

# Maximising the scientific impact of large-scale facilities using software development and scientific computing.

Jon Taylor



**Outline:**

**Scientific impact from Neutrons**

**Role of software & Development**

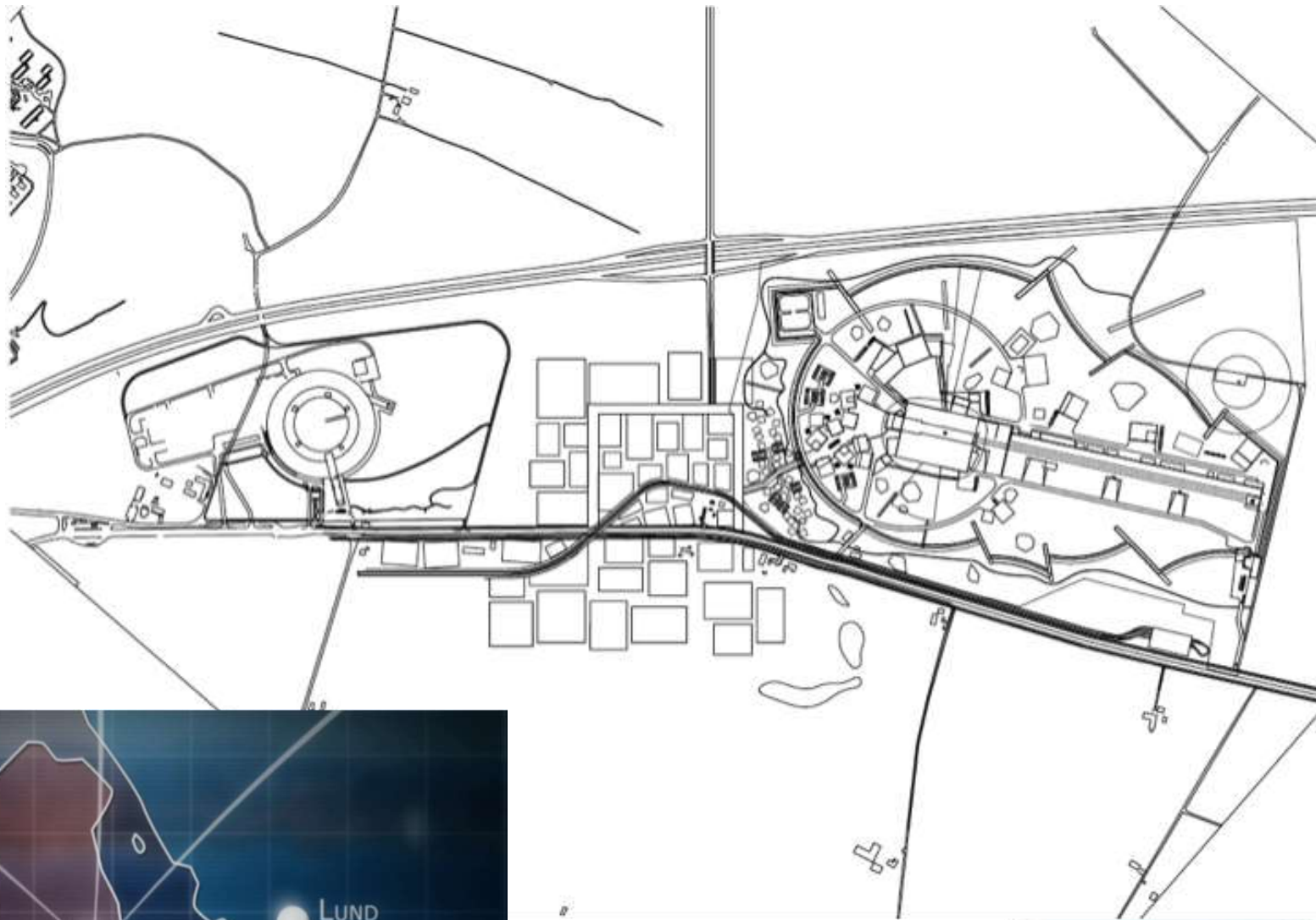
**Some key projects**

**Considerations @ day 1**



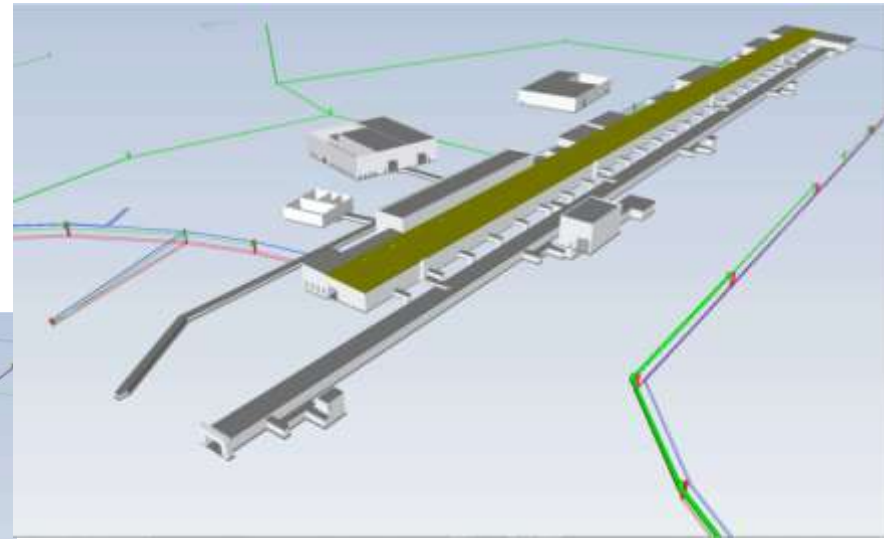
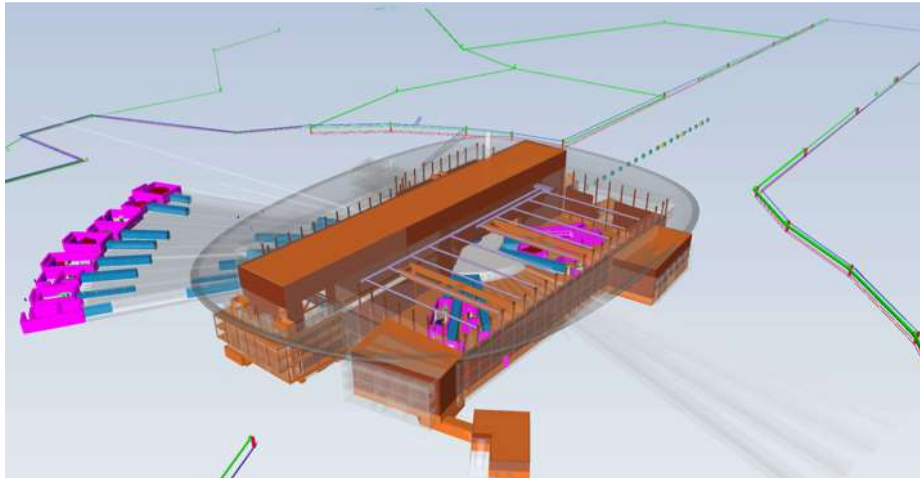


EUROPEAN  
SPALLATION  
SOURCE





EUROPEAN  
SPALLATION  
SOURCE





**DMSC**



**Data Systems & Technologies**

**Inst. Control, Data Acq. & Reduction (Jon Taylor)**

**Data Management (Tobias Richter)**

**Data Analysis & Modeling (Thomas Rod)**

**User Office Software**

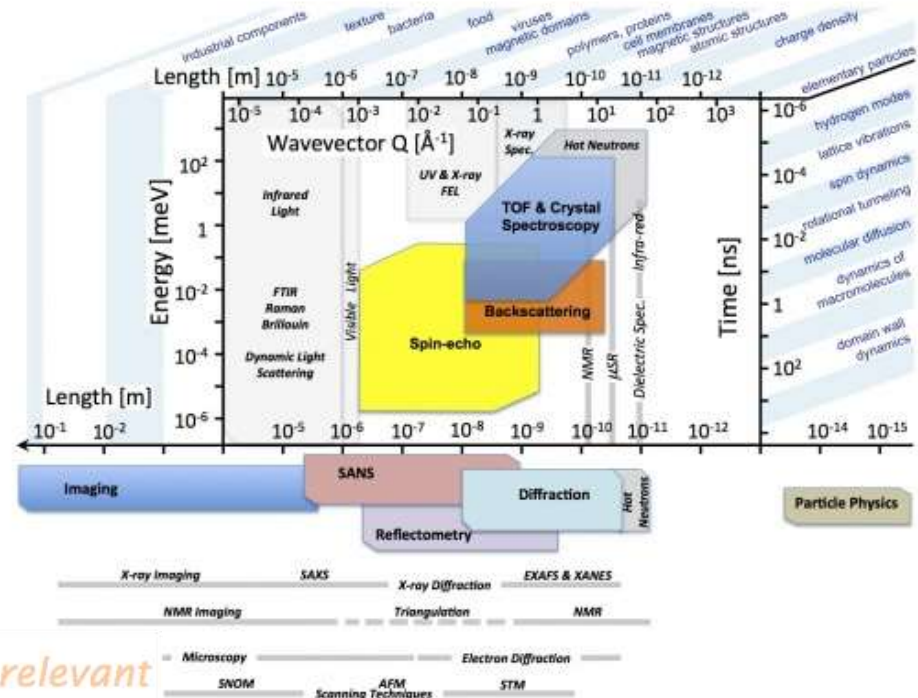
Copenhagen Data Centre  
DMSC servers in Lund  
Clusters, Workstations  
Disks, Parallel File System  
Networks (inc. Lund – CPH)  
Data transfer & Back-Up  
External Servers

Instrument Control User Interfaces  
EPICS read/write  
Streaming data (ADARA)  
Data reduction (MANTID)

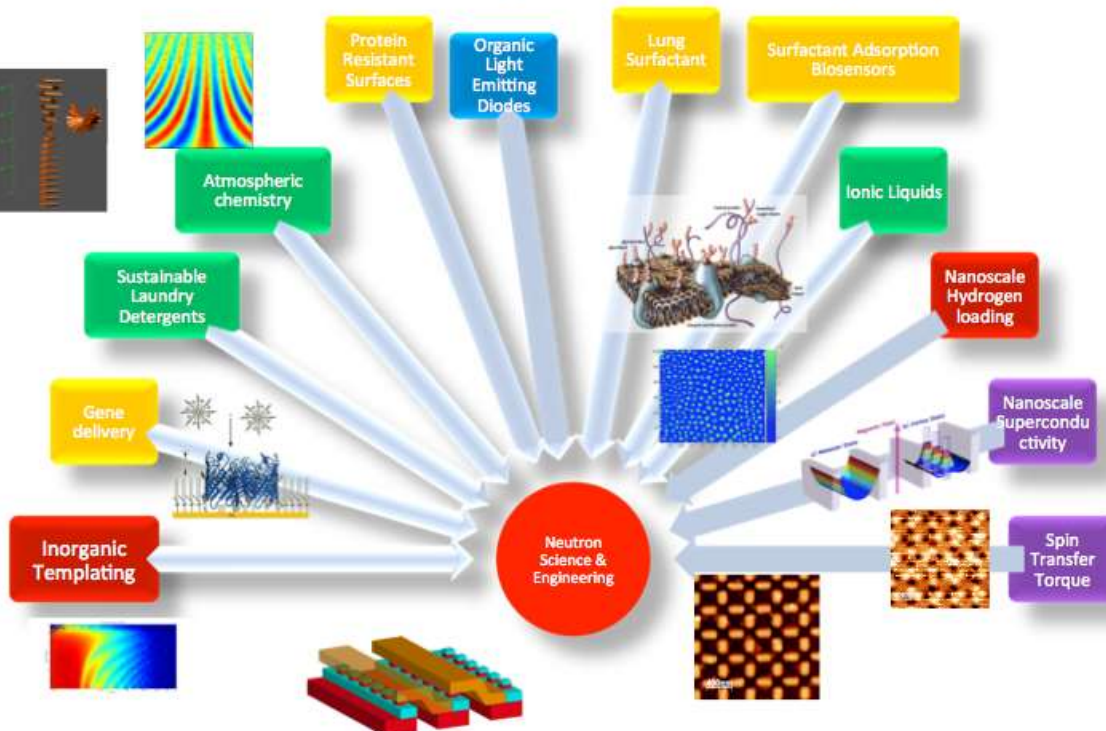
File writers (ADARA)  
Data Catalogues  
Workflow Management  
Post-Processing.....  
---- Reduction  
---- Analysis  
Messaging Services  
Web Interfaces

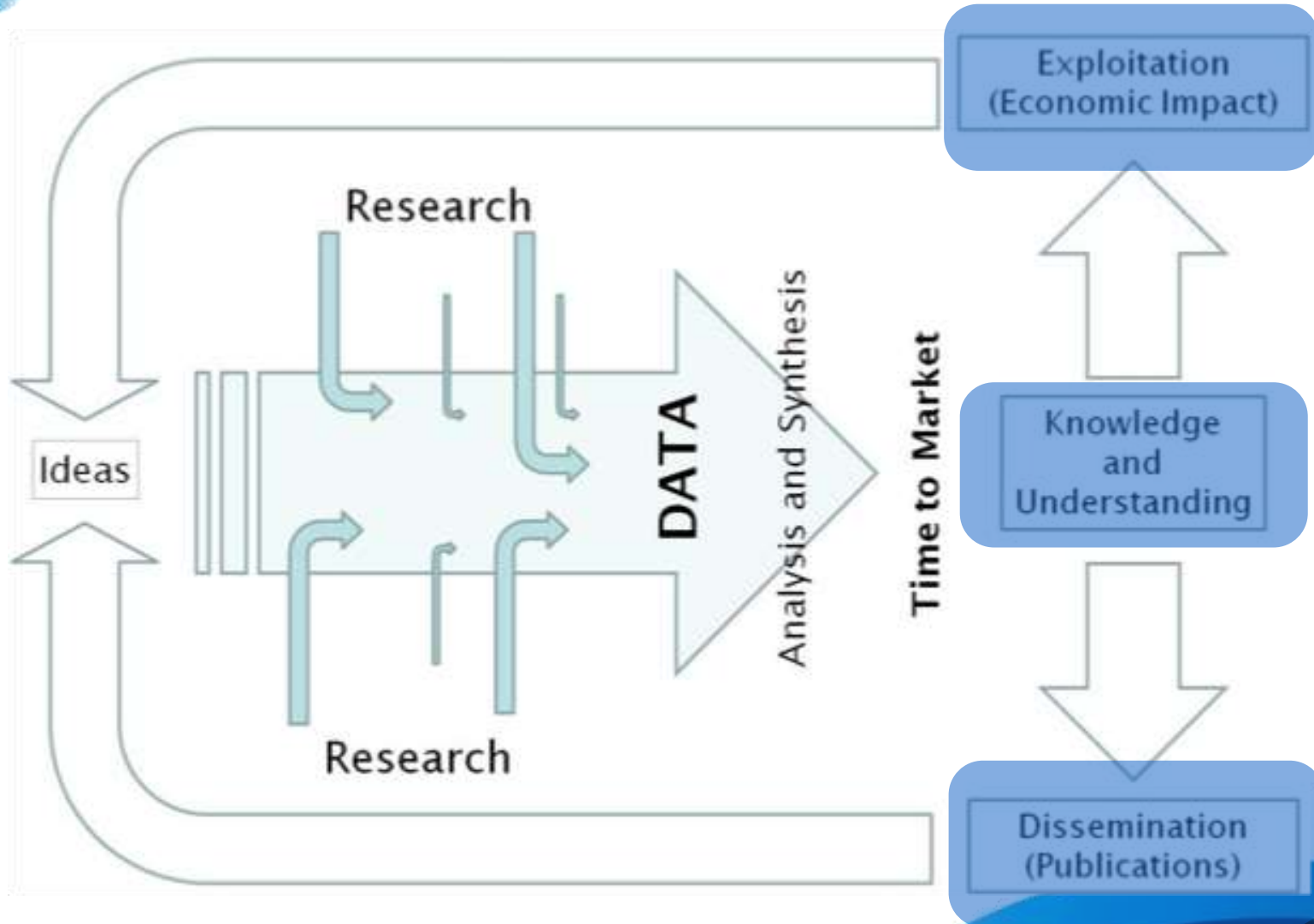
MCSTAS support + dev.  
Instrument Integrators  
Analysis codes (e.g. SANSview, Rietveld,...)  
MD + DFT Framework

User Database  
Proposal System  
Training Database  
Publications Database

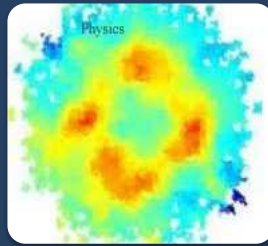


Fundamentally driven, *technologically relevant*





**PHYSICS**



## ANGSTROMS AND PICOSECONDS

- electronic and magnetic structure
- strongly correlated electron systems

**CHEMISTRY**

**SOFT MATTER  
& BIOLOGY**

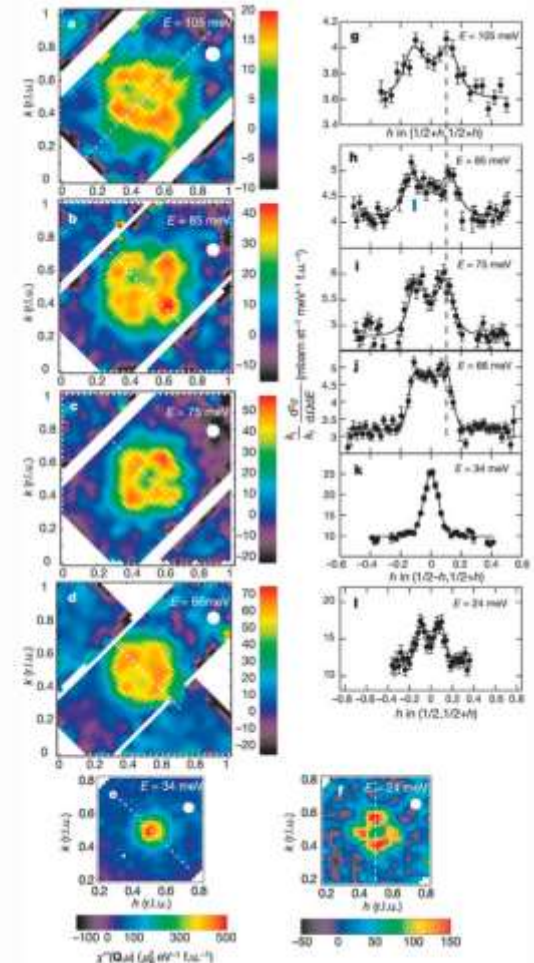
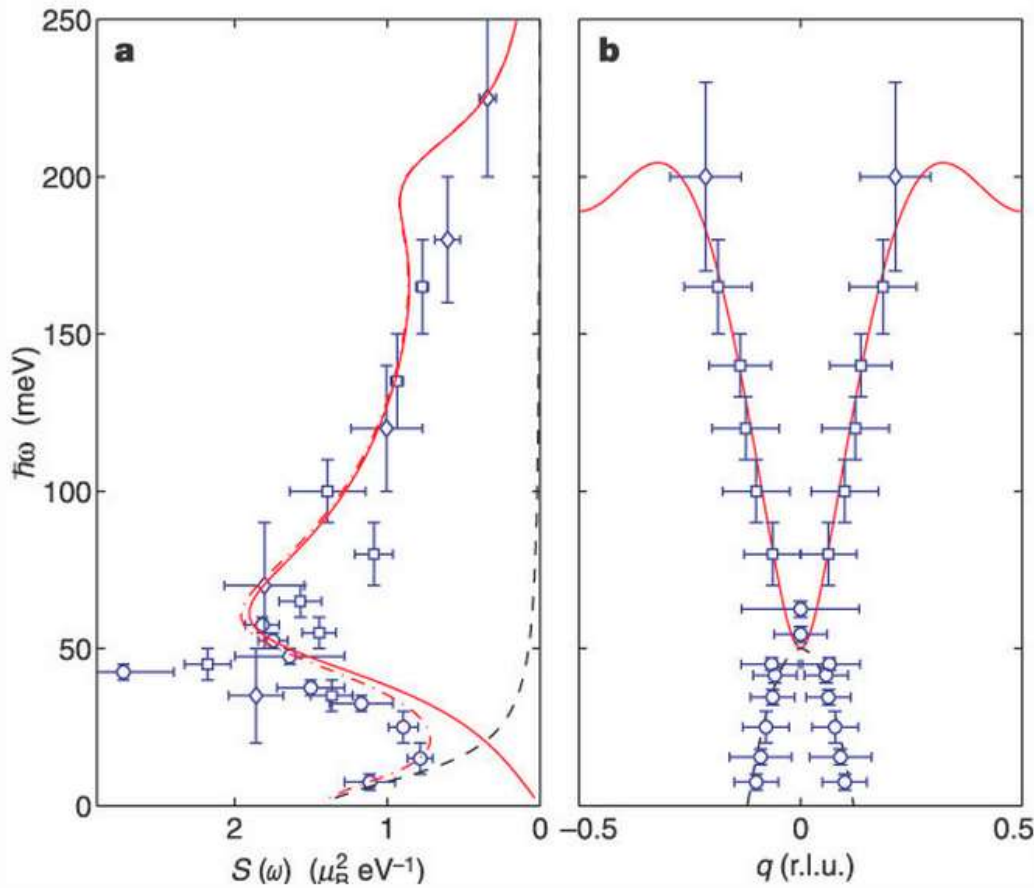
**ENGINEERING &  
MATERIALS SCIENCE**



## Quantum magnetic excitations from stripes in copper oxide superconductors

J. M. Tranquada<sup>1</sup>, H. Woo<sup>1,2</sup>, T. G. Perring<sup>2</sup>, H. Goka<sup>3</sup>, G. D. Gu<sup>1</sup>, G. Xu<sup>1</sup>, M. Fujita<sup>3</sup> & K. Yamada<sup>3</sup>

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



- High profile publications

## What is “Impact”

- Shorter lead time to publish

- Shorter lead time to publish
- Minimize barriers to publication
- Maximise efficient use of beam time
- Make life easier for users and staff
- Remove single point failures

- High profile publications
- Access to simulation software.
- Help to use simulation software.

***SC generates a factor 3 in neutron citations  
correlates to a factor 2 increase in H***

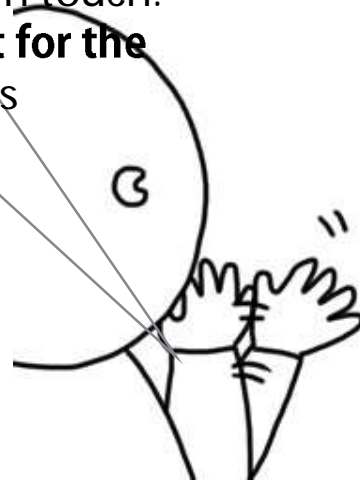
# We don't expect users to:

develop beam lines

In order to grow our user community we must be

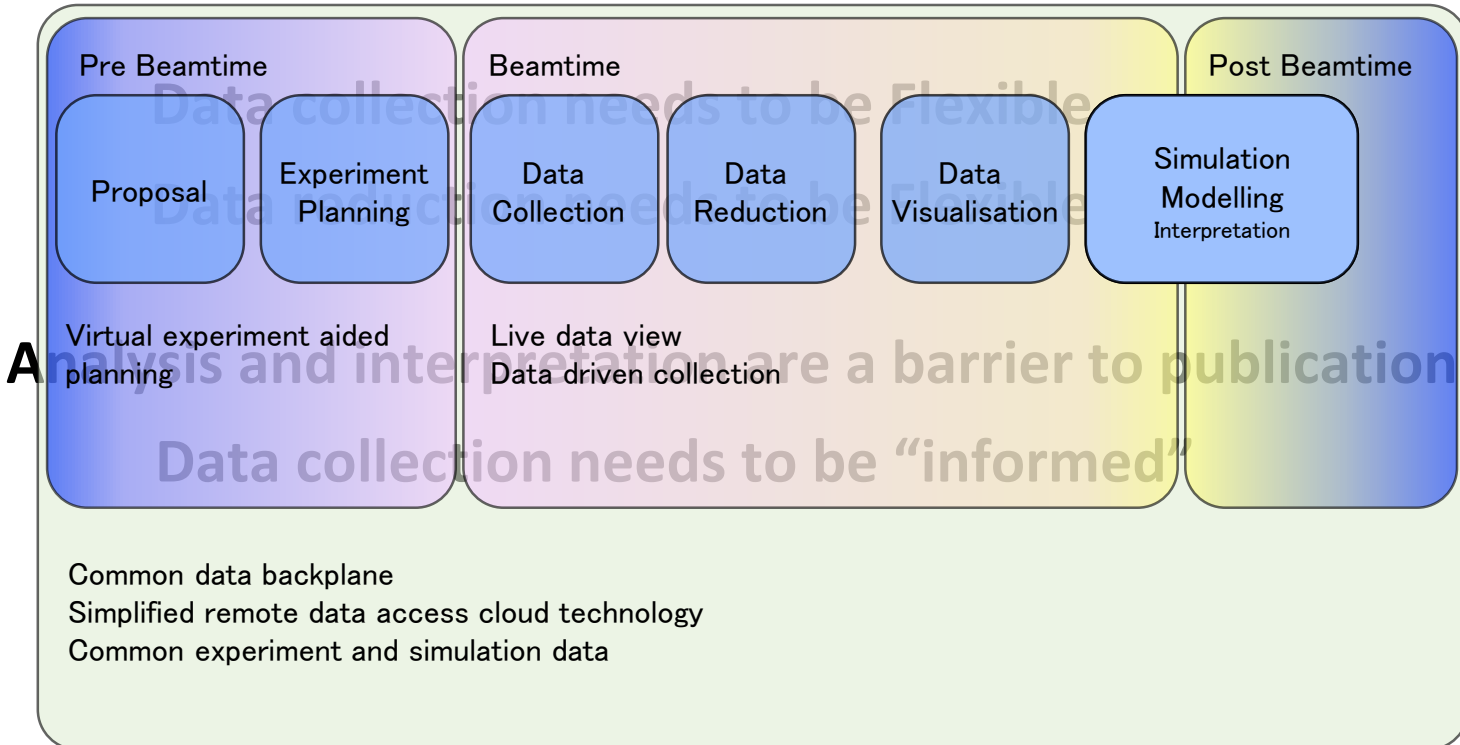
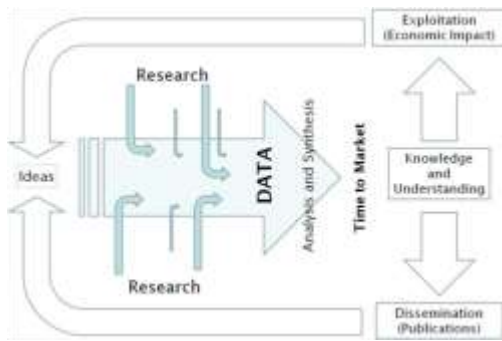
“Propose to service users who have no scientific experience of  
to make their own scattering, or scientific programme that  
does not require a priori knowledge  
but after the experiment...”

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



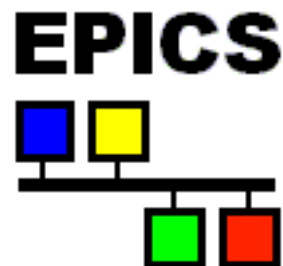
Thanks I promise to  
**publish my data... in**  
nature





# Relevant Technologies & frameworks

All open source :: develop within existing FWs



McStas



**SasView for Small Angle Scattering Analysis**  
A SAS Community Project launched from the NSF DANSE effort



Pandaas  
Sine2020





## Acknowledgements



### MANTID DEVELOPER WORKSHOP

Spallation Neutron Source • Oak Ridge National Laboratory • Oak Ridge, Tennessee, USA  
January 23, 2014

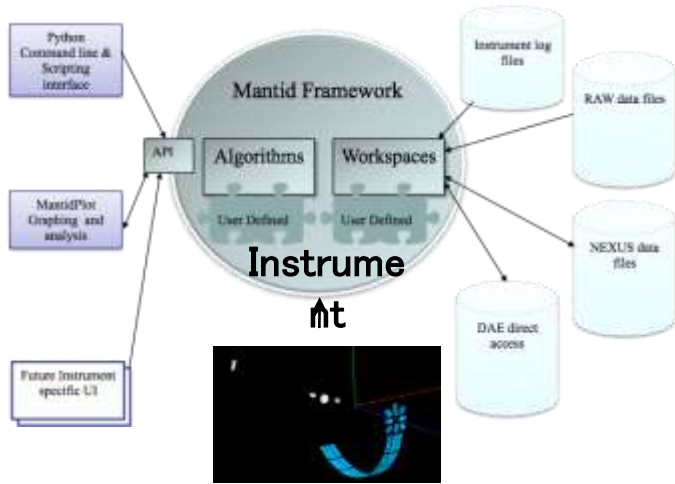


### MANTID SCIENTIFIC STEERING COMMITTEE

Spallation Neutron Source • Oak Ridge National Laboratory • Oak Ridge, Tennessee, USA  
January 15, 2014







Full Instrument description  
 Workspace history  
 Multiple workspace types  
 Box controlled rebin on nD data  
 Live event view

Algorithms event aware

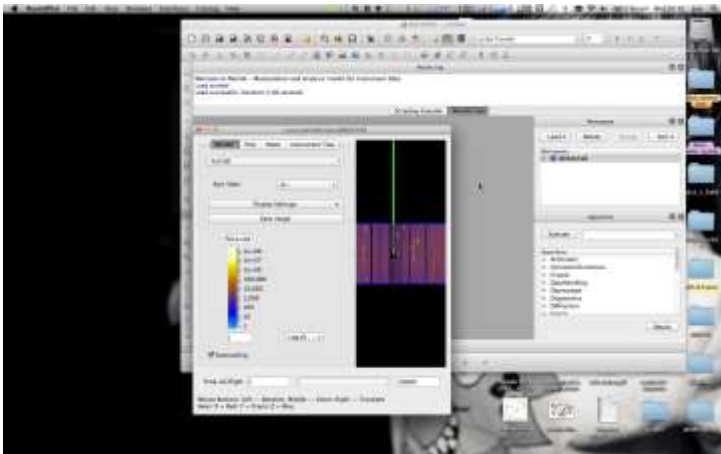
Slice viewer for 2D data

Python + IPython + Numpy + SciPy

ParaView

OpenMP

User extendable



Instrument view



# H2020 projects

- **PaNDAs**

Federated data storage and analysis infrastructure

- **SINE2020 :Data JRA (Thomas Rod)**

Automated Workflows and data analysis pipelines

# SINE2020

World class Science and Innovation with Neutrons in Europe in 2020

- EU Horizon 2020 proposal (INFRADEV-4)
- Five main partners:

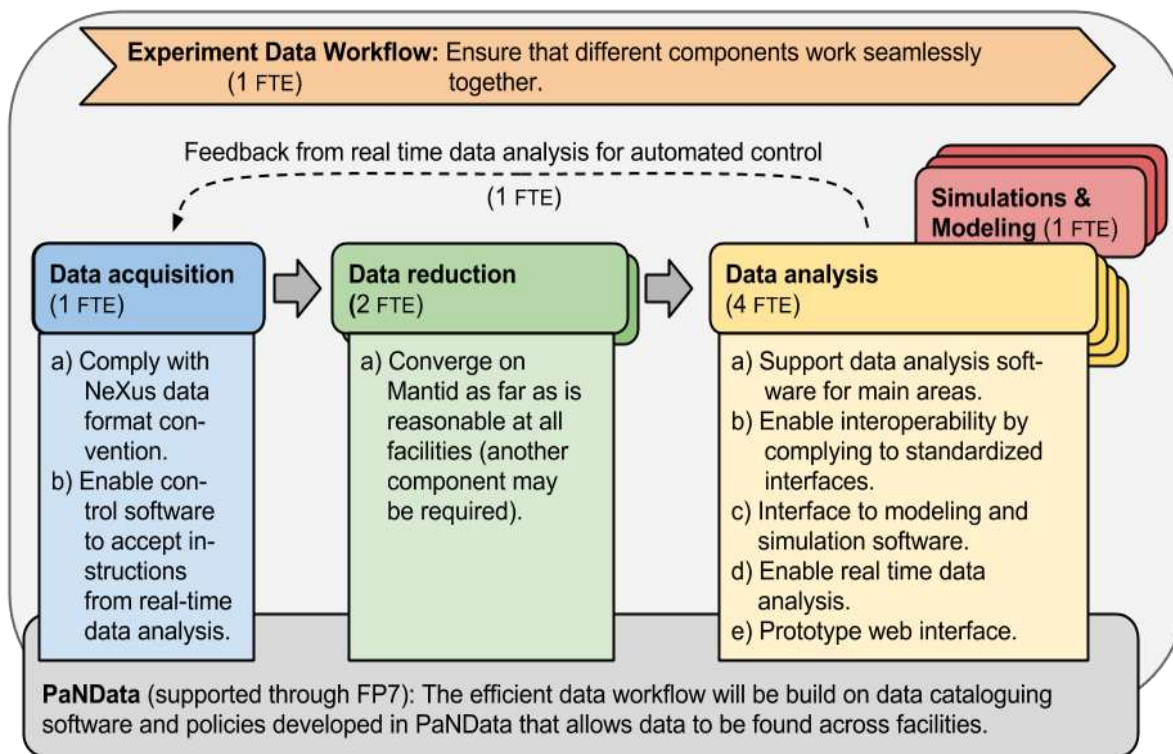


## Main topics:

- Innovation based on neutrons experiments
- Ready for ESS in 2020
- Interoperable software for data processing

Facility	Task
<i>ILL+FZJ+PSI</i>	<i>Mantid for continuum sources</i>
<i>ESS</i>	<i>SANS (SASView)</i>
<i>FZJ</i>	<i>Reflectometry (BornAgain)</i>
<i>ILL</i>	<i>Modelling (nMoldyn)</i>
<i>ISIS</i>	<i>QENS (Mantid)</i>
<i>PSI</i>	<i>Imaging (MuhRec/KipTool)</i>

# Interoperable Data Treatment Software for the European User Community



# Supporting development of existing programs

ESS will support (distributed) development of existing programs by hosting software development environments

- Web sites, repositories, build servers, etc

SASView and McStas will be the first two projects supported in this way



# High availability Infrastructure



Complexity metric



pandata

+



+



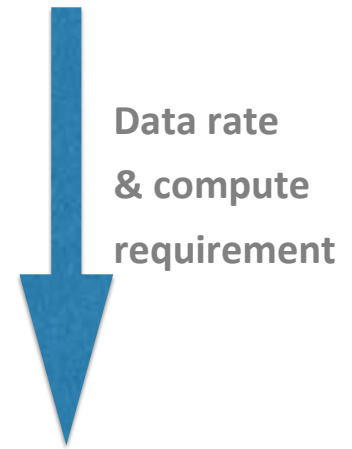
# A not extensive list of experimental requirements

## Experiments

Temperature / field / pressure dependent measurements of  
diffraction  
INS  
reflectometry  
SANS.

Generation of 4D data volumes, step scan / continuous rotation mode

Back projection reconstruction imaging



## Experiment set-up modes

Real time Laue mode.

Real time motion scan mode.

Sample location and centring.

Slit scans

# Towards “Real Time” processing / Visualisation Modelling

**Considerations::**

**Data rate**

**Compute availability**

**Architecture**

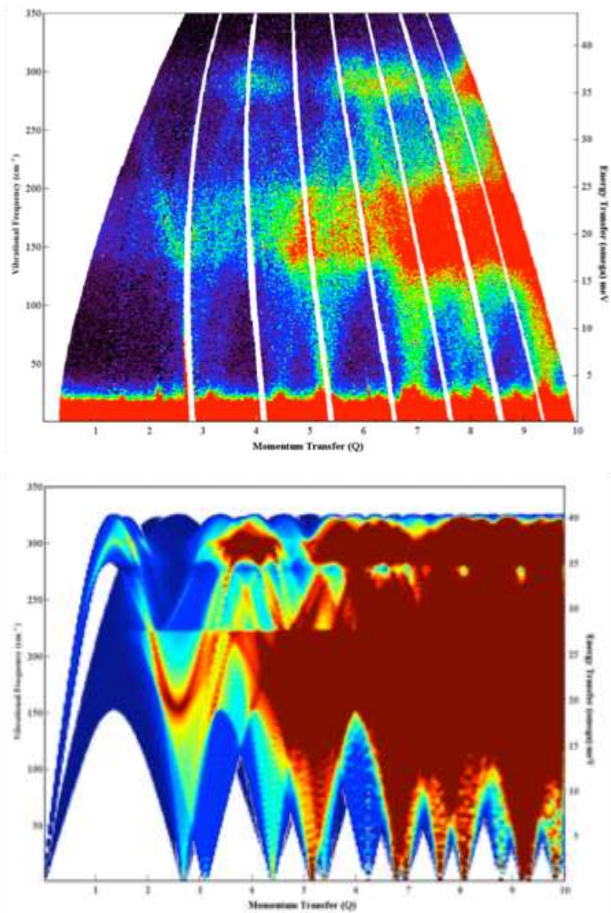
**Usability :: UX & UI**



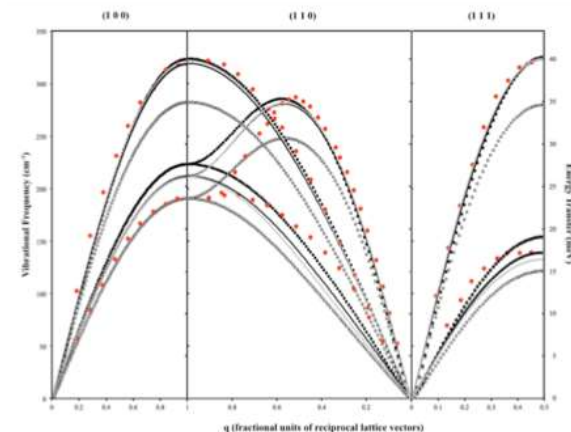
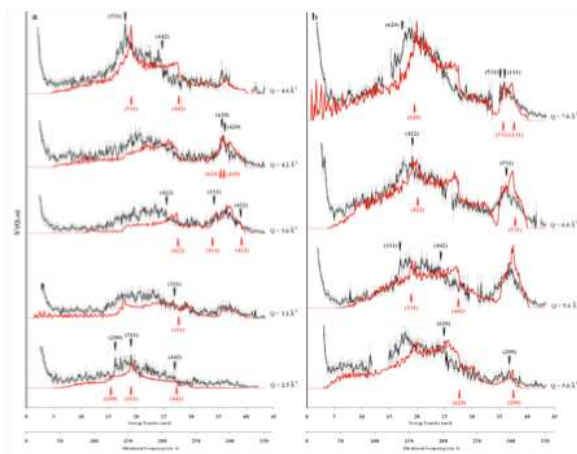
## The Interpretation of Polycrystalline Coherent Inelastic Neutron Scattering from Aluminium

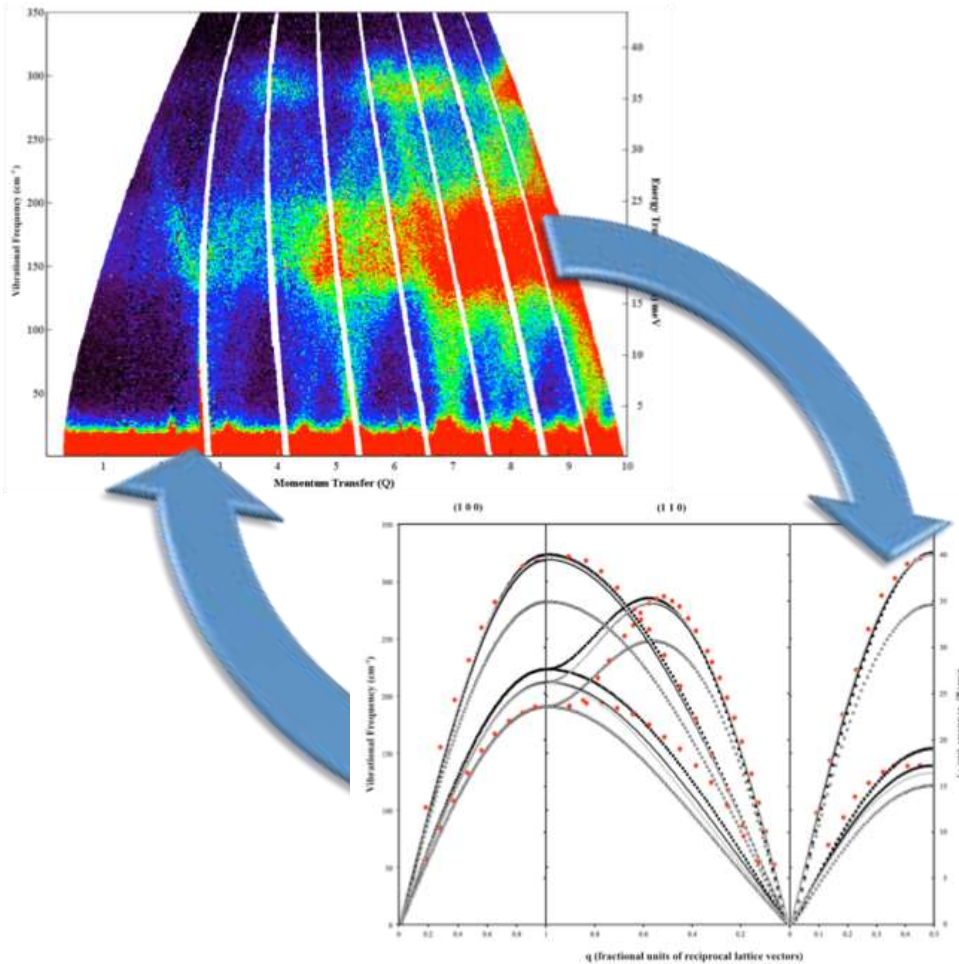
Authors

Daniel L Roach<sup>a\*</sup>, D Keith Ross<sup>a</sup>, Julian D Gale<sup>b</sup> and Jon W Taylor<sup>c</sup>



## Coherent lattice excitations from powders

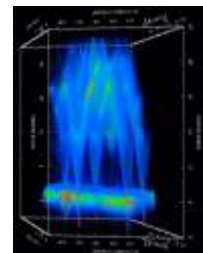
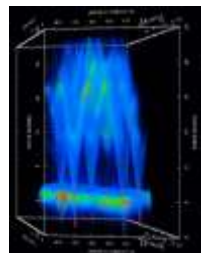




GULP fitting cycle  
~60s

# Generation of 4D data volumes in RRM

- Worst case 48 hrs for reduction



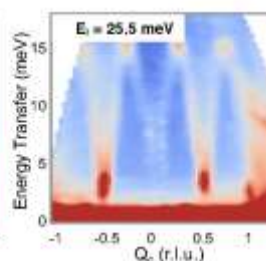
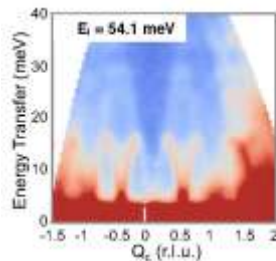
1x 200+ Gb file

1x 200+ Gb file



or **MANTiD**

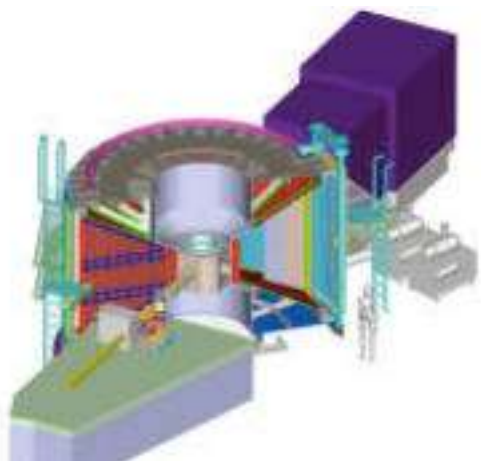
2+ hrs

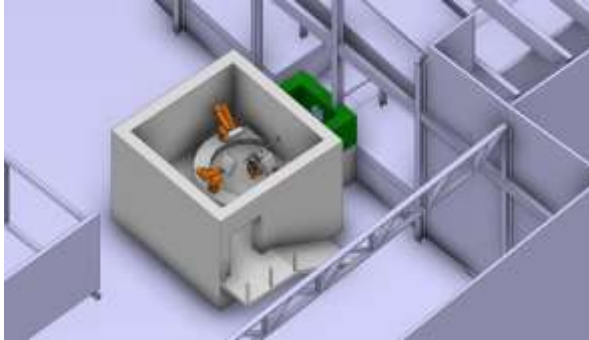


2-300 files per ei  
~200mb each

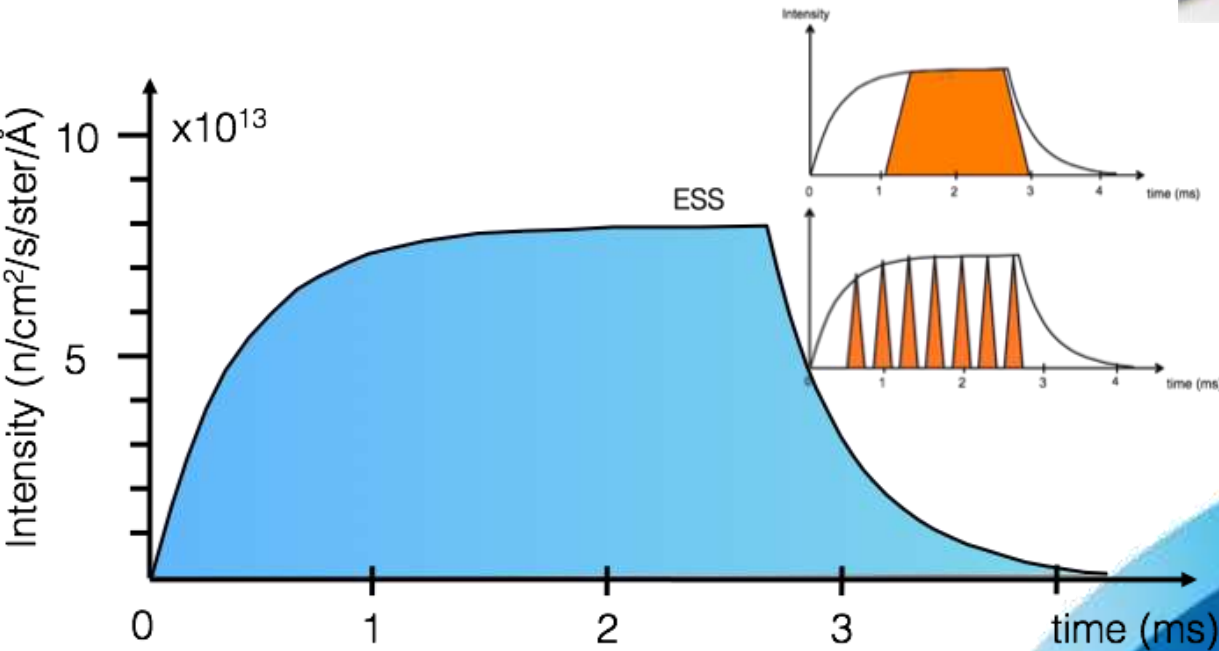
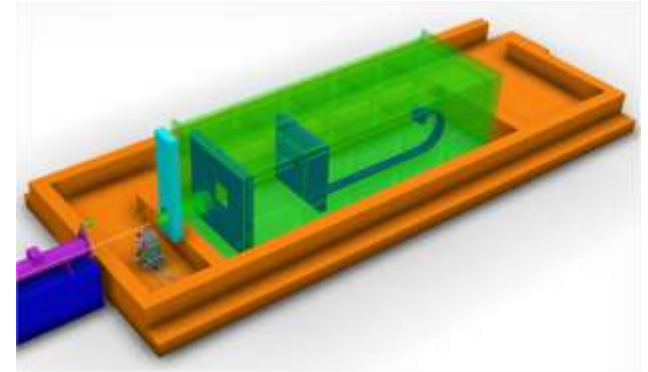
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60s

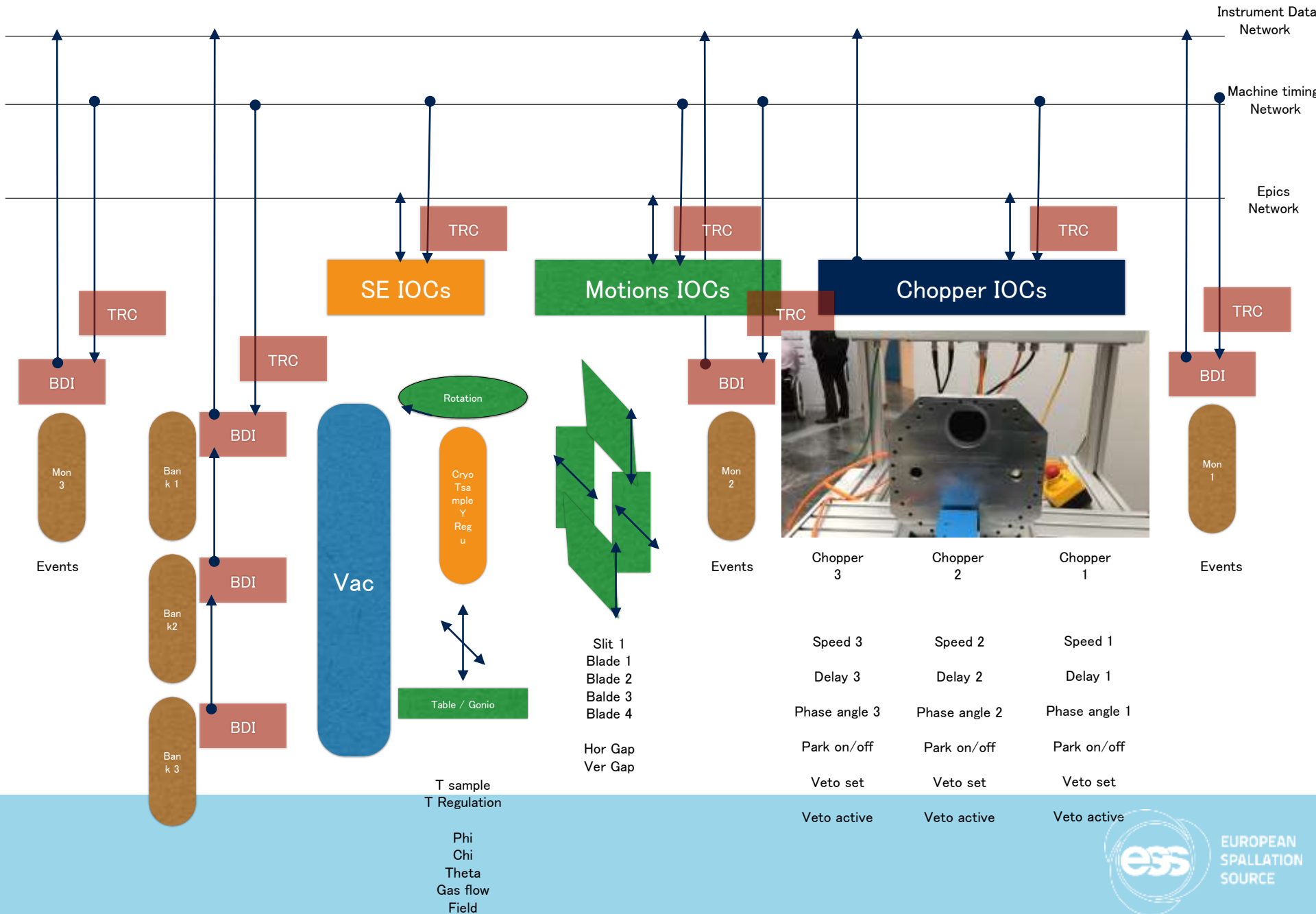




- $\sim 10^9$  n/s/cm<sup>2</sup>
- $\sim 600$ k channels



# schematic of control at a parallel event based source like ESS





EUROPEAN  
SPALLATION  
SOURCE

Instrument  
Data Network

Machine timing  
Network

Epics  
Network

Aggregator

Stream Management  
server



IC server side

IC Client side

MANTID

vm

Pandaas compatible type VM infrastructure

Live Data reduction  
Live visualisation

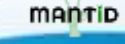


Online Data reduction

Streaming file service



ESS Instrument Data Stream



Online Data reduction

Streaming file service





# Concluding remarks

**Software is essential for impact**

**Collaborative development maximises impact**

**Existing projects essential for ESS**

