Software

Andrew Jackson
European Spallation Source

XIV School of Neutron Scattering “Francesco Paolo Ricci” (SoNS)
2nd Course of the Erice School “Neutron Science And Instrumentation”
“Designing And Building A Neutron Instrument**”**

Erice 1st – 9th April 2016

with thanks to Jon Taylor and all at ESS DMSC

I want to build a cool instrument … why do I need to worry about this software business?

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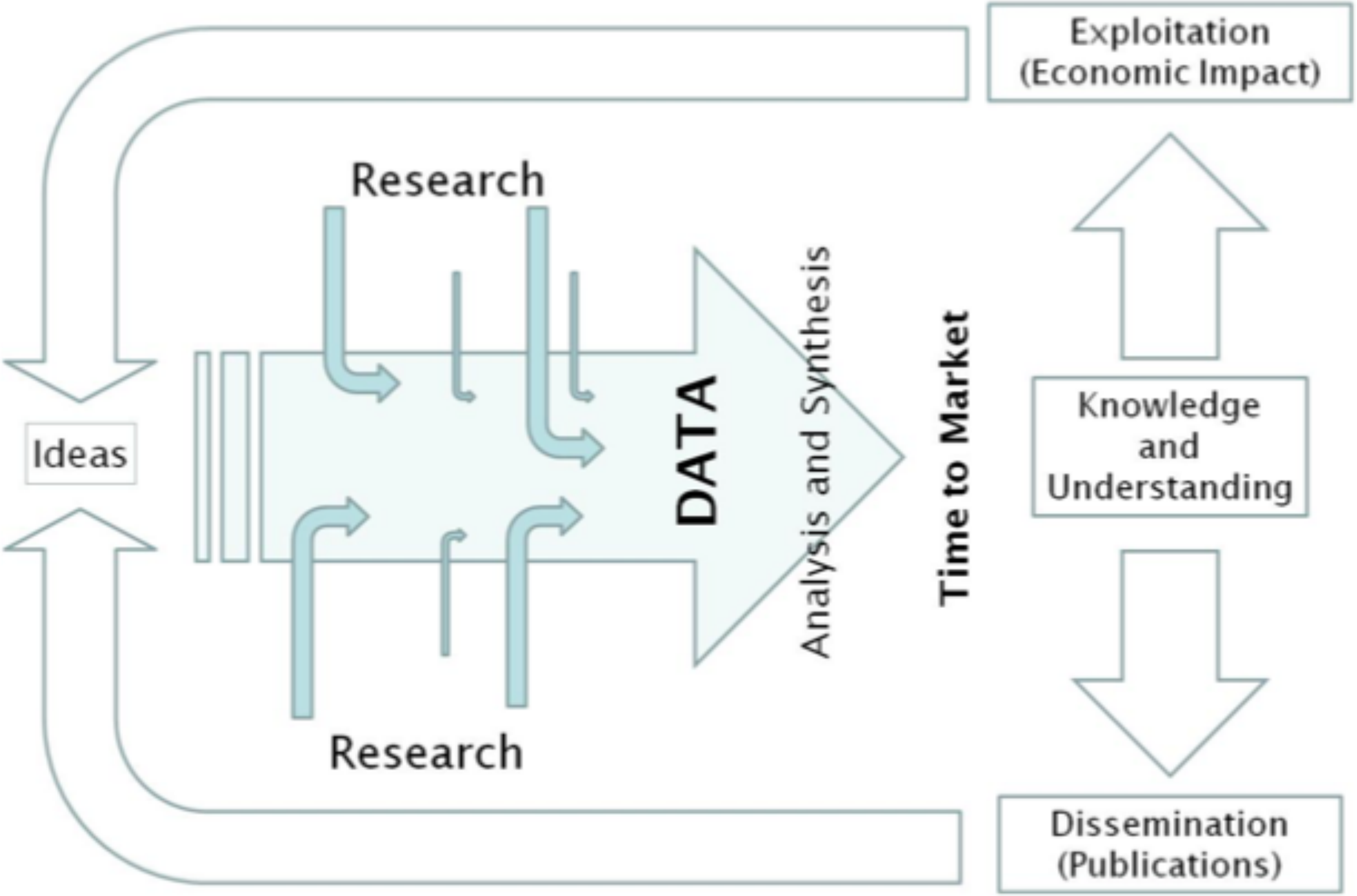
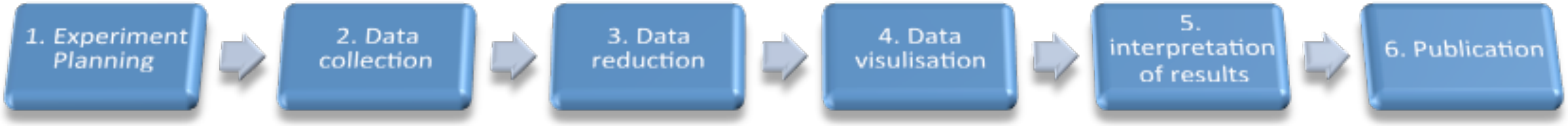
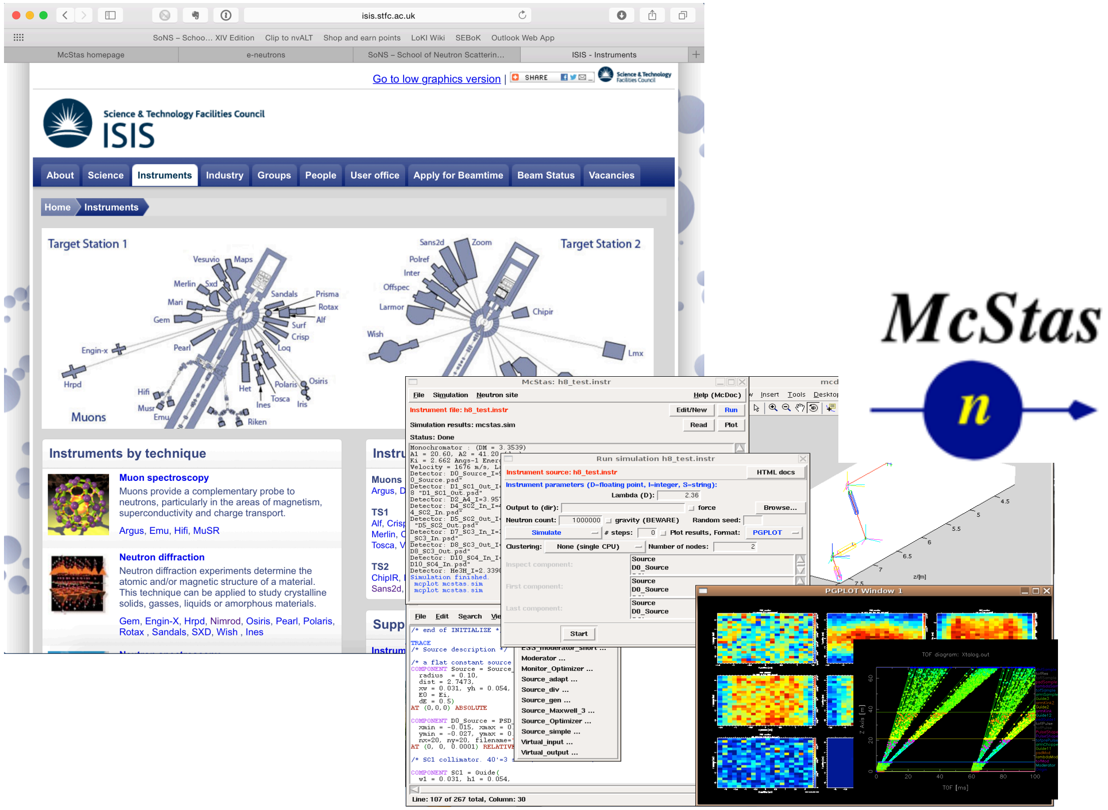
Research Information Flow



Neutron Experiment Information Flow



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



isis.stfc.ac.uk

Instruments by technique

Muon spectroscopy

Muons provide a complementary probe to neutrons, particularly in the areas of magnetism, superconductivity and charge transport.

Argus, Emu, Hifi, MuSR

Neutron diffraction

Neutron diffraction experiments determine the atomic and/or magnetic structure of a material. This technique can be applied to study crystalline solids, gasses, liquids or amorphous materials.

Gem, Engin-X, Hrpd, Nimrod, Osiris, Pearl, Polaris, Rotax , Sandals, SXD, Wish , Ines

Instru

Muons
Argus, D

TS1
Alf, Crisp
Merlin, C
Tosca, V

TS2
ChipIR,
Sans2d,

Supp

Instrum

McStas: h8_test.instr

Instrument file: h8_test.instr

Simulation results: mcstas.sim

Status: Done

```
Monochromator : (DM = 3.3539)
A1 = 20.60, A2 = 41.20
Ki = 2.662 Angs-1 Ener
Velocity = 1676 m/s, La
Detector: D0_Source_I=
0_Source.psd"
Detector: D1_SC1_Out_I=
8 "D1_SC1_Out.psd"
Detector: D2_A4_I=3.957
Detector: D4_SC2_In_I=
4_SC2_In.psd"
Detector: D5_SC2_Out_I=
 "D5_SC2_Out.psd"
Detector: D7_SC3_In_I=
_SC3_In.psd"
Detector: D8_SC3_Out_I=
D8_SC3_Out.psd"
Detector: D10_SC4_In_I=
D10_SC4_In.psd"
Detector: He3H_I=2.3390
Simulation finished.
 mcplot mcstas.sim
 mcplot mcstas.sim
```

Run simulation h8_test.instr

Instrument source: h8_test.instr

Instrument parameters (D=floating point, I=integer, S=string):

Lambda (D): 2.36

Output to (dir): ☐ force

Neutron count: 1000000 ☐ gravity (BEWARE) Random seed:

Simulate # steps: 0 ☐ Plot results, Format: PGPLOT

Clustering: None (single CPU) Number of nodes: 2

Inspect component: Source D0_Source

First component: Source D0_Source

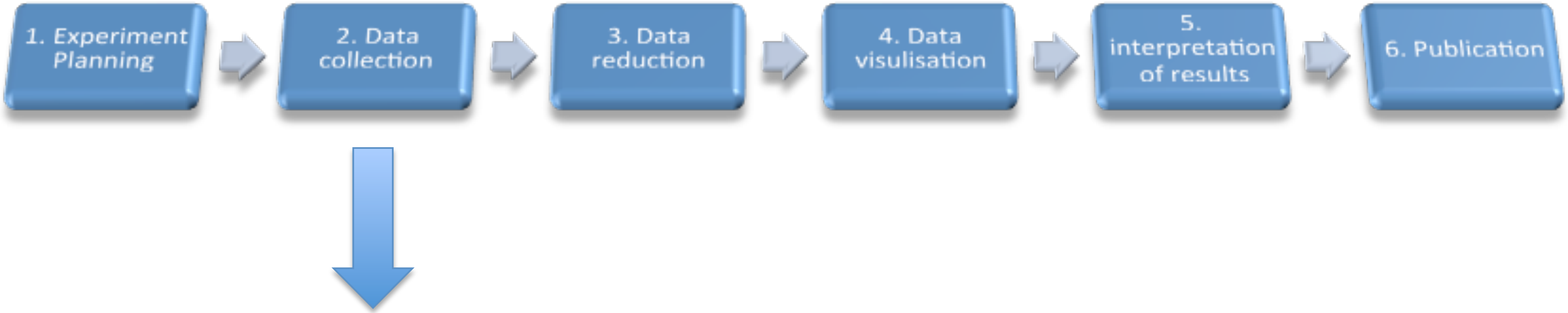
Last component: Source D0_Source

```
/* end of INITIALIZE */

TRACE
/* Source description */

/* a flat constant source
COMPONENT Source = Source_
  radius  = 0.10,
  dist = 2.7473,
  xw = 0.031, yh = 0.054,
  E0 = Ei,
  dE = 0.5)
AT (0,0,0) ABSOLUTE

COMPONENT D0_Source = PSD_
  xmin = -0.015, xmax = 0.
  ymin = -0.027, ymax = 0.
  nx=20, ny=20, filename=
AT (0, 0, 0.0001) RELATIVE

/* SC1 collimator. 40'=3

COMPONENT SC1 = Guide(
  w1 = 0.031, h1 = 0.054,
```

ESS_moderator_short ...
Moderator ...
Monitor_Optimizer ...
Source_adapt ...
Source_div ...
Source_gen ...
Source_Maxwell_3 ...
Source_Optimizer ...
Source_simple ...
Virtual_input ...
Virtual_output ...

Line: 107 of 267 total, Column: 30

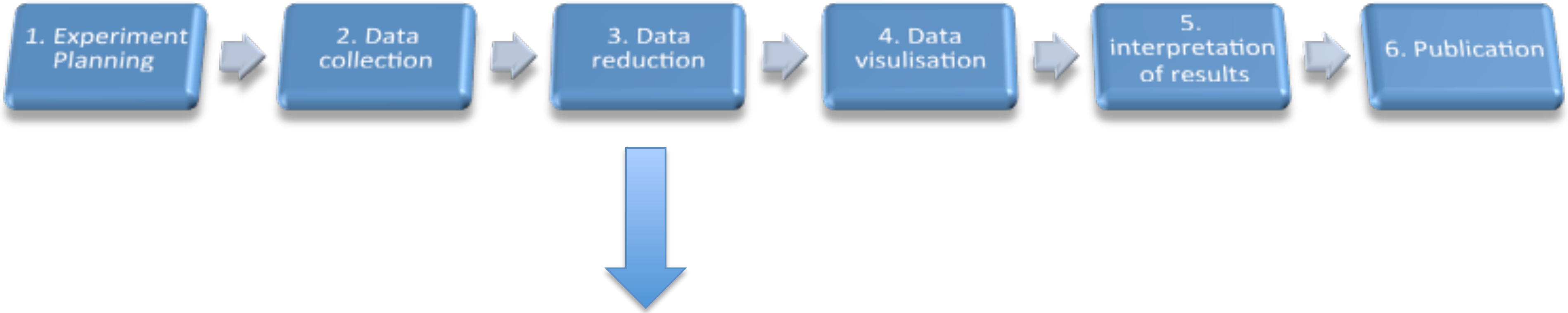
Neutron Experiment Information Flow



Do the experiment!

- Configure the instrument
- Set up sample environment
- Count neutrons on a detector
- Record data and metadata to disk
    - Keep an archive
    - Have a catalogue

Neutron Experiment Information Flow



1. Experiment Planning

2. Data collection

3. Data reduction

4. Data visulisation

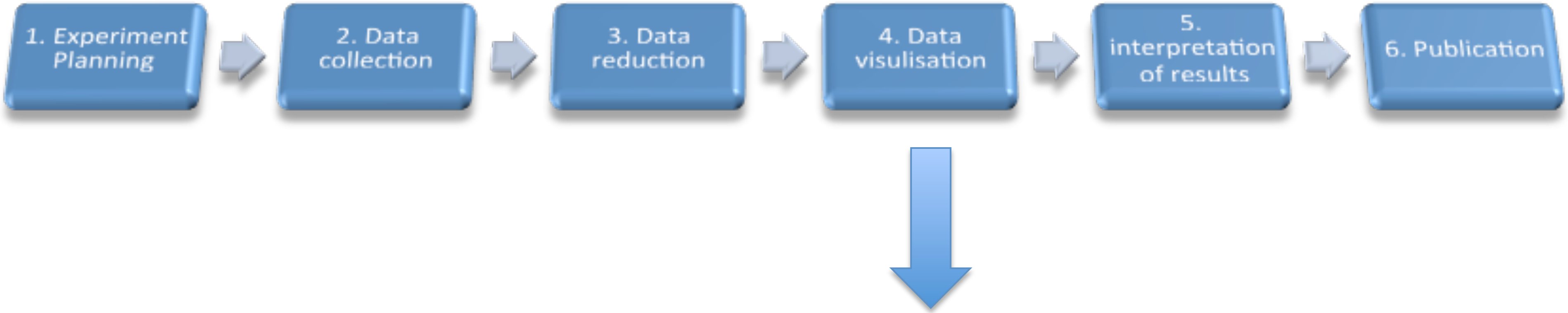
5. interpretation of results

6. Publication

Process the Data

- Convert detector data to useful space (Q, E, d, z …)
- Record processed data to disk
- Match up with sample environment data

Neutron Experiment Information Flow



1. Experiment Planning

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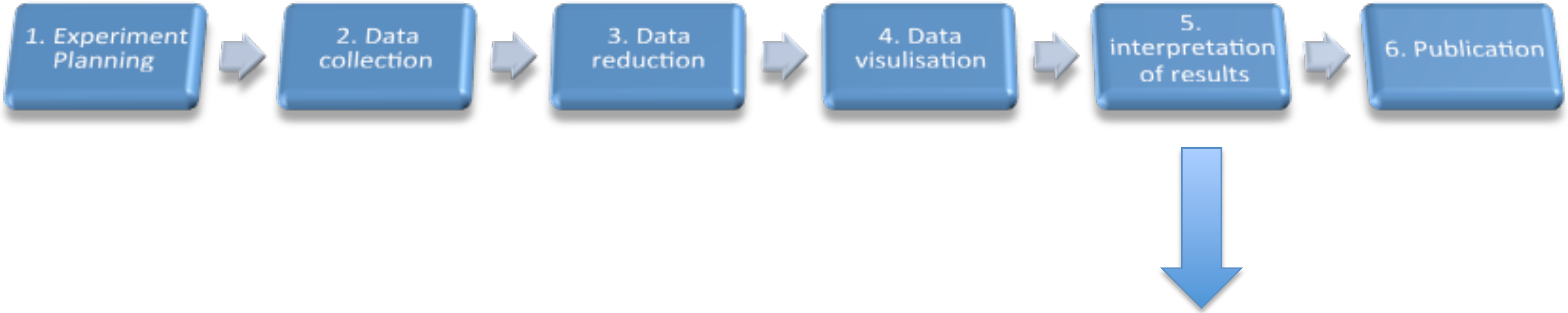
Look at the data

- Visualize data in appropriate way
- Explore data

Neutron Experiment Information Flow



1. Experiment Planning

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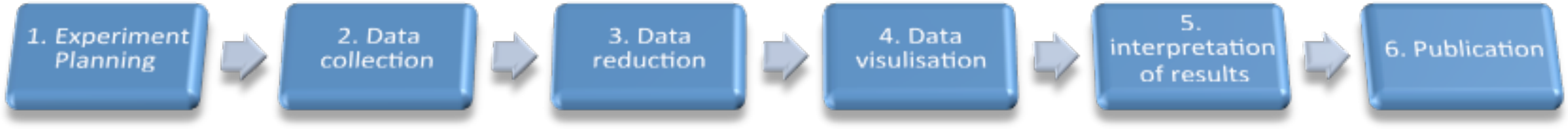
Analyze the data

- Extract scientific/physical information from neutron data
- Model fitting
- Peak finding
- Comparison with simulation results
- … ?? ??

Neutron Experiment Information Flow



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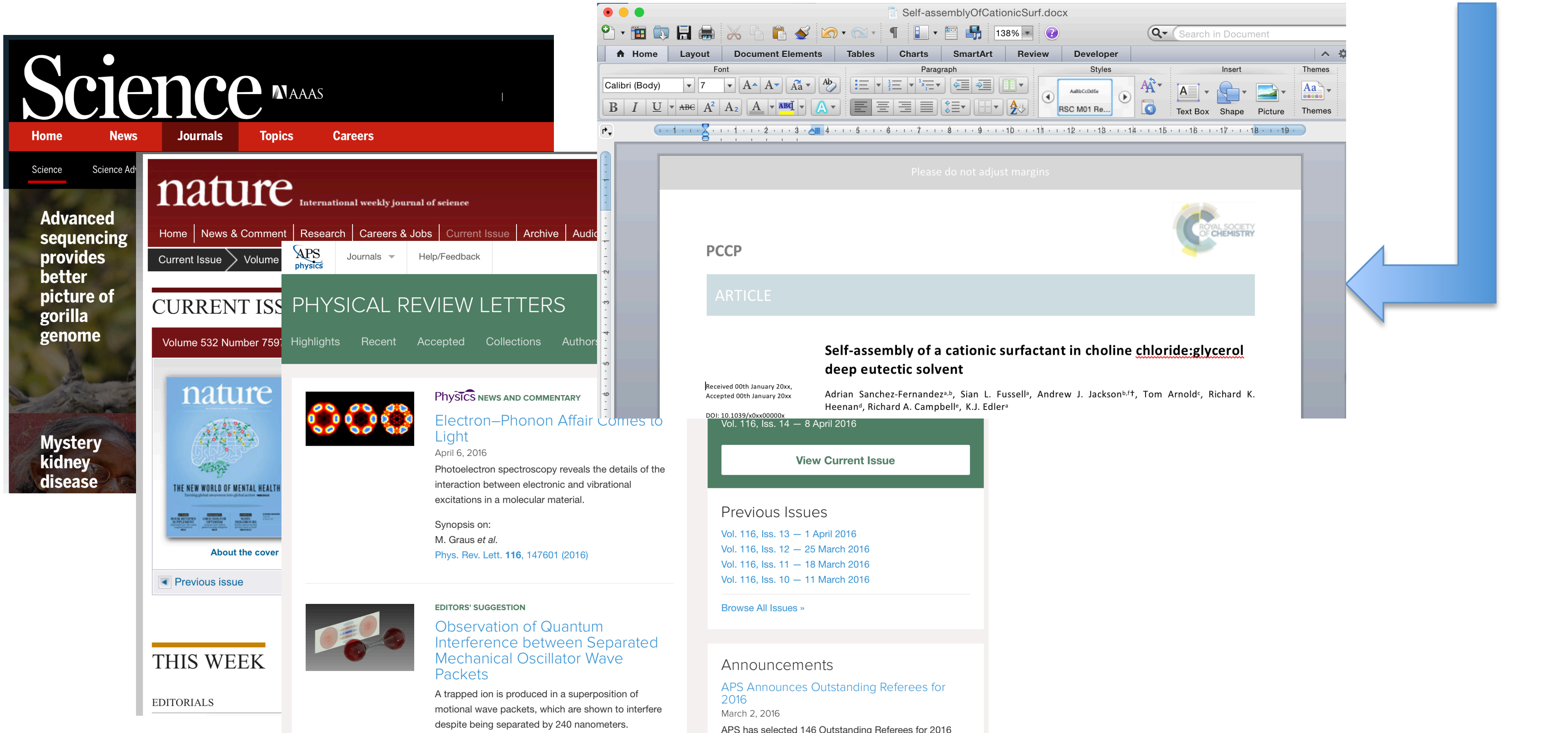

Advanced sequencing provides better picture of gorilla genome

Mystery kidney disease

CURRENT ISS

Volume 532 Number 759

nature

THE NEW WORLD OF MENTAL HEALTH

THIS WEEK

EDITORIALS

Physics NEWS AND COMMENTARY

Electron–Phonon Affair Comes to Light

April 6, 2016

Photoelectron spectroscopy reveals the details of the interaction between electronic and vibrational excitations in a molecular material.

Synopsis on:
M. Graus *et al.*
Phys. Rev. Lett. **116**, 147601 (2016)

EDITORS' SUGGESTION

Observation of Quantum Interference between Separated Mechanical Oscillator Wave Packets

A trapped ion is produced in a superposition of motional wave packets, which are shown to interfere despite being separated by 240 nanometers.

Please do not adjust margins

PCCP

ARTICLE

Self-assembly of a cationic surfactant in choline chloride:glycerol deep eutectic solvent

Received 00th January 20xx,
Accepted 00th January 20xx

DOI: 10.1039/x0xx00000x

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Vol. 116, Iss. 14 — 8 April 2016

Previous Issues

Vol. 116, Iss. 13 — 1 April 2016
Vol. 116, Iss. 12 — 25 March 2016
Vol. 116, Iss. 11 — 18 March 2016
Vol. 116, Iss. 10 — 11 March 2016

Announcements

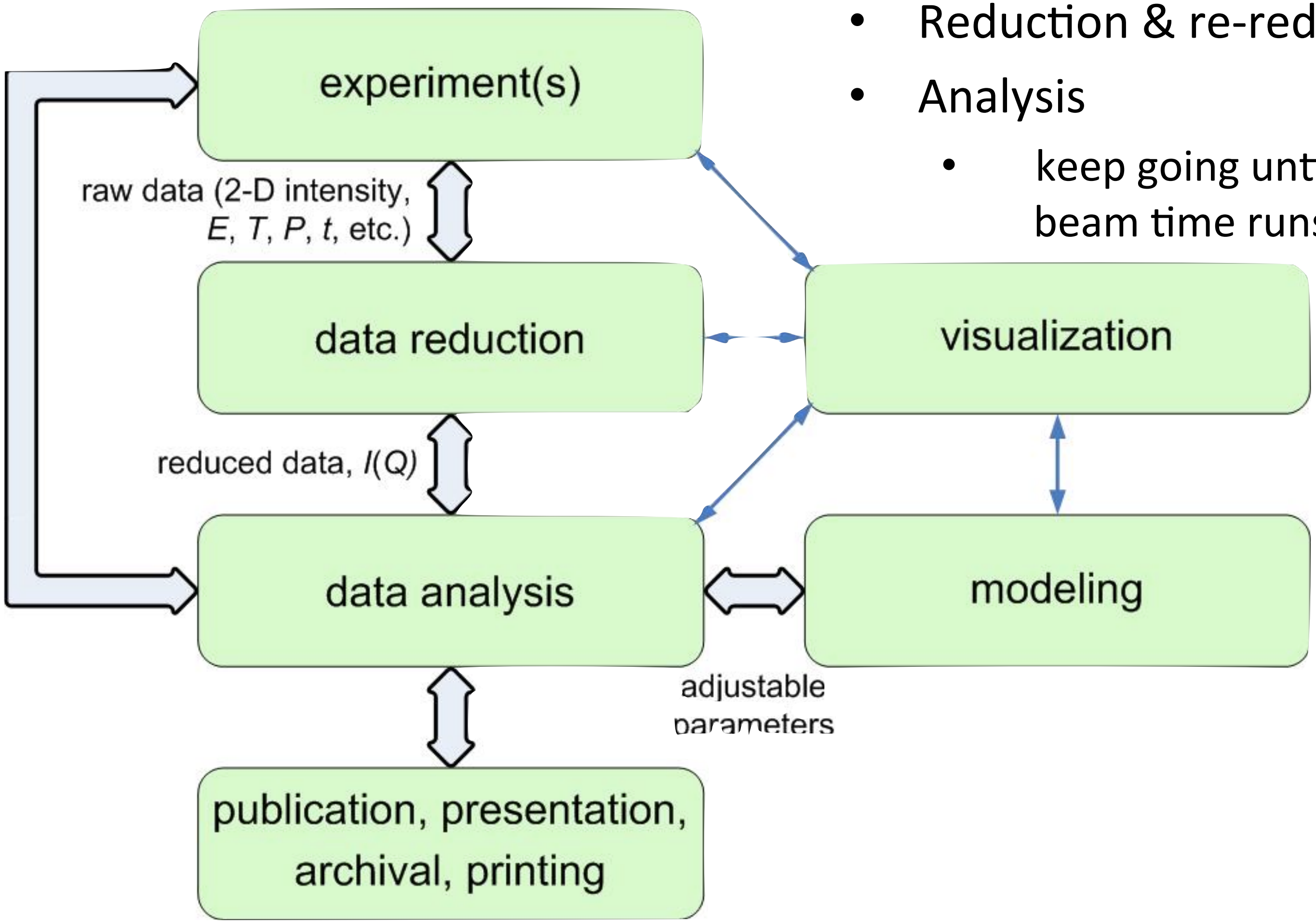
APS Announces Outstanding Referees for 2016

March 2, 2016

APS has selected 146 Outstanding Referees for 2016

What is an experiment in reality?

- Planning
- Setup
- Acquisition
- Reduction & re-reduction
- Analysis
  - keep going until either the coffee or beam time runs out



Instrument Control Architectures

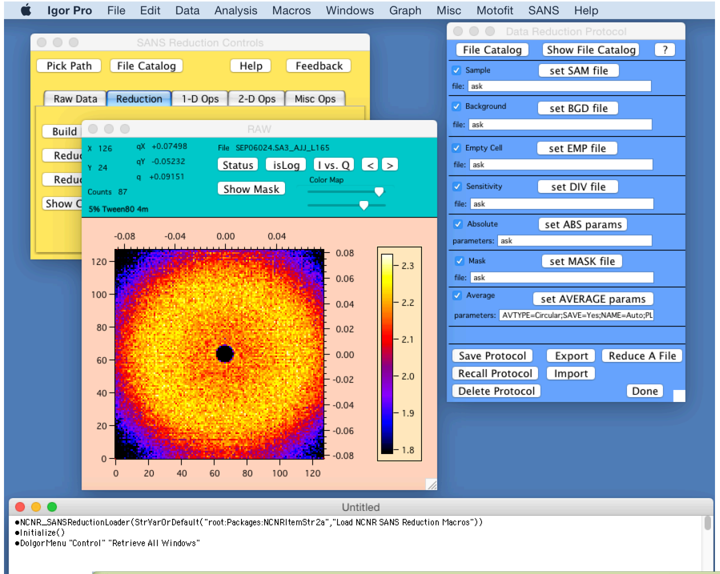
- Some existing frameworks:

  - Sardana (Photon Python/QT Tango FW)
  - NoMad (C++ VME framework)
  - GDA (Photon Java Eclipse RCP python EPICS FW)
  - SNS development (C++ epics CSS development)
  - ISIS IC development (C++ CSS BOY EPICS development)
  - GumTree (Java, EPICS, C/ObjC, Python)

Data Reduction and Visualization

- Aim to remove instrument geometry and engineering details from data
- Thus can be very instrument specific
- Often needs to be written by instrument scientist

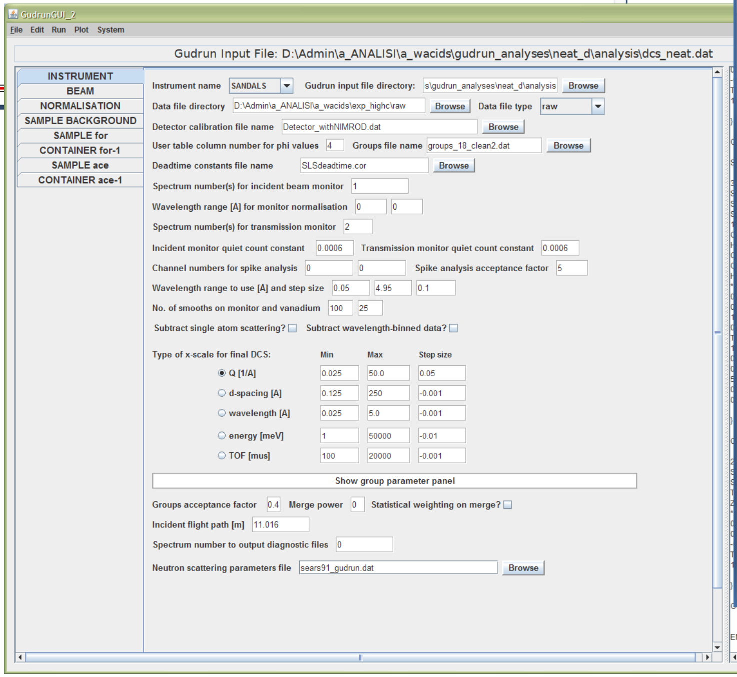
MANTID



X 126 qX +0.07498 File SEP06024.SA3_AJJ_L165
Y 24 qY -0.05232
q +0.09151
Counts 87
5% Tween80 4m

☑ Sample
file: ask
☑ Background
file: ask
☑ Empty Cell
file: ask
☑ Sensitivity
file: ask
☑ Absolute
parameters: ask
☑ Mask
file: ask
☑ Average
parameters: AVTYPE=Circular;SAVE=Yes;NAME=Auto;PL

```
•NCNR_SANSReductionLoader(StrVarOrDefault("root:Packages:NCNRItemStr2a","Load NCNR SANS Reduction Macros"))
•Initialize()
•DolgorMenu "Control" "Retrieve All Windows"
```



Gudrun Input File: D:\Admin\a_ANALISI\a_wacids\gudrun_analyses\neat_d\analysis\dcs_neat.dat

Instrument name SANDALS Gudrun input file directory: s\gudrun_analyses\neat_d\analysis

Data file directory D:\Admin\a_ANALISI\a_wacids\exp_highc\raw Data file type raw

Detector calibration file name Detector_withNIMROD.dat

User table column number for phi values 4 Groups file name groups_18_clean2.dat

Deadtime constants file name SLSdeadtime.cor

Spectrum number(s) for incident beam monitor 1

Wavelength range [A] for monitor normalisation 0 0

Spectrum number(s) for transmission monitor 2

Incident monitor quiet count constant 0.0006 Transmission monitor quiet count constant 0.0006

Channel numbers for spike analysis 0 0 Spike analysis acceptance factor 5

Wavelength range to use [Å] and step size 0.05 4.95 0.1

No. of smooths on monitor and vanadium 100 25

Subtract single atom scattering? □ Subtract wavelength-binned data? □

Type of x-scale for final DCS:	Min	Max	Step size
● Q [1/A]	0.025	50.0	0.05
○ d-spacing [A]	0.125	250	-0.001
○ wavelength [A]	0.025	5.0	-0.001
○ energy [meV]	1	50000	-0.01
○ TOF [mus]	100	20000	-0.001

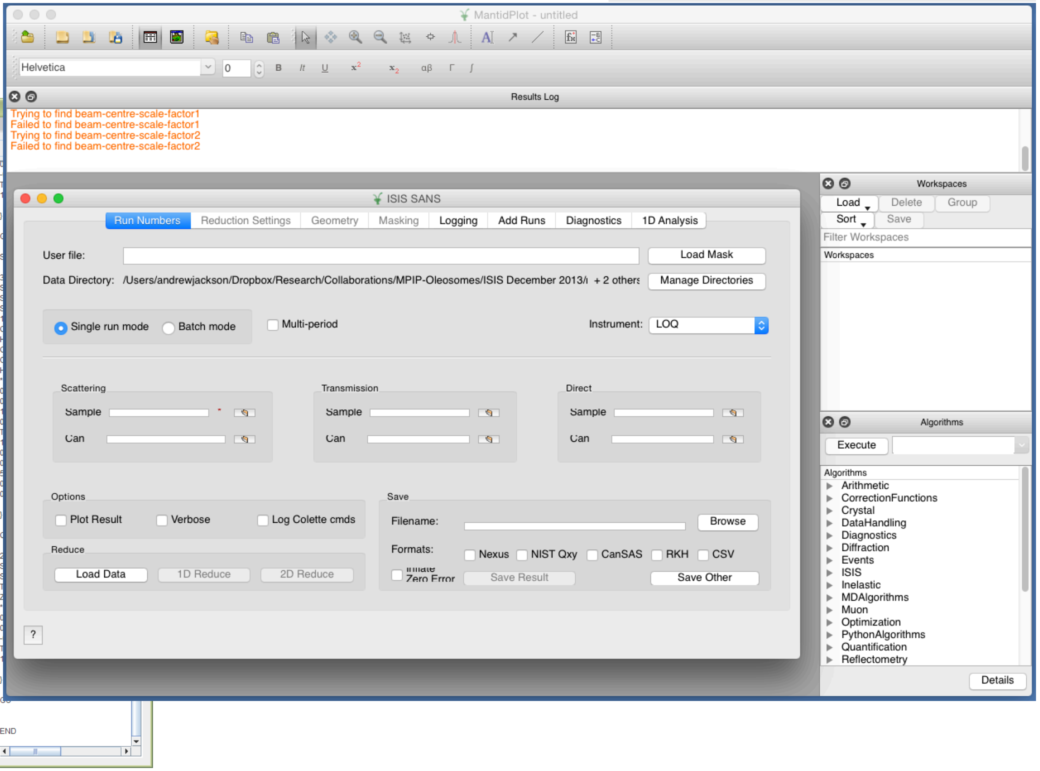
Groups acceptance factor 0.4 Merge power 0 Statistical weighting on merge? □

Incident flight path [m] 11.016

Spectrum number to output diagnostic files 0

Neutron scattering parameters file sears91_gudrun.dat

END



```
Trying to find beam-centre-scale-factor1
Failed to find beam-centre-scale-factor1
Trying to find beam-centre-scale-factor2
Failed to find beam-centre-scale-factor2
```

User file:

Data Directory: /Users/andrewjackson/Dropbox/Research/Collaborations/MPIP-Oleosomes/ISIS December 2013/ + 2 others

● Single run mode ○ Batch mode □ Multi-period Instrument: LOQ

□ Plot Result □ Verbose □ Log Colette cmds

Filename:

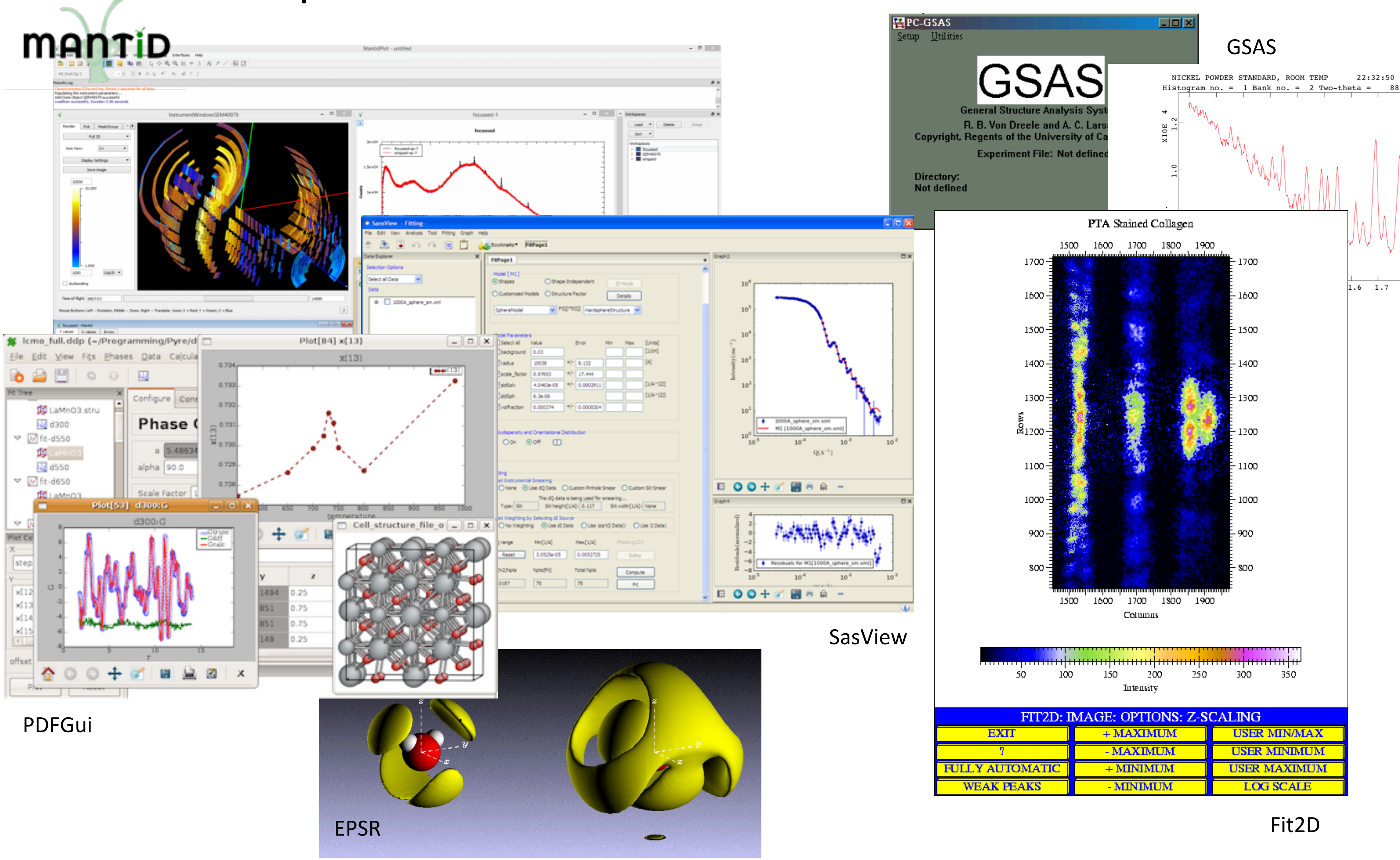
Formats: □ Nexus □ NIST Qxy □ CanSAS □ RKH □ CSV

□ Zero Error

Algorithms
- Arithmetic
- CorrectionFunctions
- Crystal
- DataHandling
- Diagnostics
- Diffraction
- Events
- ISIS
- Inelastic
- MDAlgorithms
- Muon
- Optimization
- PythonAlgorithms
- Quantification
- Reflectometry

Data Analysis

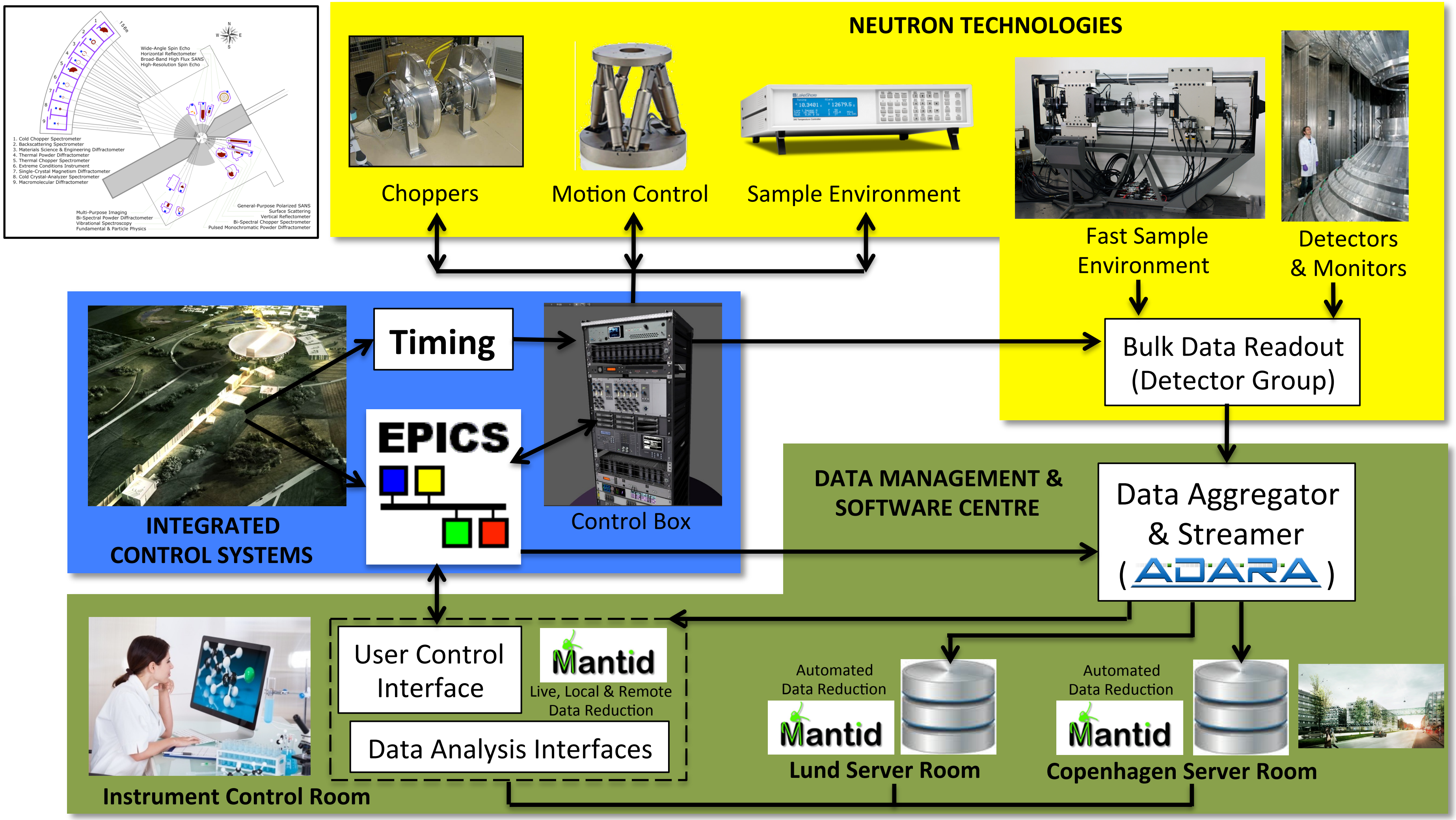
Domain Specific – users often have their own favourite tools



Data Archiving and Cataloguing

- Initial metadata (sample history, user, proposal)
- Inform automatic reduction and processing parameters (per sample, per exposure)
- Domain specific information
- Integrate external information (experimental log etc.)
- Keep a record of raw, reduced and processed data
- User interfaces required, on site and off

Instrument Control, Data Acquisition, Data Reduction and Data Storage



156m
N
W
E
S
Wide-Angle Spin Echo
Horizontal Reflectometer
Broad-Band High Flux SANS
High-Resolution Spin Echo
1. Cold Chopper Spectrometer
2. Backscattering Spectrometer
3. Materials Science & Engineering Diffractometer
4. Thermal Powder Diffractometer
5. Thermal Chopper Spectrometer
6. Extreme Conditions Instrument
7. Single-Crystal Magnetism Diffractometer
8. Cold Crystal-Analyzer Spectrometer
9. Macromolecular Diffractometer
Multi-Purpose Imaging
Bi-Spectral Powder Diffractometer
Vibrational Spectroscopy
Fundamental & Particle Physics
General-Purpose Polarized SANS
Surface Scattering
Vertical Reflectometer
Bi-Spectral Chopper Spectrometer
Pulsed Monochromatic Powder Diffractometer

NEUTRON TECHNOLOGIES

Choppers

Motion Control

Sample Environment

Fast Sample Environment

Detectors & Monitors

Bulk Data Readout (Detector Group)

Timing

EPICS

Control Box

INTEGRATED CONTROL SYSTEMS

DATA MANAGEMENT & SOFTWARE CENTRE

Data Aggregator & Streamer (ADARA)

User Control Interface

Mantid

Live, Local & Remote Data Reduction

Data Analysis Interfaces

Instrument Control Room

Automated Data Reduction

Mantid

Lund Server Room

Automated Data Reduction

Mantid

Copenhagen Server Room

Challenge : Data Rates

Data on disk is useless

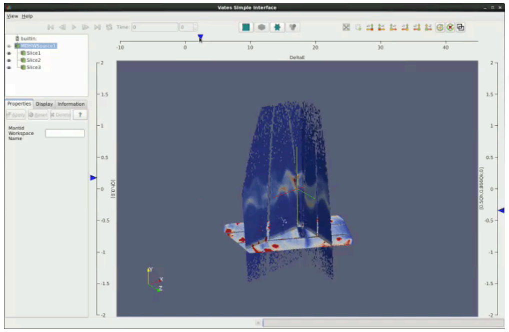
↓

Need to be able to process it to scientific results

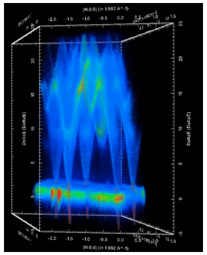
"Real Time" Processing and Visualisation

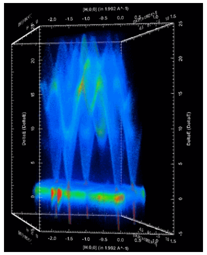
- NIST SANS VAX Data : 88 kb per detector image
- ISIS SANS Event Data File : 50 – 100 Mb
- ESS SANS Event Data Rate : 100s of Mb / s

4D Data Volumes in an RRM Spectrometer



Model fitting to sliced & diced volumes using Vates



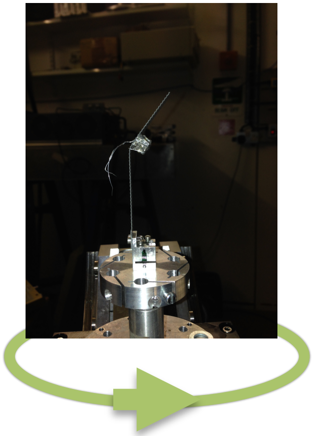


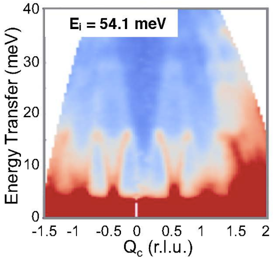
1x 200+ Gb file1x 200+ Gb file

MANTID

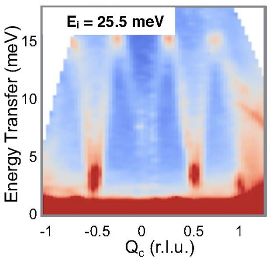
2+ hrs

Volume dataset creation





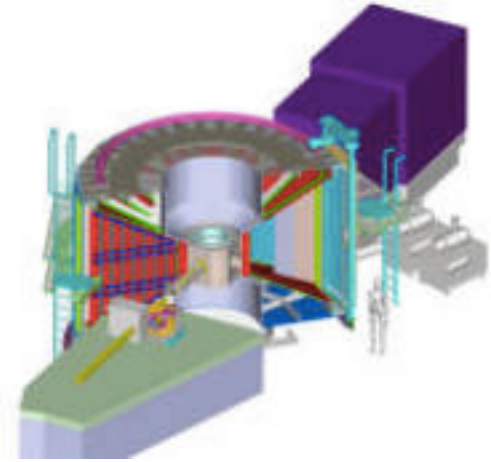
2-300 files per ei ~200mb each



2-300 files per ei ~200mb each

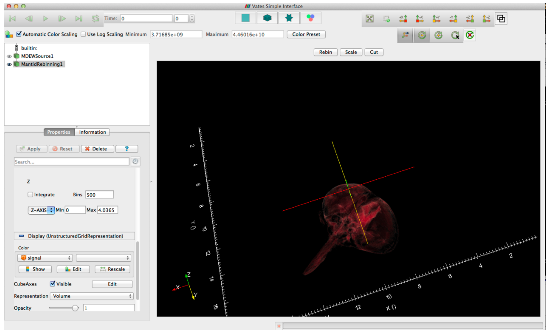
60s

Data reduction



Real Time Processing of Imaging Data

VG studio used for final render



MANTID

+ psi tools for image c

PSI / DLS and or octopus

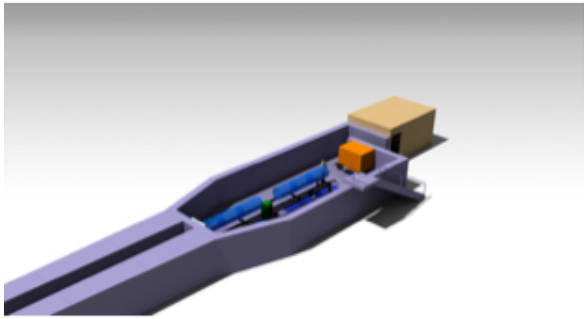
Reconstruction

Code

10+Gb/s

~14-100MB/s

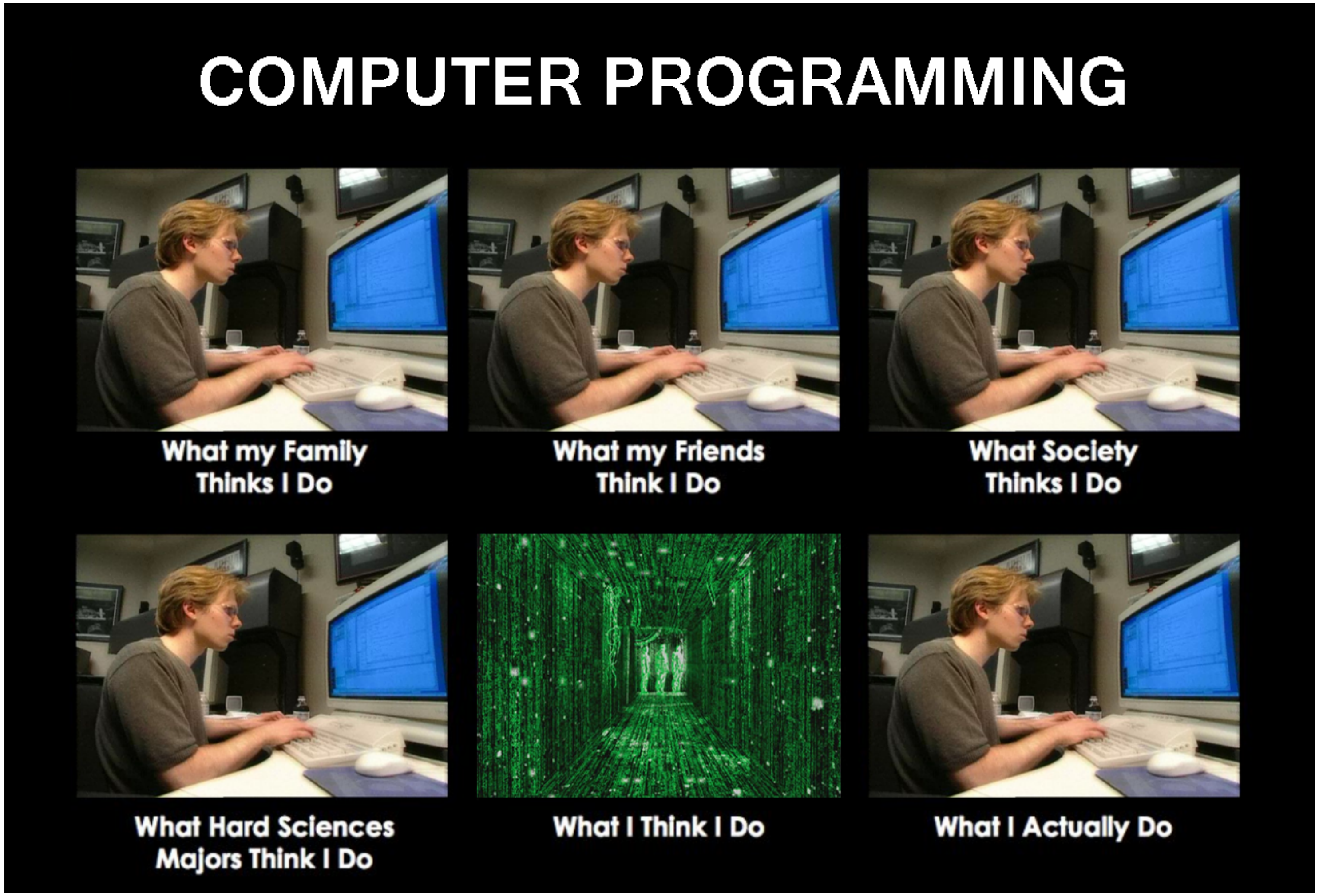
3500k images



How is our software written?

Software Wizards!

How is our software written?


COMPUTER PROGRAMMING
What my Family Thinks I Do
What my Friends Think I Do
What Society Thinks I Do
What Hard Sciences Majors Think I Do
What I Think I Do
What I Actually Do

How is our software written?

Instrument Teams must include software expertise

“Hero Developer” Model

- Domain expertise
- Direct translation of knowledge to code
- Low communication overhead

- “Hit by a bus” problem:
- Continuity
- Responsiveness

“Professional Development Team” Model

- Software engineering expertis
- Continuity
- Responsiveness

- Communication overhead
- Lack of domain expertise
- Translation required from science knowledge to code

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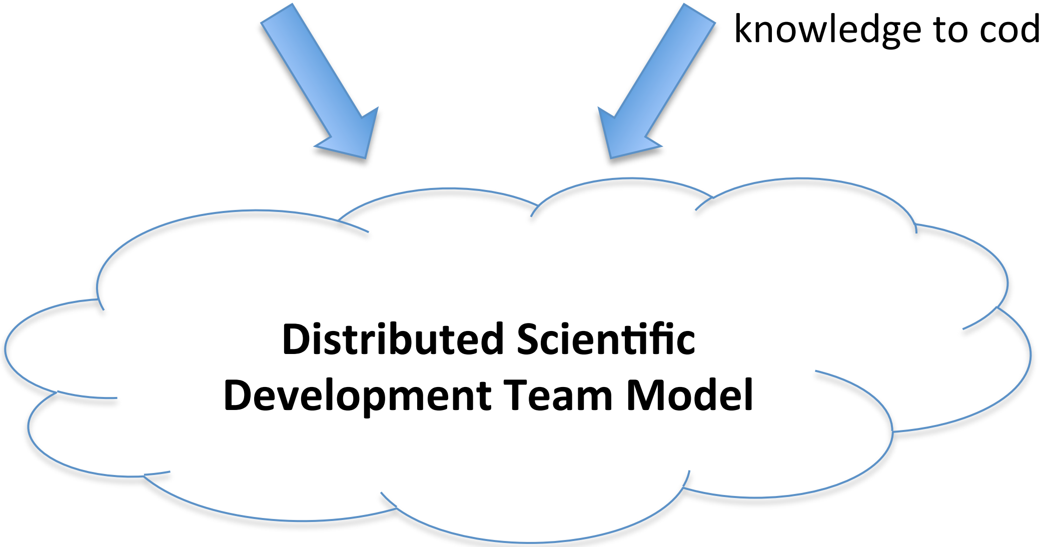

Distributed Scientific Development Team Model

Designing Software

"super users"

"most users"

"some users"

Working with software engineers …

… is the same as working with hardware engineers …

… except "everything is possible in software".

- Clear requirements in terms software engineers understand
- Iterative development model
- Understanding of manpower requirements

Summary

- Software is a vital and complex part of modern neutron scattering instruments and facilities

- Think about how **users** will interact with your instrument – what is good for the instrument scientist/engineer may not be good for the user

- Development model is moving from “hero coder” to “distributed teams” – scientists should be part of development teams

- Instrument teams must have software expertise and engage with the various software teams at facilities