Previous research track record

Professor Toby Perring *(TGP)* is an STFC Fellow and Honorary Professor of Physics at UCL, with scientific interests in strongly correlated electron materials, whose properties arise from the subtle interplay of the spin, charge, orbital and lattice degrees of freedom. His particular interest is colossal magnetoresistive manganites; his earliest works[1,2] stand as two of the ten most highly cited papers from the chopper spectrometers at ISIS. He is also part of long-standing collaborations studying the spin excitations in high-transition temperature superconductors[3,4]. Other interests include quantum fluctuations in one[5] and two[6] dimensional model magnets, spin dynamics in elemental ferromagnets and the classic weak itinerant ferromagnet MnSi, and most recently iron pnictide superconductors[7].

Most of TGP's scientific work has been carried out at ISIS. He performed the pioneering experiments which demonstrated that inelastic neutron scattering from single crystals could be performed highly effectively at pulsed sources, and was instrumental in establishing it as a routine probe of magnetic dynamics. He was project scientist responsible for the scientific and technical specification and commissioning of the MAPS spectrometer, which has formed the template for the design of instruments at ISIS, SNS (USA) and J-PARC (Japan). He wrote the TOBYFIT program to account for instrument resolution in model fitting to data from chopper spectrometers, which has been recently enhanced to exploit the computing resources of eScience and the Grid. Most recently, he has been developing methods and software to fully map the full four-dimensional wave-vector and energy dependence of magnetic and structural dynamics in single crystals. He is also a Project Sponsor of the MANTID data analysis package being developed at ISIS.

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Professor Laurent C. Chapon *(LCC)* has been a scientist at the ISIS facility since 2002, where he is now head of the crystallography group. LCC is also Visiting Professor in the CRISMAT Laboratory in Caen (France). LCC's main interest is in the field of magnetism of complex transition metal oxides[1,2] and most recently on "type-II" multiferroics[3-7]. LCC obtained his PhD in Materials Science at the University of Montpellier (France), in the field of thermoelectrics, before joining the Materials Science Division at Argonne National Laboratory (USA) as a post-doc in molecular magnetism, then the Hahn-Meitner Institut (Berlin, Germany). LCC was awarded the IOP Physical Crystallography Prize 2008 for outstanding contributions to the development of magnetic diffraction methodology and instrumentation. LCC is the project scientist for the WISH diffractometer currently under commissioning (TS-2, ISIS). LCC has a strong interest in scientific computing. He is a continuous contributor to the Rietveld package FullProf and the lead scientist for the data analysis package Mandid, currently being developed at ISIS.

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Professor Andrew Boothroyd *(ATB)* has interests in crystalline materials in which magnetic, electronic and structural interactions create exotic ground states. He has published over 130 papers on condensed matter, including polymers, superconductivity, correlated electron phenomena, magnetism and crystal growth, with emphasis on the use of neutron and X-ray scattering techniques. Recent highlights include the complete mapping of spin excitation spectra in charge-ordered materials,[1] the discovery of one-dimensional spin correlations among the charge carriers in a stripe-ordered phase,[2] direct observation of orbital order by soft x-ray resonant magnetic scattering,[3] the first observations[4,5] of spin excitations in triangular-lattice Na_xCoO_2 related to a novel unconventional superconductor, an unambiguous determination of the magnetic structure in a stripe-ordered cuprate superconductor,[6] and the first measurements of high-energy spin fluctuations in the parent phase of a new iron pnictide superconductor.[7] Work on complex oxides is supported by EPSRC grants EP/F001266/1 and EP/F020694/, and a project on multiferroic phenomena is supported by EPSRC grant EP/D053560/1.

ATB has strong links with neutron and X-ray scattering Facilities. In the mid-1990s he led an SERC-funded project to upgrade the neutron polarization on the CRISP reflectometer at ISIS. He was co-investigator on a series of EPSRC grants to build and commission the MAPS neutron spectrometer at ISIS and he was lead external applicant on a successful bid to fund the LET spectrometer at ISIS TS2. He has served many times on scheduling committees for the ISIS & ILL facilities. He is a member of the SAC for the UK CRG XMaS at the ESRF, and is Chairman of the SAC for the Swiss neutron source SINQ at the Paul Scherrer Institute.

[1] H. Woo et al., *Phys. Rev. B* **72**, 064437 (2005). [2] A.T. Boothroyd et al., *Phys. Rev. Lett.* **91** 257201 (2003). [3] S.B. Wilkins et al., *Phys. Rev. Lett.* **91**, 167205 (2003). [4] A.T. Boothroyd et al., *Phys. Rev. Lett.* **92**, 197201 (2004). [5] L.M. Helme et al., *Phys. Rev. Lett.* **94**,157206 (2005). [6] N.B. Christensen et al., *Phys. Rev. Lett.* **98**, 197003 (2007). [7] R.A. Ewings et al., *Phys. Rev. B* **78**, 220501(R) (2008).

Professor Martin Dove *(MTD)* has been Professor of Computational Mineral Physics at the University of Cambridge since 2003, and works in the two areas of neutron scattering and computer modelling. In the area of neutron scattering, he was one of the PI's that led the development of the MERLIN spectrometer at ISIS, and other strategic developments he has led include the analysis of total scattering data to measure structural fluctuations and the development of equipment to measure diffraction at simultaneous high temperatures and pressures. Much of this work has been concerned with studying structural phase transitions and materials with anomalous physical properties. In his computation work he uses a variety of techniques, including large-scale molecular dynamics, *ab initio* models and lattice dynamics, with applications to phase transitions, disordered materials, materials with anomalous physical properties, radiation damage and adsorption of pollutants on mineral surfaces. For the past six years MTD has led large eScience grants with focus on the intersection of grid computing, data and metadata management, and collaborative tools, and a similar focus on approaches to data representation. MTD is an active software developer, writing programs for the analysis of neutron scattering data and in support of computational methods.

[1] A.L. Goodwin et al., *Phys. Rev. Lett.* **93**, 075502 (2004). [2] K. Trachenko et al., *Phys. Rev. Lett.* **93**, 135502 (2004). [3] M.G. Tucker et al., *Phys. Rev. Lett.* **95**, 255501 (2005). [4] K. Trachenko et al., *Phys. Rev. Lett.* **98**, 135502 (2007). [5] A.L. Goodwin et al., *Science* **319**, 794 (2008). [6] R.P. Bruin et al.,*Concurrency and Computation: Practice and Experience* **20**, 1329–1340 (2008).

Professor Des McMorrow *(DFM)* took up a chair in the London Centre for Nanotechnology and Department of Physics and Astronomy at UCL in January 2004. Prior to this he had worked in Denmark for 10 years holding various senior posts including head of the Neutron and X-ray Group within the Physics Department at Risø National Laboratory, Director of the Danish Centre for Neutron Scattering and Senior Research Scientist. During this period he was also External Lecturer at the Niels Bohr Institute in Copenhagen.

The main theme uniting DFM's research interests is the study of different aspects of magnetism. He was awarded a Royal Society Wolfson Merit Award (2004) and won the Allan Mackintosh Prize, Niels Bohr Institute, University of Copenhagen (2003). DFM has made significant contributions to several fields, including high-temperature superconductivity, low-dimensional quantum magnetism, thin-films and superlattices, and rare-earth magnetism.

The main tools used in his research have been neutron and x-ray scattering techniques, which he has also played a significant role in developing. He has published over 150 papers, and has co-authored with Jens Als-Nielsen a major new textbook on X-ray physics "Elements of Modern X-ray Physics" (John Wiley and Sons), which has become established as the standard text in the field.

DFM has served on many committees and review panels in various countries, and is presently Secretary to the IUPAP Magnetism Commission (C9), and is a Fellow of the Institute of Physics. He is currently Deputy Director of the London Centre for Nanotechnology.

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Visualisation and quantitative analysis of massive neutron scattering data volumes

1. Background

Increasingly, the materials of interest in condensed matter physics and chemistry are characterised by the correlated interaction of the charge, lattice, spin and orbital degrees of freedom, which can lead to extreme sensitivity of physical properties to small changes in control parameters such as temperature, magnetic or electric fields. Novel properties include multiferroic behaviour, colossal magnetoresistance (CMR), metal-insulator transitions, high temperature superconductivity, and qualitatively new behaviour such as quantum criticality and topologically protected order in frustrated magnetic systems. In consequence, the investigation of strongly correlated materials is, and will continue to be, a dominant theme in solid state physics, chemistry and materials research, because of both the fundamental physics interest and for the host of functional properties.

The chopper spectrometers at ISIS have an outstanding scientific record, with high profile publications in, for example, high-temperature superconductivity [1], quantum magnetism [2], CMR pervoskites [3] and the new iron pnictide superconductors [4], in Nature, Science and Physical Review Letters. This track-record rests on the ability of the position sensitive detector arrays of the instruments to make unprecedented maps of the wavevector, $\boldsymbol{Q}$, and frequency, ω, dependency of the dynamics. The diffractometers at ISIS have an equivalently enviable reputation, with high profile publications not just in the fields above but also, for example, multiferroics [5], orbital degeneracy and charge ordering [6], frustrated magnetism [7] and hydrogen order in ice [8] and nanostructures [9].

To fully understand the materials of interest to solid state physics, chemistry and materials research, complete mapping of the four dimensional $\boldsymbol{Q}$ and ω dependency of the lattice and magnetic dynamics will increasingly be needed, as will mapping in $\boldsymbol{Q}$ of the static atomic or magnetic structure as a function of temperature, applied magnetic field, pressure or electric field. The latest generation of instruments at ISIS have this capability, with highly pixellated area detectors of 3 steradians and neutron guides that increase fluxes by an order of magnitude or more.

Scientific areas where the latest instruments can be expected to make an immediate impact include:

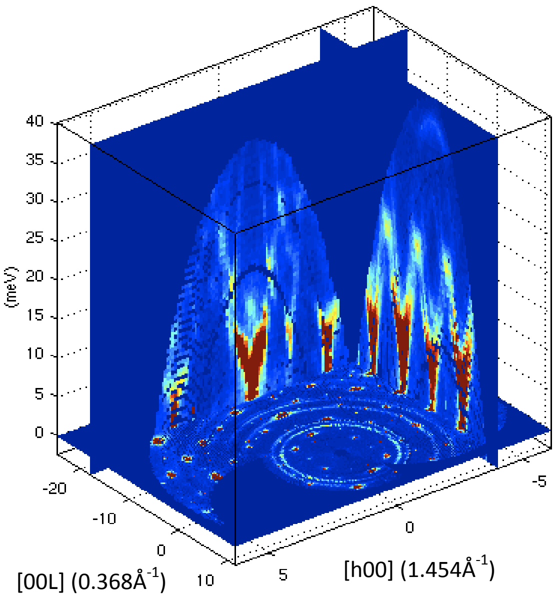
Structure of complex multifunctional materials. Materials such as type-II multiferroics and magnetoelectrics show the most complex magnetic structures, with non-collinear spin arrangements and long-wavelength modulations, often with harmonics or multi-**k** structures. Determination of the detailed spin structure, symmetry and underlying coupling mechanisms can only be tackled through analysis of massive data sets, including nuclear scattering as the onset of magnetic ordering is coupled to the lattice. WISH will have a significant impact in this area.

Quantum fluctuations and criticality in model magnets. The desire to understand the ways in which new states of matter emerge from strongly interacting many-body quantum systems is a theme uniting disparate areas of science. Examples include Bose-Einstein condensates formed in various systems, including magnons in low-dimensional quantum magnets, the anomalous electron fluid in the normal and superconducting states of the cuprates, and the fractional quantum hall effect in low-dimensional semiconductors, to name but a few. Central to the success of this endeavour is the ability to control quantum fluctuations in the vicinity of critical points at which these states form. The latest spectrometers at ISIS, especially LET and MERLIN, offer an unprecedented opportunity to address key challenges in the field of quantum criticality by performing neutron scattering experiments on model quantum magnets as a function of applied field, pressure, chemical composition, etc. Future opportunities include exploiting the excellent high-resolution of LET to perform lineshape measurements of the fluctuations in the vicinity of the quantum phase transition, studying the formation of a Bose glass which is predicted to occur upon doping, etc. Essential to realising these opportunities are the development of new software to handle the complex data sets, and the ability to quantitatively model the data by including resolution effects.

Frustrated magnetic systems. Frustration can arise from competing exchange interactions or the topology of the lattice, but in either case the result can be unexpected new ground states and strong fluctuations at temperatures well below the exchange energy. Famous examples include the triangular, Kagome and pyrochlore lattices, which can variously show spin liquid, spin glass or spin ice states, and it can be expected that other frustrating topologies will result in equally interesting and surprising magnetic ground states and dynamics. Determining the nature of the magnetic correlations is key to unravelling the physics of frustrated magnets and they are contained in the 3D diffuse part of both the elastic and inelastic magnetic scattering. The unparalleled detector coverage of WISH, LET and MERLIN will in combination make a significant impact in the field.

Lattice dynamics in functional materials. In many of the functional materials of current interest the interesting physical properties are determined by, or strongly involve, the lattice vibrations. This includes, for example, colossal negative or positive thermal expansion (TE) materials, ferroelectrics, multiferroics, and new thermoelectric materials (e.g. skutterudites and Ruddlesden–Popper oxides). A full understanding of these materials requires knowledge of the relevant lattice dynamics. For example, negative TE in the famous materials ZrW_2O_8 and $Ag_3Co(CN)_6$ is due to strong fluctuations of under-constrained rigid structural units, yet the nature of the eigenmodes responsible for this behaviour is not yet understood. MERLIN and LET will enable complete mapping of the low energy librational modes of the structural units, and in conjunction with *ab initio* and potential model calculations as baselines will enable the eigenmodes responsible for the functional properties to be identified.

Interplay between superconductivity and spin- or charge-density-wave fluctuations in super-conductors. Prediction of the two most important quantities characterising superconductivity — the transition temperature and energy gap — in the BCS framework poses a daunting challenge to first principles calculations. Recent inelastic spin-echo results for phonon lifetime and dispersion anomalies indicate that electron correlation effects beyond the local density approximation are needed to account for the observations. Suggestions include dynamic enhancement of Fermi-surface nesting via spin- or charge-density-wave fluctuations. To investigate these scenarios will require comprehensive mapping of phonon anomalies with high resolution, and comparison with DFT calculations as the benchmark against which to assess anomalies. LET is ideally suited for these studies.



Three dimensional subset of phonon data in calcite, gathered on MERLIN. This subset corresponds to approximately 2% of the full dataset.

However, the opportunities offered by the new instruments pose a severe data analysis challenge. With up to 300,000 detector elements, each resolving the scattered neutron wavelengths into 2000–4000 channels, they intrinsically collect data in three dimensions in parallel in 10^8–10^9 pixels. Their high fluxes permit crystal orientation or parameters such as temperature to be altered every few minutes (diffraction) or up to 0.25–0.5hr (spectroscopy), so that the combined data sets completely map the statics or dynamics in hours to 2–3 days. Already at ISIS, the MERLIN and MAPS spectrometers have started to collect such datasets with proven success (see Figure).

This proposal aims to address the software challenge of exploring and quantitatively analysing the massive datasets that will soon be collected routinely across several of the new ISIS instruments. These include the LET spectrometer, WISH diffractometer, phase-2 Target Station 2 instruments such as LMX, as well as the existing instruments: MAPS, MERLIN, SXD, and GEM.

2. Programme and Methodology

2.1 Overall aims and objectives

The present proposal is to create two major software applications for users of ISIS, for use both during experiments and at their home institutions:

(1) **A visualisation application** for routine, real time exploration of diffraction and inelastic data;

(2) **An analysis application** to optimise parameters in experimenter-supplied models of inelastic data, folding in the momentum- and frequency-dependent instrument resolution function.

Together with an interface to allow experimenter-supplied models to be accessed, and a library of standard simple models (e.g. spin waves and spinons in previously studied systems), three computationally intense generic modelling tools will be implemented within the analysis application:

(i) The General Utility Lattice Program (GULP, https://www.ivec.org/gulp/), which performs lattice dynamical simulations from atomic potential functions or fitted force constants;
(ii) Calculation of magnetic excitations and spectral weight for arbitrary spin and orbital Hamiltonians, using McPhase (http://www.mcphase.de/);
(iii) *ab initio* lattice dynamics calculations using CASTEP (http://www.castep.org/), which implements density functional theory (DFT) using plane wave basis sets.

These model codes will collectively cover the needs of a broad selection of the anticipated programme on the chopper spectrometers. The investigators and their groups have experience of all three of these codes; furthermore, one of the authors of McPhase works in the group of one of the co-Is (ATB), and one of the developers of CASTEP is based at ISIS.

2.2 Methodology

Two programmers are being sought to write the applications, and a PDRA to conduct a science programme that requires the applications. The PDRA will work with the analysis application programmer to interface the application to GULP, McPhase and CASTEP. The PDRA's science will focus the whole project on delivering effective and practical applications for ISIS users.

The applications will be built on top of the MANTID data analysis framework that is being written at ISIS (www.mantidproject.org). It has professional project management and core programming effort supplied by Tessella (http://www.tessella.com/), a specialist scientific computing applications developer and consultancy. Further dedicated effort from two ISIS computing staff is devoted to MANTID, amounting to approximately 6 FTE in total. ISIS has committed to fund MANTID as part of the TS-2 project and to support it for the whole of ISIS. MANTID will provide the underlying data access and management, basic manipulation (units changing, rebinning, integration etc.) and display, and full virtual instrument descriptions. The architecture has been designed to enable user supplied algorithms to be integrated into the framework. MANTID will free the programmers to concentrate on the implementation of the visualisation and analysis applications.

2.2.1 Visualisation application

An essential requirement is that users of the instruments can explore their data with real-time response, to enable them to use their own experience as the 'expert system' to identify the important static or dynamic features in their data. This is particularly the case in complex systems where the interesting pockets in $(\boldsymbol{Q},\omega)$- or $(\boldsymbol{Q},T,H,..)$-space may not *a priori* be known. Established applications at ISIS (MSLICE on the spectrometers, SXD2001 on the diffractometers), will not scale to handle the combined datasets, which will have as many as 10^{10}–10^{11} pixels, in four or more dimensions[1]. A professionally written visualisation application that will operate on multiprocessor systems, both dedicated single machines or distributed clusters, will be written. It will be available within ISIS for use during experiments, and for users to remotely access from their home institutions. It will be distributable to run at users' home institutions without requiring commercial software. Because the underlying structure and manipulations of the data are so similar, as are the requirements for GUI-driven navigation through the data, a single application with minor tailoring for diffraction or inelastic use can be written, as well as for polycrystalline and non-crystalline data.

2.2.2 Quantitative analysis of inelastic data

The track-record of the chopper spectrometers at ISIS rests not just on the their ability to map volumes of scattering in $(\mathbf{Q},\omega)$-space, but also software to perform resolution corrected least-squares fitting of models to the data (TOBYFIT *ISIS*). Just like the current visualisation software, it will not scale to handle the combined datasets, nor does its architecture allow integration of models other than simple user supplied algorithms.

The analysis application will optimise the parameters in experimenter-supplied models of the magnetic or lattice dynamics, fully accounting for the spectrometer resolution function in least-squares fitting to an arbitrary selection of sub-sections of the new massive combined data sets, generalising the formalism of the existing TOBYFIT. The application will be designed so that simple models and ones that are computationally expensive to evaluate will be supported across distributed computing environments. In particular, the selected third-party modelling software packages will be interfaced to the application as part of the development, which will ensure that the design is well-suited for integration with other third party software.

The data exploration/quantitative analysis process is iterative, with models tested on critical portions of the data until a global understanding of the data and science is built up. The applications will be designed to work together so that they will form an easy-to-use 'one-stop-shop' for analysis by both infrequent and experienced users of the Facility.

2.2.3 PDRA and science projects

Past experience shows that the development of the best scientific analysis software has been driven by individuals with a keen vested interest in the software for their own science. The PDRA will have two major scientific projects that will require the software, thereby providing the focused imperative for the development of the applications as functioning scientific tools. The two projects

[1] The combined inelastic datasets currently taken on MERLIN already have 2×10^9 pixels. With the increased flux on the LET spectrometer and the fact that it can collect data from several independent incident neutron energies simultaneously when operating in multiple repetition-rate mode, the expectation is that the pixel count with exceed 10^{10}. For inelastic data, the dimensionality is at least the four of $(\mathbf{Q},\omega)$; for diffraction it is the three of $\mathbf{Q}$ and at least one of e.g. temperature, magnetic field.

provisionally identified have been selected from the science areas described earlier: (i) The onset of dynamical critical scattering at the quantum critical points in the model spin ladder $(C_5H_{12}N)_2CuBr_4$ [10], including characterisation across the transition between the Luttinger liquid and the Bose-Einstein Condensate phases; (ii) High resolution mapping of phonon anomalies in the elemental superconductors lead and niobium, to investigate dynamical spin- or charge- density wave effects [11]. These projects have been chosen as they cover the need for surveying ($\mathbf{Q}$,ω)-space using the visualisation application, and in the latter case careful resolution correction with modelling of phonons using DFT.

The PI and co-Is will also couple the developments into some of their existing research projects, e.g. understanding of eigenmodes responsible for negative thermal expansion in ZrW_2O_8 (TGP: DFT and potential models), colossal positive and negative thermal expansion in $Ag_3Co(CN)_6$ (MTD: DFT and potential models), and spin waves in strongly correlated transition metal oxides (ATB and TGP: interface with general calculation of spin wave dispersion and intensities using McPhase).

2.3 Timeliness and novelty

With the step change in the capabilities of the latest instrumentation on both TS-1 and TS-2, a step change in data visualisation and modelling software is both timely and essential.

This is particularly the case for inelastic scattering data analysis. There is a wealth of applications to analyse neutron diffraction and total scattering data, from Reitveldt refinement code for powder data, GSAS and FullProf, to PDFgetX2 and Reverse Monte Carlo applications. Conversely, there is very little software for inelastic data analysis, and that software with a proven track-record is maintained solely as a by-product of the authors' own research programmes. This proposal aims to fill this gap.

ISIS has been the world-leading pulsed neutron source for the past 15 years. It now faces competition from new more powerful spallation sources in the USA and Japan. To defend the competitiveness of ISIS two ingredients are needed: world-leading instrumentation, and the goal of this proposal: world-leading data analysis software.

2.4 Management and programme of work

The PI and co-Is will form a scientific steering committee for the visualisation and analysis projects, which will be managed on a day-to-day basis by the MANTID Project Manager. These projects will operate on a cycle of 6 week development iterations, an established methodology in software engineering projects, and one followed by MANTID. Within the overall project framework, short term objectives will be set at the start of each iteration, and reviewed at the end. Once functioning applications are created, formal latest releases of the applications will be made at the end of each iteration for assessment by the PI and co-Is and their wider research groups, for feedback to go into the planning of the next iteration. When the releases are stable, they will be made available across ISIS for wider assessment.

Every 3 months — i.e. every second iteration meeting — the PI, co-Is and the staff on the project will meet in person together with the MANTID project manager, to review progress and set objectives for the next 3 months. At the interleaving iterations, the university-based co-Is will attend if convenient, or participate by videoconference.

The PDRA will be based at ISIS under the direct supervision of the PI.

Major milestones: *(M6 refers to 'Month 6')*
End of M6: Sign-off design of visualisation and analysis applications following review of proof-of-principle prototypes; PDRA fully trained in single crystal neutron spectroscopy.
End of M12: Beta-release of visualisation and analysis applications; PDRA using them to analyse data from the science projects.
End of M24: Visualisation and analysis applications finished, and used to complete analysis of data from the PDRA's science projects. Applications formally handed over to MANTID project (visualisation) and Excitations Group (analysis).

Programme of work for each staff member:
- *Visualisation programmer:*
(1) M1-M2: Gain understanding of problem, gather requirements.
(2) M3-M4: Investigate open source visualisation software, benchmark performance, determine pros and cons of each option, adopt one.
(3) M5-M6: Proof-of-principle prototype using chosen software tool-kit. Sign-off the design.
(4) M6-M12: Develop first release for both diffraction and spectroscopy.
(5) M12-M18: Expand/refine using feedback from PDRA, PI, co-Is and their groups, use on excitations and diffraction group instruments.
(6) M18-M24: Full deployment across ISIS, further development with priority determined by analysis sub-project and PI/co-I/PDRA.

- *Analysis programmer:*
(1) M1-M2: Gain understanding of problem, gather requirements.
(2) M3-M4: Investigate distributed computing options, use of the Grid/TeraGrid, and the integration with MANTID and visualisation application. Investigate constraints of integration

with CASTEP, McPhase, GULP and generic interface to compute intensive 3rd party software.
(3) M4-M6: Proof-of-principle application prototype. Sign-off the design.
(4) M6-M12: Develop first release with library of simple scattering models.
(5) M12-M24: Integration of 3rd party modelling software: GULP, CASTEP and McPhase. Work day-to-day with PDRA and visualisation programmer to ensure application becomes one-stop-shop for data visualisation and analysis.

- *PDRA:*
(1) M1-M6: Work with PI and one or more co-Is on one existing single crystal neutron spectroscopy project through to manuscript submission, to become thoroughly familiar with the technique and requirements of the software project.
(2) M6-M12: Perform neutron experiments as part of the new science projects. Start analysis using existing programs, and work with programmers to interface 3rd party modelling software and test the development of the prototype applications.
(3) M12-M24: Further analysis and experiments as part of the science projects, using the now beta-release software applications. Work with programmers to ensure they become user-focussed tools. Submission of scientific papers.

Risk management
- Technical risk:
Both applications will need to work on multi-processor systems and distributed computing platforms, in order to handle the vast quantities of data. This represents a significant step in the scale of the project compared to conventional data analysis programs written by scientists. However, the technical risk is minimal for several reasons:

(1) The applications will use the MANTID framework, which has secured funding as part of the TS-2 development. MANTID is already proven: the data reduction software on the ISIS powder diffractometers has been replaced with MANTID based applications, and replacement on the small-angle instruments is underway. Work to replace the data correction code on the chopper spectrometers with MANTID based applications starts in May 2009.

(2) A promising open source graphical toolkit has been identified to provide the components for the visualisation application: http://www.paraview.org/ (Paraview). It has been developed for extremely large data sets using distributed computing resources. It is supported by Los Alamos National Laboratory, Sandia National Laboratory and the U.S. Army Research laboratory, among others.

(3) The PI and the STFC e-Science Centre have written a prototype distributed computing version of TOBYFIT. Its current form will not scale to the massive datasets in this proposal but the essential problems of the resolution function formalism and parallelisation scheme have been addressed.

- Staff risk:
The software projects will be closely integrated with the Mantid project (50% of the visualisation and 25% of the analysis applications will be funded within Mantid). The Mantid team is large enough that redeployment of staff effort will minimise the impact of early departure of either programmer. The short term shortfall in effort on Mantid can be made up through the existing contract with Tessella until a replacement programmer is recruited.

2.5 Future use and maintenance

The visualisation application will be used across the whole of ISIS instrumentation, and will be fully integrated into Mantid. While the major development effort will be focussed on handling multi-Gbyte datasets in four or more dimensions, an essential part of the application is the seamless integration of 3D, 2D and 1D graphics for rapid closer inspection of smaller regions that attract interest. This part of the application development will satisfy the requirements of all ISIS instruments.

By the end of the project, the analysis application will be used by the majority of experiments on the chopper spectrometers. The Excitations Group has just appointed a staff member whose responsibility will include the continued maintenance and development of all of the Group’s software. This will include adapting the analysis application for developments in the 3rd party software (GULP, McPhase, CASTEP) and including other models as prioritised by the PI and the user community.

3. Relevance to Beneficiaries

The immediate beneficiaries will be the users of ISIS, who will be able to rapidly explore the datasets created by the latest generation spectrometers and diffractometers on the two ISIS target stations. The analysis application for spectroscopy will benefit all users of the spectrometers, who will be able to concentrate on quantitative discrimination between models while relying on a robust, maintained and documented application to look after all details of data-handling and instrument resolution.

The ISIS Facility will benefit as the capabilities of the instruments will be exploited to the maximum, resulting in faster publication of results. The software applications will be applicable to other facilities, e.g. ILL, Diamond, Spallation Neutron Source (SNS) in the USA, and J-PARC in Japan.

Studies of the atomic and magnetic structure of materials, and fundamental studies of their dynamics, underpin an understanding of new and functional materials. The science community engaged in the study of novel physical properties in condensed matter and functional materials will benefit, and ultimately that part of the economy that exploits functional materials will benefit.

The developments will be available to the wider community through web-page-based downloads, installation assistance by ISIS, and dissemination by the PI and co-Is in papers and talks.

4. Justification of Resources

4.1 Programming staff and PDRA

Development of the visualisation application requires a dedicated full time programming professional with experience of graphics applications development. The MANTID project will fund 50% of the programmer, because of the recognised benefit for the whole of ISIS.

The analysis application programmer needs to be a dedicated full time computing professional with experience of parallel programming. Development in several areas is needed: generalisation of existing TOBYFIT code to handle massive combined datasets, interfaces to 3rd party modelling code, parallelisation of GULP and seamless job submission, including just-in-time broadcast and compilation of user-supplied models to distributed computing. The ISIS resources used in the prototype development will continue, and will cover 25% of the effort.

Experience shows that a clear scientific focus with the active participation of experienced users is required for software projects to deliver genuinely useful applications. The PDRA will ensure that the software projects will deliver on their goals, and guarantees the full engagement of the PI and co-Is.

The PI will spend 10% of his time supervising the project and the PDRA, the SFTC co-I 5%. The university co-Is will attend 4 meetings per year at ISIS, and advise the PI and PDRA, averaging 1hr per week. Travel costs cover the co-Is attending the meetings, the PDRA visiting the co-Is and attending two international conferences.

4.2 Spend profile

Year 1: 50%. Year 2: 50%

4.3 Impact on operational cost of the facility

Maintenance and development of the visualisation application is already anticipated within the future cost of running MANTID as part of the ISIS Data Analysis and Computing Groups. The analysis application will be maintained using existing staff effort of the ISIS Excitations Group.

5. Fit with STFC's Strategic Direction and other Research Councils

The STFC mission is to promote and support high-quality scientific research by developing and providing facilities and expertise in support of basic strategic and applied research. This proposal is to create software applications that will result in a step change in the exploitation of many of the latest and next generation instruments on the existing and second target stations at ISIS. Instruments typically represent an investment of £5M or more each, and the second target station an investment of £140M. This is a cost-effective proposal to increase the effectiveness of this investment for studies of new materials. Development of innovative software will also be key to the operation of future facilities.

A significant component of several of EPSRC's priority areas, and to a lesser extent research councils such as NERC, depends critically on fundamental research on new materials, whether for energy, sensors, information and communications technologies etc. As well as an understanding of the structural and static magnetic properties, many new materials require an understanding of the atomic and magnetic dynamics, which are quantities that can be probed with the new generation of spectrometers at ISIS. One specific EPSRC Priority Research theme relevant to this proposal is, for example, advanced functional materials for energy, e.g. thermoelectrics and battery materials. The project will also contribute to the Digital Economy (another EPSRC Priority Research Theme) through training of manpower and the development of new computational tools and methods.

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