# VATES

*Owen Arnold, Michael Reuter, Alex Buts, Martyn Gigg, Andrei Savici, Nick Draper*

Tessella
Technology & Consulting

SNS
SPALLATION NEUTRON SOURCE

Science & Technology Facilities Council
ISIS

# VATES : The problem

- Highly pixelated instruments
- Large data volumes
- Many dimensions of interest
- Need for n-dimensional data manipulation
- One workbench required



**1520 tubes**

**x 128 pixels** 160°

**+/- 15°**

**x 5000 time channels**
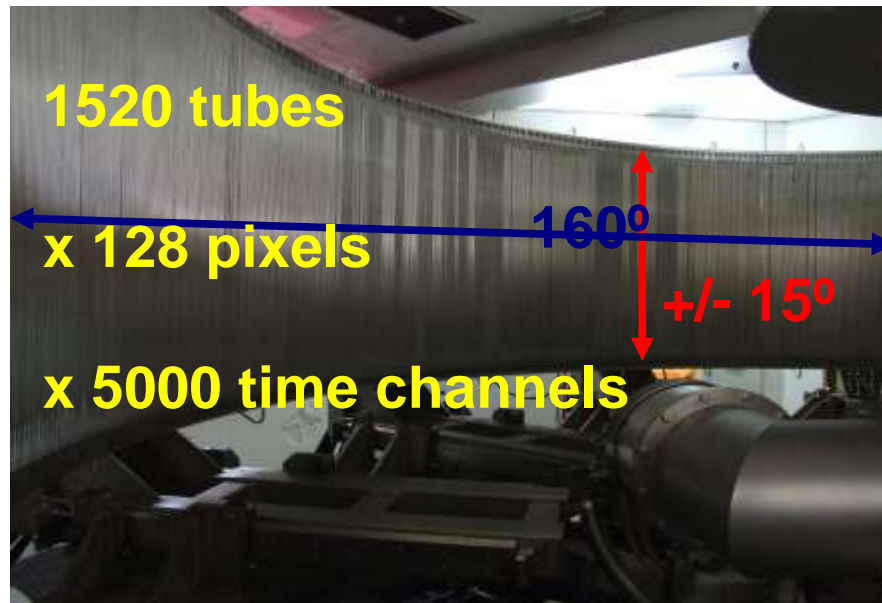
# VATES : Requirements

- Containers and pipeline for multi-dimensional data
- Visualisation of multi-dimensional data
- Simulation and fitting of multi-dimensional data
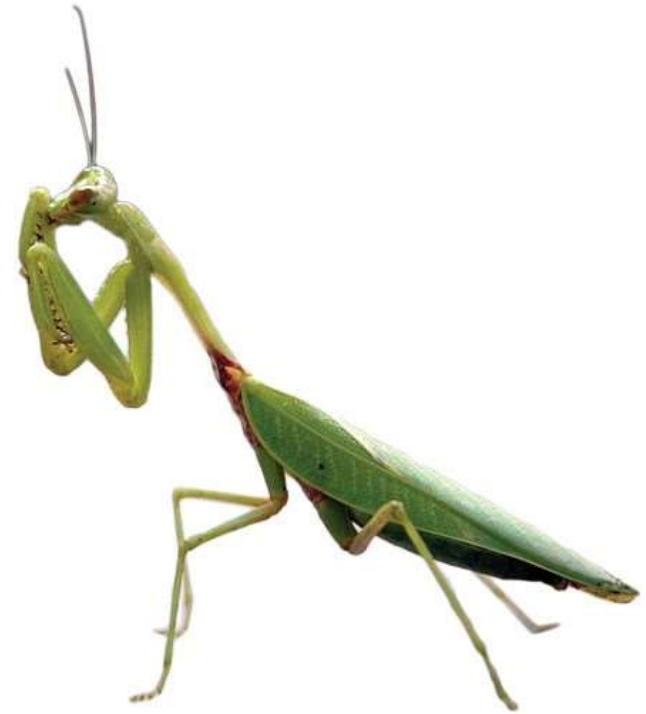- Pluggable/Extendable in many ways

# Platform Design Choice: Mantid

Mantid: Instrument and technique independent Data Reduction       and Analysis.
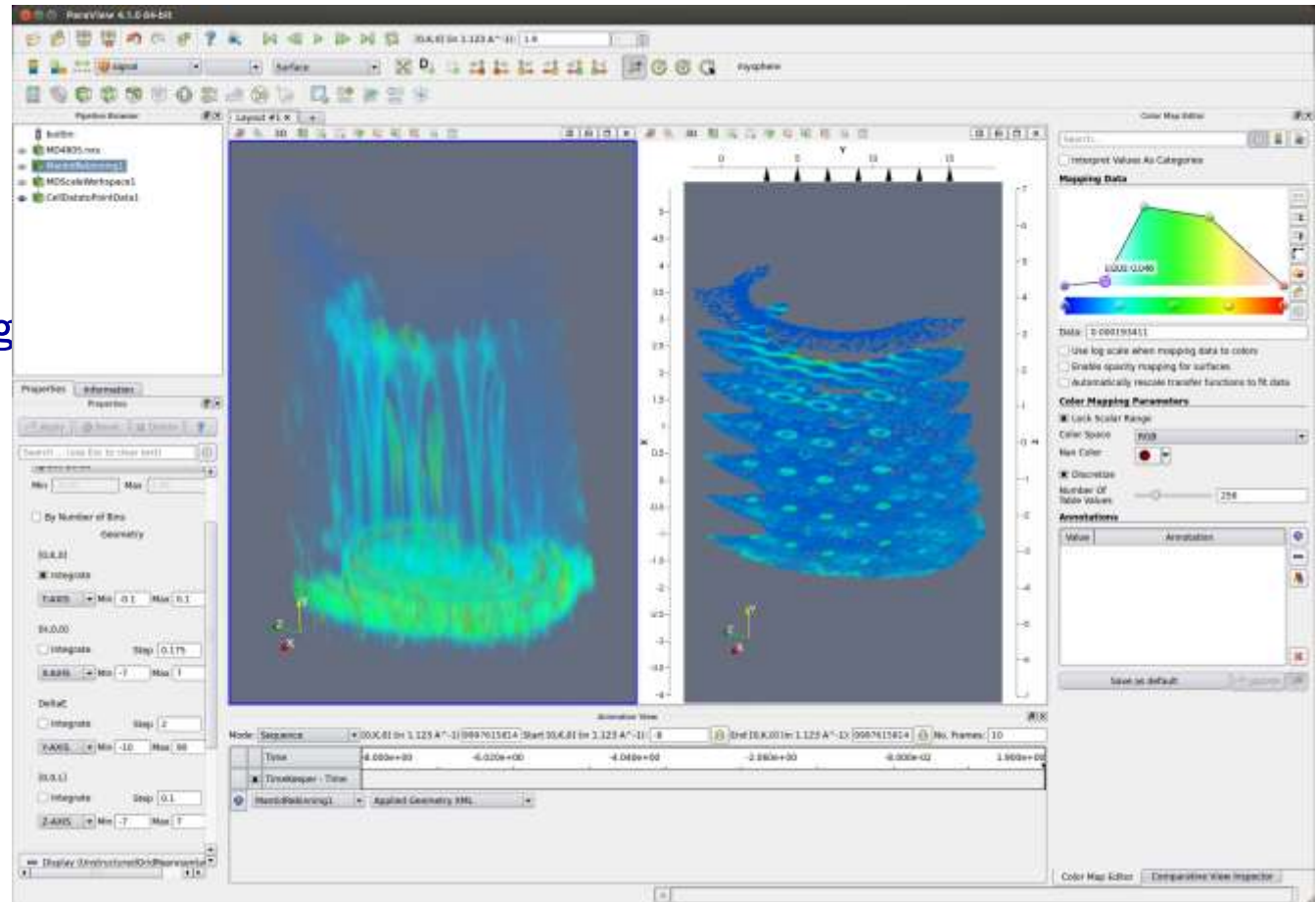
Joint project by ISIS and SNS

- Overlap in target platforms
- Overlap in common functionality
- Assemble one continuous chain
- Shared maintenance effort
- No need for another standalone tool
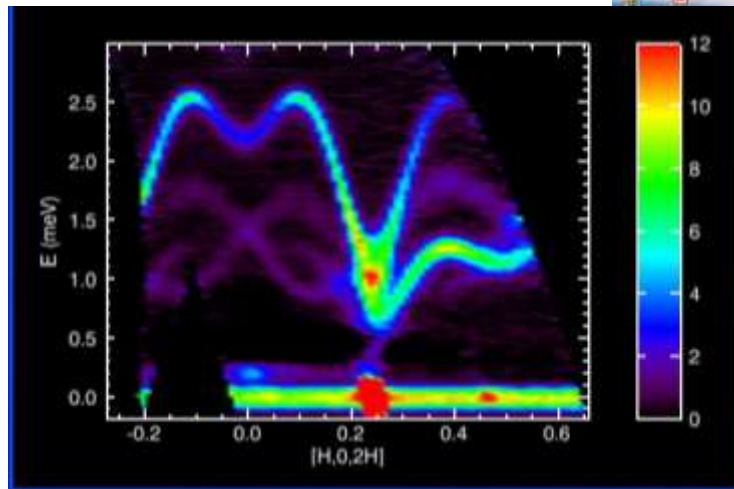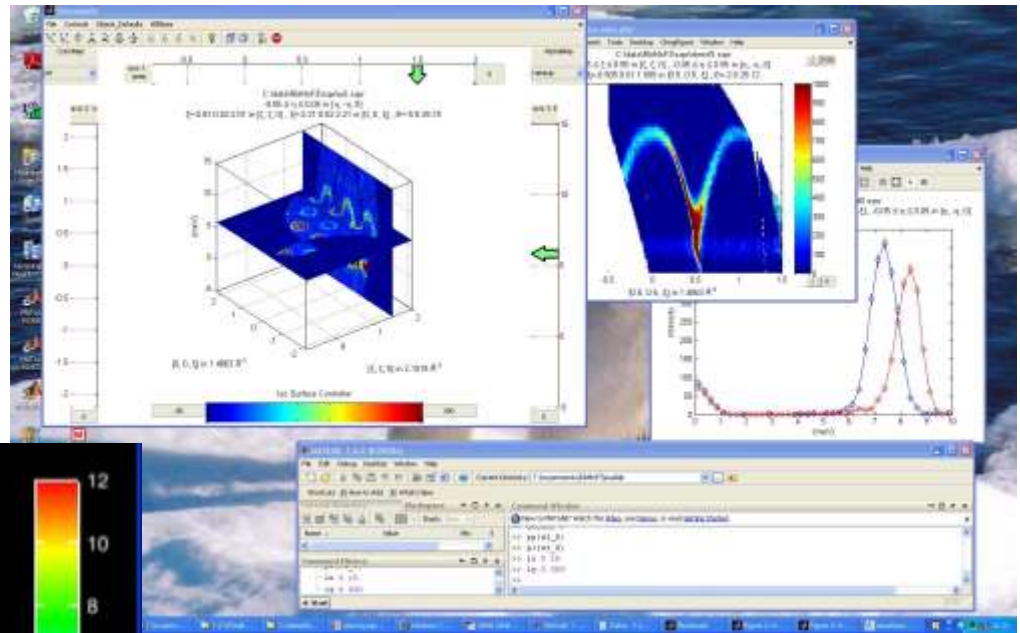
# Platform Design Choice: ParaView

- Cross-platform
- Well supported
- Open source
- Pipeline branching
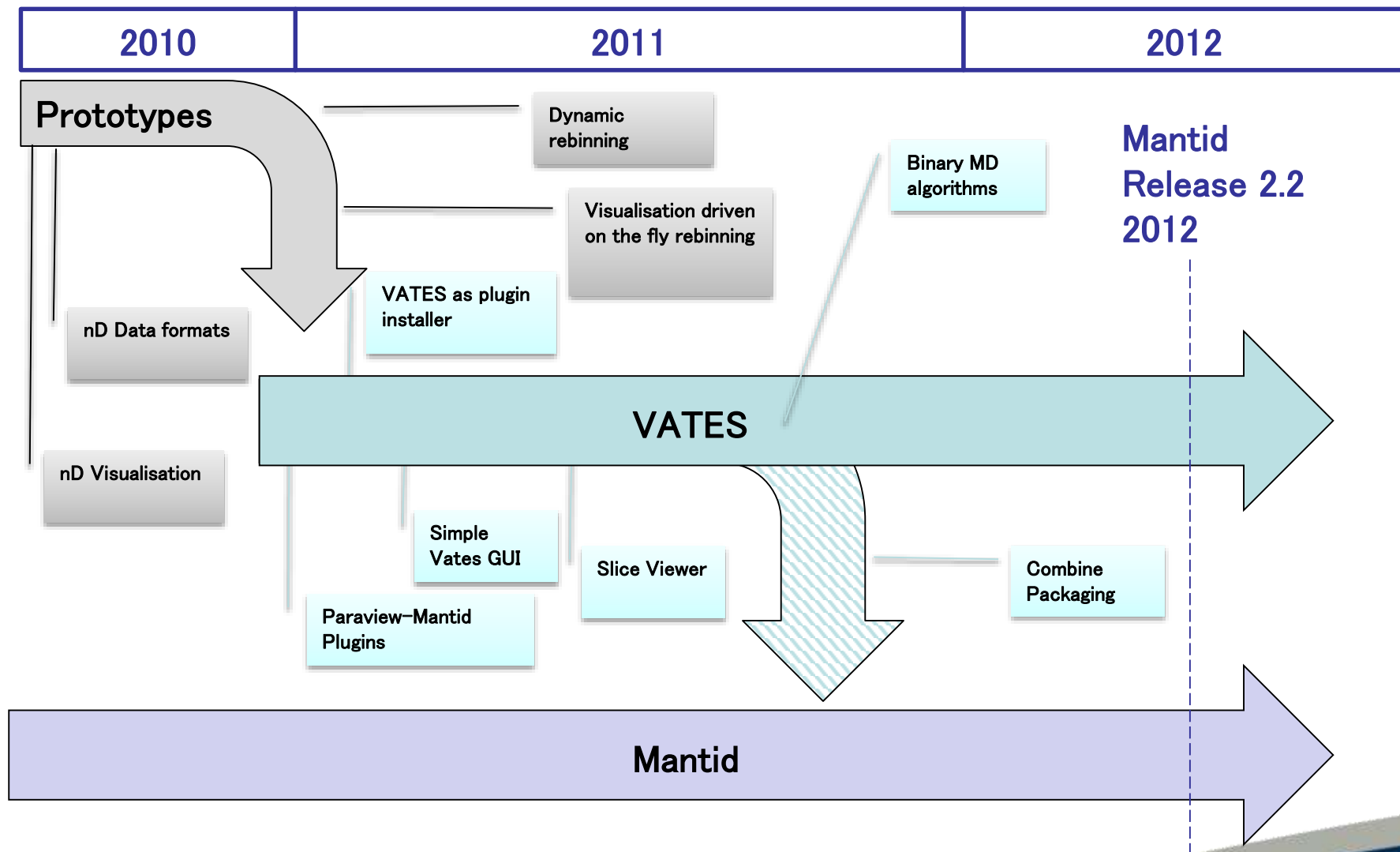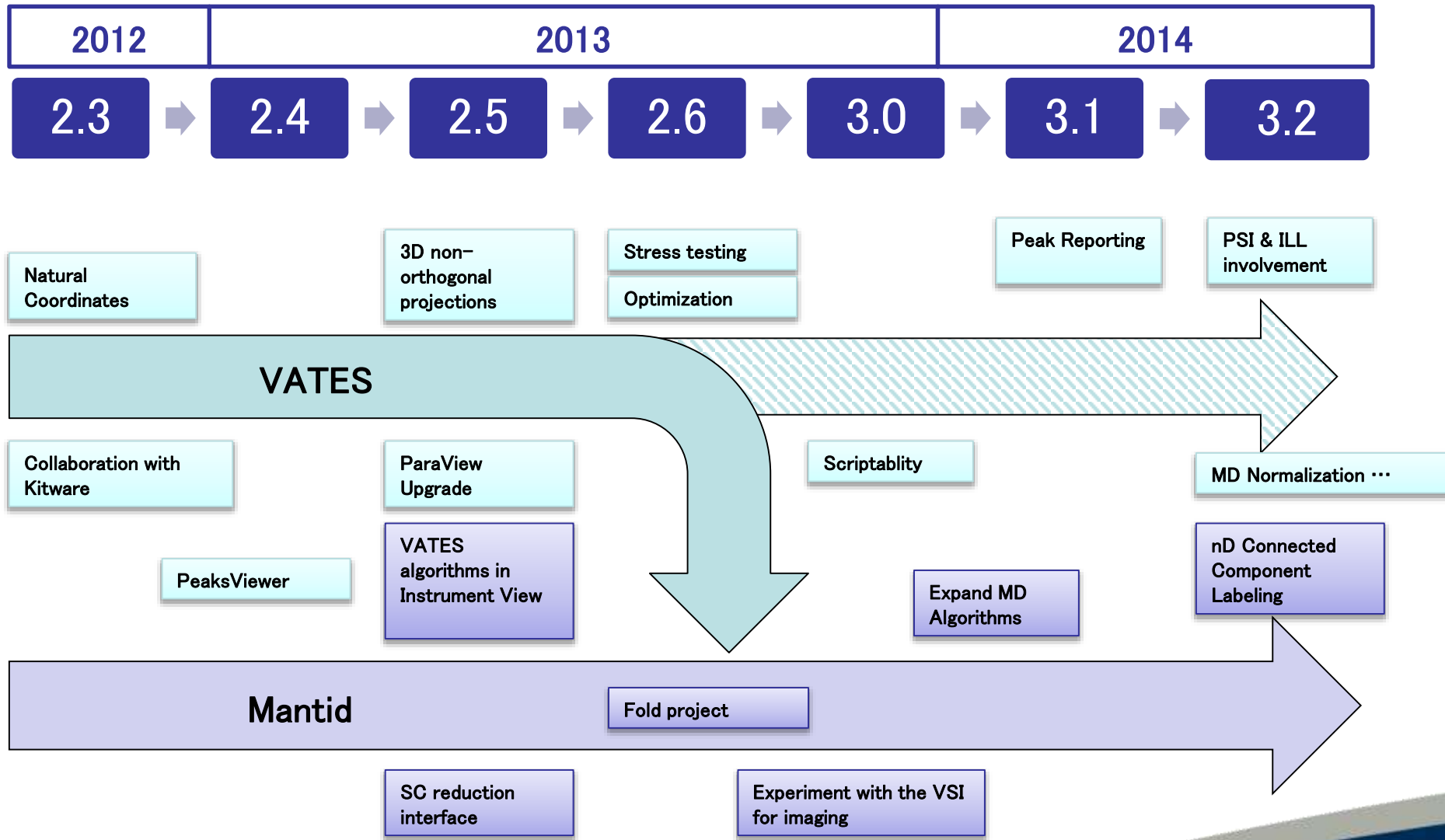- Suitable for large volumes of data

# Previous and Existing Tools

Many successful tools to
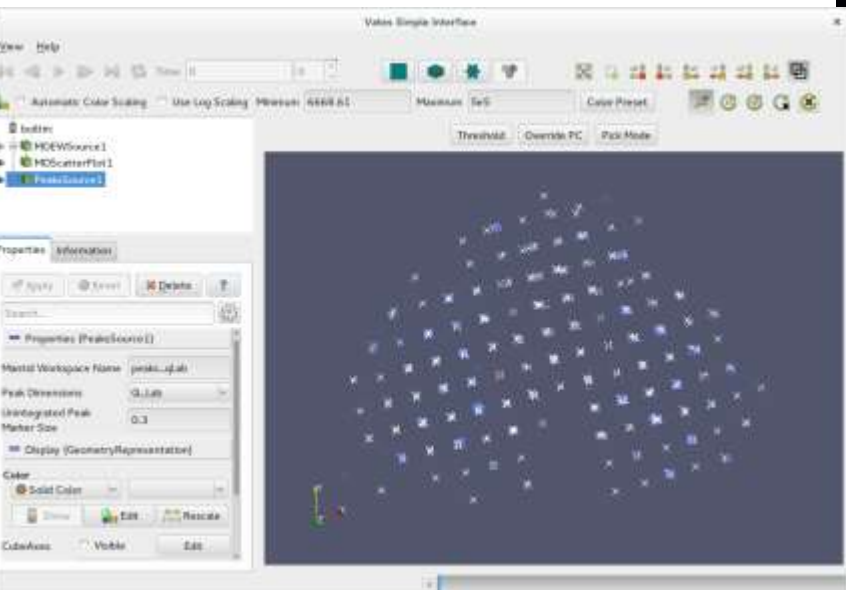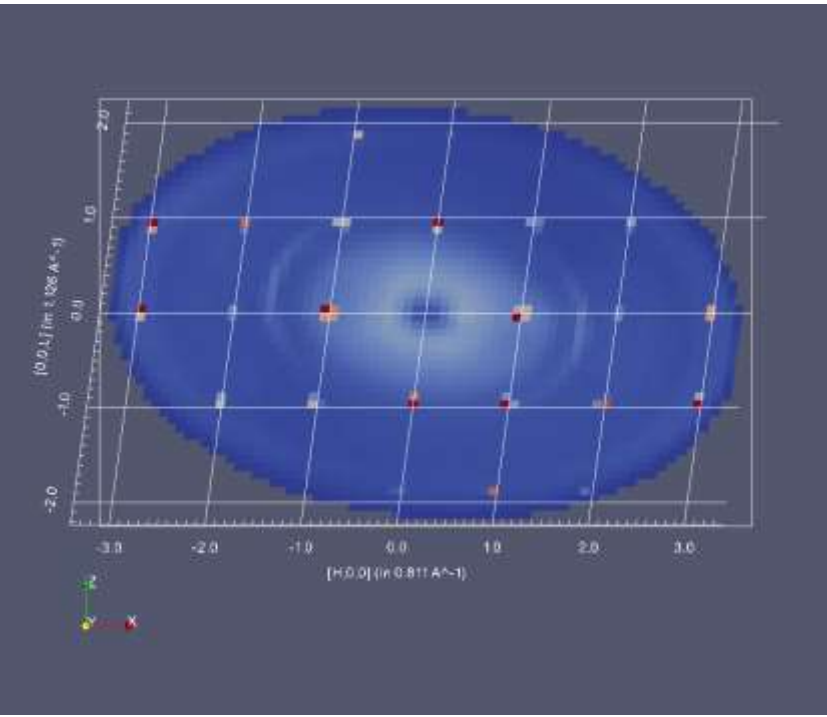draw ideas from and extend

# Historic Overview

| 2010 | 2011 | 2012 |
|------|------|------|

**Prototypes**

Dynamic rebinning

Visualisation driven on the fly rebinning

Binary MD algorithms

**Mantid Release 2.2 2012**

nD Data formats

VATES as plugin installer

nD Visualisation

**VATES**

Simple Vates GUI

Slice Viewer

Combine Packaging

Paraview-Mantid Plugins

**Mantid**

MANTiD

SNS
SPALLATION NEUTRON SOURCE

Science & Technology Facilities Council
ISIS

# Overview

| 2012 | 2013 | 2014 |
|------|------|------|

**2.3** → **2.4** → **2.5** → **2.6** → **3.0** → **3.1** → **3.2**

Natural Coordinates

3D non-orthogonal projections

Stress testing

Optimization

Peak Reporting

PSI & ILL involvement

**VATES**

Collaboration with Kitware

ParaView Upgrade

Scriptablity

MD Normalization …

PeaksViewer

VATES algorithms in Instrument View

Expand MD Algorithms

nD Connected Component Labeling

**Mantid**

Fold project

SC reduction interface

Experiment with the VSI for imaging

MANTiD

SNS
SPALLATION NEUTRON SOURCE

Science & Technology Facilities Council
ISIS

# Multi Dimensional Visualization
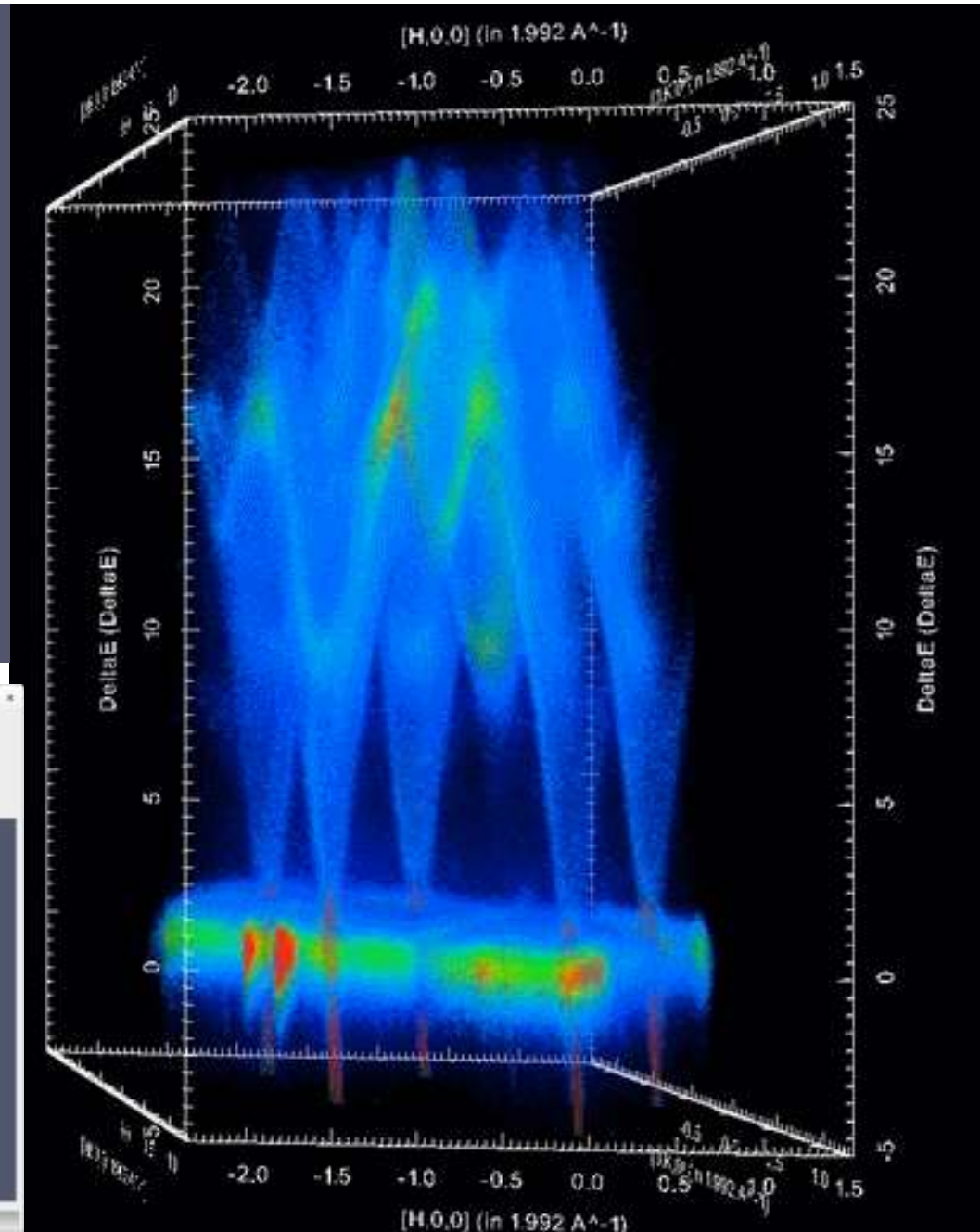
# Model Fitting and Simulation

Visualisation ⬅➡ model fitting/simulation

- Highly iterative procedure
- Require seamless integration with Mantid and visualisation
- Allow user-supplied models for scattering
  - 'foreground': typically global across dataset + resolution
  - 'background': simple (e.g. Linear background), no resolution

- Links with existing Mantid Fit framework
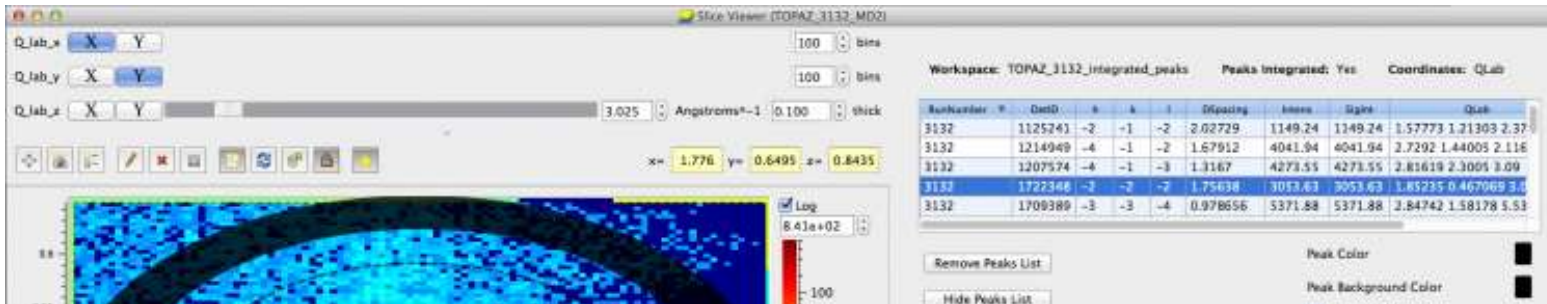- Foreground and background models are extendable

# Model fitting: current status and forward view

- Verify & expand stock foreground model library

- Speed optimisation

- User interface:
  - easy-to-use templates for simple user models
  - Work-bench interface

- Distributed computing (clusters)

- Possible investigation into using GPU resources

- Other resolution function models
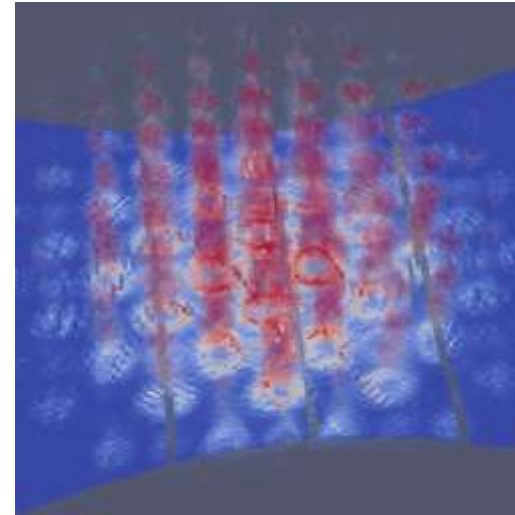


*Simulation of MERLIN instrument resolution convolved with a Strontrium122 foreground model*
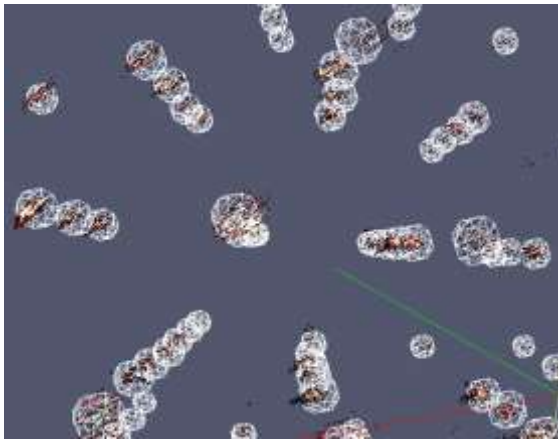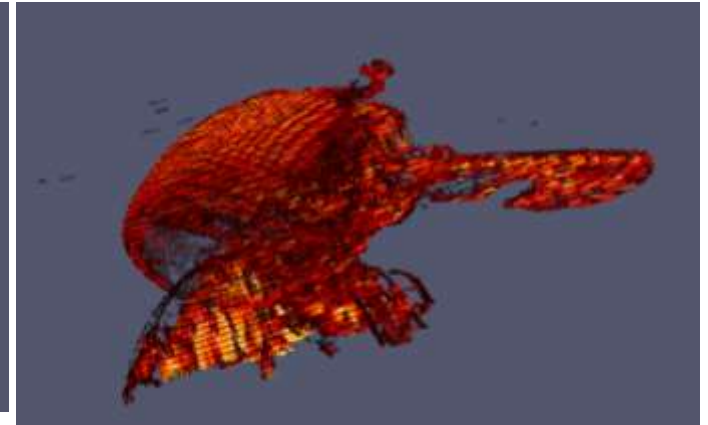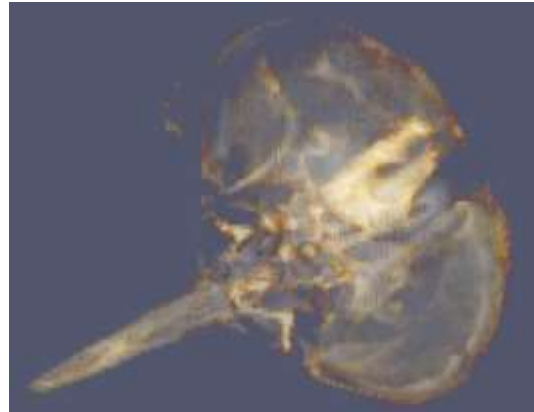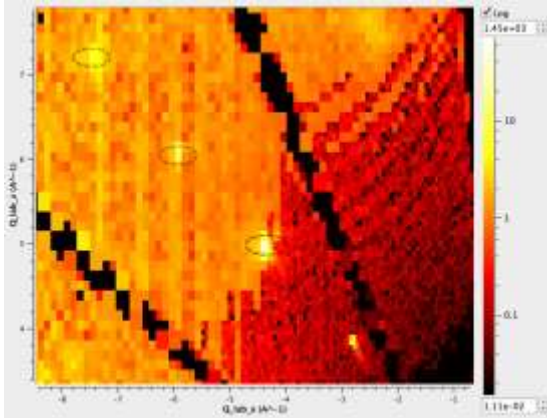
# PeaksViewer

# PeaksViewer

# Peak Integration

1. Heavily uses both Mantid and VATES
2. Started out with a spherical integration algorithm
3. Ellipsoid integration
4. Experimenting with CCL approach
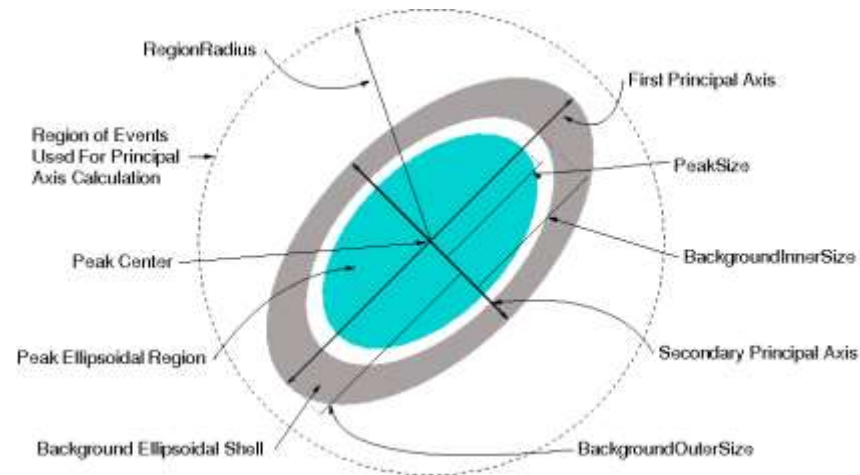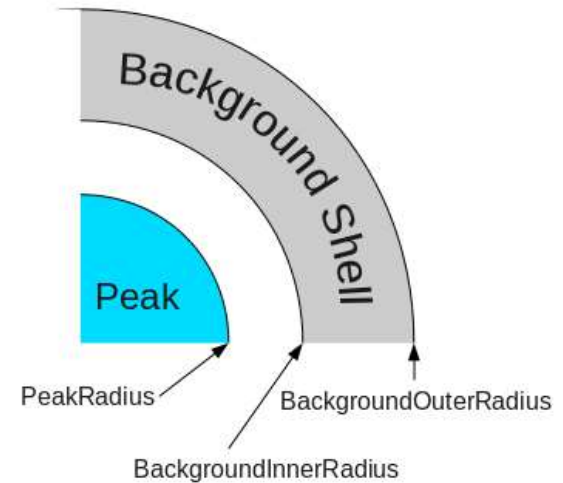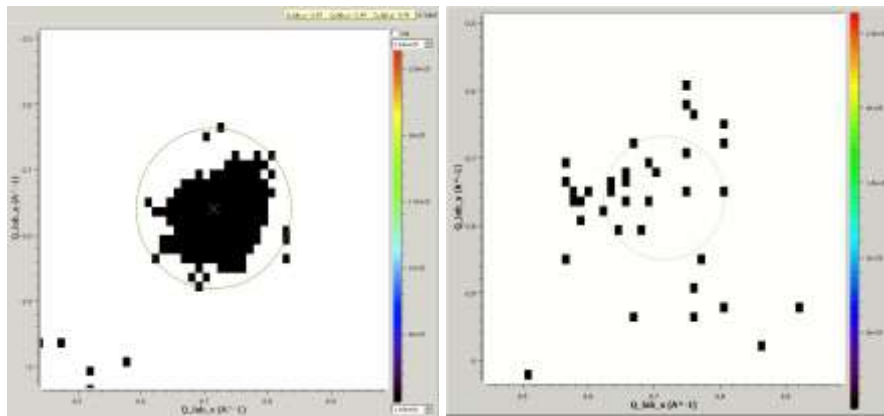
# Two way interaction
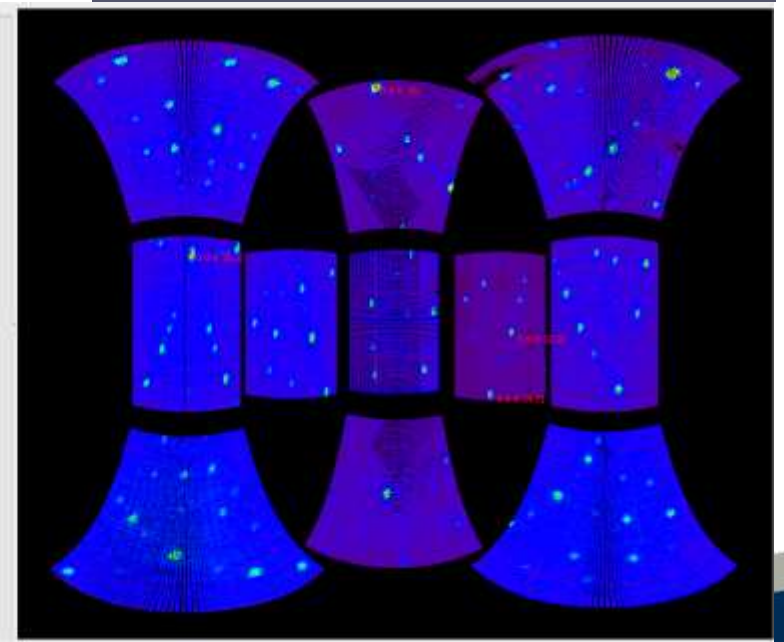
# Looking Forwards

- Complete scriptability. A well thought out API.

- Better cohesion between tools.

- MD normalization work.

  - Properly account for solid angle and flux in Horace scans

- Processing of large datafiles.

- Turning our attention to MPI and GPU processing

- Continued scientific led development

# Questions