VATES Adoption Acceleration Project

# Summary

VATES aims to provide easy-to-use, generic multidimensional data visualisation and resolution broadened model fitting within MANTID. However its adoption is not widespread because of a combination of the user experience not meeting expectations, major features that are not yet implemented, and the lack of focussed resources from within the MANTID project to provide the required functionality. The result is that non-MANTID applications (particularly HORACE and TOBYFIT within the ISIS Excitations Group) continue to be developed at the cost of considerable scientist time. (See Appendix: Background to VATES for more information.)

This project proposes a two part focussed acceleration of improvements to VATES to allow widespread adoption in the facility. Part (1) would provide improve the visualisation and manipulation of multidimensional data, and requires 6 month’s work from two additional developers, with deliverables for June 2015. Part (2) would develop the current tentative prototype for resolution broadened fitting, and requires 12 months effort from one additional developer. This part can start before the completion of Part 1, but should be staggered because of the need for significant close input from instrument scientists.

# Visualisation: Objectives and Deliverables

## Objectives

To accelerate the improvements to scripting, usability, graphical user interfaces and performance required to allow widespread adoption by the facility instrument scientists by the 2nd of June 2015.

## Deliverables

* A simple functional scripting language for graphing and manipulation as agreed with representatives of the instrument scientists.
* Improvements to the user experience of the VSI and other visualisation tools for use with the underlying multi-dimensional workspace (the MD data structure) to make it easier to visualise the data. These improvements will be defined by representatives of the instrument scientists.
* Changes to the core MD data structures to support all of these changes and to accommodate the enhanced normalisation work of Andre Savici for event mode data.
* Improvements to the performance of MD file generation (sqw) to support the needs of contemporary experiments.
* Instrument staff training, support and user documentation.

## Resources

|  |  |
| --- | --- |
| Dev Team |  |
| UK | **US** |
| Owen 70% (Overview, scripting, sliceviewer) | Michael 50% (VSI & Paraview) |
| Roman 50% (Core changes) | Andre 50% (normalisation) |
| Alex 40% (verification and validation, proxy SME) |  |
| New UI developer 100% (6 Months) |  |
| New Performance developer 100% (6 Months) |  |

|  |  |
| --- | --- |
| Scientists |  |
| UK | **US** |
| Toby Perring / Russell Ewings (10%) | inelastic ??% |
| Pasacal Manuel (10%) | diffraction ??% |
| Winfried Kockelmann? (10%) |  |

# Quantification: resolution broadened model fitting

## Objectives

To enable user-supplied models for the scattering written in Python or c/c++ to be simulated or least-squares fitted to data in an arbitrary set of MD workspaces, with account of interchangeable models for the instrument resolution. The improvement programme should be completed by 20 December 2015.

## Deliverables

* Implementation and job management on multicore commodity workstations, large scale computing (SCARF)
* A GUI interface as agreed with representatives of the instrument scientists.
* Scripting syntax fully integrated and consistent with that developed for visualisation.
* The current TOBYFIT resolution function for MAPS and MARI will be implemented, together with generalisation for MERLIN and LET. This will also cover the SNS chopper instruments.
* OSIRIS resolution function?
* Library of basic scattering models, including simple spin waves and requiring lookup tables.
* Instrument staff training, support and user documentation

## Resources

|  |  |
| --- | --- |
| Dev Team |  |
| UK | **US** |
| Martyn 50% (resolution convolution) | Michael 20% (Back end implementation for SNS) |
| Roman 20% (Core & model fitting support) | Andre 20% (verification and validation) |
| Alex 40% (verification and validation, proxy SME, models) | Jose ?% (possible alternative resolution convolution models) |
| New GUI and back end developer 100% (12 Months) |  |

|  |  |
| --- | --- |
| Scientists |  |
| UK | **US** |
| Toby Perring / Russell Ewings (10%) | Direct inelastic 10% |
| Sanghanitra? (10%) | Indirect ineslatic 10% |

## Optional extension

CUDA and other graphics card acceleration approaches hold the possibility to accelerate the quantification and model fitting of multi dimensional data. However while on paper the likelihood of significant gains is high, this cannot be guaranteed until proven and measured using a prototype.

This most sensible approach here would be to allocate 1 month of Martyn Gigg’s time to prototype and measure the improvements that can be made by graphics card processing, if successful and the improvement was agreed to be worthwhile this would be followed by a further 3 months to implement the improvement for general usage.

# Organisation

The improvement project would take place in two parts. Initially, the specification would be detailed using representatives from both facilities. Monthly progress meetings would take place for the first 3 months. Afterwards, with a working implementation, bi-weekly iterative meetings would take place. Specific example datasets would be selected as characteristic of the types of models to be fitted. Code changes will be made within the Mantid codebase, with involved scientists using the nightly builds to review progress.

# Appendix: Background to VATES

VATES is a major sub-project within MANTID designed to provide (1) visualisation tools for multidimensional data – be that multi-dataset single crystal inelastic data (‘Horace’ data) or single crystal diffraction data, and (2) a generic resolution convolution and parameterised model fitting engine. The visualisation part is generic to all neutron instrumentation – the multiple dimensions could be (vector) momentum, temperature, energy, magnetic field, shear rate etc. The resolution and fitting (hereafter called ‘quantification’) was identified at the MANTID Scientific Steering Committee meeting in January 2014 as important not just for the chopper instruments at ISIS, but also those at SNS and also indirect instruments at both facilities.

Major improvements to the user experience and multidimensional data file generation are essential for VATES to be widely adopted. For example, while the HORACE software (T.G.Perring et al.) is widely used for visualisation and analysis of inelastic data at various neutron facilities (Ewings and Perring will be running training courses at ISIS and SNS in the next few months to satisfy demand from users at ISIS and SNS), adoption of VATES for inelastic data visualisation is patchy because the user experience needs considerable improvement. Furthermore, both VATES and HORACE can take several hours to prepare the underlying multi-dimensional datasets from the latest experiments, a serious bottleneck whichever route is followed. These problems apply equally to diffraction data.

Regarding Part (2) – ‘quantification’ – a prototype implementation is in place but is incompletely tested, and has not been used in practice because Part (1) is not yet established. It is a long wished-for goal to have ‘Rietveld for inelastic’, to provide equivalent tools to those taken for granted in diffraction data analysis. From computerised calculations of linear spin wave theory, through predictions for lattice dynamics or the generalised magnetic susceptibility χ′′(**Q**, ω) from DMFT, to bespoke user models as the theory itself develops alongside the experiments, a true quantitative test against data requires proper account of the instrument resolution. A major step forward would be to implement a framework for routine substitution of user models for the scattering and instrument resolution functions. The goal of Part (2) is to provide this for simple user models, with a view to a later (and more ambitious) project as part of a wider Scientific Computing Strategy to interface with sophisticated 3rd party models once the framework is in place.

# Visualization Plan

