



PACIFIC RIM APPLICATIONS & GRID MIDDLEWARE ASSEMBLY
COLLABORATION OVERVIEW 2006-2007

“Science is international; and many other countries have expertise, data resources, computing systems, applications and systems software, and instruments (such as telescopes and particle accelerators) that need to be available more easily to international teams...”¹

Background Image: Kanakura, Japan — courtesy of Rob Reed.

“In the twenty-first century advances in science and engineering (S&E) will, to a large measure, determine economic growth, quality of life, and the health of our planet. The conduct of science, intrinsically global, has become increasingly important to addressing critical global issues...Our participation in international S&E collaborations and partnerships is increasingly important as a means of keeping abreast of important new insights and discoveries in science and engineering.”²

PACIFIC RIM APPLICATIONS AND GRID MIDDLEWARE ASSEMBLY

Institutions and Contacts	2
Overview: <i>Promoting Global Collaboration Through Cyberinfrastructure</i> . . .	5
Accomplishments	6
PRIME and PRIUS: <i>Preparing Students for the Global Workforce</i>	12
Working Groups	18
Members	23
Schedule of Workshops	38
Publications	41
Student and Postdoctoral Opportunities	43
Broader Community Interactions	43
PRAGMA Sponsors	44
Cover Image - Uncovered	45

1. Atkins, D.E., K.K Droegemeier, S.I. Feldman, H. Garcia-Molina, M.L. Klein, D.G. Messerschmitt, P. Messina, J.P. Ostriker, M.H. Wright. 2003. Revolutionizing Science and Engineering Through Cyberinfrastructure: Report of the National Science Foundation Blue-Ribbon Advisory Panel on Cyberinfrastructure (NSF, Arlington, VA, Jan. 2003); www.communitytechnology.org/nsf_ci_report

2. National Science Board. Toward a More Effective NSF Role in International Science 00-217 (Dec. 2000); www.nsf.gov/nsb/documents/2000/nsb00217/nsb00217.htm



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. To the right is a list of member institutions and key contacts. This year, four new members joined PRAGMA: Mexico's Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE); Malaysian Institute of Microelectronic Systems (MIMOS); Thai National Grid Center; and Institute of High Performance Computing (IHPC) of Singapore. More information about the Steering Committee members, noted with names in purple, may be found at www.pragma-grid.net/steering_committee.htm.

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Background Image: Ensenada, Mexico—courtesy of CICESE.

OVERVIEW 2006-2007

This fourth annual Collaborative Overview chronicles the accomplishments of the Pacific Rim Applications and Grid Middleware Assembly (PRAGMA) and its member institutions in 2006. Established in 2002, PRAGMA is an open organization that focuses on how practically to create, support, and sustain international science and technology collaborations via multidisciplinary teams of researchers. PRAGMA plays a critical role as an international *conduit* for professional interactions, ideas, information, and grid technology. Our multi-faceted *framework for collaboration* catalyzes and enables new activities through a culture of openness to new ideas. Our pragmatic approach has led to new scientific insights, enhanced technology, and a fundamental sharing of experiences manifest in our routine-use laboratory, as documented in this report.

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 laboratory* and are evaluated to uncover how the applications and middleware work on the PRAGMA testbed. These experiments lead to scientific insight and to improved middleware. Successful solutions are integrated into country-specific software stacks (e.g. NSF Middleware Initiative), Open Grid Forum (OGF) standards, or other *multi-way dissemination* vehicles, so others may benefit. Our workshops are a metronome of our progress and provide a venue to involve new collaborators in our activities. Additional outreach efforts bring our lessons learned to others, and ultimately help *build the community*.

This year's highlights include: our routine-use testbed activities; interactions between our testbed and several large production grids; accomplishments of our application working groups; engaging the next generation of scientists via educational programs such as PRIME and PRIUS; and specific community building activities. The brochure also highlights the critical contributions of each of the working groups and member institutions.

PRAGMA is heading in several new directions. Two new application communities include the geosciences, working closely with the new iGEON effort, and metagenomics researchers. We continue to expand our testbed to new sites and will establish a dedicated data infrastructure required by several applications. We will also deploy and experiment with collaborative tile display wall technology, to enhance our ability to interact and collaborate. Finally, we will team with middleware developers outside of the Pacific Rim to work toward improved interoperability of our grids.

What are the key measures of our ultimate success? There are two. First is the science that is enabled—on a routine basis. The second measure derives from the new communities that have embraced the tools and approach of collaborative science via cyberinfrastructure. Such successes will validate the global investment in tools and PRAGMA's model, which harnesses the ingenuity and leverages the resources of more than 100 individuals from 29 institutions to build sustainable collaborations and advance grid technologies through applications.



ACCOMPLISHMENTS

PRAGMA participants have successfully demonstrated the value of international collaborations in conducting applications on the grid. The following vignettes—science successes from PRAGMA’s fourth year—illustrate the grid concept that brings remotely distributed resources such as microscopes, computers, data, and expertise to researchers’ local work environments. These examples demonstrate the value of working together on the grid and reveal the barriers that need to be overcome to make the grid more accessible. Knowing where the difficulties lie will help focus the broader grid community efforts and lead to the development and deployment of improved infrastructure. For more information about most of these examples, see References.

Simulating the Australian Monsoon and the Effect of Wildfires

DAVID ABRAMSON AND AMANDA LYNCH, MONASH UNIVERSITY, AUSTRALIA

The Australian monsoon is critical to the environment and economy of the north Australian region, which produces wealth for Australia out of proportion to its population. It delivers life-sustaining moisture to a dry continent, although lightning associated with the monsoon also causes devastating fires. In the past, the monsoon has varied both spatially and in intensity. Contemporary ecosystems have adapted to these extremes, but how tightly linked are burning, vegetation, and rainfall? What might these linkages mean for future Australian water resources?

Interactions between atmosphere, ocean and land in the context of the Australian monsoon are complex, as they result from feedbacks that operate on a variety of spatial and temporal scales. Until now, computational and data volume limitations have hindered efforts to reach a full understanding of the biophysical processes and the mechanisms for long-term variation in the natural monsoon system. Performing simulations of the type and extent needed to understand monsoon dynamics requires more computational resources than one is likely to obtain from any single high-performance computing (HPC) center in Australia.

In this study we used the CSIRO climate model called CCAM in combination with our locally developed Nimrod/G tool set. Nimrod allowed us to distribute the CCAM computations across the PRAGMA testbed, while exploring a very wide range of scenarios. We are currently analyzing the scientific results of the experiment, but initial examination has revealed a significant interaction between the monsoon and wildfires.

The experiment executed on a maximum of 90 processors (out of a maximum 159) across seven PRAGMA grid resources located in Australia, Japan, Korea, Taiwan, Thailand and the U.S. The experiment ran for an elapsed time of 170 days, with an average of 37 processors in use across that period. (See graph below.)

We have performed an analysis of the log data in order to understand the dynamics of running a large, multi-organizational science-driven experiment. Importantly, there were approximately five periods of time across the execution when very little work was performed (see graph at the top of page eight). These were mainly due to:

- One week when we modified Nimrod’s file server code to improve fault tolerance;
- Two weeks when most of our testbed resources were down (for both hardware and middleware reasons);
- Two weeks when some Nimrod bugs were being fixed; and
- A further week when resources had to be devoted to another experiment because of a conference deadline.

Removing the down periods, the experiment would have finished in less than 143 days.

Had the PRAGMA testbed resources been large enough to run the whole 90 processes on a single cluster, and if we had dedicated time on those resources, the work could have been completed in 40 days on the fastest machine, and 80 days on the slowest. Based on the mix of machines we used, the average would have been 56 days. However, no single resource had 90 processors, and no single resource was up the whole time. Thus, the testbed efficiency ranges from 23% to 52% depending on the metrics that are used. Notably, the highest efficiency is less than 100% because the testbed was shared and not



Background Image: A low to moderate intensity controlled burn was set in open savanna woodland and measurements were made of the surface energy balance using eddy covariance techniques to verify the performance of the model—courtesy of Dr. Jason Beringer, Monash University.

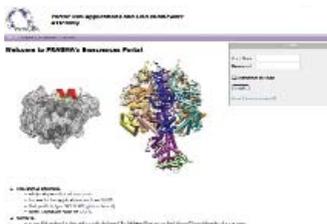
always available. Considering the resources were shared, we argue that this is a very satisfactory outcome.

Some conclusions:

1. We used the PRAGMA resources to deliver real science results. The hypothesis that burning the savanna can affect the strength and timing of the monsoon was confirmed. The findings will be published in the near future.
2. The testbed operated for 170 days, and delivered over 1.25 million processor hours! Importantly, we were able to do a live upgrade of a number of the cyberinfrastructure components during the period.
3. The experiment had a profound effect on the development of Nimrod, and caused us to incorporate a number of enhancements. Most notably, we improved Nimrod's ability to schedule computations by incorporating both data location and transport delays. This allowed it to make a better choice of resources, improving the performance of the system as well as its fault tolerance. We also enhanced Nimrod's ability to handle faults in the Grid testbed.
4. The experiment shipped some 1.6TB of data across national and international networks. This exposed some interesting features of Australia's network charging policy, and will lead to lasting improvements.

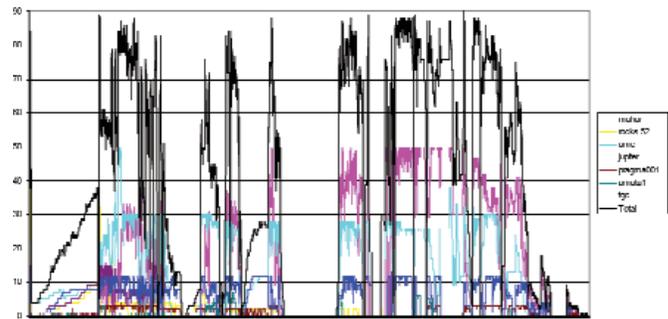
PRAGMA Biosciences Portal

In order to deliver cyberinfrastructure to the general scientific and biomedical research community, transparent access



Bioscience Portal developed by PRIUS students

and ease of use is of critical importance. Students and researchers from Jilin University, China, Osaka University and Tsukuba University in Japan, University of Queensland, Australia, and UCSD, have developed a prototype PRAGMA Biosciences Portal (PBP). The portal uses the GridSphere framework (www.gridisphere.org) to enable reuse of functionalities exposed as portlets, which are portable for different application scenarios. In this work environment, a user can apply for access to compute resources through Grid Account Management Architecture (GAMA), which automates the user X509 certificate creation, signing, and proxy management (Bhatia



Number of processors used to conduct the Savannah Burn experiment.

et al 2006), with the newly-established PRAGMA CA. A user who has never used the grid can start using it through the portal environment. To simplify the job submission process, developers have also created a prototype Community Scheduler Framework 4.0 (CSF4) portlet that allows users to submit jobs to CSF4-managed resources. The jobs are submitted to different clusters with local batch schedulers, such as SGE, dynamically based on metadata provided by Monitoring and Discovery System (MDS) or through first-come, first-served/round robin scheduling algorithm. For simple access to data and application deployment, Gfarm-Fuse (File System in User Space) is used to enable a familiar Unix environment in which installation of software is only required once per platform. User data appears as a unified filesystem even though the data could be distributed worldwide.

Into the Gfarm-Fuse data grid, PBP has compiled and deployed commonly used bioinformatics software such as MEME and BLAST, and other computational mathematics, biology and chemistry applications (including FFTW, APBS, and AutoDock). Since then PRAGMA members have profiled the performance of such applications in the PBP environment (Ding 2006). Going forward developers will explore integrating CSF4 into other web-service toolkits such as Opal (Li, Krishna et al 2006), to enable different clients to take advantage of the transparent computational data grid infrastructure.

PRAGMA Leads Application Experiments of Grid Interoperation in GIN Testbed

Many scientists work across different grid projects and their applications should not be restricted by grid boundaries. Expanding collaborations among grids is important and beneficial to global scientific communities. But how can different grids interoperate and how can we make it easier for scientists to use multiple grids? PRAGMA is addressing these issues to create solutions by working

under the umbrella of the Multi-grid Interoperation (<https://forge.gridforum.org/projects/mgi>, charter document by C. Catlett and M. Satsuoka) activity in the Global Grid Forum. PRAGMA has also led in the establishment and operation of the Grid Interoperation Now (GIN) testbed.

The four focus areas in GIN include: data location and movement; authentication/authorization and identity management; job description and execution; and information services.

As with the PRAGMA Grid testbed, the grid interoperability experiments are driven by applications. In little more than six months, five grids have joined the GIN testbed. In addition, we have successfully run Time Dependent Density Functional Theory (TDDFT)—a quantum chemistry application based on grid middleware Ninf-G—on four of those grids (PRAGMA Grid, TeraGrid, Open Science Grid and NorduGrid). This was not an easy task. We encountered interoperability problems with every grid. The result of discussion and experimentation is a much better understanding of the differences among grids. Working with other grids, we developed and tested various strategies and middleware interfaces, ran TDDFT across grids, and thereby achieved interoperation. Our experiments resulted not only in some immediate solutions but also provided knowledge and motivation for future standardization work and thoughts on the long-term direction of grid interoperation.

In addition to applications, grid interoperation issues were also tested with cross-grid infrastructure services. Using SCMSWeb software, we set up an infrastructure testing matrix, testing and monitoring key services of each GIN testbed site. Globus authentication, gridftp and job submission all helped provide real-time status reports at goc.pragma-grid.net/cgi-bin/scmsweb/probe.cgi.

Differences among grids posed interoperability problems for cross-grid monitoring as well. Our SCMSWeb software team, part of the National Thai Grid project, implemented more flexible strategy in SCMSWeb software (www.opensce.org/components/SCMSWeb) to handle a variety of



GIN and PRAGMA grid locations

grid-service configurations and tests. We are also leading the collaborative effort among various grid monitoring software developers, who are developing a common schema upon which interoperable, cross-grid monitoring capabilities can be built.

PRAGMA also collaborated with the EGEE project which developed a grid map for GIN (maps.google.com/maps?q=http://field.home.cern.ch/field/gin.kml) and PRAGMA Grid (maps.google.com/maps?q=http://goc.pragma-grid.net/cgi-bin/scmsweb/glue.cgi?format=kml&compat=1).

This was achieved by overcoming an incompatibility issue between BDII/LDIF and SCMSWeb/XML schema. Our SCMSWeb team developed an XML-to-LDIF translator which has enabled interoperation between BDII and SCMSWeb and achieved information sharing among grids. This new feature and other changes will be part of the persistent SCMSweb package.

To explore data-related grid interoperability issues, the PRAGMA Savannah application team is preparing to run their application soon on the GIN testbed. This application is based on the Nimrod/G middleware. PRAGMA is also contributing to the GIN testbed documentation effort. GIN testbed contact information, resources information, interoperability issues, lessons learned, solutions and discussions are documented at forge.gridforum.org/sf/wiki/doc/viewPage/projects.gin/wiki/GinOps.

PRAGMA Establishes Certificate Authority (CA) Using NAREGI-CA Software

PRAGMA Grid has expanded to 26 sites in 14 countries this year. Currently there are 12 applications being tested and run on the grid globally, driven by users from various institutions around the world. PRAGMA Grid is also leading the Grid Interoperation Now (GIN) testbed effort, where trust among grids is an essential first step for grid interoperation. Participation in the International Grid Trust Federation (IGTF) extends global trust in both the PRAGMA and GIN testbeds. Yet some sites and users who would like to join and work in these testbeds do not have the ability to obtain a certificate through an IGTF-accredited certificate authority (CA). Addressing this need, PRAGMA established its own certificate authority—PRAGMA CA—linked to IGTF via APGrid PMA. PRAGMA will move to production CA by the end of 2006.

GIN infrastructure testing matrix

Site	Summary	Authentication (v10)	DNS (v10)	GridFTP (v10)	GridFTP (v10)	JobRun (v10)	JobAuth (v10)
OSG	osg-ops-013.acs.utd.edu	(v10)	(v10)	(v10)	(v10)	(v10)	(v10)
TeraGrid	tsckp-02.adnc.edu	(v10)	(v10)	(v10)	(v10)	(v10)	(v10)
PRAGMA	prg-grd1.us.tengrid.org	(v10)	(v10)	(v10)	(v10)	(v10)	(v10)
NorduGrid	ngc-train.org	(v10)	(v10)	(v10)	(v10)	(v10)	(v10)
EGEE	www.tpcsc.jp	(v10)	(v10)	(v10)	(v10)	(v10)	(v10)
	shvred1.hq.hi	(v10)	(v10)	(v10)	(v10)	(v10)	(v10)
	gpc3.hpc.phh.ac.uk	(v10)	(v10)	(v10)	(v10)	(v10)	(v10)

The PRAGMA CA service was set up by UCSD with the NAREGI-CA software developed by Japan's National Research Grid Initiative (NAREGI). Several PRAGMA member institutions participate in NAREGI.

To ensure that PRAGMA CA qualifies for IGTF accreditation, setup and the NAREGI-CA software development are being done under the direction of APGrid PMA. AIST, a member of PRAGMA, chairs the APGrid PMA, which in turn is one of three founders of IGTF and has led this effort for the PRAGMA community.

To implement PRAGMA CA and IGTF requirements, NAREGI-CA is being adapted to add functionalities to let the CA server run in offline mode. Feedback from PRAGMA CA administrators and users has helped improve the NAREGI-CA software as well as the PRAGMA CA user guide and operation procedures.

Expanding the Collaboration Grid

The advent and deployment of optical networks has fundamentally changed how researchers are using the network, developing the grid, and ultimately conducting collaborative research. Through our collaboration with the NSF-funded OptIPuter, PRAGMA partners are expanding the PRAGMA “experimental framework” to optical networks and lambda grids, in which the optical networks themselves (or “lambdas,” where a “lambda” is a wavelength of light) are schedulable grid resources. An early focus of this expansion is the use of tile display wall (TDW) infrastructure as the portal into the grid and as the interface into collaborative cyberinfrastructure. The TDW is being used with high definition video conferencing as a tool coupled with Telescience (see Telescience Working Group).

On September 20, 2006 an HD video conference session was successfully conducted between Osaka University, Japan and UCSD. The test involved two Sony HD prosumer cameras and Scalable Adaptive Graphics Environment (SAGE) driven tile displays. The video streams were transmitted at 1080i and 25 frames per second along with audio and the streams used approximately 25 Mbits per second of network bandwidth in each direction. The test was successful as the video quality was flawless and there were no packet

losses during the hour-long session. There was a 2.5 second delay between the end-points but the majority of this delay was due to the MPEG encoding hardware in the cameras. However since this delay is consistent, it is not a deterrent for video-conference style meetings.

This set the stage for a successful demonstration of this technology between NECTEC and Osaka during the PRAGMA 11 Workshop, where the President of Osaka University, who was opening an office of Osaka University in Bangkok, addressed the PRAGMA members in Osaka. The success was based on the collaboration of four PRAGMA sites (Osaka University, UCSD, NECTEC and NCHC) and on a PRIME student in Osaka as well as a PRIUS student to NCHC who helped build the technology and knowledge that underpinned this demonstration.

We expect future versions of HD cameras to have faster hardware to reduce this delay significantly. This will be tested with the Korea Institute for Science and Technology Information (KISTI) and the National Institute of Advanced Industrial Science and Technology (AIST), both PRAGMA and OptIPuter partners, as well as with the National Center for High-performance Computing (NCHC).

Building Communities, Catalyzing Collaborations

PRAGMA and its members are engaged in broadening the use and impact of grid technologies by building communities and catalyzing collaborations. The involvement of new communities and new scientific collaborations is essential to PRAGMA's mission because it brings in new talent as well as new applications—improving routine use of the grid.

The NCHC in Taiwan, with funding from the National Science Council of Taiwan, hosted the 1st South Asia International Joint Research and Training Workshop (www.nchc.org.tw/event/2005/1128), including

researchers from Vietnam, Malaysia, and the Philippines. The goal was to build better understanding of researchers in this region, and encourage them to participate more broadly in international activities. In addition, PRAGMA members participated in efforts to build bridges to communities in Central and South America, participating in an NSF



Osaka University President Miyahara greeting PRAGMA 11 participants from Bangkok—courtesy of Teri Simas, UCSD.

Workshop on Cyberinfrastructure for International Biodiversity Research Collaboration, Panama, and later in the World Computer Congress and Center for Mathematical Modeling (www.cmm.uchile.cl) workshop, hosted by the University of Chile, which has been leading the Chilean National Grid initiative. In all cases, these interactions have led to new interactions with PRAGMA researchers.

PRAGMA has been working collaboratively with two research communities. With the Geosciences Network (GEON), which is building cyberinfrastructure for the geosciences, we helped launch a complementary international activity, iGEON. To date there have been efforts to build these collaborations with PRAGMA partners in three locations:

- India organized a special workshop after PRAGMA 9, hosted by the University of Hyderabad (UoH);
- China co-organized a workshop in Beijing, working with the Computer Network Information Center (CNIC) and the Graduate University of the Chinese Academy of Sciences (GUCAS); and
- Japan, through collaboration with the National Institute of Advanced Industrial Science and Technology, is planning a GEO Grid workshop at PRAGMA 12 in coordination with local host National Electronics and Computer Technology Center (NECTEC). There are also plans to have an established Geo Working Group within PRAGMA, focused on the data and computing needs of this community. To date, there are GEON nodes in the PRAGMA testbed at three sites (see Resources).

The EcoGrid effort of NCHC (and the Telescience Working Group) spawned the Global Lake Ecological Observatory Network (GLEON) and the Coral Reef Ecological Observatory Network (CREON). At PRAGMA 10, a second meeting of the GLEON/CREON groups was held. NCHC organized a successful third meeting in October 2006. These community-building workshops focused on common measurements from instruments, as well as the appropriate grid technologies, and interfaces for sharing data, instrument control, and automating processes in observing systems. The lake group is analyzing data on diel oxygen from GLEON lakes to gain a better understanding of lake metabolism. Two manuscripts from earlier work on Yuan Yang Lake and the impact of typhoons on the resetting of ecosystems have been submitted for publication.



Background Image: Yuan Yang Lake, Taiwan. Yuan Yang Lake is among the lakes being monitored through GLEON in collaboration with Academia Sinica, NCHC, and the Taiwan Forest Research Institute—courtesy of Dong-kuan Liao.

PRIME & PRIUS *Preparing Students for the Global Workforce*

PRIME and PRIUS are programs that engage students from PRAGMA institutions in project-based learning via an international educational exchange program. The educational visions for PRIME and PRIUS are similar: to prepare students for the challenges of working globally, while also advancing PRAGMA's goals. The PRIME program continued to build strong, project-based teams in new and continuing research areas during its third year. Meanwhile, PRIUS finished its first year after engaging several researchers from PRAGMA institutions as lecturers and mentors of PRIUS students. Future plans call for expanding these activities to include more institutions, a wider set of grid applications and technologies, and students at different stages of their careers.

Overview

In 2004 UCSD and PRAGMA partners in Japan (CMC), Taiwan (NCHC), Australia (Monash University), and China (CNIC) launched PRIME—the Pacific Rim Undergraduate Experiences program (prime.ucsd.edu). The program provides opportunities for UCSD students and host-site mentors and colleagues to participate in international research and cultural experiences. The activities of the student researchers contribute to the growth of the cyberinfrastructure through developing, testing, and running application codes in this internationally distributed environment. PRIME prepares students for the global workplace of the 21st century and has created stronger collaborations among participating PRAGMA institutions and researchers. PRIME was developed with three years of support from the National Science Foundation (NSF) Office of International Science and Engineering (OISE) and Office of Cyberinfrastructure (OCI), and with additional support from the California Institute for Telecommunications and Information Technology (Calit2), as well as support from the partner and host institutions.

The success of PRIME over the last three years has sparked other activities to cultivate human resources in the framework of PRAGMA. In August 2005 Osaka University received funding 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. This new project 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. To this end, the new project will establish a persist-

ent educational infrastructure called PRIUS—Pacific Rim International UniverSity (prius.ist.osaka-u.ac.jp)—for graduate students from Osaka University. The program 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.

The PRIME and PRIUS programs are models for nurturing students' abilities to take a leadership role in next-generation integrated 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.

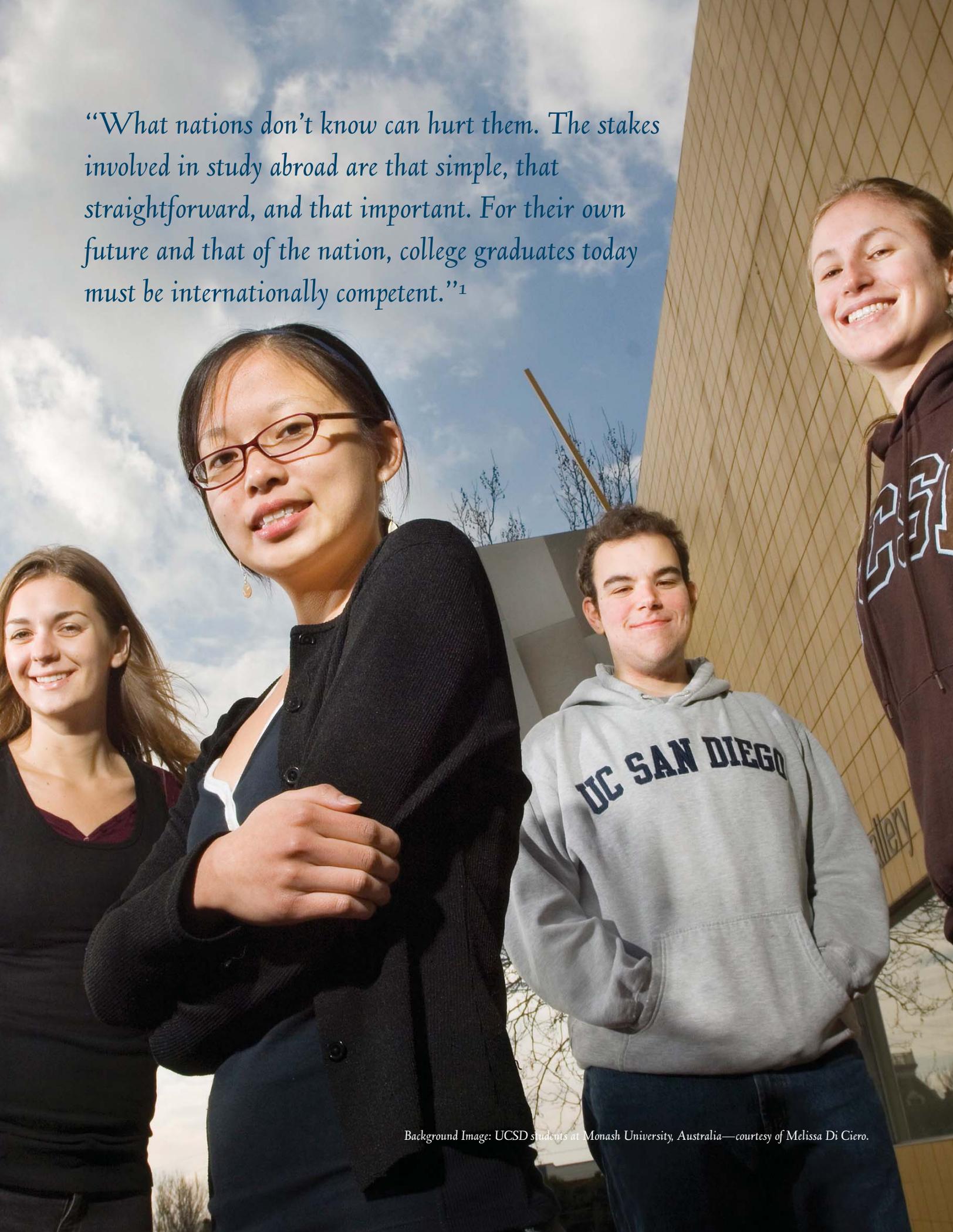
PRIUS Year One Highlights

In its first year, PRIUS launched both components of its program. Ten international instructors—all PRAGMA members—lectured on grid computing and applications topics ranging from grid and web services, clustering tools, optical network computing, grid accounting systems, biomedical applications of grid computing, and the economic and social impact of cyberinfrastructure. The lecturers interacted with PRIUS students for a few days to provide them with insights into the technological issues as well as topics of importance in other regions. The interactions allowed students to meet foreign researchers and establish collaborations and internships.

INSTRUCTORS: Mark Ellisman, Jason Haga, Wilfred Li, Tomas Molina, Philip Papadopoulos (UCSD); Fang-Pang Lin (NCHC); Bu-Sung (Francis) Lee (Nanyang Technological

1. *Global Competence and National Needs: Commission on the Abraham Lincoln Study Abroad Program* 2005, p. ii, www.lincolncommission.org/report.htm

“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.”¹



Background Image: UCSD students at Monash University, Australia—courtesy of Melissa Di Ciero.

University, Singapore); Rajesh Kumar Chhabra (Queensland University of Technology, Australia); Rajkumar Buyya (Melbourne University); Sun-In Lin (NCHC).

There were four graduate students and one undergraduate student along with mentors and a team of researchers from each of four host institutions:

San Diego Supercomputer Center (SDSC) and the National Biomedical Computation Resource (NBCR) at the University of California, San Diego (UCSD), U.S.
Ph.D. Candidate: Kohei Ichikawa

Kohei Ichikawa developed a QM/MM hybrid simulation program for protein research using OPAL (NBCR), a web service to wrap existing applications. Also, he developed an OPAL operation provider, allowing the interoperation of OPAL-based web service and Gt4-based service. Upon his return to Osaka, he worked with the Protein Data Bank Japan (PDBJ) to install Opal-based services and presented a poster on his work at the Life Science Grid 2006 conference.

Team: Wilfred Li, Peter Arzberger, Srirum Krishnan, Tomas Molina (UCSD); Shinji Shimojo, professor and director of the Cybermedia Center at Osaka University, and Susumu Date, a specially-appointed associate professor of the PRIUS project.

Nanyang Technological University (NTU), Singapore
Ph.D. Candidate: Shingo Takeda

Shingo 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.

Team: Francis Lee, Junwei Zhang (NTU); Shinji Shimojo and Susumu Date (Osaka University)

Queensland University of Technology (QUT), Australia
Master's Students: Yohei Sawai, Junya Seo

Yohei Sawai and Junya Seo worked on the development of a BioScience Portal for PRAGMA. The single-sign-on portal was constructed by integrating middleware portlets (JSR 168) such as GAMA (UCSD), CSF4 (Jilin University),

GridPortlets (GridSphere group) and several application portlets, including NAMD, that were provided by PRAGMA research groups. This portal is configured to utilize the PRAGMA testbed resources at the back end. This project exemplifies PRAGMA's emphasis on re-using software and hardware resources within the community.

Team: Rajesh Kumar Chhabra, Ashley Wright, Matthew J. Watts (QUT); Susumu Date (Osaka University); members of the PRAGMA Bioscience Working Group.

National Center for High-Performance Computing, Taiwan

Undergraduate student: Seiki Kuwabara

Seiki Kuwabara learned various tiled-display technologies such as the parallel system for OpenGL (Chromium), and applied them to high-definition-quality streaming video over a high-speed network. The team performed a preliminary experiment between Taiwan and Japan, thus suggesting directions for further collaboration between Osaka University and NCHC.

Team: Fang-Pang Lin, Sun-In Lin, Yi-Haur Shiau, Jer-Huang Shiau and Shi-Wei Lo (NCHC); Shinji Shimojo, Susumu Date, Takuji Nakagawa, Shuo Yang (Osaka University)

PRIME Year Three

In its third year, the PRIME program supported research experiences abroad for 14 UCSD undergraduate students. Projects ranged across biological, chemical, and engineering applications and involved developing and applying many aspects of cyberinfrastructure, including visualization, distributed computing, and distributed data handling. This year several students worked together on joint projects, which increased the productivity of the group and their ability to create a finished product. Several projects involved using or developing software for tile display walls. These projects provided a vehicle to engage more researchers at PRAGMA sites and to diversify applications within the PRAGMA community, including such new areas as cardiac physiology and systems biology.

PRIME also refined its cross-cultural training program this year to help prepare the students for their experiences in Asia and Australia. The program draws heavily on the work of the University of the Pacific's Dr. Bruce LaBrack and materials on his website "What's Up with Culture?" (www.pacific.edu/culture).

UCSD also hosted two graduate students from China's Jilin University who are working on the iGAP/Gfarm/CSF4 project (see Accomplishment: Bioscience Portal and Ding et. al. 2006).

YEAR THREE HIGHLIGHTS OF PRIME STUDENT ACTIVITIES

Cybermedia Center, Osaka University

Students: Robert Sy, Ao 'Cathy' Chang; Daniel Goodman, Marshall Levesque

Cathy Chang, Daniel Goodman and Marshall Levesque worked as a team this year, interacting with Susumu Date and Kohei Ichikawa of the BioGrid project, and their UCSD mentors, Phil Bourne (Chang and Goodman) and Jason Haga (Levesque). This team was focused on using computational tools in a grid environment to study aspects of protein structure and docking with ligands. In particular Chang worked on homology modeling of the protein kinases and binding site prediction; Goodman conducted docking simulations of protein kinases and the virtual screening of ligands for inhibitors; Levesque's work was similar to Goodman's, with protein phosphatase as his focus. Protein kinases and protein phosphatase are enzymes that modify other proteins by respectively adding or removing phosphate groups. Kinases have profound effects in cells, and when some kinases are not regulated, they lead to diseases. Phosphatases also play an important role in regulating the signaling pathways in cells and have been hypothesized to play a role in cancer. Knowing how to regulate them is an important challenge in biomedicine. The team used the program Dock in their work. Moreover, the team has succeeded in plugging Dock into the PRAGMA Grid testbed for the distribution of its computational workload. They developed WSRF services for Dock using Opal Operation Provider and enabled access to Dock programs on multiple cluster systems from remote sites. As a result, the team has been continuing work on the project even after returning to San Diego. The team benefited from computational power provided by as many as 130 PRAGMA testbed processors in total for their analyses.

Visual Arts major Robert Sy worked with Shinji Shimojo and Kohei Ichikawa of the Telescience team at Osaka University, and with UCSD's Mark Ellisman, Tomas Molina, and Raj Singh, to help establish a tiled display wall in Osaka. Sy installed Scalable Adaptive Graphics Environment (SAGE), a program developed at the Electronic Visualization Lab (EVL) at the University of Illinois at Chicago. SAGE manages the flow of pixels onto

different parts of the display wall and allows researchers to treat the display as one contiguous desktop. It provides researchers with the ability to zoom into large datasets and view them in great detail, while providing enough screen real estate to allow for a contextual reference of the zoomed area in the large 2D or 3D data. Sy also installed several visualization packages on the wall, including JuxtaView, MagicCarpet, VNCviewer, and more. This work sets the stage for broader interactions between UCSD and Osaka in building collaborative environments based on tiled-display technology.

TEAM LEADERS AND MEMBERS

OSAKA UNIVERSITY: Shinji Shimojo, Director, Cybermedia Center and Principal Investigator, Biogrid Japan; Susumu Date, Associate Professor, Graduate School of Information Science and Technology and Project Lead, PRIUS; Toyokazu Akiyama; Kazunori Nozaki; Tomomi Takao; and PRIUS student researcher Kohei Ichikawa.

UCSD: Mentors include Mark Ellisman, Director, NIH-supported NCMIR and CRBS; Steve Peltier, Executive Director, NCMIR; NCMIR researchers Tomas Molina and Raj Singh (for Robert Sy); Philip Bourne, Professor of Pharmacology (for Cathy Chang and Daniel Goodman); Jason Haga, Postdoctoral Researcher, Bioengineering (for Marshall Levesque). Additionally, Nicholas Schwarz of EVL assisted Robert Sy.

National Center for High-performance Computing (NCHC), Taiwan

Students: Stephen Chen, Mahboubeh Hashemi

National Center for Research on Earthquake Engineering (NCREE)

Student: Bryan Lin

Mahboubeh Hashemi and Stephen Chen joined forces to address the problem of implementing image-processing software developed at NCHC, to detect accurately the location of cells in a neural network, and to understand how the cells communicate. They worked with images of astrocytes, the largest and most numerous of the supporting, or glia, cells in the brain and spinal cord. A variety of algorithms (converging squares, thresholding) to improve the image processing/detection software (e.g. for gray space segmentation) were identified, studied, implemented, and evaluated for accuracy. If successfully implemented, this would automate the process of cell location, and collapse the time-consuming process from days to seconds. Work continues in the fall.

Bryan Lin split his time between NCHC and NCREE. He worked on an experiment with classrooms in a decommissioned elementary school building in Taoyuan. The experiment replicated aspects of earthquakes to better understand their impact on specific structural units. The work entailed customizing GISA3D, a graphical user interface for structural analysis, and creating visualization plug-ins with indicators for monitoring and analyzing the results of the experiments. The custom modification of GISA3D gave Lin a crash course in the basic principle of networked pseudo dynamic testing in NCREE. In addition, Lin joined the image-based displacement measurement team in the school building experiment. With NCREE members, he helped design and make a set of distortion calibration checkerboards for image analysis. Lin also photographed and witnessed the experiment.

TEAM LEADERS AND MEMBERS

NCHC: Fang-Pang Lin, Manager, Grid Computing Division; Sun-In Lin; Shi-Wei Lo; Hsui-Mei Chou; Chien-Lin Huang, Yao-Tsung Wang, Po-Wen Chen, Jyh-Horng Wu, Tom Ho, Grace Chau-Wei Hong, Vicky Yang, Anne Wang.

NCREE: Ming-Chieh Chuang, Yuan-Sen (Vincent) Yang and Keh-Chyuan Tsai.

UCSD: Host mentor Gabriel Silva, Assistant Professor, Bioengineering and Ophthalmology (for Mahboubeh Hashemi); Jurgen Schulze, Researcher, Calitz (for Stephen Chen); and Chia-Ming Uang, Professor, Structural Engineering (for Bryan Lin).

Monash University

Students: Angelina Altshuler, Celia Croy, Iwen Wu, Noah Ollikainen

A common thread in the research of these four students is the application of the parameter-sweep middleware, Nimrod, in three different applications. This exposes the students to the power of distributed resources, even as the students provide feedback to developers—thus leading to improvements in the middleware itself.

Angelina Altshuler and Iwen Wu assisted in the development of more stable ionic models in rabbit (LabHEART) and human ventricular myocytes. This work continues the work of previous PRIME students in each of the preceding two years. The students worked on determining Nimrod/G parameter values to improve the model stability over long time periods and at different frequencies of stimulation. In turn, those improvements enable calculation of, for exam-

ple, ionic currents, Ca-transients, and action potentials. They also permit testing of hypotheses about the mechanisms regulating the excitation-contraction coupling in cardiac cells of epicardial and endocardial origin.

Celia Croy worked on a combination of studies involving computational analysis of biological structures using the GAMESS/APBS/Nimrod programs. The GAMESS and APBS tools enable computational chemistry studies using quantum chemical and electrostatic theories, respectively. This activity extends work of other PRIME students from previous years and deepens the collaboration between David Abramson's lab at Monash and Kim Baldridge's group at SDSC and at the University of Zurich. In particular Croy worked on establishing a workflow pipeline for high-throughput computations of structure and property of a sequence of molecules. Users can specify computational level and property type and a set of molecular structures that are targets for study, and the pipeline—using the GAMESS and APBS computational chemistry software, and the Nimrod parameters sweep tool—does the necessary processing to get the results. Additionally, Nimrod/O tools can be invoked for analysis of data and refocusing of computations. The UCSD student used the set of amino acids as her test set of molecules.

A new interaction between UCSD and Monash was started this year by Noah Ollikainen. His goal was to develop an efficient method for large-scale virtual screening of ligands, by linking Nimrod/G and AutoDock. AutoDock simulates the binding of a specific target protein to a large set of ligands. Ollikainen conducted virtual screening experiments on the bacterial aminoglycoside phosphotransferase (APH), which resembles ACAD10, a novel protein kinase. This experiment docked the first 2,000 compounds from the ZINC drug-like dataset as well as kanamycin, an antibiotic that binds to APH. These results were compared with similar experiments run by Daniel Goodman, a PRIME student at Osaka University, who used DOCK as the docking program.

TEAM LEADERS AND MEMBERS

MONASH: David Abramson, Professor, School of Computer Science and Engineering, Lead Developer of Nimrod; Colin Enticott; Slavisa Garic; Rob Gray; Tom Peachey; UCSD: Mentors Anushka Michailova and Roy Kerckhoffs, Senior Researchers, Bioengineering; Andrew McCulloch, Professor, Bioengineering (for Altshuler and Wu); Kim Baldridge, Researcher, SDSC and Professor, Organic Chemistry Institute, University of Zurich (for

Celia Croy); and *Philip Bourne*, Professor of Pharmacology (for *Ollikainen*).

Computer Network Information Center (CNIC), Chinese Academy of Sciences (CAS)

Students: Lily Cheng, Elaine Liu, Danjing Lisa Zhao

Lily Cheng and Lisa Zhao worked on complementary aspects of an initial study on avian influenza virus, subtype H5N1, screening neuraminidase and hemagglutinin proteins, respectively, against two libraries of ligands. 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 has stimulated a broader collaboration between UCSD, CNIC and other PRAGMA partner sites, which will continue through the next year.

Elaine Liu's project was to visualize high-resolution astronomical images remotely on UCSD's tile display wall while controlling it from CNIC. The viewing platform was an LCD-based tile display wall. Liu accomplished this objective over the summer, setting up the opportunity for future collaborations, in particular in developing a visual collaboration environment within PRAGMA.

TEAM LEADERS AND MEMBERS

CNIC: *Kai Nan, Kevin Dong, Yihua Zheng, Hua Zhao (for Elaine Liu); Zhonghua Lu, Bin Shen, Ze Luo, Jinyi Wang, Guihua Shan, Qi Chen (for Lily Cheng and Lisa Zhao); Haiyan Xu, Wei Chen (for Elaine Liu, Lily Cheng and Lisa Zhao).*

CAS: *Dan Wang, Scientist, National Astronomical Observatories (for Elaine Liu).*

UCSD: *Wilfred Li, Research and Executive Director, NBCR (for Lily Cheng and Lisa Zhao); Jurgen Schulze, Research Scientist, Calit2 (for Elaine Liu).*

University of California, San Diego

Gabriele Wienhausen, one of three program coordinators for PRIME, is the principal investigator of the NSF PRIME award, and provost of Sixth College, which is focused on the integration of culture, arts, and technology. She is joined by co-PI Linda Feldman from the Academic Internship Program, who has broad experience internation-

ally in establishing and evaluating internship programs, and co-PI Peter Arzberger, who is PI of the PRAGMA award, which provides a source of projects as well as the essential human network of PRAGMA sites. Teri Simas assisted with project management. With their partners, they are looking to expand the program to more students and sites next year and are exploring ways to host internships for students at UCSD from PRAGMA sites.

TEAM LEADERS AND MEMBERS

UCSD: *Gabriele Wienhausen, Provost, Sixth College and Academic Participant, Calit2; Linda Feldman, Director, Academic Internship Program; PRAGMA Principal Investigator Peter Arzberger, Director, UCSD Life Sciences Initiative and Director, National Biomedical Computation Resource; Teri Simas, Project Manager, PRAGMA.*

2006 STUDENTS: *Robert Sy, Ao 'Cathy' Chang; Daniel Goodman, Marshall Levesque (Osaka University); Stephen Chen, Mahboubeh Hashemi (NCHC); Bryan Lin (NCREE and NCHC); Angelina Altshuler, Celia Croy, Iwen Wu, Noah Ollikainen (Monash); Lily Cheng, Elaine Liu, Danjing Lisa Zhao (CNIC)*

2006 MENTORS: *Andrew McCulloch, Anushka Michailova, Roy Kerckhoff, Jason Haga, Gabriel Silva (Bioengineering); Wilfred Li (NBCR); Mark Ellisman, Steve Peltier, Tomas Molina, Raj Singh (NCMIR); Philip Bourne, (Pharmacology); Jurgen Schulze (Calit2); Chia-Ming Uang (Structural Engineering); Kim Baldrige, (U Zurich and SDSC).*

WORKING GROUPS

The working groups below reflect the interests of current PRAGMA members. Each group has a lead or co-leads who coordinate the activities of that group at and between meetings. The groups have projects that bring a focus to their activities, working towards milestones and holding demonstrations at PRAGMA workshops and other meetings. This structure allows for the inclusion of new applications as well as new areas of interest. New working groups are being considered for geo-grid/geosciences activities.

Biological Sciences

The Bioscience Working Group has established several projects that are of interest to participating members. The goal? To reach a common goal of conducting routine scientific investigations using the evolving grid infrastructure, while developing the necessary missing components in collaboration with other working groups, and disseminating the lessons learned.

Seven different institutes contributed to the CCGrid 2006 publication on the deployment of scientific applications on the grid. The lessons learned came from using Nimrod/G, Gfarm, MPICH-G2, and Ninf-G on applications ranging from quantum chemistry to computational biology and bioinformatics.

Members of the Bioscience Working Group actively participated in the PRIME and PRIUS projects, and the interactions among the programs' students and mentors have developed several important research and software development programs. Over the summer, PRIME researchers from UCSD at China's CNIC did research on virtual screening of new inhibitors for avian flu surface proteins. Another part of the project involves the initial planning for an avian flu database. UCSD and Osaka PRIUS teams extended the Opal web service toolkit to the Web Service Resource Framework (WSRF) as Opal operation provider.

Additional interactions among PRIUS host sites (University of Queensland and UCSD) through PRIUS students, and among summer interns from Jilin University at UCSD, contributed to the development of the PRAGMA Bioscience portal, with applications such as MEME and NAMD available as portlets. Additional applications will come from contributions from other participating members as GridSphere portlets. The Jilin University team developed a visual interface to CSF4 using GridSphere portlet technology. As part of the

ongoing experiment using Gfarm, UCSD, JLU and Tsukuba University teams deployed native bioinformatics applications such as MEME and continue to improve the performance and scalability of the Gfarm/CSF4 environment for biological applications.

The metagenomics annotation effort will begin to drive future development efforts of the Bioscience Working Group.

BIOSCIENCE: K. Jeong, Konkuk Univ., Chair; A. Krishnan, F. Tang, A. Shahab, BII Singapore; S.T. Hwang, Kookmin Univ.; J. Lee, K. Kee, K. Cho, KISTI; W. Li, SDSC at UCSD; K. Baldridge, SDSC and Univ. Zurich, P. Arzberger, UCSD; S. Hatano, Y. Qin, E. Zhang, Z. Lu, Chinese Acad of Sci; S. Shimojo, S. Date, S. Takeda, Osaka Univ.; X. Wei, Jilin Univ.; H. Lee, ASCC; collaborator E. McMahon, U Wisconsin.

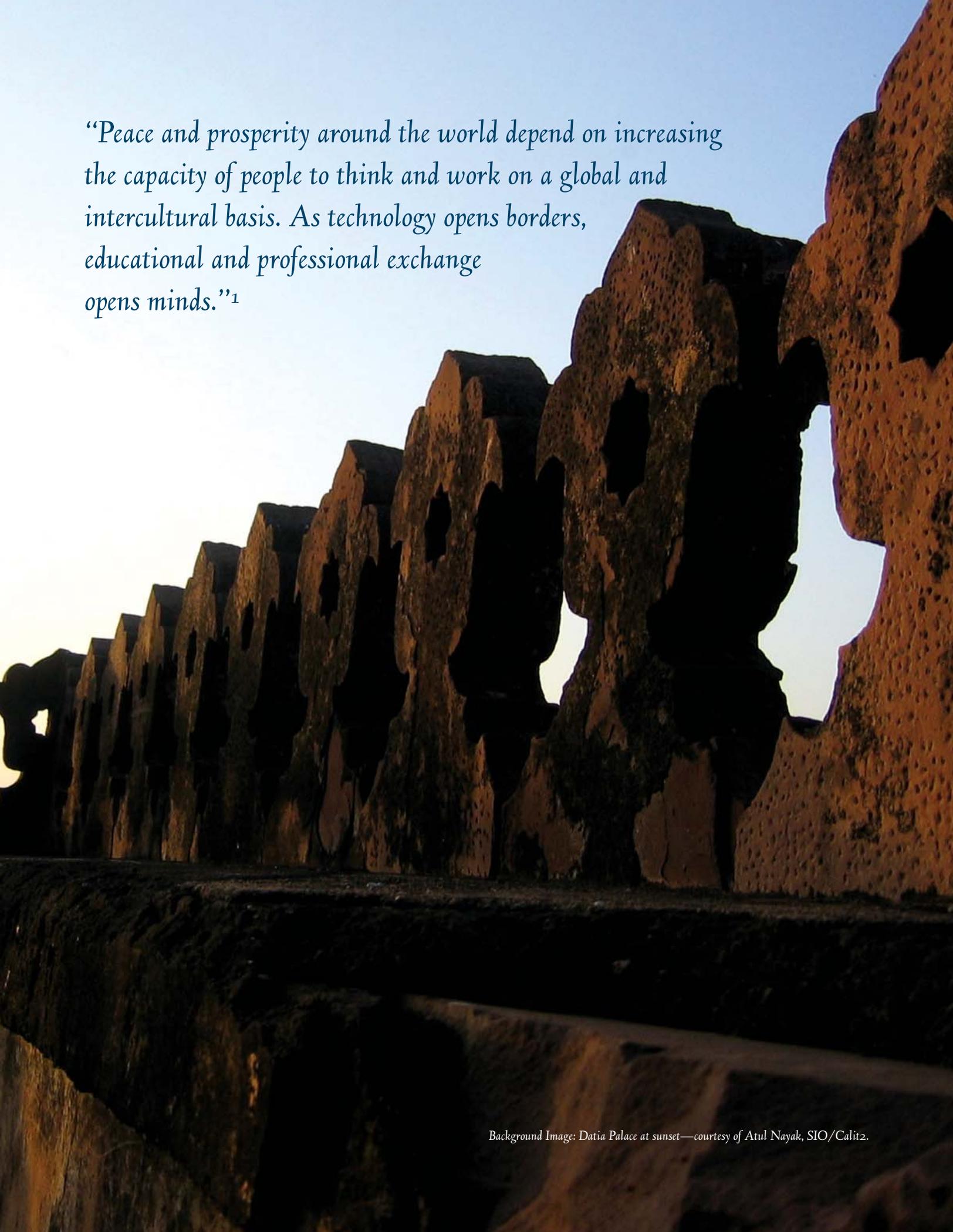
Telescience

The Telescience Working Group aims to create and develop new information technology that allows scientists to remotely use advanced, scientific devices and to show a form of 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. 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 two types of projects. The first—and traditional—activity is the establishment of a grid workbench for neuroscience, which would allow experts to use electron microscopes and control them remotely. The second is Ecology Grid which originated in Taiwan.

1. Annual Report IIE 2005, and www.iie.org "About"

“Peace and prosperity around the world depend on increasing the capacity of people to think and work on a global and intercultural basis. As technology opens borders, educational and professional exchange opens minds.”¹



Electron tomography is a powerful technique that draws on advanced instrumentation, networking, and grid computing to derive 3D structural information from biological specimens. The Telescience portal was developed by the National Center for Microscopy and Imaging Research (NCMIR) as a web-based portal solution for end-to-end electron tomography. It centralizes applications and seamlessly interfaces with the grid to accelerate the throughput of data results. The possibility indicated by the portal has promoted participation in the working group. Until today, the partnership has incorporated the Cybermedia Center at Osaka University's expertise in IPv6 networking, NCMIR's advances in Telescience infrastructure, and NCHC's expertise in visualization, advanced volume segmentation, and web-based visualization tools. As a result, the telemicroscopy systems of the Osaka ultra-high voltage electron microscope and the NCMIR intermediate voltage electron microscope have been enhanced and extended by digital video over end-to-end IPv6 networks, providing end-users with dramatically improved visual feedback during remote microscopy experiments. The working group has subsequently facilitated the integration of the new 1.25 MeV electron microscope at the Korea Basic Sciences Institute (KBSI) with the Telescience system. The working group won the Application Bandwidth Challenge award at SC03 by demonstrating the ability to use high-quality, low-latency HDTV to navigate a specimen in Osaka University's 3.0 MeV electron microscope via IPv6.

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. The Global Lake Ecological Observatory Network (GLEON) grew out of these activities, and could help as a testing ground as PRAGMA extends its testbed to sensors.

A new wave is coming to the Telescience Working Group in the form of tiled display walls. Scientists and other researchers in the group hope that the 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 areas of collaboration.

TELESCIENCE: F. Lin and S. Shimajo, Co-chairs; S. Kato, T. Akiyama, K. Nozaki, Osaka Univ.; M. Lee, KISTI; D. McMullen, Indiana Univ.; K. Mikami, Cray Inc.; B. Durnota, Complexibotics; M. Ellisman, S. Peltier, A. Lin, D. Lee, T. Molina, NCMIR at UCSD; I. Kim, KBSI; H. Chou, S-I Lin, S.Cheng, NCHC; S. Ninomiya, NARC and APAN; B. Pailthorpe, N. Bordes, U Queensland; T. Fountain, S. Tilak, UCSD; H. King, Taiwan Forest Research Inst; T. Kratz, N. Temperate Lakes LTER; D. Hamilton, U Waikato.

Resources and Data

The Resources and Data Working Group's goal is to improve the interoperability of grid middleware around the world and to make grids easier to use for scientists.

During the past year, the group has expanded PRAGMA's Grid testbed and routine-basis experiments, taking the lead in establishing Grid Interational Now (GIN) application testbed and in conducting GIN experiments in the GIN application testbed. Furthermore, the Data Computing Working Group has been combined with the Resources Working Group, to begin to build a data-grid as part of the routine-basis testbed.

The PRAGMA testbed grew from 19 sites in 13 countries to 26 sites in 14 countries, with a total of 726 CPUs, more than half a terabyte of memory, and 13.2 terabytes of online storage.

Applications have grown from three last year to 12 this year, ranging from climate simulation and quantum mechanics to genomics, organic chemistry and molecular simulation. Most of the applications utilize a grid middleware, either Ninf-G, Nimrod/G, MPICH-GX or Gfarm. Some applications, such as Savannah/Nimrod (see Accomplishments) and FMO/Ninf-G (pragma-goc.rocksclusters.org/applications/FMO/Results.html), have achieved long runs and produced meaningful scientific results. These routine-use experiments also resulted in significant enhancements for all application middleware involved. In particular, Ninf-G, Nimrod (see Accomplishments) and MPICH-GX all made significant improvements in scheduling algorithms, fault-tolerance and performance.

The same is true for grid infrastructure middleware. The grid monitoring software, SCMSWeb, and the grid accounting system, MOGAS, have made many important enhancements and have deployed to most testbed sites. They have become the key information systems in PRAGMA Grid.

Application users employ SCMSWeb regularly to check the resources availabilities and jobs status; and MOGAS provides critical accounting data for application and job analysis. For site administrators, SCMSWeb is essential for monitoring their systems and helping to locate and fix problems; and MOGAS data is not only handy for reporting resource usages to funding agencies, but also provides insight for grid infrastructure software design and development and supplies statistics for making resource configuration and policy adjustments to improve resource utilization.

Grid meta-scheduling is a big technical challenge to the grid community. Two teams in the resources group have been working on meta-scheduling solutions from two different approaches. The team at Jilin University in China has been working on Community Scheduling Forum (CSF), developed interfaces to commonly used local job schedulers, SGE, PBS and LSF, and demonstrated successful job submissions with basic resources selection. The team continues to work on more complete and automated resource selection capabilities by interfacing MDS with CSF. The other team is at the Institute of High Performance Computing in Singapore, which has developed a more self-contained meta-scheduling software and will test it on the PRAGMA Grid testbed soon.

While expanding our existing computational grid, the resources group has also taken steps to build a data grid in the testbed with Gfarm software. A Gfarm meta-server for the data grid has been setup at the testbed site National Institute of Advanced Industrial Science and Technology (AIST) in Japan. SDSC and NCHC are among the first few sites to install Gfarm file system and client nodes.

The group also participated in the GEON workshop in Beijing this July, discussed how GEON, AIST GEO Grid and PRAGMA testbed interoperate, what software is needed for geoscience applications, and how to run applications and share geoscience data. GUCAS and CNIC took action immediately. With help from the GEON team, GUCAS set up a compute node with geon roll and joined PRAGMA testbed. CNIC is building a geon data node which will join PRAGMA testbed, and both will also be linked to the GEON data network.

To enable interoperation with other grids and to enable users around the world to use grids, the group has established PRAGMA Certificate Authority (PRAGMA CA) using NAREGI-CA software, which was developed by National Research Grid Initiative (NAREGI) in Japan, in

which several PRAGMA member institutions participate. Working closely with APGrid PMA, PRAGMA CA joined International Grid Trust Federation (IGTF) to gain and maintain trust among global grids. (See Accomplishments.)

Since November 2005, PRAGMA has been involved with the Grid Interoperations Now (GIN) activity, led by Charlie Catlett and Satoshi Matsuoka that takes place at the GGF (now OGF) meetings. In early February this year, the resources group led the establishment of GIN application testbed (involving AIST, SDSC, and TeraGrid) and conducted the grid interoperation experiments. In a little more than six months, five grids have joined the GIN testbed. Working together, the GIN-ops team successfully ran TDDFT (Time Dependent Density Functional Theory—a quantum chemistry application based on grid middleware Ninf-G) on four of those grids—PRAGMA Grid, TeraGrid, Open Science Grid and NorduGrid. In addition, the team also explored grid interoperation issues with cross-grid infrastructure monitoring. Using SCMSWeb software, the team has set up an infrastructure testing matrix, tests and monitors key services of each GIN testbed site, providing real-time status. Furthermore, it collaborated with CERN and developed a grid map. (See Accomplishments)

The group has always been very active in knowledge sharing with broader grid communities. This year, its members gave numerous presentations and tutorials, published and documented issues, solutions and lessons learned on many major projects they involved in. You can learn about PRAGMA Grid activities at goc.pragma-grid.net. Four research papers based on PRAGMA Grid testbed work have been published this year (see Publications)

The group also welcomed institutions that are contributing to PRAGMA but have not yet become official members:

- State University of New York, Binghamton (SUNY-Binghamton, www.binghamton.edu), located in New York, U.S., has contributed resources to the testbed, attended the PRAGMA 10 workshop and is developing a grid-enabled sensor network application to run in the testbed.
- The Laboratory of Computational Geodynamics, Graduate University of Chinese Academy of Sciences (GUCAS, www.gucas.ac.cn/gscasenglish/index.aspx), located in Beijing, China, has contributed resources to the testbed as a GEON compute node and is developing a grid-enabled geoscience prototype to run in the testbed.

- The HCMC Institute of Information Technology (IOIT-HCM, www.ioit-hcm.ac.vn/english), is a scientific research institution of the Vietnamese Academy of Science and Technology (VAST), located in Ho Chi Minh City, South Vietnam. IOIT-HCM is one of the five leading organizations of VNGrid project. It has contributed resources to the testbed, attended PRAGMA 9 and PRAGMA 10 workshops, and developed and tested grid applications in the testbed. IOIT-HCM researchers have been involved in grid-based applications, including a national bioinformatics project and computational fluid dynamics. research.
- Queensland University of Technology (QUT, www.qut.edu.au), located in Brisbane, Australia, has contributed resources to the testbed, attended many PRAGMA workshops, and developed and tested grid portals in the testbed. QUT has also hosted two PRIUS students for two months while supervising the development of the PRAGMA BioScience Portal in collaboration with SDSC. This portal will utilize the PRAGMA testbed resources.
- Universidad de Chile (UCHile, www.uchile.cl), located in Santiago, has contributed resources to the testbed, attended the PRAGMA 7 workshop and has since become the lead of Chile's national grid initiative (CLGrid). In January 2006 the Center for Mathematical Modeling (www.cmm.uchile.cl) of Universidad de Chile invited all the Chilean universities to participate in the local grid initiative. The objective was to develop grid scientific applications of national interest. Currently 18 universities are participating and have carried out two workshop, an Intel software college, and grid programming testbeds.
- Universidad Nacional Autónoma de México (UNAM, www.unam.mx), located in Mexico City, has contributed resources to the testbed, attended the PRAGMA 7 workshop, and was an original lead of Mexican grid efforts via CUDI.
- Organic Chemistry Institute (OCI), University of Zurich (UniZH, www.oci.unizh.ch), located in Zurich, Switzerland, has contributed resources to the testbed and been involved in PRAGMA meetings from early on. Researchers at OCI are involved in the computational chemistry activities mentioned in the Accomplishments section, including projects with Nimrod, GAMESS/APBS, and Kepler software.

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

RESOURCES AND DATA: M. Katz, Co-chair, SDSC at UCSD; Y. Tanaka, Co-chair, AIST; Y. Tanimura, H. Takemiya, T. Ikegami, AIST; H. Shih, Eric Yen, ASGC; L. W. Kit, S. Wong, BII Singapore; O. Tatebe, CCS; S. Castañeda, J. Delgado, R. Hazas, CICESE; K. Dong, K. Nan, CNIC; S. Chen, H. Zhang, Y. L. Shi, GUCAS; Z.H. Ding, X. Wei, JLU; H. V. Nguyen; V. D. Hieu; T. V. Lang, M. Trang, T. Du, IOIT-HCM; D. Ta, H. M. Chan, IHPC; S. Kim, P. Lee, KISTI; S. Sriprayoosakul, S. Phatanapherom, P. Uthayopas, KU; J. Y. Luke, W. Hassan, MIMOS; C. Eenticott, D. Abramson, MU; C. L. Huang, W. Huang, NCHC; T. Roney, R. Nandkumar, NCSA; S. Prueksaaron, S. Vannarat, NECTEC; N. Teou, H. Y. Lee, NGO; F. Lee, J. W. Lee, NTU Singapore; S. Takeda, S. Date, Osaka U; A. Wright, R. Chhabra, QUT; C. Zheng, P. Papadopoulos, SDSC at UCSD; T. Chiba, S. Matsuoka, TITECH; A. Garcia, UBC; J. C. Maureira, A. Jofre, Univ. Chile; H. Zhang, M. Liu, UMC; E. Murrieta Leon, J. L. Gordillo Ruiz, UNAM; R. Wankar, N. Reddy, A. Agarwal, UoHyd; B. Yaik, F. Haron, C. H. Yong, Suhaini Ahmad, Habibah Wahab, USM; K. Baldridge, UniZH and SDSC; C. Amoreira, M. Packard, UniZH; X. Fan, T. N. Truong, U. Utah.



MEMBERS

PRAGMA is an institution-based organization. It brings together, leverages, and integrates expertise, tools, and resources from its member institutions. Below is a description of key institutional strengths and recent activities that have made PRAGMA a success.

Academia Sinica Grid Computing

www.twgrid.org

As the major grid computing and e-infrastructure center in Taiwan, the Academia Sinica Grid Computing (ASGC) center provides grid computing service and support for a variety of application areas in Taiwan and Asia. Acting as the World-wide LHC Grid Tier-1 center and Asia Regional Operation Center and Global Grid User Support, ASGC provides grid-related technology, certification authority and operation services as well as e-science infrastructure support for the Large Hadron Collider experiment in Asia.

Other than grid applications for high-energy physics, ASGC has been developing various life science applications since 2002 in collaboration with domain experts on grid systems, including BioPortal, CRASA, mpi-BLAST-g2, and others. ASGC is also extending grid technology to such fields as biomedical informatics, digital archives, Earth science and biodiversity informatics.

In April 2006, a collaboration of ASGC and European laboratories analyzed 300,000 possible drug components against the avian flu virus H5N1 using the EGEE Grid infrastructure. For the docking of 300,000 compounds against eight different target structures of Influenza A neuraminidases, 2,150 computers were used over four weeks in April—the equivalent of 137 years on a single computer. More than 1,400 gigabytes of 60,000 data output files were created and stored in a relational database.

Through participation in PRAGMA as well as its Bioscience and Grid Working Groups, Academia Sinica Grid Computing shares its expertise and enlarges the scope of its grid activities, including application development, grid middleware development and deployment, cross-grid integration and validation, along with grid operation and monitoring.

Key Contacts: Simon Lin, Eric Yen

Asia-Pacific Advanced Network

www.apan.net

With 15 primary, five associate, 11 affiliate, five liaison and two industry members, the Asia-Pacific Advanced Network (APAN) is a non-profit international consortium that provides an international, high-performance network infrastructure for research and educational activities in the Asia-Pacific region. Currently 15 countries and regions are connected through APAN's high-bandwidth links. The link between the U.S. and Japan operates at 20 gigabits per second (Gbps). The TransPAC2 link between Tokyo and Los Angeles operates up to 10 Gbps, and JGN2 offers up to 10 Gbps between Tokyo and Chicago.

APAN's working groups and committees promote projects that utilize that high-bandwidth infrastructure. The organization's Natural Resource Area has working groups in agriculture. The Earth Observation and Earth Systems Working Groups have been pursuing grid-orientated applications through collaboration with the grid committee. Examples of these applications include a data grid for satellite image archives, a high-per-

formance computing grid for climate prediction, a middleware and web-service grid for heterogeneous weather databases, and a high-density grid for wireless field sensors. In addition to PRAGMA, APAN maintains close relationships with active grid organizations in Asia including the Asia Pacific Bioinformatics Network, ApGrid, and Global Grid Forum. The grid committee coordinates APAN's grid-related activities and its links with external organizations.

Key Contacts: Seishi Ninomiya, Kento Aida

Australian Partnership for Advanced Computing

www.apac.edu.au

With its eight partners, the Australian Partnership for Advanced Computing (APAC) provides advanced computing facilities to the Australian research community, government, and industry. APAC is integrating these facilities into a national grid that allows researchers to gain seamless access to advanced computational, data and visualization resources. The APAC National Grid supports research communities in the areas of astronomy, high-energy physics, bioinformatics, chemistry, geophysics, and Earth sciences. It also facilitates participation by these communities in national and international research programs.

APAC is a silver sponsor of the Open Grid Forum. APAC representatives have attended PRAGMA workshops. Further, APAC and Monash University co-hosted PRAGMA 4 in Melbourne, Australia. With its partner QPSF, APAC also co-hosted the APAC Conference and Exhibition on Advanced Computing, Grid Applications and eResearch on Queensland's Gold Coast, September 2005. They also co-hosted PRAGMA 10 at Townsville in March 2006 and an associated follow-on meeting for lakes (GLEON) and coral-reef observatories.

APAC member Monash University hosted four PRIME students in 2006. It is also an active partner in the PRAGMA testbed and the routine-use experiment.

Key Contacts: John O'Callaghan, David Abramson, Bernard Pailthorpe

Bioinformatics Institute, Singapore

www.bii.a-star.edu.sg

Scientists from the Bioinformatics Institute (BII) have been involved in application development, creation of middleware necessary for grid-enabled biological applications, and National Grid (Life Sciences) activities. These activities resulted not only in a scalable, secure, and user-friendly national grid resource, but it has also strengthened Singapore's role in grid-based, bio-computing applications and analyses.

In recent years, BII staff and scientists have produced numerous bioinformatics manuscripts and applications on microbial genome analysis, systems biology, high-end computing, and protein structure analysis. BII also has been actively involved in providing a computational arm to laboratory-based biological science research at various departments in the National University of Singapore, National University Hospital, Singapore, and such research institutes as the Genome Institute of Singapore and Institute for Molecular and Cell Biology. The BII team is currently deploying grid-based technologies to serve as the Informatics core for the Singapore Gastric Cancer Biomarker Discovery Program, the Singapore Stem Cell Consortium and the Biopolis-wide Imaging Informatics Program.

BII contributed to PRAGMA with its involvement in the PRAGMA testbed. With the National Grid Office, Singapore, BII co-hosted the PRAGMA 8 workshop in Singapore in May 2005, and participates in the Bioscience Working Group. PRAGMA provides BII and other PRAGMA members with a platform for collaborations that foster research in such interdisciplinary sciences as bioinformatics and computational biology. BII proposes to extend its expertise in analytical and computational bioinformatics to other PRAGMA members.

Key Contact: Gunaretnam Rajagopal

Center for Computational Sciences, University of Tsukuba

www.ccs.tsukuba.ac.jp

Based at the University of Tsukuba, the Center for Computational Sciences (CCS) is a research institute for high-performance computing technology. It is working to open the grid to new areas and methodologies of discovery and analysis in computational science. The center is working on several grid projects in Japan and other countries.

CCS has strong ties with other PRAGMA partners in Japan, including the National Institute of Advanced Industrial Science and Technology (AIST), Titech, Osaka University, and ApGrid.

CCS researchers have developed several grid middleware tools such as a grid RPC system, OmniRPC for parallel programming, and the Grid-enabled Heterogeneous Multi-Computer System (HMCS-G) for sharing a special-purpose computer, GRAPE-6, on the grid, and computational chemistry applications for the grid. CCS is also involved in the International Lattice Data Grid Project to develop an international data grid for the lattice field theory community.

In 2006 Osamu Tatebe was appointed Associate Professor in CCS; previously he worked at AIST's Grid Technology Research Center. He continues to work on extensions of Gfarm. PRAGMA provides a forum for exchanging ideas and resources through the promotion of broader collaborations with PRAGMA partners.

Key Contacts: Osamu Tatebe, Taisuke Boku, Mitsuhsa Sato,

Centro de Investigación Científica y de Educación Superior de Ensenada

www.cicese.mx

The Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE), the Center for Scientific Research and Higher Education of Ensenada, is a research institution established in 1973 in Ensenada, Baja California, Mexico, with Masters- and Ph.D.-granting programs. CICESE scientists perform basic and applied research on areas such as oceanography, ecology, marine biology, geophysics, seismology, biotechnology, optics, electronics, telecommunications and computer science. For years, several groups in these fields have carried out joint projects with various U.S. universities from neighboring states including California and Arizona, in particular with those in the San Diego area.

Out of those collaborations, CICESE received an invitation to attend PRAGMA 7 and subsequently joined the PRAGMA testbed. CICESE contributed a Sun Microsystems server-based cluster to the testbed and worked with Dr. Putchong Uthayopas' High Performance Computing and Networking Center at Kasetsart University (KU), in porting the SCMSWeb monitoring tool to Solaris OS.

Under the auspices of its partnerships with Calit2, San Diego Supercomputer Center, San Diego State University,

and the National Science Foundation, CICESE participated in iGrid 2005 with a demo grid running a compute-intensive, meteorological forecasting model, MM5, using a high-bandwidth, optical-fiber link between San Diego and Tijuana, Mexico. A paper outlining the demonstration's results was published in the journal *Future Generation Computer Systems*.

Most recently CICESE has been working with the Korea Institute of Science and Technology Information (KISTI) on using MPICH-GX for applications like MM5. Many applications like the latter requiring real-time communication among its processes run well on a single cluster or a dedicated grid with all nodes on public IP addresses, yet most Beowulf-type clusters on the PRAGMA testbed use private IP addresses for the compute nodes.

Key Contacts: Raúl Hazas, Salvador Castañeda

College of Computer Science and Technology, Jilin University

www.jlu.edu.cn

Jilin University (JLU), one of the key research universities directly administered by the Chinese Ministry of Education, is ranked among the top 10 universities in China. The College of Computer Science and Technology (CCST) of JLU is a top-tier educational and research institution in computer science in China. CCST's study of parallel computation can be traced to the 1980s, and since then it has built a team of experienced researchers, with ties in the field of grid computing to PRAGMA members at the University of California, San Diego (UCSD) and Japan's National Institute of Advanced Industrial Science and Technology (AIST). The grid computing research team at CCST has developed CSF4 (Community Scheduler Framework), the first WSRF meta-scheduler, as a contribution component of GT4 with Platform Inc.

CCST has been collaborating with UCSD and AIST since 2003. To provide a grid testbed for data-intensive applications, researchers at JLU, UCSD, and AIST are working on integrating a meta-scheduler (CSF), local scheduler (LSF/SGE), and Gfarm. In 2006, JLU researchers implemented a web portal for CSF to provide a friendly interface to end users. Working with Platform, JLU researchers implemented a web service gateway service for Platform EGO which was released recently. Since 2005, JLU has augmented PRIME by sending its students (Zhaohui Ding and Yuan Luo) and faculty—whose work has contributed to the Bioscience Working Group—to UCSD.

CCST is actively engaged in PRAGMA's Resource and Data Working Groups to build a daily use grid testbed for data-intensive applications.

Key Contact: Xiaohui Wei

Computer Network Information Center, Chinese Academy of Sciences

www.cnic.ac.cn

As a founding institutional member of PRAGMA, the Computer Network Information Center (CNIC) has been actively participating in the organization's activities and promoting international cooperation around the Pacific Rim. CNIC researchers are involved in most PRAGMA working groups, providing a 36-CPU IA64 cluster for the PRAGMA testbed; participating in remote visualization activities with other PRAGMA members with a 5x4 tiled display wall situated at CNIC; and organizing science applications in such disciplines as astronomy, biology, and high-energy physics in China. As part of its commitment to collaborative training among PRAGMA members, CNIC held a distance-training workshop with UCSD in February 2004. PRAGMA 6, hosted by CNIC in May 2004, was a tremendous success. As part of the PRIME program, CNIC hosted three students from UCSD in summer 2006, and two the previous summer. The center will also co-host the twentieth CODATA conference in October 2006 in Beijing.

CNIC is a subsidiary research institute under the Chinese Academy of Sciences (CAS). It was founded in 1995 and plays a significant role in grid computing and applications in China. In particular, it has been deeply involved in such key projects as the China National Grid (CNGrid) and the Scientific Data Grid (SDG). In these projects, CNIC is one of the two main nodes providing a 4TFLOPS supercomputer Lenovo DeepComp 6800 and is the leading SDG site among the 45 CAS institutes across the country. Version 2.1 of SDG Middleware was released in August 2005 as a set of grid middleware to support data access and integration for distributed, heterogeneous and multidisciplinary scientific data. The programs, activities, and partnerships launched in the past few years form the foundation on which CNIC researchers will build on past achievements in grid computing and applications.

Key Contacts: Baoping Yan, Kai Nan

Cray Inc.

www.cray.com

Cray Inc., a global leader in supercomputers purpose-built for high-performance computing (HPC), is the first Industrial Affiliate member of PRAGMA and sponsor of PRAGMA workshops. In addition to participating in PRAGMA workshops, Cray provides expertise in HPC and demonstrates ways in which grid technologies can be used to provide access to scarce HPC resources.

Cray is involved with PRAGMA's Resources Working Group and provides support for grid middleware and application porting activities. By utilizing technical expertise obtained through its association with PRAGMA, Cray has facilitated the successful implementation of grid software at customer sites.

Such projects include Globus Toolkit integration on the Cray XT3 system at Japan's National Institute of Advanced Industrial Science and Technology (AIST), which supports campus-wide access via Globus to the XT3 system. Another such project involved UNICORE integration on the Cray X1E system at the Korean Meteorological Administration, which supports multi-model ensembles as a remote service using grid technology within the center's infrastructure and in pilot studies.

Key Contacts: Geert Wenes, Kazunori Mikami

Cybermedia Center and Research Center for Ultra-High Voltage Electron Microscopy, Osaka University

www.cmc.osaka-u.ac.jp

www.uhvem.osaka-u.ac.jp

prius.ist.osaka-u.ac.jp

Osaka University has been contributing to PRAGMA in terms of both R&D and education since the consortium's creation. The university's grid R&D activities are based heavily on Japanese national projects such as the Japan Gigabit Network (JGN2), governed by the National Institute of Information and Communication Technology (NICT), and the BioGrid project, funded by MEXT. As for educational activities at Osaka University, the PRIUS program started in 2005 and the university continues to participate in UCSD's PRIME program.

In PRAGMA, Osaka University is co-leading the Telescience Working Group, and is an active participant in the Bioscience Working Group. Through collaboration with the Telescience group, the university has developed a

grid system that allows scientists to perform their analyses by remotely controlling the world's largest ultra-high voltage electron microscope, located in the Research Center for Ultra-High Voltage Electron Microscopy. As a participant in the Bioscience group, Osaka University brings its expertise from the BioGrid project. In addition, the university recently installed two sets of 4x5 tiled display facilities to create a collaboration environment for e-science with the PRAGMA community. The facilities are expected to be part of the PRAGMA cyberinfrastructure.

With regards to education, Osaka University has been working for the establishment of an educational network on the PRAGMA R&D infrastructure through the framework of UCSD's NSF-funded PRIME program and the Japanese university's PRIUS educational project. Osaka University has accepted ten students in total from UCSD over three years, and sent three students to Nanyang Technological University and Queensland University of Technology as part of its investment in PRAGMA.

The Cybermedia Center co-hosted the third PRAGMA workshop with the National Institute of Advanced Industrial Science and Technology (AIST) in January 2003, and hosted the PRAGMA 11 workshop in October 2006.

Key Contacts: Shinji Shimojo, Susumu Date, Kazunori Nozaki, Toyokazu Akiyama

Global Scientific Information and Computing Center, Tokyo Institute of Technology

www.gsic.titech.ac.jp

The Tokyo Institute of Technology (Titech) is one of Japan's premier universities, specializing in advanced fields of science and technology. Since Titech's Global Scientific Information and Computing Center (GSIC) was established in April 2001, it has been responsible for deploying advanced informational infrastructure for the entire institute. GSIC aims to host a world-class supercomputing facility and to research, develop, and deploy grid-computing infrastructures for high-end scientific computing. GSIC's grid deployment project, called the Titech Grid, and centered around the new cluster supercomputer TSUBAME that embodies 10480 Opteron processors plus the Clear-



Background Image: Kyoto fountain—courtesy of Rob Reed.



Background Image: UCSD's Stuart Collection "Bear" sits in front of the Calitz building.

Speed accelerator, exhibiting peak performance at 85Teraflops, along with memory capacity of 21.4 TB, and on-line disk capacity of 1.1 Petabytes that demonstrate 50GB/s of I/O bandwidth. It is currently the fastest supercomputer in Japan as well as Asia Pacific. GSIC also serves as a consolidated compute/datacenter hosting other resources in the grid in a central fashion, including its Windows cluster of 300 CPUs, a data-oriented cluster of 350 processors, etc. The clusters are connected internally as well as with the high-speed multi-gigabit campus network, SuperTITANET.

The Titech Grid, initiated in April 2002, has deployed various grid middleware, including the Globus Grid Toolkit, Condor job management system, and the Ninf GridRPC middleware, jointly developed with AIST. In 2003 a Memorandum of Understanding was signed between SDSC and Titech to foster collaborative research and share experiences of grid infrastructures. The MoU has led to several successful collaborative projects, including those in the Encyclopedia of Life project, highlighted at SC03. Also, it is the leading institution in deploying the grid middleware developed by the NAREGI project—the Japanese national project that is implementing Japan's CyberScience Initiative led by the National Institute of Informatics. Titech is currently participating in the PRAGMA Testbed and routine-use experiment. Furthermore, Titech leadership has encouraged the formation of GIN and inclusion of PRAGMA in the GIN activity.

Key contacts: Satoshi Matsuoka, Takeshi Nishikawa, Toshio Endo

*Grid Technology Research Center,
National Institute of Advanced Industrial
Science & Technology www.gtrc.aist.go.jp/en*

As part of the National Institute of Advanced Industrial Science and Technology (AIST), the Grid Technology Research Center (GTRC) is dedicated to the research and development of state-of-the-art grid programming tools, international verification experiments, grid-building technologies, and ultra-high-speed networks.

Six GTRC teams cover every facet of R&D. The center's mission is to collaborate on international standardization with research organizations in Asia-Pacific countries. GTRC also aims to turn research and development results into deliverables and provide them to users, while accelerating the commercialization of grid technology through industrial, academic, and government collaboration.

The GTRC, founded in 2002 with a limited term of 6.75 years, has grown to include 64 members, including regular, postdoctoral, visiting, and temporary staff. At the Tsukuba Central 2 and Akihabara offices, GTRC conducts studies on requirements for a reliable grid in efforts to make a quantum leap in sophistication and systematization of grid technology.

PRAGMA provides opportunities to encourage the use of AIST-developed grid middleware, such as Ninf-G and Gfarm. AIST, which co-hosted the third PRAGMA workshop in Fukuoka, has provided a cluster to the PRAGMA testbed. AIST researchers have been involved in all PRAGMA working groups, including the Resource group, in which AIST researchers led the first routine-use experiment on the PRAGMA testbed using Quantum Computational Chemistry and Molecular Simulation with Ninf-G. This months-long experiment provided a basis for fault-tolerant research. Ninf-G was included in NSF Middleware Initiative core releases, and Gfarm has been selected by several PRAGMA applications. Furthermore, AIST researchers have forged new interactions with GEON, OptIPuter, and the California Institute for Telecommunications and Information Technology (Calit2), including establishment of a persistent presence within Calit2's headquarters at UCSD and a letter of intent to explore new areas of collaboration.

Key Contacts: Satoshi Sekiguchi, Yoshio Tanaka

Institute of High Performance Computing, Singapore

www.ihpc.a-star.edu.sg

The prime charter of the Institute of High Performance Computing (IHPC) is to power scientific discoveries in multi-disciplinary domains through advanced methodologies, techniques and new tools in modeling, simulation and visualization. To support the computational needs of that agenda, IHPC researchers work on high-performance and grid computing technologies, and explore end-to-end solutions for scientific applications. Researchers investigate innovative approaches in grid middleware, including infor-

mation and execution management, distributed data file management, workflow execution, grid deployment and a template-based approach for automated generation of Java-based user interfaces.

In addition to middleware work, IHPC works with the user community to grid-enable applications using their components. Target applications include: fire and smoke modeling; multi-physics solving; digital-media content rendering; multi-disciplinary engineering design optimization; electromagnetic simulation; hydrodynamic simulation; and life science applications such as motif discovery, which have also been successfully grid-enabled.

In July 2006, IHPC initiated the Agency for Science, Technology and Research (A*STAR) Digital Nervous System (ADNS) initiative. ADNS strives to establish a grid-enabled scientific computing platform that will integrate across A*STAR's resources while offering access to the diverse scientific and engineering applications for A*STAR-wide institutions. Technologies to be integrated include high-performance computer servers, high-bandwidth networks, data storage systems, sensor networks, lab equipment as well as high-fidelity visualization facilities. ADNS will also provide technology for geographically distributed scientists to collaborate remotely and more effectively.

A newly inducted member, IHPC is working on integrating its computing resources with those of other PRAGMA organizations. It also plans to contribute its existing grid components to PRAGMA and to work with the Resources Working Group.

Key Contacts: Terence Hung, Hoong Maeng Chan, Quoc Thuan Ho

Kasetsart University

www.ku.ac.th

Through PRAGMA, researchers at Kasetsart University (KU) have been working closely with leading counterparts throughout the Asia-Pacific region. As part of the Resources Working Group, the KU High-Performance Computing and Networking Center (HPCNC) has helped develop the powerful and comprehensive monitoring tool called SCMSWeb. This tool enables near-real-time capture of PRAGMA testbed system characteristics, leading to the detection and solution of problems and resulting, in turn, in a much more stable and practical grid system. KU developers are responding to feedback from the routine-use test by adding job monitoring and process accounting

features, and porting SCMSWeb to many new platforms. KU researchers are working together under PRAGMA leadership in exploring Grid Interoperation Now (GIN) issues. This collaboration inspired KU team members to add new features to SCMS, including geographic mapping, bandwidth probing, GLUE interface, and better service probing.

KU also dedicated its AMATA cluster to PRAGMA flagship routine-use applications, including a Savannah burn simulation using Nimrod, as well as QM-MD and TDDFT simulations using Ninf-G. Another collaboration—with the Asia Institute of Technology and Titech—uses Ninf-G as middleware in handling remote-sensing data to enhance agriculture. The experiences learned from the development, deployment, and use of these applications represent best practices for using grid systems in large-scale applications.

Kasetsart University is actively promoting NPACI Rocks technology in southeast Asia. NPACI Rocks team leader Mason Katz visited Thailand and helped set up a successful workshop in May 2006. The KU team also contributes development work to NPACI Rocks, notably in the development of Diskless Roll, which enables users to set up diskless compute nodes as a compute spool for a ROCKS cluster.

Going forward, KU, the Thai National Grid Center and the country's National Electronics and Computer Technology Center (NECTEC) are working together on hosting PRAGMA in Thailand in 2007.

Key Contacts: Surasak Sanguanpong, Putchong Uthayopas

Korea Basic Science Institute www.kbsi.re.kr

The Korea Basic Science Institute (KBSI) is the largest provider of state-of-the-art and large-scale research equipment in Korea. The JEM-ARM 1300S—dubbed the Morning Star—is the first Ultra-High Voltage Transmission Electron Microscope (UHV-TEM) installed in Korea. Its atomic resolution can exceed 1.2 Å (point-to-point). With its precise stage control, the UHV-TEM is able to tilt more than $\pm 60^\circ$ within $\pm 0.1^\circ$ error, which allows for 3D structure analysis of complex materials. The UHV-TEM can also operate remotely without losing its atomic resolution.

The UHV-TEM is remotely operated in collaboration with Telescience experts at the UCSD-based National Center for Microscopy and Imaging Research (NCMIR) and grid experts at the Korea Institute of Science and Technology Information (KISTI) Supercomputing Center. At PRAGMA 6, researchers demonstrated the UHV-TEM's remote control and data acquisition capabilities. The goal of the UHV-TEM e-science project is to develop methods for grid-based imaging, telemicroscopy and automated electron tomography.

As part of the PRAGMA Telescience Working Group, KBSI is collaborating with KISTI, NCMIR, SDSC and Osaka University to expand the remote operation system of UHV-TEM. KBSI is an active participant in many PRAGMA workshops.

Key Contacts: Inho Gim, Jung-Eok Gu

Korea Institute of Science and Technology Information

www.kisti.re.kr
www.ksc.re.kr

The Korea Institute of Science and Technology Information (KISTI) is the leading organization of K*Grid, an initiative that aims to construct a Korean national grid infrastructure of geographically distributed high-performance computers, high-technology instruments and scientific experts, all in support of middleware and application research. In 2005, Korea launched the six-year Korea e-Science Project, providing Korean researchers with an international e-science infrastructure. During the first three years, activities will focus on five application projects (Bio, Nano, Metrology, Aerospace, and Telescience). The initiative also calls for the development of a Science Gateway in 2010, comprised of middleware that can be applied to all five application projects.

Through K*Grid and e-Science, KISTI researchers are involved in research activities including implementation of a computational grid and access grid and the development of the grid middleware toolkit, grid applications, and high-performance networking of interest to PRAGMA. KISTI is establishing a grid testbed with domestic and international researchers in a variety of applications, and it also operates the secretariat of Grid Forum Korea, which provides a venue for grid researchers in Korea to communicate and collaborate. In addition, KISTI actively participates in other grid-related organizations such as Global

Grid Forum and the Asia-Pacific Advanced Network (APAN) consortium.

KISTI has been actively involved in PRAGMA workshops, working groups, testbed, routine-use experiment (contributing 80-node and 16-node Linux clusters), and projects including: MGrid (www.mgrid.or.kr), a cost-efficient and reliable grid computing system for biomolecular simulations; and e-AIRS (obiwan.kisti.re.kr/escience/eairs), an integrated system for the aerospace research system, in which some developed modules have been utilized in collaboration with the U.S. National Center for Supercomputing Applications (NCSA). Researchers also tested MPICH-GX with MM5 running on Kgrid, a collaboration linking KISTI to the partner PRAGMA testbed site at Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE).

KISTI also produced a Korean version of the Rocks cluster software. KRocks 4.0.0 for x86, x86_64t, and ia64 was released in August 2005 and is distributed through krocks.cluster.or.kr.

Future collaborations will include running the CFD simulation on the e-science testbed run by KISTI and PRAGMA members in Japan and China, and investigating network performance measurement with NCSA and the National Center for High-performance Computing (NCHC).

Key Contacts: Jysoo Lee, Kum Won Cho

Malaysian Institute of Microelectronic Systems

www.mimos.my

MIMOS is a leading research and developing organization in Malaysia, and is developing a new approach to steering the nation's premier applied R&D centre into frontier technologies. Through technology innovation, MIMOS is striving to stimulate Malaysia's economic growth by producing novel products which eventually benefits the Malaysian and global society. MIMOS focuses in applied research areas based on the real-world trends. These research areas include: Cyberspace Security; Encryption Systems; Grid Computing; Wireless Broadband; Micro Energy; MEMS/NEMS Systems; Advance Informatics; and Knowledge Technology. MIMOS invites collaboration and partnerships with industry, universities, and governments.

MIMOS' major thrust of the Grid Computing laboratory is to research and develop major grid infrastructures as well as data mining applications that will benefit the research

community. The priority of the research will therefore focus on investigating and developing middleware tools, enablers, applications and grid facility, infostructure, and security.

MIMOS is actively engaged in several PRAGMA activities by contributing resources to the PRAGMA testbed and participating in the Bioscience Working Group.

Key Contacts: Thillai Raj T. Ramanathan, Jing-Yuan Luke, Irdawati Ab Rahman

National Agricultural Research Center

narc.naro.affrc.go.jp/narc-e/index.htm

The National Agricultural Research Center (NARC) is one of the 11 research institutes under Japan's National Agriculture and Bio-oriented Research Organization. It covers a wide range of research fields in agricultural and life science. NARC's department of Information Science and Technology is a global leader in the application of information technology and science to agriculture and natural resource-related fields.

Given the data resources handled by NARC, important issues include the integration of various kinds of comparatively small-scale distributed data sets, as well as overcoming the heterogeneity of even the same kind of data resources. Therefore, data grid technology for such resources has been a focus of the NARC group. Data mediation middleware that provides client applications with consistent access to heterogeneous databases is one of the solutions promoted by NARC. One middleware implement for meteorological databases, MetBroker, provides such access to the weather data of more than 20,000 weather stations from almost 200 countries in 23 databases around the world. To address issues of high-quality and spatially dense data acquisition in the field, NARC has targeted the development of efficient sensor networks or grids. The Field Server—a low-cost and high-quality wireless field monitoring robot—is one of the products for the sensor network, which has deployed more than 100 sets in seven countries. These products of NARC are partially contributing to the lake metabolism project launched by PRAGMA.

Key Contacts: Seishi Ninomiya, Masayuki Hirafuji

National Center for High-performance Computing, National Applied Research Laboratories

www.nchc.org.tw

The National Center for High-performance Computing (NCHC) has led development of Taiwan's national grid project, the Knowledge Innovation National Grid (KING), from 2003 to 2006. KING is an advanced and collaborative high-performance computing environment for scientific applications and technology development. Its twin project, the TaiWan Advanced Research & Education Network (TWAREN) is a world-class, island-wide R&D network made up of a high-bandwidth 20Gbps backbone. NCHC's three resource centers at Hsinchu, Taichung, and Tainan are all linked via the TWAREN network and therefore able to share fully in grid resources such as high-end networking, cluster computing, storage and supporting grid technologies (including sensor network technology, access grid, and advanced visualization technologies such as virtual reality and tile display walls). KING is an applications-driven project that focuses on such life-improving applications as the e-learning grid, eco-grid, healthcare grid, flood mitigation grid, and biology grid. KING collaborates with various Taiwan-based high-performance computing and domain-technology experts, and with international grid-related organizations.

Many KING application projects collaborate on PRAGMA-related initiatives, including the Telescience project, the SARS grid project, GLEON, and Coral Reef Observatory Network (CREON), and NCHC hosted the third GLEON and CREON joint workshop in 2006. Further, NCHC's parent organization, the National Applied Research Laboratory of Taiwan, has fully supported NCHC and National Center for Research on Earthquake Engineering (NCREE) to join in the Earthquake Engineering Network workshop organized by PRAGMA.

NCHC hosted the PRAGMA 5 workshop, provides dedicated resources to the PRAGMA testbed, and hosted three PRIME students in 2004 and 2005. In 2004, NCHC hosted the Sensor Network Forum, where PRAGMA members and Taiwan researchers delivered speeches and shared knowledge. In 2005 NCHC hosted the first Southeast Asia Workshop to provide a venue to further develop ties among regional grid-research institutions. NCHC also helps organize the Workshop on Grid Technologies and Applications, Taiwan's first academic grid workshop.

Key Contacts: Whey-Fone Tsai, Fang-Pang Lin

National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign

www.ncsa.uiuc.edu

The National Center for Supercomputing Applications (NCSA) at the University of Illinois at Urbana-Champaign, funded in part by the NSF's Office of Cyberinfrastructure, is the largest high-end computing center with almost 50 TFlops of computing power for open scientific research to advance discoveries in science, engineering, arts and humanities. NCSA serves a broad community of researchers, and is engaged in offering services and conducting R&D in cyber-resources for enabling discovery at the leading edge, cyberenvironments for harnessing the power of the national cyberinfrastructure, innovative computing systems for defining the path to petascale computing, scientific visualization for scientists and engineers providing critical insights and for educating the public, and cybereducation—bringing cyberinfrastructure into the classroom.

NCSA is dedicated to developing and deploying cyberinfrastructure in collaboration with others. NCSA is one of the original NSF-funded supercomputing centers, and has been one of the two original partners in the NSF Partnerships for Advanced Computational Infrastructure program. NCSA is part of the TeraGrid, and leads the National Center for Advanced Secure Systems Research, a project funded by the Office of Naval Research. It is also involved with a wide range of collaborative research projects, including LEAD (Linked Environments for Atmospheric Discovery), GridChem (Computational Chemistry Grid portal), CLEANER (Collaborative Large-scale Engineering Analysis Network for Environmental Research), Mae Viz (Mid America Earthquake Center) and LSST (the Large Synoptic Survey Telescope).

NCSA works with numerous PRAGMA member institutions and participates in the Resources and Data Working Groups, while providing access to its high-performance computing environment to the PRAGMA testbed. NCSA's International Affiliates Program hosted two researchers from KISTI for two months in 2006. Similar exchanges are planned with APAC. NCSA also hopes to sponsor students as part of PRAGMA's PRIME program and a similar PRIUS program in Japan. In October 2007, NCSA will host PRAGMA 13 in Urbana-Champaign.

Key Contacts: Radha Nandkumar, Danny Powell

National Electronics and Computer Technology Center

www.hpcc.nectec.or.th/pragma

National Electronics and Computer Technology Center (NECTEC) has been involved in Thailand's development of cluster and grid computing technology from the beginning. NECTEC's Thai Social/Scientific Academic and Research Network (ThaiSARN) connects and supports grid collaboration among Thai research communities and international research networks and forums. On the application side, NECTEC focuses its information grid research on agriculture and natural resources, bioinformatics, computational science, and engineering. In addition, NECTEC participates in a number of international forums on grid-related activities, such as ApGrid, Asia-Pacific Advanced Network (APAN), Internet2, and PRAGMA.

PRAGMA provides a venue in which NECTEC and Thai researchers can expand and share activities and resources in grid technology with Asia-Pacific colleagues. NECTEC is a founding member of PRAGMA actively participates in all PRAGMA meetings, and is actively engaged in the testbed activity. NECTEC will co-host the PRAGMA 12 workshop with Thai National Grid Project and Kasetsart University in March 2007. Prior to PRAGMA 12, NECTEC will host a GEO Grid workshop to promote this potential new area in PRAGMA in collaboration with the Grid Technology Research Center of Japan's National Institute of Advanced Industrial Science and Technology

Key Contacts: Piyawut Srichaikul, Chalermopol Charnsripinyo, Sornthep Vannarat

National Grid Office

www.ngp.org.sg

The National Grid Office (NGO) in Singapore has a vision of a high-speed network connecting computer resources that are shared in a secure, reliable, and efficient manner by authenticated users. Such resources will be shared for a variety of application domains and sectors, in an effort to improve the economic and technological competitiveness and quality of life in Singapore. NGO aims to achieve this vision by formulating a framework and policies, planning and developing a secure platform, adopting common open standards, encouraging grid computing, demonstrating compute resource-on-tap commercial viability, and laying the foundation for a vibrant grid-computing economy.

Via a high-speed gigabit network, the National Grid Pilot Platform (NGPP) connects resources at the Bioinformatics

Institute (with which NGO co-hosted PRAGMA 8 in Singapore in May 2005), Institute of High Performance Computing, Nanyang Technological University, National University of Singapore, Singapore-MIT Alliance, Singapore Management University, Ngee Ann Polytechnic, and Sun Asia-Pacific Science & Technology Center. Two clusters are connected as a part of the Large Hadron Collider Computing Grid at CERN. The NGPP also has Internet2 connectivity to the U.S., Europe, Taiwan, Japan, and Korea. The working groups focus on such areas as middleware and architecture, grid security, networks, applications, and governance. Domain-specific groups (virtual grid communities) have been established for life sciences, physical sciences, digital media, and manufacturing.

Besides establishing a computational grid, NGO's grid-related activities include access grid, certification authority, meta-scheduler deployment, undertaking grid-enabling of applications, development of a grid accounting system, co-organizing the annual GridAsia meeting, raising competency through seminars and training courses, and fostering international collaborations with Japan's National Institute of Advanced Industrial Science and Technology (AIST), Korea Institute of Science and Technology Information (KISTI), Asia-Pacific Advanced Network (APAN), UK-Singapore Partners In Science, and Gelato Federation.

Key Contacts: Lawrence Wong, Hing Yan Lee

Pacific Northwest Gigapop

www.pnw-gigapop.net

The Pacific Northwest Gigapop (PNWGP) plays a pivotal role as a state-of-the-art network infrastructure and communication-services hub for advanced network organizations of the Pacific Rim and North America.

Building on strategic partnerships and its strengths in network engineering and high-end multimedia, PNWGP provides a fertile breeding ground for innovative approaches needed to meet the escalating resource demands of the research community.

In addition to its collaborations with other PRAGMA participants, PNWGP is an APAN associate member and is a co-steward (with Japan's Widely Integrated Distributed Environment) of the Internet Educational Equal Access Foundation 10Gbps circuit between Seattle and Tokyo. As a parent organization of the Pacific Wave international exchange facility, PNWGP supports peering and Global Lambda Integrated Facility (GLIF) services for its network

peers throughout the Pacific Rim. These include AARNet, CANARIE, GEMNET, KAREN (NZ), KREONet2/GLO-RIAD, MIMOS, National University of Singapore, SINET, TANet, TransPAC, TWAREN, and WIDE/T-LEX.

PNWGP is a key partner in the NSF-funded TransLight Pacific Wave. This initiative will exploit new, high-bandwidth network infrastructures to provide expanded resources for research. This will include making the massive amounts of data collected through the billion-dollar global investment in astronomy facilities on the Big Island of Hawaii readily available through GLIF-like, high-capacity paths from the summit of Mauna Kea to other astronomers, processing centers and distributed data repositories around the world.

PNWGP is a founding member of Internet2 and National LambdaRail. Together with the University of Washington, PNWGP supports advanced grid applications in high-definition IP broadcasting and immersive collaboration tools for biotechnology, medical sciences, geology, deep ocean sciences, high-energy physics, astronomy, and so on.

As an advanced communications services gateway between the Pacific Rim, the Americas, and Europe, and with the resources and expertise it has to offer, PNWGP is ideally positioned as a collaboration hub for PRAGMA.

Key Contact: Jacqueline Brown

STAR TAP/*StarLight* Initiative

www.startap.net/starlight

As the foremost 1Gbps-to-10Gbps optical exchange in North America, StarLight supports high-performance computing experiments of a global community of researchers. As an advanced optical infrastructure, StarLight is a proving ground for network services optimized for high-performance applications. StarLight currently provides services to 25 national, international, and regional research and education networks, as well as federal agency networks and network testbeds that have 1Gbps, 2.5Gbps, and 10Gbps circuits. The StarLight facility supports network connectivity both for production-related research and education traffic, and for computer science, advanced networking and e-science basic research and experiments. It provides co-location space for the placement of high-performance networking, database, visualization, and computer cluster equipment, much of which is shared by teams of researchers. The environment facilitates advancements in middleware (transport

and signaling protocols) as well as network measurement and monitoring research for e-science applications. StarLight is a member of the Global Lambda Integrated Facility (GLIF) consortium and is a model for GLIF Open Lightpath Exchanges (GOLE).

TransLight/StarLight and TransLight/Pacific Wave (a joint project with Pacific Northwest Gigapop) are complementary efforts funded by the National Science Foundation (NSF) to provide multi-gigabit links and supporting infrastructure to interconnect U.S., European and Pacific Rim research and education networks, and to supplement the available bandwidth that is being provided by other countries. TransLight/StarLight and TransLight/Pacific Wave are now directly connected through a 10Gbps lightpath connection donated by Cisco Systems and deployed by National LambdaRail (NLR) in support of the TransLight project, enabling participating networks to easily configure direct connections whenever they are needed.

StarLight encourages PRAGMA members to join GLIF and work with colleagues worldwide to share new LambdaGrid techniques and tools such as those being developed for the OptIPuter project with UCSD and University of Illinois at Chicago (UIC).

StarLight is being developed by UIC's Electronic Visualization Laboratory, the International Center for Advanced Internet Research at Northwestern University, and the Mathematics and Computer Science Division at Argonne National Laboratory, in partnership with Canada's CANARIE and the Netherlands' SURFnet.

Key Contacts: Maxine Brown, Tom DeFanti

Thai National Grid Center (TNGC)

www.thaigrid.or.th

Thai National Grid Center (TNGC) is a leading organization of the national initiative Thai National Grid Project (TNGP). The aim is to construct a strong cyberinfrastructure from a geographically distributed resources using grid technology. This infrastructure can be used to drive the next generation research and development in both academics and industry. Moreover, under TNGP, an alliance of 13 leading universities and one government agency has been formed. Applications for bioinformatics, cheminformatics, computational fluid dynamics, digital media animation, and large-scale simulation will be ported onto the newly built Grid infrastructure by TNGP members.

Through TNGP, TNGC researchers play a vital role in the design and construction of a national grid system in Thailand. TNGC team conducts the research and development of Grid software technology for the deployment, management, and monitoring of large scale Grid using NPACI ROCKS. Furthermore, TNGC also works with partner-institutes to grid enabling key strategic applications. The goal is to enable a routine-basis usage of these strategic applications on the Grid. Currently, TNGC researchers also work closely with Uninet, the main academics network provider from Ministry of Education, to develop a national-scale bandwidth analysis infrastructure.

Under PRAGMA, TNGC team has been engaged in PRAGMA monitoring and management system under Resources Working Group by driving SCMSWeb software development. This software is now widely used by PRAGMA members and is also used as a part of the GIN Project. As a new member in 2006, TNGC is now looking for more collaboration, activities, and exciting projects with PRAGMA.

Key Contacts: Putchong Uthayopas

TransPAC2, Indiana University

www.transpac2.net

TransPAC2, a part of the NSF-funded International Research Network Connections (IRNC) program, is a high-performance network connecting scientists in the U.S. with their counterparts in the Asia-Pacific region. TransPAC2 provides fundamental network infrastructure to support e-science collaborations between these researchers in a broad range of scientific disciplines.

Architecturally, TransPAC2 connects the U.S. research and education infrastructure to Asia, specifically to the Asia-Pacific Advanced Network (APAN) consortium in Tokyo, with extensions to Hong Kong and Singapore. TransPAC2 provides a 10 Gbps connection from Tokyo to Los Angeles, an OC-48 connection (link owner NICT-Japan) from Tokyo to Hong Kong, and an OC-12 connection (link owner NII-Japan) from Tokyo to Singapore.

TransPAC/TransPAC2 is a founding member of PRAGMA and co-hosted PRAGMA 7 in San Diego with UCSD. TransPAC2 actively supports e-science and grid activity via its partnerships with PRAGMA, APAN, and ApGrid. TransPAC2 also leads and participates in measurement and security partnership activities between Asia and the U.S.

Key Contacts: James Williams, Donald McMullen, John Hicks, Chris Robb

Universiti Sains Malaysia

www.usm.my

Universiti Sains Malaysia (USM), the Science University of Malaysia, is one of the first universities to embark on grid-computing research in Malaysia. In 2002 the first grid testbed was established through an e-science project involving USM, Universiti Teknologi Malaysia (UTM) and Universiti Malaya (UM) in drug discovery and liquid crystal simulation. The e-Science Grid Portal integrates both e-science grid components and applications, and enables secure access for researchers to a set of applications and data. Components of the e-Science Grid include grid resource monitoring, allocation, metering and prediction. The e-





Background Image: Singapore Chinese Gardens
—courtesy of the Singapore Tourism Board.

Science Grid's applications include the iterative solver agent, molecular simulation, and molecular docking. The Malaysian Biogrid testbed has been established in collaboration with the Malaysian Biotechnology and Bioinformatics Network, Universiti Kebangsaan Malaysia and Sun Microsystems.

Through PRAGMA and as part of the newly-formed Malaysia Research and Education Network (MyREN), USM is committed to taking grid-computing applications and research in Malaysia to the next level. These interactions were enabled by the Asia Pacific Science and Technology Center, and initiated further collaborations with Nanyang Technological University, Singapore. As a founding member in PRAGMA, USM is actively participating in the Bioscience and Resource Working Groups. Collaborations with other PRAGMA members include Kasetsart University—USM Grid colloquium. PRAGMA members also attended the launch in May 2005 of the USM Campus Grid, which provides high-performance computing to USM academics and researchers.

USM has contributed Aurora and Hawk clusters, each providing a stable high-performance grid environment to the PRAGMA testbed. A molecular dynamics simulation, AMBER, has been tested and deployed as the AMBER Multiple Execution on the Grid (AMEX-G) on the PRAGMA testbed involving institutions from Taiwan, Vietnam, the U.S. and Mexico. USM also actively participates in routine-use PRAGMA testbed applications such as SCMSWeb, MOGAS, QM/MD Ninf-G and Savannah. Finally, USM will host the PRAGMA 15 workshop in Fall 2008.

Key Contacts: Ahmad Yusoff Hassan, Habibah A. Wahab, Chan Huah Yong

University of California, San Diego

www.ucsd.edu

Researchers at the University of California, San Diego (UCSD) are involved in application and grid activities of interest to PRAGMA. Those activities include the NSF-funded OptIPuter, Geosciences Network, Network for Earthquake Engineering Simulation, and TeraGrid, NIH-funded activities include the Biomedical Informatics Research Network, National

Biomedical Computation Resource, and National Center for Microscopy and Imaging Research. The Global Lake Ecological Observatory Network has been funded by the Gordon and Betty Moore Foundation, as has been the Community Cyberinfrastructure for Advanced Marine Microbial Ecology Research and Analysis (CAMERA).

UCSD hosted the inaugural PRAGMA workshop in 2002 and PRAGMA 7 in 2004 (with TransPAC). The university provided a dedicated cluster to the PRAGMA testbed and its researchers collaborated on projects with a variety of PRAGMA partners: Osaka University, Korea Basic Science Institute (KBSI), Korea Institute of Science and Technology Information (KISTI), the National Center for High-Performance Computing (NCHC), and the National Center for Microscopy and Imaging Research on the Telescience project; Monash University, Universiti Sains Malaysia (USM), Kasetsart University (KU) and the University of Zurich on Computational Chemistry; the National Institute of Advanced Industrial Science and Technology (AIST), Jilin University (JLU), KISTI, Computer Network Information Center (CNIC) and University of Tsukuba on the Integrated Genome Analysis Pipeline; and NCHC, Trout Lake Station of the University of Wisconsin, University of Waikato, and several other sites on GLEON. UCSD also launched the PRIME program with partners Osaka University, NCHC, Monash, and CNIC, and is actively supporting Osaka University's new project, PRIUS.

In 2006 UCSD began working within PRAGMA on a Geo grid working group with AIST and others. In addition the university's researchers have started a data grid activity and have participated in the Grid Interoperation Network activity, with AIST, NCSA, and TNGC.

UCSD organizations involved in PRAGMA include the California Institute for Telecommunications and Information Technology (which provides a headquarters on the UCSD campus for PRAGMA and space for AIST and PRAGMA participants), the San Diego Supercomputer Center, the Center for Research in Biological Systems, the National Biomedical Computation Resource, and the National Center for Microscopy and Imaging Resource.

Key Contacts: Peter Arzberger, Philip Papadopoulos, Mason Katz, Teri Simas, Cindy Zheng, Kim Baldrige, Chaitan Baru, Mark Ellisman, Tony Fountain, Wilfred Li, Tomas Molina, Steven Peltier, Raj Singh

University of Hyderabad www.uohyd.ernet.in

Researchers from the University of Hyderabad (UoH) are involved in grid-related activities, including biosciences, nanotechnology, drug design and discovery, geosciences, weather modeling and more. It also hosts the High Performance Computing Facility in the Centre for Modelling, Simulation and Design (CMSD), with substantial support from the University Grants Commission (UGC) and Department of Science and Technology (DST). It is further involved in the iGRID initiative of the Centre for Development of Advanced Computing (C-DAC).

UoH is a founding member of PRAGMA and has dedicated an 8-node cluster to this initiative. It is also contributing to PRAGMA's resource and middleware initiatives as well as its weather modeling demonstration.

After submitting a proposal to the Indo-U.S. Science and Technology Forum, UoH received funding approval for the formation of a "knowledge R&D networked" center between the U.S. and India as an extension of the Geosciences Network (GEON) project led by UCSD. The funding was announced at the U.S.-India Summit on Education, Research & Technology in San Diego in May 2006. The iGEON-India activities will be coordinated in India via UoH through its Center for Earth and Space Sciences (CESS) and CMSD. Project activities will include establishment of a GEON node at the University of Hyderabad to serve as the GEON entry point for accessing datasets and tools hosted by the Indian geosciences community participating in GEON. A major activity will be an annual GEON workshop to train geoscientists in the latest advances in geoinformatics.

UoH collaborates with UCSD and the iGEON-India partnership was catalyzed by a pre-existing memorandum of understanding with UCSD's San Diego Supercomputer Center signed in 2002.

The University of Hyderabad expects to participate in the coming year in two PRAGMA-related programs to prepare students for tomorrow's global workforce: UCSD's PRIME and Osaka University's similar PRIUS program, both of which send students to work at a partner PRAGMA site on cyberinfrastructure research.

Key Contact: Arun Agarwal

SCHEDULE OF WORKSHOPS

PRAGMA Workshops are working meetings held biannually to allow members to review accomplishments and plan for future activities. To ensure continuity between subsequent meetings, the co-chair of one meeting is the chair of the next one.

Future Meetings

PRAGMA 12 20-22 March 2007, Bangkok, Thailand
Hosted by National Electronics and Computer Technology Center, High Performance Computing and Network Center at Kasetsart University, and the Thai National Grid Project. This meeting will be held in conjunction with a GEO Grid workshop on 19-20 March 2007. *Chairs: Piyawut Srichaikul (NECTEC), Putchong Uthayopas (KU); Co-chair: Radha Nandkumar (NCSA).*

PRAGMA 13 Fall 2007, Urbana-Champaign, Illinois, USA
Hosted by National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign. *Chair: Radha Nandkumar (NCSA), Co-Chairs: Whey-Fone Tsai and Fang-Pang Lin (NCHC).*

PRAGMA 14. Spring 2008, Hsinchu, Taiwan
Hosted by the National Center for High-performance Computing. *Chairs: Whey-Fone Tsai and Fang-Pang Lin (NCHC).*

PRAGMA 15. Fall 2008, Penang, Malaysia
Hosted by the Universiti Sains Malaysia. *Chair: Muhammad Idiris Saleh.*

Past Meetings

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



PRAGMA 10 26-28 March 2006, Townsville, Australia
Hosted by the Queensland Parallel Supercomputing Foundation, Australian Partnership for Advanced Computing (APAC), James Cook University, and Australia Institute for Marine Science.

PRAGMA 9 20-23 October 2005, Hyderabad, India
Hosted by the University of Hyderabad.

PRAGMA 8 2-4 May 2005, Singapore
Hosted by the Bioinformatics Institute in Singapore and the National Grid Office.

PRAGMA 7 15-17 September 2004, San Diego, U.S.
Hosted by the University of California, San Diego, San Diego Supercomputer Center, California Institute for Telecommunications and Information Technology (Calit2), and TransPAC.

PRAGMA 6 16-18 May 2004, Beijing, China
Hosted by the Computer Network Information Center, Chinese Academy of Sciences.

PRAGMA 5 22-23 October 2003, Hsinchu/Fushan, Taiwan
Hosted by National Center for High-performance Computing.

PRAGMA 4 4-5 June 2003, Melbourne, Australia
Hosted by Monash University and APAC.

PRAGMA 3 23-24 January 2003, Fukuoka, Japan
Hosted by the National Institute of Advanced Industrial Science and Technology and Osaka University.

PRAGMA 2 10-11 July 2002, Seoul, Korea
Hosted by the Korea Institute of Science and Technology Information.

PRAGMA 1 11-12 March 2002, San Diego, U.S.
Hosted by the San Diego Supercomputer Center and University of California, San Diego division of Calit2.



Background Image: Fog rising in the Snow Mountain range near Yuan Yang Lake, Taiwan—courtesy of Peter Arzberger, UCSD.

PUBLICATIONS 2006

The references below augment material summarized in this brochure. These have been selected to reflect activities among PRAGMA partners (*), key technologies upon which PRAGMA activities are based, or member-related activities. They have been grouped by topic. More publications about PRAGMA and associated technologies can be found at www.pragma-grid.net.

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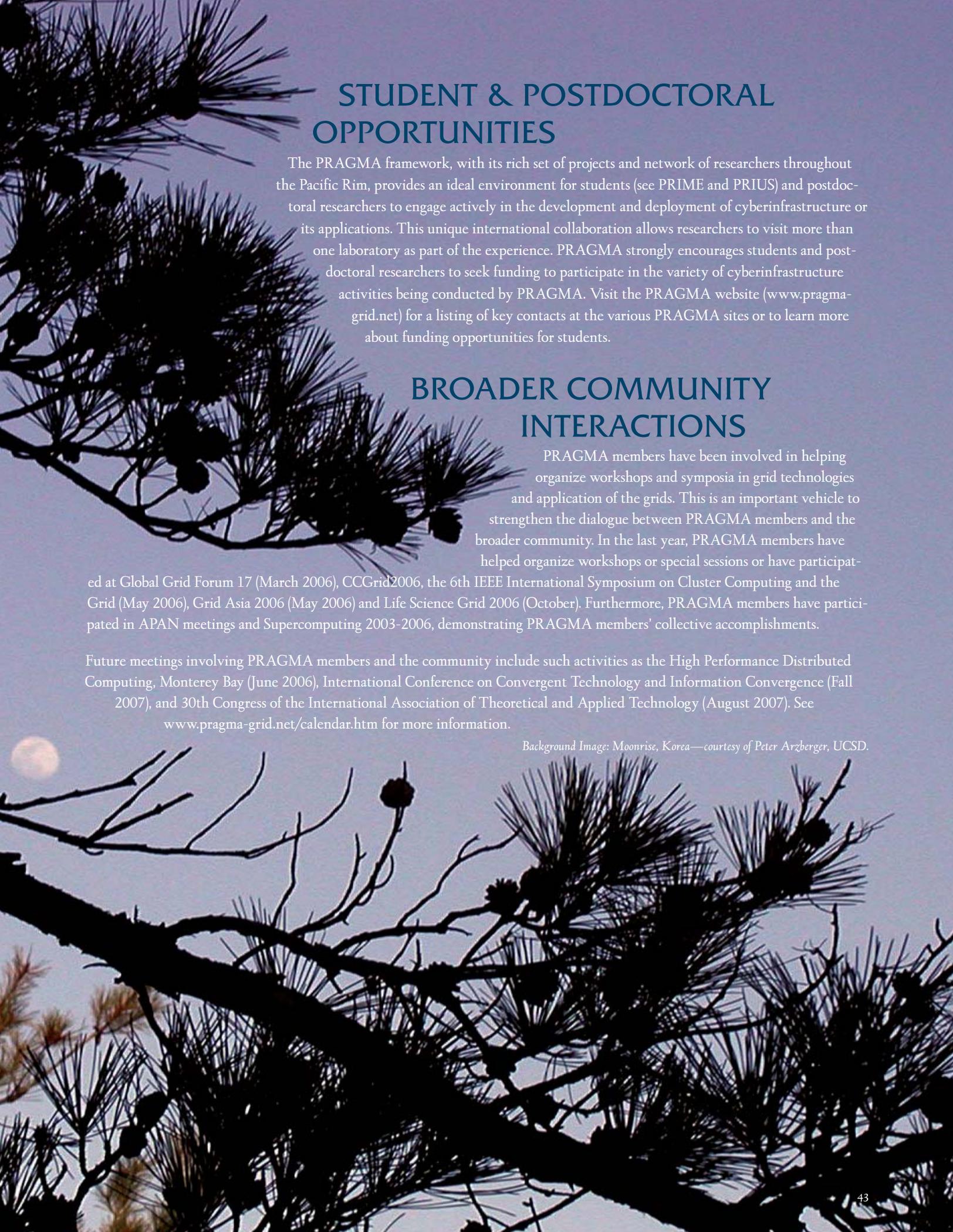
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STUDENT & POSTDOCTORAL OPPORTUNITIES

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 and PRIUS) and postdoctoral researchers to engage actively in the development and deployment of cyberinfrastructure or its applications. This unique international collaboration allows researchers to visit more than one laboratory as part of the 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 or 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 is an important vehicle to strengthen the dialogue between PRAGMA members and the broader community. In the last year, PRAGMA members have helped organize workshops or special sessions or have participated at Global Grid Forum 17 (March 2006), CCGrid2006, the 6th IEEE International Symposium on Cluster Computing and the Grid (May 2006), Grid Asia 2006 (May 2006) and Life Science Grid 2006 (October). Furthermore, PRAGMA members have participated in APAN meetings and Supercomputing 2003-2006, demonstrating PRAGMA members' collective accomplishments.

Future meetings involving PRAGMA members and the community include such activities as the High Performance Distributed Computing, Monterey Bay (June 2006), International Conference on Convergent Technology and Information Convergence (Fall 2007), and 30th Congress of the International Association of Theoretical and Applied Technology (August 2007). See www.pragma-grid.net/calendar.htm for more information.

Background Image: Moonrise, Korea—courtesy of Peter Arzberger, UCSD.

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COVER IMAGE - UNCOVERED

PRAGMA 11 Participants, Osaka, Japan, October 2006. Workshop organizer, Susumu Date, is featured in the image at right.



PRAGMA SPONSORS - CONTINUED

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