

PACIFIC RIM APPLICATIONS AND GRID MIDDLEWARE ASSEMBLY

www.pragma-grid.net

Institutions and Contacts

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.

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Contents

In the 21st 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]^I

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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 to 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

This brochure highlights 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

In 2004 PRAGMA has made great strides on many fronts. A broad experiment was mounted, using dedicated machines in a PRAGMA grid, to understand how to make the grid usable to researchers on a routine basis. Key to this goal is having middleware that can interoperate. To this end, researchers at KISTI took preliminary steps to localize a cluster software, Rocks. Researchers at the UCSD's SDSC have developed and are maintaining Rocks Rolls of Ninf-G and Gfarm middleware created at AIST. As a result, a broader set of users gained easy access to software created in other countries. Leveraging previous NCHC activities in the EcoGrid, PRAGMA has forged international partnerships that are launching the first-ofits-kind Global Lake Metabolism Observatory Network for Research and Education.

PRAGMA also focuses on building human expertise for collaborations. A collective effort among Osaka University, NCHC, Monash University, and UCSD, funded by NSF and PRAGMA partner Cal-(IT)², created a research internship program, PRIME, for UCSD students to work at one of three PRAGMA sites. Many PRAGMA members also participated in and led special sessions at key international conferences, such as SC'03, HPCAsia 2004, and the Life Science Grid workshop. PRAGMA's first project-based distance training between UCSD and the Computer Network Information Center (CNIC) focused on web services. Other training conducted within the PRAGMA community focused on middleware produced by its members.

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, PRAG-MA 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. 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.

Accomplishments: Achieving Success Through Partnership

Telescience Technologies deployed on the Pacific Rim

The Telescience Portal is the grid entry point through which scientists have been providing access to their unique scientific instruments. Developed initially at the National Center for Microscopy and Imaging Research (NCMIR), the Telescience Portal has been installed at collaborating institutions and extended through collaborative efforts of PRAGMA partners, allowing the centers to exchange resources and data as NCMIR has for more than a decade.

Most recently, at the Korea Basic Science Institute (KBSI) in Daejon, South Korea, NCMIR scientists working with KBSI researchers constructed a working Telescience environment that grants KBSI scientists the capacity to perform end-to-end tomography. The Telescience package includes a grid portal, data grid, and imaging applications and tools that allow investigators at remote institutions to control KBSI's newly installed 1.25 MeV electron microscope via the Internet. This collaborative effort involving KISTI was a first step of the K*Grid project to make instruments remotely available.

Building on a long standing interaction, researchers from NCMIR and the Cybermedia Center (CMC) integrated an IPv6 version of Telemicroscopy software and other applications within CMC's existing grid environment. This integration project also involved the efforts of two undergraduate students participating in the PRIME program (see PRIME Section), funded by the National Science Foundation. The IPv6 project continues the success of earlier



Left: The Center for Ultra-High Voltage Electron Microscopy at Osaka University in Japan houses the world's largest microscope, the 3 MeV. Center: Telescience allows researchers to operate high-performance microscopes via the Internet to access images like this spiny dendrite from a mouse brain. Right: KBSI's 1.25 MeV ultra-high voltage electron microscope is remotely accessible and integrated into the Telescience architecture.

ventures involving CMC's expertise and its 3 MeV microscope, in which NCMIR has been sending video from the 3 MeV using IPv6 technology. Current efforts are integrating control of this microscope—the world's largest and most powerful high voltage electron microscope—and its camera systems for automatic 3D reconstruction of data.

The collaborations have resulted in a rich exchange of data, resources, and knowledge. NCMIR researchers have been training KBSI scientists in electron tomography techniques, including most probable loss tomography, which, when applied to intermediate voltage electron microscopy, dramatically enhances image resolution and reduces chromatic aberration in thick sections compared to standard unfiltered transmission electron microscopy techniques.

Data collected using these advanced methods and deposited automatically into the Cell Centered Database *(ccdb.ucsd.edu)* provides 3D microscopic imaging data available to the structural biology and neuroscience communities.

Computational Chemistry Merges Grid Technology and Application

Computational Chemistry Methods, a PRAGMA collaborative initiative, has been designing and automating workflow processes for computational chemistry 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.

By coupling SDSC's KEPLER workflow system with the Nimrod grid distribution tool, researchers can build complex workflows that include a parameter sweep, configuration optimizations, or integrated calculations involving more than one type of calculation and often more than one chemistry software package in a way that automates and distributes the calculations. This appealing tool combination can be applied to any workflow involving complex calculations performed on different resources of a computational grid. Moreover, grid technologies combined with chemistry software allow researchers to choose separate, optimal calculations for each portion of a study, all built into one workflow scheme.

For example, GAMESS/APBS (electrostatic evaluation code)+Nimrod software can be used to perform molecular docking studies. Nimrod/O contains state-of-the-art optimization algorithms Telescience Technologies Development Participants: NCMIR at UCSD, Cybermedia Center of Osaka University, Kore, Basic Science Institute, KISTI

COMPUTATIONAL CHEMISTRY PARTICIPANTS: Monash University, SDSC at UCSD, University of Zurich. Resources for testing and experiments come additionally from Victorian Partnership for Advanced Computing, Kasetsart University, National Institute of Advanced Industrial Science and Technology, Cray Inc.

Lake Metabolism and EcoGrid Participants:

National Center for High-perfori ance Computing; Taiwan Forest Research Institute; Academia Sinica; North Temperate Lakes LTER; SDSC at UCSD; Asia-Pacific Advanced Network; National Agricultural Research Center

BANDWIDTH CHALLENGE

PARTICIPANTS: The Trans-Pacific Grid Datafarm team included members or resources from National Institute of Advanced Industrial Science and Technology, Tokyo Institute of Technology, University of Tsukuba, KEK, APAN Tokyo XP, and TransPAC/Indiana University, SDSC at UCSD, Kasetsart University. The Multi-continental Telescience team included members and resources from NCMIR and SDSC at UCSD, Universidad de Buenos Aires, Karolinska Institute, Osaka University, Center for Ultra-High Voltage Microscopy, KDDI R&D Labs, Korea Basic Science Institute, KISTI, National Center for High-performance Computing

Middleware Interoperability Participants: SDSC at UCSD AIST, KISTI.

IGAP AND GFARM INTEGRATION PARTICIPANTS: UCSD at SDSC, Bioinformatics Institute of Singapore, National Institute of Advanced Industrial Science and Technology (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 KEPLER-Nimrod system has enabled further investigations into protein-ligand interactions by giving insight into how a ligand may bind into a pocket of a protein, or how residue mutation can influence dynamics in a protein structure. The behavior of ligands in proteins and the dynamics involved in protein-protein interactions are important for understanding biological processes and the design of pharmaceutical agents.

Wireless and Internet Technologies in Ecogrid Transform Study of Lake Metabolism

PRAGMA researchers have begun creating a first-of-its-kind global lake monitoring network to investigate lake metabolism by establishing wireless connections to field sensors in lakes on both sides of the Pacific Ocean. Sensors deployed in Trout Lake in Wisconsin and Yuan-Yang Lake in Taiwan have enabled measurements of gross primary production, respiration, and net ecosystem production.

Wireless communication with the sensors from anywhere in the world via the Internet allows for real-time, frequent measurements of barometric pressure, dissolved oxygen, wind speed, and temperature at various lake depths. While previously published studies examined mostly northern temperate lakes and relied on short sampling durations, new technologies have promoted the study of such sub-tropical lakes as the Yuan-Yang, which experiences many typhoons each year. Sensors in that lake captured minute-by-minute data during a typhoon, yielding exciting results and recording phenomenon not seen in Wisconsin lakes *(lakemetabolism.org)*.

Future efforts will focus on developing web services to automate the reduction of raw buoy data to estimate daily respiration, gross primary production, and net ecosystem production. As the project matures, other services will be developed to automate aspects of the system for quality control of the data, intelligent signal detection (e.g., major external meteorological events), and analyses and visualizations.

This project, initiated by PRAGMA collaborations, leverages the information management experience of North Temperate Lakes Long-Term Ecological Research project, combined with the infrastructure and wireless experience of the Ecogrid Project (ecogrid.nchc.org.tw) in Taiwan led by the Taiwan National Center for High-performance Computing (NCHC) in collaboration with the Taiwan Ecological Research Network, the Taiwan Forest Research Institute, and Academia Sinica. The project also involves interactions between the U.S. Long-Term Ecological Research Network and SDSC/UCSD in building web services. To build interoperating web services for meteorological data, the project has relied on the technologies of PRAGMA collaborating with NCHC, the Chinese Network Information Center (CNIC), the Asia-Pacific Advanced Network (APAN), and the National Agricultural Research Center in Japan.

BANDWIDTH CHALLENGE AWARDS WON AT SC'03

During the High-performance Bandwidth Challenge, a highlight of SC'03, contestants from science and engineering research communities around the world demonstrated the latest technologies and applications for high-performance networking, many of which are so demanding that no ordinary computer network could sustain them. The awards won for demonstrations by two PRAGMA teams emphasized that collaborative science applications are a significant force behind the development of high-performance networking



Buoy in Yuan-Yang Lake, Taiwan contains sensors and is integrated into the EcoGrid infrastructure.

The Trans-Pacific Grid Datafarm team won the Distributed Infrastructure Award for a geographically distributed file system that took advantage of multiple physical paths to achieve high performance over long distances. For the competition, the National Institute of Advanced Industrial Science and Technology of Japan (AIST) replicated terabyte-scale experimental data between the U.S. and Japan over several OC-48 links. Five clusters in Japan, three in the U.S., and one in Thailand constituted a Grid virtual file system of 70-terabyte capacity and 13 Gbps of parallel disk I/O performance using the Grid Datafarm Data Grid Middleware. Worldwide parallel and distributed data analysis of an astronomical object survey was performed for the terabyte-scale archive data using the testbed. For replicating I.I terabyte data, the team achieved stable 3.79 Gbps network flow out of theoretical peak 3.9 Gbps (97%) using II node pairs.

The Multi-Continental Telescience team's entry, which earned the Application Award, showcased multidisciplinary technology and partnerships encompassing Telescience, microscopy, biomedical informatics, optical networking, next-generation protocols, and collaborative research. High network bandwidth using the IPv6 protocol allowed participants to control the multiple high-energy electron microscopes, demonstrating the ability to use high-quality, low-latency HDTV to navigate a specimen in Osaka University's 3.0 MeV electron microscope via IPv6. The demonstration was performed in synchrony with parallel processing and visualization of data from the Biomedical Informatics Research Network over a global grid of heterogeneous resources located at five institutions worldwide.

Middleware Made Interoperable, Redistributed, and Localized

The unique promise of e-science and cyberinfrastructure begins with the ease of assembling such disparate resources as experimental instruments, distributed computing resources, and large volumes of data from observations and simulations. Ultimately, such an integration will allow researchers to work with all of these resources as needed. Necessary for this vision is the transparent and sustainable interoperability of middleware.

Achieving sustainable interoperability and persistent grid development involves addressing both technical and non-technical factors, including funding boundaries, incentives for researchers to devote time to make tools work together, and trust. PRAGMA provides an environment in which different groups can address practical interoperability and the wider variety of non-technical and equally critical factors. Examples where PRAGMA has brought software together include the GAMESS/Nimrod-G/KEPLER initiative, Telescience instrument control and portal technology, and integrative Genome Annotation Pipeline (iGAP) and Grid Datafarm (see Accomplishments). Two additional activities, described below, expand the user base of Rocks cluster software.

To complement the Rocks cluster software, "Rolls" for Ninf-G and Gfarm, middleware developed by Grid Technology Research Center of the National Institute of Advanced Industrial Science and Technology, have been developed and is being maintained to bring AIST work to a new audience of Rocks users. Rolls allows Rocks users to install other middleware applications on their clusters at start-up. In addition, Rolls provides more users of Rocks with easy access to software developed elsewhere, and in a way that ensures the software will function on a cluster. Another example is the scalable cluster environment (SCE, developed by Kasetsart University) roll, currently being deployed to build many grid ready cluster systems.

In addition, the Korea Institute of Science and Technology Information (KISTI) has been working with SDSC to produce a localized version of Rocks, distributed through *krocks.cluster.or.kr* especially for use in a grid environment by the cluster user community in Korea. The Korean version, named KRocks, provides an easyto-use guide for Korean researchers to install Rocks.

These types of efforts will help expand the user base of the software internationally. Over the coming year PRAGMA will begin to develop systems that will allow for persistence of these activities through all of the new versions that will be released.

BIOINFORMATICS AND GRID DATA TOOLS INTEGRATED

The Integrative Genome Annotation Pipeline (iGAP) is a suite of bioinformatics software developed for annotation of protein structure and functions. It has been used to analyze more than 140 complete or partial genomes *(eol.sdsc.edu)*. The grid deployment of iGAP has been a exemplar collaborative effort among SDSC, BII, Titech, and AIST within the PRAGMA community. A four day demonstration at SC'03 involved grid-enabled iGAP running at six different sites on as many as 400 cpu's at a time to provide updated annotation for more than 36,000 proteins from 70 different proteomes. The new architecture takes advantage of the parameter sweep template APST developed at UCSD, and the GridMonitor web interface developed by BII for monitoring the grid workflow. The annotation process may also be initiated from an iGAP application portal developed using GridSpeed from Titech.



Gfarm is a global parallel file system developed by AIST in collaboration with KEK, University of Tokyo, and Titech. A new feature of Gfarm enables the execution of existing applications within the Gfarm virtual filesystem with no modification required. This new development, important for many bioinformatics applications, allowed for the successful running of iGAP in Gfarm using distributed compute and storage resources transparently and efficiently. Running iGAP inside Gfarm not only offered a real life science application suite using a new technology not available before to life sciences applications, but also provided the new sparks and momentum for Gfarm software development and code hardening. During the past year, PRAGMA augmented its activities by directly involving students in projects and working groups. PRIME is a first step 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.

PRIME: Preparing Undergraduates for the Global Workforce

Overview

In April 2004, UCSD with several PRAGMA partners launched Pacific Rim Undergraduate Experiences Program (PRIME: *prime.ucsd.edu*). PRIME provides an opportunity for students from UCSD to participate in international research and cultural experiences that will better prepare them to participate in the global workplace of the 21st century. In addition, PRIME will create 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). Collaborators in PRIME are PRAGMA partners at the Cybermedia Center (CMC), Osaka University, Osaka, Japan; the National Center for High-performance Computing (NCHC), Hsinchu, Taiwan; and the Department of Computer Science, Monash University, Melbourne, Australia.

The research and activities conducted by the student researchers will contribute to the growth of the cyberinfrastructure. Through the development of code to be used by others and by testing and running application codes in this internationally distributed environment, e-science activities will be enhanced 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; 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.

During this first year—with additional support from NSF's Division of Shared Infrastructure and Cal-(IT)² (*www.calit2.net*) the program supported the research experiences for nine students, with three each at CMC, NCHC, and Monash. The students were selected based on a wide variety of criteria, including scholastic accomplishment, previous research or working experience, their research plan's inclusion of defined goals, and statements from UCSD and host-site mentors. Selected students were also required to return 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 first 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, systems biology, and earthquake engineering.

The anticipated deadline for the summer 2005 PRIME application is early March 2005. PRIME aims to increase funding to allow the program to include more students and additional sites.

YEAR I HIGHLIGHTS OF STUDENT ACTIVITY Cybermedia Center, Osaka University

Undergraduates Stephen Geist and Ramsin Khoshabeh worked with the Cybermedia Center team in Osaka, 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, to continue developing components of the Telescience infrastructure. Geist migrated code from a CCD camera on an electron microscope at UCSD's NCMIR to the same camera on the Osaka 3 MeV electron microscope. Khoshabeh explored the next-generation IPv6 protocol with respect to key components of the telescience middleware infrastructure.

PRIME student Takumi Takahashi worked with UCSD Bioengineering chair Shu Chien, researcher Jason Haga, and the Osaka team to adapt tools to provide a user interface for grid computing that will facilitate the analysis of gene microarray data. He created an interface that enables microarray data to be submitted to the grid and normalized using different mathematical schemes. This will lead to new tools that will benefit from the high speed computational power of grid computing and integrate data from different genomic databases relevant to cellular function when exposed to different biochemical and biomechanical stimuli.

Теам Leaders and Members: Shinji Shimojo, Cybermedia Center vice-director, Biogrid Japan PI; Susumu Date, assistant professor in the Graduate School of Information Science and Technology; Toyokazu Akiyama; Kazunori Nozaki; Tomomi Takao

National Center for High-performance Computing (NCHC) and National Center for Research on Earthquake Engineering (NCREE)

PRIME student Robert Ikeda worked with the NCHC team and UCSD Bioengineering Assistant Professor Trey Ideker to develop a graphical user interface for viewing and navigating large molecular interaction networks based on hyperbolic space projections. Ikeda then integrated the interface into Cytoscape, a large-scale, computer-aided modeling program for biological signaling and regulatory networks.



Images from left to right: Takumi Takahashi (third from left), Ramsin Khoshabeh (fourth from left), and Stephen Geist (far right) pose with members of the PRAGMA Osaka team during their summer visit to Osaka University; Left to right: John Colby, Christopher Kondrick, and Duy Nguyen, pictured above during a visit to the shore in Australia, conducted research at Monash University in Melbourne; Left to right: Jared Bell, Brandon Smith, and Robert Ikeda stand in front of Chiang Kai-Shek Memorial Hall in Taiwan

Undergraduate Brandon Smith enhanced software used to check the quality of data coming from sensors deployed in the environment, including the Collaborative Lake Metabolism project (lakemetabolism.org), thereby extending the Ecogrid infrastructure in Taiwan's Ecological Parks. His new code is easily adapted by other projects, extensible for other features, and faster than existing code. Smith worked with the NCHC and UCSD team Peter Arzberger, Tony Fountain, director of Knowledge and Information Discovery Laboratory within the Data and Knowledge Systems program at the San Diego Supercomputer Center (SDSC), and Longjiang Ding, SDSC.

PRIME student Jared Bell worked with the NCHC and NCREE teams and Chia-Ming Uang, professor and vice-chair of UCSD's Structural Engineering department. Bell bridged the two centers in Taiwan and UCSD by comparing the Internet based Simulations for Earthquake Engineering (ISEE) and National Earthquake Engineering Simulation (NEES) model, both virtual laboratories for testing earthquake resistance of structures. In addition, he wrote a Linear Analysis Engine Simulator and gained a deeper understanding of the ISEE system.

NCHC TEAM LEADERS AND MEMBERS: Fang-Pang Lin, Grid Computing Division manager; Hsui-Mei Chou; Sun-In Lin; Shi-Wei Lo; Grace Hong

NCREE TEAM LEADERS AND MEMBERS: Keh-Chyuan Tsai, director; Wei-Choung Cheng; Yuan-Sen Yang

Monash University

All three Monash students worked on aspects of the Nimrod family of tools, developed by David Abramson's group. John Colby and his UCSD mentors Andrew McCulloch, Bioengineering vice-chair and Anushka Michailova, Bioengineering researcher, employed Nimrod to investigate and optimize the dynamics of a simulated cardiac cell. By sweeping large parameter spaces with Nimrod/O, John identified parameters that improved the stability of the complex cellular model and its agreement with experimental measurements under a wide variety of conditions. Christopher Kondrick, 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. Using two computational chemistry codes, GAMESS and APBS, he investigated some preliminary ideas in protein/ligand docking using first principles methodologies. Duy Nguyen incorporated Nimrod tools, complete with the Nimrod Portal, into the Rocks cluster software, to create a ready-to-use system for scientific data computing. He also ported Nimrod to the Apple Macintosh and developed new Globus components. Nguyen worked with Philip Papadopoulos, SDSC program manager of Grid and Cluster Computing and PRAGMA coprincipal investigator.

TEAM LEADERS AND MEMBERS: David Abramson, professor, School of Computer Science and Engineering; Colin Enticott; Slavisa Garic; Rob Gray

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: Gabrielle Wienhausen, founding provost of Sixth College and the Cal-(IT)² 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 (NBCR); Teri Simas, PRAGMA Project Manager. Students in 2004: Stephen Geist, Ramsin Khoshabeh, Takumi Takahashi, Duy Nguyen, Christopher Kondrick, John Colby. Mentors in 2004: Mark Ellisman, Steve Peltier, Tomas Molina (NCMIR); Kim Baldridge, Longjiang Ding, Tony Fountain, Philip Papadopoulos (SDSC); Shu Chien, Jason Haga, Trey Ideker, Andrew McCulloch, Anushka Michailova (Bioengineering); Chia-Ming Uang (Structural Engineering). 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.

Working Groups: Integrating PRAGMA's Diversity

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 endto-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 (see Accomplishments).

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 metabolisms (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 have joined PRAGMA this year and are active in Telescience and EcoGrid, respectively.

BIOLOGICAL SCIENCES

As biological research continues to drive grid development in many areas, the Biological Sciences Working Group pursues a wide range of activities, including the Encyclopedia of Life (EOL) project, the Gfarm distributed file system, and the integration of various biogrids within the PRAGMA community.

The EOL project, demonstrated at SC'03 as a successful use of the grid, moved towards routine use by researchers with the improvement of the user interface. The output of the EOL computation at SDSC is mirrored at the Bioinformatics Institute (BII). The EOL application also has been integrated with the AIST Gfarm distributed file system middleware through a collaboration between researchers in the Biological Sciences and Data Computing Working Groups.

In another example of successful collaboration, the integration of various bio-grids within the PRAGMA community has allowed investigators to share knowledge and exchange ideas, reducing the likelihood of duplicate efforts and leveraging the strength and output of all participants. For example, researchers at the Korean Konkuk University and BII in Singapore have made comparative assessments and technology evaluation of the grid portal tools used in the molecular simulation, which have resulted in greater labor and resource efficiencies.

Working Group members have been involved in organizing critical biological grid workshops, providing a broader interface for PRAG-MA members and reaching a wider community. The BioGrid Workshop, held in conjunction with HPC Asia 2004 and co-organized by Osaka University and BII, was a resounding success. Member institutions were also involved in organizing the First International Life Science Workshop in Japan in May 2004. Such workshops remain an integral part of PRAGMA training and knowledge-sharing activities.

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 2003, the working group established a Trans-Pacific Grid Datafarm testbed consisting of three clusters in the U.S., five clusters in Japan, and one cluster in Thailand, creating a wide-area virtual file system with a 70-terabyte capacity and 13 Gbps of parallel disk I/O performance using the Grid Datafarm Data Grid Middleware. As a result, the working group earned a "Distributed Infrastructure Award" at the SC'03 high-performance bandwidth challenge (see Accomplishments).

The Data Computing Working Group encourages collaborations around data computing in the Pacific Rim region, expanding the testbed to several hundreds of terabytes of high-performance shared virtual file system. Current activities include the Belle Data Grid, the Spatial Data Grid, the Scientific Data Grid, and the Virtual Observatory Grids. Belle, a data grid focusing on high energy physics, includes the University of Melbourne, National Institute of Advanced Industrial Science and Technology (AIST), and the High Energy Accelerator Research Organization (KEK). The Spatial Data Grid involves the NCHC and SDSC, and the Scientific Data Grid is a partnership between Chinese Academy of Sciences and SDSC. The Virtual Observatory Grids project is a collaboration among NCSA, AIST, and the Australian National University.

Resources Working Group

Improving the interoperability of grid middleware in the Pacific Rim and throughout the world will lead to increased productivity and effectiveness in the use of the grid for research. To this end, the Resources Working Group has taken several steps to construct a PRAGMA grid testbed.

This year, PRAGMA researchers focused on enhancing usability of scientific applications by automating scheduling, access, and the launching of jobs. The group investigated these issues by running a single application, the Time Dependent Density Functional Theory Calculation, over the heterogeneous testbed. This calculation, developed by Dr. Nobusada of Hokkaido University (www.tddft.org), was executed using Ninf-G as the key middleware to manage the calculations. During this routine use experiment, which lasted from June 1, 2004 to August 31, 2004, a prototype grid operations center was established to monitor all of the nodes on the routine use testbed using SCMSWeb (See pragma-goc.rocksclusters.org/ scmsweb/scms_home.html). A report that can be accessed at pragma-goc.rocksclusters.org/ tddft/Lessons.htm outlines the lesson learned from this activity that will be applied to PRAGMA's next step in moving towards a pro-

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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, Korea Basic Science Inst; H. Chou, J. Chen, G. Hong, NCHC; S. Ninomiya, Nat'l Agriculture Res. Center and Asia Pacific Advanced Network; B. Pailthorpe, N. Bordes, Univ of Queensland; D. McMullen, L. Ding, T. Fountain, UCSD; H. King, Tawain Forest Research Inst, T. Kratz, North Temperate Lakes LTER

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SCMSweb monitoring the PRAGMA grid

Resources: M. Katz, Co-chair, SDSC at UCSD: K. Sakharkar. Co-chair, BII Singapore; Y. Tanaka, Co-chair, AIST; P. Papadopoulos, C. Zheng, SDSC at UCSD; R. Buyya, Univ Melbourne; J. Lee, J. Kwak, KISTI; F. Lin, W. Huang NCHC; K. Mikami, Cray Inc.; K. Nan, K. Dong, CNIC, Chinese Acad of Sci; K. Shirose, Tokyo Inst of Tech; S. Shimojo, Osaka Univ; O. Tatebe, Y. Tanimura, AIST; P. Uthayopas, S. Sriprayoonsakul, Kasetsart Univ; H. Wahab, Univ Sains Malaysia; J. Williams, D. McMullen, J. Hicks, Indiana Univ; E. Yen, ASCC; A. Agarwal, Univ Hyderabad; J.L. Gordillo, Univ Nacional Autónoma de México; N. Teow, BII; T. Roney, NCSA

duction grid, which will involve more sites, will expand the number of diverse applications being run simultaneously on it, will implement more tools to monitor the testbed and the usage patterns on it, and will develop a set of strategies and good practices for the global grid.

A secondary goal of the working group is to promote, deploy, integrate, and test grid middleware developed by PRAGMA members, such as Ninf-G, SCMSWeb, and Ganglia. This year, concrete examples of software being integrated into a single distribution include Ninf-G and Rocks (see Accomplishments). In keeping with the PRAGMA philosophy, the Resource Working Group interacts closely with ApGrid to test software more broadly, share experience, and adopt the best software.

With the existence of a testbed, future challenges will include seeding new grid-aware applications, pushing deployment of software environments better tuned to applications, enhancing the coupling of distribution of software from various PRAGMA sites into a single release, and installing accounting systems to track use of the testbed and the barriers to sharing resources internationally. This experience will help inform all funding agencies interested in understanding how the global grid will be used and will benefit researchers within funding boundaries to link national and regional production grids.

PRAGMA "Routine Use Testbed" Resources consists of dedicated hardware for this activity: The first instantiation took place at AIST, SDSC, KISTI, Titech, USM, KU, NCHC, NCSA, BII, and UNAM. The second instantiation is expected at AIST, SDSC, KISTI, KU, NCSA, NCHC, and UNAM. 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.

Members: Providing Expertise, Tools, and **Resources**

ACADEMIA SINICA COMPUTING CENTRE

www.ascc.net, www.twgrid.org

ASCC is one of the major high-performance computing and communication centers in Taiwan. ASCC provides service and support for academic computing at Academia Sinica and its collaborating institutes. ASCC began investigating



and deploying grid technology in 2000. Since then, ASCC has established grid-based infrastructure for research and education in Academia Sinica and other institutes, and has conducted grid-related training and workshops. PRAGMA will enable ASCC to collaborate with other leading institutions in building and maintaining an advanced production grid environment for various applications.

ASCC is one of the two Large Hadron Collider Computing Grid regional centers in Asia, supporting Data Challenge 2004 of ATLAS, CMS, and ALICE experiments in High Energy Physics, serving as the second Grid Operations Center of LCG starting from April 2004; and working with Forschungszentrum Karlsruhe since June 2004 to provide global Grid user support services. ASCC researchers are working at CERN in middleware development, resource management, integration of HEP analysis and Grid, distributed database discovery, and certification and testing.

In addition to the High Energy Physics, ASCC is also in charge of the information technology and infrastructure support, including deployment and service, for the National Digital Archive Program and National Research Program for Genomic Medicine.

Grid technology development at ASCC includes: PC Cluster and grid system, middleware, certification authority, and grid applications in high-energy physics, bioinformatics, digital archive, biodiversity, eLearning, and the Access Grid. ASCC would like to both share its expertise and enlarge the scope of its grid activities by participating, through PRAGMA, in the following areas: grid application development, grid middleware development and deployment, cross-grid integration and validation, grid operation and monitoring, and hosting future PRAGMA meetings.

Key contacts: Simon Lin, Eric Yen

ASIA-PACIFIC ADVANCED NETWORK www.apan.net

APAN is a non-profit international consortium, comprising 14 primary, ten affiliate, five liaison, two associate, and two industry members, that provides an international high-performance network infrastructure for research and educational



activities in the Asia-Pacific region. Currently 14 coun-

tries 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 12.4 Gbps (2.4 Gbps on the TransPAC link between Tokyo and Los Angeles [Abilene]; 10 Gpbs on the JGN2 link between Tokyo and Chicago [Starlight]).

APAN's working groups promote projects that utilize the infrastructure. The Natural Resource Area of APAN has working groups in agriculture. Earth observation and Earth systems have been pursuing grid-orientated applications under collaboration with the grid working group 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 recently 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 partners provide advanced computing facilities to the Australian research comapac munity, government, and industry. APAC is integrating these facilities into a grid over the next three years. The APAC Grid will allow Australian researchers to get seamless access to the computational and data resources in the APAC facilities as well as a new range of services to support national and international research collaboration. The APAC Grid will support research communities in the areas of astronomy, high-energy physics, bioinformatics, chemistry, geophysics, and earth sciences.

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. The APAC partners are participating in GrangeNet projects to deploy and demonstrate grid and advanced communications services.

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

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

BIOINFORMATICS INSTITUTE, SINGAPORE

www.bii.a-star.edu.sg

BII scientists and engineers are involved in application, middleware, and National Grid (Life Sciences) activities with the aim of leveraging grid computing technology to build a scalable, secure, and easy-to-use national grid resource



that will support Singapore's use and regional collaborations under the ambit of PRAGMA. The National Grid (Life Sciences) serves the newly integrated biomedical research park called the Biopolis, which houses BII, four other sister institutes, plus two blocks of commercial biotech R&D entities. The National Grid (Life Sciences) research and development work is completely incorporated with the research objective of BII.

PRAGMA provides BII with a platform for research collaborations to develop biomedical applications, middleware, and tools. BII researchers are involved in all PRAGMA workshops and will host PRAGMA 8 in Singapore in May 2005. BII collaborations with PRAGMA member institutes include the integration of AIST's Gfarm with the integrated Genome Analysis Pipeline (iGAP), collaborating with AIST and SDSC at UCSD. BII's most significant contribution is to participate in the routine use of grid compute resources to run the Encyclopedia of Life (EOL) project.

Key contacts: Larry Ang, Santosh Mishra

CENTER FOR COMPUTATIONAL SCIENCES, UNIVERSITY OF TSUKUBA

www.ccs.tsukuba.ac.jp

The Center for Computational Sciences (CCS) is a research institute for computational science and high-performance computing technology designed to open the grid to new areas and methodologies of discovery and analysis in computa-



tional 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, and University of Osaka, in Japanese grid projects and ApGrid.

Researchers at CCS 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. We are 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.

Computer Network Information Center, Chinese Academy of Sciences www.cnic.ac.cn



CNIC is a founding institutional member of PRAGMA and has been an active participant in PRAGMA activities. CNIC researchers are involved in most PRAGMA working groups, providing an 8-node cluster for the testbed and organizing science applications in such disciplines as astronomy, bi

science applications in such disciplines as astronomy, biology, and chemistry in China. CNIC is also helping develop collaborative training among PRAGMA members. There was a distance training workshop involving UCSD and CNIC in February 2004.

CNIC is a leading institute in grid computing and applications in China. It is involved in such key projects as China National Grid (CNGrid) and the Scientific Data Grid (SDG). CNIC is one of the two main nodes of CNGrid for which it provides a 4TFLOPS supercomputer Lenovo DeepComp 6800 and the leading site of SDG, which is composed of 46 institutes of CAS across the country. CNIC researchers have been developing a set of grid middleware to support data access and integration, in particular, for distributed, heterogeneous, and multi-disciplinary scientific data.

CNIC researchers have been involved in all workshops except PRAGMA4 due to the SARS crisis. CNIC hosted the successful PRAGMA6 workshop in Beijing in May 2004.

Key contacts: Baoping Yan, Kai Nan

Cray Inc.

www.cray.com

Cray Inc. is the global leader in supercomputers that are purpose-built for HPC and is also the first Industrial Affiliate member of PRAGMA and sponsor of the PRAGMA7 workshop. In addition to participation in PRAGMA meetings and workshops, Cray contributes to the organization



by providing expertise in high-performance computing and demonstrating how grid technologies can be used to provide access to scarce HPC resources.

Cray is actively involved with the Resources Working Group of PRAGMA, including access to Cray supercomputers located in the Cray-Japan office aiming at supporting 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 and a grid-based remote procedure call tool, Ninf-G. These efforts resulted in the development of a grid-based finite element structural application that executes over multiple Cray systems. The ability to utilize Cray systems for specific kernel computations as a remote library system call from a local desktop system proved to be an efficient method for executing computationally intensive simulations.

Key contacts: Mitsuhisa Sato, Taisuke Boku

Cray plans to continue efforts to place Cray systems into large-scale supercomputing grids and verify that the approach can be used effectively to handle computationally challenging scientific problems.

Key contacts: Kazunori Mikami, Christy Adkinson

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

activities are classified into the following two major categories: education and R&D. As the contributing member in the former category, Osaka University took an important role in pro-

🗘 OSAKA UNIVERSITY

moting the UCSD PRIME program in 2004. In

the program, three students from UCSD were hosted by Osaka University for about nine weeks to build skills in Grid system development.

The Grid R&D activities in Osaka University are strongly characterized in terms of international collaboration because CMC is involved 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 around international collaboration. Osaka University has participated in all PRAGMA workshops since the foundation of PRAGMA and is actively engaged in PRAGMA's Telescience and Biological Science working groups. In the Telescience working group, Osaka University has developed a Grid system that allows scientists to perform their analyses by remotely controlling the world's biggest ultra-high voltage electron microscope located in the Research Center for Ultra-High Voltage Electron Microscopy. In the Biological Sciences working group, Osaka University has knowledge on the system development for Biology, accumulated in the BioGrid Project. IPv6-based Grid technologies such as the IPv6 Globus Grid toolkit, GUIDE, a Grid portal to Gridified biological tools, and GSI-SFS, a secure file system on the Grid, have been developed and further improved through the participation of these two working groups.

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

Tokyo Institute of Technology (Titech) is one of the premier universities in Japan, specializing in advanced fields of science and technology. Its Global Scientific Information and Computing Center (GSIC) was established in April 2001.



GSIC is responsible for deploying advanced informational infrastructure for the entire institute. One of GSIC's major emphases is to host a world-class supercomputing facility, as well as conduct research and develop and deploy grid computing infrastructures for high-end scientific computing. GSIC's grid deployment project is called the "Titech Grid," seeding the entire campus (15 sites) with more than 800 processors of high-performance PC blade servers and interconnecting them with a campus Gigabit backbone to construct a large production-level testbed. With recent participation of nodes from other projects and labs, 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 was initiated in April 2002, and 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 for itself and its industrial partners, including the IBM "SUR (Shared University Research)" award, and the Nikkei IT Product award for partner NEC in 2002. In 2003 an MoU was signed between SDSC and Titech aiming for further fostering of collaborative research as well as sharing experiences of grid infrastructures. This has led to several successful collaborative projects, including those in the Encyclopedia of Life (EOL) project, highlighted at Supercomputing 2003.

Key contacts: Satoshi Matsuoka, Hidemoto Nakada, Kouji Tanaka



GRID TECHNOLOGY RESEARCH CENTER, NATIONAL INSTITUTE OF ADVANCED INDUSTRIAL SCIENCE AND TECHNOLOGY

www.gtrc.aist.go.jp

The GTRC of AIST is dedicated to the R&D of the state-of-the-art grid programming tools, international verification experiments, grid-building technologies, and ultra-high speed networks, as well as studies on requirements for a reliable grid.

Seven teams at the GTRC cover every facet of research and devel-

opment (as of 2004). 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 demonstrable manner, and to accelerate the commercialization of grid tech-



nology through industrial, academic, and government collaboration.

The GTRC, founded in 2002 with a limited term of 6.75 years, has 65 members, as of January 2004, including regular, postdoctoral, visiting, and temporary staff. At the Tsukuba Central 2 and the Ueno Office, GTRC is pursuing efforts aimed at making a quantum leap in sophistication and systematization of grid technology.

PRAGMA provides opportunities to encourage the use of AISTdeveloped grid middleware such as Ninf-G and Gfarm. In addition, PRAGMA is 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 helping developments of grid-enabled applications.

AIST researchers have been involved in all workshops. AIST hosted the third PRAGMA workshop in Fukuoka and continues to provide three clusters as a part of the PRAGMA testbed. PRAGMA projects selected the Gfarm as a challenge of PRAGMA Applications. Satoshi Sekiguchi and Yoshio Tanaka are PRAGMA Steering Committee members. Osamu Tatebe is one of the leaders of the Data Working Group.

Key contacts: Satoshi Sekiguchi, Yoshio Tanaka

Kasetsart University www.ku.ac.th

In the past year, PRAGMA collaboration has brought many benefits to KU. As part of the Resources Working Group, the High-Performance Computing グ Networking Center (HPCNC), KU has worked to establish a monitor-



ing infrastructure using the KU-developed SCMSweb monitoring tool that enables near real-time capturing of PRAGMA testbed system performance and utilization. KU has also dedicated a cluster for PRAGMA use to help testbed activities.

Under a PRAGMA exchange program, KU researcher Thadpong Pongthavonkamol worked at SDSC for two months. SCE Roll, a port of the OpenSCE cluster environment *(www.opensce.org)* to run on the Rocks system, was developed as a result. SCE roll, designed to run on the Rocks system, is being deployed to build clusters at SDSC, KU, and SUT (Thailand) and is critical to the success of the Thailand National Grid Project. PRAGMA's exchange program has also sent KU student Ittichok Jangjaimon to the Grid Research Center, AIST for two months to work on the Gfarm project.

KU has successfully deployed GAMESS to build a drug discovery infrastructure on ThaiGrid. This infrastructure is now heavily used to study thousands of chemical compounds obtained from Thai medicinal herbs. KU-developed SQMS scheduler is used to distribute GAMESS, and auto dock jobs in a grid environment. This infrastructure helps speed the work of scientists in KU.

KU is working with PRAGMA members to promote Grid use. KU has conducted workshops to promote Rocks to educate Thai researchers on grid and cluster technology. A total of 100 researchers have completed this workshop training, a critical step toward broad scale adoption of grid and cluster technology in Thailand.

Data-intensive applications are an important driving force for the grid. KU is working with the National Institute of Advanced Industrial Science and Technology in Japan on the Gfarm project to explore the viability of building wide area data-intensive application using grid technology. The target applications are GIS, remote sensing, and large data and knowledge management.

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) as well as precise stage control, able to tilt more than $\pm 60^{\circ}$ within $\pm 0.1^{\circ}$ errors. This allows for 3-D structure analysis of complex materials. The UHV-TEM can also operate remotely without losing its atomic resolution.

The remote use of the UHV-TEM is being conducted 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. Telescience participants at PRAG-MA 6 demonstrated remote control and data acquisition. The activities of the "UHV-TEM e-Science" project aim to develop methods for grid-based imaging, telemicroscopy, and automated electron tomography.

KBSI has participated in PRAGMA workshops and is actively engaged in PRAGMA's Telescience working group for expansion of the remote operation system of the UHV-TEM, collaborating with NCMIR, SDSC, Osaka University, and KISTI.

Key contacts: Inho Gim, Jung-Eok Gu

Korea Institute of Science and Technology Information

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

KISTI is the leading organization of the K*Grid project whose goals are to construct the Korean national grid infrastructure to carry out grid middleware and application research. K*Grid aims to implement a high-performance computing



infrastructure that combines geographically distributed high-performance computers, high technology instruments, scientific experts, and the next generation internet to operate as a single virtual system.

Through K*Grid, KISTI researchers are involved in research activities including implementation of computational Grid and Access Grid and the development of the Grid middleware toolkit, Grid applications, and high performance networking of interest to PRAGMA. KISTI establishes a Grid testbed by collaborating with domestic and international researchers, and runs applications in fields such as biotechnology, computational fluid dynamics, and nano technology. KISTI operates the secretariat of the Grid Forum Korea, which provides the venue for Grid researchers in Korea to communicate and collaborate, and actively participates in other grid related organizations such as GGF and APAN.

KISTI has been actively involved in PRAGMA since its inception. It has participated in all seven PRAGMA workshops, and it hosted the PRAGMA2 workshop in Seoul, Korea, where over 60 members from nine countries were present. KISTI has been involved in PRAGMA projects such as MGrid (imc.konkuk.ac.kr/~mgrid), which aims to develop a cost-efficient and reliable grid computing system for simulations of biomolecules, Telescience, which involves the transmission electron microscope (TEM) of the Korea Basic Science Institute (KBSI), and application of Ninf-G to simulations of nano-material. KISTI is currently contributing an 80-node linux cluster to be shared by PRAGMA members, and has provided a 16-node linux cluster of the KISTI testbed for PRAGMA routine-use experiments from June to August, 2004. For the cluster user community in Korea, especially for use in a grid environment, KISTI has been working with SDSC to produce a localized version of Rocks, and distributing it through rocks.cluster.or.kr. Future collaborations will include running the CFD simulation on the e-Science testbed run by Korea (KISTI), Japan (AIST), and China (CNIC). Furthermore, KISTI will collaborate with NCSA and NCHC for network performance measurement.

Key contact: Jysoo Lee

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

National Agriculture Research Center (NARC), one of the eleven research institutes under 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. Department of Information Science and Technology



of NARC is a global leader in 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 we have to handle in agriculture and natural resources. Therefore, data grid technology for such data resources has been a big target of the NARC group. Data mediation middleware that provides client applications consistent accesses to heterogeneous databases is one of the solutions promoted by NARC. MetBroker (www.agmodel.org), one middleware implement for meteorological databases, now provides such accesses to the weather data of more than 14,000 weather stations from almost 200 countries in 16 databases of the world. To address issues of high quality and spatially dense data acquisition in the field, our group 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/FieldServerEn/default.htm), is one of the products for sensor network, which has deployed more than one hundred sets in seven countries. These products of NARC are partially contributing to ClimDB/LTER and the lake metabolism project launched by PRAGMA.

Key Contacts: Seishi Ninomiya, Masayuki Hirafuji

NATIONAL CENTER FOR HIGH-PERFORM-ANCE COMPUTING, NATIONAL APPLIED RESEARCH LABORATORIES //

www.nchc.org.tw

NCHC researchers are involved in application and grid activities of interest to PRAGMA, such as the Taiwan Advanced Research and Educational

Network, Knowledge Innovation National Grid, Asthma and SARS Grids, EcoGrid, International Collaborative Lake Metabolism Project, World Wide Metacomputing, National Initiative in Hazard Mitigation and Emergency Response, National Biodiversity Program, National Science and Technology Program for Nanoscience and Nanotechnology, and various outreach efforts for grid applications.

NCHC researchers have been involved in all PRAGMA workshops, have hosted PRAGMA5, and provide a dedicated cluster to the PRAGMA testbed. PRAGMA projects involving NCHC researchers include: Telescience, EcoGrid/EcoInformatics; Pacific Rim Undergraduate Experiences (PRIME); and the PRAGMA Testbed.

PRAGMA provides a platform for sharing resources between its members; establishing a testbed for grid applications; understanding practice and policy issues of sharing resources; advancing science via collaborations; linking current projects with international collaborations; interacting with experts in applications and grid middleware and increasingly wireless extensions to the grid; and for sharing in experiences and lessons learned.

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) is a globally recognized leader in high-end computing and integrated

innovative systems and software, and it is defining and establishing the high-performance cyberinfrastructure for the future. NCSA develops and deploys cutting-edge computing, networking, and information technologies in support of research. By 2004, NCSA will deploy more than 30 teraflops of computing power, making it one of the largest facilities serving the open scientific research community. It is one of the four original partners in the NSF funded TeraGrid project, and it is also a leading-edge site for the NSF funded National Computational Science Alliance.

NCSA researchers enable exemplary scientific research in various disciplines through its national and international partnerships. As such, NCSA researchers are involved in a variety of activities of interest to PRAGMA in cluster computing, grid computing, middleware, and applications research. NCSA co-leads the National Laboratory for Applied Network Research network measurement monitoring and the NSF National Middleware Initiative, and is involved with the National Virtual Observatory, a data grid for astronomy.

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 currently 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 testbed, involving experiments to make the grid routinely usable. At the PRAGMA5 workshop, NCSA co-organized a subset of researchers associated with the Virtual Observatory activities in a virtual forum to discuss the state of the field. NCSA anticipates being an active participant in all of the other PRAGMA working groups. Finally, 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.

Key contacts: Radha Nandkumar, Danny Powell

NATIONAL ELECTRONICS AND COMPUTER TECHNOLOGY CENTER

www.hpcc.nectec.or.th/pragma

NECTEC's Computing Research and Development Division has been involved in Thailand's development of Cluster and Grid computing technology from the beginning.

Through NECTEC's Thai Social/Scientific Academic and Research Network project (ThaiSARN) we connect and support grid collaboration between Thai research communities (known as Thaigrid) with international research networks and forums. On the application side, NECTEC focuses on information grid research aiming toward agriculture and natural resources, bioinformatics, computational science, and engineering. In addition, NECTEC participates in a number of international forums, which concern grid-related activities such as ApGrid, Asia Pacific Advanced Network (APAN), Internet2, and PRAGMA.

NECTEC

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.

Key Contacts: Piyawut Srichaikul, Royol Chitradon, Sornthep Vannarat



NATIONAL GRID OFFICE

www.ngp.org.sg

The National Grid's vision is the realization of a Singapore where computer resources may be connected via a high-speed network to be shared in a secure, reliable, efficient manner by authenticated users for a variety of application domains and



sectors 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 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 BII, Institute of High Performance Computing, Nanyang Technological University, National University of Singapore, and Singapore-MIT Alliance via a high-speed gigabit network. NGO is in the process of linking up to be a part of the Large Hadron Collider Computing Grid at CERN. We have Internet2 connectivity to the U.S., Taiwan, Japan, and Korea. NGO's working groups focus on areas, such as middleware and architecture, grid security, networks, applications, and governance. Domain specific groups (virtual grid communities) have been established for life sciences, physical sciences, and digital media.

Key contacts: Lawrence Wong, Hing Yan Lee

STAR TAP/StarLight Initiative

www.startap.net/starlight

As the foremost IGbps-to-IoGbps 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.

ST * RLIGHT

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, Europe, and Asia.

StarLight is a founding member of the Global Lambda Integrated Facility (GLIF: *www.glif.is*), and 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 next major event, iGrid 2005, to be held in San Diego, September 2005.

TransPAC, Indiana University www.transpac.org

TransPAC is a high-performance network connecting scientists in the U.S. with their counterparts in the Asia-Pacific region. TransPAC provides fundamental network infrastructure to support e-science collaborations between these



researchers in a broad range of scientific disciplines. Architecturally, TransPAC connects U.S. research and education infrastructure to Asia, specifically to the Asia Pacific Advanced Network Consortium in Tokyo. Following the most recent upgrade (October 2004), TransPAC will provide an OC-48 connection from Tokyo to Los Angeles and an OC-192 connection, via the JGN2 international link, from Tokyo to Chicago, with additional direct connectivity to Europe possible via TransLight.

TransPAC was a founding member of PRAGMA and co-hosted with UCSD the PRAGMA7 meeting in San Diego. TransPAC actively supports e-Science and grid activity via its partnerships with PRAGMA, APAN, and ApGrid. TransPAC also leads and participates in measurement and security partnership activities between Asia and the U.S.

Key contacts: James Williams, Donald McMullen, John Hicks

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 2000, 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 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.

USM researchers have communicated with other PRAGMA participants about experiences in understanding practice and policy issues concerning sharing resources and the establishment of collaborations with other PRAGMA institutions. A recent example includes Kasetsart University-USM Drug Discovery Grid. PRAGMA activities involving USM researchers include cheminformatics and contributing resources to the PRAGMA testbed.

Key contacts: Ahmad Yusoff Hassan, Habibah A Wahab

Key contacts: Maxine Brown, Tom DeFanti

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 and National Partnerships for Advanced Computational Infrastructure, the NSF Middleware Initiative, OptIPuter, Geosciences Network, Network for Earthquake Engineering Simulation, National Laboratory for Applied Network Research network measurement monitoring, and the NIHfunded Biomedical Informatics Research Network, National Biomedical Computation Resource, and National Center for Microscopy and Imaging Research.







NCMIR

CRBS

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 current projects with international collaborations
- interact with experts in applications and grid middleware and increasingly wireless extensions to the grid, to 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, NCHC, and

NCMIR; Computational Chemistry, with Monash

University, USM, KU; Workflows and the Encyclopedia of Life with BII, Titech, and AIST; EcoGrid and Lake Metabolism with NCHC and the PRAGMA Testbed. Furthermore, UCSD helped launch the Pacific Rim Undergraduate Experiences (PRIME) with Osaka University, NCHC, and Monash University. In addition, 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 San Diego Supercomputer Center, the California Institute for Telecommunications and Information Technology, 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, Tony Fountain, Wilfred Li, Mason Katz, Tomas Molina, Steven Peltier, Ronn Ritke, Cindy Zheng

University of Hyderabad www.uohyd.ernet.in

UoH researchers are involved in grid-related activities, such as biosciences, nanotechnology, drug design and discovery, I-GRID initiative, and Centre for Modelling, Simulation and Design, supported by the University Grants Commission (UGC) and the High Performance Computing



Centre in conjunction with the Department of Science and Technology (DST) and Centre for Development of Advanced Computing (C-DAC).

UoH is a founding member of PRAGMA. PRAGMA serves as a mechanism through which information and resources can easily be exchanged. PRAGMA resource-sharing agreements will allow scientists and researchers to concentrate on solutions without having to perform ad hoc resource collection, installation, and testing. PRAGMA is playing a catalytic role of promoting such collaborations. UoH is dedicating an 8 node cluster to this initiative and is contributing to PRAGMA's resource and middleware initiatives and weather modeling demonstration.

UoH efforts will now be centered around creating active collaborations and exchanging researchers/students between the PRAGMA members. UoH will host the PRAGMA9 workshop *(in Fall, 2005)*.

Key contact: Arun Agarwal



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.

Schedule of Workshops

Future Meetings

PRAGMA 8: 2-4 May 2005, Singapore

Hosted by the Bioinformatics Institute in Singapore and the National Grid Office. Chair: Larry Ang (BII); Co-chair: Arun Agarwal (University of Hyderabad)

PRAGMA 9: FALL 2005

Hosted by the University of Hyderabad, Chair: Arun Agarwal (University of Hyderabad)

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. Chairs: Mason Katz (UCSD) and Jim Williams (TransPAC), Co-chair: Larry Ang (BII).



Design: NCHC



Design: CNIC



Photo: John Wooley; Design: J. Matthews

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.

References

Ninf-G

*Takemiya H, Shudo K, Tanaka Y, Sekiguchi S. Constructing Grid Applications Using Standard Grid Middleware, *J Grid Comput*, 1(2), 117-131.

Tanaka Y, Takemiya H, Nakada H, and 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*, Nov. 2004. In press.

Gfarm

*Tatebe O, Ogawa H, Kodama Y, Kudoh T, Sekiguchi S, Matsuoka S, Aida K, Boku T, Sato M, Morita Y, Kitatsuji Y, Williams J, Hicks J. The Second Trans-Pacific Grid Datafarm Testbed and Experiments for SC2003, *Proceedings of 2004 International Symposium on Applications and the Internet-Workshops* (SAINT 2004), 26-30 January 2004, Tokyo, Japan.

More information at datafarm.apgrid.org/paper.en.html

OmniRPC

Sato M, Boku T, Takahashi D. OmniRPC: A Grid RPC System for Parallel Programming in Cluster and Grid Environment, *Proceedings of CCGrid2003*, May 2003.

NIMROD, GAMESS, AND OTHER GRID TECHNOLOGIES IN COMPUTATIONAL CHEMISTRY

*Sudholt W, Baldridge KK, Abramson D, Enticott C, Garic S. Parameter Scan of an Effective Group Difference Pseudopotential Using Grid Computing. *New Generation Computing (Special Feature Grid Systems for Life Sciences)*, 22(2).

*Sudholt W, Baldridge K, Abramson D, Enticott C, Garic S. Applying Grid Computing to the Parameter Sweep of a Group Difference Potential, *The International Conference on Computational Sciences, ICCS04*, June 6-9, 2004, Krakow, Poland.

Baldridge KK, Greenberg JP, Sudholt W, Bhatia K, Mock S, Altintas I, Amoreira C, Potier Y. The Computational Chemistry Prototyping Environment. *Special Issue of IEEE on Grid Computing*, 2004. In press.

Integrated Genome Annotation Pipeline, including GridSpeed and Encyclopedia of Life

*Li WW, Byrnes RW, Hayes J, Birnbaum A, Reyes VM, Shahab A, Mosley C, Pekurovsky D, Quinn GB, Shindyalov IN, Casanova H, Ang L, Berman F, Arzberger P, Miller MA, Bourne PE (2004) The Encyclopedia of Life Project: Grid Software and Deployment. *New Generation Computing (Special Feature Grid Systems for Life Sciences)*, 22(2)

More information at www.ohmsha.co.jp/ngc/ngc2202.htm

*Shahab A, Chuon T, Suzumua WW, Li R, Byrnes W, 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. *First International Workshop on Life Science Grid (LSGRID2004)*

Telescience

*Akiyama T; Shimojo S, Nishio S, Kitatsuji S, Peltier S, Hutton T, Lin F-P (2003) Telecontrol of ultra-high voltage electron microscopy over global IPv6 network. *SAINT2003 IPv6 Workshop*. 184-187. (Acknowledges PRAGMA)

*Lee D, Lin AW, Hutton T, Akiyama T, Shinji S, Lin FP, Peltier S, Ellisman MH (2003) Global Telescience Featuring IPv6 at iGrid2002. *Future Generation of Computer Systems*, 19(6): 103139. (PRAGMA)

Peltier S, Lin AW, Lee D, Mock S, Lamont S, Molina T, Wong M, Martone ME, Ellisman MH (2003) The Telescience Portal for Advanced Tomography Applications. *Journal of Parallel and Distributed Applications, Special Edition on Computational Grids* 63(5): 539-550.

LAKES METABOLISM PROJECT

*New Wireless Sensor Network for Studying Lake Metabolism. The Network News, Vol 17 No.1 Spring 2004. See *intranet.lternet.edu/archives/documents/Newsletters/NetworkNews/sprin* g04/spring04_pg13.htm. (also see *lakemetabolism.org*)

OVERVIEW OF PRAGMA

*Arzberger PW, Farazdel A, Konagaya A, Ang L, Shimojo S, Stevens RL, Life Sciences and Cyberinfrastructure: Dual and Interacting: Revolutions That will Drive Future Science. *New Generation Computing (Special Feature Grid Systems for Life Sciences)*, 22(2) February 2004

*Arzberger, P; Papadopoulos P. PRAGMA: A Community-Based Approach to Using the Grid. *AG Focus*, 2(2) June 2004. *www.accessgrid.org/community/agfocusjune04.pdf*

Student and Postdoctoral Opportunities

The PRAGMA framework, with its rich set of projects and its network of researchers throughout the Pacific Rim, provides an ideal environment for students (see PRIME) and postdoctoral researchers to engage actively in the development and deployment of cyberinfrastructure, or in 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. The PRAGMA website (*www.pragma-grid.net*) lists funding opportunities for students as well as key contacts at the various PRAGMA sites.

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 broaden the dialog between PRAGMA members and the broader community. In the last year, PRAGMA members have helped organize workshops at APAN (January 2004), Life Sciences Grid (May/June 2004), HPC Asia 2004 (July 2004), Clusters 2004 - IEEE International Conference on Cluster Computing (September 2004), and APEC Tel (September 2004). Furthermore, many PRAGMA members actively participate in Supercomputing 2003 and 2004, demonstrating what PRAGMA members collectively have been able to accomplish.

In the coming year PRAGMA members will continue to be involved in the community, with such activities as LSG2005 in May 2005 in Singapore and the iGRID 2005 scheduled for September 2005 in San Diego CA (contact: Maxine Brown).

PRAGMA Sponsors

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APAC is supported by the Systemic Infrastructure Initiative as part of the Australian Government's Backing Australian Ability; funding for the Nimrod project is provided by the Distributed Systems Technology Research Centre (DSTC), GrangeNet, and the Australian Research Council (ARC); the Bioinformatics Institute (BII) receives its funding mainly from A*Star (Agency for Science and Technology Research), Singapore; CMC/Osaka University sponsors include the "Asia Grid Initiative," Special Coordination Funds for Promoting Science and Technology (MEXT, Japan), the IT program of the Ministry of Education, Culture, Science and Technology of Japan (MEXT, Japan), a Grant-in-Aid for Scientific Research on the Priority Area, "Informatics Studies for the Foundation of IT Evolution (13224059)" (MEXT, Japan) and JGN2 (NiCT, Japan); the major funding of Scientific Data Grid (SDG) is supported by the Chinese Academy of Sciences, while CNIC also receives funding from the Ministry of Science and Technology of China through China National Grid (CNGrid); GTRC/AIST sponsors include the "Asia Grid Initiative," Special Coordination Funds for Promoting Science and Technology (MEXT, Japan); Korean Grid Infrastructure Implementation and Middleware Development Project (K*Grid) is supported by the Ministry of Information and Communication (MIC); NARC receives major funding from the Ministry of Agriculture, Forestry and Fishery, Japan and Japan Science and Technology Agency; NCHC receives major funding support from the National Science Council, Taiwan, through the Knowledge Innovation National Grid (KING) project; NCSA is one of the high end computing centers funded by the National Science Foundation; NECTEC receives its funding through the National Science and Technology Development Agency (NSTDA); StarLight receives major funding support from the National Science Foundation (NSF ANI-9980480 and ANI-0229642); TransPAC receives major funding from the U.S. National Science Foundation and the Communications Research Laboratory in Japan. Grid Activities in USM are funded mainly through E-science and Marine Genomics and Natural Product Discovery National Top Down Projects and USM Central Funding. NGO receives funding from Agency for Science and Technology Research (A*STAR), Defense Science and Technology Agency (DSTA), Economic Development Board (EDB), Infocomm Development Authority (IDA), Nanyang Technological University (NTU), National University of Singapore (NUS), and Singapore-MIT Alliance (SMA). KBSI receives major funding from the Ministry of Science and Technology (MOST), the Ministry of Information and Communication (MIC), and the Ministry of Planning and Budget (MPB) in Korea.

Several projects at UCSD contribute to and enhance PRAGMA activities: NLANR/MNA, a participant in PRAGMA and funded by NSF award ANI-0129677, is supportive of efforts to bridge the Pacific and encourage collaboration. PRIME is supported by NSF OISE 0407508 with additional support from the Division of Shared Cyberinfrastructure and the California Institute for Telecommunications and Information Technology (Cal-(IT)²); PI G.Wienhausen, co-PIs L. Feldman and P. Arzberger. Support for the PRAGMA 7 Workshop came from NSF INT-0314015, SDSC, Cal-(IT)², Cray Inc, and TransPAC/Indiana University.



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