



Mantid

VATES

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ISIS

VATES

Visualisation &
Analysis
Toolkit
Extensions



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Vates pectinicornis

Why?

- Handling new Instruments
 - Highly pixelated
 - Large data size
- Large accumulated datasets
 - Many properties of interest (highly sensitive)
 - Large data space
 - 100+GB size
- Consolidate Existing Knowledge



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- Bespoke tools
 - Tobyfit, Horace ...



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Project Goals

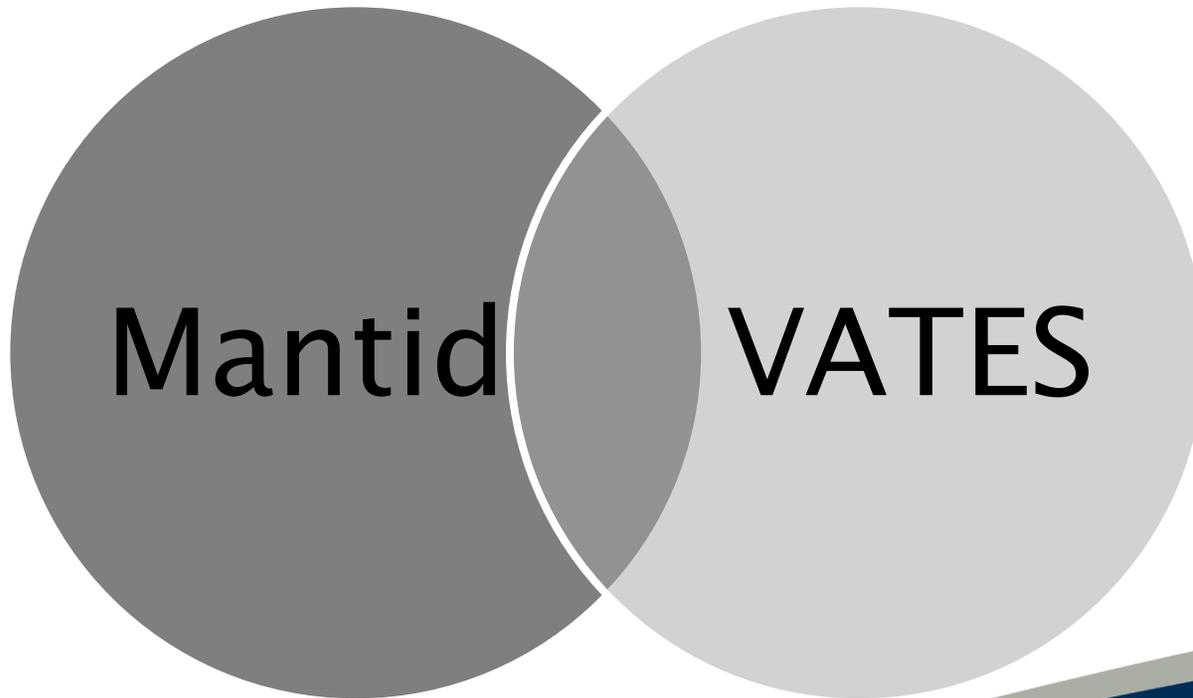
- Visual Data Reduction
 - Terascale Visualisation
 - Exploration of nD Datasets Q_x , Q_y , Q_z , ω temp, field, etc
 - On-the-fly rebinning of sparse data
- Consolidation of Existing tools
 - TobyFit, Horace knowledge
 - Build upon and extend Mantid
- Seamless working environment



Design Choice: Mantid

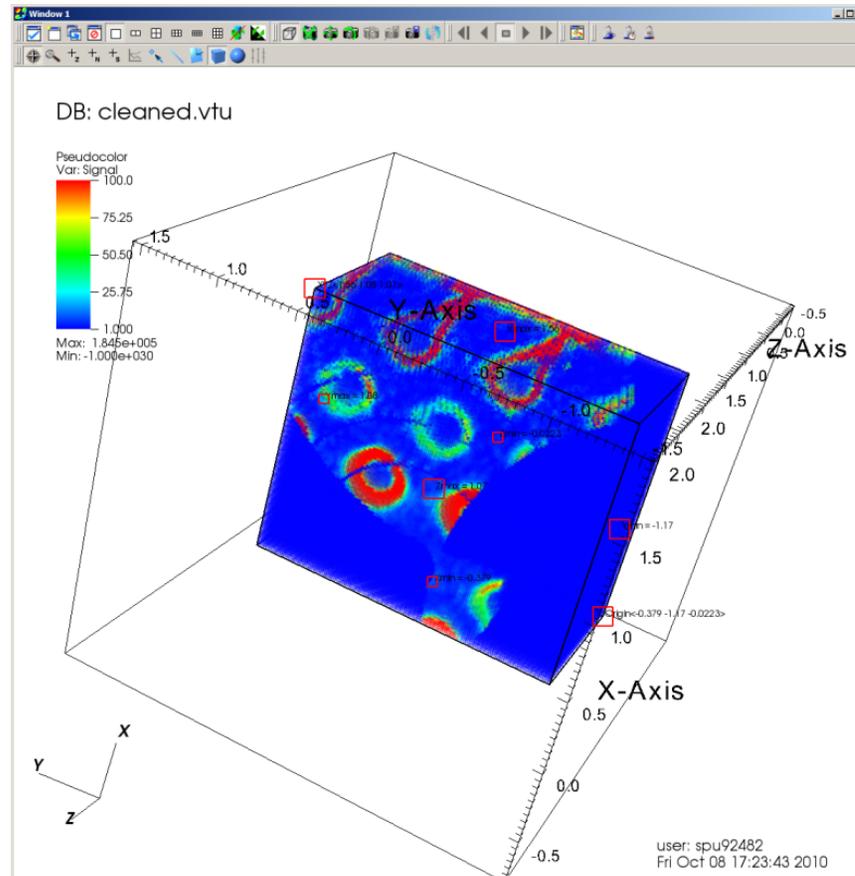
Mantid: Instrument and technique independent Data Reduction and Analysis.

- Overlap in end-goals
- Overlap in common functionality

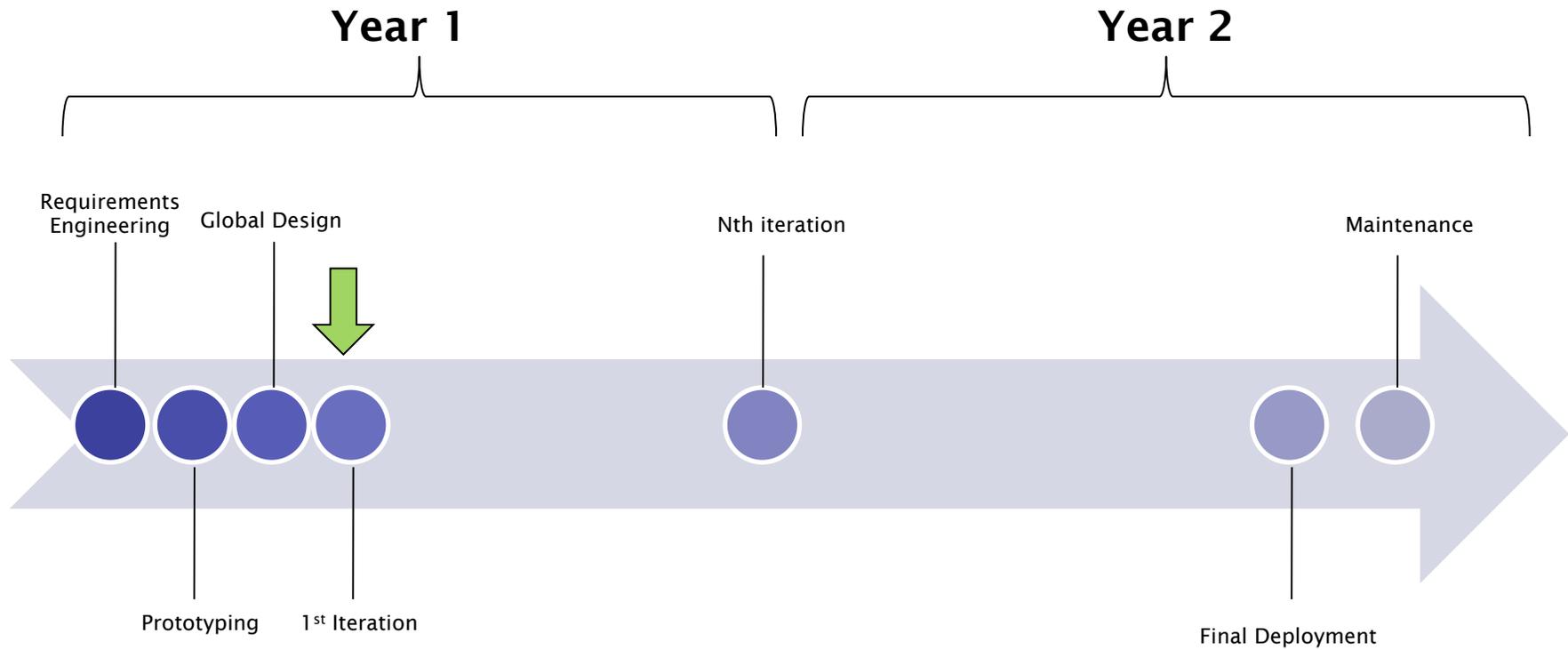


Design Choice: VisIT

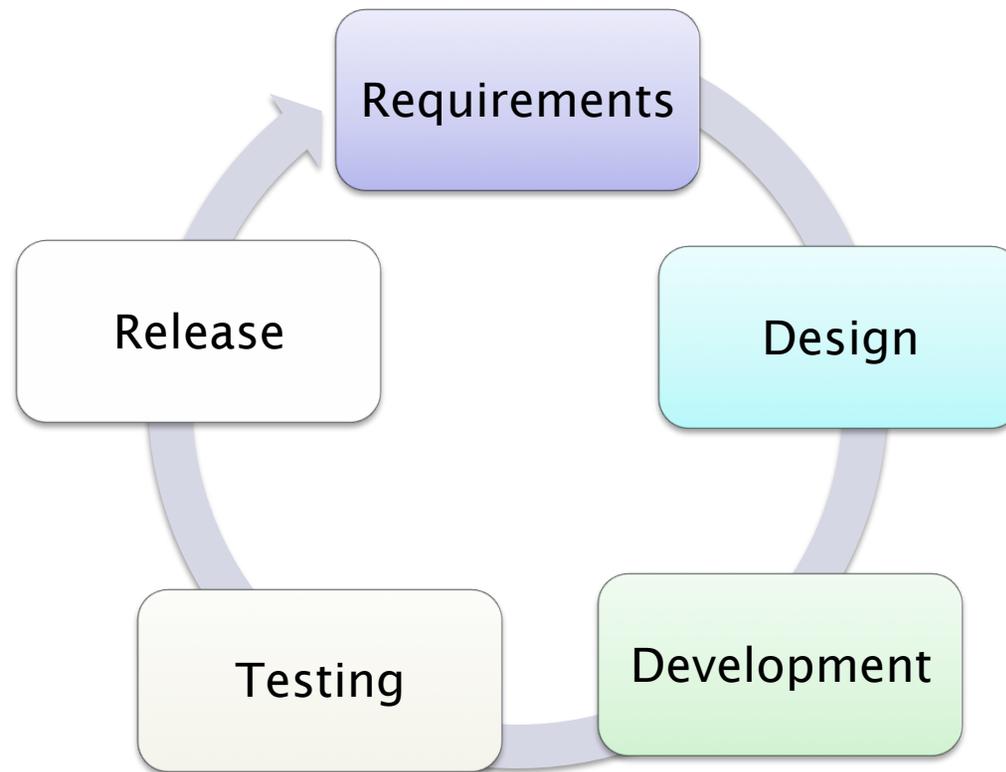
- Designed for scalable visualisation out-of-box
- Pluggable mechanism for bespoke interaction with processing pipeline
- Highly portable
- Mature
- Open Source



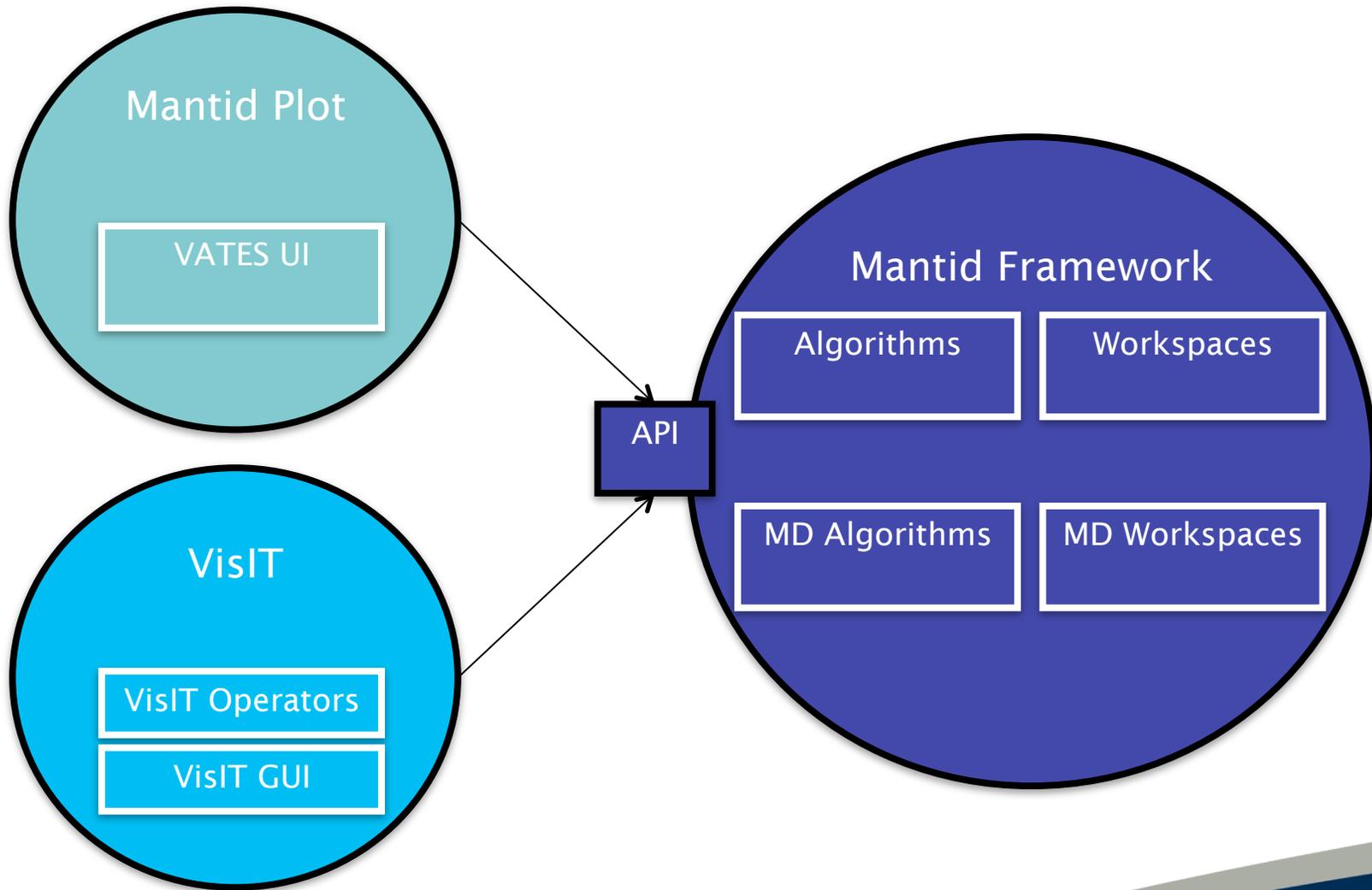
Project Plan



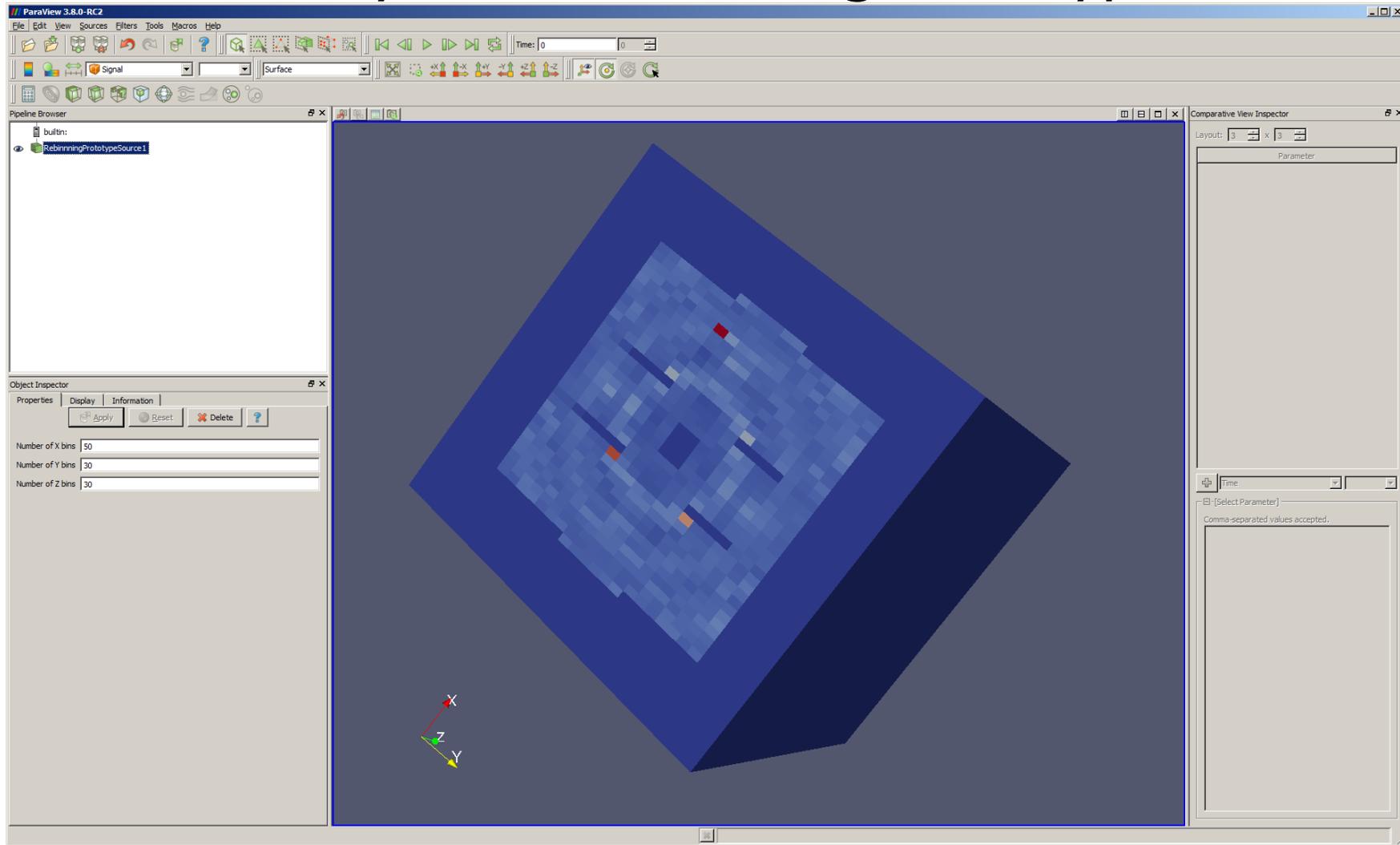
Evolutionary Development Process



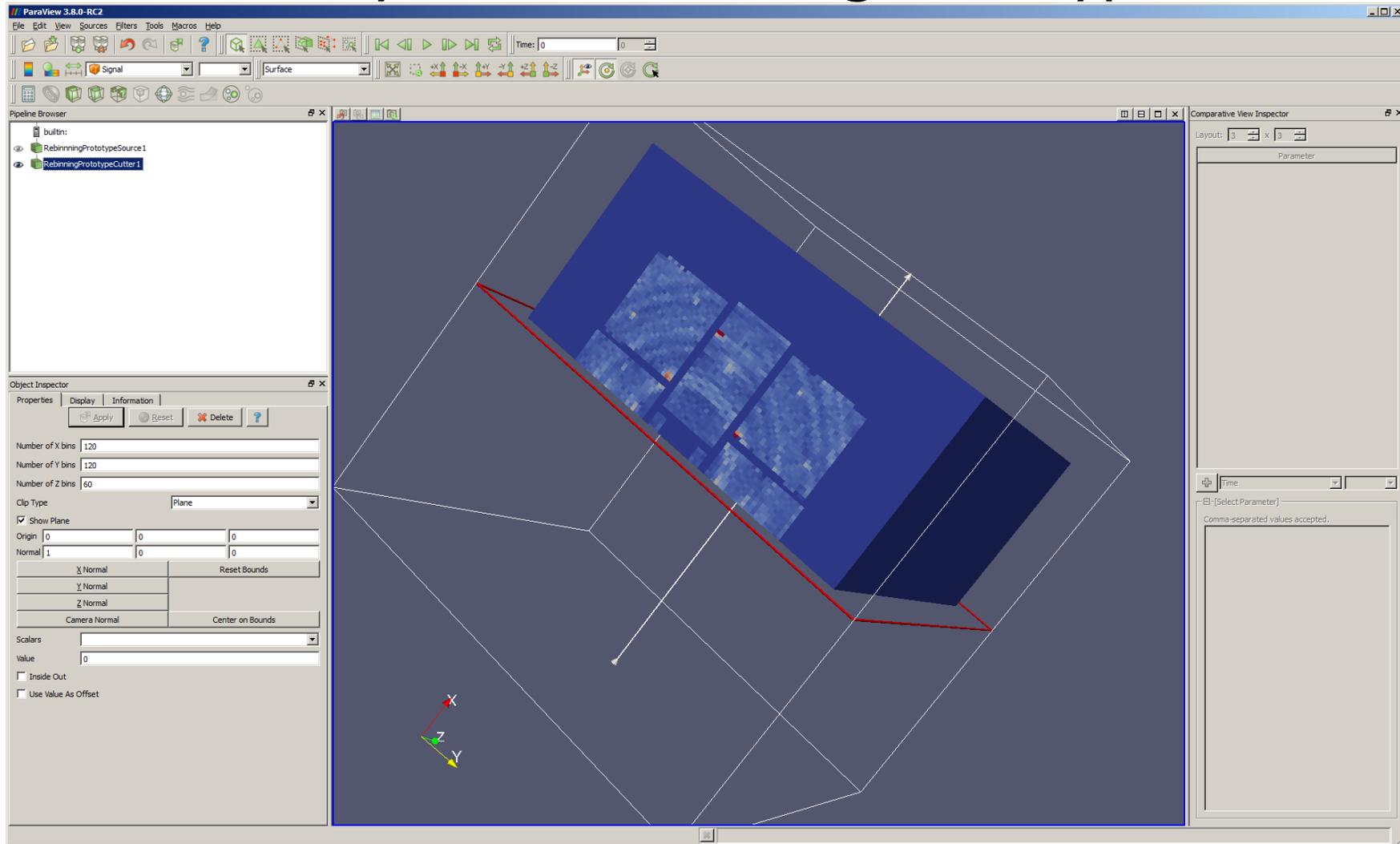
Architectural Design - Overview



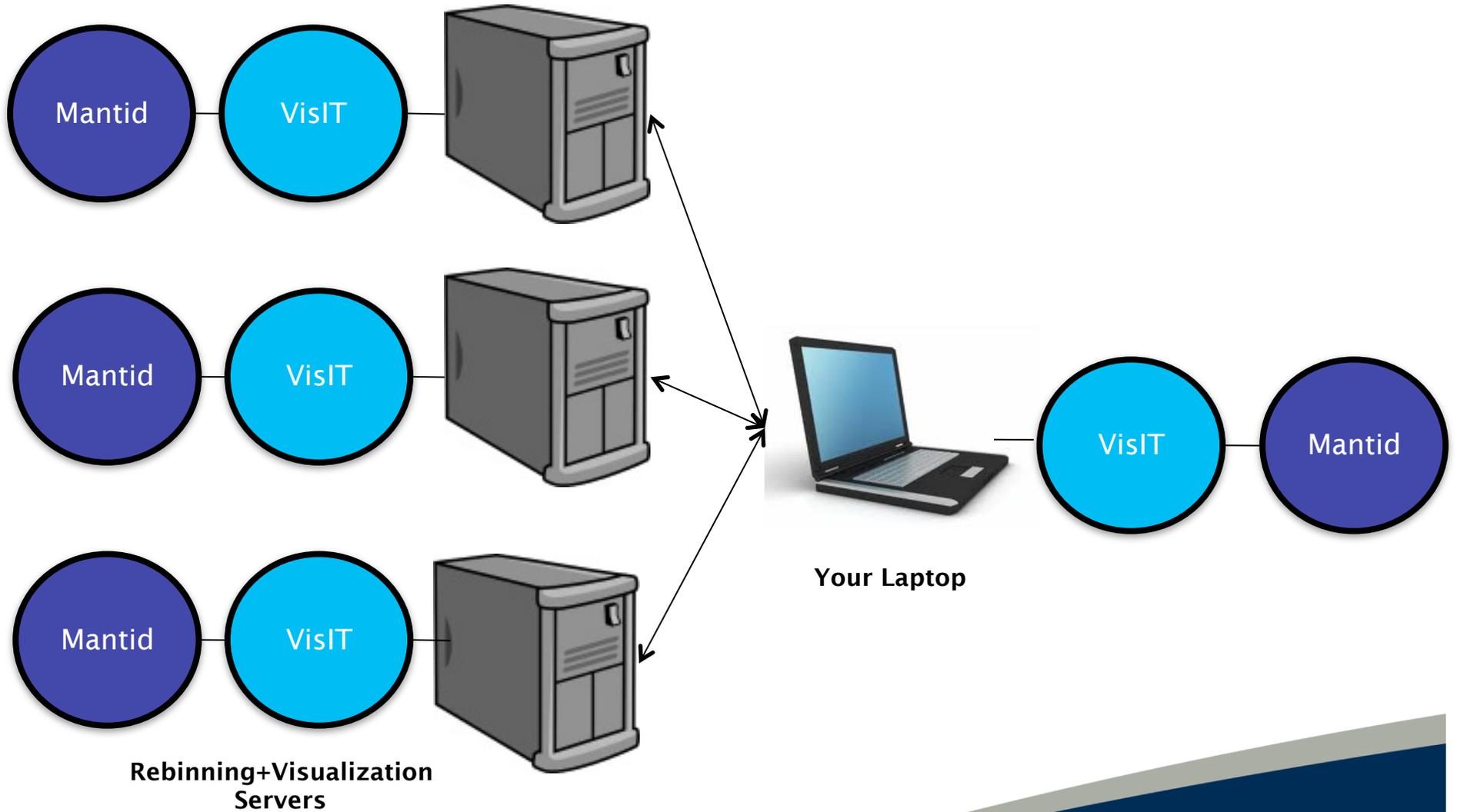
Dynamic Rebinning Prototypes



Dynamic Rebinning Prototypes



Visualisation Cluster



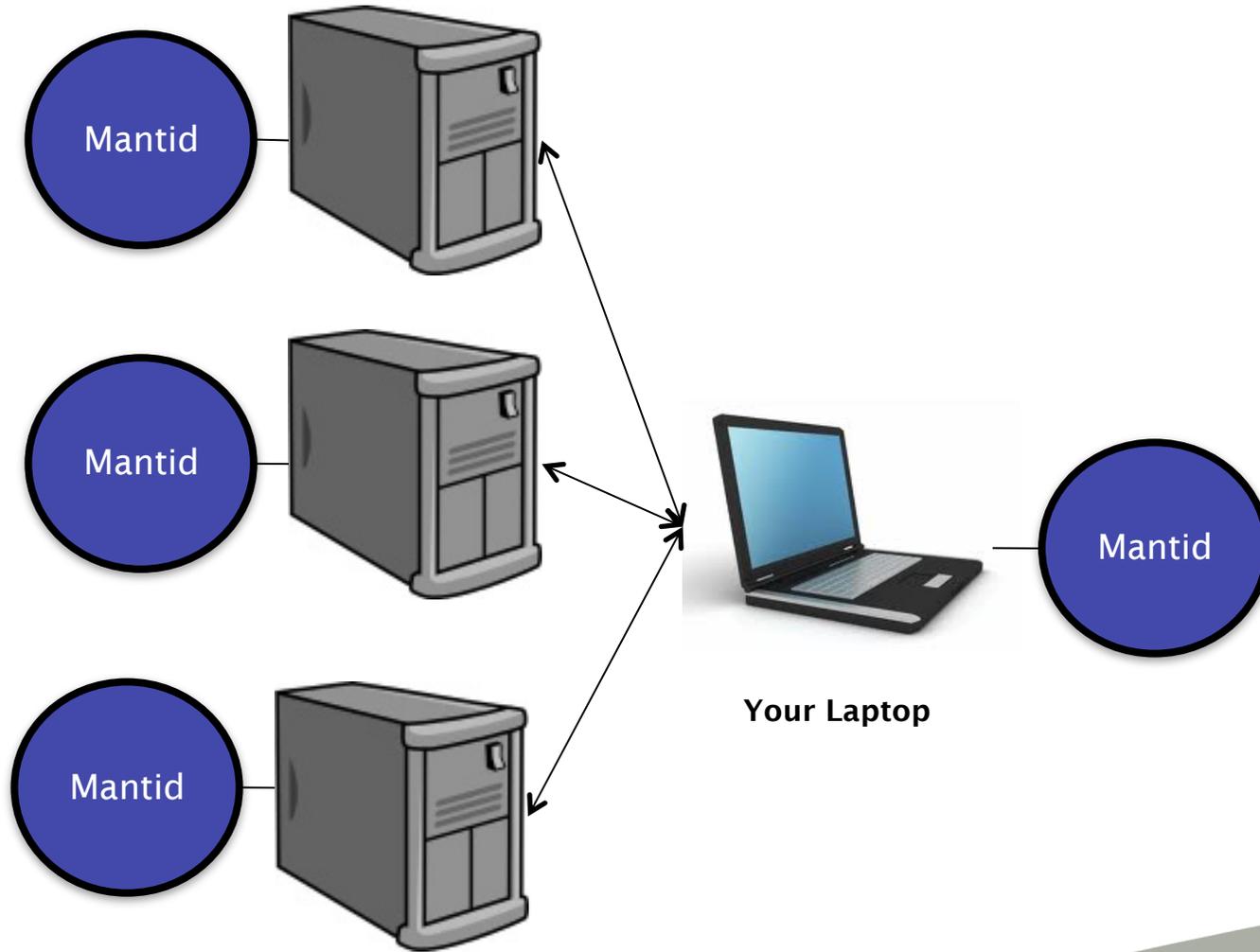
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Analysis

- Visualisation specifies cuts
 - Multi dimensional cut operations expressed in a hierarchical format
- Tobyfit
 - Simulate spectrum from model sqw model
 - Generate resolution function according to user defined sqw model
 - Optimise predicted scattering results to experimental scattering results by modifying model parameters
- Third Party Packages
 - McPhase, CASTEP, GULP
 - Optimise parameters in 3rd party model

Analysis Cluster



Further Information

- Project Web Page
 - www.mantidproject.org
- User Requirements Document
 - http://svn.mantidproject.org/mantid/trunk/Documents/Requirements/Visualisation_and_Analysis/Visualisation_and_Analysis_URD.doc
- Architectural Design Document
 - http://svn.mantidproject.org/mantid/trunk/Documents/Design/VATES/VA_ADD.doc

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Application History

