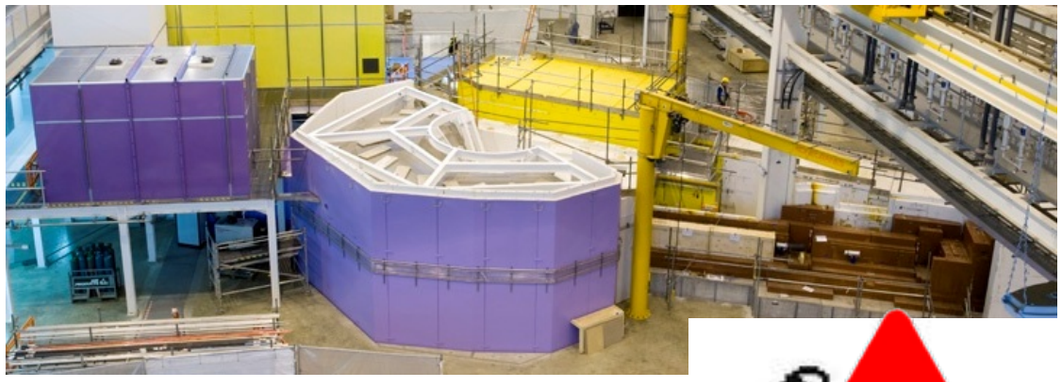

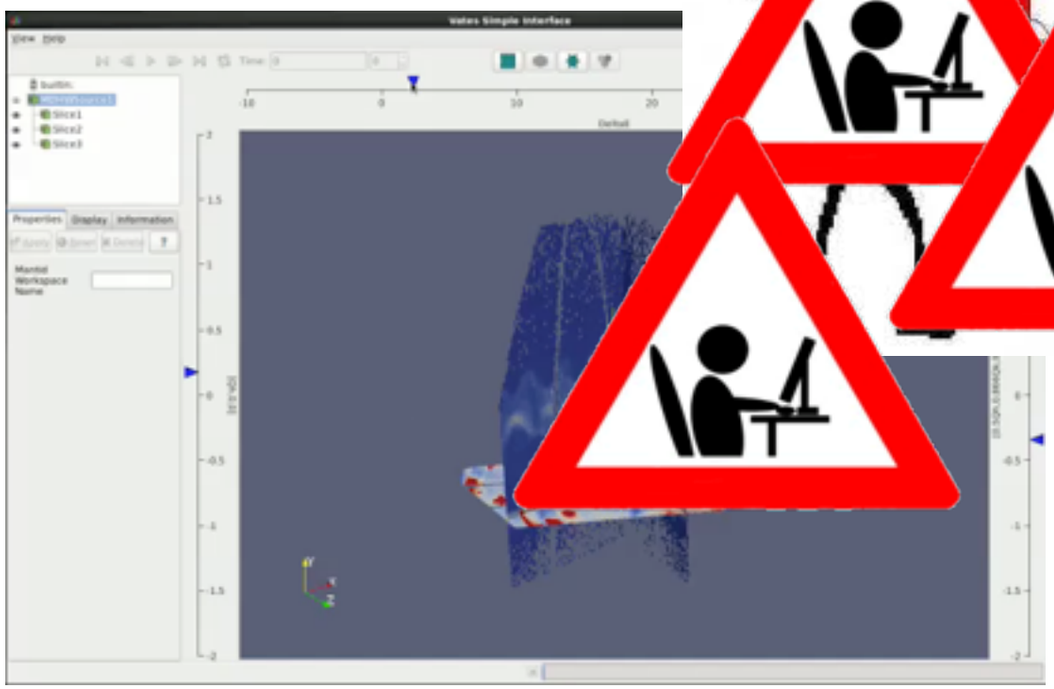

Lots of bespoke software

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We don't expect users to:

"Proposal to publication support for scientific computing to maximise the impact of the ISIS science programme that does not require any support."

In order to grow our user community we must be able to service users who have no prior experience of other neutron scattering, MUSR or scientific computation

develop beam lines

run experiments without support.

but after the experiment…

If you need help get in touch. but i'm local contact for the next 6 months

Thanks I promise to publish my data… in nature

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Create tools that form a flexible workflow

Develop a flexible scattering specific framework

Make data access simple (and fast)

Give users access to data analysis tools

What is MANTID

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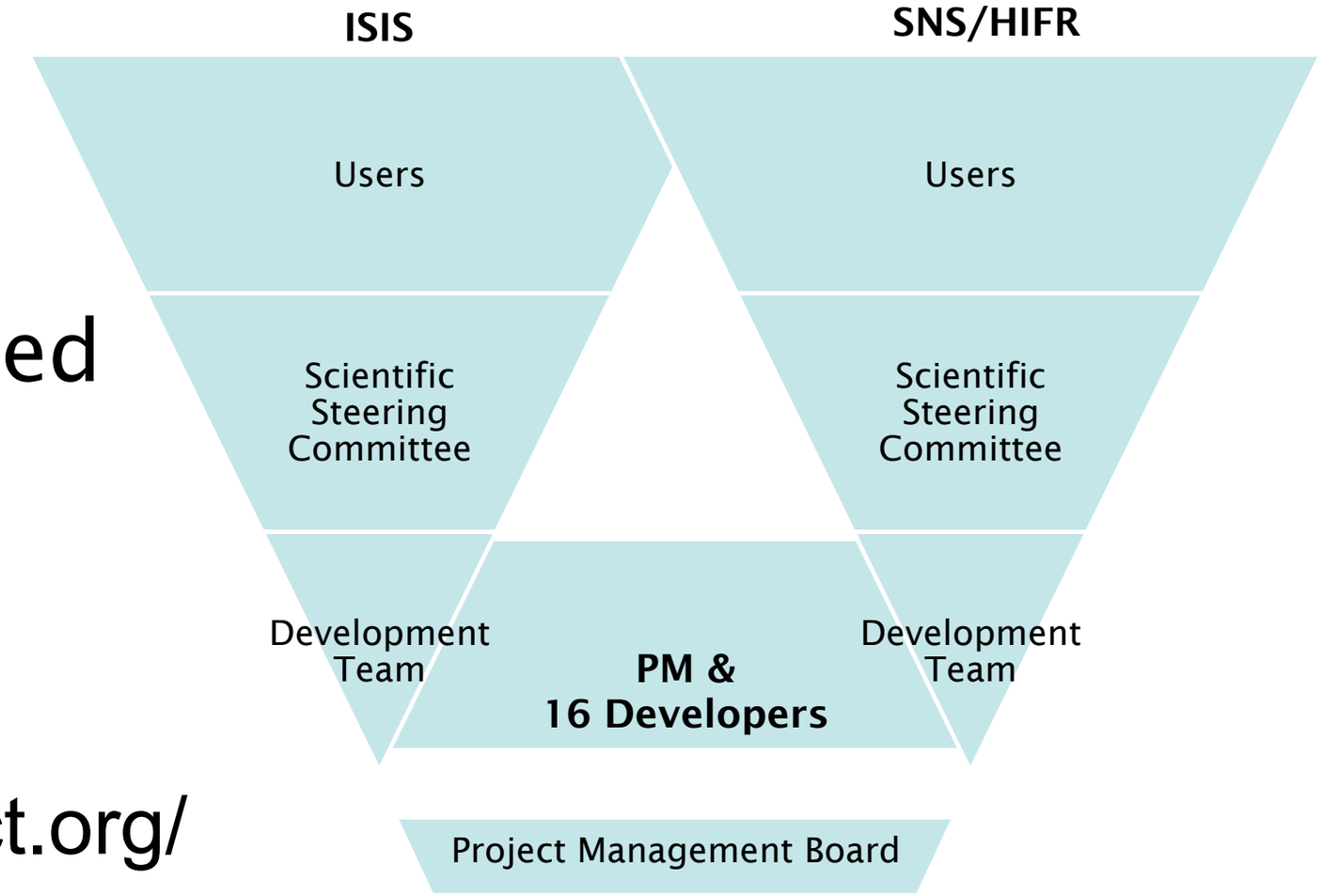
What is MANTID

- A ***common*** framework for:
  - Reduction
  - visualisation
  - analysis
- Collaboratively developed



http://download.mantidproject.org/

Cross platform **OSX** 64 **Linux** x64

and **Windows** 32 &64

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Project History

July 2007
Requirements
& Design

April 2008
V 1.0
First instrument
support

Feb 2010
V1.1
Support multiple
techniques

April 2010
Collaboration with
SNS & HFIR

Jan 2012
V2.0

Scientist validated
results. VATES
integration

Jan 2014
TOF xtal diffraction
Continued funding
Proposed use at ESS

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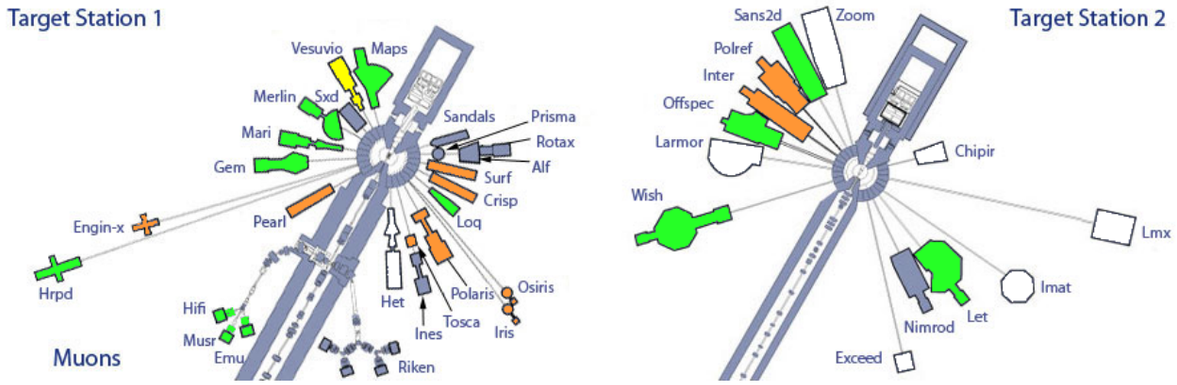
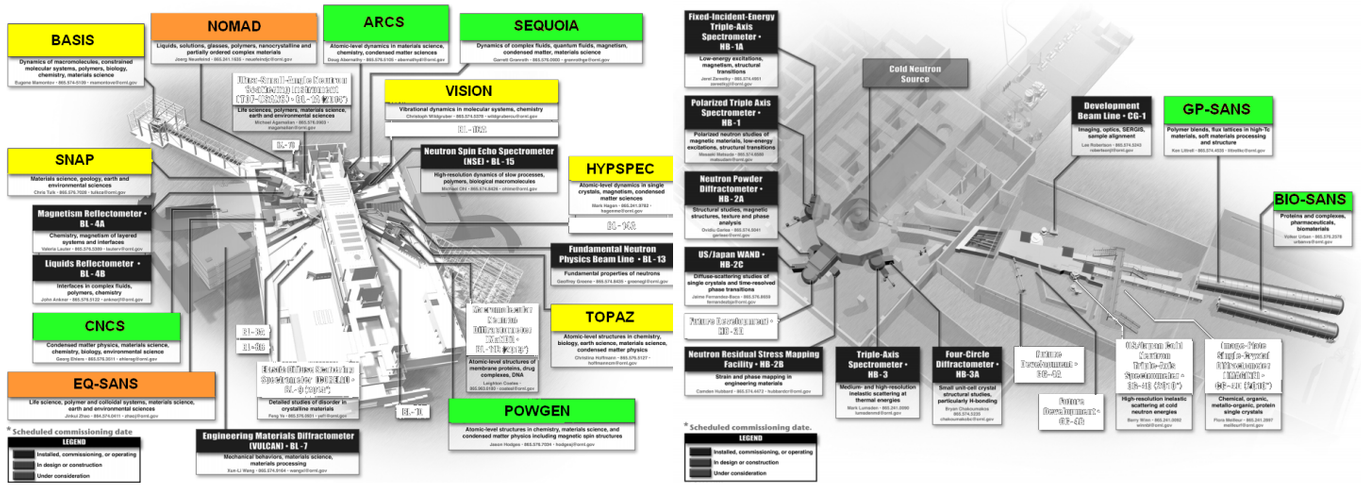
Where is Mantid used

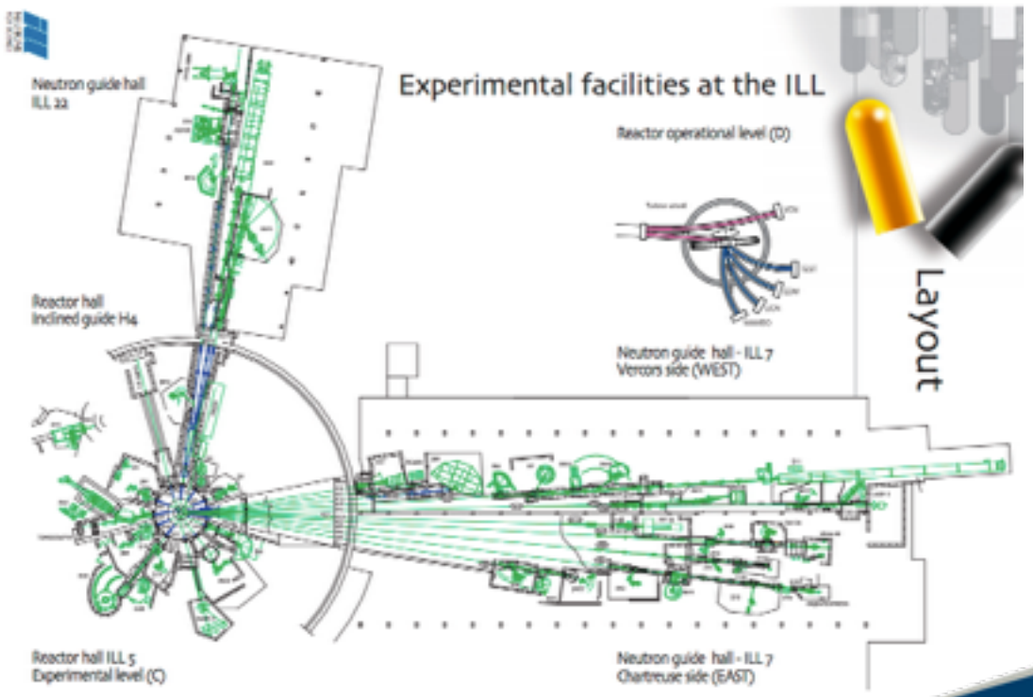
ISIS



SNS



HFIR



PAUL SCHERRER INSTITUT

PSI

ESS EUROPEAN SPALLATION SOURCE

Los Alamos NATIONAL LABORATORY EST. 1942

LANSCE Los Alamos Neutron Science Center

Australian Government | ansto

Australian Nuclear Science and Technology Organisation

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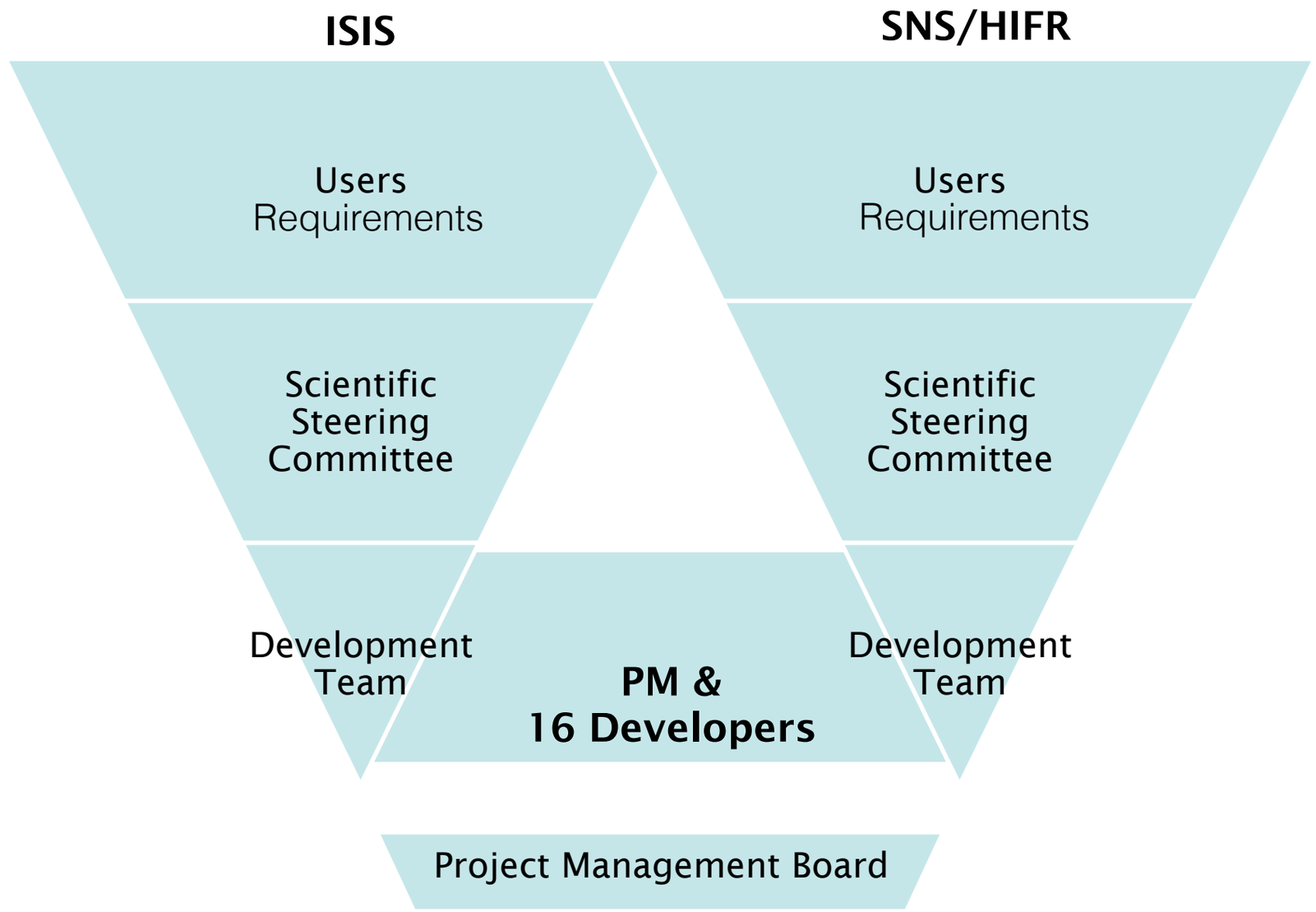

Single project manager
All core algorithms abstracted
Iterative agile development

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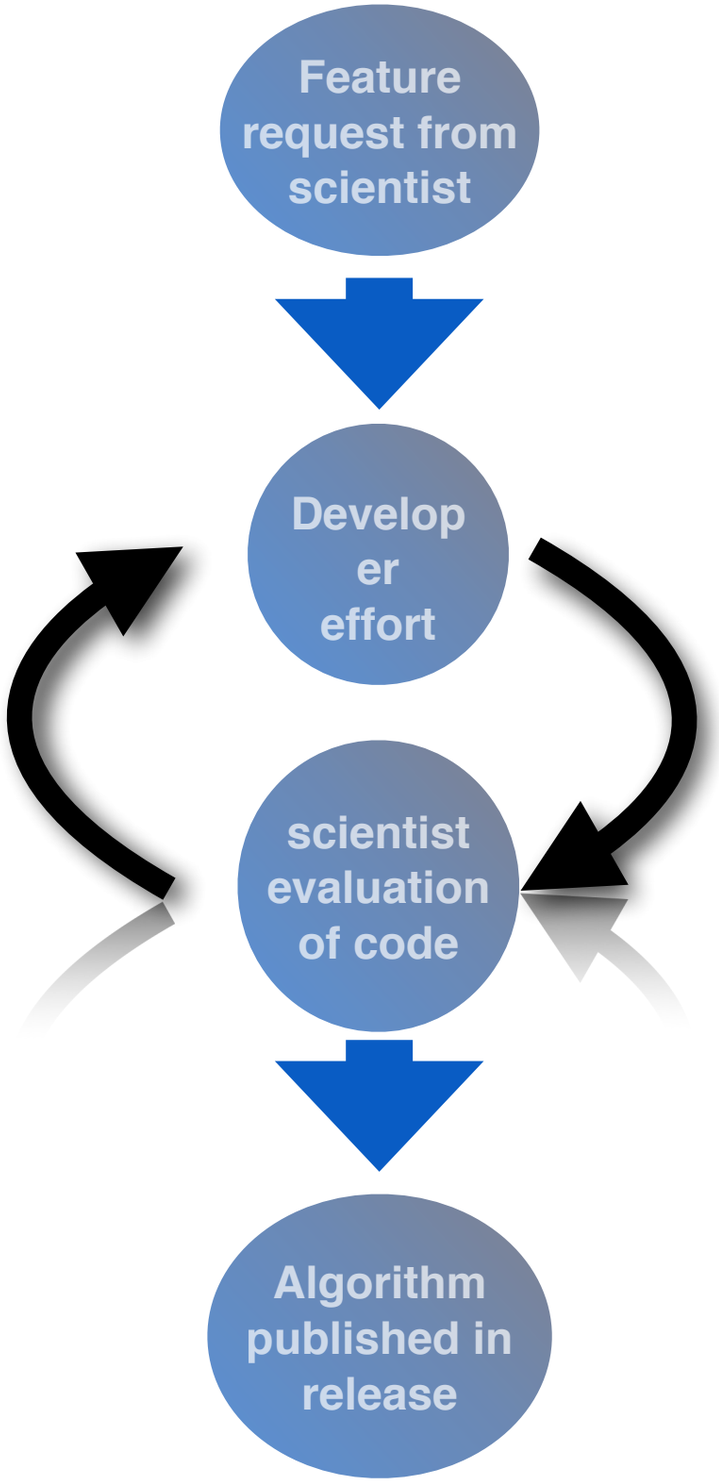
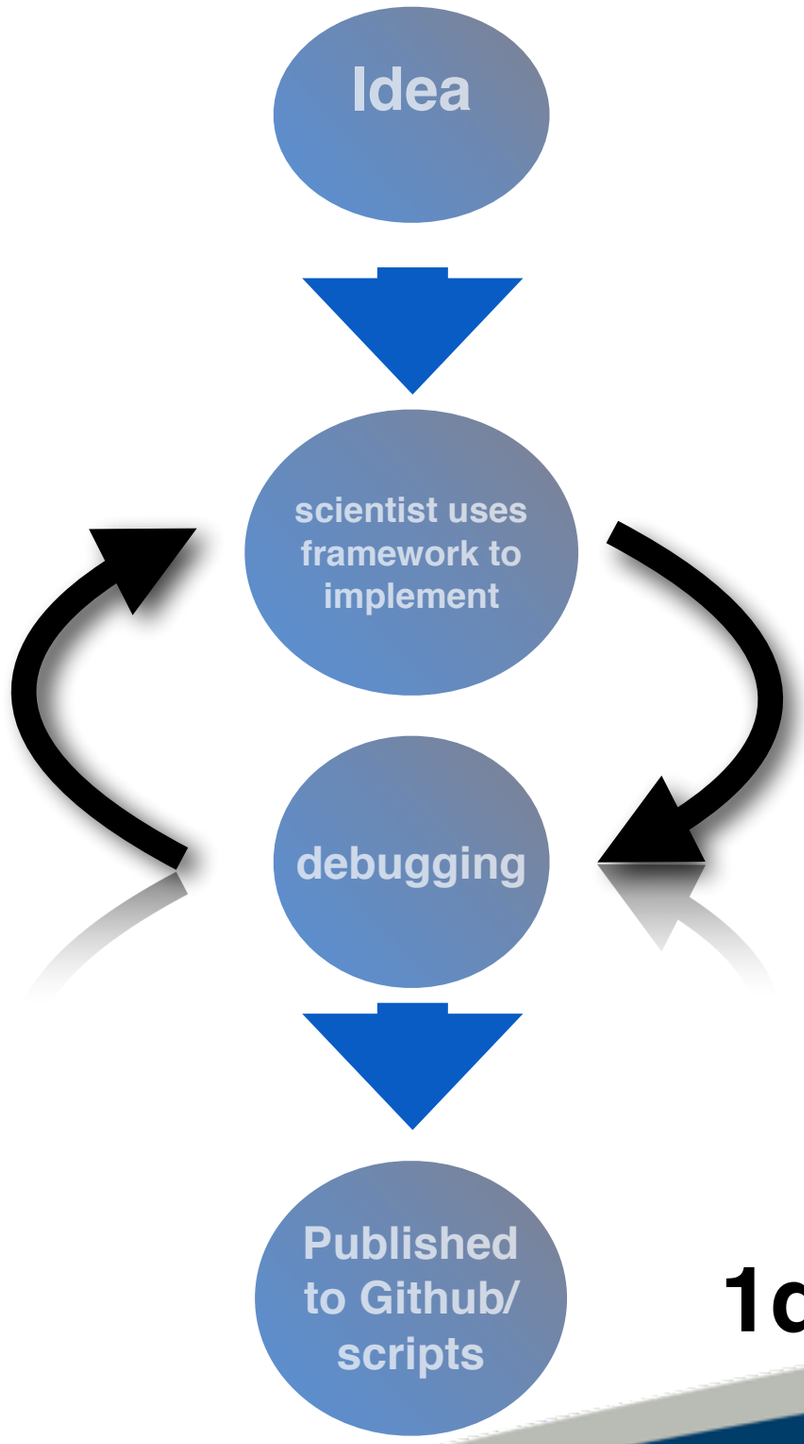
Iterative focused development



6-8weeks



1day+

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MANTID Features

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Plug in extensions

Python
Command line &
Scripting
interface

Framework

Deploy to
Download site

Instrument log
files

data files

faces

nus

API

Mantid Project Wiki

Algorithms

Worksp

User Defin

GitHub
Repository

Automated
System test

NEXUS data
files

Build + unit test
-Linux (RHE & Ubuntu)
-Mac OSX
-Windows 32
-Windows 64

DAE direct
access

trac
Issue
tracking
system

strument

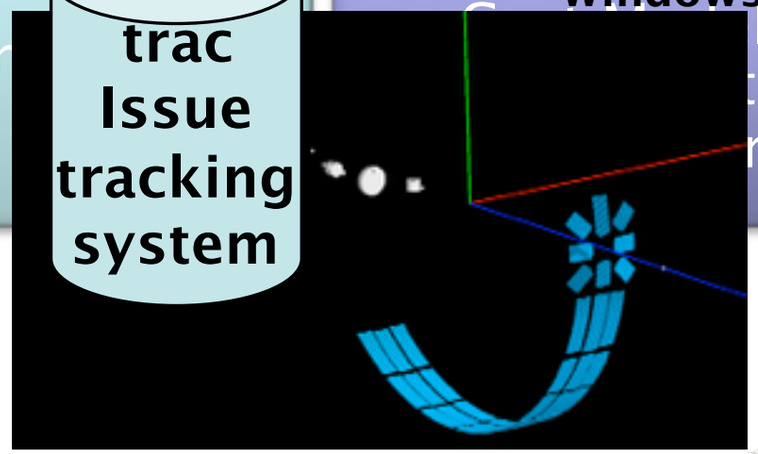
Fit Functions

nive Searching
Data Listeners
ata Catalogs

Unit Cor

Utility

Developers



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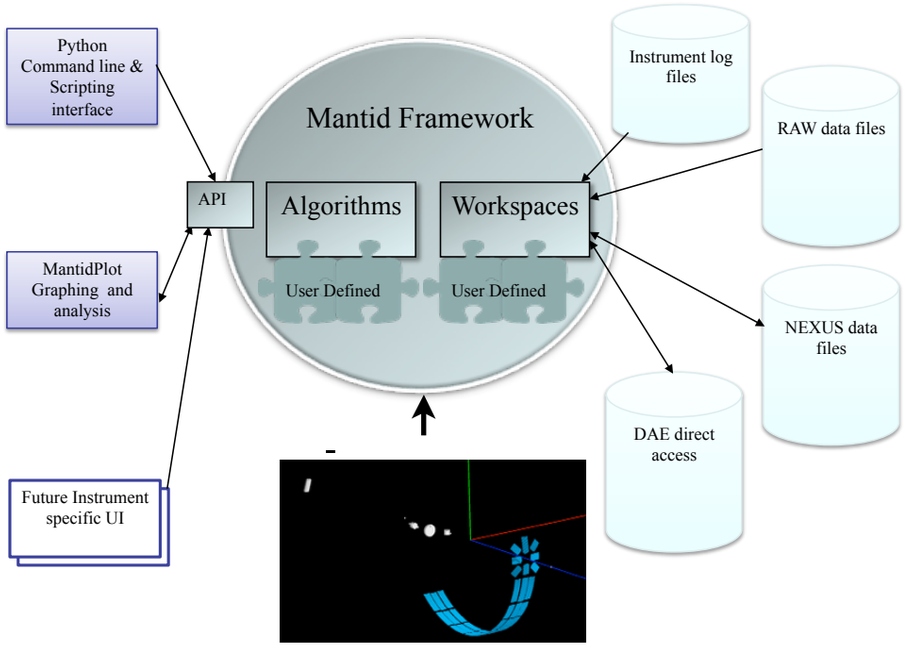


Novel features

Full Instrument description

Workspace history

Multiple workspace types

Box controlled rebin on nD data

Live event view

Algorithms event aware

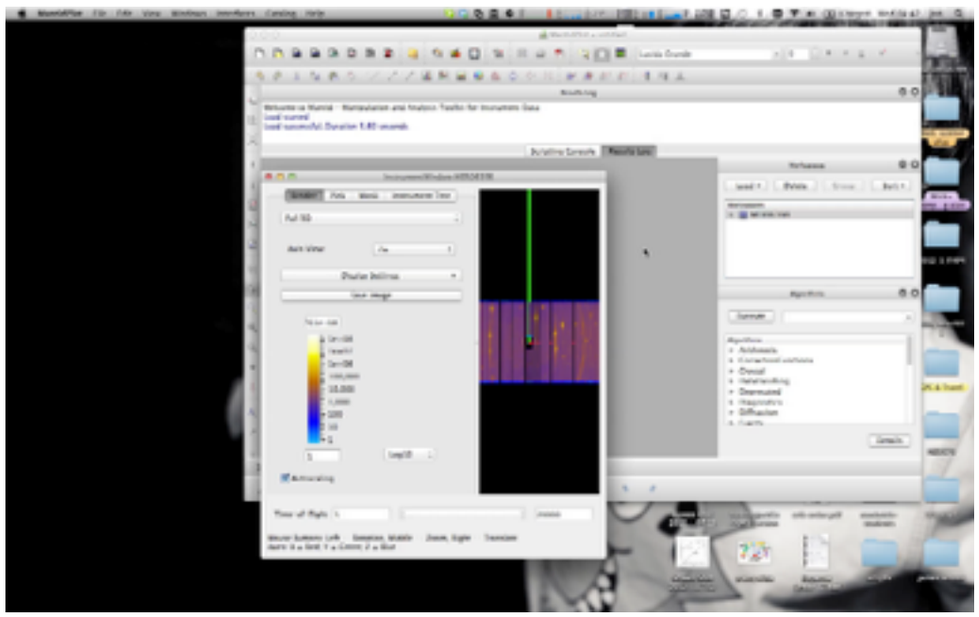
Slice viewer for 2D data

Python + IPython + Numpy + SciPy

ParaView

OpenMP

User extendable



Instrument view

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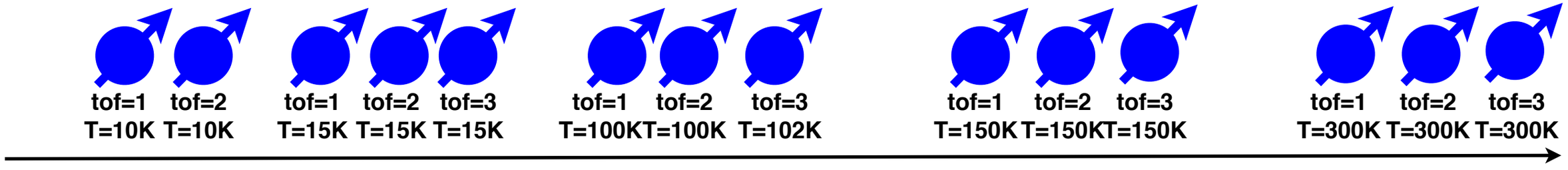
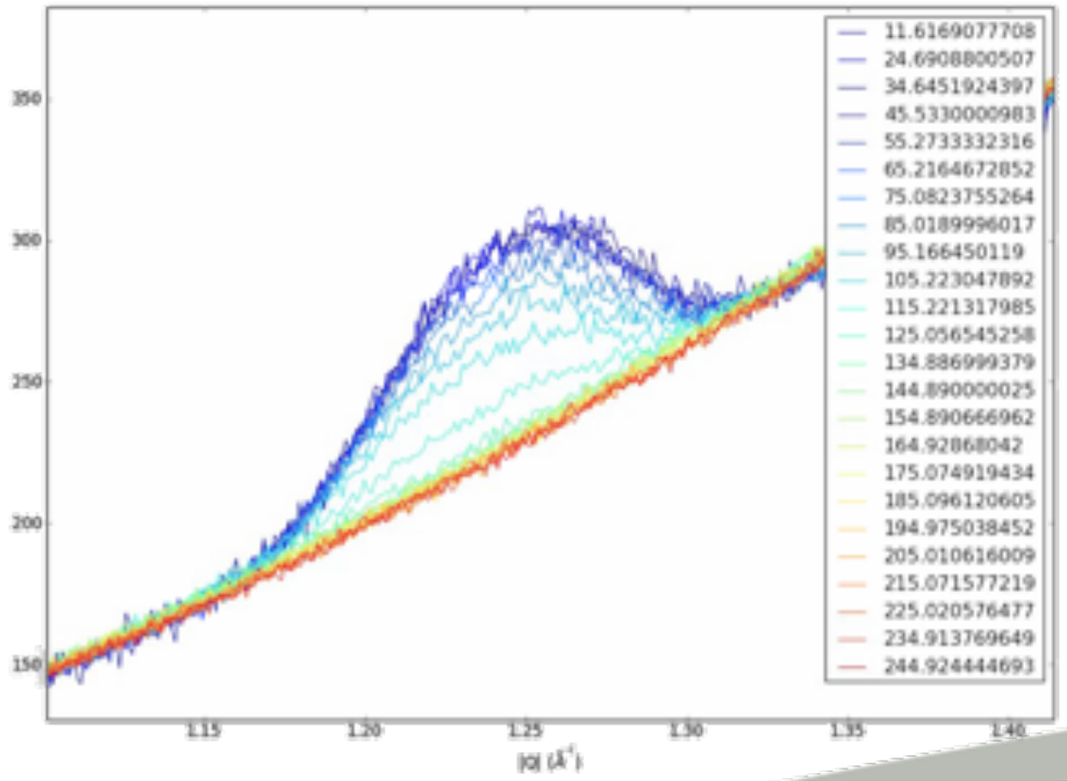
Maximize the benefits of event mode data collection



Filter data on Log values

Sparse data for INS

RMM



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What is MANTID used for

General data treatment

Advanced visualisation

Experiment setup & instrument control

Powder diffraction

Single crystal diffraction

Reflectometry

SANS

Direct geometry INS

Indirect geometry INS

MUSR

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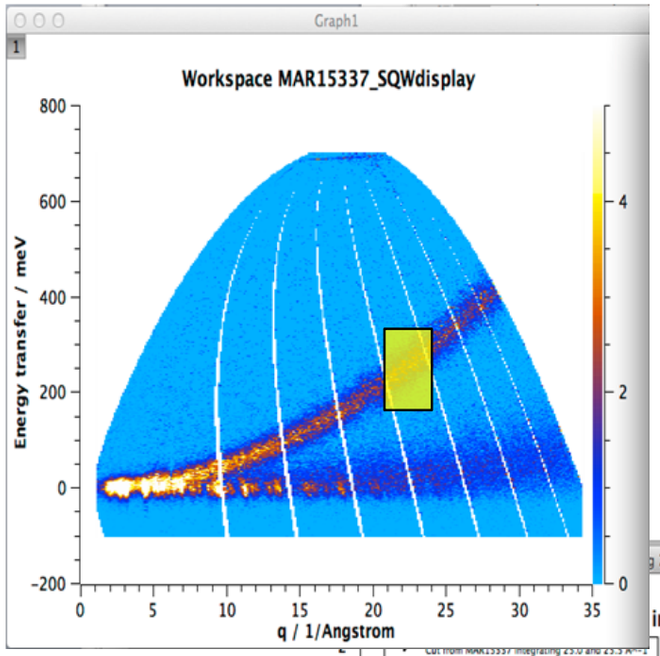
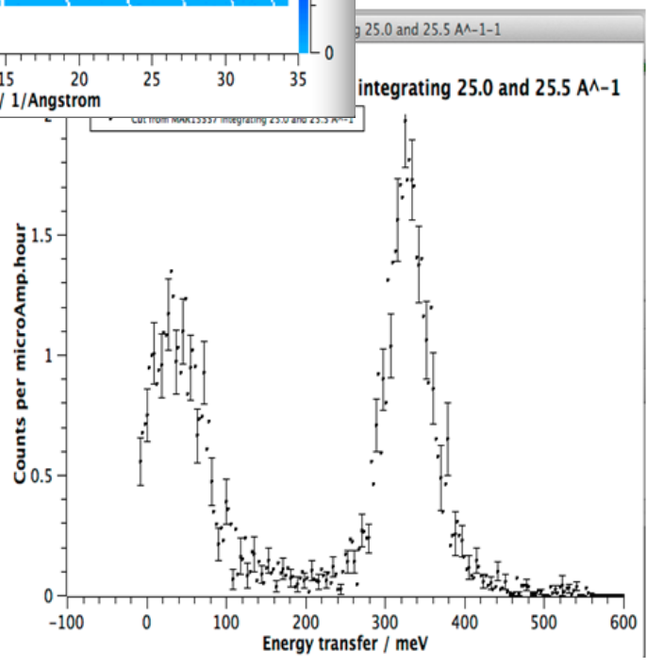
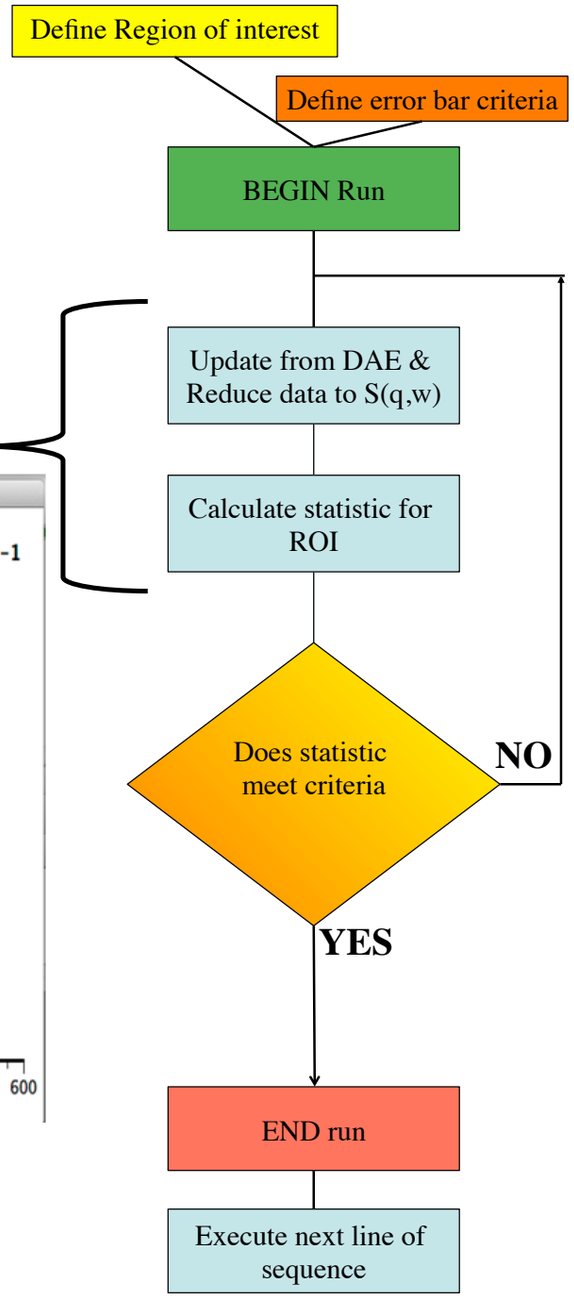
Data collection & instrument control







USER interface

- MantidPlot Python interface
- SECI interface

Developer

- PyGenie API
- SECI API

Instrument control program → DAE	SECI → Sample environment & chopper control	NI LabView → device control

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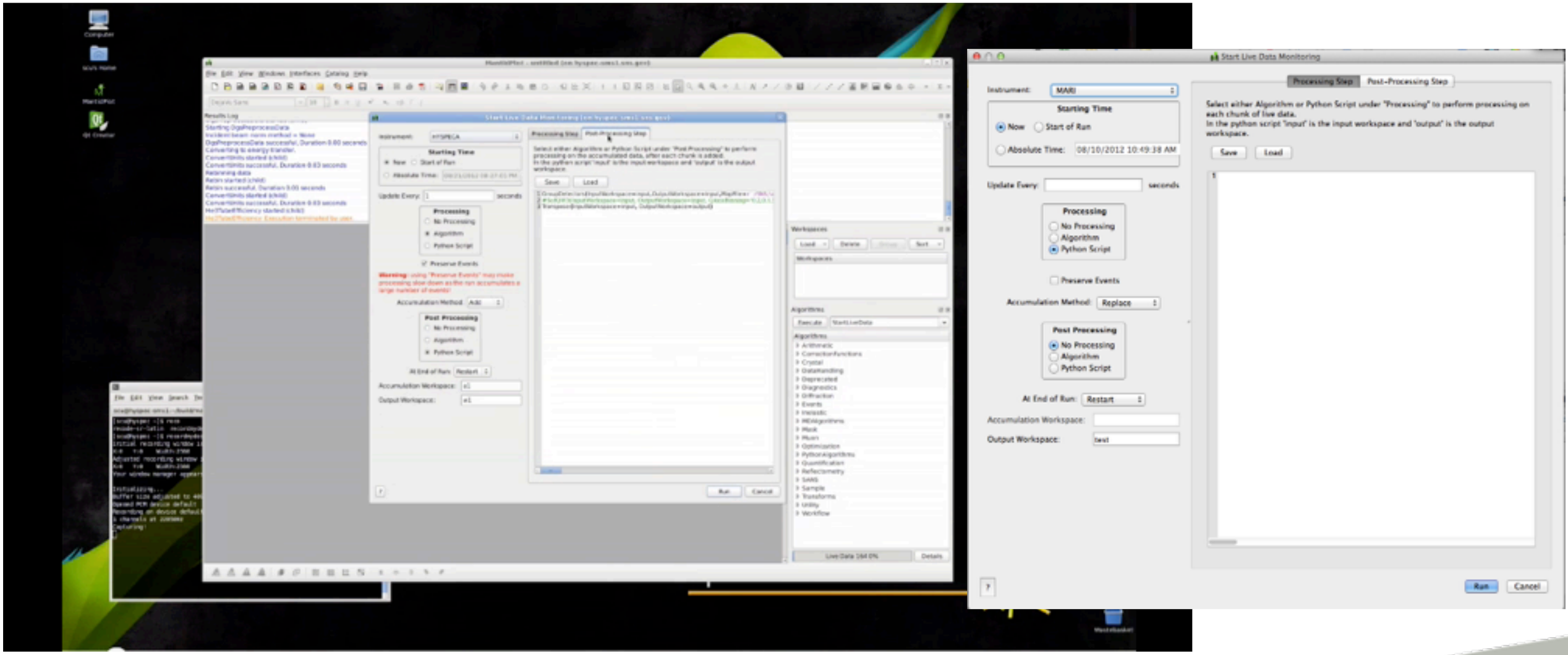
Live Reduction

- **Live view.**
- **Live reduction.**



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Data access: ICAT4 interface

My Data Search Results

Search Results : 20 Investigations Found

InvestigationId	Proposal	Title	Instrument	Run Range
24003209	720264	A μSR study of the charge density wave superconductor CuxTiSe2.	MUSR	16006-16041, 16076-16164, 16984-17014, 17041-17092, 20205-20239
24070161	910145	A μSR study of the charge density wave superconductors	MUSR	23912-23964, 24485-24496
24003232	720379	An investigation of the interplay between the charge density wave state and superconductivity	MARI	
24081518	920207	Bose-Einstein Condensation in Liquid Helium under Pressure	MARI	
24077946	910179	Bose-Einstein Condensation in solid helium confined in porous media	MARI	15313-15359
24079138	920283	CaTiO3 cooling from 291 K 30-130 ms jaws 15*20	HRPD	45112-45203, 46469-46632, 46637-46640, 48622-48737, 48740-48753, 50
24079683	1010108	Copy of: Magnetic excitations in the one dimensional (1D) spin-chain systems: Ca3TMnO6 (T=Ni and Zn)	OSIRIS	86032-86184
24088386	1120487	Copy of: Solvation dynamics of the phospholipid 1,2-dipropanoyl-sn-glycero-3-phosphocholine.	MARI	17115-17211
24077435	920285	Copy of: Structural and Magnetic Studies of Mixed-Valence Iron Silicates	OSIRIS	81518-81580
24086051	1110548	Determination of the low temperature crystal structure of Fe3O4	SXD	24189-24301
24086050	1110547	Dynamics of Confined CO2	MARI	16592-16611
24003338	720327	Dynamics of L-Proline and Glycyl-L-proline in solution	MARI	
24003157	720070	Dynamics within the Plastic Crystal Phases of Hydrogen Chloride	IRIS	36414-36781
24081574	910577	High pressure Dynamics of Urea	MARI	
24079547	1010597	Melting point dynamics of Confined fluids	MARI	15807-15934, 16082-16102, 16124-16133, 16237-16248, 16636-16637
24003150	720068	Proton Delocalization in Liquid Hydrogen Chloride	MARI	13688-13694
24003156	720069	Proton Delocalization in Liquid Hydrogen Chloride	IRIS	
24003071	720332	Search for Antiferromagnetic order in ZrMn2	MUSR	15808-15858
24083817	1110522	Solvation dynamics of the phospholipid 1,2-dipropanoyl-sn-glycero-3-phosphocholine.	MARI	16472-16513
24088079	1110529	The role of spin fluctuations, disorder and non-colinearity in the INVAR effect	HIFI	29856-29923, 30095-30114, 35963-35971, 37412-37509

Find data

Investigation Data

Data: 195 DataFiles found

Data:
- ProposalId: 1110529
  - Title: The role of s...
  - Instrument: HIFI
  - Run Range: 2985...
  - Runs
    - Status: com...
    - Type: exper...
    - Description...

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Help | Controlled loading | DataFiles | Select All Files | Download | Load | Close

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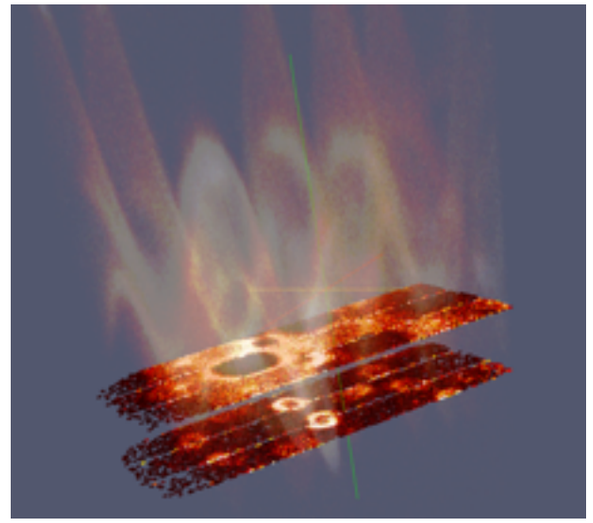
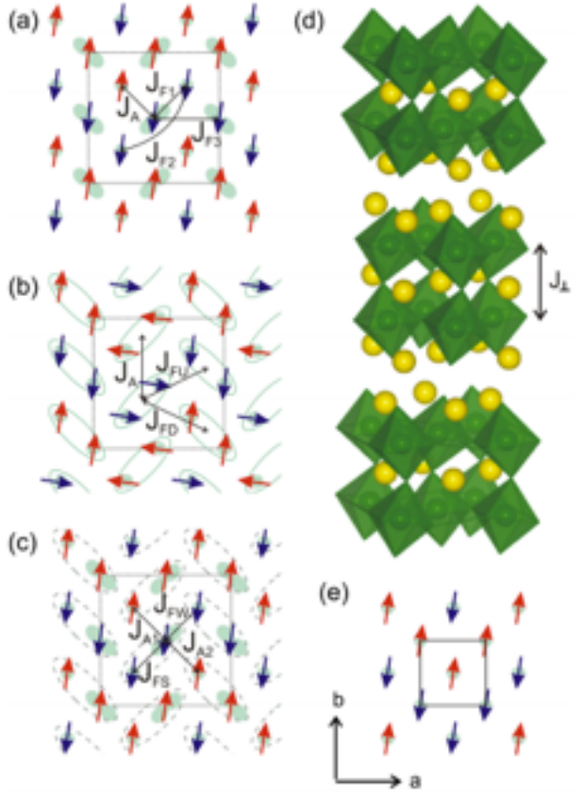
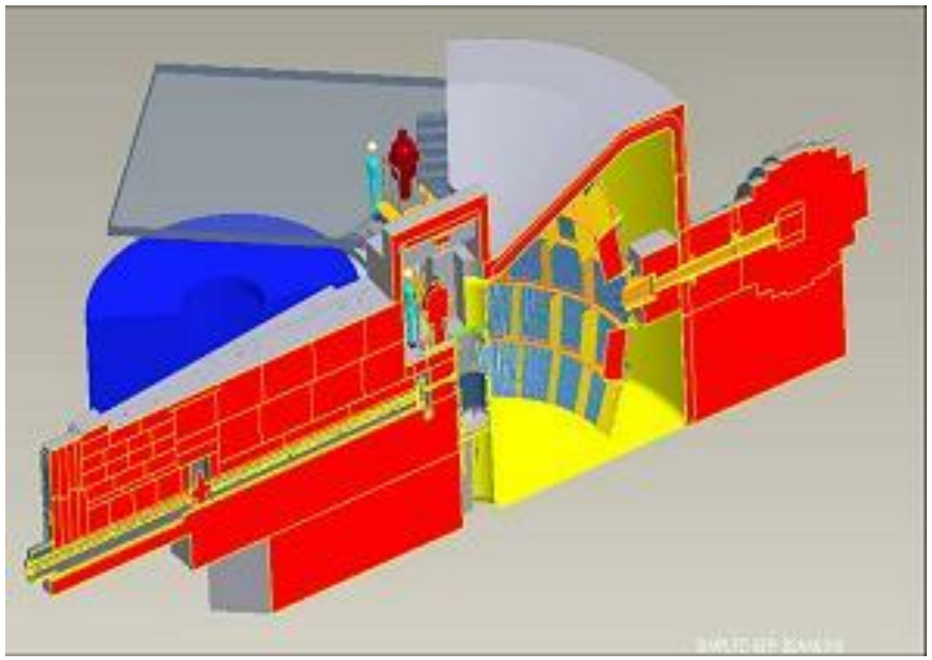
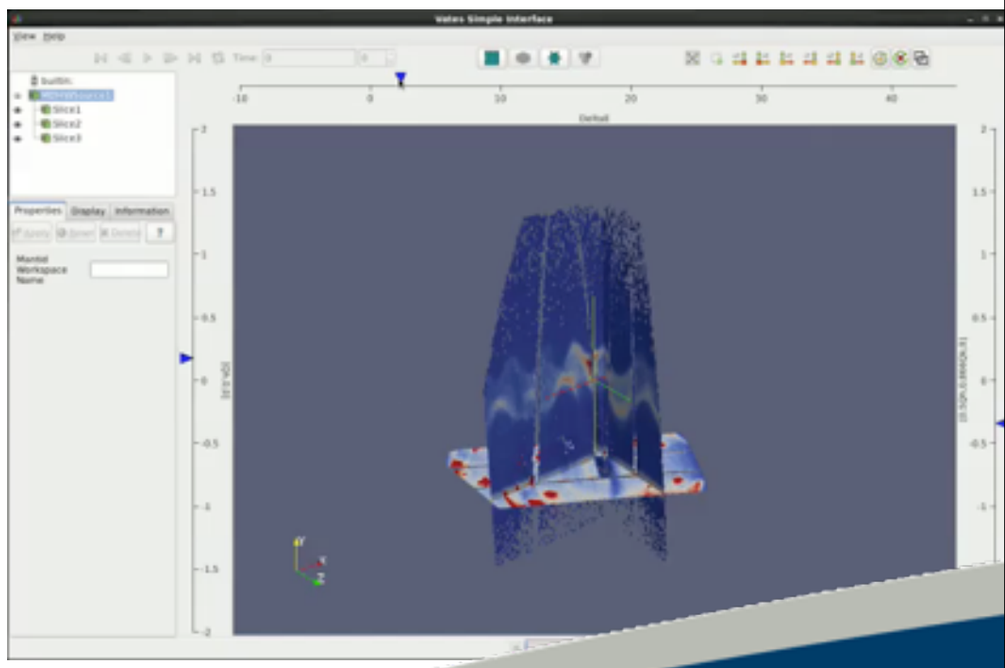
Advanced Visualisation

3D or 4D reciprocal space volume









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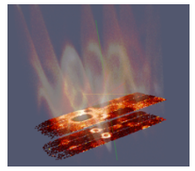
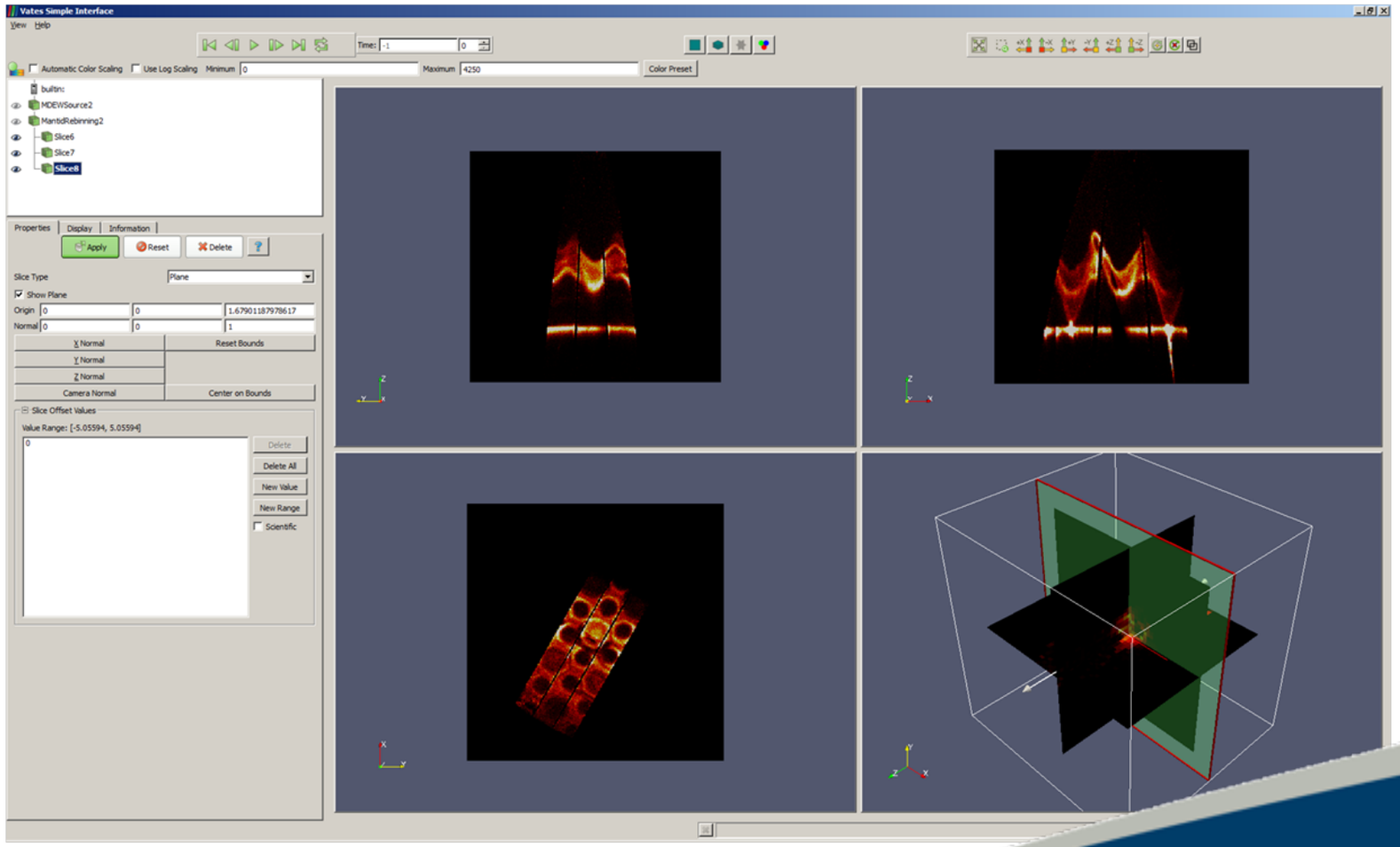


Visualisation

- Efficient re-binning of sparse data sets
- Visualisation is distributable
- Enough resource to request features from kitware



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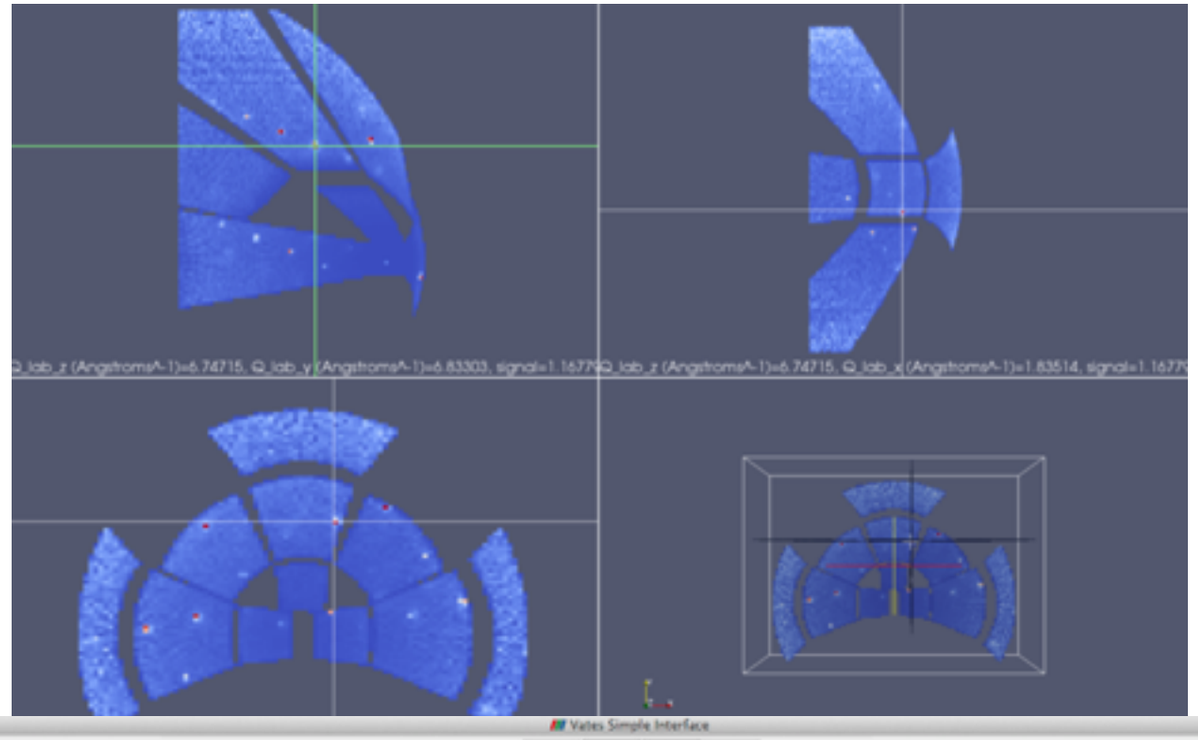
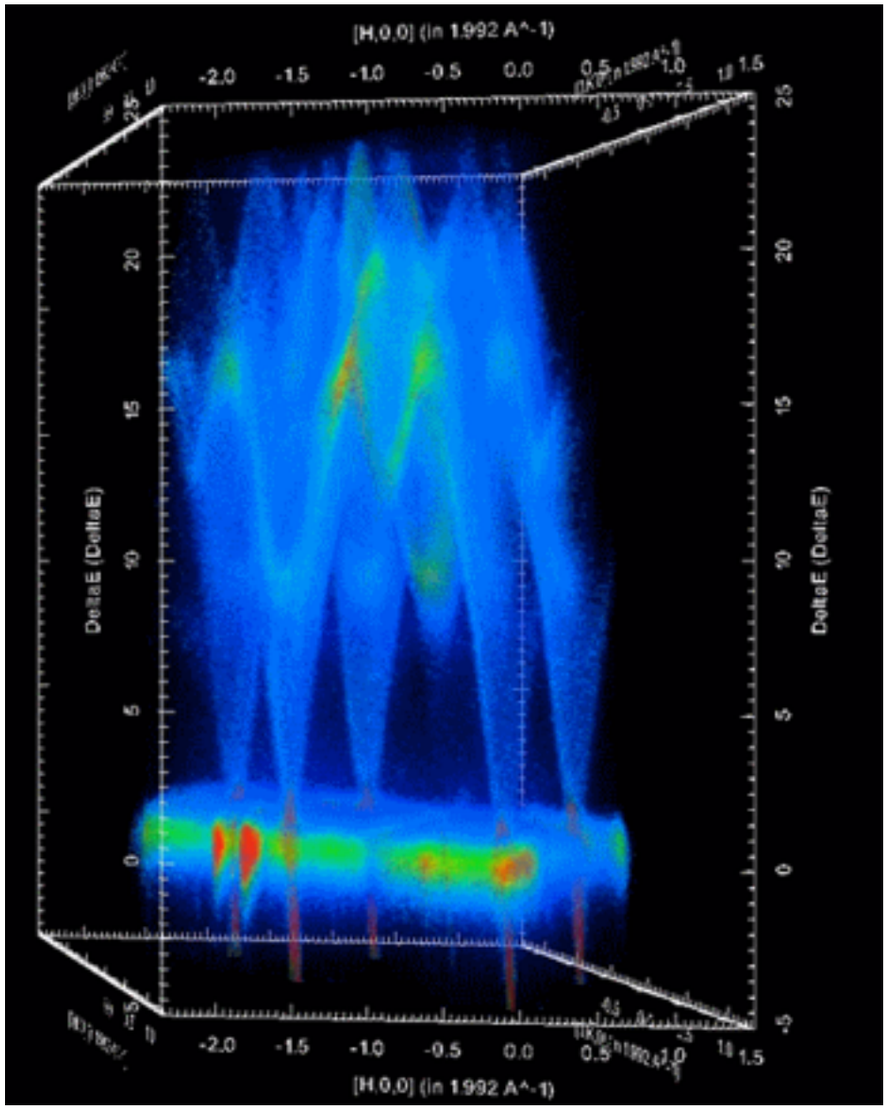
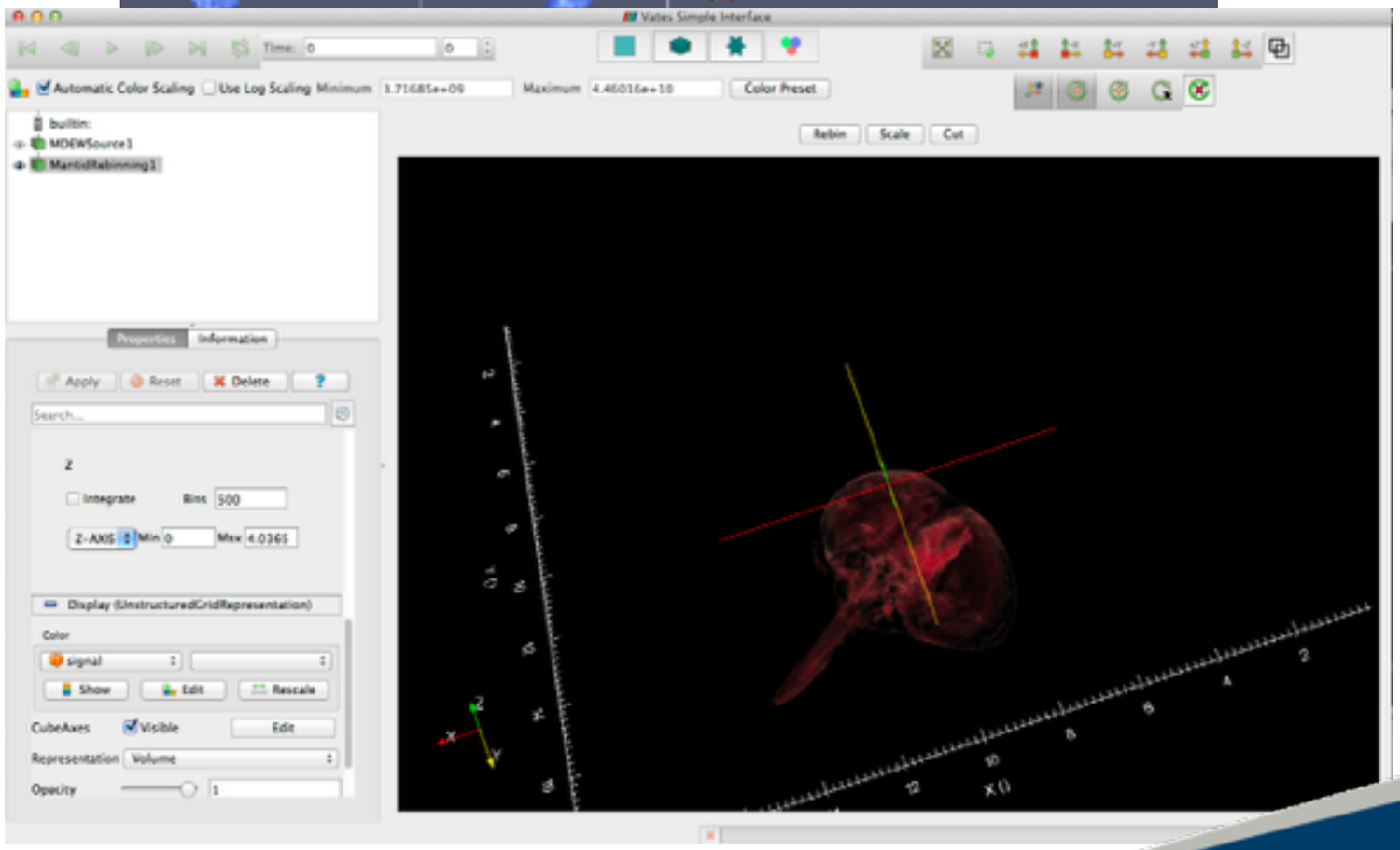
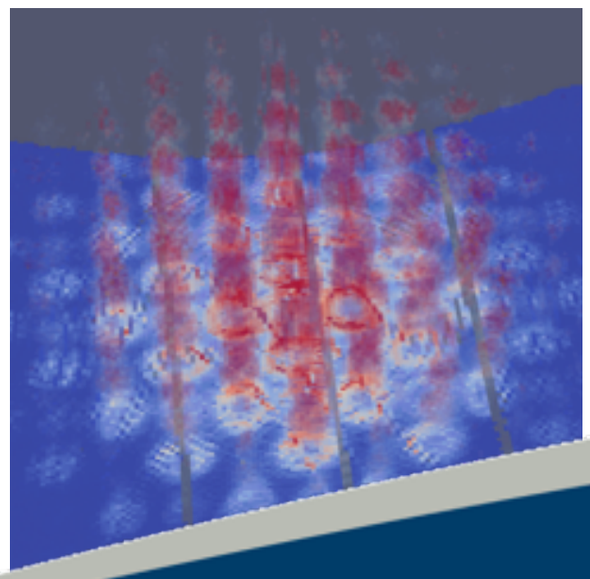
Flexible data structure









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Data analysis: scientific computing

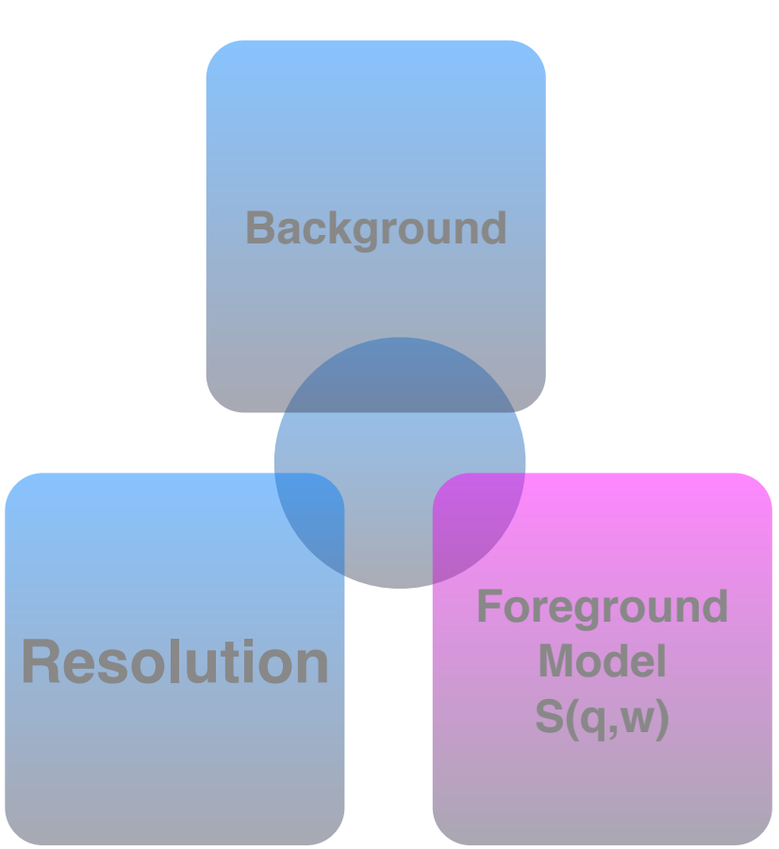
Generate a physical model

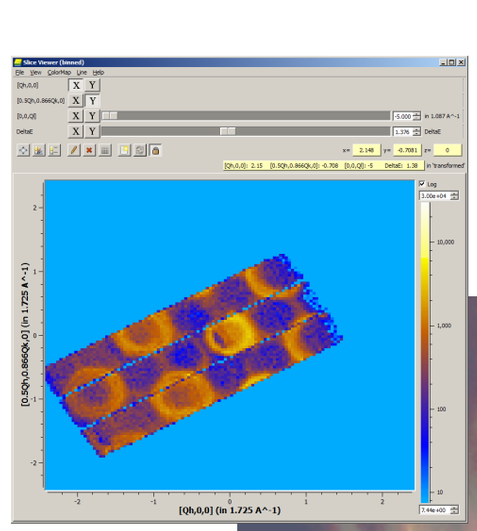
Simulate or calculate the ground state properties or dynamics

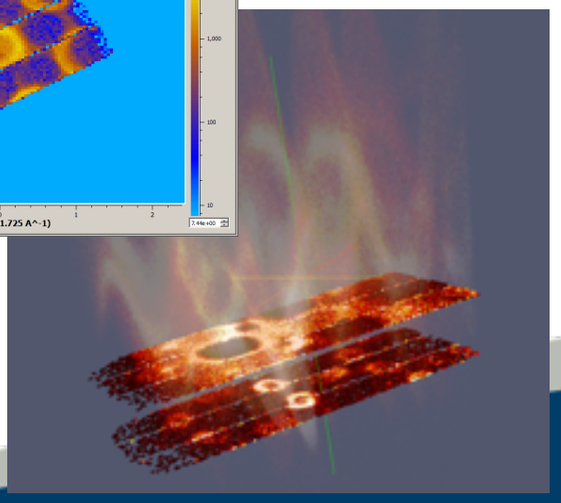
Calculate S(q,w) accounting for neutron cross-sections

Fold in instrument resolution

Iterate a fit on a parametrised model







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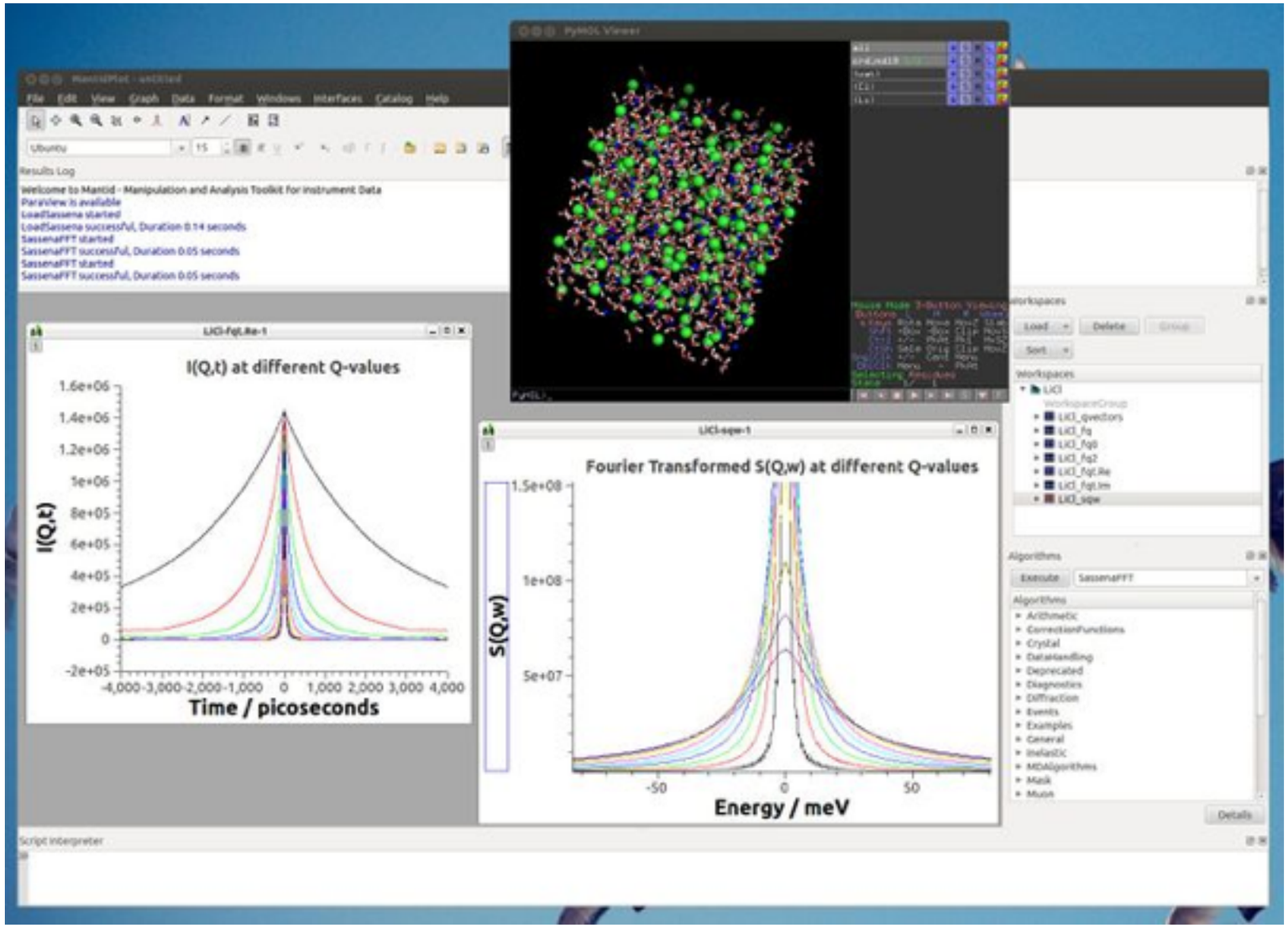
Visualising simulation data



Sassena & NMoldyn

McVine & VNF

McStas

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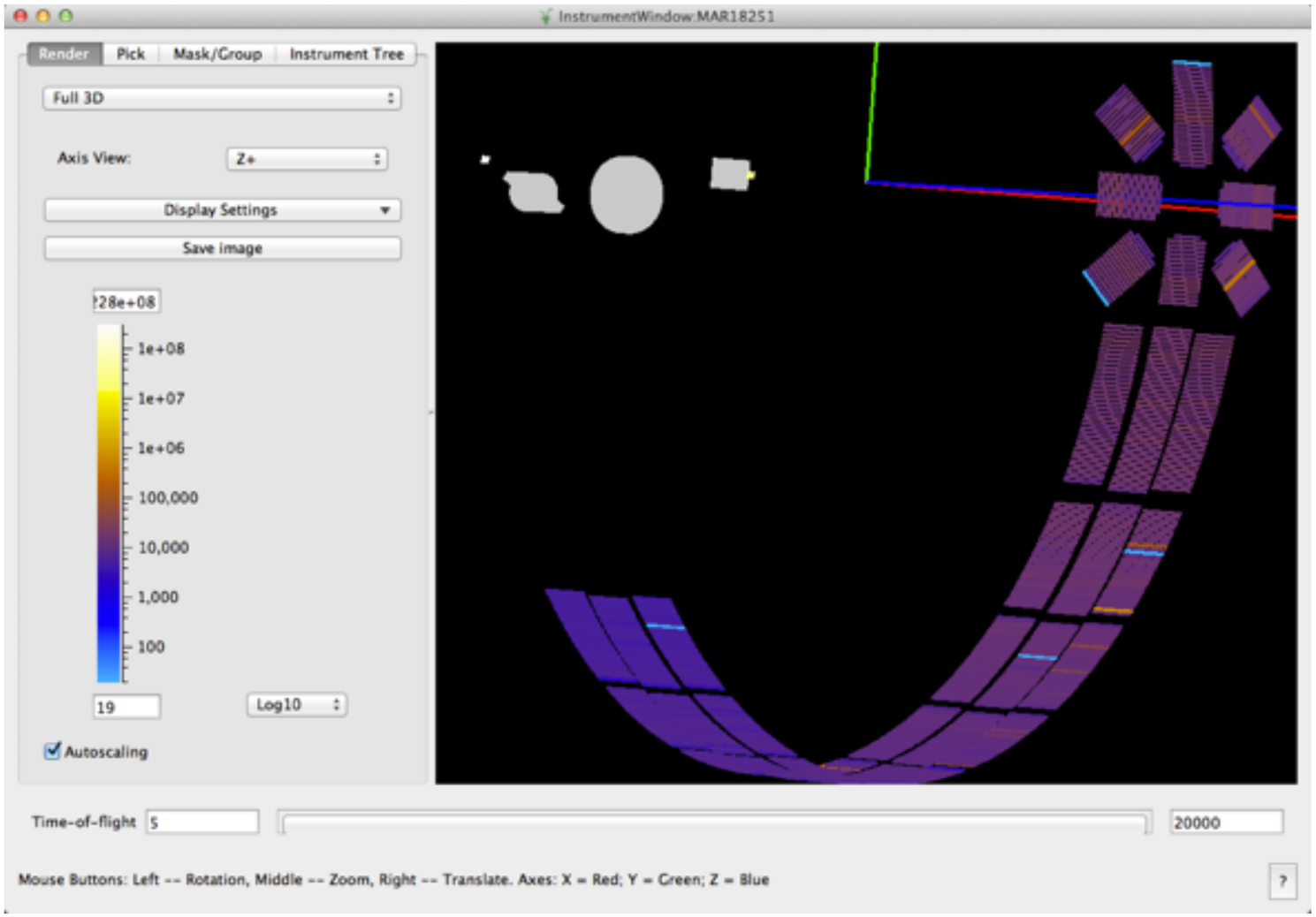
MANTID + McStas



Calculation of:

Flux
Resolution
Multiple scattering

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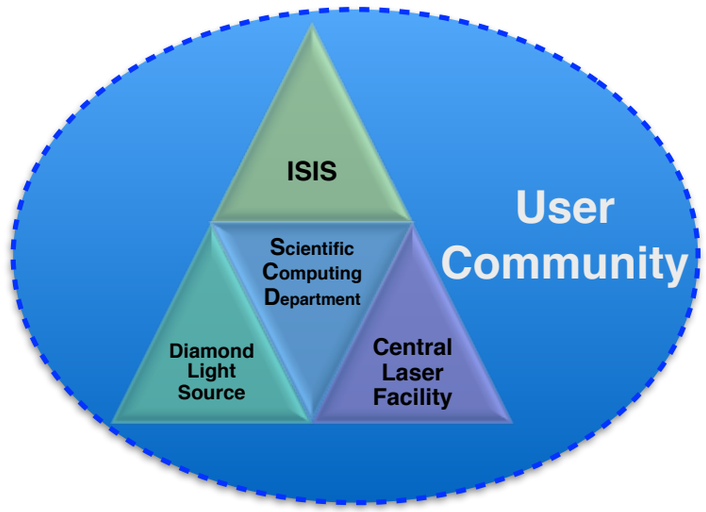
Scientific computing @ Harwell Oxford



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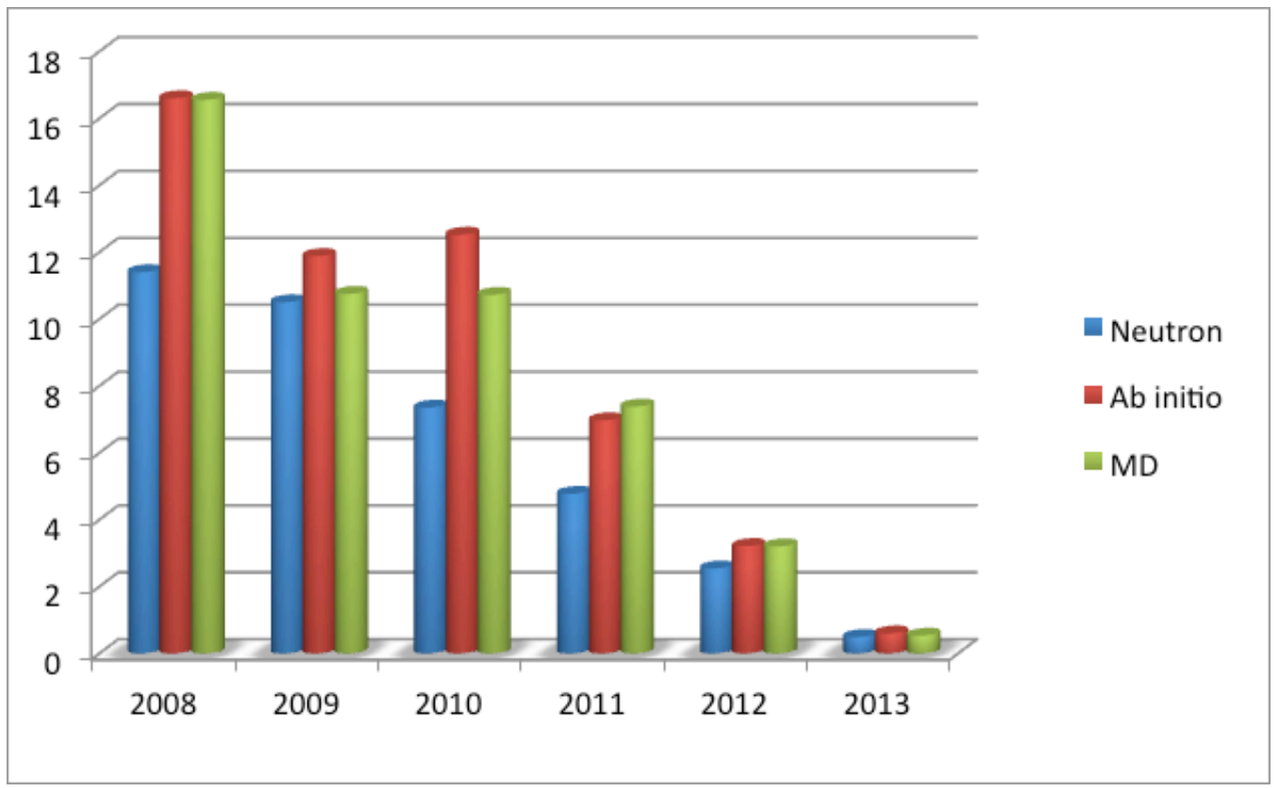
"What scientific impact does scientific computing add to data from experiments conducted at ISIS"

	Total sample	Significant use of Scientific computing
Number of records	57	15 (26%)
Ave. Citation per year	37	16
Ave. Citation per item	4	5.3
H index for sample	8	6

	Total sample	Significant use of Scientific computing	No significant use of scientific computing
Number of records	40	22 (55%)	18
Ave. Citation per year	62.2	48.7	15.8
Ave. Citation per item	10.9	15.50	5.3
H index for sample	12	11	5



The headline for this analysis is that SC generates a factor 3 in citations which correlates to a factor 2 increase in H

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Scientific Computing Project.

Infrastructure

Storage

Compute

Software development

“Modelling toolkit”

Common Framework /API Mantid

Programme delivery staff.

Computational scientists

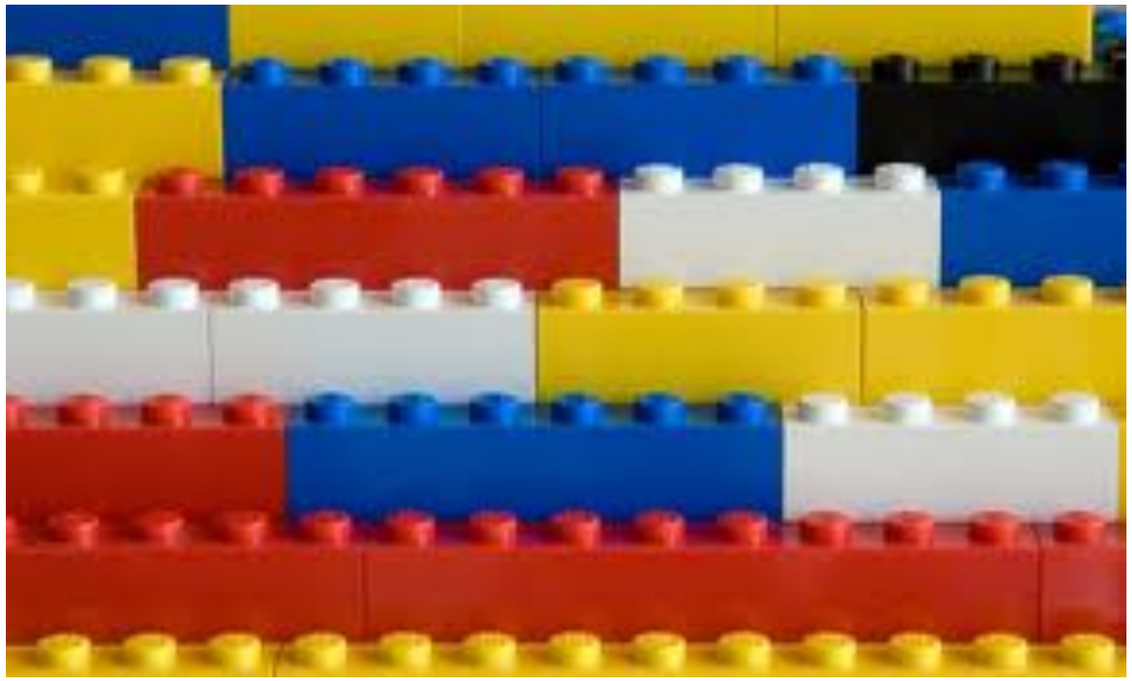
Programme managers

Science areas:

Functional materials programme
Life science programme

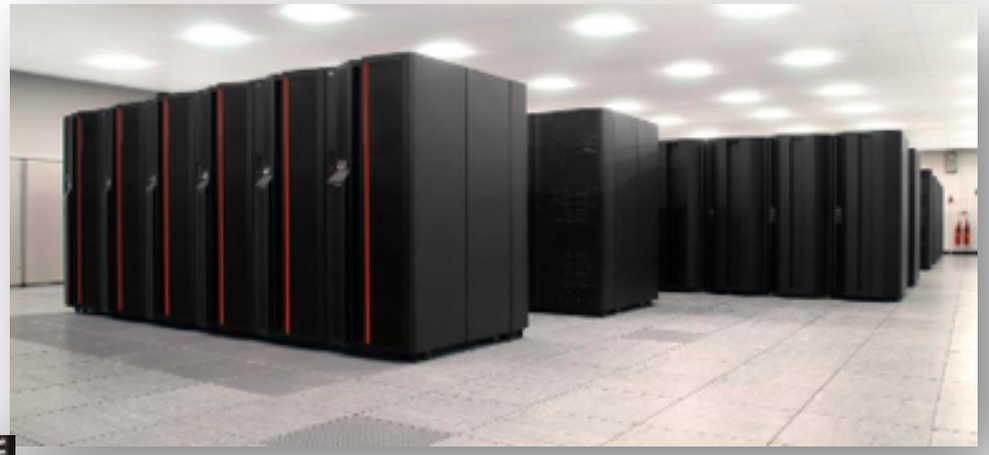
Tools in the toolkit

Package	Description
CASTEP	DFT
DL_POLY & DL_MESO	Molecular dynamics
GULP	Lattice dynamics
Aclimax	generates S(q,w) from DFT simulation output, generating overtones and multiple scattering effects
NMoldyn	converts MD trajectories to S(q,w)
TobyFit	Convolution with the correct resolution function is often ignored, there is one well know package TobyFit that convolutes model scattering functions with the correct direct geometry model for resolution.
McStas corrections	The data must be "correct". We must be certain that the experimental data used in comparison and validation of simulated models is correct. This requires corrections for absorption and multiple scattering to be common place.
Data analysis & mining tools	Tools to generate and extract meaningful information from simulation output. For example molecule flexion or bond angle correlation from MD trajectories.



pandata++

High availability Infrastructure



Complexity metric

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In order to grow our user community we must be able to provide a service to users who have no prior experience of either the source or the technique

or previous knowledge of analysis, simulation and modelling data.

Proposal to publication support for scientific computing will maximise the impact of the facility science programme

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