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### **MMSN Goals and 2005 Strategy and Activity**

The principal focus of the multi-disciplinary ARC Molecular and Materials Structure Network (MMSN) in 2005, has been to develop and establish a basis for primary goal achievements. A central and thematic goal of the MMSN that was introduced with the successful 2003 SRI seed funding application, is the collaborative development of eScience resources for the structural sciences, particularly collaborative access to remote instruments and data, and complementary visualisation and database services. Key areas of interest identified as offering enabling technologies are the emerging Grid and Semantic Web, and Network activity in 2005 has reflected the foundation focus of the MMSN. Planning for 2006 continues this theme, and in addition there will be a broadening of activity with respect to the interests of the molecular and materials structure sciences.

Following the announcement of ARC funding, a MMSN steering committee meeting was held in December 2004 to define an appropriate strategy for 2005. The strategy adopted, and subsequently endorsed at a Network meeting in March 2005, was to appoint management and programmer staff in support of the Network goals, undertake discussions and negotiations to develop a pilot national database service, organise and host meetings and workshops to both inform the community and establish or reinforce national and international linkages, and to undertake collaborative and, where appropriate, coordinated grant applications in support of the Network goals.

As reported below, particularly challenging research endeavours directly enabled by the funding of the Network include the collaborative exploration and development of Web and Grid Services as a basis for secure access to remote instruments and data (monitoring and steering). Collaborative linkages have also been established for the exploration of the potential and application of Semantic Web technologies for the benefit of the structural sciences. Particularly noteworthy are now well established and strong links with the Common Instrument Middleware Architecture (CIMA) group in the US and the UK eScience CombeChem group. The Network meetings and workshops have stimulated national and international collaborations, and made researchers and students more aware and appreciative of the potential and real benefits of eResearch for the structural sciences. In short, the funding of the MMSN has made possible meetings, workshops and collaborative research that would not otherwise have eventuated.

### **Highlights of 2005**

- Organization and hosting of March 2005 International Workshop on Remote Access and Automation, Marysville Victoria (mmsn.net.au). Twenty two presentations from high profile researchers, 17 from leading overseas facilities and institutions, and 70 delegates including 13 students and ECRs. Presentations including robot videos are available from mmsn.net.au. The meeting was attended by representatives of NANO, OPAL and the Australian Synchrotron.
- Presentations at the International Union of Crystallography Congress in Florence in August 2005. A major international meeting with some 3000 delegates.

- Contribution to organization and support for eighth International Conference on Neutron Scattering ICNS2005 in Sydney November 2005 (<http://www.icns2005.org>), with 780 attendees.
- Contribution to organising and support for first IEEE eScience and Grid Computing conference December 2005 Melbourne (<http://www.gridbus.org/escience/>). Some 350 people attended the meeting, which was held in conjunction with the International Conference on Intelligent Sensors, Sensor Networks and Information Processing.
- Organization of Instruments and Sensors on the Grid (ISOG) Workshop held as part of the IEEE eScience and Grid Computing conference. Attended by representatives of NANO, OPAL and the Australian Synchrotron ([mmsn.net.au](http://mmsn.net.au)). Peer reviewed papers of the conference and workshop have been published by the IEEE.
- Contribution to organising and support for the X-ray Absorption Spectroscopy tutorial-workshop held in conjunction with the December 2005 ASRP and Australian Synchrotron Users Workshop. Support was provided for 11 postgraduate students to attend the XAS workshop, and for the participation of expert presenter Dr Matt Newville from GSE-CARS at the Advanced Photon Source in the US.
- Series of workshops for the Grid enabling of OPAL, culminating in APAC project support for development of Grid based management of OPAL data.
- Appointment of Manager and Programmer staff for the Network.
- Negotiations with Cambridge Crystallographic Data Centre and the Inorganic Crystal Structure Database for national network access to these databases.
- Successful ARC eResearch, LIEF and Discovery and GrangeNet applications in support of MMSN goals and interests.
- Support for visits by 23 overseas experts.
- Comprehensive 30 page submission to NCRIS on behalf of the MMSN community, including appended submissions from individual participants. Subsequently the NCRIS committee reported with respect to Characterisation: “Strong support was received in response to the Exposure Draft for all three capability areas ... “.
- Initiation of a remote access network of instruments based on Web Services (in particular the Common Instrument Middleware Architecture) linked into an embryonic global network. A preview is available at <http://156.56.94.164:8080/gridsphere/gridsphere>.

A core goal of the MMSN put forward in the 2004 ARC application is to “Establish remote access for a network of molecular and materials structure determination and analysis instruments, ultimately providing the basis for developing a Grid enabled network linkable to other instrument, data and computation grids; national and international.” As described below, several grant applications in 2005 targeted this goal in particular. Significantly, the DEST funded *Dataset Acquisition, Accessibility, and Annotation e-Research Technology* project (DART), has adopted crystallography as an exemplar application, and synergistic linkages with eResearch and GrangeNet funded MMSN projects have accelerated the establishment of the proposed remote access network. Installations of CIMA remote access middleware have taken place at James Cook University and Sydney University, and further development of the middleware is underway at these sites. Installations at Queensland and Monash University sites are to follow soon. Grid technologies are to be used for data management, and the network of instruments will partner a similar network in the US and similar developments are anticipated for the UK.

### Strategy and Activity Plans for 2006

- Enhanced support, including programmer support, for eResearch initiatives with a continuing focus on Web Services based, and Grid and Semantic Web enhanced, remote access, collaboration and database systems.
- Continued dialogue with APAC.
- Further support for visits by overseas experts.
- International eResearch workshop with a focus on the Australian Synchrotron and OPAL.
- Further support for structural science conferences and workshops.
- Annual MMSN meeting.
- Following discussions and negotiations in 2005, set-up of a pilot national database service based on the CCDC Crystal Structure Database and possibly the ICSD inorganic structure database.
- Introduction to Australia of the UK eBank system for open access to structure data.
- Employment of a second Network programmer.
- Support for students and ECRs to visit participant eResearch and structure science laboratories having capabilities not available at the home institution.
- A national diffraction school-workshop for postgraduate and ECR postdoctoral researchers, following on from the December 2005 X-ray absorption spectroscopy tutorial-workshop. Support for an overseas presenter.
- Build up of the MMSN web site as a community resource. Services would include listing of structure characterisation resources, such as participant laboratories and a listing of relevant eResearch groups and activity, both national and international.
- Outreach through a national high school crystal growing competition, building on the NSW RACI crystal growing competition.
- Continued engagement with NCRIS and eResearch planning processes.

### Details of MMSN Activity in 2005

The inaugural MMSN event, held in March 2005, was a particularly successful and acclaimed workshop exploring the current state of research and implementation of remote access and automation technologies. There were 70 attendees and 22 presenters, with 17 presenters from international institutions and facilities, such as the UK ISIS neutron facility and the SSRL, ALS, APS, Daresbury and ESRF synchrotrons. The cross-disciplinary attendees included representatives of NANO, OPAL, ASRP and the Australian Synchrotron and the structural sciences community. Grid and Web Services methods for data analysis and remote access to major facility and conventional laboratory instruments were presented, as were state of the art robotic systems. Dr David Corney of the UK ATLAS data store provided insight into the UK's large scale data archiving and curation program. The workshop presentation by the Mike Soltis of the Stanford Synchrotron Radiation Laboratory on the SAM robotic system was noteworthy, and SAM has been selected as the robotic system for the protein crystallography beamlines of the Australian synchrotron. Also impressive was the presentation by Toyokazu Akiyama on Grid based remote access to the Ultra High Voltage electron Microscope in Japan. The workshop presentations, including videos of the robotic systems (SAM, CATS, BruNo and ACTOR), are available from the MMSN web site ([mmsn.net.au](http://mmsn.net.au)). The International Union of Crystallography provided a link to the meeting web site, as did the US Telescience Project. The response to the workshop was enthusiastically positive with comments such as “eye opening”, “impressive”, “very informative”, “excellent” from delegates with very varied backgrounds and expertise.

A general Network meeting held immediately after the close of the workshop considered and endorsed strategy options for 2005. The workshop was held in conjunction with the 24th conference for the Society of Crystallographers in Australia and New Zealand, and the network contributed significantly to the organization of this outstanding international meeting.

An overview summary of the Marysville Remote Access and Automation Workshop was presented by Dr Peter Turner to the June 2005 Beamline Advisory Group (BAG) for the Australian Synchrotron, which is comprised of representatives for the individual beamline advisory panels and Australian Synchrotron Project and ASRP representatives. MMSN participant Dr Nick Hauser who heads the computing and electronics group for OPAL, also gave a presentation at the BAG meeting on network and remote access plans for the new reactor.

Subsequently the MMSN organised on-site workshops and Access Grid meetings exploring Grid and Web Services technology options for user access and data management at OPAL. Participants in these meetings included OPAL, MMSN, APAC and GrangeNet representatives, and the leaders of the CIMA project from Indiana University and State University of New York Binghamton (international MMSN participants). As a consequence of these meetings CIMA will be further explored as a longer term Web Services underpinning for remote access to OPAL, and APAC has adopted the Grid enabling of OPAL as a development project. Discussions have also taken place with APAC for the storage of data from conventional MMSN laboratories.

The MMSN contributed to three major international conferences in 2005. Network poster presentations and demonstrations were given at the eScience session of the Software Fayre held as part of the International Union of Crystallography (IUCr) Congress held in Florence in August 2005 and attended by some 3000 delegates. Prof Stephen Hyde demonstrated the EPINET database system for 3D Euclidean crystalline networks, which is to be complemented and extended by the development of the PLEXUS database. There were also demonstrations of CIMA, the ReciprocalNet federated crystallographic laboratory management and data access system, and the CombeChem eBank system for open access to structural data. The eBank system will be installed at the University of Sydney in 2006.

Prof Syd Hall gave an IUCr conference presentation on significant extensions to the functionality of the dictionaries that underpin the machine readable Crystallographic Information File or CIF. The Australian structural sciences community continues to be a pioneer of the development of intelligent domain-specific ontologies, for example through the introduction of the STAR data language (Self-defining Text Archive & Retrieval) and its exemplar application in the CIF. Since its introduction the CIF has become the international standard for structure information storage, analysis, exchange and archiving and is used by all structural databases and journals for validation and deposition. The STAR approach is closely aligned with XML and schema, and thus provides a platform for expanding and developing scientific applications within the Semantic Web. The dictionary extensions described by Hall provide a capability for Semantic Web functionality, and the structural sciences provide an ideal platform from which to explore the potential of the Semantic Web.

The eighth International Conference on Neutron Scattering (ICNS2005) was held in November 2005 in Sydney providing an opportunity to discuss eScience in the context of neutron scattering research, and MMSN information inserts were provided as conference material. Dr Bob McGreevy from ISIS (a world leading neutron source in the UK), for instance, was particularly interested to hear how MMSN is tackling eScience issues. MMSN participant Dr Nick Hauser is the OPAL team leader for computing and electronics and a member of the NeXus International Advisory Committee. NeXus is a flexible data storage format with generable applicability, and

the OPAL team are developing NeXus in an XML basis to extend its flexibility. An MMSN goal is to explore NeXus as a general storage format for 2D detector data for diffraction, tomography and microscopy.

MMSN participants, notably Prof. Raj Buyya, played a leading role in organising the first IEEE sponsored International Conference on eScience and Grid Computing held in Melbourne in December 2005, and which was held in conjunction with the International Conference on Intelligent Sensors, Sensor Networks and Information Processing (ISSNIP 2005). Significant key-note presentations were provided by Prof Ian Foster who heads the development of Globus and is a widely acclaimed leading Grid researcher and developer, and Prof David deRoure who is a pioneering developer of the Semantic Grid. The conference included highlight presentations of relevance to the Network, such as that given by MMSN participant Prof. David Abramson and his student Tim Ho on data distribution and replication. Drs Peter Kelley, Paul Coddington and David Wendelborn provided a presentation on distributed Web Services. Abramson and Buyya presented tutorials on their flagship Grid projects.

The MMSN organised the Instruments and Sensors on the Grid (ISOG) workshop held on the first day of the IEEE conference. In addition to presentations on the use of Grid technologies for remote instrument and data access, David deRoure and then Jeremy Frey gave inspirational presentations on the application of Semantic Web and Grid to instruments and sensors. There were presentations on CIMA, and application the of Grid based remote access to synchrotrons and accelerators. There were 11 presentations with 10 being from international facilities and institutions. Introductory keynote presentations were given by Profs David deRoure and Prof. M. Paliniswami. Representatives from OPAL, NANO and the Australian Synchrotron participated in the workshop, and again the response of delegates was strongly and enthusiastically positive. Dr Roberto Pugliese who gave a presentation on the development of a virtual collaboratory for the Elettra synchrotron in Italy, and Dr Claudio Vuerli and Dr Stephen McGough, who gave presentations on Grid based remote access to major facilities, also visited the Australian Synchrotron to discuss mutual eScience interests. Of note, Pugliese has recently initiated an intriguing project to develop a cost-effective desktop immersive CAVE system for remote facility access and control.

The IEEE conference and ISOG presentation papers were peer reviewed and have been published by the IEEE Computer Society: 'Proceedings First International Conference on e-Science and Grid Computing', Stockinger, H.; Buyya, R.; Perrott, R. Eds., IEEE Computer Society, Los Alamitos, California, 2005.

The IEEE meeting coincided with the ASRP and Australian Synchrotron Users Workshop held at the synchrotron site Dec 5 to 7. The MMSN contributed to the X-ray absorption spectroscopy tutorial workshop held as part of that meeting on December 7. The workshop included presentations and participation by Dr Matt Newville from GSE-CARS at the Advanced Photon Source in the US, and the MMSN supported his participation and provided bursaries for the participation of 11 students (2 from UQ, 3 from ANU, 3 from Curtin, 1 from UNE and 2 from USyd).

### **Research Projects and Proposals in 2005**

In 2005 there were several successful grant applications put forward by MMSN participants, either explicitly as part of the MMSN program or of immediate relevance to MMSN interests and objectives.

Successful under the MMSN banner was an application to the ARCs pilot e-Research SRI program entitled “*Scientific Instruments as ICT Components in Building a GrEMLIN for e-Research*”, with \$120k being awarded for 2005 and 2006 for the development of Web/Grid Services based remote access. The international collaboration leverages middleware, Web Services and e-Science software developments in the US and UK, to provide Grid enabled remote instrument access and data analysis. This grant accompanies a successful application to GrangeNet with \$100k awarded for 2005-6. Both proposals put forward and focus on the notion of a Grid Enabled Multi-Level Instrument Network or GrEMLIN. Essentially the GrEMLIN is a network of instruments (at conventional and major facilities) linked by a common underpinning remote access technology based on Web Services and CIMA, and the CIMA project leaders are Principal Investigators for the proposals. OPAL computing and electronics group leader Dr Nick Hauser is also a participant in these grants, both with a longer term view of Web Services CIMA based remote access for OPAL and in exploring a common instrument data storage format. The proposals also seek to address the development of a synchronised multi-user molecular structure display and analysis system, a further goal put forward in the 2003 SRI seed funding and 2004 Research Networks funding applications.

A related ARC e-Research SRI application “*Real-time control and data analysis of remote synchrotron microprobe experiments*” was also successful and affirms a collaboration between Australia and Canada for developing remote access to synchrotron instrumentation. The Canadian light source is about a year ahead of the Australian Synchrotron. CIMA is the longer term candidate for the underpinning technology and this will be undertaken in collaboration with the GrEMLIN project mentioned above. Members of the two project teams have recently submitted an ARC Discovery application to extend and generalise these projects, and again this involves international collaboration.

An ARC LIEF application was submitted in 2005 as an MMSN project, with the subsequent awarding of \$1m for the provision of “*e-Research Infrastructure for the Molecular and Materials Structure Sciences*”. This is to provide robotic and remote access equipment for MMSN development sites at the University of Queensland and the University of Sydney. The sites provide models for remote instrument and data access at OPAL and the Australian Synchrotron. A noteworthy feature of the application was the appending of a large number of structural science community endorsements for the proposal.

Also noteworthy was the 2005 success of the “*Data Grid Storage Infrastructure for eResearch*” LIEF bid led by MMSN participant Prof. Bernard Pailthorpe, with the ARC awarding of \$0.8m for data storage for scientific instrumentation. The infrastructure will be available to both conventional and major facilities, and will contribute to the Grid enabling of structure determination instruments.

A cornerstone interest of the MMSN is the development of eResearch systems supporting geographically distributed collaborations using eResearch technologies. Prof Pailthorpe led a successful e-Research SRI application entitled “*Collaborative Working using Shared Applications in the Access Grid*”. This project aims to further develop an amplified collaboration environment, based on the Access Grid (AG), that will support shared software applications between geographically distributed research groups. This enhanced AG will provide a platform for collaborative and network-based, shared scientific visualisation tools.

Another noteworthy e-Research SRI project is the “*Development of a collaborative environment for high throughput biology discovery pipelines*”. Modern biological science involves the parallel

high-throughput investigation of many hundreds of different experimental targets. The project is to develop new approaches for high throughput macromolecular discovery and analysis, with MMSN participant Prof David Abramson providing Grid computing expertise. In a similar vein, Prof. Albert Zomaya led a successful 2005 Discovery application "*A Grid Enabled Meta Server for Protein Threading*" to develop a framework for the application of Grid technologies to bioinformatics problems.

MMSN participants were involved in the successful funding of the particularly significant *Dataset Acquisition, Accessibility, and Annotation e-Research Technology* project (DART), funded under DEST's ARIIC initiative *Managed Environment for Research Repository Infrastructure* (MERRI). The DART project has adopted crystallography as an exemplar application, primarily because of its well defined workflows and data structures. A/Prof. Ian Atkinson and Prof. David Abramson have played a catalytic role in accelerating the implementation of CIMA based remote access systems at James Cook University and Sydney University, with installations at Queensland and Monash University sites to follow soon. The extension of CIMA to allow remote control of an instrument (a new role for CIMA) is underway at the University of Sydney, and CIMA is being harnessed to Grid technologies through work at James Cook University, Monash and Sydney Universities. The build-up of a national network of instruments and data accessible through Web Services involves a strong collaborative relationship with the US CIMA group (A/Prof Rick McMullen and Dr Ken Chiu). The current focus is on single crystal diffraction instruments, however the system is extensible and adaptable to different instrument settings and its scope will be expanded to include other instrument types. As a founding partner to the global Crystal Grid Collaboratory project, the use of Semantic Web technologies will be explored by the MMSN in 2006, particularly in collaboration with the UK CombeChem group at Southampton (Prof Mike Hursthouse and A/Prof Jeremy Frey). The MMSN is a participant in the UK Sisters Project grant that initiated support for the CGC.

DART CI Prof. Jane Hunter is developing an innovative Wikki Wikki based collaborative electronic laboratory notebook system and a capability for synchronised molecular display sharing and annotation. Geographically distributed researchers will be able to collaboratively view and analyse a shared structural display, annotate the display and save the annotated display either for further analysis later or for publication and archiving purposes.

Prof. John Drennan led a successful application to the 2005 eResearch SRI program entitled "*A Grid-Enabled National Archive of Nanostructural Imagery (GRANI)*". The primary aim of this initiative is to provide the NANO community with a set of common, inter-operable tools and services to enable more efficient, cost-effective storage, management, analysis and sharing of generated microscopic images, video and analytical data. The project will be highly beneficial to the MMSN community.

### **Submissions**

In November 2005 the MMSN was invited to provide a stakeholder submission on the draft NCRIS Strategic Roadmap. In preparing a comprehensive submission, MMSN participants were invited to provide individual summaries of research interests and needs with the respect to the 16 prioritised capabilities given in the draft road-map. The 33 contributions provided the basis for the overall MMSN submission (10 page overview, 30 pages in total) and were appended to the submission (prior approval for the submission format was sought from the NCRIS secretariat). Areas of particular interest to the MMSN participants were the three Characterisation Capabilities (neutron scattering, X-ray techniques and optical and electron microscopy and microanalysis). In February 2006 the NCRIS Committee provided the following comment on Characterisation "The NCRIS Committee recommends that work commence as soon as possible, through an appropriate

facilitator, to bring forward a coordinated proposal by September 2006 to further develop Australia's characterisation capability. Strong support was received in response to the Exposure Draft for all three capability areas above and the Committee would expect the proposal to specifically address those elements.”

The MMSN provided a case study for the eResearch consultative process and assisted in the GrangeNet led scoping study for the Grid enabling of the synchrotron. MMSN participants serve on the Grid and eScience beamline advisory panel for the synchrotron.

### **Network Appointments**

In August 2005 Dr Peter Turner was appointed Manager for the Network, following national advertising in the Australian newspaper. Following extensive national and international advertising a computer programmer for the network was appointed in December 2005 and commenced work in late January 2006. The programmer is to provide support to MMSN projects with a current focus on setting up CIMA based remote access to MMSN facilities and assisting in the setup of a pilot national data base service in 2006. A second programmer is to be appointed in 2006.

### **MMSN supported visits and presentations in 2005**

- David Abramson, Computer Science, Monash University, Clayton, Victoria. Presentation at Marysville March 2005: **Software Development for the Computational Grid.**
- Dr Toyokazu Akiyama. Applied Information Systems Division, Cybermedia Center, Osaka University, Osaka. Presentation at Marysville March 2005: **Grid based remote access to the Ultra High Voltage Electron Microscope.**
- Dr Ken Chiu. Dept Computer Science, State University of New York at Binghamton. **Common Instrument Middleware Architecture (CIMA) and binary XML.**
- Dr Dave Corney, Group Leader Data Storage, Atlas Data Store, Rutherford Appleton Laboratory, Chilton, Didcot, Oxfordshire, UK. Presentation at Marysville March 2005: **Atlas Petabyte Datastore and UK Data Curation Program.** Marysville March 2005.
- A.R. Criswell, Rigaku-MSU, The Woodlands, Texas, USA. Presentation at Marysville March 2005: **Winners and Losers – Ranking Crystals from Diffraction Images.** Marysville March 2005.
- Prof Bill David, ISIS Neutron Facility, Rutherford Appleton Laboratory, UK. Presentation at Marysville March 2005: **Grid Computing and e-Science at ISIS.** Marysville March 2005.
- Dr Paul Davis, GrangeNet, Yarralumla, ACT. Presentation at Marysville March 2005: **Grid Enabling of the Australian Synchrotron.** Marysville March 2005
- Dr Francesco De Carlo, Advanced Photon Source, Argonne National Laboratory, USA. Presentation at Marysville March 2005: **X-Ray Tomography System, Automation and Remote Access at Beamline 2BM of the Advanced Photon Source.** Marysville March 2005.

- Prof David deRoure. Electronics and Computer Science, University of Southampton, UK. Presentation at Marysville March 2005: **Instruments, Sensors and the Sematic Grid.**
- Dr R. Durst, Bruker AXS, Madison, USA. Presentation at Marysville March 2005: **New Software and Hardware Tools for Remote Crystallography.**
- A/Prof. Jeremy G Frey, School of Chemistry, University of Southampton, UK. Presentation at ISOG December 2005: **Sensor Networks and Grid Middleware for Laboratory Monitoring.**
- Dr Peter Hines, Australian Key Centre for Microscopy and Microanalysis, The University of Sydney. Presentation at Marysville March 2005: **Remote access for NANO-MNRF Instrumentation**
- Prof Mike Hursthouse, EPSRC National Crystallography Service, School of Chemistry, University of Southampton, UK. Presentations at Marysville March and ISOG December 2005: **Grid and Remote Access for UK National Crystallography Service.**
- Dr Lilian Jacquamet, Institute of Structural Biology, Grenoble, France. Presentation at Marysville March 2005: **FIP: An Automated Beamline for Protein Crystallography at the ESRF: The CATS Robot.**
- Dr Ronan Keegan, Grid Technology Group and e-HTPX Project, Daresbury Laboratory, Warrington, UK. Presentation at Marysville March 2005: **e-HTPX Project for Grid based Automation and Remote Access to the Daresbury and Diamond Synchrotrons.**
- Dr Abel Lin, Center for Microscopy and Imaging Research, University of California at San Diego. Presentation at IEEE Conference December 2005: **The Telescience Tools: Version 2.0.**
- Colin. M. MacRae, Microbeam Laboratory, CSIRO Minerals Clayton, Victoria. Presentation at Marysville March 2005: **Telepresence Microscopy at CSIRO Minerals.**
- Dr Gerry McDermott, Advanced Light Source, Berkeley, USA: Presentation at Marysville March 2005: **Crystallography and Tomography Automation and Remote Access at the Advanced Light Source.**
- Andrew Stephen McGough, Department of Computing, Imperial College London, UK. Presentation at ISOG December 2005: **The GRIDCC Project.**
- Dr Rick McMullen, Knowledge Acquisition and Projection Laboratory, Pervasive Technology Labs. Indiana University. Presentations at Marysville March and ISOG December 2005: **CIMA: Scientific Instruments as First Class Members of the Grid.**
- Dr Ken Meacham, IT Innovation Centre, Chilworth Science Park, Southampton, UK. Presentation at Marysville March 2005: **Grid and Remote Access for UK National Crystallography Service.**

- Dr Dave Meredith, Grid Technology Group and e-HTPX Project, Daresbury Laboratory, Warrington, UK. Presentation at Marysville March 2005: **e-HTPX Project for Grid based Automation and Remote Access to the Daresbury and Diamond Synchrotrons.**
- Dr Tomas Molina, Center for Microscopy and Imaging Research, University of California at San Diego. Presentation at ISOG December 2005: **A Generalised Service-Oriented Architecture for Remote Control of Scientific Imaging Instruments.**
- Roberto Pugliese, Sincrotrone Trieste, Italy. Presentation at ISOG December 2005: **Elettra Virtual Collaboratory: the evolution of a Virtual Laboratory Software from a simple web application to the GRIDCC.**
- Dr Mike Soltis, Macromolecular Crystallography Group, Stanford Synchrotron Radiation Laboratory, USA. Presentation at Marysville March 2005: **Remote Access Tools for Macromolecular Crystallography Experiments at SSRL.**
- Prof Bob Sweet, Biology Department, Brookhaven National Lab. and National Synchrotron Light Source, USA. Presentation at Marysville March 2005: **Methods, Software, and Equipment for High-Throughput Data Collection in Macromolecular Crystallography: the Brookhaven Experience.**
- Claudio Vuerli, INAF, Trieste, Italy. Presentation at ISOG December 2005: **Monitoring and remote control of scientific instrumentation.**
- Duncan Waddell, Centre for Microscopy and Microanalysis, The University of Queensland. Presentation at Marysville March 2005: **Remote access for NANO-MNRF Instrumentation**
- Prof Nestor J. Zaluzec, Argonne National Laboratory Electron Microscopy Center, Materials Science Division Argonne, USA. Presentation at Marysville March 2005: **The Telepresence Microscopy Collaboratory: Evolving the Collaboratory Paradigm.**

### National Benefit of the MMSN

The MMSN program addresses key scientific endeavours, including those identified by the Australian Government (<http://www.dest.gov.au/priorities/>) as *National Research Priority 3: Frontier Technologies for Building and Transforming Australian Industries*. The *Research Priority 3* specification emphasises the importance of breakthrough science and smart information use, and recognises Australia's strength in fundamental science and key technologies such as biotechnology, advanced materials, and information and communications technology (ICT). The latter is seen as a critical enabling technology in *Research Priority 3*, which highlights a need to invest in smart information use and data management in contributing to productivity, growth, competitiveness and well being. The goals of the MMSN have resonance in *Priority Goal 4* of *Research Priority 3*; smart information use. The MMSN encapsulates smart and efficient information capture, its distribution, storage and analysis, and resulting knowledge generation.

Knowledge of the three dimensional arrangement of atoms, and the chemical identity of those atoms, in molecules and solid state materials is crucial to understanding their behaviour and harnessing their potential in real-world applications. Such knowledge can deliver profound scientific, technological, social and economic rewards, as recognised in *Priority Goals 1*

(*Breakthrough Science*), 2 (*Frontier Technologies*) and 3 (*Advanced Materials*) of *Research Priority 3*. Understanding the biological process that support and shape life and the disease and degenerative process that may threaten life, depends increasingly on a detailed knowledge of bio-molecular structure of proteins, viruses, DNA complexes and enzymes (eg. the SARS protease). Rational medicinal drug design, which produced the first anti-flu drug Relenza (developed by two MMSN participants) and the HIV protease inhibitors, would be impossible without a knowledge of molecular structure. The determination and rationalisation of the relatively small atomic structures comprising micro-magnets, microporous and mesoporous materials, hydrogen storage materials, novel metal oxides, ceramics, superconductors, minerals, 'smart' materials, piezoelectric materials, magneto- and electro-rheostatic materials, photonic devices, information storage devices, molecular switches and sensors, biomimetic materials, and pharmaceutical materials is crucial to their development and utilisation.

The network embraces *Priority Goal 5* in using breakthrough technology and the internet to develop a collaborative research environment in which Australian distances are no longer of consequence or disadvantage. A national collaborative eResearch based environment for the structural sciences will promote an innovative scientific culture, creating "structures and processes for encouraging and managing innovation".

### **ARC MMSN Steering Committee and Governance**

- Chair: Prof Cameron Kepert ( Dr Peter Turner)
- Synchrotron: Prof Richard Garrett (Dr Anton Stampfl)
- OPAL and other ANSTO instruments: Dr Nick Hauser (Dr Jamie Schulz)
- Diffraction: A/Prof Jenny Martin (Prof Mitchell Guss/ Dr Peter Turner)
- Spectroscopy and Scattering: Dr Bill Skinner (Dr Alan Buckley/ A.Prof Ian Gentle)
- Tomography: Prof Steve Wilkins (Dr Tim Gureyev/Dr Tomaso Aste)
- Electron Microscopy: Prof Simon Ringer (Dr Peter Hines)
- Database Development and Services: Prof Syd Hall (Prof Mark Spackman/Prof Stephen Hyde)
- Workshops, Meetings and Outreach: Dr Peter Turner (Prof Cameron Kepert)
- Web and Grid Services: Prof David Abramson (Prof Albert Zomaya/Prof Raj Buyya)
- Interfaces and Visualisation: Prof Bernhard Pailthorpe (Prof Mark Spackman)
- Other Networks and Organisations: Prof Ian Gentle ( Prof Cameron Kepert)
- Regional Institutions: Dr Michael Antolovich (Prof Richard Keene)

The Steering committee is responsible for identifying, recommending and overseeing the implementation of Network goals and priorities, including approval of expenditure for staffing, meetings and participant project applications. The size of the committee has increased from that given in the funding application, to more appropriately represent the interests of the Network..