Collaboration Overview: Annual Report 2005-2006

PRAGMA

PACIFIC RIM APPLICATIONS AND GRID MIDDLEWARE ASSEMBLY

www.pragma-grid.net

Participants

PRAGMA is an institution-based organization governed by a Steering Committee that invites new members, determines location of workshops, and sets overall direction. Below is a list of member institutions and key contacts. This year, three new members joined PRAGMA: the National Agriculture Research Center (NARC), the Korea Basic Science Institute (KBSI), and the National Grid Office (NGO) Singapore. More information about the Steering Committee members, noted with an asterisk (*), may be found at www.pragma-grid.net/steering_committee.htm.

ACADEMIA SINICA COMPUTING CENTRE (ASCC)
Simon Lin, *sclin@gate.sinica.edu.tw;* Eric Yen, *eric@sinica.edu.tw*

ASIA-PACIFIC ADVANCED NETWORK (APAN)
Seishi Ninomiya, *snino@affrc.go.jp;* Kento Aida, *aida@ip.titech.ac.jp*

AUSTRALIAN PARTNERSHIP FOR ADVANCED COMPUTING (APAC)
John O'Callaghan,* *john.ocallaghan@apac.edu.au;* David Abramson,* *davida@csse.monash.edu.au;* Bernard Pailthorpe,* *bap@acmc.uq.edu.au*

BIOINFORMATICS INSTITUTE, SINGAPORE (BII)
Santosh Mishra*, *santosh_mishra@bii.a-star.edu.sg*

CENTER FOR COMPUTATIONAL SCIENCES (CCS), UNIVERSITY OF TSUKUBA
Mitsuhisa Sato, *msato@cs.tsukuba.ac.jp;* Taisuke Boku, *taisuke@cs.tsukuba.ac.jp*

COLLEGE OF COMPUTER SCIENCE AND TECHNOLOGY (CCST), JILIN UNIVERSITY (JLU)
Xiaohui Wei, *weixh@jlu.edu.cn*

COMPUTER NETWORK INFORMATION CENTER (CNIC), CHINESE ACADEMY OF SCIENCES (CAS)
Baoping Yan,* *ybp@cnic.ac.cn;* Kai Nan,* *nankai@cnic.ac.cn*

CRAY INC.
Geert Wenes, *geertw@cray.com;* Kazunori Mikami, *mikami@cray.com*

CYBERMEDIA CENTER (CMC) AND RESEARCH CENTER FOR ULTRA-HIGH VOLTAGE ELECTRON MICROSCOPY, OSAKA UNIVERSITY
Shinji Shimojo,* *shimojo@cmc.osaka-u.ac.jp;* Susumu Date,* *date@ais.cmc.osaka-u.ac.jp*

GLOBAL SCIENTIFIC INFORMATION AND COMPUTING CENTER (GSIC), TOKYO INSTITUTE OF TECHNOLOGY (TITECH)
Satoshi Matsuoka,* *matsu@is.titech.ac.jp;* Hidemoto Nakada, *hide-nakada@aist.go.jp*

GRID TECHNOLOGY RESEARCH CENTER (GTRC), NATIONAL INSTI-TUTE OF ADVANCED INDUSTRIAL SCIENCE AND TECHNOLOGY (AIST)
Satoshi Sekiguchi,* *sekiguchi@m.aist.go.jp;* Yoshio Tanaka,* *yoshio.tanaka@aist.go.jp*

KASETSART UNIVERSITY (KU)
Surasak Sanguanpong, *Surasak.S@ku.ac.th;* Putchong Uthayopas, *pu@ku.ac.th*

KOREA BASIC SCIENCE INSTITUTE (KBSI)
Inho Gim, *inhogim@kbsi.re.kr;* Jung-Eok Gu, *jekoo@kbsi.re.kr*

KOREA INSTITUTE OF SCIENCE AND TECHNOLOGY INFORMATION (KISTI)
Jysoo Lee,* *jysoo@kisti.re.kr,* Kum Won Cho,* *ckw@kisti.re.kr*

NATIONAL AGRICULTURE RESEARCH CENTER (NARC)
Seishi Ninomiya, *snino@affrc.go.jp;* Masayuki Hirafuji, *hirafuji@affrc.go.jp*

NATIONAL CENTER FOR HIGH-PERFORMANCE COMPUTING (NCHC), NATIONAL APPLIED RESEARCH LABORATORIES
Whey-Fone Tsai,* *coowftoo@nchc.org.tw;* Fang-Pang Lin,* *fplin@nchc.org.tw*

NATIONAL CENTER FOR SUPERCOMPUTING APPLICATIONS (NCSA), UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN (UIUC)
Radha Nandkumar, *radha@ncsa.uiuc.edu;* Danny Powell, *danny@ncsa.uiuc.edu*

NATIONAL ELECTRONICS AND COMPUTER TECHNOLOGY CENTER (NECTEC)
Piyawut Srichaikul,* *piyawut.srichaikul@nectec.or.th,* Chalermpol Charnsripinyo,* *chalermpol.charnsripinyo@nectec.or.th,* Sornthep Vannarat, *sornthep.vannarat@nectec.or.th*

NATIONAL GRID OFFICE (NGO), SINGAPORE
Lawrence Wong, *lwong@i2r.a-star.edu.sg;* Hing Yan Lee, *hingyan@ngp.org.sg*

PACIFIC NORTHWEST GIGAPOP (PNWGP)
Jacqueline Brown, *jbrown@cac.washington.edu*

STAR TAP/STARLIGHT INITIATIVE
Maxine Brown,* *maxine@uic.edu;* Tom DeFanti, *tom@uic.edu*

TRANSPAC, INDIANA UNIVERSITY
James Williams,* *william@indiana.edu;* Donald McMullen,* *mcmullen@indiana.edu;* John Hicks, *jhicks@iupui.edu*

UNIVERSITI SAINS MALAYSIA (USM)
Ahmad Yusoff Hassan,* *cio@usm.my;* Habibah A. Wahab,* *habibahw@usm.my*

UNIVERSITY OF CALIFORNIA, SAN DIEGO (UCSD), *including Calit2, San Diego Supercomputer Center (SDSC), Center for Research in Biological Systems (CRBS), National Center for Microscopy and Imaging Research (NCMIR), and National Laboratory for Applied Network Research (NLANR);* Peter Arzberger,* *parzberg@ucsd.edu;* Philip Papadopoulos,* *phil@sdsc.edu;* Mason Katz, *mjk@sdsc.edu;* Teri Simas, *simast@sdsc.edu*

UNIVERSITY OF HYDERABAD (UOH)
Arun Agarwal,* *aruncs@uohyd.ernet.in*

Contents

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 [National Science Board 2000][1]

1. National Science Board. Toward a More Effective NSF Role in International Science and Engineering, National Science Board Interim Report, NSB-00-217 (Dec. 2000): www.nsf.gov/nsb/documents/2000/nsb00217/nsb00217.htm

Overview: Promoting Global Collaboration Through Cyberinfrastructure

The Pacific Rim Application and Grid Middleware Assembly (PRAGMA) is an open, institution-based organization founded in 2002 to establish sustained collaborations and advance the use of grid technologies in applications among a community of investigators around the Pacific Rim. PRAGMA was founded recognizing that

- science is a global endeavor, with many problems addressable only in an international framework
- cyberinfrastructure promises to revolutionize science as much as networking has done to our daily activities
- cyberinfrastructure, today too difficult to use by most researchers, demands the collaboration and involvement of the global community to ensure attaining the vision of e-science

PRAGMA accomplishes its mission by

- conducting joint projects that develop and integrate grid middleware to advance applications and ensure interoperability of grid resources
- sharing resources to create a grid testbed
- demonstrating routine use of the grid to move towards a stable global cyberinfrastructure
- exchanging and training researchers to build stronger, long-term collaborations
- disseminating the results of its efforts and working with the broader regional and international community to increase the interoperability of grid middleware

During its existence PRAGMA has evolved from a collection of individuals and their institutions to a strong, integrated, institution-based organization. Through a focus on concrete collaborations, PRAGMA has constructed a conduit for people, information, and grid technology; developed a framework for new collaborations; and built trust among its participants.

This brochure highlights specific accomplishments attained by working together across institutional and disciplinary boundaries, with a common focus and shared principles underlying the collaborations. These accomplishments illustrate how the grid brings together remote resources (observational equipment, computers, data, and people) to one's local work environment. The varied examples include

- controlling a microscope to reveal cell processes in the brain
- monitoring the environment to understand global patterns of change
- distributing computations that can lead to insights into drug discovery
- moving files essential to high-energy physics and high-throughput structural genomic experiments

- integrating middleware from different member institutions and making it available to a broader, international user community
- leading efforts internationally to promote standards and best practices

In 2005 PRAGMA has made great strides on many fronts. Using dedicated, distributed computational resources in a PRAGMA grid, the broad routine-use experiment was expanded from 8 sites in 7 countries to 19 sites in 13 countries, from a single application to multiple applications running concurrently, and engaged the NLANR AMP project to measure network traffic. A key to this expansion was the lessons learned by the participants. Another step was taken by initial efforts to integrate Ninf-G persistently into the NSF Middleware Initiative software release, which reflects PRAGMA's role in providing multi-way dissemination of middleware. As a result, a broader set of users gained access to software created in other countries. Finally, through our experiences, new standards in remote procedure calls have been proposed to the Global Grid Forum.

Collaborations between middleware developers and application scientist have resulted in improved codes in structural biology and new scientific insights in computational chemistry.

Leveraging previous NCHC activities in the EcoGrid, PRAGMA has forged an international partnership, the Global Lake Ecological Observatory Network (GLEON), which aims to understand and predict responses of lake ecosystems to natural processes and human activities at regional, continental, and global scales.

PRAGMA also focuses on building human expertise for collaborations. Pacific Rim Undergraduate Experiences (PRIME), a summer internship program, gives UCSD students the opportunity to conduct research overseas at one of four PRAGMA sites. This collective effort among Osaka University, NCHC, Monash University, CNIC, and UCSD is funded by NSF and PRAGMA partner Calit2. Now in its second year, PRIME has expanded to include cultural awareness training and has grown from four to five sites. Furthermore, Osaka University won an award this year to create an internship program modeled on PRIME. The program, Pacific Rim International UniverSity program (PRIUS), will send students to PRAGMA sites, and will offer classes for students at Osaka University taught by PRAGMA researchers.

Many PRAGMA members also participated in and led special sessions at key international conferences, such as Grid Asia 2005 and APAC'05. At the recent iGrid 2005 meeting, 18 of the 49 demonstrations were led by PRAGMA members, indicating the leadership role that PRAGMA members play in application on optical grids.

PRAGMA serves as a model for collectively fulfilling international scientific needs such as constructing and deploying a grid. It is based on the principles that the grid must be developed and deployed by international partnerships, that a focus on applications will produce those developments, that middleware must be designed to interoperate, and that an open organization of institutions committed to this goal is a viable approach. Moreover, open access to software and data are essential, and attribution of individual and identifiable contributions will ultimately benefit the larger effort. PRAGMA workshops are a forum for interactions, reviewing progress, and planning future activities. Most importantly, PRAGMA is building a social network and environment of trust and mutual respect, an essential component for building a grid.

In the coming year, PRAGMA plans to engage and create new applications, continue to integrate software and create software tools to ensure efforts will interoperate to build the desired global grid, expand PRAGMA on both sides of the Pacific Rim, and increase training and exchange of researchers.

PRAGMA aims to inspire other international collaborations and promote new means to nurture, sustain, and expand those collaborations so we as a global society can address critical issues and improve economic growth, quality of life, and the health of our planet.
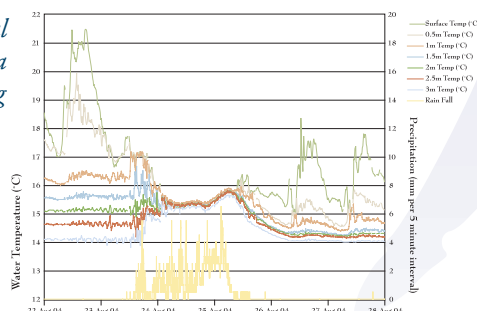
Accomplishments

PRAGMA participants have successfully demonstrated the value of international collaborations in conducting applications on the grid. The following vignettes, science successes from PRAGMA's second 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.

Lake Metabolism Project Gives Rise to Global Ecology Network

Last year PRAGMA investigators constructed a first-of-its kind global lake monitoring network by establishing wireless connections to field sensors in lakes in the U.S. and Taiwan. The network proved to be a novel way of extending the laboratory into the field by enabling frequent, long-term measurements of gross primary production, respiration, and net ecosystem production. Large-scale disturbances like typhoons—once nearly impossible to study—could now be observed remotely, with measurements of dissolved oxygen, wind speed, and temperature recorded, analyzed, and disseminated to the international science community via the Internet.

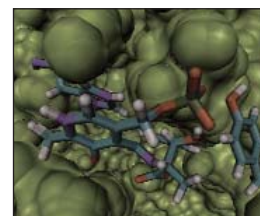The success of that pilot project, which has been chronicled in a recent article in *BioScience,* has led to the formation of a new consortium of limnologists, information technology experts, and engineers who are building a scalable, persistent network of lake ecology observatories. The Global Lake Ecological Observatory Network (GLEON, gleon.org), comprising institutions from more than 10 countries, was created to investigate key processes such as the effects of climate and landuse change on lake function, the role of episodic events such as typhoons in resetting lake dynamics, and carbon cycling within lakes. The observatories will consist of instrumented platforms on lakes around the world capable of sensing key limnological variables and moving the data in near-real time to web-accessible databases. A common web portal will allow easy access to researchers and the public.

Computational Chemistry Merges Grid Technology and Application

Computational Chemistry Methods, a PRAGMA collaborative initiative, has been designing and automating workflow processes for computational chemistry and biochemistry studies by expanding the capabilities of the GAMESS quantum chemistry code/Nimrod middleware pairing to include management tools, data visualization, and database manipulation. The applications were initially combined to conduct large parameter sweeps for large scale molecular calculations.

Engineered PLP-dependent alanine racemase from Geobacillus stearothermophillus, *for which the Baldridge group investigated the mechanism and dynamics of the reaction process involving ligand shown, in the active site.*

Rational drug design relies on computational models that determine whether and how small drug ligands interact with large molecules like proteins—in particular, whether a drug binds to a specific protein receptor. This is typically done by calculating the ligand-protein

Disruption of thermal stratification during a typhoon at Yuan Yang Lake, Taiwan

configuration that minimizes the binding energy. Software packages become complex when they combine the code that performs energy calculations with the nonlinear optimization strategies, since this means that one needs to keep track of advances in computational chemistry and nonlinear optimization, and build these into the one application.

In this work, the quantum chemistry package, GAMESS, and the electrostatic package, APBS, are used to create a hybrid method, driven by the Nimrod software, to perform molecular docking studies. Nimrod/O contains state-of-the-art optimization algorithms (with objective and subjective cost functions) that can be applied to the GAMESS and APBS software without integrating the code of one into the other. This streamlined process allows users to leverage the high molecular structure and property accuracy of GAMESS calculations with less rigorous large molecule electrostatic calculations, with the ultimate goal of establishing a procedure for ligand-protein docking that is more rigorous than is currently available using any single-use docking package.

The GAMESS-APBS-Nimrod system is being used for current investigations into key protein-ligand interactions, and has provided insight into how a ligand binds into a protein pocket, and how residue mutation can influence dynamics in protein structure. In particular, work by PRIME students (see PRIME and PRIUS) used this technology to study test systems to understand how engineered enzymes can catalyze a wide range of aldol reactions in synthetically useful scales. Experimental analysis on the particular combinations of ligand/protein system were conducted for comparison with the grid methodologies of the PRIME students. Both computational and experimental results will be published with experimental researchers at the ETH in Zürich.

Computational Chemistry Participants: Monash University, UCSD, SDSC, and University of Zurich. Resources for testing and experiments come additionally from Victorian Partnership for Advanced Computing.

Gfarm Deployed to the PRAGMA Testbed

The Integrative Genome Annotation Pipeline (iGAP), a suite of bioinformatics software for 3D structural annotation of proteins, has been deployed on the Gfarm file system for distributed proteome analysis. The Gfarm file system enables a global virtual computational data grid, which supports not only large scale I/O in petabyte, but also the execution of existing applications without modifications through a syscall hooking library.

A Gfarm v1.0.4 file system using dedicated cluster resources from seven institutes was constructed for a demonstration at SC'04. Since then, important milestones have been reached:
- The experience from SC'04 has been summarized and presented

at the Second International Life Science Grid Workshop 2005, with the performance of the Gfarm file system for iGAP evaluated for different components. In particular, the experiment motivated further optimizations and performance improvement in Gfarm.
- The optimizations and improved robustness of the Gfarm file system allow the deployment of Gfarm to the PRAGMA grid testbed, using clusters with available public IP addresses for compute nodes. The deployed Gfarm v1.2 not only addressed several performance issues observed during SC'04, but also provides full support to batch scheduler access.

The integration of batch scheduling mechanism into Gfarm is a joint effort among Jilin University, UCSD, and AIST. The efficient sharing of resources using local batch schedulers is achieved using the open source Community Scheduling Framework 4, ported by JLU to the Globus Toolkit 4 (GT4) framework.

The PRAGMA grid testbed consists of clusters of various sizes at different locations around the globe contributed by and shared among the PRAGMA members. Each resource uses a local scheduler such as the Sun Grid Engine (SGE), or Portable Batch System (PBS) or Load Sharing Facility (LSF). The use of CSF4 enables iGAP to be executed through the common shared batch scheduler, while providing the necessary user X509 proxy certificates, required for access of Gfarm filesystem nodes.

PRAGMA's Testbed Enhances Software, Forges New Collaborations

PRAGMA's rapidly expanding testbed and routine-basis experiments have generated a variety of results, from robust software enhancements to new collaborations and joint projects.

A diverse and decentralized real-world global grid that provides challenges and demands for software improvements has been created by the testbed's 19 sites residing in 13 countries on five continents. Just one year ago, the testbed comprised 8 sites in 7 countries and ran a single application. Today, multiple applications and middleware run simultaneously with new grid infrastructure software deployed. Although the testbed represents a diversity in geographical locations, languages, cultures, political, and administrative domains, each testbed site retains its own funding sources, organizational structure, and responsibility for updates to software versions, security policies, and maintenance schedules. The result is a complex global grid environment in which all levels of software share resources and interoperate.

During the past year, 10 pieces of significant software that have been running in the testbed range from applications to middleware to infrastructure software. Three middleware programs run on the testbed: Ninf-G, Nimrod/G and MPICH-G2. The testbed's four

applications include
- mpiBLAST, a Mpich-G2 based DNA/Protein sequence database alignment tool
- QM/MD, a Ninf-G based quantum mechanics application
- Savannah Study, a Nimrod/G based wildfire simulation
- iGAP, a genome annotation pipeline

Four pieces of infrastructure software are also included:
- Gfarm, a grid file system
- CSF, the Community Scheduling Framework
- MOGAS, a grid accounting system
- SCMSWeb, a grid monitoring system

Deployment of such software into the PRAGMA grid testbed revealed interoperability and fault-tolerance problems not observed in the developers' own laboratories and systems. Feedback from the experiments and testbed users have led to fast revisions and many additions of features and interfaces to the software. As a result, software usability was vastly improved, sparking greater confidence from user communities.

The routine-basis experiments and PRAGMA grid testbed also brought different software expertise together, giving rise to new collaborations:
- AIST, NMI and PRAGMA are working together on NMI/Ninf-G integration, which will provide easy deployment for both NMI and Ninf-G.
- SDSC, PRAGMA, and Naregi are working on GAMA/Naregi-CA integration to produce a grid security management system.
- NLANR and PRAGMA are working on a testbed AMP map project to provide network measurements for PRAGMA testbed networks.
- SDSC and many PRAGMA member institutions are working together to integrate SCE, Gfarm, Ninf-G, and other programs with Rocks to provide easy grid software and cluster deployment.
- PRAGMA and GEON projects are working together to expand GEON research collaborations to an international level.

AMP Project Boosts PRAGMA's Network Efficiency

The National Laboratory for Applied Networking Research (NLANR) Active Measurement Project (AMP) has taken one step toward increasing the network efficiency among PRAGMA institutions by creating an AMP mesh to measure performance aspects of the PRAGMA grid testbed. NLANR AMP, which investigates the network measurement needs of international grid-based collaborations, is known for providing the type of data required by the PRAGMA testbed: network performance testing using full mesh tests run on a widespread, controlled, and homogeneous basis.
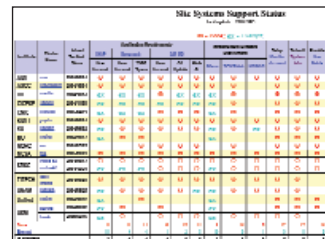
The AMP network encompasses more than 170 active measurement monitors and includes a subset of about two dozen international sites that form the NLANR International AMP mesh. Although most of PRAGMA's testbed sites already have AMP monitors deployed, NLANR AMP is working with PRAGMA members and grid testbed personnel in deploying NLANR AMP monitors throughout the grid testbed. In just the last year new AMPs were deployed: five to PRAGMA sites at CNIC, NGO Singapore, UoH, and USM. A second AMP was added in Mexico at CICESE Ensenada. Five other AMPS were deployed and are online at international, non-PRAGMA sites in Tunisia, South Africa, Switzerland, Pakistan, Indonesia, and Hong Kong.

This investigation will produce the measurements and tools necessary to impact network efficiency among PRAGMA member institutions. The PRAGMA AMP measurements will enable the quick identification of the location, extent, and duration of network performance changes. All NLANR AMP data is made publicly available as raw data and Web-based performance graphs and visualizations. A variety of performance parameters and visualizations will be available, including some to be developed specifically for the PRAGMA grid testbed.

PRAGMA Creates Multi-way Dissemination Pathways for Middleware

Ninf-G, Gfarm, and SCMSWeb were integrated this year into Rocks v4.1—a bundling of per-application requirements that can be used to deploy turnkey clusters for the PRAGMA grid. SCMSWeb has been included into Rocks in the form of the SCE Roll, which includes the complete OpenSCE software stack from Kasetsart University. One immediate user has been ThaiGrid, which deploys Rocks with the SCE Roll on the majority of end points. With about 10% of the thousands of Rocks users deploying SCE, this addition represents a significant increase in users.

The integration comes as a result of the lessons learned from routine-use experiments that showed each grid application often has its own set of software requirements. For example, iGAP requires Gfarm (AIST), QM-MD requires Ninf-G (AIST), Savannah requires Nimrod

Application Status Page

(Monash University), and the Grid Operations Center requires SCMSWeb (Kasetsart University). Enabling these application runs on the testbed has demonstrated the insufficiency of the initial minimum software requirements of Globus 2.4 configured to support the local cluster scheduling system. Software requirements are now classified as core-infrastructure requirements and per-applica-

tion requirements. To adhere to the minimal core-infrastructure requirement, the per-application requirements are managed by each application lead for runs of sub-sets of the testbed.

These per-application requirements have been difficult to deploy at some sites due to the infancy of the software and the lack of local expertise in the configuration of the software. But once deployed, several pieces of software have demonstrated their usefulness to PRAGMA and potentially the larger grid community as a whole.

This year PRAGMA has partnered with ISI to identify per-application software requirements for inclusion in the NSF Middleware Initiative (NMI) software stack. The initial candidates for inclusion were identified as Ninf-G and Gfarm, and in NMI v.8.0 Ninf-G version 2.4.0 is now included as a GPT Bundle.

iGrid 2005 Highlights PRAGMA Achievements

PRAGMA's growing presence in the global grid community became evident at iGrid 2005, where nearly half of the event's 49 application demonstrations featured the work of PRAGMA researchers.

The multidisciplinary, multicultural framework of PRAGMA was reflected in demonstrations at iGrid, a biennial community-driven international grid workshop that fosters to development and application of optical networks by academia, government, and industry. PRAGMA technologies demonstrated their benefit to a variety of disciplines, from the ocean's coral reefs, to the black holes of the cosmos, to the spiny dendrites of the brain. One demonstration featured the first live HDTV images of deep-sea venting systems associated with active underwater volcanoes, a feat accomplished by seafloor-to-ship cable transmission, coupled with a ship-to-satellite-to-shore HD link, which was then broadcasted via IP networks to viewers worldwide. In another demonstration, high-definition, uncompressed, stereo visualizations of a black hole and other galactic phenomena were streamed from the National Center for

Supercomputing Applications in Illinois to iGrid in San Diego. The microscopic universe of the brain was also explored in a multi-scale, correlated experiment where a scientist at the UCSD National Center for Microscopy and Imaging Research in San Diego viewed a sample at Osaka University in Japan and progressively magnified it, zooming from an entire rat cerebellum to an individual spiny dendrite.

PRAGMA's palpable influence on art and culture was felt in a demonstration of 4K digital cinema, which is 4 times the resolution of HDTV, and is being touted by some Hollywood studios as the next-generation movie medium. Live images captured with a special 4K digital camera, stored animations, and real-time computer-generated imagery were transmitted from Tokyo to San Diego.

Similar technologies are helping artists and researchers peer into the past. The Great Wall Cultural Heritage project allowed iGrid participants to view China's Great Wall in an interactive graphical presentation that combined high-resolution 3D scans, satellite images, and visualizations of CAD environments. And, in the Cabinet of Dreams presentation, Chinese ceremonial pieces made of wood, bronze, and clay, dating as far back as 1000 BC and on permanent exhibit at the Indianapolis Museum of Art, could be viewed in 3D virtual reality by all.

Cross-cultural partnerships cultivated by PRAGMA efforts were also evident at iGrid. Researchers from CICESE in Mexico used the newly installed optical fiber network between Tijuana and San Diego to bring Earth, oceanographic, and atmospheric science visualizations to collaborators in the US. Looking to future generations of researchers, iGrid highlighted PRAGMA's Pacific Rim Undergraduate Experiences (PRIME) program, where students from UCSD shared their experiences conducting research at PRAGMA institutions in China, Japan, Taiwan, and Australia.

PRIME and PRIUS: Preparing Students for the Global Workforce

During the past year, PRAGMA augmented its activities by directly involving students in projects and working groups. PRIME and PRIUS are initial steps in engaging students from all institutions to help advance PRAGMA's goals. 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 career.

Overview

UCSD and several PRAGMA partners launched the Pacific Rim Undergraduate Experiences Program (PRIME: prime.ucsd.edu) in

April 2004 to provide an opportunity for students from UCSD to participate in international research and cultural experiences. Besides preparing students for the global workplace of the 21st century, PRIME has been creating 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). Collaborators in PRIME include PRAGMA partners at the Cybermedia Center (CMC), Osaka University, Osaka, Japan; the National Center for

High-performance Computing (NCHC), Hsinchu, Taiwan; the Department of Computer Science, Monash University, Melbourne, Australia; and starting in 2005 the Computer Network Information Center of the Chinese Academy of Sciences, Beijing, China.

The research and activities conducted by the student researchers will contribute to the growth of the cyberinfrastructure. Specifically, activities that will develop, test, and run application codes in this internationally distributed environment will enhance e-science activities globally. PRIME is structured to leverage three key resources on the UCSD campus: Sixth College, which is focused on the integration of culture, arts, and technology; the Academic Internship Program, which has broad experience internationally in establishing and evaluating internship programs; and PRAGMA, which provides the source of projects and the critically important social network in which the students are immediately immersed.

PRIUS

The success of PRIME over the last two years has stimulated the globalization of education in universities and scientific institutions around the Pacific Rim. In fact, the educational effect of sending UCSD students abroad to an advanced R&D collaborative environment for cultural experience and skill building was more remarkable than originally estimated and has sparked movements to cultivate human resources in the framework of PRAGMA.

In August 2005 Osaka University received funding from 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 will take advantage of the PRAGMA infrastructure and a consistent educational infrastructure named Pacific Rim International University (PRIUS). The PRIUS program consists of two components: an internship experience and a class on life sciences and the grid taught by members of the PRAGMA community. For the internship, graduate students will visit UCSD, but in subsequent years, other PRAGMA sites will host interns. The life sciences class will be offered for credit to students at Osaka University.

The PRIME and PRIUS programs are models for nurturing students' abilities to take a leadership role in next-generation integrated science while offering an international perspective on both academia and industrial societies.

PRIME Year 2

During this second year—with additional support from NSF's Division of Shared Infrastructure and Office of International Science and Education and Calit2 (www.calit2.net)—the program supported research experiences for 13 students, with three each at

CMC and NCHC, five at Monash, and two at CNIC. The students were selected based on a wide variety of criteria: scholastic accomplishment, previous research or working experience, their research plans' inclusion of defined goals, and statements from UCSD and host-site mentors. Students were also required to return to UCSD in the fall to enroll at least for one quarter to continue project work and share their experiences with future PRIME candidates.

Projects for the second group of students ranged across biological, chemical, environmental, and engineering applications and involved developing and applying many aspects of cyberinfrastructure including visualization, remote control of equipment, distributed computing, and distributed data handling. The projects provided a vehicle to engage more researchers at PRAGMA sites and diversify applications within the PRAGMA community, including such new areas as cardiac physiology and systems biology.

During this second year, PRIME introduced a new cross-cultural training program to help prepare the students for their overseas experience. 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). This component of the program will be expanded next year.

Finally, PRIME members worked with researchers at the University of Wisconsin to explore the feasibility of exporting the PRIME model to other U.S. institutions. Also, UCSD hosted graduate a student from China's Jilin University who is working on the iGAP-Gfarm project. Both of these activities are expected to expand in the coming year.

The anticipated deadline for the summer 2006 PRIME application is late February 2006. PRIME seeks to increase funding to allow the program to include more students and additional sites.

Year 2 Highlights of Student Activity
Cybermedia Center, Osaka University
Year 2 Students: James Chen, Christine Liang, Eric Wang
Undergraduates Christine Liang, Eric Wang, and James Chen worked with the Cybermedia Center's BioGrid team and a team of UCSD mentors including neuroscientist Mark Ellisman, director of the NIH-supported NCMIR and the CRBS, NCMIR Executive Director Steve Peltier, and NCMIR researcher Tomas Molina. Liang and Wang worked closely with the BioGrid staff to develop a grid-based portal system and software for aiding research in computational chem-
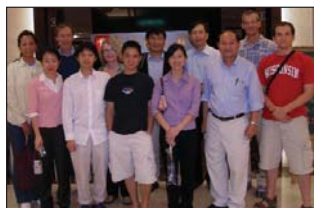

Left to Right: Eric Wang, Christine Liang, Kohei Ichikawa, Jenning King, James Chen.

istry, molecular dynamics, and quantum mechanics. Liang developed 2D visualization software applications that enable researchers to better understand protein structures and their functions using Java and XML technologies. Wang created a portal-based system using Gridsphere technology to incorporate Liang's work and several other software applications being developed and used within the BioGrid infrastructure.

PRIME student James Chen worked closely with the Cybermedia staff of Osaka University to create a simplified grid-based portal system for the Telescience project in Osaka. Chen worked to create portlets for the Cybermedia Center and to incorporate many grid-based portlets used in the Telescience infrastructure. Many of these portlets will be used to integrate functionality for remotely controlling the 3MeV electron microscope and to handle the data that comes from this microscope.

TEAM LEADERS AND MEMBERS: *Shinji Shimojo, Cybermedia Center Director, Biogrid Japan principal investigator; Susumu Date, assistant professor, Graduate School of Information Science and Technology; Toyokazu Akiyama; Kazunori Nozaki; Ichikawa Kohei, student researcher, Tomomi Takao*

National Center for High-performance Computing Year 2 Students: Charles Cheung, Shirley Lee, Daniel Leu

PRIME student Charles Cheung worked with UCSD researchers David Lee and Sunny Chow of NCMIR and University of Illinois at Chicago researchers Nicholas Schwartz and Rajvikram Singh to build a tiled TIFF extension into JuxtaView, a tool developed in the OptIPuter project for scalable tiled displays to visualize extremely high-resolution images. This extension is being used at NCMIR. Cheung's work also involves study of network connectivity, bandwidth, and loading between NCHC and NCMIR through Scalable Adaptive Graphics Environment (SAGE) framework. For a specific example, he set up and tested a TeraVision HD camera streaming to NCMIR.

Left to Right: Cheyenne Chen (NARL), Grace Shau-Wei Hong, Peter Arzberger, Charles Cheung, Gabriele Wienhausen, Daniel Leu, Fang-Pang Lin, Shirley Lee, Whey-Fone Tsai, William Chang (NSF), Timothy Kratz (U Wisconsin), Owen Langman

PRIME student Shirley Lee worked with the NCHC team and UCSD Bioengineering Assistant Professor Trey Ideker. Her work involved extending visualization capabilities of Cytoscape, a tool for modeling biological signaling and regulatory networks to analyze Internet connectivity from NCHC and optimizing the Cytoscape hyperbolic layout plug-in created by PRIME student Robert Ikeda the previous summer. The development allowed her to visualize vol-

ume results of not only what information is related but also where the information resides. She showed its usefulness by visualizing the Internet search results of the keywords "embryonic stem cell."

Undergraduate Daniel Leu worked with NCHC researchers on aspects of wireless sensor networks within the Ecogrid project. He worked to improve data transfer rates from the field to the laboratory by writing a compression algorithm that is currently employed by researchers from the Taiwan Ecological Research Network. He also assisted in adding a relay to a wireless link to transfer data from Taiwan's Yuan Yang Lake to the Research Center for Biodiversity at Academia Sinica as part of a lake metabolism research project.

NCHC also hosted a student from U Wisconsin, Owen Langman. who also worked on aspects of wireless sensor networks within the Ecogrid project. He developed a sensor interface software that allows sensors that use the SDI-12 communication interface to communicate directly with PDA's in the field. He also developed interfaces between SDI-12 sensors and the Antelope data streaming software. He visited Yuan Yang Lake to assist with field work and testing of the software.

TEAM LEADERS AND MEMBERS: *Fang-Pang Lin, Grid Computing Division manager; Sun-In Lin; Shi-Wei Lo; Hsui-Mei Chou; Chien-Lin Huang, Yao-Tsung Wang, Po-Wen Chen, Jyh-Horng Wu, Tom Ho, Grace Shau-Wei Hong, Vicky Yang, Anne Wang*

Monash University Year 2 Students: Laura Berstis, Dafna Bitton, Dorothy Dederko, James Hwang, Jordan Nevo

All five Monash students worked on aspects of the Nimrod family of tools, developed by David Abramson's group. Jordon Nevo and Dorothy Dederko, together with UCSD mentors Andrew McCulloch, Bioengineering interim chair, and Sarah Healy and Anushka Michailova, Bioengineering researchers, employed Nimrod to investigate

Left to Right: Dafna Bitton, James Hwang, Dorothy Dederko, Laura Berstis, Jordan Nevo

and optimize the dynamics of a simulated cardiac cell. They built on the work of last year's PRIME student, John Colby, who established the basic methodology and performed several experiments. By sweeping large parameter spaces with Nimrod/O, they identified parameters that improved the stability of the complex cellular model and its agreement with experimental measurements under a wide variety of conditions. By experimenting with different models, Dederko and Nevo were able to compare the behavior of the models under different conditions. Laura Berstis, who worked with Kim Baldridge of SDSC and the University of Zurich, used the Nimrod tools to experiment with different ways of performing ligand/protein docking. Last year, PRIME student Chris Kondrick experimented

with two computational chemistry codes, GAMESS and APBS, and investigated some preliminary ideas in protein/ligand docking using first principles methodologies. Building on this, Berstis extended the system to compare its performance with industry standard packages like AutoDock. James Hwang worked with colleagues Duy Nguyen who is a 2004 PRIME student, Sriram Krishnan, and Karan Bhatia from SDSC. He developed a method of linking Nimrod with a specialized GAMESS server built using the Berkeley BOINC software, thus opening opportunities to run GAMESS on traditional grid resources like clusters as well as idle workstations. Dafna Bitton worked with UCSD Professor Eleazar Eskin, as well as with David Abramson, James Whisstock, and Sarah Boyd from Monash University in the area of bioinformatics. Bitton combined Nimrod with the BLAST bioinformatics package to explore the relationship between single nucleotide permutations (SNPs) in DNA and disease.

TEAM LEADERS AND MEMBERS: *David Abramson, professor, School of Computer Science and Engineering; Colin Enticott; Slavisa Garic; Rob Gray; James Whisstock; Sarah Boyd; Tom Peachey*

Computer Network Information Center, Chinese Academy of Sciences
Students: Ian Lee, John Lee

PRIME student John Lee worked with the CNIC network team and UCSD mentors Tony McGregor and Cindy Zheng to visualize the network measurements provided by Active Measurement Project (AMP: watt.nlanr.net) with the purpose of finding an easier way to monitor the measurements among the AMP monitors. More than 170 AMP monitors throughout the world, with about 150 of those monitors residing within the United States, have been added to his visualization tool and can be monitored via the user interface.

Left to Right: Wei Zhou, Gabriele Wienhausen, Ian Lee, John Lee, Kevin Dong

As an extension of an existing project on Phylogeny Determined by Protein Domain Content, undergraduate Ian Lee worked with the CNIC bioscience team and UCSD mentors Philip Bourne and Kristine Briedis to examine incomplete collections of protein genomes to determine phylogeny by using similar tools and procedures adopted in the previous project. During his project, Lenovo DeepComp 6800 supercomputer was used to run UCSC's SAM to match the superfamily library of HMMs to the protein sequences.

TEAM LEADERS AND MEMBERS: *Kai Nan, Zhonghua Lu, Kevin Dong, Jinyi Wang, Xianyu Lang, Zhiyong Tao, Ruolin Li, Qi Chen, Beifang Niu, Ji Zhu, Hua Yang, Haiyan Xu*

University of California San Diego

Gabriele Wienhausen, one of three program coordinators for PRIME, is the principal investigator of the NSF PRIME award. She is joined by Linda Feldman and Peter Arzberger, both co-PIs of the award. 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: *Gabriele Wienhausen, founding provost of Sixth College and Calit2 Education layer leader; Linda Feldman, director of UCSD's Academic Internship Program; Peter Arzberger, PRAGMA's PI, director of the Life Sciences Initiative at UCSD, and director of the National Biomedical Computation Resource; Teri Simas, PRAGMA Project Manager. 2005 Students: James Chen, Christine Lee, Eric Wang, Charles Cheung, Shirley Lee, Daniel Leu, Laura Berstis, Dafna Bitton, Dorothy Dederko, James Hwang, Jordan Nevo, Ian Lee, John Lee Mentors in 2005: Mark Ellisman, Steve Peltier, Tomas Molina, David Lee (NCMIR); Kim Baldridge, Longjiang Ding, Tony Fountain, Philip Papadopoulos, Ronn Ritke, Cindy Zheng (SDSC); Trey Ideker, Andrew McCulloch, Anushka Michailova (Bioengineering); Philip Boure, Kristine Briedis (Pharmacy), Tony McGregor (Waikato Univ.), and Timothy Kratz (Univ. of Wisconsin).*

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 activities of middleware and training.

TELESCIENCE

Electron tomography is a powerful technique that draws on advanced instrumentation, networking, and grid computing to derive 3D structural information from biological specimens. Telescience, developed by the National Center for Microscopy and Imaging Research (NCMIR) as a web-based portal solution for end-to- end electron tomography, centralizes applications and seamlessly interfaces with the grid to accelerate the throughput of data results.

The Telescience Working Group has evolved Telescience tools by developing collaborations among experts in grid architecture and integrating scientific devices such as ultra-high voltage electron microscopes, magnetoencephalography, and synchrotron facilities to the grid. 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.

At SC'03, PRAGMA Telescience collaborators and researchers from KDDI Laboratories demonstrated the ability to use high-quality, low-latency HDTV to navigate a specimen in Osaka University's 3.0 MeV electron microscope via IPv6, winning the Application Bandwidth Challenge.

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. Working closely with PRAGMA partner KISTI, this group has also extended the Telescience application model to the Korea e-Science project (see Accomplishments). This model inspired Taiwan's Ecology Grid project, which now encompasses lake metabolism (see Accomplishments), coral reef studies, and agriculture. Collaborators from NCHC in Taiwan have also integrated the visualization and analysis capabilities of the Telescience Portal.

Both KBSI and the National Agricultural Research Center joined PRAGMA in 2004 and are active in Telescience and EcoGrid, respectively. In addition Osaka University has taken initial steps in sensor networks and participated with NCHC in a meeting on lakes and coral reefs in March 2005 in San Diego.

TELESCIENCE: *F. Lin and S. Shimojo, 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, J. Chen, G. Hong, NCHC; S. Ninomiya, NARC and APAN; B. Pailthorpe, N. Bordes, Univ. of Queensland; D. McMullen, L. Ding, T. Fountain, UCSD; H. King, Taiwan Forest Research Inst; T. Kratz, North Temperate Lakes LTER*

Biological Sciences
The Biological Sciences Working Group has been continuing to promote grid computing in the biosciences communities as it meets the increasing application requirements of the grid computing communities.

The Working Group's growing interdisciplinary R&D efforts focused on the development, deployment, and operation of software for biosciences applications to solve real-world problems. These activities have been pursued within PRAGMA working groups and

at international workshops and forums outside the PRAGMA community, from the Life Sciences Grid Research Group at GGF13 in Korea, to the special session at Grid Asia 2005 in Singapore.

Specifically, BII's Wildfire, a graphical user interface for constructing and running workflows, promotes ease of use in workflow systems to meet the application requirements of the bio-sciences communities.

Software deployment and operation efforts centered on two applications: the BioGrid Portal (Bioinformatics HTC Environment) and MGrid. Deployment of ASCC's BioGrid Portal on the PRAGMA testbed is underway following its demonstration at SC'04. The MGrid system of Konkuk University in Korea has been deployed on the Korean Grid Testbed (K*Grid) and has begun servicing molecular simulation research in Korea. MGrid will be ported to the PRAGMA testbed in the near future.

Two additional efforts are targeting real-world problems: proteome analysis and simulation database construction. The integrated system of iGAP at UCSD and Gfarm at AIST was installed on internationally distributed computing resources from six institutes in PRAGMA and was subsequently tested to analyze the complete proteome of the bacteria *Burkholderia mallei*. The results of this work were presented at the 2005 Life Sciences Grid Workshop. This interaction has been expanded to include Jilin University, KISTI, and CNIC (see Accomplishments). The MGrid system has been used to build simulation databases for glycoconjugates whose structures are available in the Protein Data Bank (PDB). This project plans to finish the construction of the simulation databases in three years and will use the MGrid system for computing and databases.

BIOLOGICAL SCIENCES: *K. Jeong, Konkuk Univ., Chair; A. Krishnan, F. Tang, A. Shahab, BII Singapore; S.T. Hwang, Kookmi 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*

Data Computing
The large-scale data generated and harbored by the Pacific Rim region covers diverse fields, providing information about climate, water, culture, spatial data, ecology, pollution, physics, chemistry, bioinformatics, medicine, astronomy, and earthquakes. The Data Computing Working Group aims to fulfill the demand for sharing and analyzing such large-scale data by introducing data grid technologies and building an international, collaborative testbed for the PRAGMA community.

In 2004, the Data Computing and Biological Sciences Working Groups jointly established an iGAP/Gfarm testbed consisting of

two clusters in the U.S., one cluster in Japan, three clusters in Korea, and one cluster in Singapore. The testbed led to the creation of a wide-area Gfarm file system that was used to analyze the distributed proteome annotation of the bacteria *Burkholderia mallei*, a known biothreat agent. This effort helped to improve functionality, performance, and robustness of the Gfarm file system into production level. The working group also investigated a batch queuing system having a capability of file location awareness by exploiting a plug-in mechanism of LSF, which improved the I/O performance of scheduled jobs. In 2005, the working group has been investigating a grid-level batch queuing system based on Community Scheduler Framework (CSF) and Globus Toolkit 4 (GT4).

The Data Computing Working Group encourages data computing collaborations around the Pacific Rim. Current activities include the iGAP/Gfarm distributed proteome analysis, the Belle Data Grid, the Spatial Data Grid, the Scientific Data Grid, and the Virtual Observatory Grids. iGAP/Gfarm distributed proteome analysis involves SDSC, AIST, Jilin University, Konkuk University, Kookmin University, KISTI, BII, and Osaka University. Belle, a data grid focusing on high-energy physics, includes the University of Melbourne, AIST, and the High Energy Accelerator Research Organization (KEK). The Spatial Data Grid involves the NCHC and SDSC; the Scientific Data Grid is a partnership between the Chinese Academy of Sciences and SDSC. The Virtual Observatory Grids project is a collaboration among NCSA, AIST, and the Australian National University.

DATA COMPUTING: *O. Tatebe, AIST, Co-chair; P. Papadopoulos, SDSC at UCSD, Co-chair; J. O'Callaghan, APAC; L. Winton, S. Melnikoff, Univ. Melbourne; P. Coddington, Univ. Adelaide; M. Sato, T. Boku, D. Takahashi, Univ. Tsukuba; A. Takefusa, Ochanomizu Univ.; F. Lin, R. Sheng-Ming Wang, NCHC; E. Yen, H. Chen, A. Chen, ASCC; P. Srichaikul, S. Vannarat, NECTEC; B. Yan, K. Nan, K. Wu, Y. Ma, H. He, D. Yang, CNIC/CAS; W. Chen, ISOC/CAS; D. McMullen, J. Hicks, Indiana Univ.; K. Kumar, Inst of HPC: K. Cho, Kyungpook Nat'l Univ.; R. Simmonds, Westgrid/Univ. of Calgary; X. Wei, L. Hu, Jilin Univ.; K. Mikami, Cray Inc; L. Headley, UCSD; S. Date, T. Tashiro, Osaka Univ.*

RESOURCES

The Resources Working Group strives to increase the grid's productivity and effectiveness by improving the interoperability of grid middleware around the Pacific Rim and throughout the world. To this end, PRAGMA has extended the routine-basis experiments and grid testbed following their launch last year.

During the past year, the PRAGMA testbed grew from 8 sites in 7 countries to 19 sites in 13 countries, with a total of 662 CPUs, nearly 1 terabyte of memory, and 7.3 terabytes of online storage. The

group has developed procedures for conducting the routine-basis experiments and has continued its grid operation center construction with increasing sophistication and effectiveness.

To build the PRAGMA testbed as a general science grid and to investigate resource-sharing issues, multiple applications were launched and run simultaneously. The group also has deployed and has been testing a grid file system—Gfarm—and a grid accounting system named MOGAS (ntu-cg.ntu.edu.sg/pragma/gridacctinfo). Development and testing of a grid-monitoring software, SCMSWeb (pragma-goc.rocksclusters.org/scmsweb), also is underway. These experiments provided insight that resulted in dramatic software enhancements in such middleware as Ninf-G and Nimrod/G and in applications including Gfarm, SCMSWeb, and MOGAS.

The routine-basis experiments also stimulated research interests and collaborations. The group has initiated many joint projects, including NMI/Ninf-G integration, GAMA/Naregi-CA integration, the NLANR/PRAGMA testbed AMP map project, Rocks/Gfarm integration, and the PRAGMA/GEON collaboration.

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

- Centro de Investigacion Cientifica y de Educacion Superior de Ensenada (CICESE, www.cicese.mx) of Ensenada, Mexico, has contributed resources to the testbed, collaborated with the SCMSWeb Team at Kasetsart University by porting SCMSWeb to the Solaris system, and brings unique oceanography applications to PRAGMA. CICESE is leading the Mexican Grid effort in Corporacion Universitaria para el Desarrollo de Internet A.C. (CUDI). CICESE members attended PRAGMA 7 and 8 Workshops and participated in iGRID2005.
- 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 the 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, UniZH 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 deploy software environments better tuned to applications, enhance the coupling of distribution of software from various PRAGMA sites into a single release, and install accounting systems that track testbed use and barriers to sharing resources internationally. This experience will help inform all funding agencies interested in understanding the grid's use and will benefit researchers within funding boundaries to

link national and regional production grids. Future challenges will include seeding real science applications and informing more scientists about the use of the grid.

RESOURCES: *M. Katz, Co-chair, SDSC at UCSD; K. Sakharkar, Co-chair, BII Singapore; Y. Tanaka, Co-chair, AIST; Y. Tanimura, H. Takemiya, AIST; M. Chiang, H. C. Lee, C.W. Wang, ASCC; L. W. Kit, S. Wong, BII Singapore; S. Castaneda, J. Delgado, R. Hazas, CICESE; K. Dong, K. Nan, CNIC; H. Zhang, Y. L. Shi, GUCAS; Z.*

H. Ding, X. Wei, JLU; J. H. Kwak, J. Lee, KISTI; S. Sriprayoonsakul, S. Phatanapherom, P. Uthayopas, KU; C. Enticott, D. Abramson, MU; C. L. Huang, W. Huang, NCHC; T. Roney, R. Nandkumar, NCSA; F. Lee, J. W. Lee, NTU Singapore; C. Zheng, P. Papadopoulos, W. Li, SDSC at UCSD; H. Aoki, S. Matsuoka, TITECH; 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, C. Amoreira, UniZH

Members

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

ACADEMIA SINICA COMPUTING CENTRE
www.ascc.net, www.twgrid.org

ASCC, a major high-performance computing and grid infrastructure center in Taiwan, provides service and support for academic computing at Academia Sinica and its collaborating institutes in a variety of application areas. ASCC also conducts grid-related training and workshops.

ASCC built the first high-speed link between Europe and the Asia-Pacific region with 2.4 Gbps bandwidth in 2004 and is now working with the Trans-Eurasia Information Network (TEIN). ASCC provides grid-related technology and infrastructure support for the Large Hadron Collider (LHC) experiment teams in Taiwan and has been acting as the Asia Regional Operation Centre and Global Grid User Support for LCG/EGEE CA. Since 2002, ASCC has been developing various life science grid applications, including the BioPortal, CRASA (a complexity reduction algorithm for sequence analysis), and mpi-BLAST-g2. ASCC is also promoting the establishment of e-science infrastructure and applications in Taiwan, extending grid technology to such fields as biomedical informatics, digital archives, earth science, and biodiversity informatics.

ASCC has participated in the PRAGMA testbed and has been responsible for driving the second routine-basis experiment by deploying and running the MPICH-g2-enabled genomic sequence alignment tool. Preliminary results have been successfully demonstrated at Supercomputing 2004. Based on these results, improvements have been made to maintenance, and the application usage threshold has been lowered.

Through participation in PRAGMA, ASCC shares its expertise and enlarges the scope of its grid activities, including application devel-

opment, grid middleware development and deployment, cross-grid integration and validation, and grid operation and monitoring. ASCC will also host future PRAGMA meetings. PRAGMA will enable ASCC to collaborate with other leading institutions in building and maintaining an advanced production grid environment for various applications.

Key contacts: Simon Lin, Eric Yen

ASIA-PACIFIC ADVANCED NETWORK
www.apan.net

APAN, a non-profit international consortium comprising 15 primary, two associate, 10 affiliate, five liaison, and two industry members, 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. As an example of the bandwidth available, the link between the U.S. and Japan operates at 20 Gbps, with 10 Gbps on the TransPAC2 link between Tokyo and Los Angeles, and 10 Gbps on the JGN2 link between Tokyo and Chicago. APAN's working groups and committees promote projects that utilize the infrastructure.

The Natural Resource Area of APAN 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 of the Application Technology Area. Examples of these applications include a data grid for satellite image archives, a high-performance computing grid for climatic 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 APBioNET, ApGrid, and GGF. APAN initiated a committee to coordinate 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

APAC and its eight partners provide advanced computing facilities to the Australian research community, government, and industry. APAC integrates these facilities into a national grid that will allow Australian 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 member of the GrangeNet program (www.grangenet.net), which has installed a multi-gigabit network between Melbourne, Canberra, Sydney, and Brisbane for research and education purposes.

APAC is a silver sponsor of the Global Grid Forum. Representatives of APAC have attended the PRAGMA workshops, and APAC co-hosted the fourth PRAGMA workshop in Melbourne, Australia.

APAC and its partner, QPSF, co-hosted the APAC Conference and Exhibition on Advanced Computing, Grid Applications and eResearch on Queensland's Gold Coast, September 26-30, 2005. They are also co-hosting PRAGMA 10 in Townsville on March 26-28, 2006, and an associated meeting for lakes (GLEON) and coral reefs observatories directly thereafter. APAC Member Monash University has hosted five PRIME students in 2005 and is 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

BII scientists have been involved in application development, creation of middleware necessary for grid-enabled biological applications, and National Grid (Life Sciences) activities with the aim of using grid-computing technology. Such activity resulted not only in a scalable, secure, and user-friendly national grid resource but also has strengthened Singapore's role in grid-based bio-computing applications and analyses. To facilitate and encourage resource contribution and collaborative efforts, BII also has developed a Goodness Index system, which allocates dynamic scores to PRAGMA sites all over the world based on their involvement and contribution. The Index is available at tglobus3.bii.a-star.edu.sg/goodness.htm.

Ongoing and previous BII collaborations with PRAGMA member institutes include the integration of AIST's Gfarm with the integrated Genome Analysis Pipeline (iGAP), collaborating with AIST, UCSD, and the Encyclopedia of Life project. Furthermore, BII

together with NGO, co-hosted the PRAGMA 8 workshop in Sinapore, May 2005.

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 sciences research at various departments in National University Singapore (NUS), National University Hospital (NUH), and such research institutes as Genome Institute of Singapore (GIS) and Institute for Molecular and Cell Biology (IMCB). Finally BII staff have developed Wildfire, a graphical user interface for constructing and running workflows, whose design focuses on ease of use in workflow systems and is motivated by application requirements from biosciences communities.

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 PRAGMA members.

Key contacts: Santosh Mishra

Center for Computational Sciences, University of Tsukuba
www.ccs.tsukuba.ac.jp

The Center for Computational Sciences (CCS), a research institute for high-performance computing technology, 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 PRAGMA partners in Japan, including 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 HMCS-G (Grid-enabled Heterogeneous Multi-Computer System) 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 (ILDG) to develop an international data grid for the lattice field theory community.

CCS shares computing resources with AIST and Titech through a grid testbed on the Japanese SuperSINET and Tsukuba-WAN. PRAGMA provides a forum for exchanging ideas and resources through the promotion of broader collaborations with PRAGMA partners. CCS has offered several PC clusters to PRAGMA as a computing resource.

Key contacts: Mitsuhisa Sato, Taisuke Boku

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 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 through the years, it has built a team of experienced researchers. CCST has strong ties with PRAGMA members UCSD and AIST in the field of grid computing.

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 test bed for data-intensive applications like iGap, JLU, UCSD, and AIST are working on integrating a meta-scheduler (CSF), local scheduler (LSF/SGE), and Gfarm. This year, JLU began participating in the Pacific Rim Undergraduate Experience by sending its students and faculty members to UCSD. Another ongoing co-research project between JLU and Platform is aimed at developing a grid operating system prototype.

CCST has attended all the PRAGMA workshops since PRAGMA 6 and is actively engaged in PRAGMA's Data Computing and Resource working groups to build a grid test bed 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, CNIC has been actively participating in PRAGMA 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 and organizing science applications in such disciplines as astronomy, biology, and high-energy physics in China. As part of its commitment to developing collaborative training among PRAGMA members, CNIC held a distance-training workshop with UCSD in February 2004. CNIC hosted PRAGMA 6, a tremendous success, in Beijing in May 2004. In the summer of 2005, CNIC hosted two students from UCSD as part of the PRIME program. Also, CNIC will co-host the twentieth CODATA conference in October 2006 in Beijing.

CNIC is a subsidiary research institute under the Chinese Academy of Sciences (CAS) and plays a leading role in grid computing and applications in China. It is 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 continue to raise achievement 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 HPC, is the first Industrial Affiliate member of PRAGMA and sponsor of PRAGMA workshops. In addition to participating in PRAGMA meetings and workshops, Cray provides expertise in high-performance computing and demonstrates ways in which grid technologies can be used to provide access to scarce HPC resources.

Cray is actively involved with the Resources Working Group of PRAGMA, providing access to Cray-Japan supercomputers that support middleware and application porting activities. Cray has worked closely with such PRAGMA members as Japan's National Institute of AIST and the Grid Technology and Research Center (GTRC) in Japan to port grid middleware such as the Globus Toolkit.

Cray plans to continue efforts to place its systems into large-scale supercomputing grids and verify that the approach can be used effectively to handle computationally challenging scientific problems. As an example of such activity, Cray is supporting the Korean Meteorological Agency (KMA) in the investigation and implementation of multi-model ensembles using grid technology within the center's infrastructure and in pilot studies.

Key contacts: Geert Wenes, Kazunori Mikami

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

www.cmc.osaka-u.ac.jp, www.uhvem.osaka-u.ac.jp

Osaka University has been contributing to PRAGMA by providing computational resources—including highly

advanced scientific devices—and expertise and experience in advanced networking and high-performance computing. CMC co-hosted the third PRAGMA workshop with AIST in January 2003. Osaka University's two major categories of activities are education and R&D. With regards to education, Osaka University played an important role in promoting the UCSD PRIME program in 2004 and 2005 by hosting three UCSD students each year to build skills in grid system development. Also, Osaka University will soon start an educational project named PRIUS (Pacific Rim International UniverSity) in tight cooperation with PRAGMA. Through PRIUS, Osaka University will establish an educational network where PRAGMA scientists and researchers can educate and nurture young scientists and researchers in the PRAGMA community.

Osaka University's grid R&D activities are based heavily on CMC's involvement in Japanese national projects such as the Japan Gigabit Network (JGN2: www.jgn.nict.go.jp), governed by the National Institute of Information and Communication Technology (NICT), and the BioGrid project (www.biogrid.jp), funded by MEXT. These projects are centered on international collaboration. Osaka University has participated in all PRAGMA workshops since its foundation, co-leads PRAGMA's Telescience Working Group, and is an active participant in the Biological Science Working Groups. Through collaboration with the Telescience Working Group, Osaka 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 Biological Sciences Working Group, Osaka University brings its expertise from the BioGrid Project. BioPfuga, a subproject of BioGrid, serves as a research workbench that allows scientists to integrate Quantum Mechanics (QM) and Molecular Mechanics (MM) simulations to reveal the detailed behavior and function of protein. In addition, Osaka University is developing security-related technology for sensor network/Grid in the JGN2 project.

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

Global Scientific Information and Computing Center, Tokyo Institute of Technology
www.gsic.titech.ac.jp

The Tokyo Institute of Technology (Titech) is one of the premier universities in Japan, 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," seeds the entire campus (15 sites) with more than 800 processors of high-performance PC blade servers and interconnects them with a campus Gigabit backbone to construct a large production-level testbed. With recent participation of nodes from other projects and laboratories, the entire infrastructure has more than 1500 processors, with 2.5 Teraflops of compute capacity interconnected by 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 and the SCore cluster operating system. This effort has been recognized internationally, winning several awards including the IBM "SUR (Shared University Research)" award and the Nikkei IT Product award for its partner, NEC, in 2002. 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 Supercomputing 2003. Titech is currently participating in the PRAGMA Testbed and routine use experiment.

Key contacts: Satoshi Matsuoka, Hidemoto Nakada, Kouji Tanaka

Grid Technology Research Center (GTRC), National Institute of Advanced Industrial Science and Technology (AIST)
www.gtrc.aist.go.jp

The GTRC of AIST 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.

Five teams at the GTRC cover every facet of research and development. The mission of the GTRC is to share the activities of international standardization in collaboration with research organizations in Asia-Pacific countries, to make research and development results into deliverable forms and provide them to users in a demonstrable manner, and to accelerate 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 79 members, including regular, postdoctoral, visiting, and temporary staff. At the Tsukuba Central 2 and the Akihabara Office, 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. In addition, PRAGMA serves as a venue for sharing resources, knowledge, and experiences; building new grid technologies via collaborations; interacting with experts in applications and grid middleware; linking PRAGMA member institutions with international grid communities; and promoting development of grid-enabled applications.

AIST, which co-hosted the third PRAGMA workshop in Fukuoka, has provided three clusters to the PRAGMA testbed. AIST researchers have been involved in all working groups, including the PRAGMA Resource Working Group, in which AIST researchers led the first routine-basis experiment on the PRAGMA testbed using a Quantum Computational Chemistry and Molecular Simulation with Ninf-G. This months-long experiment provided a basis for fault-tolerant research. Ninf-G will be included in NSF Middleware Initiative core releases, and Gfarm has been selected by several PRAGMA applications. Furthermore, AIST researchers have forged promising new interactions with GEON and OptIPuter researchers. Satoshi Sekiguchi and Yoshio Tanaka are PRAGMA Steering Committee members. Osamu Tatebe a leader of the Data Working Group.

Key contacts: Satoshi Sekiguchi, Yoshio Tanaka

Kasetsart University
www.ku.ac.th, hpcnc.cpe.ku.ac.th

Under PRAGMA collaboration, Kasetsart University's (KU) researchers have been working closely with many leading researchers in the Asia-Pacific region. As part of the Resources Working Group, the KU High-Performance Computing & Networking Center (HPCNC), together with SDSC and many other institutes, has developed a very powerful and comprehensive monitoring tool called SCMSWeb. This tool enables a near real-time capturing of PRAGMA testbed system characteristics leading to the detection and solution of problems and in turn 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. For example KU developers worked with with SDSC to create a IA-64 platform port, and a port to Solaris system developed by the Centro de Investigacion Cientifica Y de Educacion Superior de Ensendada (CICESE) in Mexico.

KU also dedicated a cluster, AMATA, to PRAGMA flagship routine use applications, including a Savannah burn simulation using Nimrod, a QM-MD simulation using Ninf-G, and TDDFT simu-

lation using Ninf-G. The experiences learned from the development, deployment, and usage of these applications show the best practice of how to use grid systems for large-scale applications.

KU successfully deployed GAMESS to build a drug discovery infrastructure on ThaiGrid, which is now heavily used to study thousands of chemical compounds obtained from Thai medicinal herbs. GAMESS and autodock are distributed by the KU-developed SQMS scheduler, helping speed the work of scientists in KU. Other collaborations exist in using remote sensing data to enhance agriculture by working with scientists from the Asia Institute of Technology, KU, and Titech, using AIST-developed Ninf-G as the middleware.

KU is actively promoting NPACI Rocks technology in the region by co-organizing a first Grid and Cluster Workshop at the University of Malaya, which was well attended by many leading researchers in Malaysia.

Finally, NECTEC, KU, and the ThaiGrid community plan to work 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—The Morning Star—is the first Ultra High Voltage Transmission Electron Microscope (UHV-TEM) installed in Korea and is capable of atomic resolution better than 1.2 A (point-to-point). With its precise stage control, the UHV-TEM is able to tilt more than ±60º within ±0.1º error, which allows for 3-D structure analysis of complex materials. The UHV-TEM can also operate remotely without losing its atomic resolution.

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

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

Key contacts: Inho Gim, Jung-Eok Gu

PRAGMA

Korea Institute of Science and Technology Information (KISTI)
www.kisti.re.kr, www.ksc.re.kr

KISTI is the leading organization of the K*Grid project, 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 6-year long 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 project also calls for the development of a Science Gateway in 2010, which comprises middleware that can be applied to all five 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 by collaborating with domestic and international researchers in a variety of applications. KISTI operates the secretariat of the 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 GGF and APAN.

KISTI has been actively involved in PRAGMA since its inception, hosting the PRAGMA 2 Workshop, participating in all nine PRAGMA workshops, and collaborating in PRAGMA working groups. For example, KISTI has been involved in such PRAGMA projects as

- MGrid (www.mgrid.or.kr), a cost-efficient and reliable grid computing system for simulations of biomolecules
- Telescience, involving the transmission electron microscope of the Korea Basic Science Institute (KBSI)
- PRAGMA testbed and routine use experiment, by contributing an 80-node Linux cluster and a 16-node Linux cluster

KISTI also has been working with SDSC to produce a localized version of Rocks especially for use in a grid environment by the cluster user community in Korea. The Korean version, named KRocks, provides an easy-to-use guide for Korean researchers to install Rocks. 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 PRAGMA members in Korea (KISTI), Japan (AIST), and China (CNIC). Furthermore, KISTI will

collaborate with NCSA and NCHC for network performance measurement. KISTI is also an OptIPuter partner.

Key contact: Jysoo Lee, Kum Won Cho

National Agricultural Research Center
narc.naro.affrc.go.jp/narc-e/index.htm

The National Agricultural Research Center (NARC), one of the 11 research institutes under the National Agriculture and Bio-oriented Research Organization (NARO: www.naro.affrc.go.jp/index_en.html) of Japan, covers a wide range of research fields in agricultural and life science. The Department of Information Science and Technology of NARC is a global leader in the application of information technology and science to agriculture and natural resource related fields. Virtually integrating various kinds of comparatively small-scale distributed data sets and overcoming the heterogeneity of even the same kind of data resources are important issues, considering the features of the data resources that NARC handles. Therefore, data grid technology for such data resources has been a focus of the NARC group. Data mediation middleware that provides client applications with consistent accesses to heterogeneous databases is one of the solutions promoted by NARC. MetBroker (www.agmodel.org), one middleware implement for meteorological databases, provides such accesses 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 (model.job.affrc.go.jp/FieldServer), 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

NCHC has been leading the development of the Taiwan national grid project, the Knowledge Innovation National Grid (KING) (2003–2006), an advanced and collaborative high-performance computing environment for scientific applications and technology development. KING's 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 fully share grid resources such as high-end networking, cluster computing, and storage and supporting grid technologies including sensor network technology, access grid, and advanced visualizations including virtual reality and the tile display wall. KING is an applications-driven project that focuses on such life-improving applications as the e-learning grid, ecology grid, medical grid, flood mitigation grid, and biology grid. KING is also collaborating with various Taiwan-based HPC and domain-technology experts and with international grid-related organizations.

Many KING application projects that have been closely collaborating with PRAGMA and its members include the Telescience project, the Global Lake Ecological Observation Network, the coral reef observatory project, and the SARS grid project. Also, 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 made significant contributions to PRAGMA: NCHC hosted the 5th PRAGMA workshop, provides dedicated resources to the PRAGMA testbed, hosted three PRIME students in 2004 and in 2005, provides space and time slots in 2003 and 2004 to support demonstrations at the Supercomputing Research Exhibitions, and is co-leading the Telescience Working Group. In 2004, NCHC hosted The Sensor Network Forum, where invited PRAGMA members and Taiwan researchers delivered speeches and shared knowledge. NCHC has been collaborating with members of academia in Taiwan to organize the Workshop on Grid Technologies and Applications, which was the first grid workshop to call for papers in Taiwan last year and will be continued this year. NCHC supports Dr. Fang Pang Lin, who has served as the PRAGMA deputy chair since March 2005.

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 is dedicated to developing and deploying cyberinfrastructure in collaboration with others, and thereby enabling new discoveries in science and engineering. NCSA is one of the original U.S. National Science Foundation (NSF) funded supercomputing centers, and one of the two original partners in the NSF Partnerships for Advanced Computational Infrastructure program. NCSA owns an international reputation in high-performance computing, visualization, data mining, and developing innovative software and systems.

NCSA researchers enable scientific research in various disciplines through their national and international partnerships. NCSA co-leads the National Laboratory for Applied Network Research network measurement monitoring, the NSF Middleware Initiative, and 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), and CLEANER (Collaborative Large-scale Engineering Analysis Network for Environmental Research).

NCSA works with several PRAGMA member institutions through its International Affiliates Program. PRAGMA provides an international venue to interact, communicate, and collaborate, and to share, beta test, and deploy infrastructure in development by NCSA and PRAGMA partners. NCSA has participated in the Resources Working Group and has provided access to its high-performance computing environment to the PRAGMA Grid testbed. NCSA co-organized with APAC an NSF funded "U.S.-Australian Workshop on High-Performance Grid Computing and Applications" that helped build stronger ties between U.S. and Australian researchers. At Supercomputing 2004, some of the flagship PRAGMA collaborative projects such as the EcoGrid and the Lake Metabolism were demonstrated at the NCSA booth. AIST researchers, with the help of NCSA, were able to access to TeraGrid resources for demonstrations at Supercomputing 2004. KISTI and NCSA applications researchers are in active discussion on joint activities in CFD and computational chemistry grids. NCSA is working towards establishing an extended node for the PRIME project by sponsoring additional students to participate in research projects in PRAGMA institutions.

Key contacts: Radha Nandkumar, Danny Powell

National Electronics and Computer Technology Center
www.hpcc.nectec.or.th/pragma

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. PRAGMA is a synergetic forum of meaningful collaboration for the greater benefit. NECTEC, one of the PRAGMA founding members, has actively participated in all PRAGMA meetings. NECTEC plans to co-host a PRAGMA workshop with Kasetsart University and the ThaiGrid in 2007.

Key Contacts: Piyawut Srichaikul, Chalermpol Charnsripinyo, Sornthep Vannarat

National Grid Office
www.ngp.org.sg

The National Grid's vision is a Singapore where computer resources connected via a high-speed network 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. The National Grid Office (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 foundation for a vibrant grid computing economy.

The National Grid Pilot Platform connects resources at the Bioinformatics Institute (BII), the Institute of High Performance Computing, Nanyang Technological University, National University of Singapore, and Singapore-MIT Alliance via a high-speed gigabit network. Two clusters have been connected as a part of the Large Hadron Collider Computing Grid at CERN. The Platform also has Internet2 connectivity to the U.S., 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 Grid Asia meeting, raising competency through seminars and training courses, and fostering international collaborations with AIST, KISTI, APAN, and Gelato Federation.

The NGO and BII co-hosted PRAGMA 8 in Singapore in May 2005.

Key contacts: Lawrence Wong, Hing Yan Lee

Pacific Northwest Gigapop
www.pnw-gigapop.net

The Pacific Northwest Gigapop (PNWGP), in cooperation with its many peer research and education groups throughout the Pacific Rim, engineers state-of-the-art networking facilities in support of research, education, and networking. Through its many strategic partnerships and unique access to a diversity of leading-edge networking resources, PNWGP catalyzes applications that utilize the latest in global lamba networking and grid network resources.

- PNWGP is a founding member of National LambdaRail.
- With the University of Washington, PNWGP supports advanced grid applications in high-definition IP broadcasting and video conferencing, medical applications, and many areas of scientific research, such as biotechnology, medical sciences, geology, high-energy physics, astronomy, and oceanography.
- As the parent organization of the Pacific Wave international exchange facility, PNWGP supports peering and GLIF services for its research and education network partners throughout the Pacific Rim including but not limited to SINET, KREONet2/GLORIAD, GEMNET, AARNet, TANet, TWAREN, TransPAC, CANARIE, WIDE/T-LEX.
- As a co-steward with WIDE of the IEEAF trans-Pacific 10Gbps circuit, PNWGP advances high-capacity, long-reach networking.

By encouraging partnerships and collaborations with its many colleagues throughout the world, PNWGP seeks to expand its knowledge and the use of networking resources into the future. The PNWGP, established in 1998, is a non-profit organization based in Seattle, Washington, USA.

PNWGP interacts with PRAGMA by assisting with networking and working collectively on application areas.

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.

As Pacific Rim research networks approach the multi-gigabit range,

the StarLight facility exists as a permanent infrastructure where PRAGMA e-scientists, computer scientists, and networking engineers may plug-in networks, co-locate equipment, and directly peer with colleagues in Canada, the U.S., South America, and Europe. StarLight founders have subsequently partnered with colleagues from Pacific Wave to create TransLight (www.startap.net/translight), an NSF-funded project to provide multi-gigabit links and supporting infrastructure to interconnect U.S., European, and Pacific Rim research and education networks, as well as to supplement the available bandwidth that is being provided by other countries. Furthermore, StarLight network engineers provide technical support to National Research Networks (NRNs) connecting to its facility, in general, and with equipment modifications and upgrades that happen most frequently prior to major demonstration events, such as the Supercomputing conferences and iGrid workshops.

StarLight, a founding member of the Global Lambda Integrated Facility (GLIF: www.glif.is), encourages PRAGMA members to join GLIF and work with colleagues worldwide to share new LambdaGrid techniques and tools. Those being developed for the OptIPuter project (www.optiputer.net) exploit and control optical networks, schedule computing resources and wavelengths, and enable new visualization and data mining collaboration techniques for complex problem solving. StarLight also encourages PRAGMA members to participate in biennial international grid (iGrid) demonstrations (www.startap.net); the last major event, iGrid 2005, was held in San Diego in September 2005, and 18 of the 49 demonstrations involved PRAGMA members.

Key contacts: Maxine Brown, Tom DeFanti

TransPAC/TransPAC2, Indiana University
www.transpac2.net

TransPAC2, the continuation of the NSF-funded TransPAC 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 Consortium in Tokyo with extensions to Hong Kong and Singapore (expected in December 2005). TransPAC2 provides a 10G connection from Tokyo to Los Angeles, an OC-48 connection (link owner NICT-Japan) from Tokyo to Hong Kong, and a planned connection (link owner NII-Japan) from Tokyo to Singapore.

TransPAC/TransPAC2 is a founding member of PRAGMA and co-hosted with UCSD the PRAGMA 7 meeting in San Diego. 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) was 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 (egrid.cs.usm.my/esportal) integrates both e-science grid components and applications and enables secure access for researchers to a set of applications and data. e-Science grid components include Grid Resource Monitoring, Grid Resource Allocation, Grid Resource Metering, and Grid Resource Prediction; e-Science Grid 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 (UKM), 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 where enabled by the Asia Pacific Science and Technology Center, and initiated further collaborations with Nanyang Technological University, Singapore.

USM researchers have communicated with other PRAGMA participants about experiences in understanding practice and policy issues concerning the sharing of resources and the establishment of collaborations with other PRAGMA institutions. Some recent examples include the Kasetsart University–USM Drug Discovery Grid colloquium and USM's contribution of two high-performance clusters to the PRAGMA testbed. Another highlight was the participation of PRAGMA members in the launching of the USM Campus Grid in May 2005.

Key contacts: Ahmad Yusoff Hassan, Habibah A. Wahab

UNIVERSITY OF CALIFORNIA, SAN DIEGO
www.ucsd.edu

UCSD researchers are involved in application and grid activities of interest to PRAGMA, such as the NSF-funded TeraGrid, the NSF Middleware Initiative, OptIPuter, Geosciences Network, Network for Earthquake Engineering Simulation, National Laboratory for Applied Network Research network measurement monitoring, and the NIH-funded Biomedical Informatics Research Network, National Biomedical Computation Resource, National Center for Microscopy and Imaging Research, and the Gordon and Betty Moore Foundation award to establish a Global Lake Ecological Observatory Network.

PRAGMA provides an international vehicle to

- share codes under development at UCSD, such as Rocks clustering software and GAMESS, a chemistry application
- establish a testbed for grid applications and understand practice and policy issues of sharing international resources
- advance science via collaborations
- link and expand current projects with international collaborations
- integrate software from partners to ensure interoperability
- interact with experts in applications and grid middleware and increasingly wireless extensions to the grid
- share in experiences and lessons learned

UCSD researchers have been involved in all workshops, including hosting the inaugural workshop; provided a dedicated cluster to the PRAGMA testbed; and provided leadership in various aspects of the organization. PRAGMA projects involving UCSD researchers include Telescience with Osaka University, KBSI, KISTI, NCHC, and NCMIR; Computational Chemistry with Monash University, USM, KU, the University of Zurich; Workflows and integrated Genome Analysis Pipeline with AIST, BII, Titech, Jilin University, KISTI, and CNIC; EcoGrid and Lake Metabolism with NCHC and Trout Lake Station of the University of Wisconsin; and the PRAGMA Testbed. Furthermore, UCSD helped launch the Pacific Rim Undergraduate Experiences (PRIME) with Osaka University, NCHC, and Monash University. In 2005, the program was expanded to include CNIC. UCSD is working to help launch the new Osaka University project call PRIUS. In addition, the National Laboratory for Applied Networking Research (NLANR, mna.nlanr.net) has been actively working with PRAGMA partners to install active and passive monitors to better understand network traffic.

UCSD organizations involved in PRAGMA include the California Institute for Telecommunications and Information Technology, the San Diego Supercomputer Center, the Center for Research in Biological Structure, the National Center for Microscopy and Imaging Research, and the National Laboratory for Applied Network Research. UCSD co-hosted, with TransPAC, the PRAGMA 7 workshop in September 2004.

Key contacts: Peter Arzberger, Philip Papadopoulos, Teri Simas, Kim Baldridge, Longjiang Ding, Mark Ellisman, Tony Fountain, Wilfred Li, Mason Katz, Tomas Molina, Steven Peltier, Ronn Ritke, Cindy Zheng

UNIVERSITY OF HYDERABAD
www.uohyd.ernet.in

University of Hyderabad (UoH) researchers are involved in grid-related activities in such fields as biosciences, nanotechnology, drug design and discovery, and weather modeling. UoH also hosts the High Performance Computing Facility Centre for Modeling, Simulation, and Design (CMSD), with liberal support from the University Grants Commission (UGC) and the 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, which recently dedicated an 8-node cluster to PRAGMA, is a founding member of the Steering Committee of PRAGMA and is contributing to PRAGMA's resource and middleware initiatives and weather modeling demonstration.

UoH hosted the PRAGMA 9 Workshop (October 20–22, 2005). With efforts centered on creating active collaborations and exchanging researchers and students between the PRAGMA members, UoH planned two special events. A tutorial preceding PRAGMA 9, titled "Deploying, Programming, and Applications of Linux Cluster Systems," demonstrated the building of a Rocks-based grid. Secondly, GEON, the Geosciences Network (www.geongrid.org), conducted the Cyberinfrastructure Workshop (October 24–27, 2005) jointly with UoH, the Centre for Modelling Simulation and Design, the Centre for Earth and Space Science, and the San Diego Supercomputer Center. This was the first formal, international collaboration that GEON has developed, with plans to launch a GEON node to host a geochemistry database and other geosciences services.

Key contact: Arun Agarwal

Schedule of Workshops

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

Future Meetings

PRAGMA 10: 26–28 March 2006, Townsville, Australia
Hosted by the Queensland Parallel Supercomputing Foundation, the Australian Partnership for Advanced Computing, James Cook University, and the Australia Institute for Marine Science. Held in conjunction with the Coral Reef and Lake Observatory community. Chair: Bernard Pailthorpe (APAC); Co-Chair: Shinji Shimojo (Osaka University)

PRAGMA 11: October 2006, Osaka, Japan
Hosted by Osaka University. Held in conjunction with the PRIUS activity. Chair: Shinji Shimojo (Osaka); Co-Chair: Piyawut Srichaikul (NECTEC)

PRAGMA 12: Spring 2007, Bangkok, Thailand
Hosted by National Electronics and Computer Technology Center, and the High Performance Computing and Network Center at Kasetsart University. Chairs: Piyawut Srichaikul (NECTEC), Putchong Uthayopas (KU); Co-chair: Radha Nandkumar (NCSA)

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

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

Past Meetings

PRAGMA 1: 11-12 March 2002, San Diego, U.S.
Hosted by the San Diego Supercomputer Center and Cal-(IT)^2 at the University of California, San Diego. Held in conjunction with the NPACI All Hands Meeting. Chair: Philip Papadopoulos (UCSD/SDSC/Cal-(IT)^2/CRBS); Co-chair: Sangsan Lee (KISTI)

PRAGMA 2: 10-11 July 2002, Seoul, Korea
Hosted by the Korea Institute of Science and Technology Information and held in conjunction with Grid Forum Korea. Chair: Sangsan Lee (KISTI); Co-chair: Yoshio Tanaka (AIST)

PRAGMA 3: 23-24 January 2003, Fukuoka, Japan
Hosted by the National Institute of Advanced Industrial Science and Technology, Osaka University, and Monash University and held in conjunction with the Asia-Pacific Advanced Network Consortium Meeting. Chair: Satoshi Sekiguchi (AIST); Co-chair: David Abramson (APAC)

PRAGMA 4: 4-5 June 2003, Melbourne, Australia
Hosted by Monash University and APAC, held in conjunction with ICCS2003. Chair: David Abramson (APAC); Co-chair: Fang-Pang Lin (NCHC)
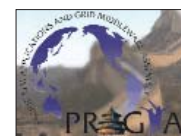
PRAGMA 5: 22-23 October 2003, Hsinchu/Fushan, Taiwan
Hosted by National Center for High-performance Computing. Chair: Fang-Pang Lin (NCHC); Co-chair: Kai Nan (CNIC)

PRAGMA 6: 16-18 May 2004, Beijing, China
Hosted by the Computer Network Information Center, Chinese Academy of Sciences. Chair: Baoping Yan; Co-chairs: Mason Katz (UCSD) and Jim Williams (TransPAC)

PRAGMA 7: 15-17 September 2004, San Diego, U.S.
Hosted by the University of California, San Diego, the San Diego Supercomputer Center, the California Institute for Telecommunications and Information Technology, and TransPAC. Held in conjunction with IEEE Cluster Computing and the Coral Reef and Lakes Observatory meeting. Chairs: Mason Katz (UCSD) and Jim Williams (TransPAC); Co-chair: Larry Ang (BII).

PRAGMA 8: 2-4 May 2005, Singapore
Hosted by the Bioinformatics Institute in Singapore and the National Grid Office. Held in conjunction with Grid Asia 2005. Chair: Arun Krishnan (BII); Co-chair: Arun Agarwal (UoH).

PRAGMA 9: 20-23 October 2005, Hyderabad, India
Hosted by the University of Hyderabad. Held in conjunction with the GEON workshop. Chair: Arun Agarwal (UoH); Co-chair Bernard Pailthorpe (APAC).

Publications 2005

The references below augment material summarized in this brochure. These have been selected to reflect both activities done between PRAGMA partners (indicated by *) as well as some key technologies upon which PRAGMA activities are based. They have been grouped by topic. More publications about PRAGMA and associated technologies can be found at www.pragma-grid.net.

Biological Sciences

Kido Y, Date S, Takeda S, Hatano S, Ma J, Shimojo S, Matsuda H. Architecture of a Grid-Enabled Research Platform with Location-Transparency for Bioinformatics, *Genome Informatics,* Vol. 15, No. 2, 3- 12 (2004).

Li WW, Quinn GB, Alexandrov NN, Bourne PE, Shindyalov IN. A Comparative Proteomics Resource: Proteins of Arabidopsis thaliana, *Genome Biol,* Vol. 4, R51 (2003).

Li WW, Arzberger PW, Yeo CL, Ang L, Tatebe O, Sekiguchi S, Jeong K, Hwang S, Date S, Kwak J-H. Proteome Analysis using iGAP in Gfarm, The Second International Life Science Grid Workshop 2005, Grid Asia 2005, Singapore, 2005.

Shahab A, Chuon D, Suzumura T, Li WW, Byrnes RW, Tanaka K, Ang L, Matsuoka S, Bourne PE, Miller MA, Arzberger PW. Grid Portal Interface for Interactive Use and Monitoring of High-Throughput Proteome Annotation. *Lecture Notes in Computer Science.* Vol. 3370, 53-67 (2005).

Wei X, Li WW, Tatebe O, Xu G, Hu L, Ju J. Implementing data aware scheduling on Gfarm by using LSFTM scheduler Plugin, International Symposium on Grid Computing and Applications, Las Vegas, NV, 2005.

Computational Chemistry

Baldridge KK,* Sudholt W, Greenberg JP, Amoreira C, Potier Y, Altintas I, Birnbaum A, Abramson D, Enticott C, Slavisa G. Cluster and Grid Infrastructure for Computational Chemistry and Biochemistry. *Parallel Computing for Bioinformatics.* A.Y. Zomaya (Ed.), John Wiley & Sons (2005) In press.

Sudholt W, Baldridge K, Abramson D, Enticott C, Garic S, Kondrick C, Nguyen D. Application of Grid Computing to Parameter Sweeps and Optimizations in Molecular Modeling. *Future Generation Computer Systems* (Invited). Vol. 21, 27-35 (2005).

Infrastructure and Testbed

Zheng C, Katz M, Arzberger P, Papadopoulos PM, Tanaka Y, Tanimura Y, Tatebe O, Abramson D, Enticott C, Garic S, Ayuub

S, Uthayopas P, Sriprayoonsakul S, Phatanapherom S, Kwak JH. Issues and Methods for Building a Multi-Application International Grid Resource 2005 (submitted to CCGrid 2006).

Ritke R, Gannis M, McGregor T. Towards a World-Wide Grid Measurement Infrastructure, APAC'05, Australia, September 2005.

Ninf-G

Tanaka Y, Takemiya H, Nakada H, Sekiguchi S. Design, Implementation and Performance Evaluation of GridRPC Programming Middleware for a Large-Scale Computational Grid, Proceedings of the 5th IEEE/ACM International Workshop on Grid Computing, 298-305, Nov. 2004, Pittsburgh, USA.

Tanimura Y, Ikegami T, Nakada H, Tanaka Y, Sekiguchi S. Proceedings of the Workshop on Grid Applications: From Early Adopters to Mainstream Users, GGF Documents (2005).

Sensors and Ecogrid.

Ma J, Hatano S, Shimojo S. Implementation of Field Monitoring System by IPv6 and GRID Authentication on the Loess Plateau. *Agricultural Information Research.* 13(4). (in Japanese) 281-290 (2004).

Porter JH, Arzberger P, Braun H-W, Bryant P, Gage S, Hansen T, Hanson P, Lin F-P, Lin C-C, Kratz T, Michener W, Shapiro S, Williams T. 2005 Wireless Sensor Networks for Ecology. *BioScience.* Vol. 55. No. 7 561-572 (2005).

Telescience

Akiyama T, Nozaki K, Kato S, Shimojo S, Peltier ST, Lin A, Molina T, Yang G, Lee D, Ellisman M, Naito S, Koike A, Matsumoto S, Yoshida K, Mori H. Scientific Grid Activities in Cybermedia Center, Osaka University, 5th IEEE/ACM CCGrid proceedings (BioGrid'05 Workshop), (to appear, 2005).

Student and Postdoctoral Opportunities

The PRAGMA framework, with its rich set of projects and network of researchers throughout the Pacific Rim, provides an ideal environment for students (see PRIME 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 at Global Grid Forum 13 (March 2005), Life Science Grid at Grid Asia 2005 (May), iGRID2005 (September 2005), and APAC2005. Furthermore, PRAGMA members have actively participated in APAN meetings and Supercomputing 2003, 2004, and 2005, demonstrating PRAGMA members' collective accomplishments.

Future meetings involving PRAGMA members and the community include such activities as the International Conference on e-Science and Grid Technologies (December 2005) in Melbourne, Grid Asia 2006 in Singapore (May 2006), and CODATA in Beijing (October 2006). See www.pragma-grid.net/calendar.htm for more information.

PRAGMA Sponsors

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CCST receives major funding support from the Chinese Natural Science Foundation."

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PACIFIC RIM APPLICATIONS AND GRID MIDDLEWARE ASSEMBLY

PRAGMA

October 2005