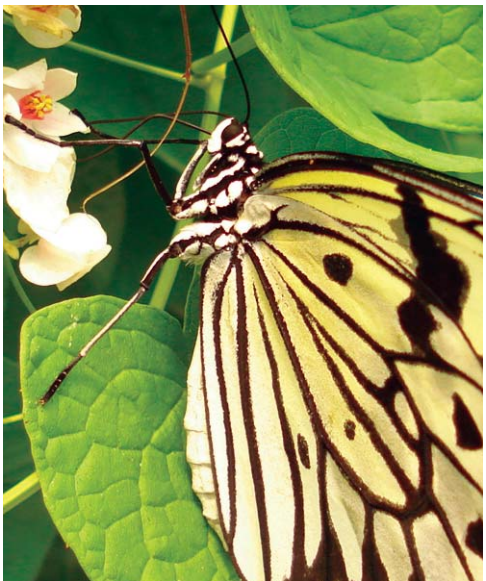
PACIFIC RIM APPLICATIONS AND GRID MIDDLEWARE ASSEMBLY

COLLABORATION OVERVIEW 2008-2009

PRAGMA

CONTENTS



Above: The Torii Gate of the Itsukushima Shrine—courtesy of Phillip Pham

INSTITUTIONS AND CONTACTS

PRAGMA is an institution-based organization governed by a Steering Committee that invites new members, determines locations of workshops, and sets overall direction. This year, three new members joined PRAGMA: Advanced Science and Technology Institute (ASTI), Republic of the Philippines, Ho Chi Minh City University of Technology (HCMUT), and High Performance Computing Center (HPCC) of Hanoi University of Technology (HUT). More information about the Steering Committee members (denoted here with an asterisk) may be found at www.pragma-grid.net/about/committee.*

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Visit www.pragma-grid.net/about/institutions for more information about PRAGMA Members.

Above: Outsite Olympic Park—courtesy of Kevin Wu
Left: Dotomburi Street city lights—courtesy of Phillip Pham

OVERVIEW

Established in 2002, PRAGMA is an open organization which focuses on practical solutions to create, support, and sustain international science and technology collaborations via multidisciplinary teams of researchers who develop or apply grid technologies to advance science. PRAGMA plays a critical role as an international *conduit* for professional interactions, ideas, information, and grid technology. Our multifaceted *framework for collaboration* catalyzes and enables new activities through a culture of openness and sharing. As documented in this report, our pragmatic approach has led to new scientific insights, enhanced technology, a fundamental sharing of experiences manifest in using the grid, and the training of the next generation of researchers.

Our approach has been to create teams of application and middleware researchers focused on a specific research challenge that requires integration of application and grid technologies. As the projects progress, they migrate to our routine-use grid and are evaluated to discover how the applications and middleware work on the PRAGMA Grid. These experiments lead to scientific insight and improved middleware. Successful solutions are then integrated into country-specific software stacks, Open Grid Forum (OGF) standards, or other wide-dissemination vehicles, so others may benefit. Our workshops provide a twice yearly venue to report on progress and to involve new collaborators in our activities. Additional outreach efforts bring our lessons learned to others, and ultimately, *help build the community.*

This year we have seen continued progress both through further development of grid technologies via applications and through ongoing enhancement to our sustainable collaborative framework. In particular, we have seen: the use of technologies to identify new possible drug targets for Avian Flu; the introduction and coupling of two technologies to assist researchers studying coral reefs; the advancement of grid interoperability between PRAGMA and the Open Science Grid to run a science application to determine protein structure from crystallographic images; integration of technologies between the Thailand SCMSWeb and the NSF-funded Condor project to utilize the information collected by the grid monitoring system - SCMSWeb, to enable Condor-G to provide more intelligent Grid-level scheduling services; and the establishment of an approved certificate authority (CA) and implementation of a virtual organization membership service (VOMS), developed by BeSTGrid with UCSD, for the use in the PRAGMA Grid to facilitate user access setup.

Critical to our sustainable collaborative framework has been our focus on developing human capital. This year we held two PRAGMA Institutes, one in Taiwan in December 2007 and the other in Malaysia in October 2008. The Institute provides a forum for training researchers on key technologies developed by PRAGMA. The PRAGMA Institute in Taiwan led to the addition of three new institutional members: Advanced Science and Technology Institute, Republic of the Philippines, Ho Chi Minh City University of Technology (HCMUT), and High Performance Computing Center (HPCC) of Hanoi University of Technology (HUT). In addition, the Institute of Information Technology—Vietnam (IOIT-VN) became a fourth new member this year.

The success of the PRIME and PRIUS programs has led to the launching of the Monash University Research Programs Abroad (MURPA) and the expansion of the PRIME program to three new sites: Universiti Sains Malaysia, University of Auckland and the University of Waikato. In addition, several of the PRIME/PRIUS students have published the results of their research.

We are pleased to note that Professor Habibah Wahab has accepted a one year term as the Deputy Chair of PRAGMA. Her interests are to continue to grow PRAGMA's involvement in building the community via ed-

[1]A. Bement 2007, Cyberinfrastructure Vision for the 21st Century Discovery. NSF Cyberinfrastructure Council, March 2007)

Above: Kyoto's Golden Temple—courtesy of Peter Arzberger. Left Below: Luging in Rotura—courtesy of Sara Richardson. Right Below: Dragon—courtesy of Rob Reed.

ucation, even at levels in primary and secondary education. We want to thank Dr. Piyawut "Joe" Srichaikul of NECTEC for serving a year and a half in this position and helping to grow the GEO Working Group effort.

What are the future directions of PRAGMA? *First*, we will continue to experiment with new technologies. At our recent meeting there was a great deal of information exchanged about how groups around the Pacific Rim are testing and implementing approaches to virtualization of resources. This is one of the values of PRAGMA, where we can be a key conduit of ideas and technologies among the participants and their constituencies. Second, we will work with social and organizational scientists to better understand how to improve our interactions to change the conduct of science through virtual organizations that transcend geographic and institutional boundaries[1]. *Finally*, we will continue to expand our impact with the results of our working groups and by explicit activities to engage the community. In particular, we will seek to broaden programs like PRIME, PRIUS and MURPA to increase the number of participants and to expand to other sites (e.g., PRIME will expand to the University of Hyderabad in summer 2009). Students who participate in these programs will become the leaders of the future.

PRAGMA GRID TECHNOLOGIES AND APPLICATION ADVANCEMENTS

- Identified new possible drug targets for Avian Flu (*See PRIME, PRIUS, MURPA section*)
- Assist researchers studying coral reefs through coupling technology.
- Advanced protein structure determination via PRAGMA and OSG interoperability
- Provide more intelligent Grid-level scheduling services via Condor SC-SMWeb integration
- Facilitate user access setup by implementation of VOMS
- Established approved certificate authority for community

PRAGMA BUILDING THE FRAMEWORK AND THE COMMUNITY

- PRAGMA Grid grown to 28 clusters at 26 institutions in 17 countries and regions, with increases in CPUs, memory, and online storage.
- The PRAGMA Institute in Taiwan in December 2007 grows the community and new members: ASTI, HCMUT, NPCC/HUT

PRIME, PRIUS, MURPA: RESEARCH AND CULTURAL EXPERIENCE FOR TOMORROWS' LEADERS

- PRIME expands program to Malaysia and New Zealand, and in 2009 to India
- MURPA launched—lectures and first students to UCSD in January 2009
- PRIUS holds meeting to coordinate research projects abroad

ACCOMPLISHMENTS

STREAMING UNDERWATER VIDEO CAMERAS TO OptIPortals

The ability of coral reef ecologists to see and sense, real time, from their desks, the biological activity in and around one or several coral reefs, will transform how they conduct their science. To realize this vision, we developed a system that integrates sensors (including underwater video cameras) with computing and storage grids to create a complete fabric for conducting e-Science. The output of multiple cameras on the grid is viewed in high-resolution on OptIPortals. The system is designed for a broad range of users including marine research scientists in Taiwan and the United States. We now describe two key technologies, namely, open source DataTurbine and SAGE-based OptIPortals, which constitute this framework. Figure 1 shows the overall system architecture. This system was demonstrated during the PRAGMA 14 meeting in Taiwan in March 2008.

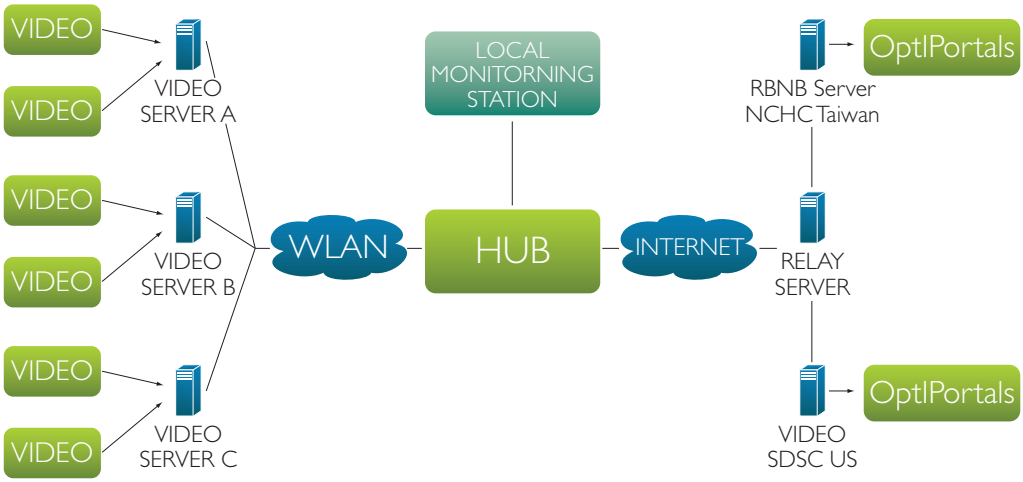

Figure 1: Setup for streaming live underwater cameras to OptIPortals

Figure 2

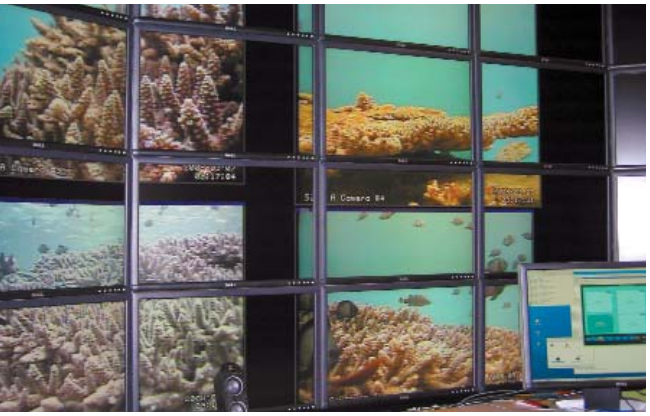

Figure 3: Tiled-display wall (TDW) at Calit2 (UCSD) showing data from underwater video cameras in Kenting (Taiwan) in real time using DataTurbine streaming data middleware.

The open-source RBNB DataTurbine provides an excellent basis for developing robust streaming data middleware. The current RBNB DataTurbine streaming data middleware system satisfies a core set of critical infrastructure requirements including reliable data transport, the promotion of sensors and sensor streams to first-class objects, a framework for the integration of heterogeneous instruments, and a comprehensive suite of services for data management, routing, synchronization, monitoring, and visualization. As a part of the PRAGMA Telescience group, researchers at the National Center for High-performance Computing (NCHC) and at UCSD deployed a DataTurbine-based system to acquire data from underwater cameras, located in the ocean at Kenting.

OptIPortals provide the ideal termination point for such content rich environments where display real estate can be used effectively. ROCKS and SAGE-based tiled display wall technologies have been widely deployed amongst multiple working groups under the PRAGMA umbrella. SAGE provides inherent support for streaming video and lets users view tiled displays as big desktops, where multiple video streams can coexist. Users can arrange the video streams on this 'desktop' and resize or maximize them for a better view. Figure 3 shows a picture of one of the tiled display walls (TDWs) at Calit2 (UCSD) showing data from underwater video cameras in Kenting (Taiwan) in real time using DataTurbine streaming data middleware.

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BRIDGING GRID ISLANDS TO DETERMINE BIOMEDICALLY RELEVANT PROTEIN STRUCTURES: *An Experiment in Grid Interoperation*

As e-Science continues to be embraced by the wider research community (i.e., not just the traditional drivers, such as computational physics), the demand for resources also increases. The capability for simple interoperation of Grids is now extremely important for the researchers and virtual organizations (VOs) that constitute their users. Only a decade ago it was common for research institutions to have a single computational cluster, if at all, whereas, now we are seeing the formulation of dedicated e-Research and e-Science centers, with their own computational clusters and needs, within these institutions.

The case study we detail here tested Grid interoperability and interoperation between: Australian EnterpriseGrid, APAC Grid, PRAGMA Grid, FermiGrid, Open Science Grid (OSG), and the University of Zurich. In order to ensure the validity and relevance of our study, the application we ran was 'real' science, a Nimrod/G experiment in structural biology. Specifically, multiple conformations of multiple proteins from the Protein Data Bank (PDB) were used in a protein crystal structure determination, using the technique of Molecular Replacement (MR). This involved testing the entire PDB using the MR application PHASER, a maximum likelihood approach (*www-structmed.cimr.cam.ac.uk/phaser*).

In order to distinguish interoperability issues from other potential problems during the case study, we followed a workflow as shown in Figure 4. This workflow shows the steps taken when adding a computational resource to the Nimrod/G experiment. We began the experiment on our known 'home' Grid (EnterpriseGrid) and started the resource discovery, testing, and application deployment steps on the remaining Grids in parallel. Finally, adding each of these Grids to the experiment with intervals of at least a week.

Resource discovery involves finding information about resources so they can be used by Nimrod/G and communication with resource providers regarding the details of the interoperation. Resource testing involves checking authorization and running automated resource checks within Nimrod/G. Application deployment was performed by a separate Nimrod/G experiment run once on each resource. After the successful completion of these steps, and gathering of interop issues along the way, resources from each Grid were added to the parent Nimrod/G PHASER experiment.

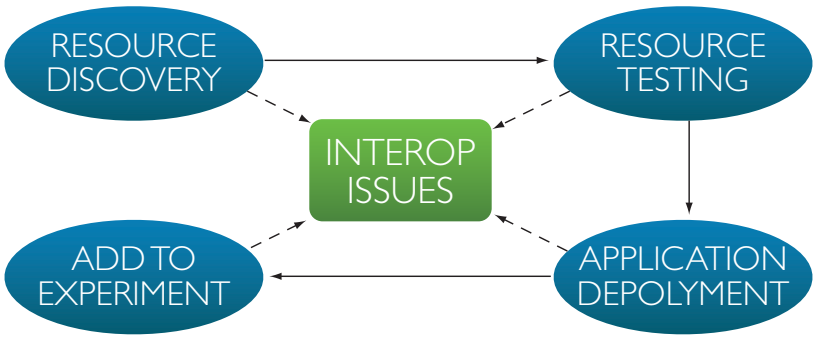

Figure 4: Interoperation Workflow

We identified five categories that the interop issues we encountered fall into: Access and Security, Resource Discovery, Usage Policies and Guidelines, Application Compatibility, and Middleware Compatibility. See Bethwaite 2008 for details. For example, under Resource Discovery, we discussed the importance of the uniform provision of information services (e.g., OSG, Fermi Grid and APAC publish information in a standard schema that can be queried programmatically). We also identified the need for tools which simplify the configuration and maintenance of these services, an area of potential future work. Please note that some monitoring software now also displays aspects of the remote system and their applications (see SCMSWeb Accomplishment section).

The experiment described above generated more than seventy thousand executions across the five Grids, requiring over half a million CPU hours. The team performed MR calculations using the entire PDB (~80,000 structures) in a reasonable timeframe. This feat was inconceivable three years ago (and many in the application community consider it still is). Our approaches have led to the structural solution of several key medically important proteins in our laboratories, many of which involve collaborations with researchers from Monash University and several international laboratories, which would otherwise have remained unsolved. Much of this data is currently being published in top international journals.

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APPLICATION-BASED GRID MONITORING DEVELOPMENT: *SCMSWeb for Application Discovery and Distributed Computing Condor*

PRAGMA's mission is to develop grid technologies through scientific applications. The Bioscience Working group has been interested in conducting virtual screening experiments (for Avian Flu virus proteins, for example). Doing this on the PRAGMA Grid requires knowing which computing resources have specific application software. Members of the Thai National Grid Project, a PRAGMA partner, who developed the grid monitoring system SCMSWeb (*goc.pragmagrid.net/wiki/index.php/SCMSWeb*), took up the challenge to augment their product with this feature. Between the 13th and 14th PRAGMA Workshops (September 2007 and March 2008), the team was able to develop and implement this feature (*goc.pragma-grid.net/cgi-bin/scmsweb/swcatalog.cgi?grid=PRAGMA*), thus addressing an important need of grid users.

The PRAGMA framework has helped catalyze collaborations and established a conduit of ideas and technologies. In early 2007, PRAGMA began experimenting with Condor, a well-known workload management system for distributed systems, developed by the Condor Project at the University of Wisconsin-Madison (UW-Madison). Condor-G was deployed as a Grid scheduler for PRAGMA Grid initially on a cluster at SDSC. Because of the diversity of resources on the PRAGMA Grid (different computer architectures, local batch schedulers, and user access and system maintenance policies), submitting jobs to the PRAGMA Grid via Condor-G placed the burden of resource selection on the user. The manual selection made it difficult for users to make efficient use of all available resources.

After the September 2007 PRAGMA 13 workshop, members of Condor and the SCMSWeb team agreed to address this challenge. A collaboration team was assembled to develop an SCMSWeb-Condor interface, which would utilize the rich information collected by the grid monitoring system of SCMSWeb to enable Condor-G to provide more intelligent Grid-level resource selection, scheduling services, and job submissions. This interface development was driven by an application of percolation theory, often used in materials science, from KISTI scientists.

With the current SCMSWeb-Condor interface, the Condor-G server can distribute jobs throughout the PRAGMA Grid according to the information provided by the sites. The team has and will continue to work on enhancements to the user interface and fault tolerance, which were raised during the user/application testing. In particular, they plan to use Condor's error handling features to deal with various fault conditions, and increase job throughput by using Condor's rank and matchmaking features.

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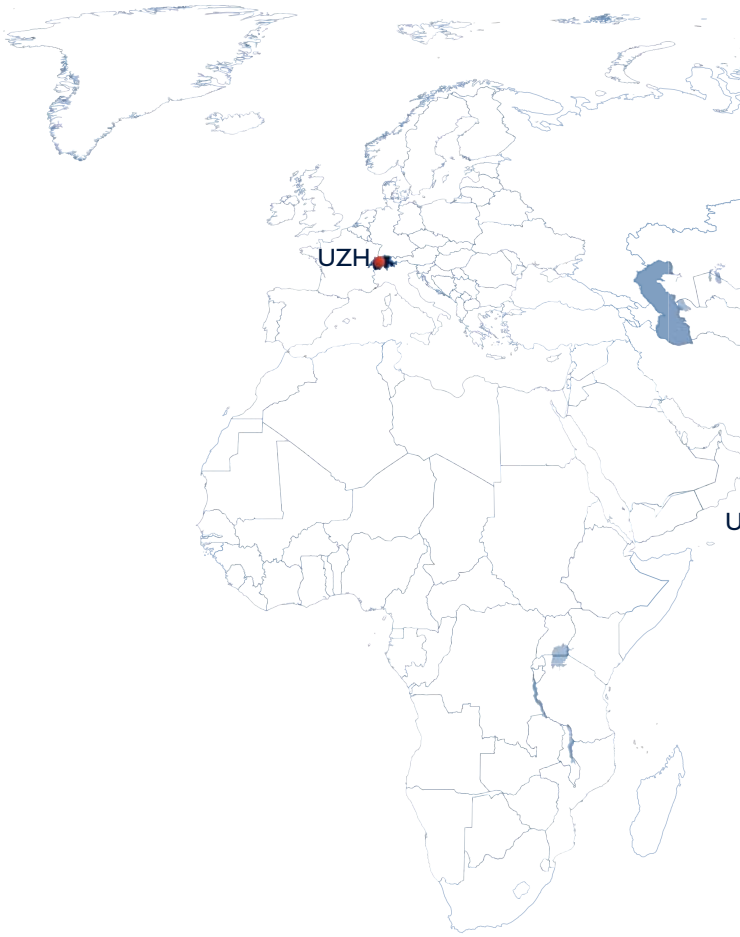
PRAGMA GRID SECURITY INFRASTRUCTURE ADVANCEMENTS: *PRAGMA CA and VOMS Setups*

The PRAGMA Grid is an active international grid interoperation environment, consisting currently of 28 clusters, 26 institutions in 17 countries and regions (*goc.pragma-grid.net/pragma-doc/pragma-grid-map.jpg* and *goc.pragma-grid.net/pragmadoc/computegrid.html*). As a grid entity, PRAGMA Grid also conducts grid interoperation experiments with other grids (See Accomplishment "Bridging Grid Islands"). To build a security infrastructure that readily and easily enables grid interoperations on a global scale; we followed the common policies, guidelines and practices established by International Grid Trust Federation (IGTF), and setup a Virtual Organization Management System (VOMS) service in the PRAGMA Grid.

Within the PRAGMA Grid, most users use their local site certificate. We had built a PRAGMA experimental CA (Certificate Authority) last year, issued certificates to users and systems at sites without local CA services. But, the PRAGMA experimental CA is not IGTF compliant and its certificates can only be used within the PRAGMA Grid. For broader grid



PRAGMA Grid: Sites contributing (red) or preparing to contribute (green) resources.

interoperations and to move towards IGTF standard within the PRAGMA Grid, a catch-all IGTF compliant CA was needed.

With the help of APGrid PMA and NAREGI-CA developers, a PRAGMA Grid team at SDSC built the PRAGMA-UCSD CA service according to the most current IGTF recommendations and guidelines (*goc.pragma-grid.net/ca*). PRAGMA-UCSD CA was accredited by APGrid PMA in April 2008. It started operation and became a part of IGTF distribution in July 2008.

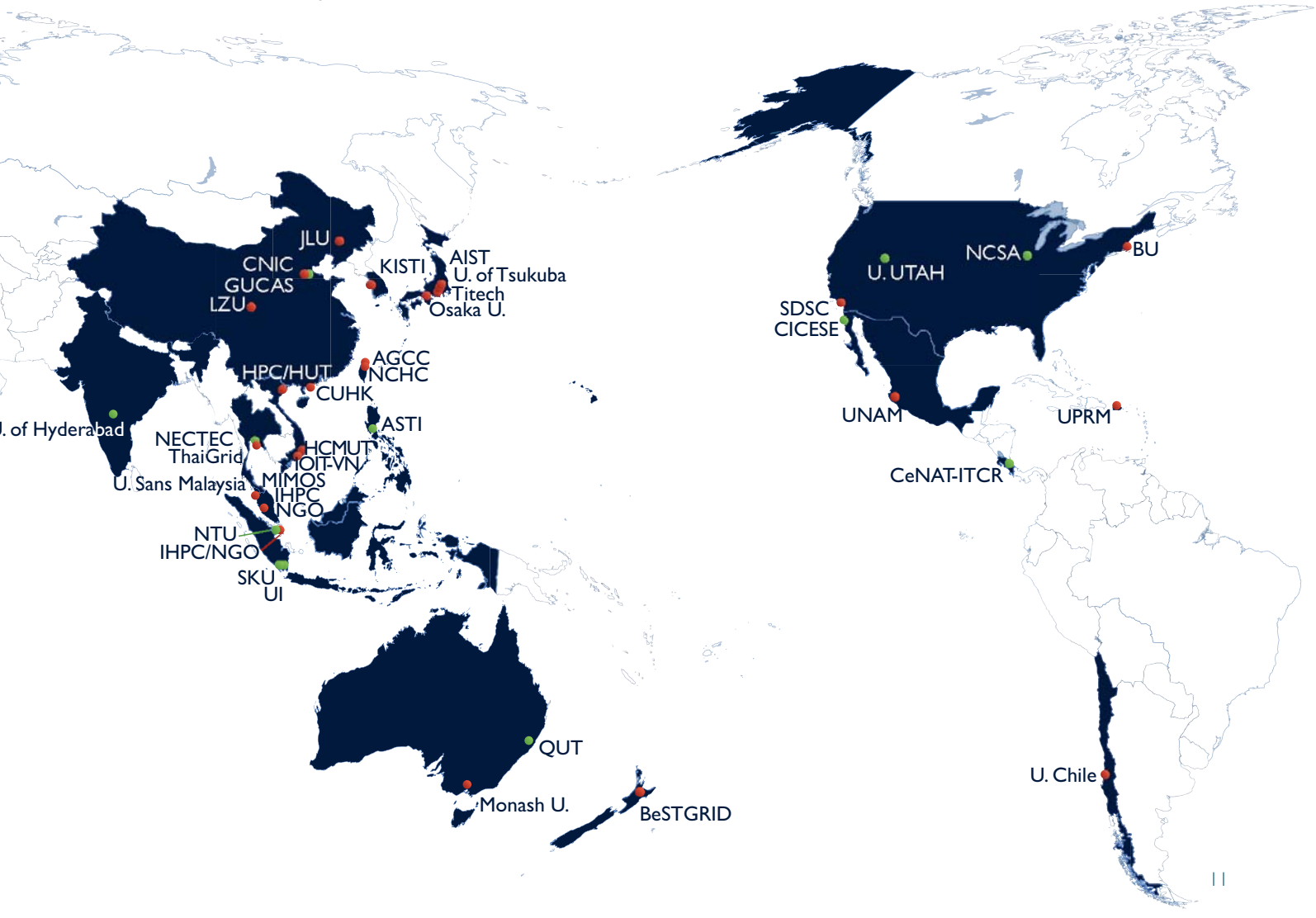
Since then, PRAGMA-UCSD CA has issued 10 host/service certificates which enabled many critical services in the PRAGMA Grid, including a Grid Operation Center, virtual organization membership service (VOMS), Condor, portals and other compute services.

PRAGMA Grid, being a "grass roots" and loosely coupled global grid, does not have a uniform infrastructure management. One aspect of this characteristic is that user access setup has been done independently at each site. Each site needs to do a new user setup for each PRAGMA Grid user. A user has to communicate and verify access with each site one-by-one. To automate the user access setup in PRAGMA Grid, but still accommodate the diversity of site management and policies, the Resources Working Group decided at PRAGMA 14 workshop to setup a VOMS service in PRAGMA Grid. Using the group management function in VOMS, we organize groups based on projects and map them to accounts at each site. Any additions or changes in existing groups only require trivial work by a VOMS administrator. This not only reduces work load for both site administrators and application users, but also speeds up and simplifies the user access setup process in PRAGMA Grid.

The BeSTGrid team in New Zealand and the SDSC team in the USA led the effort, built a VOMS server at SDSC, set up and tested the service between the BeSTGrid and SDSC sites, documented detailed examples for site administrators and application users to follow when using the VOMS service (*goc.pragma-grid.net/wiki/index.php/VOMRS*). The VOMS service has been operational since August 2008.

This work has stimulated much discussion among site administrators and users have raised many detailed questions about VOMS usage and practice policies in the PRAGMA Grid. Based on these responses, the Resources Working Group will discuss these issues at up-coming workshops and decisions will be published at *goc.pragma-grid.net/wiki/index.php/VOMRS*.

PARTICIPATING RESEARCHERS: *M. Katz, C. Zheng, A. Rajendra, SDSC; Y. Tanaka, AIST; V. Mencl, BeSTGrid; T. Okuno, NAREGI.*



MONASH UNIVERSITY RESEARCH PROGRAM ABROAD (MURPA)

The growing importance of international experiences and the success of the PRIME and PRIUS programs motivated Monash University to launch a new program, the Monash University Research Program Abroad (*infotech.monash.edu.au/about/events/2008/murpa.html*). Monash University in Australia, via David Abramson, is a founding contributor to the Pacific Rim Experiences for Undergraduates (PRIME), for which he has mentored more than 24 students over the five years of the PRIME program. Through this experience he was convinced of the need for Monash University students to have a similar experience. In the crafting of the new program, Monash University based MURPA in part on PRIME, and also on PRIUS, the Pacific Rim International Universities program developed by Osaka University (which was also modeled after PRIME).

In particular, MURPA engages faculty lectures from international sites (this first year the lectures came from UCSD). These lectures will be facilitated using the latest High Definition Video-Tele Conference equipment (HDVTC). HDVTC is a significance enhancement on existing technology, and provides a significantly superior experience than existing H323 equipment. The use of this technology has captured the imagination of many of the attendees, giving them the sense of the speakers being present. More about this first season of seminars is at *infotech.monash.edu.au/about/events/2008/murpa.html#seminars*. The first students to come to UCSD will arrive in January 2009, during the southern hemisphere summer, for a nine week stay. Applicants for MURPA will be computer science students enrolled in a fourth year honors program (in Australia, computer science undergraduates typically complete course work after three years). Likely areas of research will enforce several PRIME projects but also broaden the areas of interaction between Monash and UCSD. The areas include cardiac modeling, virtual screening, visualization and interactive displays for communications, and workflow technology.

Programs like PRIME, PRIUS and now, MURPA, have been important to PRAGMA for several reasons. *First*, these programs focus PRAGMA and the broader grid community on issues of broadening and growing the community of users and developers. This human capacity building is central to the PRAGMA mission of building sustained collaborations, not only with the students, but via the students, between various labs of PRAGMA members across the Pacific Rim. *Finally*, it demonstrates the value of PRAGMA of being a conduit of models for education and technology.

PARTICIPATING RESEARCHERS: *R. Pose, D. Abramson, Monash.* LECTURERS: *P. Arzberger, M. Ellisman, L. Smarr, I. Altintas, J. Schulze, W. Li, A. McCulloch, UCSD; Kim Baldridge, U Zurich.*

Calit2 Director Larry Smarr delivering lecture to potential MURPA students via HD camera

EXPANDING THE PRAGMA COMMUNITY

PRAGMA is a dynamic organization and community. It is continually looking for new venues to engage a broad set of participants. This year, PRAGMA undertook three types of efforts to engage new members and to initiate collaborations with new partners.

SUMMIT ON APPLICATIONS AND GRID MIDDLEWARE FOR THE PRAGMA, Swiss Grid and Euro Grid Associations *(www.oci.uzh.ch/diversa/CollaborationMeeting/meetingI.html)*: The grid, as conceived, does not know borders or boundaries. However, efforts are supported at multiple levels (local, regional, and national) and often are so occupied at that level that important interactions to help bridge these efforts are required. This Summit was hosted by the University of Zurich in March 2008, and brought together two dozen researchers from three grid efforts, to first understand the different efforts and then to explore potential points of synergy for interactions. Several areas were identified for collaboration, and progress has been made, in running applications across the grids *(see Bridging Grid Islands)*, and development of VOMS. Furthermore, U Zurich researchers have participated in a working group of the Swiss National Grid Effort (SwiNG) and have installed middleware to help bridge several grid testbeds (PRAGMA, CHEMOMENTUM, and SMSCG—Swiss multi-science computing grid). The middleware they are using include Globus, Nordugrid, and Unicore. PRAGMA, while focused on interactions in the Pacific Rim, realized that many good activities were taking place in Europe, and wanted to begin a dialog, to incorporate new developments into its own activities while also growing collaborations.

PRAGMA INSTITUTES: Initiated in September 2007 at the PRAGMA 13 meeting at NCSA, a PRAGMA Institute provided the opportunity for PRAGMA to nurture the community and those who wanted to take advantage of the many and varied technologies developed by PRAGMA members. The Institutes are hosted by PRAGMA members and the plan for the institutes are reviewed and approved by the PRAGMA Steering Committee.

The Second PRAGMA Institute *(www.nchc.org.tw/event/2007/pragma_institute)* was held in conjunction with the Southeast Asia International Joint Research and Training (SAIJRT) program hosted by NCHC in December 2007. This workshop spanned five days, and covered topics of each of the four working groups. The participants came primarily from Southeast Asia, including participants from Vietnam, Philippines, Malaysia, Thailand, and Indonesia. This combination of PRAGMA Institute with SAIJRT was successful in exposing more groups to PRAGMA, which resulting in three new PRAGMA memberships in 2008. Furthermore, the interactions with SAIJRT inspired the concept of a center of education and collaboration at NCHC that would allow for a persistent platform for education and collaboration among grid researchers in the Pacific Rim. Details are being discussed with funding agencies in Taiwan.

The Third PRAGMA Institute *(pragma15.usm.my/instituteSchedule.php)* was held in advance of the PRAGMA 15 Workshop, hosted by USM. This Institute was focused on researchers in Malaysia, both in terms of building clusters and grids, using middleware, and advancing applications in biomedicine and geosciences.

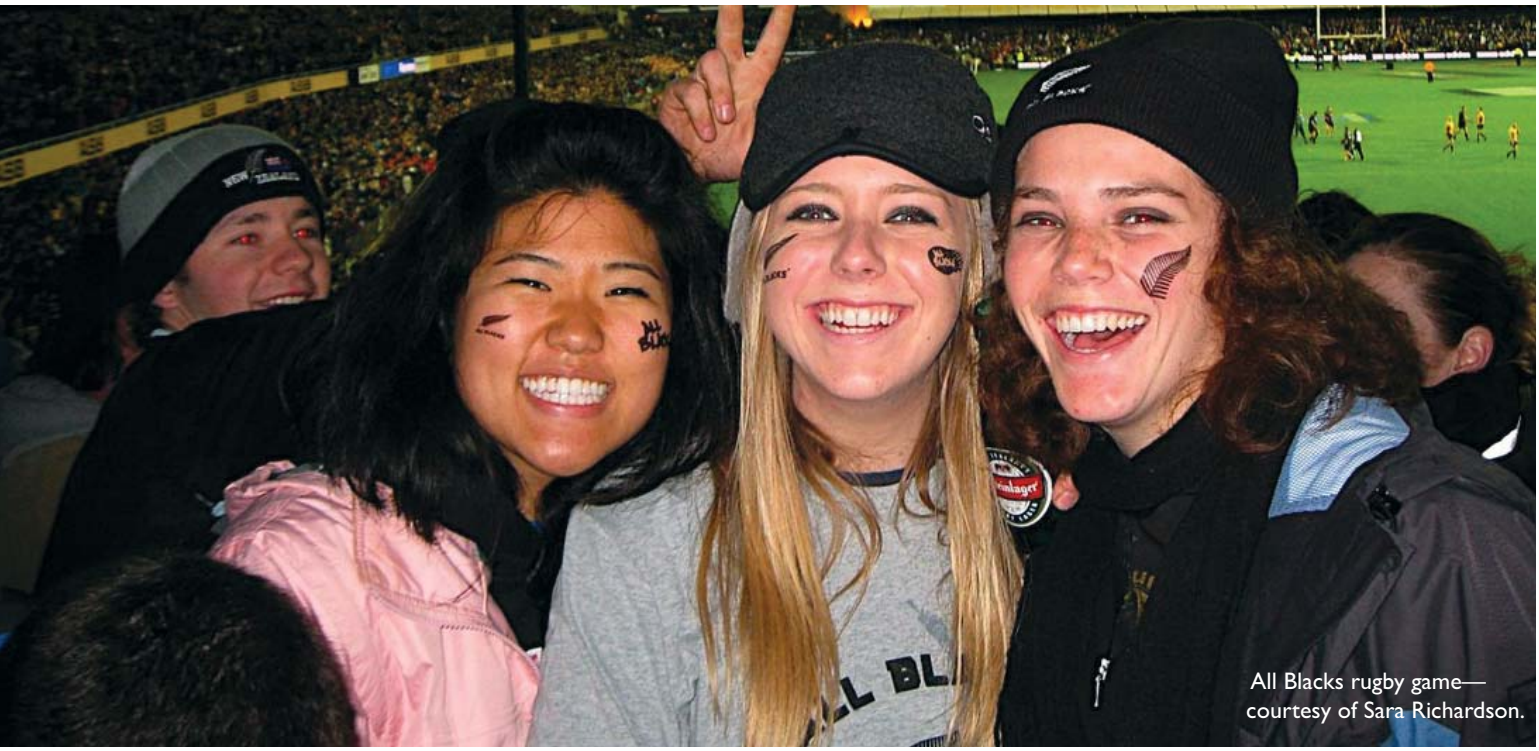
PRAGMA WORKSHOP AT IEEE CONFERENCE ON E-SCIENCE 2008: PRAGMA members have organized a workshop at the IEEE Conference on e-Science 2008, to highlight and share some of the recent advances of PRAGMA members that would be of broader interest. Our goal is to look for other collaborators. The workshop takes place in Indianapolis, Indiana, on 9 December, during the conference.

Participants at joint Southeast Asia International Joint Research and Training Program and the 2nd PRAGMA Institute. Shakadang Trail, Taroko Gorge National Park, Hualien, Taiwan

PRIME, PRIUS, MURPA

"What nations don't know can hurt them. The stakes involved in study abroad are that simple, that straightforward and that important. For their own future and that of the nation, college graduates today must be internationally competent."
From the Lincoln Study Abroad Fellowship Program Report which summarizes a growing number of calls for students, anywhere in the world, to become globally aware and internationally competent.

In 2004, against a backdrop of growing globalization of the workplace and need for international collaborations in scientific research, PRIME—the Pacific Rim Undergraduate Experiences program (prime.ucsd.edu)—was launched by UCSD and PRAGMA partners in Japan (CMC, Osaka University), Taiwan (NCHC), Australia (Monash), and China (CNIC). PRIME provides opportunities for UCSD students to participate in international research and cultural experiences with host-site mentors and colleagues, along with UCSD-based mentors. The activities of the student researchers contribute to the growth of the cyberinfrastructure through the development, testing, and running of application codes in an internationally distributed environment, including PRAGMA Grid.[1]



All Blacks rugby game—
courtesy of Sara Richardson.

The success of PRIME during its first two years sparked the establishment of PRIUS—Pacific Rim International UniverSity (prius.ist.osaka-u.ac.jp), through funding to Osaka University from Japan's Ministry of Education, Culture, Sports, Science and Technology (MEXT) for "Fostering of Globally Leading Researchers in Integrated Sciences," in tight cooperation with the PRAGMA community. PRIUS aims to nurture students' abilities to take a leadership role in next-generation integrated science, as well as offer an international perspective on both academic and industrial societies through tight collaboration with PRIME and PRAGMA. The PRIUS program,

[1]PRIME is funded by the NSF (NSF, INT 0407508), with additional support from the UCSD division of Calit2, the National Biomedical Computation Resource, the Telemedicine and Advanced Technology Research Center, the Gordon and Betty Moore Foundation, partner and host institutions.

HOST SITE *and Mentors*	PRIME Student(s)	*UCSD Mentors (Affiliation)*	Project Title
OSAKA UNIVERSITY *Susumu Date (all students), Seiki Kuwabara (RChu), Atsushi Nakazawa (RChu), Haruo Takemura (RChu)*	Rachel Chu	*Jurgen Schulze (Calit2)*	Optimized Rendering for a 3D Videoconferencing System
	Phillip Pham	*Jason Haga (Bioeng)* *Marshall Levesque (PRIME 06)*	Identification of a Specific Inhibitor for the Dual-Specificity Enzyme SSH-2 via Docking Experiments on the Grid
	Simon Han	*Jason Haga (Bioeng)* *Marshall Levesque (PRIME 06)*	Virtual Screening for SHP-2 Specific Inhibitors Using Grid Computing
NCHC *Fang-Pang Lin (both students), Kevin Lin (DT), Kathy Ma, Hsiu-Mei Chou*	Daniel Tenedorio	*Jurgen Schulze (Calit2)*	Optimized Rendering for a 3D Videoconferencing System
	Lisa Yung	*Philip Bourne (Pharm)* *Lei Xie (Pharm)*	Identifying Off-Target Protein Binding
NCREE *Keh-Chyuan Tsai, Kung-Juin Wang*	Philip Ow	*Lelli van den Einde (SDSC)* *Charles Cowart (SDSC)*	Middleware development between NCREE and NEES Data Acquisition Systems
MONASH UNIVERSITY *David Abramson, Tom Peachy, Colin Enticott, Slavic Garic, Rob Gray*	Haley Hunter-Zinck	*Philip Bourne (Pharm)* *Lei Xie (Pharm)*	Hualien Analyzing Adverse Effects of the Antidepressant Emsam in Silico
	Lynn Tai	*Kim Baldridge (U Zurich)* *Joe O'Conner (Chemistry)*	Binding Energy and Mechanisms of Conjugated Enediynes with a Ruthenium complex
	Arielle Yabolonovitch	*Anushka Michailova (Bioeng)*	Optimizing Rabbit Ventricular Myocyte Model
	Randy Lee	*Roy Kerckhoffs (Bioeng)*	Effects of Tissue Level Parameter Variation on Cardiac Output
	M. Amalia Prada Fernandez	*Roy Kerckhoffs (Bioeng)*	Transmural Heterogeneity of Mechanics in the Normal Heart
	Sirvard Nshanyan	*Jurgen Schulze (Calit2)*	Medical Research Data Visualization on Tiled Display Wall
	David Allen Wong	*Jan Talbot (Nanoeng)*	Simulation of Particle Incorporation during Electrocodeposition Process
CNIC *Kai Nan, Zhonghua Lu, Jianju Yu, Guangyuan Lu, Yanhua Sun, Haiyan Xu, Wei Chen*	Michael Wang	*Wilfred Li (NBCR)*	Secondary Target Identification for Neuraminidase Inhibitor Drugs
	Kevin Wu	*Wilfred Li (NBCR), Rommie Amaro, Dong Xu, Lily Cheng (PRIME 06), Hsing Pao (PRIME 07)*	Identification of Inhibitors against Hemaglutinin from H5N1 Influenza Virus: the Ensemble based Virtual Screening approach with Relaxed Complex Scheme
USM *Habibah Wahab; Wai Keat Yam, Dr. Hassan, Dr. Choong Yee Siew. Sy Bing, Suhaini Ahmad*	Lihua Yang	*Wilfred Li (NBCR)*	Avian Influenza Virus H5N1 Polymerase Subunit PB2 Cap-binding Site Inhibitors
	Cindy Tran	*Wilfred Li (NBCR)*	Avian Flu: Neuraminidase
	Varahenage Perera	*Kim Baldridge (U Zurich)* *David Abramson (Monash)*	Comparison of AutoDock and GAMES/APBS Methods for Performing Molecular Computations on Biological Systems
U AUCKLAND *Peter Hunter, Poul Nielsen, Martyn Nash, Xinshan Li*	Sara Richardson, Connie Hong	*Roy Kerckhoffs (Bioeng)*	Computational Modeling of the Female Pelvic Floor: Investigation of Athletic Muscle Structure
U WAIKATO *David Hamilton*	Andrea Cardenas	*Tony Fountain (SDSC)*	Control Vocabulary Study for Global Lake Research

aimed primarily at graduate students, leverages the social networks already built through R&D collaboration in PRAGMA. The educational infrastructure comprises two main components: an internship experience and a course on international integrated science, taught mainly by members of the PRAGMA community (*see Date et al., 2008*).

Building on the momentum and strengths of both PRIME and PRIUS, Monash University established the Monash University Research Program Abroad (MURPA, *infotech.monash.edu.au/about/events/2008/murpa.html*) in 2008, to provide its students with an international experience conducting research projects. MURPA will send the first students overseas in January 2009, to UCSD. In preparation, they hosted a series of presentations from host site mentors via high-definition video feeds during July-September. The program focuses on students entering their honors year (between undergraduate and graduate years).

PRIME SUMMARY AND SCIENCE

During the five years of the PRIME program, more than 70 students have participated. Each year more students have expressed an interest and more have been accepted. In addition, there have been more women each year, bringing about a change towards gender balance (see Table 2). In 2008 the program expanded from four host sites: Osaka University, NCHC, Monash, and CNIC, adding three new ones: USM, University of Auckland and University of Waikato (the latter two are in New Zealand).

While PRIME prepares undergraduates for the global workplace of the 21st century by immersing them in both a research environment and a cultural landscape outside their own, it has also created stronger collaborations among participating PRAGMA institutions and researchers through the students' research projects.

The nature of these projects has generally been the development of technologies (e.g., visualization tools for datasets) or the application of grid and other technologies to science and/or engineering problems. See the table of the 2008 PRIME students, which has their host institutions, their mentors (home and away) and the areas they investigated over the summer.

Over the years, the vast majority of the students have been engineering majors with the rest science majors. Biology is the overarching discipline of interest: nearly all the science majors are in biology and among the engineers, about half are bioengineering majors.

Following are a few examples of projects. Some are work that has evolved over the last

Table 2: Number of Students (Female|**Total**) by Host Institution and Year

	2004	2005	2006	2007	2008	TOTAL
CNIC	-	0|**2**	3|**3**	0|**3**	0|**2**	3|**10**
MONASH	0|**3**	3|**5**	3|**4**	4|**5**	5|**7**	15|**24**
NCHC/NCREE	0|**3**	1|**3**	1|**3**	1|**2**	1|**3**	4|**14**
OSAKA U	0|**3**	1|**3**	1|**4**	3|**4**	1|**3**	6|**17**
USM					3|**3**	3|**3**
U AUCKLAND					2|**2**	2|**2**
U WAIKATO					1|**1**	1|**1**
TOTAL	0|**9**	5|**13**	8|**14**	8|**14**	13|**21**	34|**71**

Top: Olympic mascot Huanhuan—courtesy of Kevin Wu. Above left to right: Fun at the Sydney Opera House—courtesy of Randy Lee; Yuanmingyuan Park—courtesy of Hai-Yan Xu; PRIME and village students together in Malaysia—courtesy of Cindy Tran.

two to three years, where students in subsequent years build upon the progress of previous students. In addition, there have been students who have continued to extend the results of their projects over the rest of their undergraduate career, and in some cases, even beyond that.

Design of a Grid Service-based Platform for In Silico *Protein-Ligand Screenings: Focus Protein Phosphatase —research at Osaka University*

This work over three generations of PRIME students has created an infrastructure for virtual screening, has identified possible inhibitors to several key protein phosphatases, and has identified practical issues of conducting virtual screening on a heterogeneous grid. It has also strengthened the collaborations between UCSD and Osaka University.

Protein phosphatases are enzymes that play an important role in regulating the signaling pathways in cells and have been hypothesized to play a role in a variety of diseases including, diabetes, neurodegeneration, and cancer. Understanding how they regulate cellular function is an important challenge in biomedicine.

The question posed to PRIME students over several years has been how to take advantage of distributed computing resources to help screen known libraries of ligands in search of chemical compounds that disrupt the function of specific proteins, in this case phosphatases. The process involves the use of a docking software program, which needs to be repeated for all of the suitable ligands in the collection (library) of interest, which can involve tens of thousands of calculations. The value of this *in silico* approach is that it is cheaper and faster to identify possible ligands in the library than attempting to perform biochemical experiments with each and every one.

PRIME 2006: At the end of the summer, Marshall Levesque, Cathy Chang, and Daniel Goodman successfully created an infrastructure that enabled access to DOCK programs on multiple cluster systems from remote sites and succeeded in plugging the docking software, Dock, into the PRAGMA Grid testbed for the distribution of its computational workload. They also used a middleware Opal Operation Provider (which was extended from Opal by Mr. Ichikawa during a PRIUS stay at UCSD).

During the following academic year, Marshall continued to work with UCSD mentor Jason Haga to improve the infrastructure and to continue to use the infrastructure for specific phosphatase screenings.

PRIME 2007: Ellen Tsai continued the project, using the improving infrastructure to identify inhibitors to phosphatases related to ones used previously, with a long-term goal of developing chemical inhibitors that would prevent the catalytic activity of the specific isoforms of these phosphatases. She performed a screening of a large database (ZINC) and via computational tools, identified 10 unique inhibitors.

The following spring (2008), Marshall Levesque had his first paper accepted, it discussed the infrastructure (*see Levesque 2008a*) developed for virtual screening. During the academic year, he continued Ellen's work with further screening to verify the accuracy of the initial results. Levesque continued by performing phosphatase activity assays to characterize the inhibitory efficacy of several of the compounds identified in the virtual screening. Marshall also served as a mentor to

his successors on the project, Ellen in 2007 and Phillip Pham and Simon Han in 2008.

PRIME 2008: Phillip Pham and Simon Han utilized the continually improving infrastructure and system on specific protein targets. Simon Han continued the work of Ellen Tsai by rescreening against a new target. Preliminary results suggest several inhibitors that can be further tested and validated in various *in vitro* laboratory experiments. Phillip Pham focused on identifying a specific inhibitor to another protein phosphatase, one which plays a significant role in different cell functions such as growth and movement. His efforts revealed a very promising inhibitor, which will be verified with wet bench testing. They have both written papers for possible publication, which discuss complications during these multiple, virtual screenings on the grid, as well as potential improvements for routine use of the grid environment for virtual screening.

Ensemble-based screening and the Avian Flu—research with CNIC and USM

Avian influenza has received worldwide attention due to its rapid global spread via migratory birds and the growing number of human cases. The highly pathogenic avian influenza virus that the World Health Organization fears may cause a pandemic in humans comprises strains from the subtype H5N1 of influenza type A. Sub types of influenza virus are named based on the observed combinations of two viral surface membrane glycoproteins, hemagglutinin (HA) and neuraminidase (NA), with 16 and 9 types known to date respectively. The challenge faced by researchers is how to quickly screen large libraries of chemical compounds to rapidly identify potential inhibitors to these proteins.

The Avian Flu research project has enjoyed the active participation of PRIME students since 2006, and has produced a number of scientific publications, including a recent one first-authored by Lily Cheng (PRIME 2006). Using a novel approach, she and her colleagues have isolated more than two dozen promising compounds from which new "designer drugs" might be developed to combat Avian Flu. In some cases, the compounds appeared to be equal or stronger inhibitors than currently available anti-flu remedies. Several are currently undergoing testing in the lab. In the press release announcing this breakthrough, Cheng noted, "Importantly, half of these compounds would have been neglected based on the crystal structure simulations alone. Many of these drug leads would only have been found through the use of this computational method."

As with the work at Osaka on phosphatases inhibitors, it is clear that a persistent approach to studying a subject yields rewards.

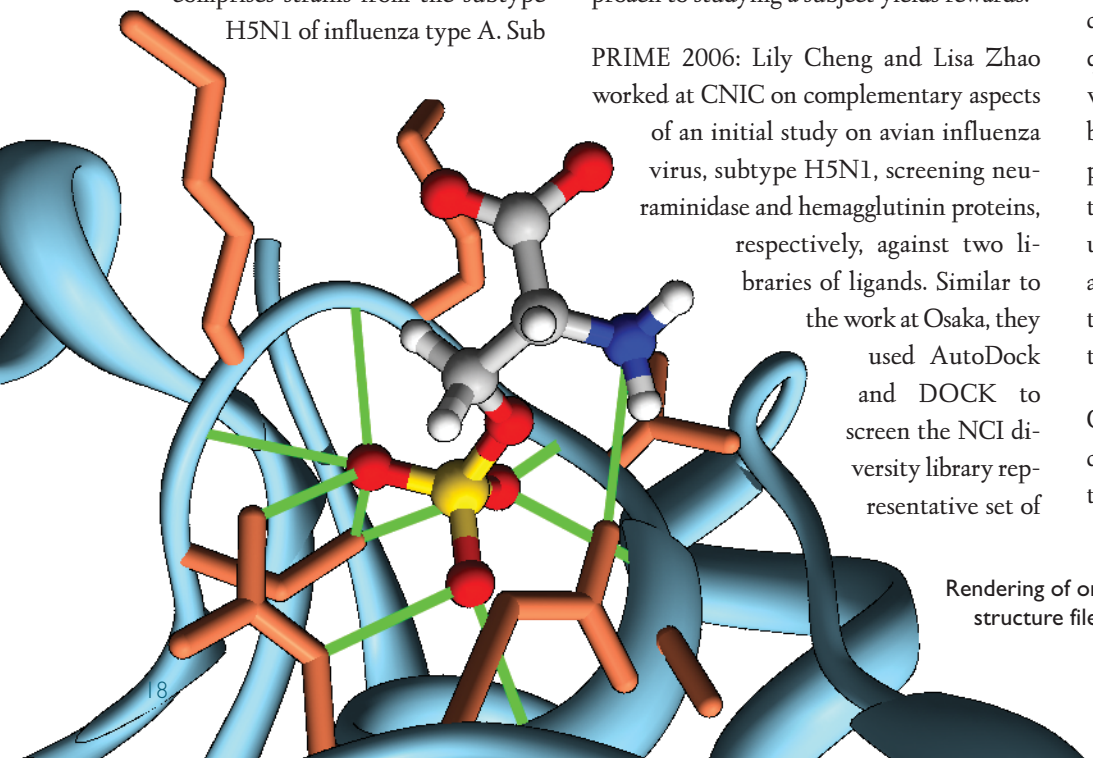
PRIME 2006: Lily Cheng and Lisa Zhao worked at CNIC on complementary aspects of an initial study on avian influenza virus, subtype H5N1, screening neuraminidase and hemagglutinin proteins, respectively, against two libraries of ligands. Similar to the work at Osaka, they used AutoDock and DOCK to screen the NCI diversity library representative set of 2,000 compounds, and 1,000,000 ZINC library compounds.

Subsequently they visualized some of the models with the best binding energy. In addition, initial steps were taken to develop a database to share the screened products. This work stimulated a broader collaboration between researchers at UCSD, CNIC, and other PRAGMA partner sites. Furthermore, these initial results helped UCSD researchers to obtain an award from TATRC (Telemedicine and Advanced Technology Research Center) to continue this work.

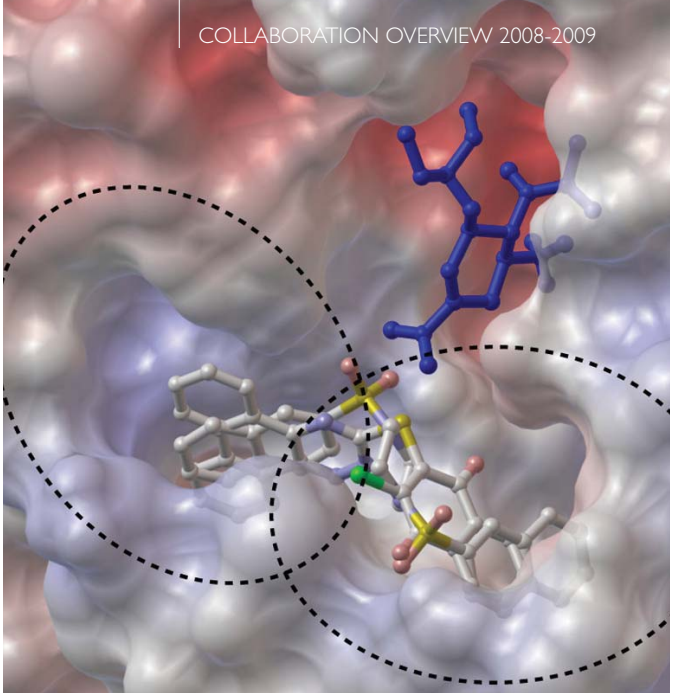
Lily Cheng continued to work on this project with a larger group of researchers associated with the National Biomedical Computation Resource (NBCR), upon returning to UCSD. She and her colleagues applied a more sophisticated approach, the Relaxed Complex Scheme (RCS) (*see Amaro 2007*), to identify more possible binding sites in NA. This RCS allows for full receptor flexibility (often missed in other virtual screening approaches).

PRIME 2007: Hsing Pao continued the work and focused on the binding affinity of hemagglutinin's receptor binding domain with the receptors containing silalic acid (SA), which exhibit different preferred glycosidic linkages for birds (SA α-2, 3-Gal) and humans (SA α -2, 6-Gal). He used a combination of tools including Modeler and AutoDock and subsequently, he visualized some of the models with the best binding energy. In addition, he built upon the efforts of the students from previous years to develop a database to share the virtual screening hits. Hsing has continued his work with the team, and is now a co-author of a paper submitted for publication that examines the relationship of glycan topology and binding ability of HA.

Cheng stayed with NBCR after graduation to complete her current work and has now entered medical school at UC Davis. Like Mar-



Rendering of one of the top molecules inhibiting the crystal structure file of SSH-2 created by Phillip Pham.



Top: Apo Crystal, Cross Cavity Binders created by Lily Cheng. Below: Monkey in the Penang Botanical Gardens—courtesy of Vicky Yang

shall Levesque, Cheng has served as a mentor to successive PRIME students working on the project (2007 and 2008).

PRIME 2008: Four students worked on aspects of the Avian Flu project, two in CNIC and two in the new site of Universiti Sains Malaysia (USM). At CNIC, Michael Wang continued the work of Lily Cheng and studied secondary target identification for neuraminidase inhibitor drugs by identifying human proteins that may have similar SA binding pockets. His work has resulted in the knowledge of a potential human secondary target that needs to be taken into consideration during drug development to avoid potential side effects. Kevin Wu, also at CNIC, worked on the identification of inhibitors against HA from the H5N1 Influenza Virus, using the RCS for ensemble-based virtual screening that incorporates molecular dynamics simulations to account for protein flexibility.

At USM, Cindy Tran studied the effectiveness of potential Avian Flu inhibitors against NA mutations by characterizing the effect of the known NA mutants resistant to oseltamivir (Tamiflu). Together with her colleague at USM, she has identified 30 natural and synthetic compounds that are effective against these mutants. Lihua (Vicky) Yang searched for inhibitors against the avian influenza virus H5N1 polymerase subunit basic protein 2 (PB2) cap-binding site. She was able to build a model of the H5N1 PB2 cap-binding domain based upon a H3N2 PB2 structure, and found 10 potential hits against this important virulence factor in H5N1. Both students explored the USM natural compound library, compiled by Dr. H. Wahab, many of which are only available in native plants in Malaysia.

Optimized Rendering for a Three-Dimensional Videoconferencing System—research with Osaka University and NCHC

Industry widely employs the two-dimensional videoconferencing system as a long distance communication tool, but current limitations such as its tendency to misrepresent eye contact prevent it from becoming more widely adopted. 2008 PRIME students Rachel Chu (Osaka) and Daniel Tenedorio (NCHC) began exploring the possibility of a three-dimensional videoconferencing system for future interactive streaming of point cloud data. While they are basing their work on only this year's activity, the development of the infrastructure was started, in part, by PRIME students at Osaka University in 2006 (Robert Sy helped establish a tile display wall) and 2007 (David Jackson and Ava Pierce developed modules for Covise). This year the students and their tri-site team were able to develop the infrastructure and algorithms to test a system with one sender.

The sender, encircled by high-definition cameras, stands and speaks in a room. A cluster of computers reconstructs each frame of the camera images into a 3-D point cloud and streams it across a high-speed, low-latency network. On the receiving end, a splat-based renderer employs a new algorithm to efficiently resample the points in real-time, maintaining a user-specified frame rate. Parallel hardware projects onto multiple screens while head tracking equipment records the viewer's movements, allowing the receiver to view a stereoscopic 3-D representation of the sender from multiple angles. The researchers can combine these visuals with appropriate use of multiple audio channels to forge an unpar-

alleled virtual experience. This next step towards immersive 3-D videoconferencing brings researchers closer to empowering worldwide collaboration between research departments (*see Chu et al., 2008*).

Modeling the Heart—research with Monash University

Five years of close collaboration between the Monash and UCSD collaborators helps grow our knowledge on the ionic and metabolic mechanisms underlining cardiac cycle with each new modification to the model.

PRIME 2004: This modelling effort began with John Colby. He identified parameters that improved the stability of the complex ATP/ADP/Mg model and its agreement with experimental measurements under a wide variety of conditions.

PRIME 2005: Jordon Nevo and Dorothy Dederko built on John's work. They identified parameters that improved the stability of the complex whole cell model in rabbits and dogs and determined their agreement with experimental measurements. By experimenting with different models, they were able to compare the behavior of the models under different conditions.

PRIME 2006: Angelina Altshuler and Iwen Wu assisted in the development of more stable ionic models in rabbit (LabHEART) and human ventricular myocytes, over long time periods and at different frequencies of stimulation. Those improvements enable calculation of, for example, ionic currents, Ca-transients, and action potentials. In agreement with the experiment the single cell model in rabbits predicted qualitatively Ca^{2+} and action potential alternans at high frequencies above the point where the model was physiologically stable.

PRIME 2007: Stephany Chang investigated the ionic properties of ventricular myocytes, and used Nimrod/O and Nimrod/G to conduct parameter searches to identify parameters that would produce a stable model in the epi- and endo- tissue sub-layers under normal conditions. Saleh Amirriazi's work focused on modeling the effects of ATP-dependent potassium current in regulating excitation metabolic coupling in endocardial ventricular myocytes under normal condition and 20 minutes of simulated ischemia. He used a new member of the Nimrod family, Nimrod/E for experimental design in conjunction with Nimrod/O, to validate a model (*see Peachey 2008*).

The Nimrod/G and Nimrod/O tools, developed at Monash, have been and are being used to find parameter values in the model that generate outputs in accordance with experimental data. There are a total of 17 parameters being analyzed and optimized so that the model to reach steady-state for a time period of 60 seconds at stimulation frequency of 0.5 Hz. Graphical analysis is being used to determine which combination of parameter values yields the most accurate outputs.

PRIME 2008: Arielle Yablonovitch further extended the ionic-metabolic model to reproduce more accurately the available experimental data in rabbit cardiac cells. Now this model is able to simulate the cell cycle during cardiac excitation-contraction coupling and its outputs predict Ca^{2+} transients in different cell regions (cleft, sub-membrane space, bulk cytosol, sarcoplasmic reticulum) as well the ATP-dependent potassium current and action potential

PRIME AT FIVE

CHANGING LIVES, CHANGING CAREER PATHS, CHANGING SCIENCE

PRAGMA met with several PRIME students from the first two years, now that they have some distance from the program, to learn from them how they feel the PRIME experience has helped shape where they are today. All are thrilled to have been part of the program and grateful for the educational and cultural opportunity it gave them. For some, the cultural immersion proved to have the deepest effect.

Robert Ikeda (2004) is now a third-year doctoral student studying computer science at Stanford University. "Before PRIME, I did not know much about computer science," he says, "But afterwards, I was encouraged to learn more, and I eventually decided to pursue a Ph.D. PRIME was my first opportunity to work on a serious software project, and I am thankful for how it has helped shape my academic interests."

While at the National Center for High-performance Computing (NCHC) in Hsinchu, Taiwan, Ikeda pursued the development of a graphical user interface for pathway editing and integration in Cytoscape, a bioinformatics software platform for visualizing molecular interaction networks and integrating them with gene expression profiles. This was for large-scale, computer-aided models of biological signaling and regulatory pathways. *Robert's work produced the Cytoscape Plug-In Hyperbolic Focus (www.cytoscape.org/plugins2.php).*

When he returned to UCSD for his junior year, he kept his electrical engineering major and took computer science courses as electives. The cultural aspect of PRIME was even more significant for him.

"The biggest effect of the program is that now I am more open-minded and aware and appreciative of the world's cultures," he explains, "I still have a lot to learn, but visiting Taiwan made me realize that there is a whole world outside of the United States. I think my willingness to be open-minded and attentive was why I had such a good time. The people I met were welcoming and made me feel like I had a story to share as well. My summer in Taiwan was my most memorable."

Shirley Lee (2005), also went to Taiwan, one year later, after hearing about PRIME from Ikeda. "The most significant aspect of participating in the program was the impact on my personal life," says Lee, "Born and raised in California, there was a disconnect between myself and my siblings, with our parents who had grown up in Taiwan," she adds, "Spending ten weeks in the country of my parents and grandparents, I came to understand my family better, which really is to understand myself better."

While at NCHC, Lee, a bioengineering junior, enhanced the display interface plug-in first developed by Ikeda for Cytoscape. Both Ikeda and Lee worked with advisors Fang-Pang Lin, NCHC's Grid Computing division manager and Trey Ideker, a bioengineering assistant professor at UCSD.

"Without question, PRIME was the most influential experience I had during my time as an undergraduate at UCSD." John Colby (2004)

"The program made me realize how software solutions can evolutionize or revolutionize most, if not all, industries," Lee adds, "If you initially spend the time required to create the program, you can save a lot of time in the long run. Currently, I am in the medical device industry which is documentation-intensive. Already, I see how software solutions are transforming my everyday work environment for the better." Lee has been a quality engineer at Abbott Vascular for over two years. She analyzes and manages risk to patients by implementing statistically-based sampling plans to ensure product quality.

Lee also looks at the world differently because of her PRIME experience; she explains, "It showed me that there is literally a world of opportunities for people who want to collaborate with others around the globe and work towards achieving a common goal. I now feel comfortable and open to the idea of living and working outside of the United States."

Laura Berstis (2005) has put that insight into action. She is living abroad, as a graduate student at the University of Zurich, currently finishing her master's degree on the way to beginning her formal Ph.D. program in theoretical computational chemistry. She is working with her advisor, Kim Baldridge, to whom she was introduced via the PRIME program. Berstis worked on computational biology tools while at Monash University in Australia, with David Abramson and Baldridge (who is also an adjunct professor at UCSD) as her mentors. Berstis' master's thesis project involves computational studies of the interactions and differences between small molecular nucleic acid systems. She expects it to be completed at the end of the year, so she can begin her doctoral work in January.

Before leaving for Monash in 2005, Laura, the then 20-year-old sophomore and aspiring bioengineer said: "I applied to PRIME because I wanted to experience different avenues of research and in general to explore possibilities for what I want to dedicate my life to." She was one of the few sophomores

accepted into the PRIME program at that time.

What she says now: "It may sound 'cheesy' said so bluntly, yet it couldn't be more true—the PRIME program truly changed my life!"

"The PRIME program definitely had a major impact on me, and my future academic choices. I had a fantastic experience working in Australia on my project," she explains, "And, I continued working on projects during my final years at UCSD, including coming to Zurich for a second academic internship position. When it came time to apply to graduate schools, I was also considering medical school and pursuing an M.D.-Ph.D. degree as my next step. However, I found that the opportunity to move to Zurich and work with Kim was another incredible chance, as with the PRIME program, to again explore a significantly different location, culture, and to simultaneously further my scientific/academic career, and expose myself to a new environment, learn a new language, and learn from the lessons and hurdles experienced when living abroad for a longer period of time."

When it came time for choosing graduate schools, John Colby (2004) opted for the M.D.-Ph.D. program and is now in his third year (of eight overall) at UCLA. He is pursuing the Ph.D. in biomedical engineering, with a specialization in neuroengineering. His thesis is in developmental neuroimaging. Before beginning medical school at UCLA, Colby worked for a year in industry at SAIC in La Jolla, where we worked with a group to develop biosensors.

Colby also went to Monash with PRIME and had Abramson as his host advisor; his UCSD advisor was Anushka Michailova, a senior research scientist in Andrew McCulloch's Cardiac Mechanics Research Group lab. He studied the impact of temporal and spatial distribution of two pacemakers around the heart to understand therapeutic optimizations. "I remember my first student [John]," recalls Michailova, "He was so excited with this program." He still is.

"Without question, PRIME was the most influential experience I had during my time as an undergraduate at UCSD," states Colby, "The foundation of knowledge in high performance computing that I acquired through PRIME is something that I have continued to use everyday in my research career—whether it be modeling mass spectrometry signals or distributing a computationally challenging MRI analysis across a cluster environment. I have no doubts that this will continue to be true in the future as well, as complex computational and informatics problems continue to be become more and more important to diverse fields of biomedical research.

"Still, to me, the most significant aspect of the program was the first-hand experience it delivered in planning and leading a research collaboration. This type of training is integral for the coming generations of scientists and clinicians, who must navigate an ever more specialized and collaborative research environment," adds Colby, "And the fact that all of this was done literally thousands of miles away from UCSD, our friends, and home mentors, simply cannot be understated. Not only did this jump start our leadership role in the collaboration, but it also helped us to develop an independent problem solving mentality that is beneficial to a career in science—and for that matter—daily life. Because these collaborations were developed at the international level, PRIME also gave us an invaluable opportunity, and one that is exceedingly rare for undergraduates in science and engineering, to experience another culture through a study-abroad type program in another country."

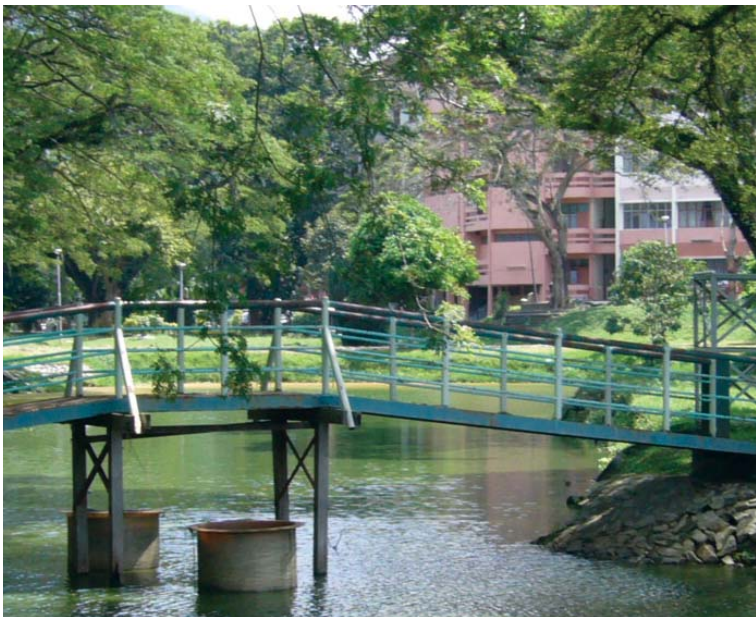
Berstis summarizes both the past experience with PRIME and the future, when she says, "My German is definitely improving; and with this I feel quite liberated, knowing that I could move to practically any country in the world, learn a new language and culture, and still thrive. In a way it makes the world feel so much more interconnected, as it truly is, in terms of research collaborations, cultural interactions, and also physically without such distinct national borders appearing as barriers anymore."

The PRIME, PRIUS, and MURPA programs are models for nurturing and preparing students to take leadership roles in next-generation collaborative international science. The internship experiences offer students a valuable perspective on society and research at the international level, thus grooming students to be effective, culturally competent members of the global science workforce.

PRIME: **prime.ucsd.edu**

PRIUS: **prius.ist.osaka-u.ac.jp/en**

MURPA: **infotech.monash.edu.au/about/events/2008/murpa.html**



time-course. It also takes into account the regional physiological differences between the cells isolated from the endocardium and epicardium and can simulate Ca^{2+} transients under both normal and ischemic conditions.

PRIUS SUMMARY AND SCIENCE

The PRIUS program has four years of experience. As noted in the table below, there have been a total of 20 students who have participated in PRIUS, and researchers from 19 institutions. This program spans 19 Institutions in 13 countries, and extends beyond PRAGMA sites. Following are two examples of PRIUS research. Note that the Opal OP work dovetails with the research by PRIME students on In Silico Protein-Ligand Screenings focusing on the protein phosphatase discussed earlier.

Opal OP—research at UCSD

Kohei Ichikawa developed the Opal Operation Provider (Opal OP). OPAL OP is based on OPAL, a web service to wrap existing applications, developed by the NBCR. He worked with mentors Wilfred Li and Sriram Krishnan of UCSD. OPAL OP allows for the interoperation of OPAL-based web services and Globus Toolkit (GT) 4-based grid service, the de facto standard middleware of the grid. Opal OP has been developed to offer the features of Opal as a plug-in module by leveraging the plug-in framework of GT4. After his stay at UCSD (winter 2005/2006), he returned to Osaka and worked with the Protein Data Bank Japan (PDBJ) to install Opal-based services.

Table 3: PRIUS Data

YEAR	VISITING LECTURERS *(no. researchers)*	INTERNSHIPS ABROAD *(no. students)*
2005	6	1
2006	13	4
2007	12	7
2008	12	8

Opal OP was tested and used by PRIME students to build a drug docking simulation service on the PRAGMA Grid. The drug docking service was deployed over five sites, seven clusters, and 150-200 processors were being used at one time depending on Grid workload and averaged 180 processors. The screening took a total of 11.56 days of laboratory time, which is the equivalent of 2,081 CPU days (over 5.5 years). Ichikawa continued his involvement with the PRIME students upon his return. This has resulted in joint publications (Levesque et al, 2008, Pham et al, 2008, Han et al, 2008). This experience has helped build strong ties between UCSD and Osaka University, it also provided components of Ichikawa's dissertation. Ishikawa is now on the faculty at Kansai University in Osaka.

Security Monitoring System—research at NTU in Singapore

Shingo Takeda, a Ph.D. student at Osaka University, was a researcher at Nanyang Technological University in Singapore in summer 2006, under the mentorship of Bu Sung (Francis) Lee. Takeda designed and prototyped a grid security monitoring system, taking advantage of the Multiple Organizational Grid Accounting System (MOGAS), developed at NTU. The prototype graphically visualizes the information aggregated from a variety of services deployed among grid resources, and has a flexible access-control mechanism based on RBAC to protect user and site privacy. The system can help grid managers and site administrators find security problems easily and quickly.

The developed security system was set up and tested on the PRAGMA testbed. More specifically, the security sensor was deployed over seven PRAGMA testbed sites, with the database located in NTU in Singapore. Results of an experiment performed from August 21,2006 to March 11, 2007, showed the system succeeded in detecting 172,150 resource requests from 30 users. Statistics based on the information recorded indicated that 75% of all requests, were successfully processed and 25 % of all requests failed (99% of failures were authentication errors, 1% were authorization failures).

This project was extremely successful in building ties with NTU and other PRAGMA sites and providing feedback to the PRAGMA community. These results were part of his thesis.

MURPA: THE PROGRAM

See Accomplishments, p. 12

Left: Universiti Sains Malaysia—courtesy of Cindy Tran.

WORKING GROUPS

The working groups below reflect the interests of current PRAGMA members. Each group has a lead or coleads who coordinate the activities of that group during and between meetings. Each group has projects that bring a focus to their activities, working towards milestones and giving demonstrations at PRAGMA workshops and other meetings. This structure allows for the inclusion of new applications, as well as new areas of interest.

RESOURCES AND DATA-WORKING GROUP

The Resources and Data Working Group's goal is to improve the interoperability of grid middleware and to make grids easier for scientists to use. During the past year, the group has expanded the PRAGMA Grid and its routine-basis experiments, as well as continued to conduct peer-grid interoperation experiments.

During the last year, the PRAGMA Grid has grown to 27 sites in 15 countries/regions with total of 1008 CPUs, more than 1.3 terabytes of memory, and over 24.7 terabytes of online storage.

Application numbers have grown to more than 20 this year, with topics ranging from biology to aerodynamics, from chemistry to sensor data analysis. Most of the applications continue to utilize grid middleware, such as Ninf-G, Nimrod/G, Gfarm, or CSF. These routine-use experiments also resulted in continuous enhancements for all application middleware involved. See Table 1 for some specific examples.

We also continued and expanded our grid interoperation effort by running a structural biology application, Phaser, across PRAGMA Grid, OSG and SwissGrid. See also *Accomplishments Bridging Grid Islands*.

PRAGMA Grid has become an essential resource and support to the PRIME program. This summer, eight students ran applications and worked on their projects using the PRAGMA Grid and getting support and learning from the experts on the PRAGMA Grid team.

Grid infrastructure middleware continues to develop and improve in the PRAGMA Grid. For example, three important new functions have been added to the grid monitoring system, SCMSWeb, in the past year: *Automated Alert* informs site administrators when a site system fails; *Software Catalog* indicates the available software on monitored resources; and *Bandwidth Measurements* provides real-time bidirectional bandwidth measurements of the mesh. Many middleware products have matured and been deployed as services in PRAGMA Grid. For example, a third Nimrod portal, a CSF server and a UNICORE system have been deployed and used during the past year. Furthermore, integration and collaboration activities among middleware developers have increased. For example, collaborating with Condor, a SCMSWeb-Condor interface was developed to provide rich resource information collected by SCMSWeb and enables Condor to perform more intelligent grid-wide scheduling services (*see also Accomplishments on Grid Monitoring Development*). Similar collaborations are in progress between SCMSWeb, CSF (Community Scheduling Forum) and MOGAS (Multi-Organizational Grid Accounting System).See Table 2 for some key middleware activities in PRAGMA.

While expanding our existing computational grid, the resources group has also been building a data grid in the PRAGMA Grid with Gfarm software. For three years, the Gfarm development team has collaborated with many PRAGMA Grid sites, testing and improving Gfarm software. The most recent version 2.1.1 was released September 2008. It added support to GSI (Grid Security Infrastructure), group management, disk usage report and replication on-demand capabilities. A Gfarm meta-server for the data grid has been set up with Gfarm v2.1.1 at the San Diego Supercomputer Center (SDSC). The U. of Tsukuba, AIST, and SDSC will lead the Gfarm testing and deployment in the PRAGMA Grid. In addition, the MOGAS team at NTU, Singapore will collaborate with U. Tsukuba and all PRAGMA Grid sites, working on integrating MOGAS with Gfarm.

To enable interoperation with other grids, with the help of APGrid PMA and NAREGI-CA developers, the group has built the PRAGMA-UCSD CA service for PRAGMA Grid at SDSC according to the most current IGTF recommendations and guidelines. (*goc.pragma-grid.net/ca*) PRAGMA -UCSD CA was accredited by APGrid PMA

in April 2008. It started operation and became a part of IGTF distribution in July 2008. Since then, PRAGMA-UCSD CA has issued 10 host/service certificates which enabled many critical services in PRAGMA Grid, including Grid Operation Center, VOMS, Condor, portal and other compute services *(see Accomplishments on* PRAGMA CA - VOMS*)*.

PRAGMA Grid, being a "grass root" and loosely coupled global grid, does not have a uniform infrastructure management. One aspect of this characteristic is that user access setup has been done independently at each site. A user has to communicate and verify access with each site, one at a time. To automate the user access setup, but still accommodate the diversity of management and policies among PRAGMA Grid sites, the group built a VOMS service at SDSC, which uses VOMS to manage groups based on projects and maps them to accounts at each site. Any additions or changes in existing groups require only trivial work by a VOMS administrator. This not only reduces work load for both site administrators and application users, but also speeds up and simplifies the user access setup process in PRAGMA Grid.

The group has always been very active in knowledge sharing with broader grid communities. Many members in this group have participated in many conferences, such as SC08, ACOMP2008, OGF, CCGrid, Grid Asia, etc. Also, in the past year, PRAGMA started organizing PRAGMA Institute training programs, where many members of the resources working group have given numerous presentations and tutorials. Many collaboration teams in the group also published papers and documented issues, solutions and lesson-learned on the many major projects in which they are involved. Finally, members of the Resources working group were involved in the Summit on Applications and Grid Middleware for the PRAGMA, Swiss Grid and Euro Grid Associations in March 2008 *(see Accomplishments, Expanding the Community)*.

Overall, the Resources Working Group aims to develop, deploy, and test all layers of grid software which can simplify and ease the use of grids for scientists. In the coming year, the group focus on developing and testing meta-scheduling software and portal services, building datagrids and linking sensor networks to the PRAGMA Grid, as well as running more diverse applications to utilize and test datagrid and sensor networks. Future challenges - include seeding real science applications and helping more scientists begin using the grid.

ACKNOWLEDGEMENTS: The Resource and Data Working Group as well as PRAGMA in general welcome and wish to acknowledge the contributions of institutions participating in PRAGMA and the PRAGMA Grid effort but have not yet become official members *(see Supporting Institutions)*.

MORE INFORMATION: See *goc.pragma-grid.net*; see *Publications* for several research publications.

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COMPUTE GRID ONLY: *AIST, ASGC, BeSTGrid, Binghamton U., CNIC, CUHK, HCMUT, HUT, IOIT-HCM, IHPC, KISTI, JLU, LZU, MIMOS, Monash, NCHC, NECTEC, NGO, Osaka U., SDSC, ThaiGrid, U. Chile, Nat. U. Mexico (UNAM), U. Chile, UoH, U. Puerto Rico Mayaguez (UPRM), USM (Computer Science and Pharmaceutical), and U. of Zurich.*

RESOURCES: *APAC (host MyProxy, NCSA), SDSC (host CA, VOMS, Nimrod portal, Bioportal, GOC, Condor-g with SCMSWeb interface, CSF, GLEON-INCA).*

Table 1: Key application activities in PRAGMA Grid

APPLICATION MIDDLEWARE	DOMAIN DRIVER	INSTITUTION	STATUS
Avian Flu/Gfarm, CSF4	Genomics	UCSD, USA	On-going
CSTFT / Ninf-G	Environmental Science	UPRM, Puerto Rico	On-going
Data Turbine	Grid Scalability	SDSC, USA	Starting
e-AIRS	Aerodynamics	KISTI, Korea	On-going
fRMI / xWFL	Grid Workflow/Scheduling	UMelb, Australia	Starting
Phaser / Nimrod	Structural Biology	MU, Australia	On-going
Sand-Winds	Air Fluid Dynamic	LZU, China	On-going
Drug Design	Medical Research	LZU, China	On-going
Percolation	Material Science	KISTI, Korea	On-going
Protein-folding	Organic Chemistry	KeioU, Korea	Completed
Siesta / Nimrod	Molecular simulation	UniZH, Switzerland	On-going

Table 2: Key middleware activities in PRAGMA Grid

MIDDLEWARE	DEVELOPER INSTITUTION	SOFTWARE INTEGRATION
CSF4	Jilin University, China	Gfarm, SCMSWeb
Gfarm	AIST/University of Tsukuba, Japan	Rocks, CSF4, SCMSWeb
MOGAS	NTU, Singapore	SCMSWeb
Naregi-CA	Naregi, Japan	GAMA
Nimrod	Monash, Australia	Unicore
Ninf-G	AIST, Japan	Rocks, NorduGrid
OptIPuter	Calit2, USA	Rocks, GLIF
Rocks	SDSC, USA	Ninf-G, Gfarm, SCMSWeb, OptIPuter
SCMSWeb	ThaiGrid, Thailand	Rocks, Gfarm, CSF4, MOGAS

BIOSCIENCES WORKING GROUP

Bioscience applications are very diverse, with different computing and data management requirements. The working group aims to conduct cutting edge scientific research using available computational resources from the PRAGMA Grid and high-performance computing clusters, such as the TeraGrid. In addition, we work with computer scientists to ensure that emerging technologies meet the requirements of biological applications through cross-working group interactions. Lastly, by engaging scientific expertise to address biological problems of common interest through international partnerships, we expedite research and development activities through seminal research, training and dissemination activities in the global community.

One major focal activity of the Biosciences Working Group has been their work on addressing the emerging pandemic threat of the avian influenza virus, in particular, the H5N1 subtype. They have established a virtual organization called Avian Flu Grid to facilitate data and resource sharing, and algorithmic development in the ongoing fight against infectious diseases. This activity has provided specific usage scenarios for middleware such as CSF4, Gfarm, Glyco-M*Grid, Opal, and their transparent access through various types of user applications and problem solving environments such as portals and workflow tools. For example, CSE-Online is an enabling online gateway for virtual screening on the PRAGMA and TeraGrid grids; Vision is a desktop workflow application that may access Opal-based web services for applications such as AutoDock4 and NAMD2.

The Biosciences Working Group has actively participated in the training and dissemination activities offered by projects such as PRIME, PRIUS, and MURPA. (See PRIME, PRIUS, MURPA section for more details.) The students from these projects have contributed to various aspects of the Avian Flu research, from the discovery of novel hits for potential Avian Flu inhibitors, to middleware components that are reusable by other researchers. They have fostered close ties between researchers around the Pacific Rim working on similar problems, and promoted both cultural and scientific exchanges.

Lastly, together with the Resources working group, we have begun to refine the requirements for the Avian Flu Grid, and identify new emerging technologies that may prove beneficial to biosciences research, and further reinforce the routine use of distributed resources.

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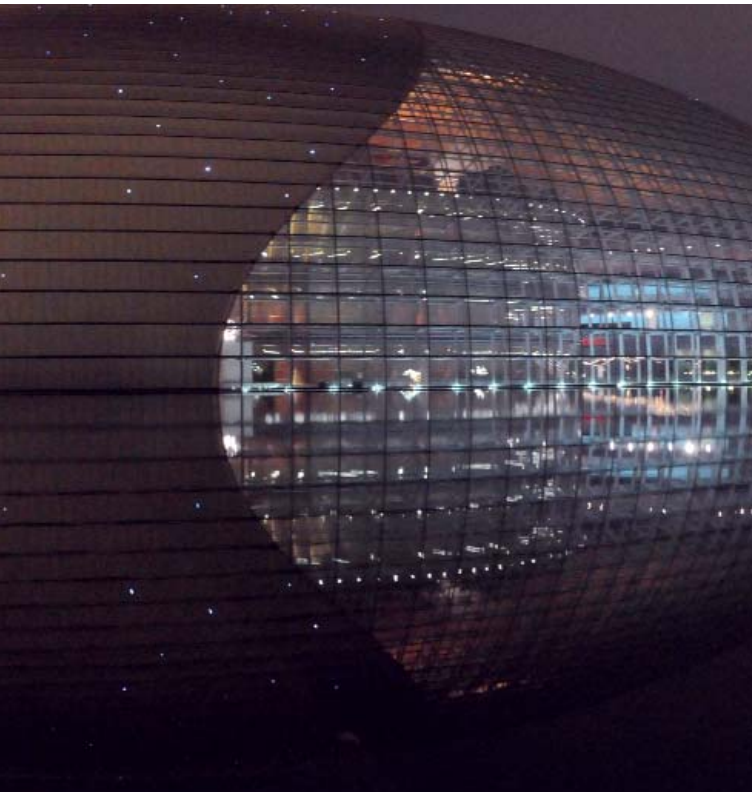
PRAGMA BY THE NUMBERS

(as of 24 October 2008)

29 clusters
27 Institutions
15 countries and regions
1008 CPUs
> 1.3 terabytes of memory
23.7 terabytes of online storage
24 compute sites in all, another 11 in preparation



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TELESCIENCE WORKING GROUP

The Telescience Working Group aims to create and develop new information technology that allows scientists to remotely use advanced scientific devices and to demonstrate future science on an advanced cyberinfrastructure. Examples of such devices include high-accuracy scientific measurement devices, such as ultra-high-voltage electron microscopes and synchrotron facilities, and highly sophisticated visualization facilities, such as tiled-display walls (TDWs). The working group's activities have gained in importance and expanded year by year because of the ubiquity and maturity of high-speed network technology.

The R&D activities in the Telescience Working Group fall into three types of projects. The first, and most traditional activity, is the establishment of a grid workbench for neuroscience, which will allow experts to use electron microscopes and control them remotely. The second is Ecology Grid which originated by NCHC's efforts and has led to other grass roots efforts and collaborations such as the Global Lake Ecological Observatory (GLEON) and the Coral Reef Ecological Observatory Network (CREON). The third and final component is the use and dissemination of tiled-display wall technology as a means for sharing information and collaborating. We summarize key progress for the past year in two of these areas.

Ecological Grid is a project inspired by the Telescience project. It aims to establish a grid environment where scientists can monitor environmental factors such as temperature and humidity using environmental sensing devices. The application area of the Ecological Grid is lake metabolism, agriculture, and coral reef studies. GLEON grew out of these activities, and could help as a testing ground as PRAGMA extends its testbed to include sensors. The GLEON activities are highlighted in video (see *gleon.org*). A recent highlight is the joint deployment of the data-streaming middleware, DataTurbine, by NCHC and UCSD, to monitor activity around the Kenting Coral Reef in Taiwan, a node of CREON *(see Accomplishments Streaming Underwater Video Cameras)*. This accomplishment linked together a data stream with the OptIPortal technology involving tiled-display walls, and was demonstrated at PRAGMA 14 in Taiwan. Furthermore, the middleware DataTurbine has been deployed at the Moorea Coral Reef Long-term Ecological Research site *(www.dataturbine.org)*. The NARC team continues to deploy Field Servers (for meteorological data collection), and their software MetBroker can now handle data from databases, predicted models, and real-time data.

Top: Beijing's Temple of Heaven. Below: Beijing's National Center for Performing Arits—both images courtesy of Hai-Yan Xu

A new wave is coming to the Telescience Working Group in the form of tiled-display walls (TDWs). Scientists and researchers in the group hope that this visualization technology not only provides an intuitive understanding of scientific results from both projects, but also establishes a multi-collaboration environment for future science. In addition to the discussion on how tiled-display technology is used for future science on a cyberinfrastructure, the development and the standardization of tiled-display technology is expected to be an area of collaboration. The Telescience Working Group also has helped incubate education and human development of internationally collaborative research groups. Through the PRIME and PRIUS projects, students from UCSD and Osaka University joined research teams of the Telescience working group in different counties for nine weeks. They experienced on-going research and cultural aspects of different countries. In particular, this year two PRIME students, one in Osaka and one in NCHC, developed and implemented algorithms in a prototype for three-dimensional video teleconferencing. See PRIME, PRIUS, MURPA section and Chu et al. in the Publications and References section.

Finally there were several cases of members of the group using high-definition (HD) cameras in their work. First, Osaka University and the University of Washington are experimenting with transferring HD images from the microscope using iVista. Second, the MURPA program is using HD video to hold lectures between UCSD to Monash *(see Accomplishments MURPA)*.

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COLLABORATORS: J. DeRoest, *U Washington*

GEO WORKING GROUP

The GEO Working Group is the youngest of the four current working groups in PRAGMA. The goal of the GEO Working Group is to develop a grid testbed to support geosciences and practical applications based on huge datasets of satellite imagery and GIS data, such as disaster prevention and environmental monitoring. During early meetings of this group, it was decided that development of the testbed should be coordinated with other international efforts, in particular, with the Global Earth Observation System of Systems (GEOSS), which seeks to achieve comprehensive, coordinated, and sustained observations of the Earth system, in order to improve monitoring of the state of the Earth, increase understanding of Earth processes, and enhance prediction of behavior.

The GEO Working Group is building on the strengths of its participants. In particular, AIST has a very strong effort on GEO Grid, which is developing an infrastructure to integrate remote sensing and GIS data from various sources. The preliminary design of GEO Grid involves integrating all the relevant data virtually as a set of services. The software architecture and its preliminary implementations are based on Grid computing, web service technologies and GIS standards defined by the Open Geospatial Consortium (OGC). The National Applied Research Laboratory (NARL) in Taiwan is a nonprofit organization with nine research institutions. NARL GEO (Global Earth Observatory)-Grid project is to deploy a high-resolution 3-D GIS platform for Taiwan. Disaster event GIS data, as well as typhoon forecasting, rainfall, and flooding data can all be displayed over the platform. NARL includes NCHC, which is integrating NARL's GEO-related projects including operating an earth-observing satellite Formosat-2 imagery, GIS information, 3-D visualization, GLEON, and typhoon monitoring and prediction. Finally, the iGEON project, which involves UCSD, UoH and CNIC, is developing tools to integrate heterogeneous databases associated with geosciences. The GEO Working Group will promote collaboration between these projects, bring more participants to this activity, and will begin technological integration of various components, with a particular focus on integration of data from various systems.

Left: Penang Butterfly Farm—courtesy of Cindy Tran. Right: Harajuku's Takeshita Street—courtesy of Rachel Chu. Below: Zurich's Fraumünster Church clock—courtesy of Rob Reed.

At the recent PRAGMA 15 Workshop (October 2008), one aspect of integration between iGEON and GEO Grid was demonstrated. At the meeting, we demonstrated inter-metadata catalog searches using standard protocols. We used Open Geospatial Consortium's (OGC) Catalog Services for Web (CS-W) standard to make distributed searches. This web services' capability and user interface allows users to make uniform queries for geoscience resources registered at PRAGMA partner sites, in this case: GEONgrid Portal and GEO Grid Portal.

In January 2008 AIST hosted the 2nd GEO-Grid Workshop. This was attended by many members of the PRAGMA community, including NARL and NCHC, as well as NECTEC.

During 2008, NARL and six of its institutes have developed a prototype "3-D GIS Taiwan" virtual-reality (VR) platform based on OpenGL, with features of volume rendering, discrete level-of detail, and high-resolution 4K VR projection system. The main purpose of this project is to deploy a high-resolution 3-D GIS Taiwan platform which can be expanded and added on for any appropriate applications. This is a key project of the GEO-Grid activity and will leverage content from several of the NARL institutes. Aspects of this activity were shown at PRAGMA 14 in March 2008. In addition, in November 2008, a demo will take place at SC08 in Austin, TX. NARL has been involved in other international and national meetings, such as Taiwan International Digital Earth (March 2008) and GRID Computing Conference 2008, held in Kuala Lumpur in May 2008. Finally, cooperation between AIST and NSPO (NARL Institute) on satellite database federations on GEO Grid using ASTER and FORMOSAT-2 is continuing.

During 2007, the iGEON activity in India began to grow and create partners between different universities (*see Accomplishments 2007*). The deployed GEON portal middleware framework at these distributed sites provides capabilities to (i) develop and deploy services, tools and serve datasets for the users at their sites and for the broader iGEON-India community, (ii) help the partner sites integrate local department or campus resources, and (iii) provide a platform for other research organizations and universities to come together and collaborate.

Several applications have been developed on GEON, such as, processing of Topomaps and integration with ArcGIS/ArcIMS (Processing of Maps). Furthermore, some users have started registering data sets, including GIS data, geochemistry data, etc.

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COLLABORATORS: C-C. Liu, *National Cheng Kung U.*; P. Bajcsy, *NCSA*

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WORKSHOPS AND INSTITUTES

FUTURE MEETINGS AND INSTITUTES

PRAGMA 16
23-25 March 2009, Daejon, Korea; Hosted by *KISTI*
Chair: Kum Won Cho, co-chair Vu Duc Thi

PRAGMA 17
October 2009, Hanoi, Vietnam; Hosted by *IOIT-VN*
Chair: Vu Duc Thi

4TH PRAGMA INSTITUTE
1-5 December 2008, Taichung, Taiwan; Hosted by *NCHC*

PAST MEETINGS AND INSTITUTES

3RD PRAGMA INSTITUTE
21- 22 October 2008, Penang Malaysia; Hosted by *USM*

2ND PRAGMA INSTITUTE
3-7 December 2007, Hsinchu Taiwan; Hosted by *NCHC*

1ST PRAGMA INSTITUTE
26-27 September 2007, Urbana-Champaign, Illinois, U.S.; Hosted by *NCSA, UIUC*

PRAGMA 15
22-24 October 2008, Penang, Malaysia; Hosted by *USM*

PRAGMA 14
10-12 March 2008, Taichung, Taiwan; Hosted by *NCHC*

PRAGMA 13
23-25 September 2007, Urbana-Champaign, Illinois, U.S.; Hosted by *NCSA, UIUC*

PRAGMA 12
20-22 March 2007, Bangkok, Thailand; Hosted by *NECTEC and ThaiGrid (TNGC), SIPA*

PRAGMA 11
15-18 October 2006, Osaka, Japan; Hosted by *Osaka U.; Held in conjunction with PRIUS activities*

PRAGMA 10
26-28 March 2006, Townsville, Australia; Hosted by the *Queensland Parallel Supercomputing Foundation, APAC, James Cook U.*, and the *Australia Institute for Marine Science*

PRAGMA 9
20-23 October 2005, Hyderabad, India; Hosted by the *UoH*

PRAGMA 8
2-4 May 2005, Singapore; Hosted by *BII-Singapore and NGO*

PRAGMA 7
15-17 September 2004, San Diego, U.S.; Hosted by *UCSD, SDSC, Calit2* and *TransPAC*

PRAGMA 6
16-18 May 2004, Beijing, China; Hosted by *CNIC, CAS*

PRAGMA 5
22-23 October 2003, Hsinchu/Fushan, Taiwan; Hosted by *NCHC*

PRAGMA 4
4-5 June 2003, Melbourne, Australia; Hosted by *Monash and APAC*

PRAGMA 3
23-24 January 2003, Fukuoka, Japan; Hosted by *AIST* and *Osaka U.*

PRAGMA 2
10-11 July 2002, Seoul, Korea; Hosted by *KISTI*

PRAGMA 1
11-12 March 2002, San Diego, U.S.; Hosted by *SDSC* and the *UCSD* division of *Calit2*

Japanese woman picking rice—courtesy of Phillip Pham

STUDENT AND POSTDOCTORAL OPPORTUNITIES

The PRAGMA framework, with its rich set of projects and network of researchers throughout the Pacific Rim, provides an ideal environment for students (*see PRIME, PRIUS, MURPA*) and postdoctoral researchers to engage actively in the development and deployment of cyberinfrastructure and its applications. This unique international collaboration allows researchers to visit more than one laboratory as part of their experience. PRAGMA strongly encourages students and postdoctoral researchers to seek funding to participate in the variety of cyberinfrastructure activities being conducted by PRAGMA. Visit the PRAGMA website (www.pragma-grid.net) for a listing of key contacts at the various PRAGMA sites and to learn more about funding opportunities for students.

BROADER COMMUNITY INTERACTIONS

PRAGMA members have been involved in helping organize workshops and symposia in grid technologies and application of the grids. This vehicle strengthens dialogue between PRAGMA members and the broader community. In the last year, PRAGMA members have helped organize workshops or special sessions and have participated at IEEE 4th Conference on e-Science (December 2008). Furthermore, PRAGMA members have participated in *Supercomputing* 2003-2008, demonstrating PRAGMA members' collective accomplishments. For future meetings involving PRAGMA members and the community see *www.pragma-grid.net/events-calendar* for more information.

Background: Kapitan Kling Mosque—courtesy of Varahenage Perera

PRAGMA SUPPORTING INSTITUTIONS AND SPONSORS

In addition to our members, many institutions participate, or have participated, actively in PRAGMA. We welcome and value their contributions in extending the PRAGMA Grid to new sites.

- State University of New York, Binghamton (SUNYB, *www.binghamton.edu*, New York), contributed resources to PRAGMA Grid, attended the PRAGMA 10 workshop and is developing a grid-enabled sensor network application to run in the PRAGMA Grid.
- Chinese University of Hong Kong (UCHK, w*ww.cuhk.edu.hk/v6/en*, Hong Kong), has contributed resources to the PRAGMA Grid and attended PRAGMA 10, 12, 13 and 14 workshops.
- LanZhou University (LZU, *www.lzu.edu.cn*, LanZhou), has contributed resources to PRAGMA Grid and attended PRAGMA 12 and 13 workshops.
- Nanyang Technological University (NTU, *www.ntu.edu.sg*, Singapore), develops and maintains MOGAS—a grid accounting software system in PRAGMA Grid and has attended PRAGMA workshops since 2006.
- National Applied Research Laboratory (NARL, *www.narl.org.tw/en*) established in 2003 to consolidate nine national laboratories into a single nonprofit organization to construct, operate and maintain the large-scale R&D facility or platform in support of the academic research and foster the necessary manpower in various advanced fields focused by the nation. NCHC is one of the laboratories in NARL. NARL provides leadership in the GEO working group, and can bring to bear several other laboratories at NARL for PRAGMA collaborations.
- Universidad de Chile (UChile, *www.uchile.cl*, Santiago), has contributed resources to the PRAGMA Grid, attended the PRAGMA 7 workshop and become the lead of Chile's national grid initiative (CLGrid). In January 2006, the Center for Mathematical Modeling (CMM, *www.cmm.uchile.cl*) of UChile invited Chilean universities to participate in the local grid initiative. The goal was to develop grid scientific applications of national interest, with PRAGMA as the main reference to follow. Eight universities are participating and have carried out four workshops, an Intel software college, and programming PRAGMA Grids. CMM contributes to the development of a multi-user data farm (based onGfarm) in conjunction with UPRM and CPTEC. Now, CMM is getting funding to push CLGrid to the next level of grid deployment, test-beds and international collaboration.
- Universidad Nacional Autónoma de México (UNAM, *www.unam.mx*, Mexico City), has contributed resources to the PRAGMA Grid, attended the PRAGMA 7 workshop, and was an original lead of Mexican grid efforts via CUDI.
- University of Puerto Rico at Mayaguez (UPRM, *www.uprm.edu*, Mayaguez), has contributed resources to PRAGMA Grid, attended the PRAGMA 13 workshop and runs a sensor data analysis application in PRAGMA Grid.
- Organic Chemistry Institute Grid Competence Center (GC3), UniZH (*www.oci.unizh.ch*, Zurich), has contributed resources to the PRAGMA Grid and been involved in PRAGMA meetings from early on. GC3 researchers focus on computational chemistry activities, including projects with Nimrod, GAMESS, APBS, Unicore and Kepler. They have mentored PRIME students. Furthermore, OCI co-organized and hosted the Summit on Applications and Grid Middleware for the PRAGMA, Swiss Grid and Euro Grid Associations.

OTHER PROJECTS AND ORGANIZATIONS

Other projects and organizations have collaborated with PRAGMA activities.

The California Institute for Telecommunications and Information Technology (Calit2; *www.calit2.net*) has provided space for PRAGMA activities and visitors at Atkinson Hall, the home of its UCSD division. Calit2 is promoting the use of OptIPortal Technology and invites participation in the CAMERA project (*camera.calit2.net*). Furthermore, Calit2 has provided support for students of PRIME.

The National Biomedical Computation Resource (NBCR; *nbcr.net*) is a National Institutes of Health National Center for Research Resources project and involves researchers at UCSD, The Scripps Research Institute, and Washington Univ. NBCR's goals are to conduct, catalyze and enable multiscale biomedical research through development, deployment and use of advanced cyberinfrastructure. NBCR has developed software (OP, an application wrapper) extended by PRIUS students (Opal OP) and its researchers are central to the Avian Flu Grid project. Further, an NBCR researcher codeveloped GAMA, a complete GSI credential management software, being used by the Resources and Data, as well as the GEO, Working Groups.

National Center for Imaging and Microscopy Research (NCMIR, *ncmir.ucsd.edu*) is an NIH National Center for Research Resource at UCSD. NCMIR's interdisciplinary staff develops state-of-the-art 3-D imaging and analysis technologies to help biomedical researchers understand biological structure and function relationships in cells and tissues in the dimensional range between 5 nm^3 and 50 μm^3. NCMIR has helped pioneer remote control of instruments via information technology and has played a fundamental role in many Telescience Working Group activities.

The Global Lake Ecological Observatory Network (GLEON, *www.gleon.org*) is a grassroots network of limnologists, information technology experts and engineers who have a common goal of building a scalable, persistent network of lake ecology observatories. GLEON is built on earlier projects in the Telescience Working Group and PRAGMA catalyzing a relationship between the EcoGrid project of NCHC's and the North Temperate Lakes Long Term Ecological Research project at the Univ. of Wisconsin (*www.lternet.edu/sites/ntl*). It has been supported by the NSF, Gordon and Betty Moore Foundation, National Science Council Taiwan, and member institutions. An additional key partner in launching GLEON is at the Center for Biodiversity and Ecology Research, Univ. of Waikato, New Zealand (*cber.bio.waikato.ac.nz*).

The Coral Reef Ecological Observatory Network (CREON; *www.coralreefeon.org*) is a collaborating association of scientists and engineers from around the world striving to design and build marine sensor networks. Similar to GLEON, it also grew out of Telescience Working Group activity. Its growth has been supported by the Gordon and Betty Moore Foundation, NSF, National Science Council Taiwan, and member institutions. There are strong collaborations between NCHC, Academia Sinica, the Moorea Coral Reef Long Term Ecological Research site (mcr.lternet.edu), and the Australian Institute for Marine Science and James Cook Univ., Australia.

The Open Source DataTurbine Initiative (OSDT, *www.dataturbine.org*) is an NSF-sponsored project to develop and deliver streaming data middleware to the science and engineering communities. The OSDT Initiative includes national and international collaborators from universities, private companies, and government agencies. The OSDT Initiative publishes the DataTurbine software and participates in numerous sensor network and environmental observing system projects. The OSDT central office is located at UCSD.

Above: Sunset at Batu Ferringhi Beach—courtesy of Vicky Yang

The Open Science Grid (OSG; *www.opensciencegrid.org*) is a collaboration of science researchers, software developers and computing, storage and network providers. OSG members come from universities, national laboratories and computing centers across the U.S. OSG's mission is to help satisfy the ever-growing computing and data management requirements of scientific researchers, especially collaborative science requiring high-throughput computing.

The Global Cyberbridges Project (GCB; *www.cyberbridges.net*), located at Florida International Univ., is a U.S. implementation of multinational efforts to improve technology training for a new generation of scientists, and increase the rate of discovery for all domains. The project has committed participation from CNIC of CAS, City Univ. of Hong Kong, and Univ. of Sao Paulo's School of the Future in Brazil.

SPONSORS

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CMC/Osaka Univ. is supported by JGN2 of the National Institute of Information and Communications Technology (NICT), Japan. Support for "Fostering of Globally-leading Researchers in Integrated Sciences" (PRIUS) is provided under the MEXT framework of "University Education Internationalization Promotion Program," and is promoted by the Grad School of Information Science and Technology at Osaka Univ.

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CNIC receives funding from the Ministry of Science and Technology of China through the China National Grid (CNGrid). Scientific Data Grid's (SDG) major funding is supported by the Chinese Academy of Sciences.

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IHPC receives its funding mainly from Singapore's Agency for Science and Technology Research (A*STAR).

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NCHC receives major funding support from the National Science Council, Taiwan, through the Knowledge Innovation National Grid (KING) project.

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TNGC receives support under the Software Industry Promotion Agency (SIPA), Ministry of Information and Communication Technology.

TransPAC2 receives major funding from the NSF and Japan's National Institute of Information and Communications Technology.

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Other UCSD projects enhancing—and benefiting from—PRAGMA activities include: PRIME is funded by NSF OISE 0407508 with additional support from the Office of Cyberinfrastructure, and OISE 0710726 additional support from the Division of Information and Intelligent Systems (IIS) and the Div of Chemical, Bioengineering, Environmental, and Transport Systems (CBET) and Calit2; PI: G Wienhausen, coPI: P. Arzberger. Work to build GLEON is supported in part by an award from the Gordon and Betty Moore Foundation, which also funded a PRIME student in 2008; Collaborative Research: Automating Scaling and Data Processing in a Network of Sensors: Towards a Global Network for Lake Metabolism Research and Education DBI-0446802; National Biomedical Computation Resource (NIH, NCRR P 41 RR08605), which funded a PRIME student in 2008. Finally, the work on the Avian Flu Grid is supported by Telemedicine and Advanced Technology Research Center (TATRC; award W81XWH-07-2-0014). This support also supported PRIME students in 2007 and 2008.

www.pragma-grid.net