



PRAGMA

PACIFIC RIM APPLICATIONS AND GRID MIDDLEWARE ASSEMBLY
COLLABORATION OVERVIEW 2007-2008

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PRAGMA



INSTITUTIONS AND CONTACTS

PRAGMA is an institution-based organization governed by a Steering Committee that invites new members, determines locations of workshops, and sets overall direction. This year, four new members joined PRAGMA: Korea's Konkuk University, Australia's Monash University, CSE-Online, and BeSTGRID New Zealand. We also note that the Australia Partnership for Advanced Computing (APAC) is a founding member and active participant. APAC ceased operations at the end of October 2007. More information about the Steering Committee members (*) may be found at www.pragma-grid.net/about/committee.

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Image: Roof painting, north gate at Gyeongbok Palace, Seoul, Korea

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More Information about each of the PRAGMA Institutional Members can be found at www.pragma-grid.net/about/institutions.



Image: PRAGMA 12 Group Photo (Source: NECTEC)

OVERVIEW 2007-2008

This fifth annual Collaborative Overview chronicles the accomplishments of the Pacific Rim Applications and Grid Middleware Assembly (PRAGMA) and its member institutions for 2007.

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

Our approach has been to create teams of application and middleware researchers focused on a specific research challenge that requires integration of application and grid technologies. As the projects progress, they migrate to our routine-use grid and are evaluated to uncover how the applications and middleware work on the PRAGMA grid. These experiments lead to scientific insight and improved middleware. Successful solutions are integrated into country-specific software stacks (e.g., NSF Middleware Initiative), Open Grid Forum (OGF) stan-

dards, or other wide-dissemination vehicles, so others may benefit. Our workshops are a metronome for our progress and provide a venue to involve new collaborators in our activities. Additional outreach efforts bring our lessons learned to others, and ultimately, help build the community.

This year's highlights include: 1) expanding our routine-use grid activities to more institutions and more applications; 2) demonstrating interoperation between the PRAGMA Grid and the Open Science Grid; 3) generating accomplishments via our application working groups; 4) launching a new GEO working group, whose long-term goal is the development of a grid testbed to support geosciences and practical applications based on huge datasets of satellite imagery and GIS data, such as disaster prevention or environment monitoring; 5) engaging the next generation of scientists via educational programs such as PRIME and PRIUS; and 6) broadening our community building activities, specifically, hosting the first PRAGMA Institute at NCSA. PRAGMA Institutes are intended as intensive education and training workshops to increase the use of grid technologies around the Pacific Rim.

PRAGMA has been a very successful platform for launching new collaborations and projects. First, the Pacific Rim Experiences for Undergraduates (PRIME) program at UCSD and the Pacific Rim International UniverSities (PRIUS) program at Osaka University (inspired by PRIME), were started several years ago to create research apprenticeships, provide students with immersive cultural experiences, and develop stronger linkages among PRAGMA researchers across institutions. PRIME recently received a three-year renewal from the US National Science Foundation (NSF) to continue the program and enhance its cultural awareness materials. The success of PRIUS partly contributed to Osaka University's participating in the Global COE (Centers of Excellence) program, funded by the Ministry of Education, Culture, Sports, Science and Technology, Japan (MEXT). The Global COE program aims to establish education and research centers that perform at the apex of global excellence, in order to elevate the international competitiveness of the Japanese universities, (see www.jsps.go.jp/english/e-globalcoe/index.html).

Second, the early work of the Telescience Working Group led to a collaboration between NCHC's Ecogrid Project and University of Wisconsin researchers on lake metabolism. Subsequent funding from the Gordon and Betty Moore Foundation (GBMF) helped create the Global Lake Ecological Observatory Network (GLEON) and led to a Research Coordination Network award by the US NSF to support GLEON activities.

Third, early work by the Biosciences Working Group, which focused on integrating data grid tools (Gfarm), a community scheduler (CSF4), and other tools developed by PRAGMA members, led to efforts to create an integrated infrastructure to screen for potential binding compounds to known binding sites of infectious diseases. This work led to funding from the Telemedicine and Advanced Technology Research Center (TATRC), part of the U.S. Army Medical Research and Materiel Command, to continue integration of these tools into an Avian Flu Grid.

These accomplishments illustrate how the grid enables opportunities for researchers to work collectively across distances. PRAGMA's grass-roots effort is a model for a collaborative framework and platform, which we believe will be more prevalent in the future.

PRAGMA is proceeding with several new directions. We continue to develop ties with metagenomics researchers throughout the world, and have distributed CAMERA project data to the new PRAGMA Gfarm test-bed. We continue to deploy and experiment with collaborative tiled-display wall technology to enhance our ability to interact and collaborate. Several PRIME students have worked on this and an award has been made to Florida International University for Global Cyberbridges to incorporate this technology for team teaching and interactions.

This year we also established a rotation of the Steering Committee. Founding members who rotated off of the Steering Committee include Maxine Brown, UIC; John O'Callaghan, APAC; and Guna Rajagopal from BII. We thank them for their service to PRAGMA and for helping us succeed during our first five years. New members of the Steering Committee include Radha Nandkumar of NCSA and Putchong Uthayopas of TNGC. Members of the Steering Committee are listed at www.pragma-grid.net/about/committee.

In addition, we wish to officially congratulate Fang-Pang Lin, the recipient of Taiwan's Executive Yuan for the "2006 Award for Outstanding Contributions in Science and Technology." He has always asked the question: "How can our technology help address key questions being asked by society, from SARS to improvement in the environment?"

We note that Fang-Pang served as Deputy Chair of the PRAGMA Steering Committee from 2005-2007. His successor is Piyawut "Joe" Srirachaikul of NECTEC, who helped organize an early workshop on GEOGrid.

What are the key measures of our ultimate success? There are three. First is the science that is enabled—on a routine basis. The second measure comes from the new communities that have embraced the tools and approach of collaborative science via cyberinfrastructure. Third is the professional growth and development of both the individuals in PRAGMA and its collaborative network. Such successes validate the global investment in tools and PRAGMA's model, which harnesses the ingenuity and leverages the resources of more than 100 individuals from 33 institutions to build sustainable collaborations and advance grid technologies through applications.

PRAGMA'S GRASS-ROOTS EFFORT *A Model for a Collaborative Framework and Platform*

PRAGMA has been a very successful platform for launching new collaborations and projects, especially ones which have in turn generated additional activities and results. (Details are in full text to the left.)



1. Programs developed to engage and train students: PRIME at UCSD and PRIUS at Osaka University.

⌘ The creation of PRIUS was inspired by PRIME.

⌘ The success of PRIUS partly contributed to Osaka University's participating in Japan's Global Centers of Excellence program (MEXT), which will establish education and research centers, to elevate the international competitiveness of the Japanese universities.

2. Early work of the Telescience Working Group led to

⌘ A collaboration between NCHC's Ecogrid Project and University of Wisconsin researchers on lake metabolism.

⌘ Subsequent funding (GBMF) to create the Global Lake Ecological Observatory Network (GLEON).

⌘ Additional funding (NSF) for a Research Coordination Network to support GLEON activities.

3. Early work by the Biosciences Working Group focused on integrating data grid tools (Gfarm), a community scheduler (CSF4), and other tools developed by PRAGMA members, and led to

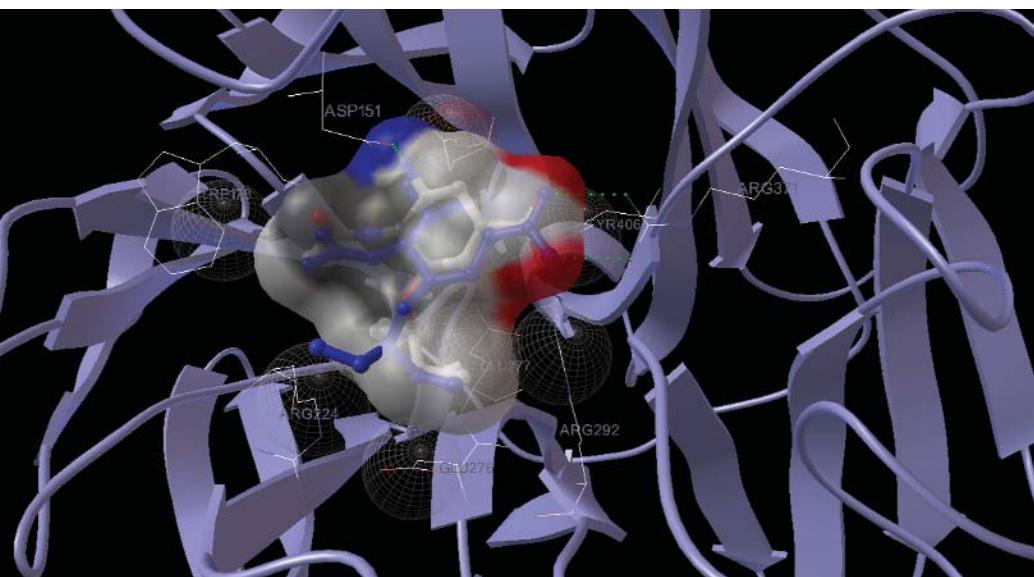
⌘ Efforts to create an integrated infrastructure to screen for potential binding compounds of infectious diseases;

⌘ Funding (TATRC) to continue integration of these tools into an Avian Flu Grid.

Image above: PRIME 2007 Students, Osaka Castle, Osaka, Japan (Source: Young Chun)

ACCOMPLISHMENTS

PRAGMA participants have successfully demonstrated the value of international collaborations in conducting applications on the grid. The following vignettes—science successes from PRAGMA's fifth year—illustrate the grid concept that brings remotely distributed resources such as sensor, tiled-display walls, 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 Publications.



AVIAN FLU GRID

The world's population will experience more encounters with infectious diseases as the globe warms. One of these is the avian flu H5N1, already an emerging threat to many countries around the world. Hemagglutinin (HA) and neuraminidase (NA), two viral surface proteins involved in the entry into and release from human cells, are important therapeutic targets for H5N1 vaccines and inhibitor development.

The PRAGMA Biosciences working group has begun efforts to create an infrastructure to do rapid screening of potential drugs to bind sites of proteins. With a grant from the

Telemedicine and Advanced Technology Research Center (TATRC), researchers from the National Biomedical Computation Resource (NBCR), and the University of Hawaii, USA; Jilin University (JLU) and the Chinese Network Information Center (CNIC), China; Konkuk University and the Korea Institute for Science and Technology Information (KISTI), Korea; Advanced Industrial Science and Technology (AIST), Japan; Universiti Sains Malaysia, Malaysia (USM); Academia Sinica, Taiwan; and Computational Science and Engineering Online (CSE-Online) have begun work to build a computational grid for Avian flu research using research and technology

from our member institutes and PRAGMA grid resources. The Avian Flu Grid (avian-flugrid.pragma-grid.net) aims to provide a drug discovery platform and a data sharing environment for research on avian flu, with potential application to other infectious diseases. The specific tools include technology such as CSE-Online, CSF4, Gfarm, MGrid, and research tools such as AutoDock and NAMD. A PRIME student who was hosted by CNIC participated in the modeling of HA mutations and host selectivity studies this past summer.

Initial organization: JLU will support the scheduling of multiple clusters (CSF4) to distribute jobs transparently at multiple sites around the region. AIST will support the deployment of Gfarm in conjunction with researchers at the University of Tsukuba; KISTI, in conjunction with researchers at Konkuk, will create an integrated portal environment for the computational pipeline using results of Korea's National e-Science Project by the Korean Ministry of Science and Technology (MOST). CNIC will develop a transparent web service layer for data access. CNIC will also become the central repository for the project's research data. Researchers associated with the National Biomedical Computation Resource (NBCR) at UCSD and the Academia Sinica in Taiwan will help implement the relaxed complex method for identifying various configurations of the proteins to use in the screening. USM will conduct virtual screenings of the Natural Compound Library and validate top candidates. CSE-Online will enable broad participation in the virtual screening efforts by providing transparent access to PRAGMA grid computing resources.

More information about aspects of this activity can be found in Amaro *et al.* 2007, and Choi *et al.* 2007

Image Above: The orientation of oseltamivir in the binding pocket of neuraminidase is shown for the crystal structure (opaque) and the docked structure (transparent). Receptor-ligand interactions were predicted by AutoDockTools include the following amino acids: R118, E119, R224, E276, R292, N294, R371, Y406. The ribbon structure of the receptor is shown and important residues are labeled. (Cheng *et al.*, unpublished results). L Cheng was a 2006 PRIME student at CNIC.



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STREAMING DATA MANAGEMENT AT KENTING'S UNDERWATER ECOLOGICAL OBSERVATORY

The fate of coral reefs, the spread of invasive species or infectious diseases, the role of lakes in global biogeochemical cycles, and changes in climate and land-use are some of the many environmental challenges that large-scale sensor-based observing systems hope to address. Environmental observing science is undergoing dramatic changes through revolutions in information technologies including sensor networks and cyberinfrastructure. Wireless sensor networks capable of measuring environmental variables in an *in situ* fashion, and operating at unprecedented temporal and spatial granularities, are being deployed to obtain highly detailed insight into complex physical worlds.

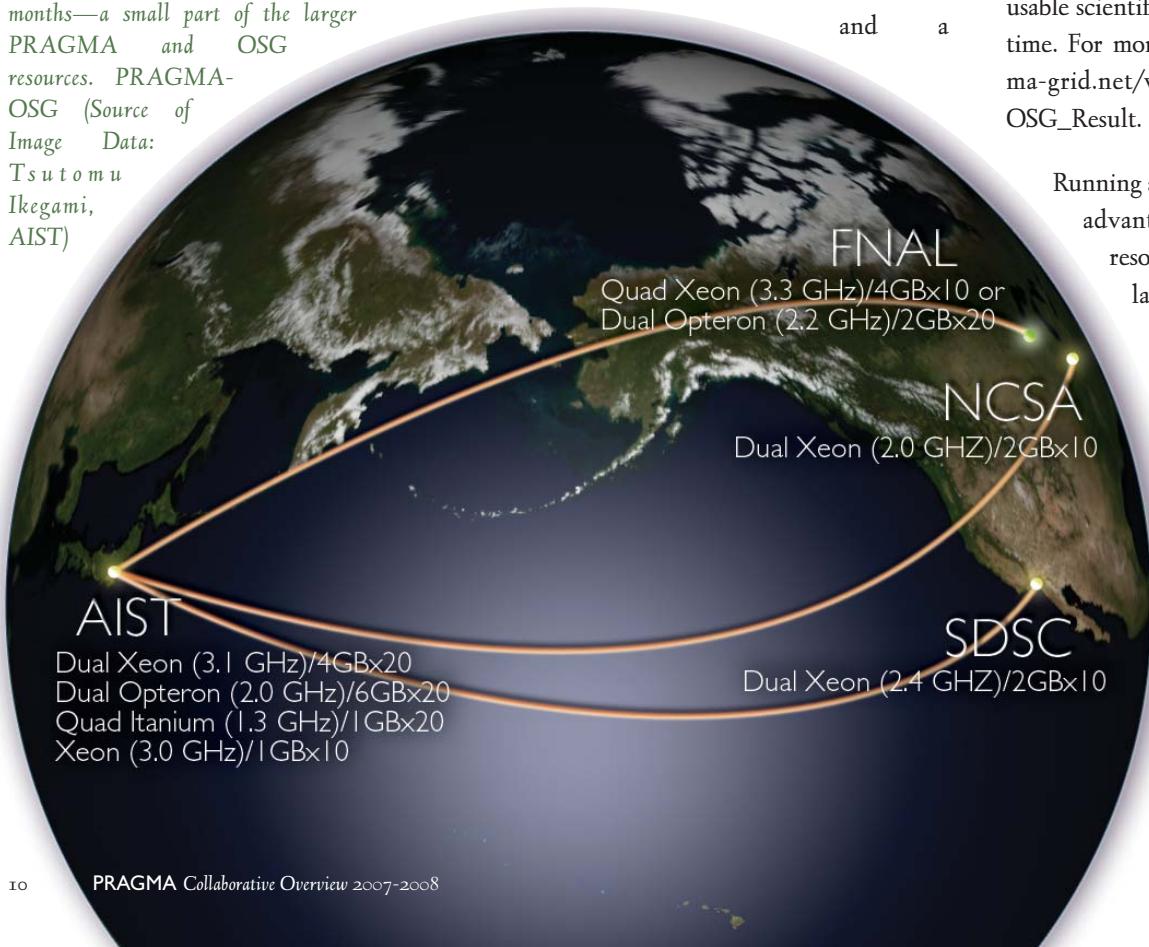
The EcoGrid project in Taiwan has been working to deploy sensors to lakes and coral reefs. As part of the PRAGMA telescience activity, researchers at the National Center for High-performance Computing (NCHC) and UCSD deployed an open-source streaming-data middleware, DataTurbine, to help monitor the coral reef at Kenting, Taiwan. Kenting's national park is located on the southernmost tip of Taiwan. The area has a tropical climate with diversified terrain, plentiful wildlife and a dazzling coral reef, which is the subject of active research. A system of underwater cameras facilitates marine researchers in monitoring the coral reef and the life around it. This effort focused on building a system to integrate sensors (more specifically, underwater video cameras) with computing and storage Grids to create a complete fabric for conducting e-Science. The system is currently used for observation by marine research scientists at the Biodiversity Research Center of Academia Sinica in Taiwan.

The management of real-time streaming data in large-scale collaborative applications presents major processing, communication and administrative

Image: Coral reefs are great interest for the biodiversity around their locations and their ability to shelter shorelines near them from erosive forces of storms. Coral are also under stress from environmental changes. This coral, Favites flexuosa, which is widely distributed across the Indian and Pacific Ocean, is captured spawning, in Kenting National Park (KNP, www.ktnp.gov.tw/eng/home/index.asp) of Taiwan. While photographed by human, it is typical of the type of observation that we will be studying by the EcoGrid and DataTurbine combine technology. The KNP Bio-database is contains information about other coral (bio.ktnp.gov.tw). (Image from Dr. Tung-Yung Fan's group National Museum for Marine Biology and Aquaria)

challenges. The current DataTurbine streaming-data middleware system satisfies a core set of critical infrastructure requirements including reliable data transport, the promotion of sensors and sensor streams to first-class objects, a framework for the integration of heterogeneous instruments, and a comprehensive suite of services for data management, routing, synchronization, monitoring, and visualization. New features for DataTurbine (www.dataturbine.org) will be further developed via a grant from NSF. Its usability will be extended by collaboratively working with the Global Lake Ecological Observatory Network (GLEON), on deployments at Lake Erken in Sweden and Lake Sunapee in New Hampshire, for example, as well as the Coral Reef Ecological Observatory Network (CREON), via a new award from the Gordon and Betty Moore Foundation, as an early step toward creating a truly integrated global network of sensors to understand critical environmental processes.

Image: Interoperation between PRAGMA (yellow dots) and OSG (green dot). The PRAGMA-OSG Virtual Organization boasts ~240 CPUs x three months—a small part of the larger PRAGMA and OSG resources. PRAGMA-OSG (Source of Image Data: Tsutomu Ikegami, AIST)



More information about this activity can be found in Strandell *et al.* 2007 and Tilak *et al.* 2007 a b.

PARTICIPATING RESEARCHERS: E. Strandell, H.-M. Chou, Y-T Wang and F-P Lin, NCHC; S. Tilak and T. Fountain, UCSD

PRAGMA-OSG GRID INTEROPERATION EXPERIMENT

Many scientists work across different grid projects. Their applications should not be restricted by grid boundaries. This requires grids to interoperate and provide ease of access for applications running across grids. To address this goal, PRAGMA Grid collaborated with Open Science Grid (OSG) and successfully completed a peer-grid interoperation experiment this year.

The experiment was driven by a real science application. Yoshio Tanaka and Tsutomu Ikegami at the National Institute of Advanced Industrial Science and Technology, Japan, developed a grid middleware—Ninf-G and a

Ninf-G-based quantum chemistry application: GridFMO. GridFMO is a Grid implementation of the Fragment Molecular Orbital (FMO) method which enables a first-principle calculation of macromolecules, such as proteins; energy of the molecules can be obtained accurately, including polarization effect, and their chemical reactions can be described with few assumptions. The FMO method is now used to study a reaction mechanism of enzymes, for use in drug design, or to study the electronic structure of the photosynthetic systems. The long-term calculations are supported by Ninf-G's fault tolerance and resource management facility.

For the large-scale calculations, PRAGMA and OSG resources were united as a VO (virtual organization). A series of GridFMO calculations ran on this combination of PRAGMA and OSG resources. A total of seven calculations were conducted from 2007/02/28 through 2007/05/18, utilizing a maximum of 240 CPUs. The fault-tolerance of GridFMO supported the stability of the calculations, each of which took 10 days on average. This produced meaningful and usable scientific results in a relatively short time. For more information, see goc.pragma-grid.net/wiki/index.php/PRAGMA-OSG_Result.

Running applications across grids takes advantage of multiple available resources and thus makes very large scale calculations like these possible. However, grid environments differ, and the differences can be learning opportunities for all involved. Working with our peers provided opportunities to exchange good ideas and tools between grids. For example, we have since setup a Condor-G server in the PRAGMA Grid and are working

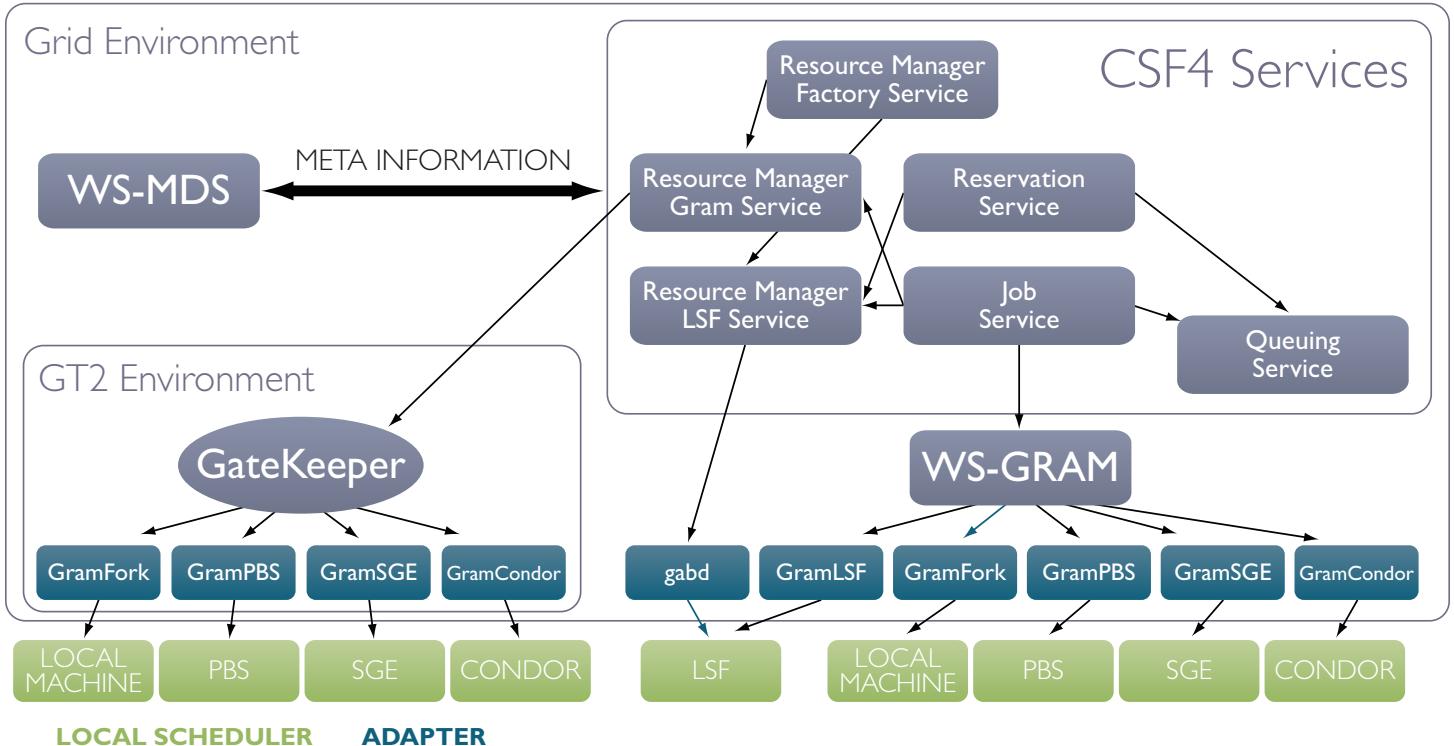


Image: Community Scheduler Framework (CSF4) provides grid meta-scheduling capability, either via globus tool kit or directly with individual schedulers. The CSF4 development team has been working with other science and development teams to integrate several other services. (Image provided by CSF4 development team at JLU)

with OSG to integrate Virtual Data Toolkit (VDT) with our software.

On the other hand, differences can also be a source of difficulty and confusion for both applications and users. Two key challenges include security policies and job submission procedures. Through the grid interoperation experiments, we were able to learn what the differences are and obtained a much better understanding of the issues involved. We have worked together to try to provide some interfaces and workarounds to enable interoperability in the short term. Long-term and strategic solutions to grid interoperability require much more collaborative work and a much better understanding of these and other issues. Grid interoperation experiments like these are essential in paving the way to long-term solutions, by revealing issues and developing solutions.

PARTICIPATING RESEARCHERS: Y. Tanaka and T. Ikegami, AIST; N. Sharma, Fermilab; C. Zheng, SDSC at UCSD

PRAGMA DEPLOYED AND SETUP A COMMUNITY SCHEDULER FRAMEWORK (CSF) SERVICE AND PORTAL

In the PRAGMA grid, heterogeneous resources are distributed in multiple virtual organizations (VOs) around the globe; each VO has different local policies. Hence, scheduling and resource management are among the key obstacles for making a global grid easier to use. The Community Scheduler Framework (CSF) is an open-source implementation of a number of Grid services, which together perform the functions of a grid meta-scheduler or community scheduler. It provides a virtualized resource access interface to end users and enforces global policies for both resource providers and consumers. The CSF is playing more and more important roles in computational grids.

Over the past two years, the CSF develop-

ment team at JLU, China, has been working with many other science teams within PRAGMA, developing and testing CSF, as well as integrating with Gfarm and SCMSWeb. Gfarm is a grid file system developed by AIST, Japan and SCMSWeb is a grid monitoring system developed by ThaiGrid, Thailand. All three organizations—JLU, AIST and ThaiGrid—are PRAGMA member institutions.

This year, the JLU and UCSD teams worked together to setup a production CSF service and portal in the PRAGMA grid. This service is able to utilize the resource information from SCMSWeb, support GT2 and GT4, and various local schedulers, PBS, SGE, LSF and Condor, as well as provide job submission and reservation services.

For more CSF4 information, see Ding *et al.*

PARTICIPATING RESEARCHERS: X. Wei, Z. Ding, and Y. Luo, JLU; W.W. Li NCSR at UCSD; C. Zheng and L. Clementi, UCSD

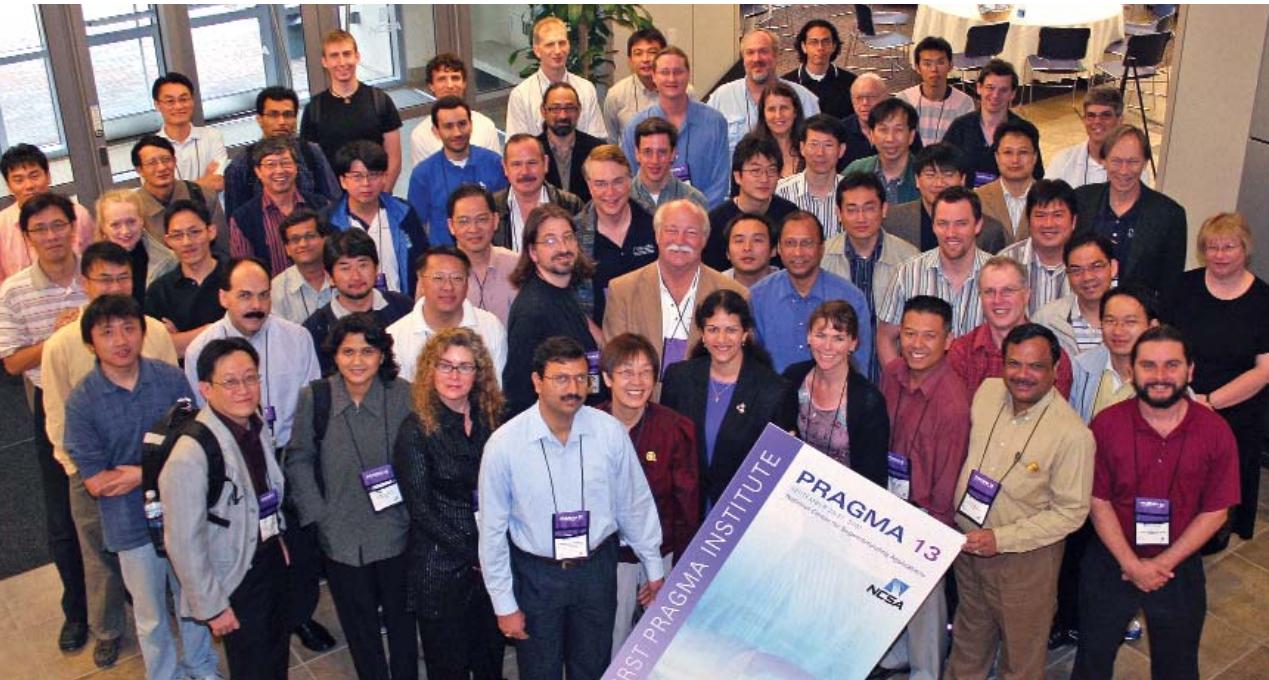


Image: 1st PRAGMA Institute, NCSA (Source T. Simas and NCSA)

PRAGMA INSTITUTES AS A MEANS TO BUILD A COMMUNITY

A cornerstone of PRAGMA's success has been its focus on people, in particular in building sustained collaborations among its members. As an additional dimension to this focus, PRAGMA has launched a PRAGMA Institute program aimed at developing a broader awareness and user-base for grid technologies thereby creating a broader set of potential collaborators and increasing feedback on existing tools.

Our first PRAGMA Institute was hosted by the National Center for Supercomputing Applications (NCSA) and sponsored by the Institute for Advanced Computing Applications and Technologies at the University of Illinois at Urbana-Champaign (UIUC) in September 2007 (www.ncsa.uiuc.edu/Conferences/PRAGMA13/i-agenda.html), following the PRAGMA 13 Workshop hosted by NCSA. The participants heard keynote talks on new areas of science (metagenomics) being

enabled by optical network technology, new collaborations (geosciences network), impact of future of theory and modeling in biology, including the use of petascale technology, global climate change, and grass roots approach to development of middleware in science (Condor). In addition, the participants received tutorials on a variety of tools created by PRAGMA members, including Nimrod—a parameter sweep middleware developed at Monash University; CSF4—a community grid scheduler developed at JLU; Opal—a web service wrapper; GridChem of NCSA and its partners; Floodgrid—a national grid project of Taiwan using a system of live cameras linked with simulations; MPICH-GX—a grid enabled MPI developed by KISTI, MaeViz of NCSA/UIUC; SP2LEARN of NCSA and D2K of NCSA.

In attendance were more than 80 participants, approximately 40 from more than 14 international institutions, and the rest from seven US institutions.

The 2nd PRAGMA Institute will be held

in concert with the Southeast Asia International Joint Research and Training (SAIJRT) Program, hosted by NCHC 3-7 December 2007 and supported in part by the National Science Council of Taiwan. This SAIJRT Program includes researchers from Vietnam, Malaysia, and the Philippines.

In the long-run, PRAGMA Workshops, the PRAGMA Institutes and other forms of training will be invaluable to strengthening the community of collaborators around the Pacific Rim. These individuals will be part of our legacy.

GRASSROOTS APPROACH TO BUILDING A GEOSCIENCES NETWORK IN INDIA

India is rich in data related to the geology and geosciences of its region. The data are gathered by several different sources, which independently handle and distribute their data to government research laboratories and universities. However, if combined together, these data could serve important applications, such as providing greater insights for disaster mitigation, in the case of earthquakes, or early warning systems, in the case of tsunamis.

In October 2005, during a workshop following the PRAGMA 9 Workshop hosted by the University of Hyderabad (UoH), researchers from around India interacted

Image Left: In the Argra (Red) Fort, Agra, India

with leaders of the GEoscience Network (GEON) from the United States, to see what technologies had been developed, which scientific problems had begun to be addressed with this new technology, and whether and how UoH should set up a GEON node. The GEON node, a collection of hardware and software, would allow for international collaboration between researchers in India and the United States. This was an early international GEON (iGEON) activity. Other iGEON activities are underway at AIST (Japan), CNIC (Beijing), and with the Russian Academy of Sciences in Moscow (Russia).

Subsequent to this workshop, Arun Agarwal, Professor-in-Charge of the Center for Modeling Simulation and Design (CMSD) at UoH, launched an initiative, inspired by PRAGMA's grassroots approach, to bring together the different sectors of the Indian geosciences community, with the goal of building a set of GEON PoP nodes in India. Through a grant from the Indo-US Science and Technology Forum to UoH and the San Diego Supercomputer Center (SDSC) at UCSD, he organized a week-long workshop in August 2007, which brought together both computer scientists and geoscientists. This workshop and his efforts are already beginning to bear fruit with the establishment of several stable iGEON point of presence nodes in India (Hyderabad, Pune, and Rajamundhry) that will provide data, information, and knowledge dissemination to the Indian, as well as the international, geosciences communities. The PIs for this Indo-US grant are Profs. K V Subbarao and Arun Agarwal (UoH, India), and Dr. Chaitan Baru (SDSC at UCSD, USA).

This activity is part of a larger effort embodied in the PRAGMA GEO Working Group, as well as the iGEON effort in the GEON project, exploring the technology, as well as the policy, of sharing data. We are hopeful that this grassroots approach will inspire even greater participation in the future.



PRIME AND PRIUS

PREPARING STUDENTS FOR THE GLOBAL WORKFORCE

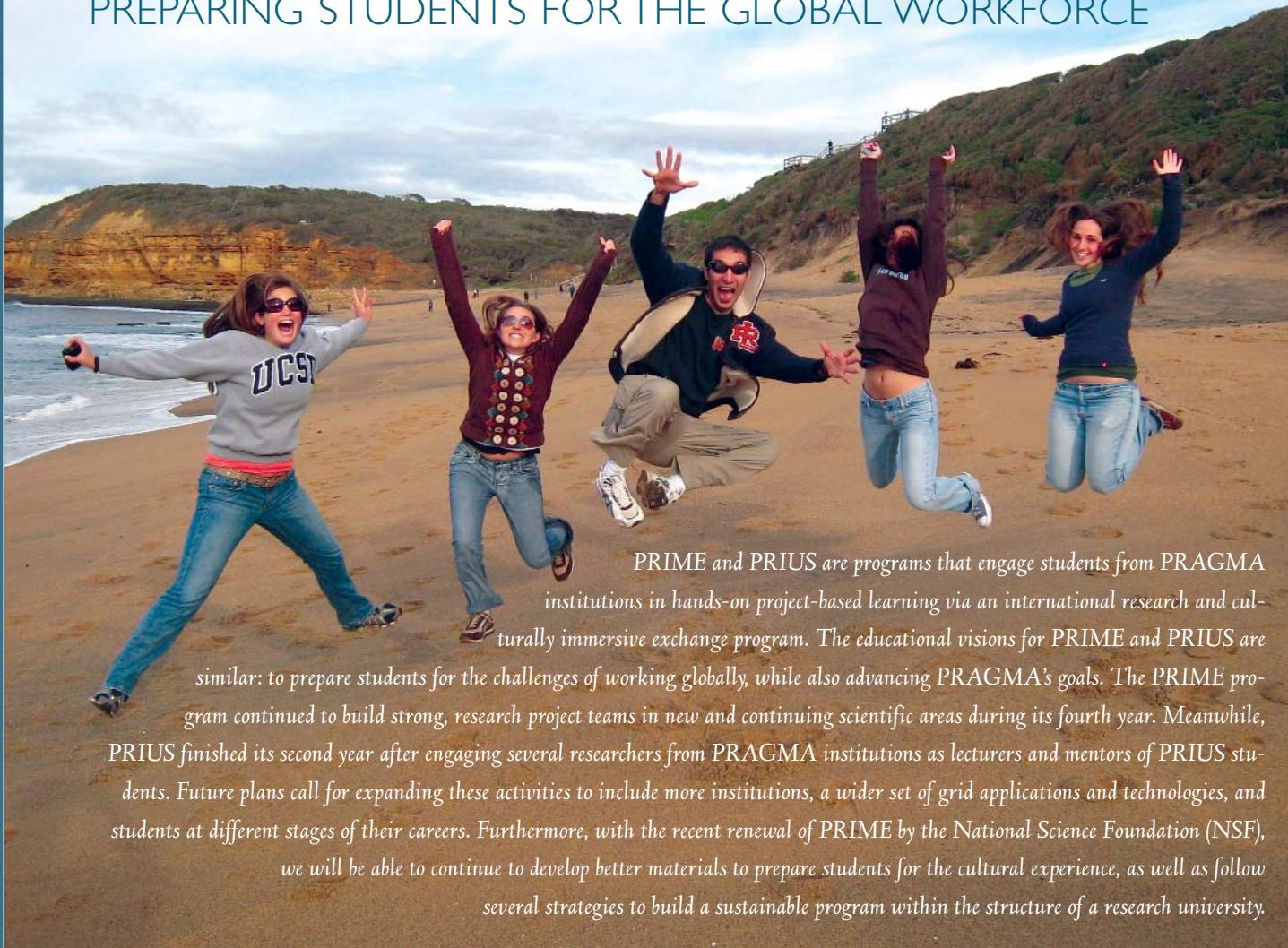


Image: PRAGMA 2007 Students, Melbourne (Source: Heather Griffith)

PRIME and PRIUS are programs that engage students from PRAGMA institutions in hands-on project-based learning via an international research and culturally immersive exchange program. The educational visions for PRIME and PRIUS are similar: to prepare students for the challenges of working globally, while also advancing PRAGMA's goals. The PRIME program continued to build strong, research project teams in new and continuing scientific areas during its fourth year. Meanwhile, PRIUS finished its second year after engaging several researchers from PRAGMA institutions as lecturers and mentors of PRIUS students. Future plans call for expanding these activities to include more institutions, a wider set of grid applications and technologies, and students at different stages of their careers. Furthermore, with the recent renewal of PRIME by the National Science Foundation (NSF), we will be able to continue to develop better materials to prepare students for the cultural experience, as well as follow several strategies to build a sustainable program within the structure of a research university.

OVERVIEW

In 2004, UCSD and PRAGMA partners in Japan (CMC, Osaka University), Taiwan (NCHC), Australia (Monash), and China (CNIC) launched PRIME—the Pacific Rim Undergraduate Experiences program (prime.ucsd.edu). PRIME provides opportunities for UCSD students to participate in international research and cultural experiences with host-site mentors and colleagues. The activities of the student researchers contribute to the growth of the cyberinfrastructure through the development, testing, and running of application codes in this internationally distributed environment. PRIME prepares students for the global workplace of the 21st century. In addition,

it has created stronger collaborations among participating PRAGMA institutions and researchers. PRIME was developed with three years of support from the NSF Office of International Science and Engineering (OISE) and Office of Cyberinfrastructure (OCI), with additional support from the UCSD division of Calit2, as well as from the partner and host institutions.

The success of PRIME during its first two years sparked the establishment of PRIUS—Pacific Rim International UniverSity (prius.ist.osaka-u.ac.jp), through funding to Osaka University from Japan's Ministry of Education, Culture, Sports, Science and Technology (MEXT) for “Fostering of Globally Leading Researchers in Integrated

Sciences,” in tight cooperation with the PRAGMA community. PRIUS aims to nurture students’ abilities to take a leadership role in next-generation integrated science, as well as offer an international perspective on both academic and industrial societies through tight collaboration with PRIME and PRAGMA. The PRIUS program, aimed primarily at graduate students, leverages the social networks already built through R&D collaboration in PRAGMA. The educational infrastructure comprises two main components: an internship experience and a course on international integrated science, taught mainly by members of the PRAGMA community.

During this past year, PRIME received a

three-year renewal from the NSF to continue the program and enhance its cultural awareness materials.

In addition, the success of PRIUS partly contributed to Osaka University's participating in the Global Centers of Excellence (COE; www.jsps.go.jp/english/e-globalcoe) program, funded by MEXT. The Global COE program aims to establish education and research centers that perform at the apex of global excellence to elevate the international competitiveness of Japanese universities. As a result of the successful competitive selection process by MEXT, the Graduate School of Information Science and Technology of Osaka University was accepted as a "Center of Excellence for Founding Ambient Information Society Infrastructure." Through this program, Osaka University will foster highly creative young researchers who will go on to become world leaders in their respective fields. They are expected to be fostered through experiencing and practicing research of the highest world standard from now forward.

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

PRIUS 2007 HIGHLIGHTS

PRIUS has been steadily expanding and taking advantage of the researcher network within PRAGMA since the 2005 launch of its classes—"Studies on International Integrated Sciences" and internship abroad. At the time of reporting, the PRIUS framework has become an educational network where 13 institutions and universities in nine countries—of which, nine are PRAGMA member institutions and universities

in six countries—are engaged in developing human resources for the sciences.

To date, 17 instructors from PRAGMA member institutions and universities have visited the Graduate School of Information Science and Technology of Osaka University and lectured on grid computing and applications topics. The topics of classes ranges from grid and web services, clustering tools, optical network computing, grid accounting systems, tiled-display wall systems, biomedical applications of grid computing, and the economic and social impact of cyberinfrastructure. The lecturers interact with PRIUS students for a few days to provide them with insights into the technological issues as well as topics of importance in other regions. The interactions allow students to meet foreign researchers and establish collaborations and internships.

INSTRUCTORS: Peter Arzberger, Mark Ellisman, Jason Haga, Mason J. Katz, Wilfred Li, Tomas Molina and Philip Papadopoulos, UCSD, USA; Luc Renambot, UIC, USA; Fang-Pang Lin and Sun-In Lin, NCHC, Taiwan; Bu-Sung (Francis) Lee and Chai Kiat Yeo, Nanyang Technological Univ., Singapore; David Abramson, Monash Univ., Australia; Rajkumar Buyya, Melbourne Univ., Australia; Rajesh Kumar Chhabra, Queensland Univ. of Technology, Australia; Habibah A. Wahab, USM, Malaysia; Kim Baldridge, UniZH, Switzerland

Over the course of its existence, PRIUS has provided internship opportunities to twelve graduate students and one undergraduate. In summer 2007, five graduate students stayed and collaborated with mentors and a team of researchers from each of two host institutions. Following, are the highlights of this year's students.

Nanyang Technological University (NTU), Parallel and Distributed Computing Centre (PDCC), Singapore

TEAM: Francis Lee, Chai Kiat Yeo and Junwei Zhang, NTU, Singapore; Shinji Shimojo and Susumu Date, Osaka Univ.

MASTERS STUDENTS: Naoya Hori and Shusuke Yamazaki

Naoya Hori and Shusuke Yamazaki designed and developed a web services application to facilitate the access to a Multiple Organizational Grid Accounting System (MOGAS) database by the public using standard web browsers. The new prototype features include ease of user access, speed of data retrieval, ease of future extension, as well as an attractive, intuitive and informative Graphical User Interface (GUI). JSR181 and Spring framework were used to develop the user-friendly web-based application. Database users can easily indicate the desired information to be extracted via the Java annotations designed by the students. Users no longer need to use JDBC to connect to the database nor do they need to understand the database structure. The users do not even need to know how to query the database. Moreover, the new prototype registers a hefty 400% improvement in access time over the existing system owing to vast improvements made in the SQL requests.

Nanyang Technological University (NTU), Centre for Multimedia and Network Technology (CeMNet), Singapore

TEAM: Chai Kiat Yeo and Francis Lee, NTU, Singapore; Shinji Shimojo, Yuuichi Teranishi and Susumu Date, Osaka Univ.

PHD STUDENT: Tomoya Kawakami

Tomoya Kawakami proposed a P2P-based mechanism for retrieving location-dependent contents in a dynamic ubiquitous environment. In a dynamic environment, peers join and leave the system or simply fail. Peer failure and departure will lead to loss of content, as well as hindering, and in the worst case, inhibiting content discovery totally. Tomoya developed an algorithm for quick detection of peer departure and failure through the appropriate use of duplicate links so that orphaned peers can be quickly grafted to the system. Moreover, to improve the robustness of the system in the event of

peer failure, he made use of content duplication at selected peers to boost the success rate of content retrieval. His algorithm is aimed at nearly complete retrieval of matched contents (i.e., more than 95%) with a minimum number of overhead messages. He has implemented his algorithm in a simulator using multithreading in Java using Location-based Logical Network (LL-Net) (Kaneko *et al.* 2005) to build the P2P system.

*University Sains Malaysia (USM),
School of Pharmaceutical Sciences,
Malaysia*

TEAM: Habibah A Waha and Suhaini Ahmad, USM, Malasia; Shinji Shimojo, Toru Fujiwara and Susumu Date, Osaka Univ.

MASTERS STUDENTS: Masafumi Tominaga and Mitsuru Jikeya

From August to September 2007, Masafumi Tominaga and Mitsuru Jikeya joined the School of Pharmaceutical Sciences of USM as non-graduating students as part of the PRIUS internship program. Throughout the two months Tominaga and Jikeya helped to develop Natural Product Drug Discovery - Virtual Screening In the Grid Environment (NADI-VISAGE), a web portal for high throughput docking implemented on the grid, incorporating many JAVA servelets. The system connects to two different MySQL NADI databases —one a receptor database and the other a small molecules (ligands) database—that have been setup for AutoDock calculations. It also has a functionality to submit docking jobs to clusters in the PRAGMA Grid. The submitted jobs are processed independently and in parallel by each CPU in the clusters.

This system also provides a user-friendly Graphical User Interface, easy access to clusters (in the grid), a decreased latency in job submission and most interesting of all, it does not need any special software. Users can use this system by simply choosing one protein/receptor from the pull out menu and one small molecule or a plant (with

many ligands) or all the ligands in the NADI database. Once the job is submitted, the results can be viewed by users where the 3D structures of protein/ligand complex and the rank of free energies of binding can be obtained by following specific links.

Finally, PRIUS is producing not only young talented human resources with international perspective, but also research achievements. Classes and internship abroad opportunities brought by PRIUS allow students to obtain knowledge on how to internationally collaborate as well as to learn cutting-edge technological skills as on the job training. Already, some PRAGMA-member joint papers (Takeda *et al.* 2007, Ichikawa *et al.* 2007a) and derivative papers (Kuwabara *et al.*, Ichikawa *et al.* 2007b) have been published as a result of classes and internships in the first two years. Furthermore, the joint international collaborations started by PRIUS educational activities have been accelerating by benefiting from PRAGMA. Therefore, more research achievements are expected in near future.

PRIME YEAR FOUR HIGHLIGHTS

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

PRIME also refined its cross-cultural train-

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

UCSD also hosted a graduate student from China's JLU who is working on the iGAP/Gfarm/CSF4 project (see Accomplishments Avian Flu Grid).

Finally, PRIME experimented with multimedia to capture the experiences of PRIME students for future understanding of the benefit of the experience (see www.youtube.com/watch?v=4lY6x0S3IoA&feature=PlayList&p=A19401D562B6417C&index=4), produced in collaboration with Calitz2.

Cybermedia Center (CMC), Osaka University

TEAM LEADERS AND MEMBERS

OSAKA UNIVERSITY: Shinji Shimojo, CMC; Susumu Date, Graduate School of Information Science and Technology and Project Lead, PRIUS; Eisaku Sakane; Kazunori Nozaki; PRIUS student researchers Kohei Ichikawa and Seiki Kuwabara

UCSD: Mentors Mark Ellisman, NCMIR and CRBS; Steve Peltier, Masahiko Hoshijima Takeharu Hayashi and Tomas Molina, NCMIR (for Young Chun and Ava Pierce); Jürgen Schulze, Calitz (for David Jackson and Ava Pierce); Jason Haga, Bioengineering; PRIME student researcher Marshall Levesque (for Ellen Tsai).

STUDENTS: Young Chun, David Jackson, Ava Pierce and Ellen Tsai

Ellen Tsai's work with Susumu Date and Kohei Ichikawa of the BioGrid project extended the efforts of PRIME 2006 student Marshall Levesque under the continued mentorship of Jason Haga. She was focused on using computational tools in a grid environment to study aspects of pro-

tein structure and docking with ligands. In particular she focused on a class of proteins known as phosphatases, which are enzymes that modify other proteins by removing phosphate groups. Phosphatases play an important role in regulating the signaling pathways in cells and have been hypothesized to have regulatory roles in cancer. Her objective was to identify inhibitors to Src homology 2 domain—containing phosphatases (Shp), with a long-term goal of developing chemical inhibitors that will prevent the catalytic activity of specific isoforms of these phosphatases. She performed a screening of a large database (ZINC) and identified via computational tools 10 unique inhibitors to Shp2. Future experiments will test the efficacy of these inhibitors *in vivo*.

Young Chun engaged in a new collaboration between UCSD and Osaka University to acquire high-resolution microscopic images of heart cells by utilizing the world's largest high-voltage electron microscope located at Osaka to establish realistic models of this cell type in 3D, using mathematical computation. The project was built on the existing collaboration between the CMC and NCMIR at UCSD. With the help of CMC mentors, Young established a new server environment in CMC that was used to acquire, store, process, and transfer large-volume electron-microscopic image data to NCMIR. Young worked with researchers at Osaka and successfully captured the first set of electron microscopic images of four micro-meter thick sections of mouse heart tissues and reconstructed tomography of them at CMC.

David Jackson and Ava Pierce worked as a team on visualization using the tiled-display wall technology. They worked with the COllaborative VIualization and Simulation Environment (COVISE), and added features to make COVISE more usable. David and Ava worked on a File Browser Plugin with a suite of image processing functions for COVISE, which can graphically show all files in a directory, navigate to other directories, and load any COVISE file to their respective plugins. Ava worked on aspects of this, in particular on data imaging tools, while David worked on the framework. They were able to implement a version of this File Browser Plugin during their stay.

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

TEAM LEADERS AND MEMBERS

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

UCSD: Hyonny Kim, Structural Engineering (for Samson Hang), Jürgen Schulze, Calitz (for Ya Kao)

STUDENTS: Samson Hang and Ya (Betsy) Kao

Ya (Betsy) Kao explored visualization of scientific data, using tiled-display wall technology and volume rendering tools. Her application was to explore the rich data sets on fly brain images of researchers in Taiwan. Betsy created a method to layout large image sets as they occur in brain



Image: Silver Temple, Kyoto Japan (Source: Young Chun)

imaging on a tiled-display wall. Her software allows the user to change the layout parameters interactively in order to achieve the desired result.

Samson Hang worked on simulation of an evaporation-based procedure for fabricating conductive composite film of multi-walled carbon nanotube and polyethylene oxide composite. The resultant composite film can be applied to sense strains in critical materials, such as aircraft wings. Samson was able to build models of a tube, created multiple of these tubes that avoid collision in three dimensions, and render the spatial distribution of these tubes.

Monash University, Australia

TEAM LEADERS AND MEMBERS

MONASH: David Abramson, School of Computer Science and Engineering; Colin Enticott, Slavisa Garic, Rob Gray and Tom Peachey

UCSD: Mentors Andrew McCulloch, Anushka Michailova and Roy Kerckhoffs, Bioengineering (for Saleh Amirriazi, Stephany Chang, Heather Griffith); Kim Baldridge, SDSC and Organic Chemistry Institute, UniZH (for Michelle De Fiore); and Cindy Zheng, PRAGMA Grid (for Elizabeth Kain)

STUDENTS: Saleh Amirriazi, Stephany Chang, Michelle De Fiore, Heather Griffith and Elisabeth Kain

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

Saleh Amirriazi, Stephany Chang and Heather Griffith continued a program-long interaction between the Cardiac Mechanics Research Group at UCSD and Distributed Systems and Software Engineering at



Monash. Heather's work explored how changing two existing default parameters on a cardiac model (the time-to-peak strain and the relaxation duration) affects the model behavior, specifically, the dp/dt_{max} , dp/dt_{min} , and ejection fraction. The model is used to test different types of CRT (Cardiac Resynchronization Therapy) in order to improve treatments for people with heart failure. Understanding the relationship between these two parameters and overall hemodynamic functions of the heart may help expand the ability of the model to test varying heart conditions with greater accuracy. She was able to set up the computational experiment, which required access to several PRAGMA Grid resources and some changes in the software Continuity, a computational tool for continuum problems in bioengineering and physiology, especially those related to cardiac mechanics and electrocardiology research. One result is that Nimrod can run Continuity jobs. Stephany Chang's work investigated the ionic properties of ventricular myocytes, and used Nimrod/O and Nimrod/G to conduct parameter searches to identify parameters that would produce a stable model. Similar to Heather's project, she used a variety of PRAGMA Grid resources. Saleh Amirriazi's work focused on modeling the effects of ATP-dependent potassium current in regulating excitation-metabolic coupling in endocardial ventricular myocytes under normal condition and

20 minutes of simulated ischemia. He used a new member of the Nimrod family, Nimrod/E for experimental design in conjunction with Nimrod/O, to validate a model with experimental data.

Michele Di Fiore extended the work of PRIME 2006 student Celia Croy, who initiated the establishment of a computational pipeline for high-throughput molecular modeling using GAMESS, APBS, or GAMESS/APBS hybrid, using Nimrod programs. The GAMESS and APBS tools enable computational chemistry studies using quantum chemical and electrostatic theories, respectively. This activity builds on and extends the work of other PRIME students from previous years and deepens the collaboration between David Abramson's lab at Monash and Kim Baldridge's group at the University of Zurich (UniZH). In particular, Michele studied the binding energy and the orientation of the phenyl rings in the binding site and how rotation by 30 degrees of side rings affect the binding energy.

Elizabeth (Liz) Kain focused on how to take a large application code (in her case, on climate modeling) and have it run across resources in the PRAGMA Grid as well as on platforms in Europe. While earlier work ran the CSIRO climate modeling code CCAM on the PRAGMA Grid (see Accomplishments 2006, joint work between

*Image: Calit2 building at dusk.
(Source: Philipp Rittermann)*



Amanda Lynch, CSIRO, and David Abramson. Also see Görgen, *et. al.*), Liz wanted to extend this work, conceptually, to interact with a different grid environment, running Unicore (Uniform Interface to Computing Resources). This work falls within the Grid Interoperations Now (GIN) activity (see *Resources and Data Working Group*). Liz succeeded in getting the Nimrod interface to Unicore working, an essential step to using the broader resources for the climate simulation. She was also able to test the climate code on the resources associated with PRAGMA at MIMOS, UniZH, IOIT-HCM, LZU, AIST, ThaiGrid, and Singapore.

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

TEAM LEADERS AND MEMBERS

CNIC: Kai Nan, Kevin Dong, Yihua Zheng (for Alex Liu); Zhonghua Lu, Xianyu Lang, Beifang Niu (for Lynn Greiner); Jianjun Yu, Yanhua Sun (for Hsing Pao); Haiyan Xu, and Wei Chen (for Lynn Greiner, Alex Liu and Hsing Pao)

UCSD: Wilfred Li, NBCR (for Hsing Pao); Jürgen Schulze, Calit2 (for Alex Liu); Tomas Molina, NCMIR (for Lynn Greiner).

STUDENTS: Lynn Greiner, Alex Liu and Hsing Pa

Hsing Pao continued work started by Lily Cheng and Lisa Zhao, 2006 PRIME students, who worked on complementary aspects of an initial study on avian influenza virus, subtype H5N1, screening neuraminidase and hemagglutinin (HA) proteins, respectively, against two libraries of ligands. Hsing's work focused on the binding affinity of hemagglutinin's receptor binding domain with the receptor sialic acid (SA), which prefers different glycosidic linkages in birds (SA a-2, 3-Gal) and humans (SA a-2, 6-Gal). He screened various strains of HA for affinity to sialic acid, using a combination of tools including Modeler and AutoDock. Subsequently he visualized some of the models with the best binding energy. In addition, he built upon the efforts of the students from previous years to develop a database to share the screened products. This work has stimulated a broader collaboration between UCSD, CNIC and other PRAGMA partner sites, which will continue through the next year (see *Accomplishments*).

Lynn Greiner's work focused on clustering algorithms used in multivariate statistics. The project was to apply these clustering algorithms on gene expression patterns, which were available at the host site. Lynn reviewed eight known algorithms, and began implementation of two of them in the computational infrastructure at CNIC. He succeeded in getting one of these two implemented, and ran some preliminary tests with the code. The next task is to conduct parallel optimization of the program and improve the performance. The ultimate aim of the project is to establish an integrated program package based on eight kinds of clustering algorithms. Users can flexibly select any one of these eight clustering algorithms according to data characteristics needed clustering.

Alex Liu's work built on a project and collaboration from the 2006 PRIME student Elaine Liu. Alex worked on programs to display high-resolution time-series images. He was able to take steps towards achieving

this goal, and achieved some degree of compatibility with the software SAGE, the Scalable Adaptive Graphics Environment, which was developed at the Electronics Visualization Laboratory of the University of Illinois Chicago.

University of California, San Diego

TEAM LEADERS AND MEMBERS

UCSD: Gabriele Wienhausen, Sixth College and Calit2; Linda Feldman, Academic Internship Program; Peter Arzberger, PRAGMA and NBCR; Teri Simas, PRAGMA.

STUDENTS: Young Chun, David Jackson, Ava Pierce and Ellen Tsai, Osaka University; Samson Hang and Ya Kao, NCHC; Saleh Amiriazi, Stephany Chang, Michelle De Fiore, Heather Griffith, and Elisabeth Kain, Monash; Lynn Greiner, Alex Liu, and Hsing Pao, CNIC.

MENTORS: Andrew McCulloch, Anushka Michailova, Roy Kerckhoff, and Jason Haga, Bioengineering; Wilfred Li, NBCR; Mark Ellisman, Masahiko Hoshijima, Steve Peltier, Tomas Molina and Raj Singh, NCMIR; Jürgen Schulze, Calit2; Hyonny Kim, Structural Engineering; Kim Baldridge, UniZH and SDSC; Cindy Zheng, PRAGMA Grid

Gabriele Wienhausen, one of three program coordinators for PRIME, is the principal investigator of the NSF PRIME award, and Associate Dean for Education, Division of Biological Sciences. She is joined by co-PI Linda Feldman from the Academic Internship Program, who has broad international experience in establishing and evaluating internship programs, and co-PI Peter Arzberger, who is PI of the PRAGMA award, which provides a source of projects, as well as the essential human network of PRAGMA sites. Teri Simas assisted with project management. With their partners, they are looking to expand the program to more students and sites next year and are exploring ways to host internships for students at UCSD from PRAGMA sites.

WORKING GROUPS

The working groups below reflect the interests of current PRAGMA members. Each group has a lead or co-leads who coordinate the activities of that group during and between meetings. The groups have projects that bring a focus to their activities, working towards milestones and giving demonstrations at PRAGMA workshops and other meetings. This structure allows for the inclusion of new applications, as well as new areas of interest. This year PRAMGA launched a new GEO working group whose long-term goal is the development of a grid testbed to support geo-sciences and practical applications based on huge datasets of satellite imagery and GIS data, such as disaster prevention or environment monitoring.



Image: Formosat-2 image, a true color composite in visible wavelengths, captured on September 12th, 2007. Ivanpah Playa, the target area, is located south of Las Vegas, Nevada in the US. The GEO Working Group compared this image with one using Aster data, taken on the same day. AIST members in the ASTER science team obtained the ground-truth concurrently with the satellites' overpass. The radiometric accuracy of Formosat-2 can be greatly improved through the comparison with the ASTER and ground truth. A grid middleware, developed by GEO working group, will help users to find such pairs through federation of huge data archives of ASTER and Formosat-2. (Source of image: NARL)

RESOURCES AND DATA WORKING GROUP

The Resources and Data Working Group's goal is to improve the interoperability of grid middleware around the world and to make grids easier to use for scientists. During the past year, the group has expanded the PRAGMA Grid and its routine-basis experiments, as well as continued to conduct peer-grid interoperation experiments as part of the Grid Interoperation Now (GIN) activity. Furthermore, the Resources and Data Working Group has been building a Gfarm data-grid as part of the routine-basis PRAGMA grid.

During this last year, the PRAGMA grid grew from 26 sites in 14 countries/regions to 30 sites in 17 countries/regions, with a total of 1109 CPUs, more than one terabyte of memory, and 26.7 terabytes of online storage.

Application numbers have grown from 12 last year to 20 this year, topics ranging from climate simulation and quantum chemistry to metagenomics, fluid dynamics, molecular simulation and sensor data analysis. Most of the applications continue to utilize grid middleware, such as Ninf-G, Nimrod/G, MPICH-GX, Gfarm, or CSF. These routine-use experiments also resulted in continuous enhancements for all application middleware involved. See Table 1 for some specific examples. See also *Accomplishments PRAGMA OSG Grid Interoperations Experiment*.

PRAGMA Grid has become an essential resource and support to the PRIME program. Eight students ran applications and worked on their projects using the PRAGMA Grid and getting support and expertise from the PRAGMA Grid team.

Grid infrastructure middleware continues to develop and improve in the PRAGMA grid. More importantly, integrations with other middleware, services, and applications have increased. For example, new functions—such as Gfarm and WSGRAM

Table 1. Key application activities in PRAGMA grid

APPLICATION	MIDDLEWARE	DOMAIN	DRIVER INSTITUTION	STATUS
Amber	Gfarm	Molecular simulation	USM, Malaysia	Completed
Avian Flu	Gfarm/CSF4	Genomics	UCSD, USA	On-going
CSE-Online		Computational chemistry	University of Utah, USA	Starting
CSTFT	Ninf-G	Environmental science	UPRM, Puerto Rico	Starting
e-AIRS		Fluid dynamics	KISTI, Korea	Starting
GridFMO	Ninf-G	Quantum chemistry	AIST, Japan	Completed
MM5, WRF	Mpich-GX	Climate simulation	CICESE, Mexico	Completed
Savannah	Nimrod	Climate simulation	Monash, Australia	On-going
Siesta	Nimrod	Molecular simulation	UniZH, Switzerland	On-going

monitoring, bandwidth measurements amongst sites—have been added to the grid monitoring software, SCMSWeb. Other services, such as CSE-Online and CSF, have also been integrated with SCMSWeb, and rely on SCMSWeb to provide essential resources information in order to make choices and decisions. See Table 2 for some key middleware activities in PRAGMA.

Application users employ SCMSWeb regularly to check resource availability and jobs status, and MOGAS provides critical accounting data for application and job analysis. For site administrators, SCMSWeb

is essential for monitoring their systems and helping to locate and fix problems. MOGAS data is not only handy for reporting resource usages to funding agencies, but also provides insight for grid infrastructure software design and development and supplies statistics for making resource configuration and policy adjustments to improve resource utilization.

This year, many grid services have been developed and deployed in PRAGMA Grid: CSE-Online, Condor-G server, bio-science portal, CSF server and portal.

CSE-Online provides user-friendly access to a wide range of remote data stores, computational tools and modeling and visualization resources for both research and education. This year, the CSE-Online team worked with another PRAGMA Grid team—ThaiGrid team—integrating CSE-Online with SCMSWeb and ThaiGrid, which extended the grid access to a portal architecture and improved security to grid resource providers that have community users. Subsequently, several workshops in computational chemistry have been successfully organized in Thailand to introduce CSE-Online and ThaiGrid infrastructure to the chemistry community. From there, the CSE-Online team worked with all PRAGMA grid sites and integrated CSE-Online with the PRAGMA grid for the Avian Flu Grid project.

As a result of this year's Grid Interoperation experiment with OSG, the PRAGMA Grid UCSD team set up a Condor-G server in the PRAGMA grid which provides a simple job submission service to all PRAGMA grid users.

Based on last year's work by Queensland University of Technology and UCSD teams, a bioscience portal has been permanently established at portal.pragma-grid.net this year. This portal provides an easy interface for researchers to run bioscience applications.

In a heterogeneous and diverse global grid environment like PRAGMA grid, scheduling and resource management are among the key challenges in making it easier to use. Our efforts with the Community Scheduler Framework (CSF) are described in *Accomplishments*.

While expanding our existing computational grid, the resources group

Table 2. Key middleware activities in PRAGMA grid

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

has also been building a data grid in the PRAGMA grid with Gfarm software. A Gfarm meta-server for the data grid has been setup at the PRAGMA grid site National Institute of Advanced Industrial Science and Technology (AIST) in Japan. AIST and SDSC are setup as big storage sites. Currently, the datagrid consists of 19 clusters from 14 institutions across ten countries/regions, and will continue to expand among PRAGMA Grid sites. More importantly, the USM-AIST team successfully demonstrated the running of AMBER application using Gfarm and is working to expand the test to more Gfarm datagrid sites. In addition, the CUHK-AIST team also started AMBER/Gfarm testing on “x86_64” sites within the PRAGMA Gfarm datagrid. Furthermore, the UniZH team has developed a Gfarm roll for the Rocks cluster system. This will greatly simplify the deployment of Gfarm on Rocks clusters, which more than half of PRAGMA grid sites are running.

To enable interoperation with other grids and to enable users around the world to use grids, the group has established PRAGMA Certificate Authority (PRAGMA CA) using NAREGI-CA software, which was developed by the National Research Grid Initiative (NAREGI) in Japan, in which several PRAGMA member institutions participate. Working closely with APGrid PMA, PRAGMA CA joined International Grid Trust Federation (IGTF) to gain and maintain trust amongst global grids.

This year, the resources group continues to lead the GIN application PRAGMA grid effort. The GIN PRAGMA grid has grown from last year's seven sites from five grids across six countries, to this year's 17 sites from seven grids across 11 countries.

Working together, the GIN-ops team started to run Savannah fire simulation, a data-intensive climate application based on grid middleware Nimrod, on three of those grids—PRAGMA Grid, TeraGrid and Open Science Grid—and worked on developing a

Nimrod interface to Unicore and NorduGrid, via PRIME student Liz Kain (see *Accomplishments*).

The group has always been very active in knowledge sharing with broader grid communities. This year, its members gave numerous presentations and tutorials, published and documented issues, solutions and lessons learned on the many major projects in which they are involved.

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

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

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

RESOURCES AND DATA: M. Katz, Co-chair, SDSC at UCSD; Y. Tanaka, Co-chair, AIST; Y. Tanimura, H. Takemiya and T. Ikegami, AIST; D. Bannon, G. Jenkins and C. Kendrick, APAC; E. Yen and H. Shih, ASGCC; K. Chiu, J. Skovronski and M. Head, SUNY-B; O. Tatebe, CCS; R. Hazas, S. Castañeda and J. Delgado, CICESE; K. Nan and K. Dong, CNIC; R. Yeung, S. Tang and C. Chu, CUHK; H. Zhang and S. Chen, GUCAS; X.H. Wei, Z.H. Ding and Y. Luo, JLU; T. V. Lang, H. V. Nguyen; V. D. Hieu; IOIT-HCM; T. Hung, H. M. Chan, B. Yeo, IHPC; S. Kim, P. Lee, B. Kim, J. Moon and

K.W. Cho, KISTI; W.B. Chen, Y. Zhang and H. Yan, LZU; H. Kauthary, J. Y. Luke, MIMOS; D. Abramson and C. Enticott, MU; W. Huang, C. L. Huang and M. Yu, NCHC; R. Nandkuma and T. Roney, NCSA; S. Vannarat and S. Prueksaaron, NECTEC; H. Y. Lee, J. Lau, N. Teow, and N. Chalakornkosol, NGO; F. Lee and J. W. Lee, NTU; S. Dat and, S. Takeda, Osaka U; P. Papadopoulos, C. Zheng, SDSC; P. Uthayopas, S. Sriprayoonsakul and S. Phatanapherom, ThaiGrid; A. Garcia and L. Zoppi, UBC; A. Jofre and J. C. Maureira, Univ. Chile; J. L. Gordillo Ruiz, E. Murrieta Leon, P. Martinez and P. Palacios, UNAM; R. Wankar, B. Sandhya, A. Agarwal, UoH; D. Rodriguez, W. Rivera, K. Cruz and J. Sanabria, UPRM; H. Wahab, F. Haron, C. H. Yong, B. Yaik, M. Cheng and S. Ahmad, USM; T. Truong and, X. Fan, U. Utah; K. Baldridge, UniZH and SDSC; W. Sudholt, N. Williams, C. Amoreira and M. Packard, UniZH

COMPUTE GRID ONLY: Binghamton University, BII, CICESE, IHPC, JLU, Monash, KISTI, Osaka University, NCHC, National University of Mexico (UNAM), U Chile, UoH, University of Puerto Rico at Mayaguez (UPRM), USM (Computer Science and Pharmaceutical)

COMPUTER AND DATA GRIDS: ASGCC, Chinese University of Hong Kong (CUHK), CNIC and CAS, Graduate University of Chinese Academy of Sciences (GUCAS), Ho Chi Minh City Institute of Information Technology (IOIT-HCM), Lan Zhou University (LZU), MIMOS, NCSA, NECTEC, NGO, AIST, ThaiGrid, UCSD and SDSC, UniZH

SERVICE PROVIDERS: APAC (host MyProxy [NCSA] and VOMS services)





Image: From Wat Chaiwattanaram, the great Thai-Cambodian style temple near the Chaophraya river, Ayutthaya, Thailand

BIOSCIENCES WORKING GROUP

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

One major activity of the Biosciences Working Group has been their work on building a grid to address infectious diseases. The initial focus is on the avian flu H5N1, which is an emerging threat to

many countries around the world. See Accomplishments section for more information on the Avian Flu Grid and its approach to integrating technologies such as CSF4, Gfarm, MGrid, and research tools such as AutoDock and NAMD. Work has begun using CSE-Online as an enabling gateway for virtual screening on the PRAGMA and TeraGrid grids. Such a gateway will encourage much broader participation in this effort beyond that of the PRAGMA community.

Another project which has begun to leverage some of the infrastructure developed for the Avian Flu Grid, is the development of a pipeline for metagenomics studies on phosphate removal bacteria in sludge and waste water treatment plants. Several phylogenetic analysis tools are deployed on the PRAGMA grid, and the resulting workflows would be exposed as web services, made easily accessible to metagenomics researchers, and contributed to the community-based tools for the CAMERA project. This work will also benefit the efforts of the

Global Lake Ecological Observatory Network (GLEON) in their general interest in the role of microbes in lake dynamics.

Lastly, with the Resources working group, we have established a production portal environment, portal.pragma-grid.net, which serves as a place of entry to PRAGMA resources and access to the CSF metascheduler and Gfarm data grid.

PARTICIPATING RESEARCHERS: K. Jeong, Chair, Konkuk Univ; H. Wahab, Co-Chair USM, co-chair; W. W. Li, NBCR at UCSD, co-chair; K. Baldridge, SDSC at UCSD and UniZH; L.Cheng and D. Xu, UCSD; T. N. Truong, CSE-Online, U of Utah

COLLABORATORS: R. Amaro, UCSD; M. Alam, U. Hawaii; E.McMahon, U. Wisconsin; J.H. Lin, Academia Sincia, National Taiwan Univ

RESOURCES: K. Nan and Z. Lu, CNIC and CAS; X. Wei, CCST, JLU.; Y. Tanimura, AIS; O. Tatebe, CCS, U Tsukuba; S.T. Hwang, Kookmin Univ; J.Lee, K. Kee and K. Cho, KISTI; H. Lee, ASGCC; T. N. Truong, Center for High-Performance Computing, U of Utah

TELESCIENCE WORKING GROUP

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

The R&D activities in the Telescience Working Group fall into three types of projects. The first, and most traditional, activity is the establishment of a grid workbench for neuroscience, which will allow experts to use electron microscopes and control them remotely. The second is Ecology Grid which originated in Taiwan and has led to other grass roots efforts and collaborations such as the Global Lake Ecological Observatory (GLEON) and the Coral Reef Ecological Observatory Network (CREON). The third and final

component is the use and dissemination of tiled-display wall technology as a means for sharing information and collaborating.

Electron tomography is a powerful technique that draws on advanced instrumentation, networking, and grid computing to derive 3D structural information from biological specimens. The Telescience portal was developed by the National Center for Microscopy and Imaging Research (NCMIR) at UCSD as a web-based portal solution for end-to-end electron tomography. It centralizes applications and seamlessly interfaces with the grid to accelerate the throughput of data results. The potential revealed by the portal has promoted participation in the working group. To date, the partnership has incorporated the Cybermedia Center at Osaka University's expertise in IPv6 networking, NCMIR's advances in Telescience infrastructure, 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 dur-

ing remote microscopy experiments. In addition, researchers from KBSI and Seoul National University have continued to develop a datagrid for the High Voltage Electron Microscope at KBSI.

Ecological Grid is a project inspired by the Telescience project. It aims to establish a grid environment where scientists can monitor environmental factors such as temperature

and humidity using environmental sensing devices. The application area of the Ecological Grid is lake metabolism, agriculture, and coral reef studies. GLEON grew out of these activities, and could help as a testing ground as PRAGMA extends its testbed to include sensors. A recent highlight is the joint deployment of the data streaming middleware, DataTurbine, by NCHC and UCSD, to monitor activity around the Kenting Coral Reef, a node of CREON (See Accomplishments). The NARC team continues to deploy FieldServers (for meteorological data collection), and their software MetBroker can now handle data from databases, predicted models, and real-time data.

A new wave is coming to the Telescience Working Group in the form of tiled-display walls. Scientists and researchers in the group hope that this visualization technology not only provides an intuitive understanding of scientific results from both projects, but also establishes a multi-collaboration environment for future science. In addition to the discussion on how tiled-display technology is used for future science on a cyberinfrastructure, the development and the standardization of tiled-display technology is expected to be an area of collaboration. Another spin-off activity from the Telescience Working Group is education and human development of internationally collaborative research groups. Through the PRIME and PRIUS projects, students from UCSD and Osaka University joined research teams of the Telescience working group in different countries for nine weeks. They experienced on-going research and cultural aspects of different countries. This technology was used to provide a live broadcast between the President of Osaka University, who was in Thailand, to participants at the PRAGMA 11 meeting in Osaka, via collaboration between Osaka University, Thailand's National Electronics and Computer Technology Center (NECTEC), NCHC and UCSD (See Accomplishments 2006-2007). Additionally,



Image: Screen-shot of the File Browser Plugin developed by PRIME students David Jackson and Ava Pierce (see page 17).

tiled-display wall technology is being used by the Global Cyberbridges Project (www.cyberbridges.net) to conduct joint classroom experiences between students at Florida International University (FIU) and CAS, CNIC. The goal of the Global Cyberbridges Project is to improve the technology training for a new generation of scientists and to increase the rate of discovery for all domains. (NSF supports Global Cyberbridges via an award to FIU.) Participants from FIU and CNIC took part in a tutorial on SAGE (Scalable Adaptive Graphics Environment, www.evl.uic.edu/cavern/sage/description.php) which helps drive the tiled-display wall technology. In addition, participants had a hands-on session where they learned how to build tiled-displays based on ROCKS (www.rocksclusters.org/wordpress) and how to configure the software.

PARTICIPATING RESEARCHERS: F. Lin and S. Shimojo, co-chairs; S. Date, T. Akiyama, E. Sakane, and K. Nozaki, CMC, Osaka Univ.; S. Kato, Hyogo Univ. of Health Sciences; M. Lee, KISTI; D. McMullen, Indiana Univ.; B. Durnota, Complexibotics; M. Ellisman, S. Peltier, A. Lin, T. Molina and R. Singh, NCMIR at UCSD; K.M. You and H.S. Kweon, KBSI; H Yeom, Seoul National Univ.; J.H. Woo, Konkuk Univ.; H. Chou, S-I Lin and S.Cheng, NCHC; S. Ninomiya, NARC and APAN; B. Pailthorpe and N. Bordes, U. Queensland; T. Fountain and S. Tilak, UCSD; K. Nan and K Dong, CNIC.

COLLABORATORS: H. King, Taiwan Forest Research Inst; T. Kratz and N. Temperate, Lakes LTER; D. Hamilton, U Waikato; Heidi Alvarez and Julio Ibarra, FIU

GEO WORKING GROUP

The GEO Working Group is the youngest of the four current working groups in PRAGMA. The initiative to start such an activity began during the PRAGMA 10 meeting in Townsville (March 2006); it came to fruition at the PRAGMA 12 meeting in Bangkok (March 2007), when a proposal by members of the working group was

approved by the PRAGMA Steering Committee. The goal of the GEO Working Group is to develop a grid testbed to support geosciences and practical applications based on huge datasets of satellite imagery and GIS data, such as disaster prevention and environment monitoring. A first activity of this group was to organize the 1st GEO Grid Workshop in Bangkok alongside PRAGMA 12. Subsequently, members of the GEO Working Group organized a session at the 5th Taipei International Digital Earth Symposium on GEO Grid. The group realized during both workshops that development of the testbed should be coordinated with other international efforts, especially with Global Earth Observation System of Systems (GEOSS). GEOSS seeks to achieve comprehensive, coordinated, and sustained observations of the Earth system, in order to improve monitoring of the state of the Earth, increase understanding of Earth processes, and enhance prediction of the behavior.

The GEO Working Group is building on the strengths of its participants. In particular, AIST has a very strong effort on GEO Grid, which is developing an infrastructure to integrate remote sensing and GIS data from various sources. Challenges include the wide varieties of existing data sets in the community for which each data owner insists on determining their own licensing policy. In addition, there are many related projects that will be configured as virtual organizations (VOs). AIST completed the preliminary design of GEO Grid to integrate all the relevant data virtually as a set of services. The software architecture and its preliminary implementations are based on the Grid computing, web service technologies and GIS standards defined by Open Geospatial Consortium (OGC). The National Applied Research Laboratory (NARL) in Taiwan is a non-profit organization with nine research institutions. NARL GEO (Global Earth Observatory)-Grid project is to deploy a high-resolution 3-D GIS platform for Taiwan. Disaster event

GIS data, as well as typhoon forecasting, rainfall, and flooding data can all be displayed over the platform. Users can easily perceive disaster event scenarios with this 3-D GIS visual presentation. A total of six research centers under the NARL are involved in this project. In particular, NARL includes NCHC, which is integrating NARL's GEO-related projects including operating an earth-observing satellite Formosat-2 imagery, GIS information, 3-D visualization, GLEON, and typhoon monitoring and prediction. Finally, the iGEON project, which involves UCSD, UoH and CNIC, is developing tools to integrate heterogeneous databases associated with geosciences (See Accomplishments). The GEO Working Group will promote collaboration between these projects, bring more participants to this activity, and will begin technological integration of various components, with a particular focus on integration of data from various systems.

At the PRAGMA 13 meeting, an example of the satellite data integration was demonstrated. AIST and NARL coordinated simultaneous observations of a test site in Nevada by two satellite sensors, namely ASTER and Formosat-2. If users can find many pairs of such simultaneous observations in the huge data archive, the synergy enables them to obtain Formosat-2 images with high spatial/temporal resolutions, which are very accurately calibrated using ASTER images. The group plans to conduct similar experiments of database federation for geological datasets provided by iGEON nodes and Geological Survey of Japan in AIST.

PARTICIPATING RESEARCHERS: Co-leads: R. Nakamura, AIST; G-S. Chang, NARL; A. Memon, UCSD; S. Vannarat, NECTEC

COLLABORATORS: C-C. Liu, National Cheng Kung Univ.; W-F Tsai, NCHC; P. Srichaikul, NECTEC; A. Agarwal, U. Hyderabad; K. Nan, CNIC; K. Won Cho, KISTI; P. Bajcsy, NCSA; Y. Tanaka and S. Sekiguchi, AIST.

PUBLICATIONS AND REFERENCES

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

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Image: From Wat Phrasisanphet, the ruins of the royal temple, Ayutthaya, Thailand



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WORKSHOPS AND INSTITUTES

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

FUTURE MEETINGS

PRAGMA 14

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

Chairs: Whey-Fone Tsai and Fang-Pang Lin

PRAGMA 15

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

Chair: Muhammad Idris Saleh

PRAGMA 16

March 2009, Daejon, Korea; Hosted by KISTI

Chair: Kum Won Ch

FUTURE PRAGMA INSTITUTE

2nd PRAGMA INSTITUTE

3-7 December 2007, Hsinchu Taiwan; Hosted by the NCHC

PAST MEETINGS

1st PRAGMA INSTITUTE

26-27 September 2007, Urbana-Champaign, Illinois, U.S.; Hosted by NCSA, UIUC

PRAGMA 13

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

PRAGMA 12

20-22 March 2007, Bangkok, Thailand; Hosted by NECTEC and ThaiGrid (TNGC), Software Industry Promotion Agency (SIPA)

PRAGMA 11

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

PRAGMA 10

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

PRAGMA 9

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

PRAGMA 8

2-4 May 2005, Singapore; Hosted by the BII in Singapore and the NGO

PRAGMA 7

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

PRAGMA 6

16-18 May 2004, Beijing, China; Hosted by the CNIC, CAS

PRAGMA 5

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

PRAGMA 4

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

PRAGMA 3

23-24 January 2003, Fukuoka, Japan; Hosted by AIST and Osaka Univ.

PRAGMA 2

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

PRAGMA 1

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

STUDENT AND POSTDOCTORAL OPPORTUNITIES

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



Image: Taro Gorge, Hualien, Taiwan



PRAGMA SUPPORTING INSTITUTIONS AND SPONSORS

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

- * State University of New York, Binghamton (SUNY-B, www.binghamton.edu), located in New York, U.S., has contributed resources to the PRAGMA grid, attended the PRAGMA 10 workshop and is developing a grid-enabled sensor network application to run in the PRAGMA grid.
- * The Chinese University of Hong Kong (UCHK, www.cuhk.edu.hk/v6/en), located in Hong Kong, China, has contributed resources to the PRAGMA grid and attended PRAGMA 10, PRAGMA 12, and PRAGMA 13 workshops.
- * The Laboratory of Computational Geodynamics, Graduate University of Chinese Academy of Sciences (GUCAS, www.gucas.ac.cn/gscasenglish/index.aspx), located in Beijing, China, has contributed resources to the PRAGMA grid as a GEON compute node and is developing a grid-enabled geoscience prototype to run in the PRAGMA grid.
- * The Ho Chi Minh City Institute of Information Technology (IOIT-HCM, www.ioit-hcm.ac.vn/english), is a scientific research institution of the Vietnamese Academy of Science and Technology (VAST), located in Ho Chi Minh City, Vietnam. IOIT-HCM is one of the five leading organizations of VNGrid project. It has contributed resources to the PRAGMA grid, attended PRAGMA 9, PRAGMA 10 and PRAGMA 12 workshops, and developed and tested grid applications in the PRAGMA grid. IOIT-HCM researchers have built Grid-based applications including bioinformatics, geoinformatics, telemedicine, as well as e-Science in computational fluid dynamics research.
- * Ho Chi Minh City Univ. of Technology (HCMUT, www.hcmut.edu.vn), located in Ho Chi Minh City, Vietnam, has contributed resources to PRAGMA grid and attended PRAGMA 11 and PRAGMA 12 workshops.
- * LanZhou University (LZU, www.lzu.edu.cn), located in LanZhou, China, has contributed resources to PRAGMA grid & attended PRAGMA 12 workshop.
- * Nanyang Technological University (NTU, www.ntu.edu.sg), located in Singapore, has been developing and maintaining MOGAS—a grid accounting software system in PRAGMA grid and attended PRAGMA workshops since 2006.
- * National Applied Research Laboratory (NARL, www.narl.org.tw/en) was established in 2003 to consolidate nine national laboratories into a single non-profit organization to construct, operate, and maintain the large-scale R&D facility or platform in support of the academic research and foster the necessary manpower in various advanced fields focused by the nation. NCHC is one of the laboratories in NARL. NARL has provided leadership in the GEO working group, and can bring to bear several other laboratories at NARL for PRAGMA collaborations.
- * Universidad de Chile (UChile, www.uchile.cl), located in Santiago, has contributed resources to the PRAGMA grid, attended the PRAGMA 7 workshop and has since become the lead of Chile's national grid initiative (CLGrid). In January 2006 the Center for Mathematical Modeling (CMM, www.cmm.uchile.cl) of UChile invited all Chilean universities to participate in the local grid initiative. The objective was to develop grid scientific applications of national interest having PRAGMA as the main reference to follow. Currently, eight universities are actively participating and have carried out four workshops, an Intel software college, and grid programming PRAGMA grids. CMM is contributing to develop a multi-user data farm (based onGfarm) in conjunction with UPRM and CPTEC. Nowadays CMM is getting funding to push CLGrid to the next level of grid deployment, test-beds and international collaboration.
- * Universidad Nacional Autónoma de México (UNAM, www.unam.mx), located in Mexico City, has contributed resources to the PRAGMA grid, attended the PRAGMA 7 workshop, and was an original lead of Mexican grid efforts via CUDI.
- * University of Puerto Rico at Mayaguez (UPRM, www.uprm.edu), located in Mayaguez, Puerto Rico, has contributed resources to PRAGMA grid, attended the PRAGMA 13 workshop and is running a sensor data analysis application in PRAGMA grid.
- * Center for High-Performance Computing (www.chpc.utah.edu) at the University of Utah has contributed resources to the PRAGMA grid for use with the CSE-Online cyberenvironment.
- * Organic Chemistry Institute Grid Competence Center (GC3), UniZH (www.oci.unizh.ch) located in Zurich, Switzerland, has contributed resources to the PRAGMA grid and been involved in PRAGMA meetings from early on. GC3 researchers are involved in computational chemistry activities, including projects with Nimrod, GAMESS, APBS, Unicore and Kepler. They have mentored PRIME students.

BROADER COMMUNITY INTERACTIONS

PRAGMA members have been involved in helping organize workshops and symposia in grid technologies and application of the grids. This vehicle strengthens dialogue between PRAGMA members and the broader community. In the last year, PRAGMA members have helped organize workshops or special sessions or have participated at *International Workshop on Advanced Computing and Applications 2007, Taipei Int. Digital Earth Symposium* (May 2007), *30th Congress of the Int. Association of Theoretical & Applied Technology* (Aug 2007), and *High Performance Computing Asia* (Sept 2007). Furthermore, PRAGMA members have participated in *Supercomputing 2003-2007*, demonstrating PRAGMA members' collective accomplishments. Future meetings involving PRAGMA members and the community include such activities as the *Int. Conference on Convergent Technology & Information Convergence* (Fall 2007) and the *3rd IEEE Int. Conference on e-Science & Grid Computing* (Dec 2007). See www.pragma-grid.net/calendar.htm for more information.



OTHER PROJECTS AND ORGANIZATIONS

Other projects and organizations have collaborated with PRAGMA activities.

- The California Institute for Telecommunications and Information Technology (Calit2; www.calit2.net) has provided space for PRAGMA activities and visitors at Atkinson Hall, the new home of its UCSD division. Calit2 is promoting the use of OptIPortal Technology and invites participation in the CAMERA project (camera.calit2.net). Furthermore, Calit2 has provided support for students of PRIME.
- The National Biomedical Computation Resource (NBCR; nbcr.net) is a National Institutes of Health National Center for Research Resources project and involves researchers at UCSD, The Scripps Research Institute, and Washington University. NBCR's goals are to conduct, catalyze and enable multiscale biomedical research through development, deployment and use of advanced cyberinfrastructure. NBCR has developed software (OP—an application wrapper) extended by PRIUS students (Opal OP) and its researchers are central to the Avian Flu Grid project. Further, an NBCR researcher co-developed GAMA, a complete GSI credential management software, which is being used by the Resources and Data, as well as the GEO Working Groups.
- National Center for Imaging and Microscopy Research (NCMIR, ncmir.ucsd.edu) is a National Institutes of Health National Center for Research Resource at the University of California San Diego. NCMIR's interdisciplinary staff develops state-of-the-art 3D imaging and analysis technologies to help biomedical researchers understand biological structure and function relationships in cells and tissues in the dimensional range between 5 nm³ and 50 fm³. NCMIR has helped pioneer the remote control of instruments via use of information technology, and have played a fundamental role in many of the Telescience Working Group activities.
- The Global Lake Ecological Observatory Network (GLEON, gleon.org) is a grassroots network of limnologists, information technology experts, and engineers who have a common goal of building a scalable, persistent network of lake ecology observatories. GLEON is built on earlier projects in Telescience Working Group and PRAGMA catalyzing a relationship between the EcoGrid project of NCHC's and the North Temperate Lakes Long Term Ecological Research (www.lternet.edu/sites/ntl) project at the University of Wisconsin. It has been supported by the US National Science Foundation, the Gordon and Betty Moore Foundation, National Science Council Taiwan, and member institutions. An additional key partner in launching GLEON is at the Center for Biodiversity and Ecology Research, University of Waikato, New Zealand (cber.bio.waikato.ac.nz).
- The Coral Reef Ecological Observatory Network (CREON; www.coralreefeon.org) is a collaborating association of scientists and engineers from around the world striving to design and build marine sensor networks. It also grew out of the Telescience Working Group activity. Its growth has been supported by the Gordon and Betty Moore Foundation, the US National Science Foundation, the National Science Council Taiwan, and member institutions. There are strong collaborations between NCHC, Academia Sinica, the Moorea Coral Reef Long Term Ecological Research site (mcr.lternet.edu), and the Australian Institute for Marine Science and James Cook University, Australia.
- The Open Science Grid (OSG; www.opensciencegrid.org) is a collaboration of science researchers, software developers and computing, storage and network providers. OSG members come from universities, national laboratories and computing centers across the United States. OSG's mission is to help satisfy the ever-growing computing and data management requirements of scientific researchers, especially collaborative science requiring high-throughput computing.
- The Global Cyberbridges Project (GCB; www.cyberbridges.net), located at Florida International University (FIU) is a U.S. implementation of multi-national efforts to improve the technology training for a new generation of scientists, and to increase the rate of discovery for all domains. The project has committed participation from the Computer Network Information Center of the Chinese Academy of Sciences, the City University of Hong Kong, and the University of Sao Paulo's School of the Future of Brazil.

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Image: PRAGMA 12 Bangkok (Source: NECTEC)

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