
PRAGMA
COLLABORATION OVERVIEW
2011-2012
KEY
PRIME
EXPERTISE
CHEMISTRY
MANY
GROW
RESEARCH
MULTIPLE
SUCCESS
INVOLVED
CENTER
BUILDING
TOGETHER
DEMONSTRATED
SDSC
MAKE
RECOVERY
NEW
PARTNERS
UNDERGRADUATE
UNIVERSITY
REGION
CYBERINFRASTRUCTURE
MAN-MADE
TECHNOLOGY
APPLICATIONS
COLLABORATION
HIGH-PERFORMANCE
REEF
INSTITUTIONS
EARTHQUAKES
SCIENTISTS
INFORM
SARS
GEOGRID
BUILD
CONTINUE
NATIONAL
CONTRIBUTE
HOSTI
FU
INTERNATIONAL
SCIENCE
NETWORK
PEOPLE
REGIONAL
EXPLOITING
STRONG
GLOBAL
ASIA
PRAGMA
WORK
ACTIVITIES
COMPUTING
STUDENTS
UNDERSTANDING
COLLABORATIONS
AREAS
USE
VARIETY
CHALLENGES
KNOWLEDGE
REGARDLESS
RANGE
ONE
ENABLE
MEMBERS
TECHNOLOGIES
FOCUS
RESOURCE
WELL
KOREAN
MODELS
BASED
AIST
UCSD
ADVANCED
ECOLOGICAL
SENSORS
INFORMATION
NEEDS
SYSTEMS
MODELING
NATURAL
ENSURE
NOW
MURPA
PRACTICES
DISPLAY
LEVELS
YEARS
SITES
SCIENTIFIC
AMONG
RANGING
PROGRESS
APPROACHES
ENVIRONMENT
PROGRAMS
SENSOR
EASIER
IMPACT
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MARCH
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VARIOUS
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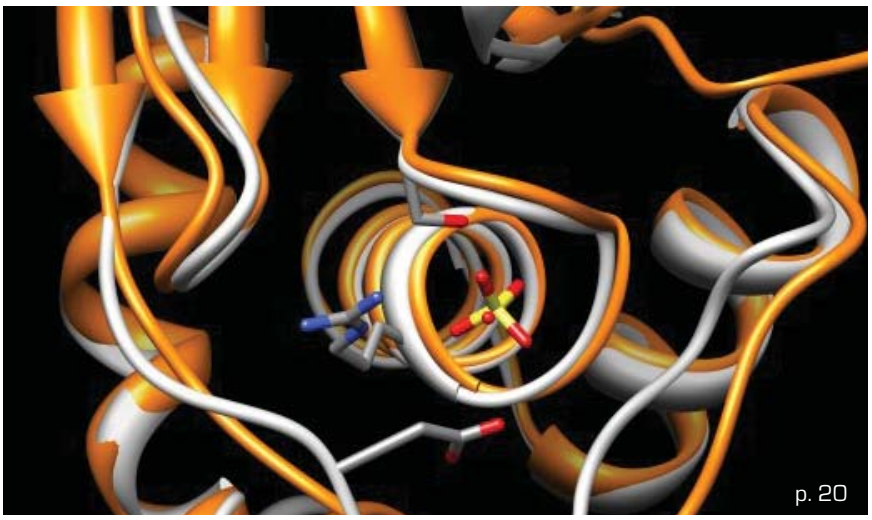
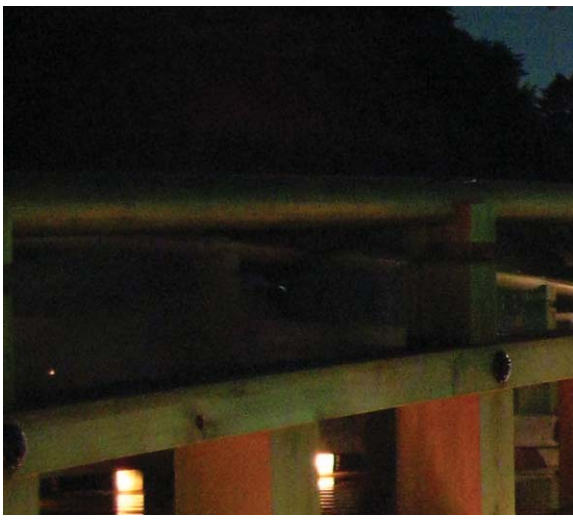


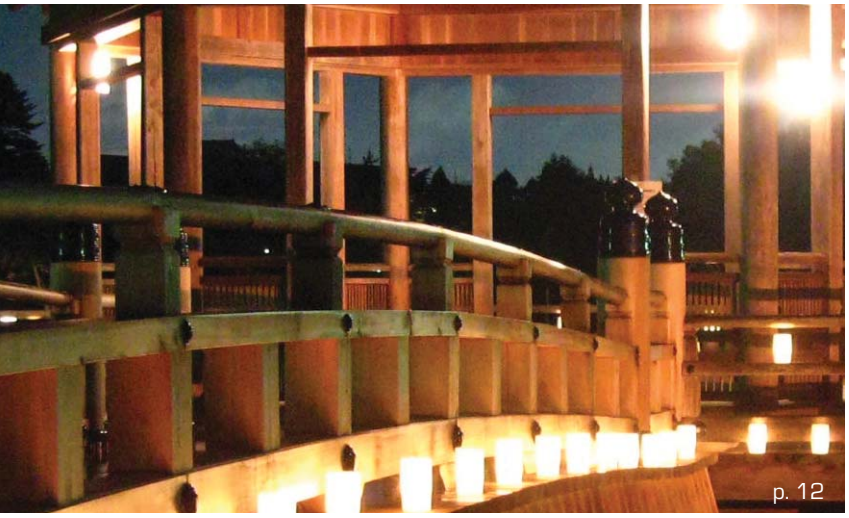


PRAGMA will be 10 years old in March 2012!

INTRODUCTION

In 2002, we started small with just 13 institutions involved; now we have more than 30 member or affiliate institutions. More than numbers, what began as a few relationships has grown into a very strong and vibrant community based on a project- and people-focused collaboratory environment which supports and advances a diversified range of scientific research and trains the scientists of today, as well as tomorrow, for current and future technological challenges. Bringing together both the expertise and scientific needs of each participant and research group or institution, PRAGMA has accomplished a great deal during our first 10 years. Here are some of our highlights:

- Mobilized a global response to the needs of colleagues at the National Center for High-performance Computing (NCHC) in Hsinchu, helping to apply technology solutions to the healthcare crisis caused by the SARS virus.
- Contributed to launching local and regional grid efforts of PRAGMA members at Universiti Sains Malaysia (USM), ThaiGrid, NCHC, Jilin University (JLU), Lanzhou University (LZU), GEO Grid of the National Institute for Advanced Industrial Science and Technology (AIST), as well as Advanced Science and Technology Institute (ASTI), Institute of Information Technology (IOIT), and Universidad de Chile.
- Improved and globally disseminated multiple cluster and grid software applications from members, covering a wide range of fields: Ninf-G (AIST), Gfarm (AIST and U Tsukuba), Nimrod (Monash U), Duckling (Computer Network Information Center [CNIC]), Rocks (San Diego Supercomputer Center [SDSC]), CSF4 (JLU), e-AIRS (Korea Institute for Science and Technology Information [KISTI]), SCE (Kasetsart U [KU]), Opal (National Biomedical Computation Resource [NBCR]), DataTurbine (University of California, San Diego [UCSD]), and SAGE (UIC).
- Collaborated with the Asia Pacific Grid Policy Management Authority (APGrid PMA) and promulgated security standards and practices among our members and affiliates.
- Engaged application scientists and supported applications on the PRAGMA Grid. Examples include: modeling the spread of volcanic ash in Costa Rica (Núñez 2010); understanding the impact of Savannah burns on climate (Lynch 2007); and gaining insights into a variety of computational chemistry applications (Ikegami 2007, Sudholt 2004).
- Provided a testbed platform from pilot work of NCHC's EcoGrid activities, which lead to the Global Lake Ecological Observatory Network (GLEON) organization (now with more than 300 members), the Coral Reef Environmental Observatory Network (CREON), and other regional activities such as the Korean Lake Ecological Observatory Network (KLEON).
- Created training programs for members and students, ranging from the Southeast Asia International Joint Research and Training Program in High-Performance Computing Applications and Networking Technology (SEAIP), to programs that support undergraduate and graduate student internships abroad: PRIME, PRIUS, and MURPA.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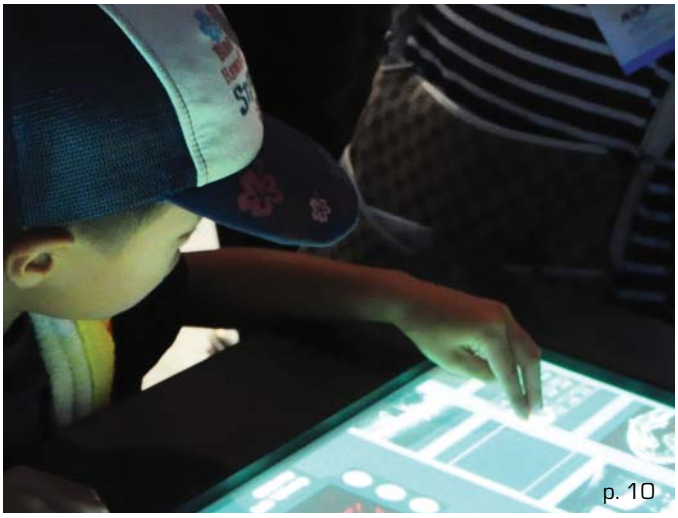
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One of the motivations for creating PRAGMA was to ensure that the vision of a truly global grid was realized, one where grids from different locations would work together to advance science, despite being funded from different sources at local or regional levels. This entailed building a forum for both an open exchange of ideas as well as a framework to work towards that vision. We use applications to drive forward the development of those technologies using multi-institutional collaborations. Success required building up expertise, creating an environment of trust, and establishing best practices to MAKE THE GRID USEFUL FOR APPLICATIONS (Zheng 2007, Abramson 2006). Still, using the heterogeneous multi-grid remains difficult at best.

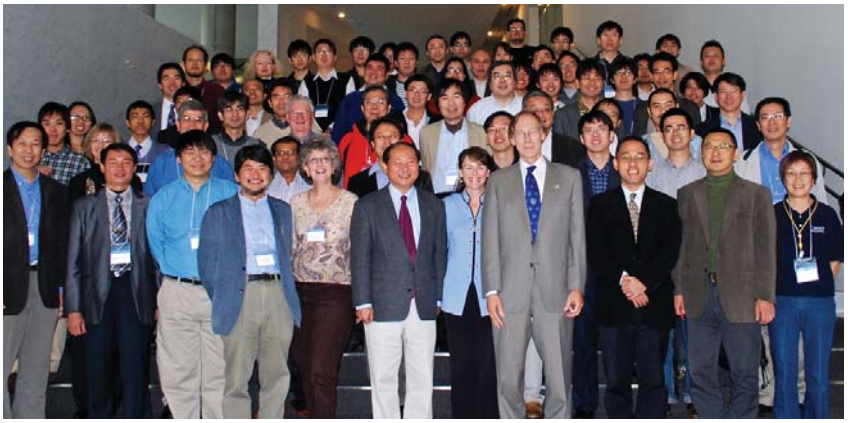
Keeping on top of the ever-changing technology landscape, PRAGMA has built its expertise in virtualization over the past two years, moving its focus from grids to cloud computing, with the goal of making them more readily useful for applications. Last year, PRAGMA demonstrated how to replicate a virtual machine (VM) image onto several hosting servers with a common hosting environment. In this Collaborative Overview we highlight PRAGMA's success in migrating images to multiple sites that use different operating systems and different hosting environments. This approach makes possible the availability of more applications by and for users (through PRAGMA-authored images), easier access to more resources (via providers such as Amazon's EC2), and the ability for resource providers to migrate services during times of natural disasters such as earthquakes or man-made disruptions such as power outages. As explained in this overview, this technology approach has allowed AIST's GEO Grid to provide disaster recovery services via PRAGMA partners NCHC and SDSC in the aftermath of the March 11, 2011 earthquake in Japan (Matsuoka 2011).

Another high point this year is the contribution of PRIME and MURPA undergraduate students to a variety of areas, including enhancing multi-touch display table technology in order to display photographs from the Museum of Photographic Arts (in San Diego, CA) at the Knowledge Capital Trial in Umeda, Osaka. The display at this exhibit represents the culmination of a multiyear collaboration with multiple partners. Students also contributed to earthquake research following significant events in New Zealand this year and Taiwan last year. Collectively, the PRIME and MURPA students have helped build collaborations among PRAGMA partners, enhanced the PRAGMA infrastructure, and generated new knowledge in a variety of fields.

Future PRAGMA activities will build on our past successes and will focus on three key thematic areas:

1. EXPERIMENTING WITH AND EXPLOITING NEW TECHNOLOGIES, VIA THESE THREE ACTIVITIES:
   - Building the computational and data cloud, to make the use of applications easier.
   - Exploiting the ubiquity of sensors throughout our natural and man-made environments and the explosion of sensor and instrument data, to inform our models and understanding of the world.
   - Utilizing visualization and collaboration technologies to understand the data and models, collaborating regardless of whether researchers are together in one location or geographically dispersed.
2. ADDRESSING APPLICATION AREAS IMPORTANT TO THE SOCIETAL CONCERNS OF THE REGION. THE FOUR CHALLENGE AREAS ARE:
   - Disaster Mitigation: Beyond disaster recovery of key services and systems is understanding the impact from earthquakes and flooding on structures and transportation, as well as modeling responses using sensor and other data input.
   - Environmental Observing and Modeling: We will continue to grow strong ties with lake and coral reef ecologists, and will expand into the areas of biodiversity and understanding chemical or molecular distribution based on soil chemistry.
   - Health: This is a concern, not only because of the SARS and Avian Flu outbreaks, but also because many of the world's neglected diseases (a group of tropical infections) originate in the region. We have already taken steps to create tools that will enable better approaches to identifying possible candidate targets to active sites of the proteins involved, and now plan to integrate various tools from across PRAGMA.
   - Cultural Interaction and Preservation: Finally, as our globe becomes increasingly connected, sharing local and regional cultural heritage allows for greater understanding of a region and the variety of people in it.

3. CONTINUING TO GROW COLLABORATIONS AND PEOPLE: WE ARE PURSUING TWO APPROACHES
   - To make progress in these application areas requires building a broader group of expertise in areas ranging from the application sciences to computer and information science and engineering.



Images, above: A view of Amanohashidate, one of the "three views" of Japan—courtesy of Wesley Hsu; below left to right: Burmese Buddist Temple, Penang Malaysia—courtesy of Peter Arzberger; PRAGMA 21 group photo—courtesy of Teri Simas

The technologies of both cloud computing and sensors have many unanswered questions, and the driving areas require multidisciplinary approaches to make progress.

- Furthermore, we will engage students at various levels of their careers to demonstrate the excitement of these areas and the value of international collaboration, thus growing our community for the future.

Technology changes and applications evolve; the one constant is the people. Our approach will continue to focus on building the people connections to ensure the creation of sustainable, adaptable collaborations. Retaining the creativity of people to address the new challenges, bringing in new people to PRAGMA, and providing others with the technology are all critical for continued success in our future.

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HIGHLIGHTS

The Virtual Machine (VM) Migration Experiment: From Grid to Cloud – Phase 2

OVER THE LAST TWO YEARS, PRAGMA HAS SHIFTED ITS FOCUS FROM GRID TO CLOUD COMPUTING. The PRAGMA Cloud infrastructure is heterogeneous, consisting of different architectures, based on local needs and decisions. We continue to pursue the goal of making new technology easy to use for researchers, enabling them to advance science and global-scale collaborative research. Pursuing this goal requires us to seek out methods to ensure interoperability of many different architectures and clouds. Our approach is to allow users to author their own application virtual machines (VMs) using their preferred VM platforms, then deploy these application VMs and make them available on demand via various PRAGMA Cloud sites. To achieve this objective, we set out to develop automated VM migration systems.

Earlier this year, we explored the practical issues involving VM migrations between different platforms starting with a pilot project among three PRAGMA sites: SDSC/UCSD, AIST, and NCHC. UCSD and AIST were running Rocks Xen VM hosting servers; NCHC was running KVM hosting servers. We manually migrated three different application VMs among the three sites: (F-motif—authored on KVM, GEO Grid and Bloss (a parallel eignesolver developed by AIST, based on the block Sakurai-Sugiura methods), both authored on Rocks Xen. We found that it is not only possible to migrate VMs among different platforms, but quite easy to do so. Detailed steps are documented at **goc.pragma-grid.net/mediawiki-1.16.2/index.php/VM_deployment**.

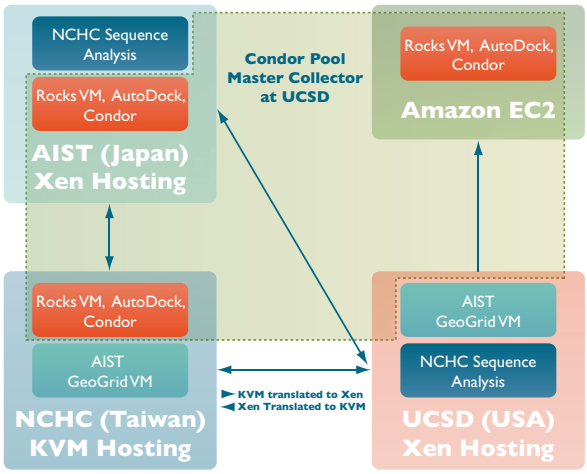

Figure 1: Three-site VM Portability Experiment. Each site authored a virtual machine (VM) and ran it at the other two sites. Conversions of VM formats were also managed

At PRAGMA 20 (March 2011, Hong Kong), the three pilot sites demonstrated this Phase 1 experiment and findings. These results have excited many PRAGMA sites and motivated them to join this effort. Since then, seven more sites have set up VM hosting services and migrated the three application VMs. These sites are: Indiana University (IU), ASTI, MIMOS, LZU, Osaka University, CNIC and University of Hyderabad (UoHyd).

Inst.	Region	Host Name	nodes	CPUs	Mem.	Disk Space	CPU Speed	VM Platform	System	VM Manager	OS Release
AIST	Japan	pragma-v	32	64	768GB	600TB	2400MHz	KVM	Cluster	OpenNebula	Linux kernel 3.0.4
ASTI	Phillipines	one	10	80	160GB	5TB	2000MHz	Xen	Server	OpenNebula	2.6.18-238.19.1.el5
CNIC	China	cluster	1	2	128GB	2TB	2400MHz	Xen	Server	Rocks 5.4.3	2.6.18-238.19.1.el5xen
IU	USA	pragma	8	16	128GB	12TB	2000MHz	Xen	Cluster	Rocks 5.4	2.6.18-194.17.4.el5xen
LZU	China	vm	1	8	16GB	1TB	4122MHz	KVM	Server	Rocks 5.4	2.6.18-238.12.1.el5
MIMOS	Malaysia	vm	6	12	192GB	1TB	2400MHz	KVM	Cluster	Eucalyptus	2.6.18-194.11.1.el5
NCHC	Taiwan	Snowfox	8	64	128GB	2TB	2500MHz	KVM	Cluster	OpenNebula	2.6.18-194.11.1.el5
OSAKA U	Japan	cider	3	24	34GB	3TB	2270MHz	Xen	Cluster	Rocks 5.4	2.6.18-194.17.4.el5xen
SDSC	USA	fiji	18	25	380GB	10TB	2261MHz	Xen	Cluster	Rocks 5.4	2.6.18-194.17.4.el5xen
SDSC	USA	rockstar	32	64	512GB	16TB	2000MHz	Xen	Cluster	Rocks 5.4.3	2.6.18-238.19.1.el5xen
SDSC	USA	pragma-kvm	1	4	32GB	1TB	3200MHz	KVM	Server	Rocks 5.4	2.6.18-238.12.1.el5xen
UoHyd	India	venus	4	4	16GB	4TB	2400MHz	Xen	Cluster	Eucalyptus	2.6.18-194.11.1.el5
Totals			124	367	2494GB	657TB					

Table 1. PRAGMA Cloud Resources. Note: All systems employ CPU model x86_64.

> "Above all, PRAGMA brings great value to CCST in terms of broadening international collaboration, engaging applications, publishing scientific papers, and cultivating student." **Jilin University**

PRAGMA Cloud Resources

During the PRAGMA 20 Workshop, in addition to expanding the number of sites involved in the experiment, the Resources Working Group set its sights on automating the VM deployment process, and decided to use Gfarm to deposit and share VM images among PRAGMA Cloud sites.

For the second phase of the VM migrations experiment to implement a PRAGMA Cloud, the three pilot sites (AIST, NCHC, and SDSC/UCSD) led the development on three fronts that (1) automated the VM migration process, (2) authored application VMs, and (3) built Gfarm file system. Descriptions follow.

Automating the VM Migration Process

Based on what we learned from our VM migration Phase 1, the SDSC/UCSD team developed the vm-deploy script which fetches a user-specified VM image from Gfarm, modifies it, then boots it up on a VM hosting server (**goc.pragma-grid.net/mediawiki-1.16.2/index.php/VM_deployment_script**). The performance to date is acceptable; our testing showed that for a 1GB VM image file in Gfarm, it takes the script a total of about 2.5 minutes to get the VM instance up and running. AIST and SDSC/UCSD worked together closely to test the script with new application VMs on an Open-Nebula platform, thus enhancing its functionality and portability. NCHC worked on automating the process of packaging applications into VM images, so that domain scientists can easily create application VMs without having to learn about VM technology. The QEMU Copy On Write (qcow) is used to implement the differential backup for the application VM image which will use the existing image as the base, and thus

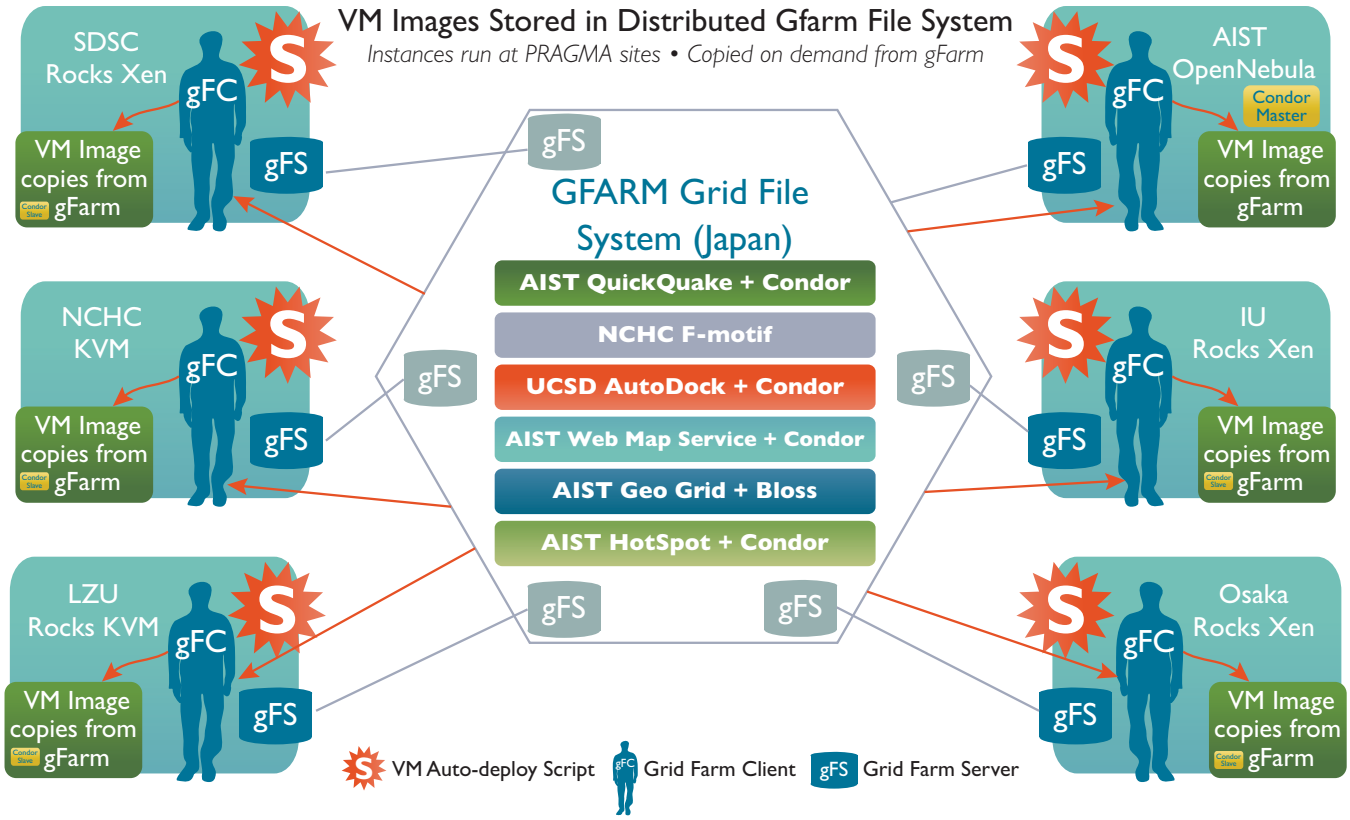

Figure 2: VM Migration Experiment, Phase 2

to reduce the storage space needed for the VM storage. In addition, the boot up speed of the virtual machine will be largely increased.

Authoring real science application VMs

Since the PRAGMA 20 Workshop, AIST has authored three timely and important application VMs that aid recovery from and scientific investigation of the earthquake/tsunami disasters that impacted Japan in March 2011 (see the next highlight, Disaster Recovery of Critical IT Infrastructure and Services, for details):

1. Web Map Service: Geological research service
2. Hot Spot: Enables real-time high-temperature detection from satellite data
3. QuickQuake: Generates ground motion map of earthquake

Building Gfarm file system

Working closely with the University of Tsukuba (U Tsukuba), the Gfarm development team, UCSD/SDSC built a Gfarm metaserver, tested the Gfarm file server and Gfarm client setup, and developed a Gfarm roll, i.e., the Gfarm software is packaged to install easily and be operated in the Rocks environment (**goc.pragma-grid.net/mediawiki-1.16.2/index.php/Gfarm**). This facilitated speedy deployment of Gfarm among PRAGMA sites. By PRAGMA 21 (October 2011, Sapporo), a total of seven sites (SDSC, AIST, NCHC, IU, LZU, Osaka U, and CNIC) have installed and setup Gfarm software, of those, four sites (SDSC, LZU, Osaka U, and IU) used the Gfarm roll.

At the time of the PRAGMA 21 Workshop, we have merged all these efforts together, deposited three new important application VM images in Gfarm, and deployed them on demand among the six sites with automated deployment tools, such as vm-deploy script and other mechanisms including cluster toolkit and cloud middleware (e.g., Rocks, OpenNebula, etc.). The new application VMs include Condor. When a VM instance boots up on a VM hosting server, it contacts a Condor master node running at a user site (in Fig.2, located at AIST). Application users are able to take control of scheduling and run jobs through Condor. We have included Amazon's EC2 in the mix of resources.

With this technology now tested we will work to encourage users to author VMs, and to use the growing PRAGMA Cloud infrastructure. Furthermore, we will continue to develop solutions to the general issue of cloud interoperability and experiment with approaches to expand the handling of larger data sets.

The approach described above for VM migration has implications for disaster recovery of critical services during major disruptive events.

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Disaster Recovery of Critical IT Infrastructure and Services

Disruptive and destructive events are a reality of our world, both through natural forces and man-made actions (intentional or accidental), e.g., earthquakes, tsunamis, hurricanes and storms, subsequent flooding, fires, power outages, and large-scale equipment or systems failures. In 2011, one of our PRAGMA members, AIST, suffered a sustained power outage (along with structural damage to buildings) due to the major earthquake and resulting tsunami on 11 March 2011 that devastated parts of Japan. Less catastrophic, but with negative impact, SDSC/UCSD has recently suffered two power outages within a five-week window (5 August 2011 and 8 September 2011). Both AIST and SDSC operate essential services for the global research community, which were severely disrupted.

In addition, the impact of the flooding in Thailand and ensuing destruction of property and the disruption of services from NECTEC and at Kasetsart University is not fully understood, but will be extremely high.

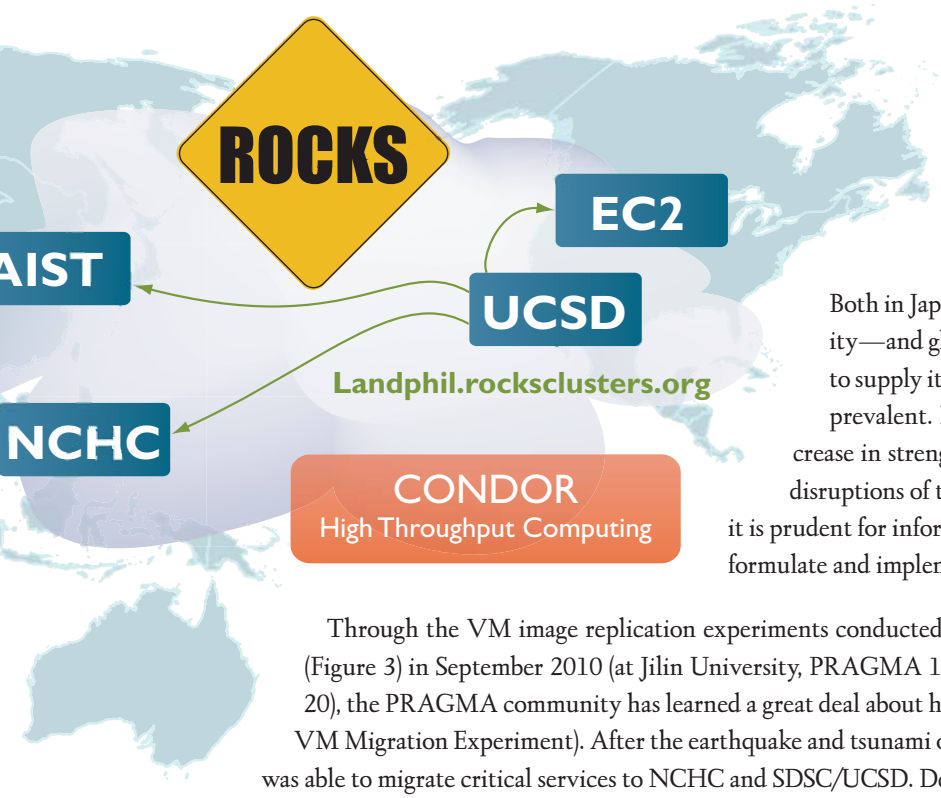


Figure 3: The VM migration experiment efforts involving AIST, NCHC and SDSC/UCSD enables quick migration of critical services in response to disasters.

Both in Japan—where the country is rethinking its sources of electricity—and globally, as the demand for energy increases while the ability to supply it stays constrained, power outages are likely to become more prevalent. In addition, if storms such as typhoons and hurricanes increase in strength (as many believe they will), there will likely be further disruptions of the power supply in an increasing number of regions. Thus, it is prudent for information technology infrastructure and services providers to formulate and implement procedures for disaster recovery of key services.

Through the VM image replication experiments conducted by PRAGMA members AIST, NCHC, and SDSC/UCSD (Figure 3) in September 2010 (at Jilin University, PRAGMA 19) and March 2011 (at Hong Kong University, PRAGMA 20), the PRAGMA community has learned a great deal about how to migrate services in a cloud (see previous highlight on VM Migration Experiment). After the earthquake and tsunami of 11 March 2011, AIST, through its GEO Grid Task Force, was able to migrate critical services to NCHC and SDSC/UCSD. Details of specific contributions follow.

The GEO Grid activity offers several services: satellite imagery (including observation of stricken areas); geological maps; and hazard information, which includes a strong ground motion map based on observation records of seismic networks and geomorphologic conditions in Japan. These tools support a range of critical uses: emergency response, research into tsunamis and structural damage, and restoration and rehabilitation of civilian life and economic activities to the broad-scale and long-term disaster. The services have been designed and developed based on three requirements. The first is "redundancy." Several services, such as the data processing procedures and distribution computational functions of the GEO Grid, were migrated to external servers and a cloud system to obtain stable and redundant operations. The second requirement is "rapidity." High-speed automatic data processing requires using high-performance computers. The third requirement is "standardization." Most of the geographic information is open to the public as Web Map Service (WMS) and Google Earth Keyhole Markup Language (.kml/.kmz), which are international standard protocols for geographic data. Beginning in May, updating of the GEO Grid services content is again being performed at AIST. The contents and footsteps are shown on the specially created disaster website (**disaster-e.geogrid.org**).

The need to have persistence of services during and after a disaster motivated the current experiment to provide flexibility of cloud resources. It will continue to influence PRAGMA's research directions on issues of interoperation of clouds, trustworthiness of systems, and in the use of the PRAGMA Cloud.

Specific Contributions of PRAGMA Partners NCHC and UCSD

Within a few days of the request for help, NCHC began allocating resources (Naruto cluster, details below) and set up a Gfarm platform for AIST. AIST then migrated its applications, including QuickQuake, Hot Spot and WMS Server onto the VM cluster—dynamically generated by the Ezilla-Cloud WebOS by NCHC (Figure 4). The VM cluster is running on an existing cluster and shares resources with other applications. In addition to the

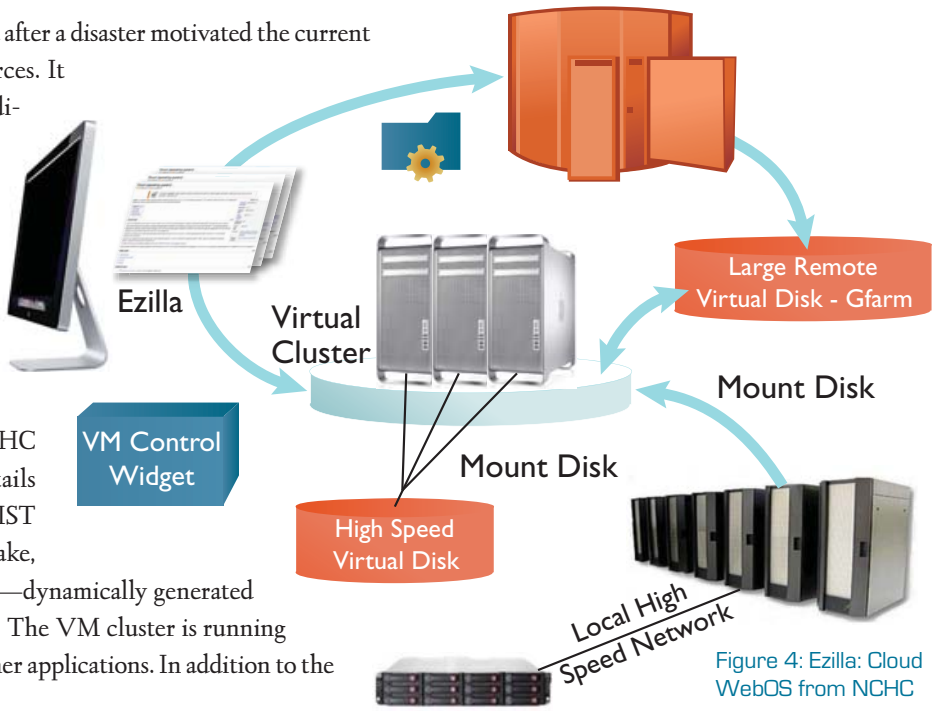
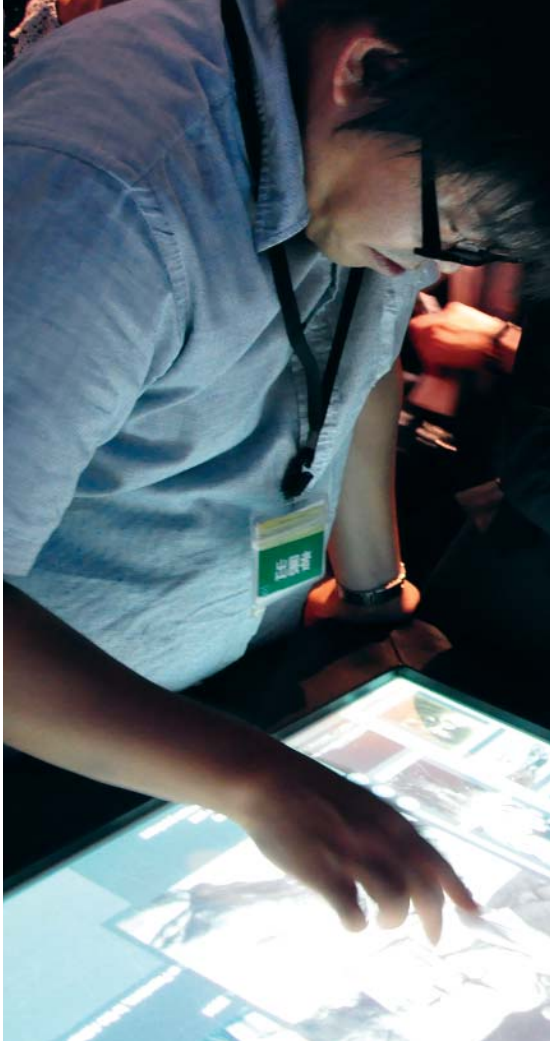


Figure 4: Ezilla: Cloud WebOS from NCHC



storage space provided by Gfarm, the "high speed virtual disk" was also mounted from the NCHC storage system once the VM was generated by the Ezilla. With the experience of VM migration from the experiments between AIST, SDSC/UCSD, and NCHC, the environment to host the critical services from AIST was in place without much effort. The services were fully implemented and stable in July and are still running today.

NCHC provided the Naruto cluster, consisting of 16+1 nodes, with the following specifications:

- CPU: 4-core 2.0 GHz Intel Xeon E5335 * 2 (8 cores/node)
- MEMORY: Total 32x16 GB = 512GB
- DISK: 2TB
- INTERCONNECT: DDR InfiniBand +1GE

We use eight nodes for daily operation and another eight nodes for R&D and testing. The daily-operation WMS servers provide information about the disaster area. The average daily access numbers for the WMS servers on Naruto for April through September 2011 are summarized below:

	Hit	Files	Pages	Visits
April	16828	14514	13241	485
May	14514	14132	12766	500
June	12560	12038	11736	782
July	12406	11997	11951	1095
August	9628	9132	9164	888
September	6928	6537	6639	674

SDSC/UCSD provided the Triton cluster (**tritonresource.sdsc.edu**). Triton requires job submission to be done via the batch system; therefore it is not appropriate for interactive and emergency use. So, Triton was used for generation of the ground motion map of the March11 Tohoku Pacific Ocean Earthquake covering all of Japan to observe and analyze the earthquake. The movie is available on the GEO Grid Disaster Task Force website. Approximately 1500 jobs were submitted to Triton, each of which took 3-4 hours to process, utilizing one CPU.

PARTICIPATING RESEARCHERS: *AIST*: Masashi Matsuoka, Satoshi Sekiguchi, Yoshio Tanaka, and the GEO Grid Disaster Task Force (Lead M Matsuoka); *NCHC*: Weicheng Huang, Serena Pan; *SDSC/UCSD*: Philip Papadopoulos.

Note: Many other groups in Japan and internationally provided resources and software, including Open Cloud Consortium (OCC)/University of Illinois at Chicago (UIC), R. Grossman

My Gallery Interactive: Engaging Museum Audiences with Technology

New technologies are allowing museums to engage visitors through innovative and interactive exhibitions. As part of this movement to enhance the visitor experience, the goal of this project is to create a crowd-sourced experience using a novel multi-touch table interface that allows users to experience and participate in the curatorial process in a fun and interactive way. This project was a unique collaboration between the Pacific Rim Undergraduate Experiences (PRIME) program at UCSD, the Museum of Photographic Arts (MOPA) in San Diego, and the National Institute of Information and Communications Technology (NICT) in Tokyo and Kyoto.

The hardware consisted of a frustrated total internal reflection (FTIR) touch table, developed by an undergraduate PRIME student from the previous year, Kevin Nguyen (PRIME 2010), that displayed the multi-touch interface and was coupled with a tiled-display-wall (TDW) to display user created photography galleries. The interface was based on the Open Exhibits multi-touch framework (Ideum, Corrales, NM) using ActionScript and Adobe Flash. This open source framework facilitated the construction of the interface and allowed for more creativity with

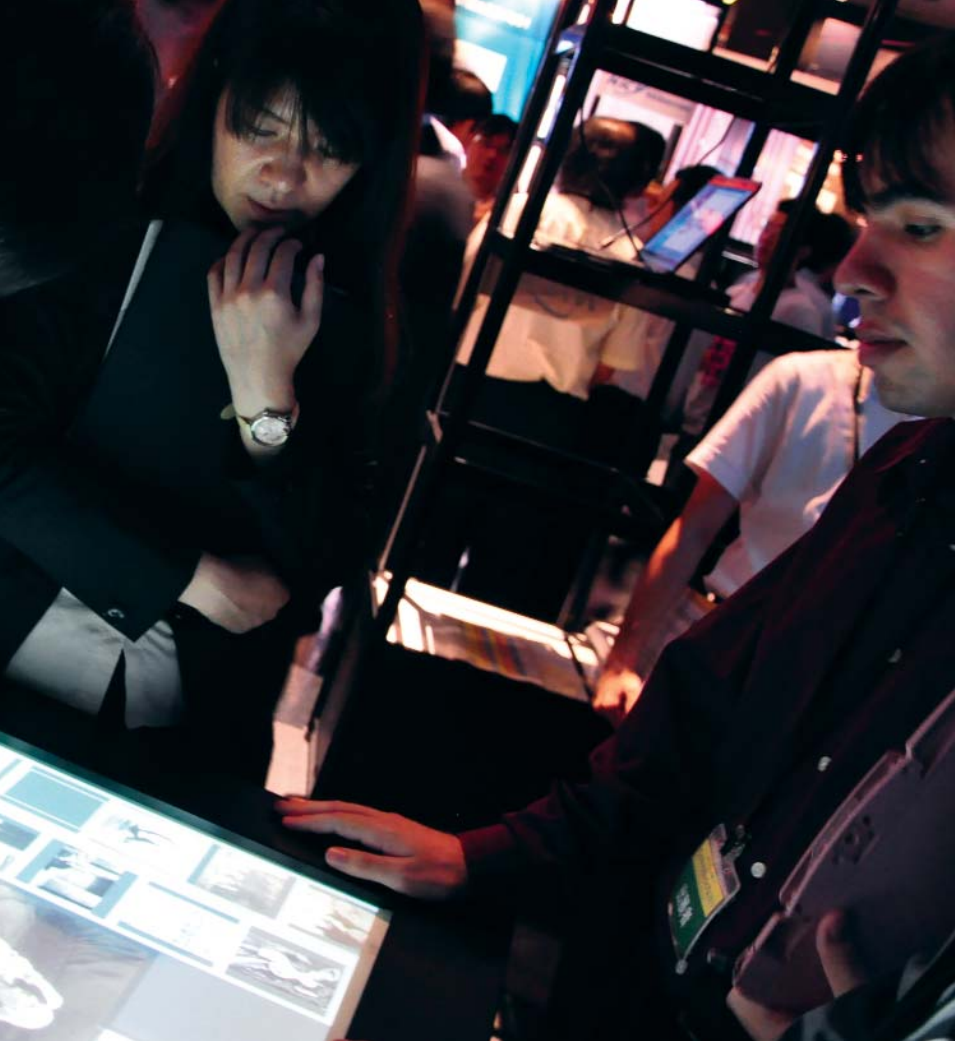


Image: MOPA touch-screen display at Knowledge Capital 2011 Exhibition, Osaka, Japan—courtesy of NICT

the user interface. Additionally, it was compatible with the FLOSC touch output data from the hardware.

The functionality of the My Gallery Interactive interface features three interactive screens. The main screen displays 50 images hand selected from MOPA's photography collection that are to be used for viewing and selecting images to create a user's mini gallery. Users can select up to 10 photographs to add to their own personal collection. A second screen enables the user to title their gallery in English or Japanese and subsequently save it. Finally, the third screen allows the user to view past collections that had been saved by other users. Collections can be sent to and shown on a 24-screen TDW, allowing a larger audience to view and engage with My Gallery Interactive.

The culmination of this work was demonstrated at the Knowledge Capital 2011 technology exhibition held in Osaka, Japan where NICT successfully showcased the fully functional interface to the public. There were over 12,000 visitors to the exhibit, and many became photography museum curators by creating their own galleries in an interactive manner, with over 50 individual galleries being created. This project harnesses the expertise of undergraduate PRIME students to complete the work and presents a new, exciting model for collaboration between museums and academic institutions interested in merging art and technology. For more information, see **www.calit2.net/newsroom/release.php?id=1915**.

PARTICIPATING RESEARCHERS: *PRIME 2011 Students:* Wesley Hsu, Lance Castillo; *MOPA:* Amber Lucero-Criswell, Joaquin Ortiz, Vivian Kung Haga; *NICT:* Masaki Chikama, Yoshinori Kobayashi, Tomoaki Takata, Shinji Shimojo; *UCSD:* Jason H. Haga

> "[While working on this project,] I was exposed to interface design, interdisciplinary collaboration, cross-cultural collaboration, gesture technology, team work, interpersonal communication, Japanese language, Japanese cuisine, business culture, [and] independence, just to name a few! It's fantastic to be given the opportunity to be exposed to all these things at once—it's a really great learning experience." **Wesley Hsu, PRIME 2011**

"Several of our students have benefitted by interacting with [PRIME students]. This has helped us to evolve a very vibrant academic and research group here in our department where every year several students register to work on problems related to grid and cloud computing." **University of Hyderabad**

PRIME & MURPA

MONASH UNIVERSITY, MELBOURNE

COMPUTER NETWORK INFORMATION CENTER (CNIC), CHINESE ACADEMY OF SCIENCES, BEIJING

DOSHISHA UNIVERSITY, KYOTO

NATIONAL INSTITUTE FOR INFORMATION AND COMMUNICATIONS TECHNOLOGY (NICT), TOKYO

OSAKA UNIVERSITY, OSAKA

UNIVERSITI SAINS MALAYSIA (USM), PENANG

UNIVERSITY OF AUCKLAND, AUCKLAND

NATIONAL CENTER FOR HIGH-PERFORMANCE COMPUTING (NCHC), HSINCHU

NATIONAL CENTER FOR RESEARCH ON EARTH-QUAKE ENGINEERING (NCREE), TAIPEI

NATIONAL TAIWAN UNIVERSITY (NTU), TAIPEI

TAIWAN FOREST RESEARCH INSTITUTE (TFRI), TAIPEI

TRAINING THE NEXT GENERATION OF RESEARCH LEADERS: PRIME AND MURPA

The Pacific Rim Experiences for Undergraduates (PRIME) program was created in 2004 to provide project-based, hands-on research internship program, combined with a cultural awareness experience for science and engineering undergraduates at UC San Diego. PRIME grew out of the PRAGMA collaborative framework and people network. PRIME's projects are based on PRAGMA collaborations, as well as additional collaborations between UCSD and PRAGMA researchers. 2011 was the eighth year of the program, sending 23 students to the 11 sites listed here, on the left. (For an overview of this year's students, please see **prime.ucsd.edu/PRIME2011_table.html**). To view the PRIME 2011 students' progress and final reports on their research and cultural interactions, please visit: **prime.ucsd.edu/student_collections2011.htm**). To date, more than 150 students have participated in PRIME.

In the summaries to follow, students report on results from several of this year's PRIME projects. Noteworthy in this year's students is their interest to make a difference to society in the work that they do. You can see this in the biomedical applications highlighted here as well as the examples where state-of-the-art technologies are used to help understand disasters or to bring cultural heritage to more members of society. Also of note this year is PRIME's partnership with the Network for Earthquake Engineering Simulation (NEES) in which we prototyped a joint program by accepting a NEES Research Experience for Undergraduate (REU) student from the University of Delaware into the PRIME program. This has helped us to understand the logistical challenges of creating such a joint program.

To strengthen the cultural aspect, PRIME has instituted a curriculum that begins students on a path of cultural awareness. We use the Intercultural Development Inventory (IDI) to measure the students' attitudes towards cultural differences. More about this index, as well as about PRIME, MURPA, and PRIUS programs, can be found in the following publications:

Images, background opposite page: Because I Was Thirsty," painted by an atomic bomb survivor, Hiroshima Peace Memorial Museum—courtesy of Iris Shieh; left to right: The Ukimi-do during Nara Light Festival in Nara Park—courtesy of Wendy Hsu; PRIME students Sarah Larsen and Matthew Religioso—courtesy of NICT; Sean Luong and Christopher Manco abseiling down Waitomo Caves—courtesy of Christopher Manco.

"Prime: An Integrated and Sustainable Undergraduate International Research Program" Arzberger, P., Wienhausen, G., Abramson, D., Galvin, J., Date, S., Lin, F-P., Nan, K., Shimojo, S. *Advances in Engineering Education*. 2010, Vol. 2, No. 2. (advances.asee.org/vol02/issue02/05.cfm).

Abramson, D., Arzberger, P., Wienhausen, G., Date, S., Lin, F-P., Nan, K. and Shimojo, S., "Cyberinfrastructure Internship and its application to e-Science," to appear, *e-Science 2011*, Stockholm, Dec 2011.

We are convinced that engaging students in research is essential to grow the next generation of scientists and that challenging them with an international experience prepares them to excel in the global workplace and participate in the forefront issues of science and society.

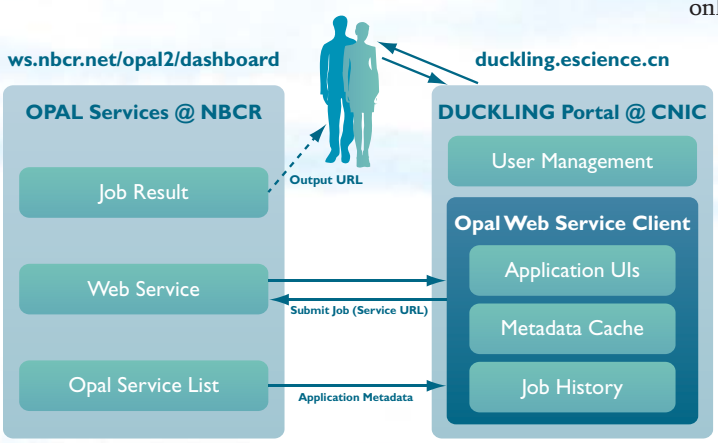
Integration of the Opal Web Service Client in Duckling Portal

The Opal Dashboard service, provided by the National Biomedical Computational Resource (NBCR) at UCSD, is a routine service for NBCR biomedical community users. The web services are also available to support remote access by a third party portal, DUCKLING. The DUCKLING portal, based on the open-source software DUCKLING, is a collaboration environment suite as well as a portlet container, which enables comprehensive resource sharing and collaboration specifically for research groups. DUCKLING is developed by the Collaboration Environment Research Center (CERC) at CNIC. PRAGMA has used the DUCKLING portal for all of its workshops beginning with PRAGMA18 (January 2010).

The goal of the project is to integrate an Opal web service client into the DUCKLING portal via the Opal web service interface. For this project, we have developed an Opal Dashboard with Duckling Portal, called the OPAL-DUCKLING Portal, which connects NBCR's OPAL web services and CERC's DUCKLING portal environment.

The OPAL-DUCKLING portal loads each application's metadata by the web service protocol and automatically generates all user interfaces and forms for the applications which are deployed at NBCR; it also submits remote jobs to NBCR OPAL servers according to the collected information and tracks job output URLs. It is designed to be an environment to integrate various remote services, such as job submission, service monitoring, and content publishing. User authentication and authorization are also available in the OPAL-DUCKLING Portal.

The integration of the Opal Web service client into the DUCKLING portal provides an open source collaboration environment where authenticated users may access scientific applications exposed as web services using the Opal toolkit. Because Opal servers cache user job output for only a limited amount of time, future development of OPAL-DUCKLING may support user data management, including access to the data cloud from the DUCKLING portal.



The dataflow between the DUCKLING portal and NBCR OPAL services.

ADDITIONAL INFORMATION: Opal Dashboard: ws.nbcr.net/opal2/dashboard; DUCKLING: duckling.sourceforge.net; OPAL-DUCKLING Portal: opal-duckling.escience.cn

PARTICIPATING RESEARCHERS: *PRIME 2011 Student, UCSD*: Brian Zhang; *CNIC*: Guangyuan Liu, Jianjun Yu, Kejun Dong, Kai Nan; *NBCR/UCSD*: Jane Ren, Wendy Fong, Wilfred Li

Background image: the Richmond Range, located in the South Island of New Zealand—courtesy of Christopher Manco

Augmented Reality in Android System with Disaster Response Application

The National Center for High-performance Computing (NCHC) has developed large tiled-display-walls (TDW), which are capable of very high resolution image display. Traditionally, the user interface with these large display walls includes a keyboard and mouse—just like those used with a regular PC. However, to take full advantage of such super high resolution display walls, a dynamic controller must be used so that a user can firmly engage with the space. Given the proliferation of new sensor-enabled, network-connected, portable devices, such as smart phones and tablets, this project explored a novel controller application using such a device. A tablet was chosen specifically for its large form factor and high computing power.

NCHC has a large dataset involving the Morakat Typhoon and its aftermath. Our application uses the tiled-display-wall to display a "before" image of an area in Kaohsiung, Taiwan. The "after" image is displayed on the tablet. The goal is that the user can hold up the tablet to the display wall and see the "after" image of the area on the wall which is covered by the tablet. By moving the tablet around the wall, the image on the tablet updates to always show the "after" image of the area behind the tablet. This project uses the Acer Iconia Tab A500 a 10.1 inch tablet running Android 3.0 (Honeycomb) and comes equipped with a gyroscope, accelerometer, compass, and both rear and front facing cameras. Also the Iconia boasts a Dualcore 1GHz ARM Cortex-A9 processor, a ULP GeForce GPU and a Tegra 2 T20 chipset. While our software reads out all of the sensors, currently only accelerometer and camera data are used for most of the application. The result is that the application works, but the tracking of the tablet location in front of the display wall needs improvement. Future work will include combining different sensor data for more robust findings, as well as filtering to smooth out jittery data.

PARTICIPATING RESEARCHERS: *PRIME 2011 Student, UCSD*: Jeanne Wang; *NCHC*: Fang-Pang Lin; Calit2/UCSD: Jurgen Schulze.

Developing a Database of Damage and Structural Performance of New Zealand Christchurch Earthquake-affected Bridges

The city of Christchurch, New Zealand experienced a series of destructive earthquakes over the past year. On September 4, 2010 a magnitude 7.1 earthquake struck the Darfield region of Canterbury, New Zealand. The epicenter of the earthquake was 40 km from the city of Christchurch, resulting in minor damage to the area's infrastructure. Subsequently, the area had hundreds of aftershocks, more than two dozen were 5.0 M or more, the worst of which was on February 22, 2011 (6.3 M). This one took place only 10 km south of Christchurch and caused more than 180 deaths, as well as significant damage to the surrounding area.

In order to better assess the seismic performance of bridges under earthquakes of this magnitude and frequency and help to inform decisions on the retrofit or replacement of damaged bridges, PRIME students Christopher Manco and Sean Luong developed a detailed database to collect damage and performance data on a small group of bridges affected by the recent earthquakes. Their responsibilities included documenting information on the foundation of each structure, calculating the mass of bridge components, traveling into the field to collect concrete samples and measurements, and categorizing evidence of damage progression. The compiled work was reviewed by researchers who will use the information to determine which bridges will be selected for detailed inspections. These case studies may reveal new findings about soil-structure interaction as a result of seismic activity and solutions to mitigate bridge damage.

During this project the PRIME students had the unique opportunity of traveling to Christchurch, New Zealand to gain hands-on field experience in structural engineering. The undergrads were able to observe firsthand how much the city was affected by the recent earthquakes. The seismic activity significantly damaged many of the multi-story buildings, deeming them unsafe. Most streets were blocked by fences and army patrols were positioned at street corners allowing access only to those who had authorization. The students also traveled to a suburban part of the area where many of the houses had been abandoned, leaving the streets desolate. Some of the homes only contained internal damage, but others leaned towards one side or displayed large cracks and gaps between their walls and the ground. The opportunity to participate on a reconnaissance mission following an earthquake is something many earthquake engineers dream of having the opportunity to do (including their UCSD mentor, Lelli Van Den Einde, from UCSD's department of Structural Engineering). This field experience demonstrated the significance an earthquake can have not only on structural systems, but on the community providing the students with a hands-on opportunity to learn about earthquake engineering, the technical requirements needed to design resistance to future earthquakes, and their devastating impact on communities.

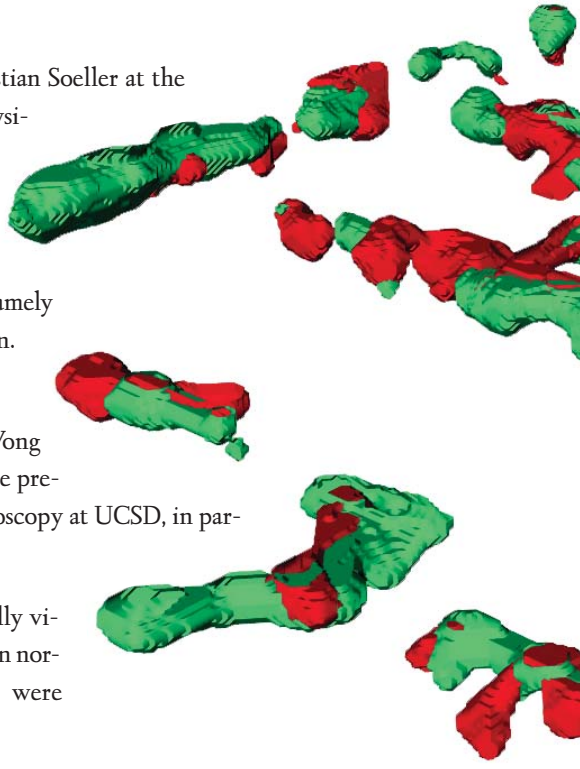
This PRIME project was part of a joint pilot program between PRIME and the Network for Earthquake Engineering Simulation (NEES) in an effort to develop an 'international research experience for undergraduates' program in earthquake engineering that will leverage the expertise of PRIME in the hopes of establishing long term ties between the two. Specifically, Christopher Manco is the first non-UCSD student to participate in PRIME.

ADDITIONAL INFORMATION: For more about their work as well as that of another PRIME 2011 student, Monica Chan, working at the National Center for Earthquake Engineering in Taipei, please see **www.calit2.net/newsroom/release.php?id=1890**.

PARTICIPATING RESEARCHERS: *2011 PRIME Students:* Sean Luong *(UCSD)*, Christopher Manco *(U Delaware); U Auckland:* Liam Wotherspoon; *UCSD:* Lelli Vande Einde

Super-resolution Microscopic Imaging of Excitation-Contraction Coupling Regulatory Machinery in Heart Muscle Cells

The rhythmic contraction of heart muscle, i.e., the heart beat, is controlled by a uniquely developed regulatory unit made of membranes, which translates the electric excitation of the plasma membrane to dynamic fluxes of calcium ions, which then spread throughout the cell and induce robust cell contractions. The malfunction of this regulatory machinery is known to cause heart failure and loss of coordination among units, and results in arrhythmias.



A UCSD laboratory lead by Masa Hoshijima and the biophysics laboratory directed by Christian Soeller at the University of Auckland have had a shared interest in determining the structure and patho-physiological function of this muscle regulatory unit. However, this task has been extremely challenging, mainly due to the fact that the size of this unit is smaller than the resolution limit of conventional light microscopes. Hoshijima and Soeller have each taken completely different approaches to solve the problem. While Hoshijima uses various three-dimensional (3-D) electron microscopic tools, Soeller has adapted a novel super-resolution light microscopy method, namely direct stochastic optical reconstruction microscopy (dSTORM). Neither uses direct visualization. Both rely on extensive computational data processing.

Hoshijima and Soeller decided to bring their technologies together and assigned Joseph Wong (PRIME 2011) to work in Soeller's laboratory to apply dSTORM to heart samples, which were prepared by Hoshijima and shipped to Auckland. The samples were studied in 3-D electron microscopy at UCSD, in parallel.

With technical support provided by colleagues in the Soeller lab, Wong was able to successfully visualize calcium flux regulatory units as nanometer-scale clustering of ryanodine receptor (RyR) in normal and disease model mouse cardiac myocytes, using dSTORM. RyR clusters were

three-dimensionally mapped along with tubular membrane invaginations of surface cell membrane. The geometry of the clusters was remarkably heterogeneous; yet, they were densely assembled at the enlarged bifurcation loci of branches. This was entirely an unprecedented finding, but is well-supported by Hoshijima's 3-D electron microscopy.

The achievement of Wong and this PRIME 2011 project is significant, as it is not limited to descriptive observation. The dSTORM data are readily useful for a variety of simulation work, combined with geometry determined by electron microscopy.

PARTICIPATING RESEARCHERS: *PRIME 2011 Student, UCSD:* Joseph Wong; *U Auckland:* Christian Soeller, Vijay Rajagopal; *UCSD:* Masa Hoshijima

Automated Image Classification for the Vespidae Family of Wasps

PRIME 2011 student Adrian Teng-Amnuay, hosted by the Taiwan Forest Research Institute (TFRI), worked closely with TFRI scientists Chau Chin Lin, Sheng-Shan Lu, and Yu-Huang Wang to develop a computer vision and analysis system for automated taxonomic identification of wasps. Taxonomic identification has traditionally been carried out by individuals with years of experience and in-depth knowledge of the particular taxa. The process of identifying specimens can often be time-consuming and tedious. Working with his TFRI and UCSD mentors (Tony Fountain and Serge Belongie), Adrian developed a system for automated image classification on a small subset of the Vespidae family of wasps. This system utilizes a combination of computer vision and machine learning tools including the OpenCV library for computer vision. Adrian developed an analysis workflow for transforming raw images into quantitative features and then conducted experiments with various feature selection and machine learning algorithms. His experiments produced high classification accuracy on the target problem and confirmed the feasibility of this approach. While this system still has much room for improvement, it provides a demonstration of how image classification can be automated and provides a foundation for further studies in this area.

ADDITIONAL INFORMATION: OpenCV library: **opencv.willowgarage.com/wiki**

PARTICIPATING RESEARCHERS: *PRIME 2011 Student, UCSD:* Adrian Teng-Amnuay; *TFRI:* Chau Chin Lin, Sheng-Shan Lu, Yu-Huang Wang; *Calit2/UCSD:* Tony Fountain, Serge Belongie

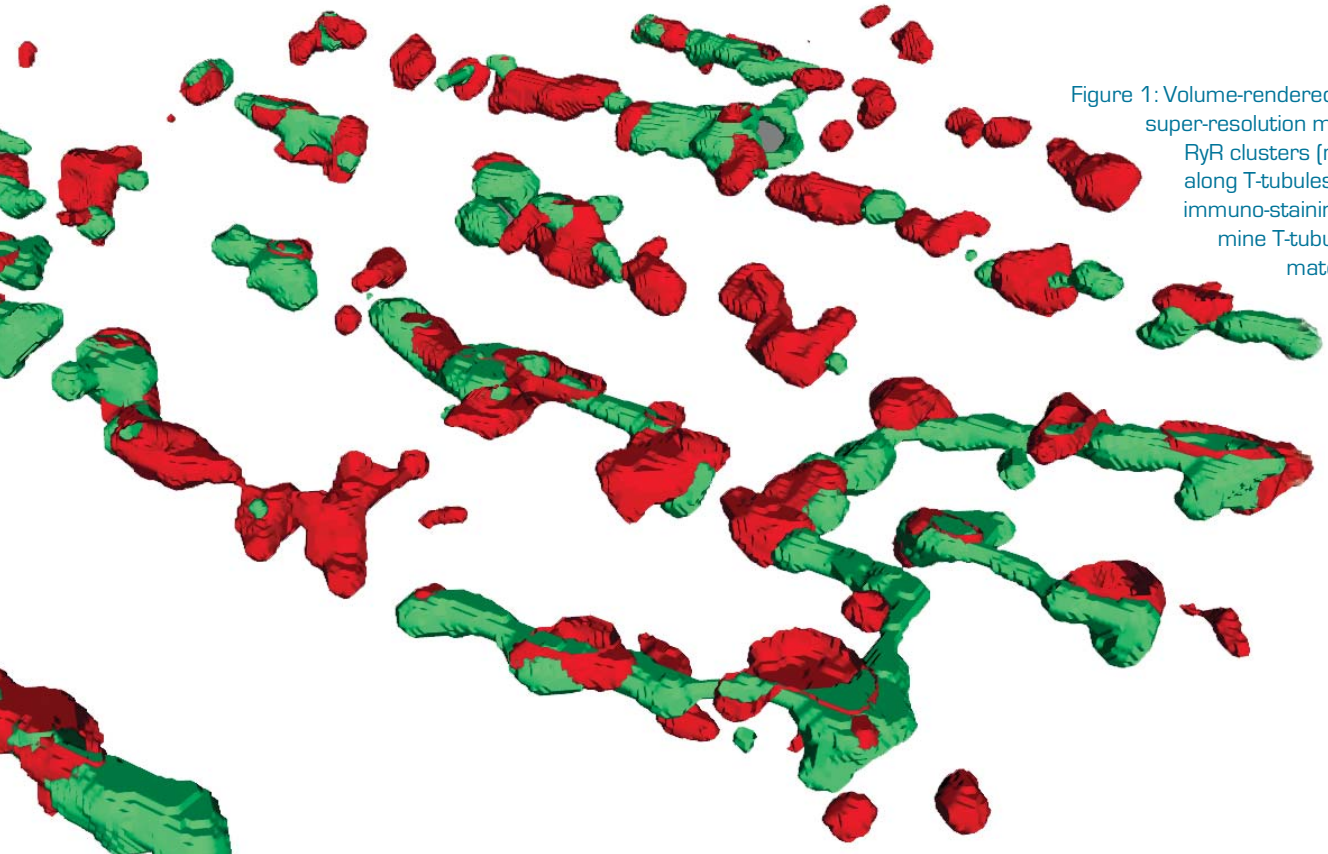


Figure 1: Volume-rendered 3-D dSTORM super-resolution microscopic image. RyR clusters (red) are distributed along T-tubules (green). Caveolin-3 immuno-staining is used to determine T-tubule structure. Estimated resolution of this image is ~30 nm, which is approximately 10 times better than that of conventional light microscopy.

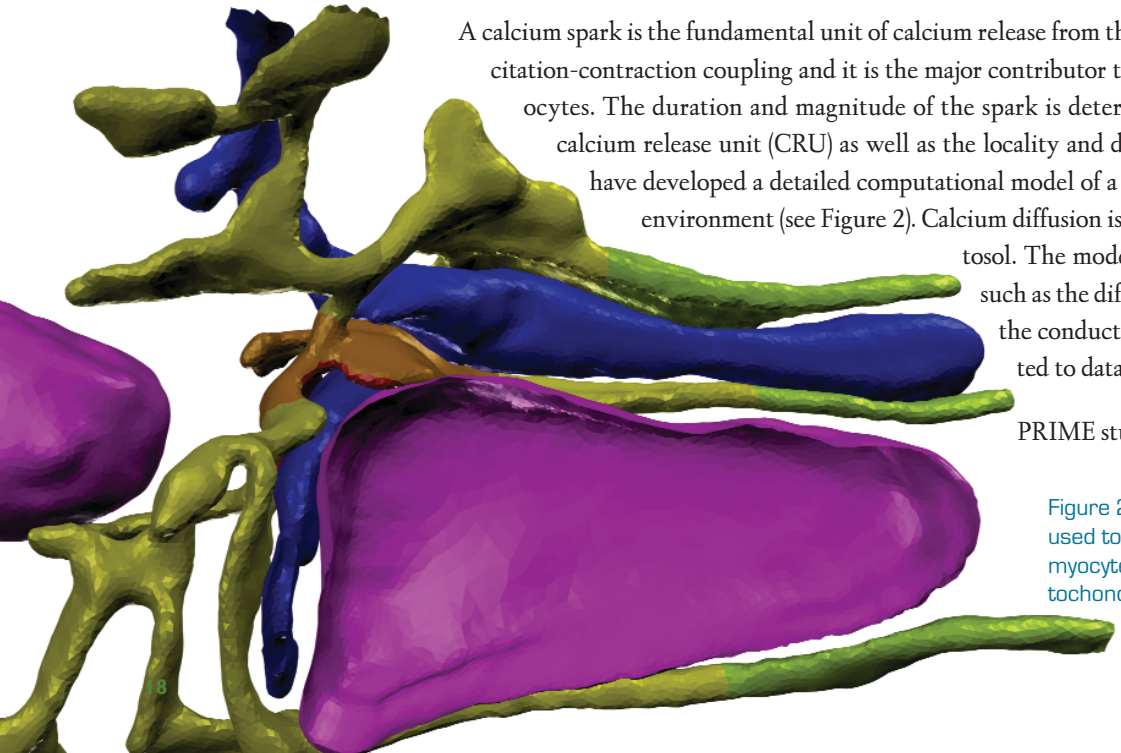
Navi: Covise-Kinect Navigation Interface with a Cultural Heritage Application

Images, left to right: Temple at Shinlin Night Market in Jiantan—courtesy of Howard Li; Sarah Larsen teaching gestures to a user (out of sight) of NAMI in order to navigate the NexCAVE—courtesy NICT; Great Ocean Road—courtesy of Jennifer Kaehms

Two prime students, Sarah Larsen at NICT and Matthew Religioso at Osaka University, worked together on a project called Navi: Covise-Kinect Navigation Interface. Kinect is a motion capture device sold by Microsoft with their game engine; COVISE—COllaborative Visualization and Simulation Environment—is an extendable distributed software environment to integrate simulations, postprocessing and visualization functionalities. In this project, they created a navigation plug-in to interface a Kinect device with COVISE to enable users to explore a Virtual Reality Modeling Language (VRML) model through movements and gestures. They also tackled and resolved problems with flickering and texture exportation on a large-scale model of old Osaka Doutonbori (道頓堀). The model was made by Kansai University; it represents the most popular entertainment district in Osaka. The plug-in they created was combined with a viewpoint plug-in to make it easier to reset and change views, and they combined it with a texture optimization plug-in. Navi works well on the NexCAVE system at the NICT Keihanna Research Center. The Navi system was successfully shown at the Knowledge Capital Trial 2011 technology exhibition for the North Umeda district project. More than 12,000 visitors attended the exhibition in Osaka.

PARTICIPATING RESEARCHERS: *PRIME 2011 Students, UCSD*: Sarah Larsen, Matthew Religioso; *Osaka U*: Kiyoshi Kiyokawa, Haruo Takemura; *NICT and Osaka U*: Shinji Shimojo; *NICT*: Masaki Chikama, Yoshinobu Kobayashi, Tomoaki Takata, Taku Morinobu; *Calit2/UCSD*: Jurgen Schulze.

Computational Modeling of Local Calcium Handling in Cardiac Myocytes



A calcium spark is the fundamental unit of calcium release from the sarcoplasmic reticulum (SR) during excitation-contraction coupling and it is the major contributor to the diastolic calcium leak in cardiomyocytes. The duration and magnitude of the spark is determined by the local geometry of a single calcium release unit (CRU) as well as the locality and density of calcium handling proteins. We have developed a detailed computational model of a single CRU situated in its native cellular environment (see Figure 2). Calcium diffusion is modeled both within the SR and the cytosol. The model includes several unknown parameters, such as the diffusion constant of calcium within SR and the conductance of the CRU, which needed to be fitted to data from Zima et al. (2008).

PRIME student Jerry Tsai used the Nimrod system

Figure 2: The reconstructed geometry that was used to model local calcium handling in cardiac myocytes: t-tubule (blue), SR (yellow/orange), Mitochondria (violet)

on a 220-core cluster at Monash University to fit the unknown parameters. He then proceeded to investigate the effect of different locations of calcium handling protein close to the release unit. He found that the sarco-endoplasmic reticulum calcium ATPase (SERCA) pump affects the duration of the release by pumping already-released calcium back into the SR. Tsai also found that using a simplistic model of the sodium/calcium exchanger on the cell membrane inside the CRU does not work as it drains calcium out of the cell before it can trigger contraction. These findings will help us to better understand what regulates the size and duration of a single calcium spark.

REFERENCE: Zima, A.V., Picht, E., Bers, D.M., and Blatter, L.A. 2008. Termination of cardiac Ca sparks: role of intra-sr [Ca], release flux, and intra-sr Ca diffusion. Circ Res 103:e105-e115.

PARTICIPATING RESEARCHERS: *PRIME 2011, UCSD:* Jerry Tsai; *Monash U:* David Abramson, Blair Bethwaite; *UCSD:* Johan E Hake

Grid-based 3-D Protein Model Building for Small Molecule Docking

In previous years, PRIME students have identified possible chemical inhibitors of the slingshot-2 (SSH-2) protein using high-throughput docking. This protein is part of the large dual specificity phosphatase (DSP) family, which consists of seven subfamilies that exhibit high homology with a characteristic HX5R(S/T) catalytic site that is able to dephosphorylate phosphoserine/threonine or tyrosine residues. SSH-2 is a regulatory enzyme that affects the actin depolymerizing protein cofilin, which in turn controls various cellular processes and makes it an invaluable protein target for pharmaceutical studies. However, high homology within the DSP family requires thorough screening of each DSP member to help determine SSH-2 inhibitor specificity. Due to the time and complexity required to do this, only about one-third of the DSP family have experimentally-determined protein structures, therefore, it was vital to create accurate 3-D protein structure models in order to obtain a complete database for virtual docking of the remaining DSP family members. Utilizing a grid-enabled 3-D modeling program, MODELLER, PRIME 2011 students Daniel Li and Brian Tsui created a streamlined workflow that can rapidly produce accurate 3-D models of DSPs that do not have known three-dimensional structures. These models were then applied to further docking studies in order to complete screening of the entire DSP family.

The modeling workflow consisted of four major steps. 1) A protein blast was applied in order to find template sequences with similar alignment to the protein of interest. 2) Top candidates were selected and arranged into groups based on phylogenetic similarity and applied to a target-template sequence and structural alignment via MODELLER. The program accounted for global and local atom pair distances, as well as solvent accessibility at the residues. 3) The top alignment was generated and selected through MODELLER and a set of 600 protein structure models was

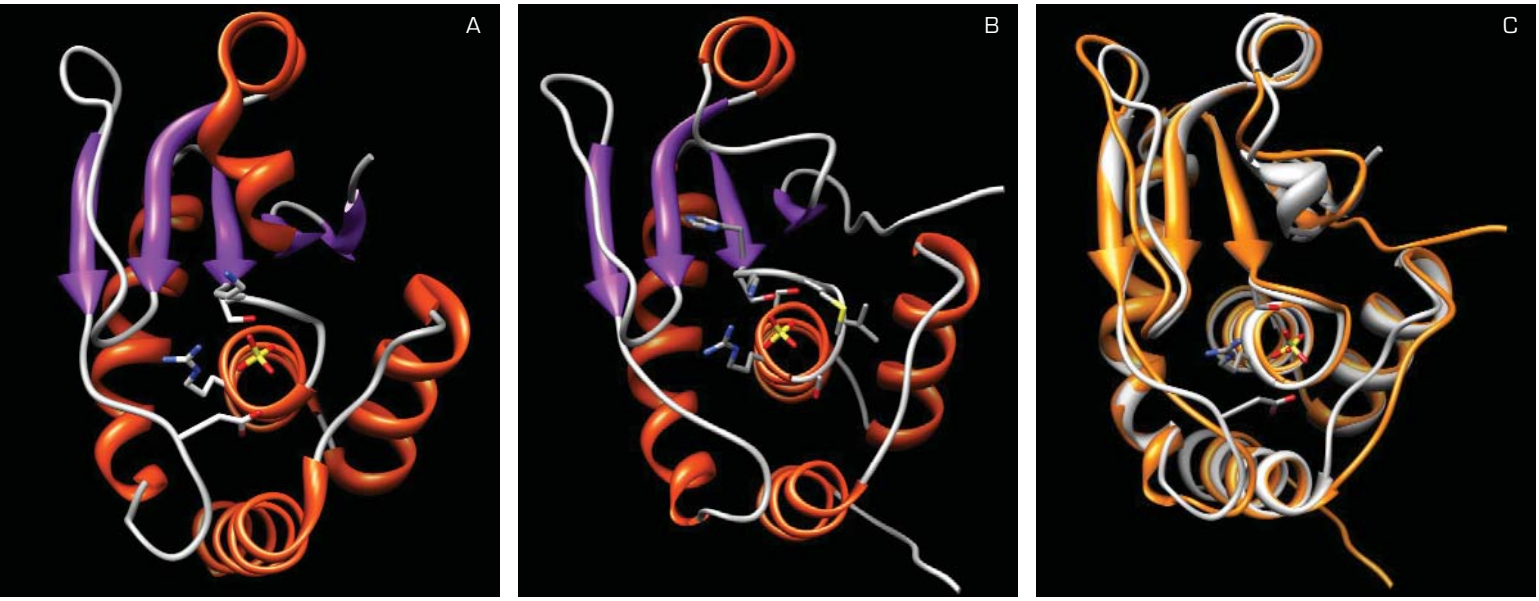


Figure 3: Visualization of (A) actual and (B) modeled three-dimensional structure of SSH-2 (2nt2) from the improved workflow. (C) is the overlay of the actual and modeled structures. Note the very close agreement of the two structures. The colors have been changed (grey=actual, orange=modeled) for clarity.

created. Each model was built through distance and angle restraints provided by the alignment with the template structures. The model structures were evaluated through GA341, a composite score that helps distinguish between good and bad protein folds, as well as an energy score evaluation via DOPE and molpdf scores. Additional models were generated if the results did not meet a predetermined cutoff (0.7 out of 1). 4) Finally, the best 3-D structure models were optimized via loop refinement (MODELLER) and energy minimization (Chimera). MolProbity analysis was then applied to verify that minimal intra-atomic clash and realistic protein folds were present in our modeled 3-D structure and the protein models were ready for subsequent docking applications. Through this workflow, 43,800 total protein structure models were produced in just four weeks time, completing the database of DSP structures. Docking experiments are now underway to test for SSH-2 inhibitor specificity.

ADDITIONAL INFORMATION: The previous summer, Charles Xue (PRIME 2010), established a grid-enabled implementation of MODELLER. MODELLER was developed and is maintained by Andrej Sali, University of California, San Francisco.

PARTICIPATING RESEARCHERS: *PRIME 2011 Students, UCSD:* Daniel Li, Brian Tsui; *PRIME 2010 Student, UCSD:* Charles Xue; *PRIME 2009 Student, UCSD:* Matthew K. Mui; *Osaka U:* Susumu Date, Kohei Ichikawa; *UCSD:* Jason H. Haga

Advances in Influenza Virus Research

The influenza virus is still a widely prevalent threat to global public health and the world-wide economy. During the summer of 2011, four UCSD PRIME students worked on various aspects of influenza biology at three host sites: CNIC, Beijing; USM, Penang; and National Taiwan University (NTU), Taipei. Victor Chu, working at CNIC, continued virtual screening studies using new target sites in hemagglutinin (HA), while Pek Ieong and Alexandra Delaney at USM, explored the glycobiology and immunology of HA; and at NTU, Howard Li focused on novel scaffolds for inhibitor design against neuraminidase (NA).

Reflecting on his summer research at NTU, Howard Li describes the novel finding that adamantane, a known influenza inhibitor rendered obsolete due to viral resistance, may contain a scaffold effective for synthesis of new inhibitors against drug resistant forms of NA.NA is an enzyme that mediates the budding and release of daughter viral particles from host cells, it is essential for the spread of influenza infections, and thus a key target for antiviral drug development. Li investigated a scaffold-based, fragment-growing method to identify molecular scaffolds for Group 1 neuraminidase inhibition. Premising this study are two assumptions: 1) effective inhibitors possess not only an optimal combination of functional groups but also a fundamental molecular geometry, dictated by a core scaffold, that allows the molecule to better access the binding site; and 2) the potential of a molecular scaffold to be developed into an effective inhibitor can be explored through fragment-growing algorithms.

> My trip to Christchurch was both educational and eye-opening. I hope that the city makes a quick recovery and grows to become an even better than it was before. **Christopher Manco** (see p.15)

An initial set of basic geometric scaffolds along with the core ring structures of Zanamivir and other known NA inhibitors were inputted into AutoGrow, the fragment-growing application used in his study. AutoGrow randomly mutates an initial input molecule with substituents from a fragment library. Using AutoDock Vina as a scoring function by docking mutated compounds to a known oseltamivir-resistant NA protein structure, AutoGrow mutations that lead to a greater binding affinity are preserved for the next generation and cycle of mutation; selection continues until an effective inhibitor eventually evolves. After eight cycles, all scaffolds showed a general increase in binding affinity; however, some clearly showed more successful evolutionary trajectories and evolved into ligands of significantly higher binding affinity. Adamantane was thus identified by this study as a novel scaffold for possible development into a potential inhibitor. Analyzing the substituents of adamantane derivatives revealed a consistent trend: the top endpoint molecules of multiple parallel evolutions all resulted in the attachment of a sulfate-containing branch, as well as an alcoholic branch exactly four bonds away. As validation for this method, ligands derived from the core scaffold of Zanamivir had nearly identical fragment attachment sites as the original Zanamivir ligand.

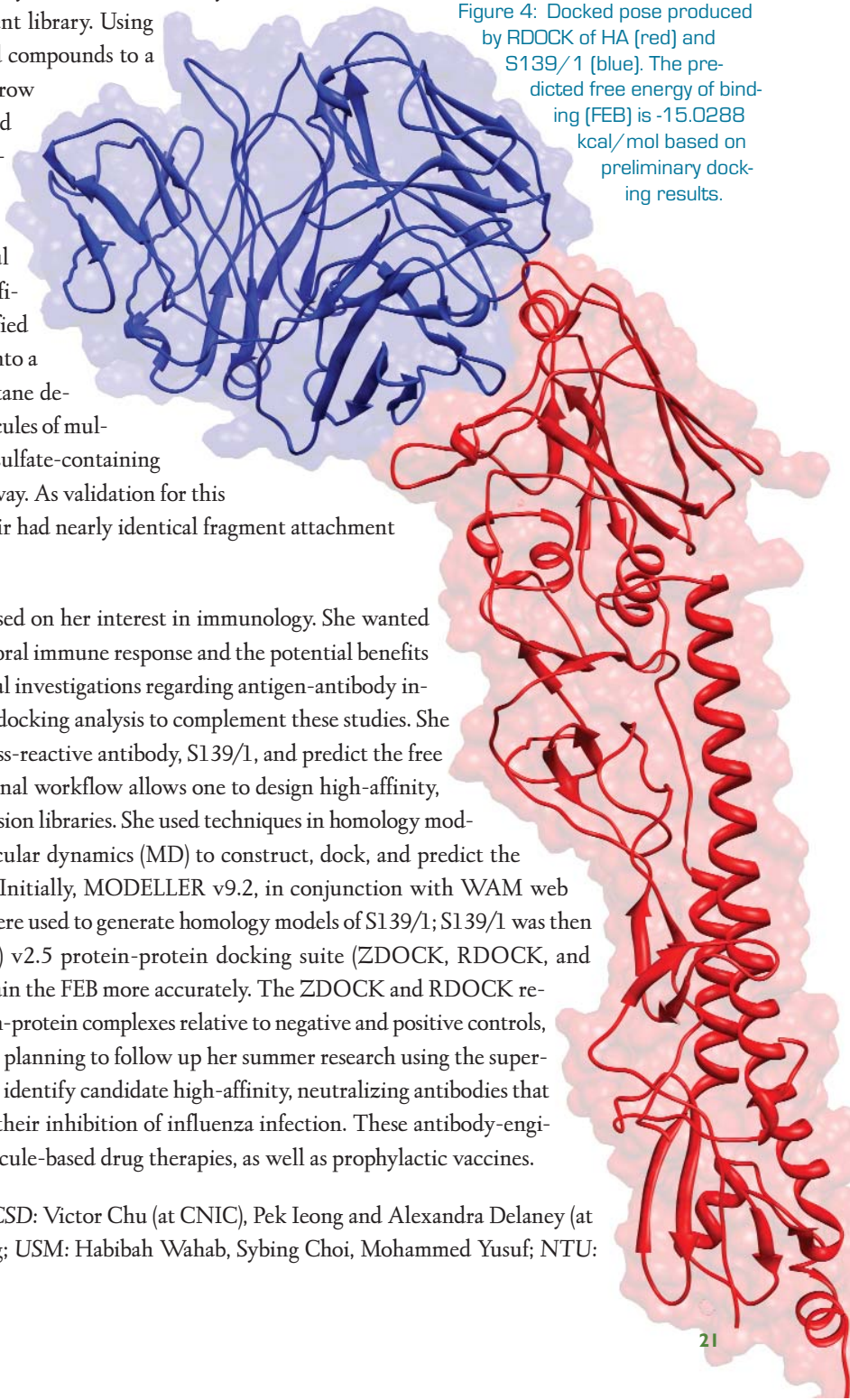


Figure 4: Docked pose produced by RDOCK of HA (red) and S139/1 (blue). The predicted free energy of binding (FEB) is -15.0288 kcal/mol based on preliminary docking results.

At USM, Alexandra Delaney chose a challenging topic based on her interest in immunology. She wanted to study antigen recognition, an integral aspect of the humoral immune response and the potential benefits of antibody engineering. Despite the large body of biological investigations regarding antigen-antibody interactions, there is a noticeable absence of in silico protein docking analysis to complement these studies. She developed in silico protocols to construct a model for a cross-reactive antibody, S139/1, and predict the free energy of binding (FEB) of S139/1 to HA. The computational workflow allows one to design high-affinity, neutralizing antibodies without the use of biological expression libraries. She used techniques in homology modeling, protein-protein docking and refinement, and molecular dynamics (MD) to construct, dock, and predict the binding energy of S139/1 to hemagglutinin H3 subtype. Initially, MODELLER v9.2, in conjunction with WAM web server and Rosetta Antibody structure prediction server, were used to generate homology models of S139/1; S139/1 was then docked to H3 using the Accelrys Discovery Studio (DS) v2.5 protein-protein docking suite (ZDOCK, RDOCK, and ZRANK). Finally, MD simulations were completed to obtain the FEB more accurately. The ZDOCK and RDOCK results indicated that it is possible to predict the FEB of protein-protein complexes relative to negative and positive controls, and engineer theoretical antibodies that bind to HA. She is planning to follow up her summer research using the supercomputing facilities at UCSD. Ultimately, she would like to identify candidate high-affinity, neutralizing antibodies that can be synthesized for further biological investigations of their inhibition of influenza infection. These antibody-engineering techniques would complement existing small molecule-based drug therapies, as well as prophylactic vaccines.

PARTICIPATING RESEARCHERS: *PRIME 2011 Students, UCSD:* Victor Chu (at CNIC), Pek Ieong and Alexandra Delaney (at USM), Howard Li (at NTU); *CNIC:* Kai Nan, Kevin Dong; *USM:* Habibah Wahab, Sybing Choi, Mohammed Yusuf; *NTU:* Jung-Hsin Lin; *SDSC/UCSD:* Wilfred Li.

MURPA Advances – This Year

As with PRIME, the Monash Undergraduate Research Projects Abroad (MURPA) program supports summer (i.e., January-March down under) internships with leading research groups overseas. It not only provides a hands-on research experience to undergraduates, but does so in an international context. Students are placed for a period of eight weeks, allowing them to integrate into the research groups as team members. MURPA also involves an advanced seminar scheme, in which students attend seminars given by world-leading experts; this is particularly helpful before they embark on their research adventures abroad. The seminar structure is novel because it uses high-definition interactive video links, making it feasible to attract some of the world's best researchers "virtually" to Monash. These seminars also allow students to "meet" potential MURPA mentors and learn more about potential projects.

MURPA has entered its fourth year; fourteen students have gone through its ranks to date. In 2011, the National Center for Supercomputing Applications (NCSA) at the University of Illinois, Urbana-Champaign, USA was added as a target destination for students. During 2012, we will also extend MURPA-related seminars to include the Technion (Israel Institute of Technology, Haifa) and the University of Warwick (UK), and may offer internships at these universities as well.

Some MURPA students have continued their summer internship projects into their fourth-year honors research project after they return to Australia, providing a much longer, and more internationally relevant, research project than the norm. We have further leveraged research projects across the two undergraduate programs (MURPA and PRIME): PRIME students who arrive in June, (hosted at Monash) have continued projects conducted by MURPA students in January and February (at UCSD). This has allowed more than one student to contribute to the project's outcome, while still providing continuity and progress on the project during the year.

MURPA seminars are a key component of the scheme, and serve multiple purposes. In addition to allowing students to meet potential mentors, the lectures are integrated into two undergraduate courses, one in Distributed Computing, and another in Computational Science. These provide a valuable research focus for courses, broadening the relevance and reach of the material taught. Typically, over 40 students and staff attend MURPA lectures, at times, the attendance has been as high as 80. Archives of talks are available on the MeSsAGE Lab website (link below). A link to learn more about past MURPA projects is also below.

Images, background: Sydney Opera House—courtesy of Xiaolong Qiu; left to right: Jumping PRIME stars—courtesy of Xiaolong Qiu; Roo Crossing—Jennifer Kaehms

Recognition of MURPA is growing, and the program now attracts students from the Faculties of Engineering and Science, in addition to Information Technology students.

We wish to acknowledge the financial support of the Faculty of Information Technology and the Monash e-Research Centre, and in 2011, we gained additional external support for MURPA from the Cybec Foundation, for which we are grateful.

ADDITIONAL INFORMATION: Monash Undergraduate Research Projects Abroad (MURPA): **messagelab.monash.edu.au/MURPA**; Monash eScience and Grid Engineering (MeSsAGE) Lab: **www.messagelab.monash.edu.au**; MURPA Past Projects: **messagelab.monash.edu.au/MURPA/PastProjects**

MEMBER BENEFITS AND SOFTWARE CONTRIBUTIONS

Members are the most important asset of PRAGMA and our activities reflect this: supporting individuals to participate in PRAGMA, hosting exchanges of researchers and students, organizing workshops, and contributing resources to the PRAGMA Grid. A complete list of active members together with their sponsors is provided at the end of the brochure, (also listed are networking, industry and other types of members).

In this section we highlight software tools developed by PRAGMA members and tested by other members over our 10 years, including two contributions new this year (EDISON and KNSG). In addition, we highlight the benefits of PRAGMA membership to five institutions.

Selected Software Enhanced by PRAGMA Use During Our First 10 Years

Throughout our nearly ten years, we have used and enhanced software developed by PRAGMA members. The table below is an overview of some of this software and how it is used. It is through use and feedback to the developers that enhanced software results. This is a benefit for PRAGMA members: feedback on the software and the use of tools designed for specific purpose.

Software	Developer Institution	Description	PRAGMA Enhancement/Use
Ninf-G	AIST / NAREGI	Reference implementation of Grid RPC, using Globus First international software into the NMI software stack	Many applications
Gfarm	AIST and U Tsukuba	Grid file system	Virtualization Tests; Avian Flu Grid
Duckling	CNIC	Resource sharing and collaboration platform	PRAGMA Workshops
CSF4	Jilin U	WSRF compliant community meta-scheduler	Avian Flu Grid
SCMSWeb	Kasetsart U	Grid monitoring system	GOC
e-AIRS	KISTI	e-Aerospace Integrated Research System	Tested on PRAGMA Grid
Mgrid	Konkuk/Kookmin	Grid computing system for collaborative molecular simulation	Avian Flu Grid
Nimrod Toolkit	Monash	Parameter sweep tools on grids	Savannah experiment; Volcanic Ash Distribution; PRIME students
MOGAS	NTU - Singapore	Grid Accounting System	Grid Operations Center
SAGE	UIC	Scalable Adaptive Graphics Environment	PRIME
DataTurbine	Calit2/UCSD	Robust real-time streaming data engine	PRIME, KEON, CREON/Thailand
CADD	NBCR/UCSD	Computer-aided Drug Discovery pipeline, using relaxed complex scheme	Avian Flu Grid
Opal Toolkit	NBCR/UCSD	Toolkit for wrapping scientific applications as web services	Avian Flu Grid
INCA	SDSC/UCSD	User Level Grid Monitoring System	Grid Operations Center
Rocks	SDSC/UCSD	Cluster (real and virtual) management system, with application rolls	Virtualization Tests

EDISON

EDISON (EDucation-research Integration through Simulation On the Net) is a computer-simulation-based cyber learning and research environment and science gateway (or portal) for computational science communities especially in the areas of computational fluid dynamics (CFD), chemistry, physics, structural dynamics, and computational design. This project officially started in July 2011; it is funded by the Ministry of Education and Science Technology in Korea and executed by KISTI. This project is a spin-off from KISTI's e-AIRS (e-Aerospace Integrated Research System) that was developed for research and education on CFD. The first purpose in constructing such a virtual experimental education

> PRAGMA led us to become a member of APGrid PMA, which became a significant component in our development of Thailand National e-Science Infrastructure Consortium...to becom[ing] a part of GEO Grid collaboration...and helped with the setting up of [a CREON site at Racha Island] **NECTEC**

and research system is to accelerate research activities and advance the level of the education environment by building a converged research and education cyber environment for advanced research outcomes and software development from academic and research labs. The second purpose is to enable computational scientists and professors in science and engineering application areas to spend less time getting help on issues regarding information technologies and practical experiments from experts and more time on research discoveries and lecture preparations. Utilizing such a system in classrooms and research labs is will definitely increase the synergistic effect by directly applying recent advanced R&D results, and decreasing the costs and efforts associated with reeducation and training.

e-AIRS has been supported on the PRAGMA testbed. We are looking forward to continuing that collaboration with this new project. For more information about e-AIRS, see the PRAGMA Collaborative Overview 2010-2011.

PARTICIPATING RESEARCHERS: *KISTI:* Kumwon Cho (PI), JongSuk Ruth Lee

Developing the Semantically-aware and Web-enabled KNSG (KISTI-NCSA Science Gateway) Application Framework

KISTI and the National Center for Supercomputing Applications (NCSA) have developed a prototype non domain-specific platform called KNSG (KISTI-NCSA Science Gateway) Application Framework for building non-domain-specific HPC applications. The KNSG Application Framework provides a core set of reusable components for building new applications as demonstrated by e-AIRS rich client platform (RCP). The e-AIRS RCP uses the framework for setting up and submitting HPC jobs on both TeraGrid and KISTI supercomputing resources and then monitors the job progress through job monitoring components provided by the framework.

This project will enhance the KNSG Application Framework by pursuing the following goals (see Figure 1):

1. Enable KNSG Application Framework to be semantically-aware.
2. Enable KNSG Application Framework to develop web applications.
3. Enable Middleware Services (PTPFlow) to support multi-users and heavy concurrent connections.

Adding semantic capabilities to the framework will provide the framework with a more complete set of content management capabilities that will allow users to collate, annotate, and run analytics on their datasets. The web application extension will allow users to setup, launch, and monitor jobs in a web-enabled environment as well as access their data and tools from any location.

Figure 1. Collaboration Structure for the KNSG Application Framework

The first two goals will be lead by NCSA with collaboration from KISTI and the third goal will be lead by KISTI with collaboration from NCSA. Both groups will ensure the quality of the final deliverables. The development and testing of the framework will be performed using both the TeraGrid environment and the KISTI environment with the help of collaborating KISTI researchers to ensure the final product works in both environments. In addition, we will develop an e-AIRS web application using the KNSG framework's enhancements and it will be tested with current e-AIRS users at KISTI.

PARTICIPATING RESEARCHERS: *KISTI:* Kum Won Cho *(ckw@kisti.re.kr)*, Dukyoon Nam *(dynam@kisti.re.kr)*; *NCSA:* Danny Powell *(danny@ncsa.uiuc.edu)*, Jong Lee *(jonglee@ncsa.illinois.edu)*

> "The exchange of ideas and culture that happened throughout these years prepare our researchers to be ready to work in a new globalized world." **Kasetsart University**

Member Benefits

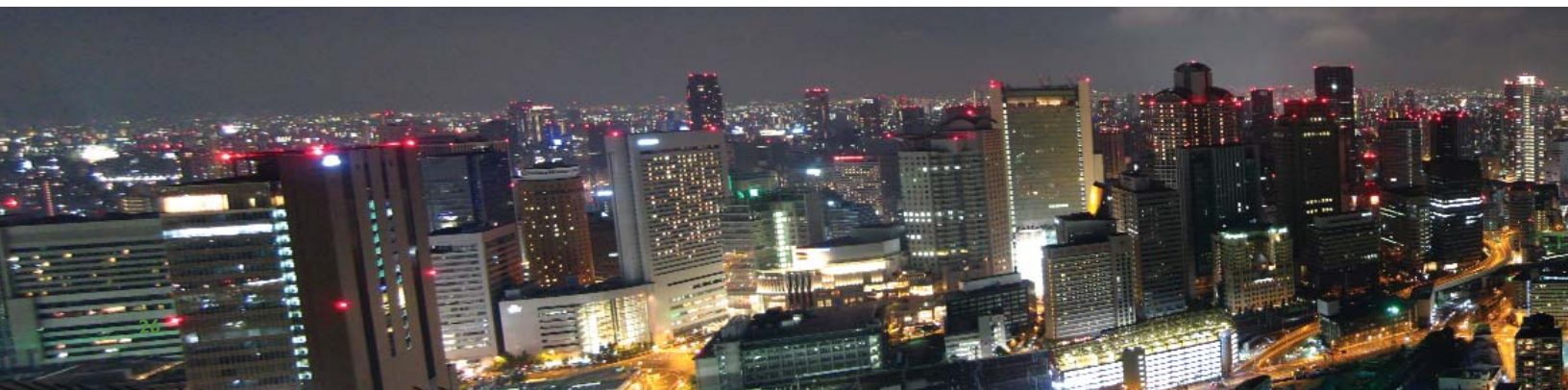
University of Hyderabad (UoHyd)

The University of Hyderabad (UoHyd) is a founding member of PRAGMA and an initial member of the PRAGMA Steering Committee. PRAGMA serves as a mechanism through which information and resources can easily be exchanged. It is playing the catalytic role of promoting collaborations. We found that with its participative sessions, PRAGMA encourages people to connect with each other quickly and seamlessly. Networking is easier and fruitful partnerships are being initiated in a relatively short time. PRAGMA has a focus and a mission to accomplish tasks and test new ideas.

Recent efforts of UoHyd have centered on exchanging students under the PRIME program, which provides undergraduates at UCSD with hands-on, full-time research experiences in internationally collaborative settings. Several of our own students have benefitted by interacting with them. This has helped us to evolve a very vibrant academic and research group here in our department (Computer/Information Sciences) where every year several students register to work on problems related to grid and cloud computing.

PRAGMA has been providing a great opportunity to connect to the grid research community and landscape of cultures as it moves from one location to another.

Images, above: Yoshio Tanaka, host and general chair of the PRAGMA 21 Workshop, enjoying a piece of akebia fruit—courtesy of Weicheng Huang, NCHC; below: A panoramic view southeast of Umeda from Umeda Skytower—courtesy of Wesley Hsu



National Electronics and Computer Technology Center (NECTEC)

The National Electronics and Computer Technology Center (NECTEC) is a statutory government organization under the National Science and Technology Development Agency (NSTDA), Ministry of Science and Technology. Our main responsibilities are to undertake, support, and promote the development of electronics and computer technologies through research and development activities. The range of our applications spans from supporting agriculture, healthcare, ecology and environment, manufacturing and the service industry, to bridging the digital divide, cultural preservation, disaster mitigation, and development of R&D human resource. We also play role in the development of IT related research infrastructure.

NECTEC has been an active member of PRAGMA since 2002. We have found that the collaboration with PRAGMA is very beneficial to our missions. Close relationships with the Resource Working Group have given us good technical support for our computing resource setup. This has been one of our strengths in building the computing infrastructure for computational research in Thailand. Collaborations within PRAGMA led us to become a member of APGrid PMA, which became a significant component in our development of the Thailand National e-Science Infrastructure Consortium. Our development of an environmental information portal called "Environment Informatorium" has become part of a GEO Grid collaboration. This is a result of the interaction within the GEO Working Group. Participation in PRAGMA's Telescience Working Group has led to recent collaborations on coral reef monitoring with the Australian Institute of Marine Science (AIMS), NCHC, NECTEC, Walailak University (WU), and UCSD. Researchers from collaborating partners and a student from PRIME have visited the study site at Racha Island, Southern Thailand; Michael Nekrasov, PRIME 2009, returned there to help with setting up the site. The equipment and software system have been set up and the site has already been registered as the fourth CREON coral reef site. A paper on this will be presented by the lead author, Professor Mullica of WU at the upcoming Environmental Information Management (EIM) conference.*

*ADDITIONAL INFORMATION: **https://eim.ecoinformatics.org/eim2011**

Kasetsart University (KU)

During our engagement in PRAGMA activities, Kasetsart University (KU) has gained many benefits from our interactions. First, the experiences in the building of a large international cyberinfrastructure help deepen our understanding of how large and complex infrastructure can be built and operated reliably. As we collaborate in building a monitoring infrastructure called SCMSWeb, there are many technical challenges that enable us to gain many valuable insights into the monitoring technology. Moreover, the exchange of ideas and culture that has happened throughout these years prepares our researchers to be ready to work in a new globalized world. We look forward to more future work with PRAGMA members in the move towards large-scale deployment of cloud and virtualization technology. This is an exciting transition and will create new potential for many areas of application and we hope that we can be a part of this effort.

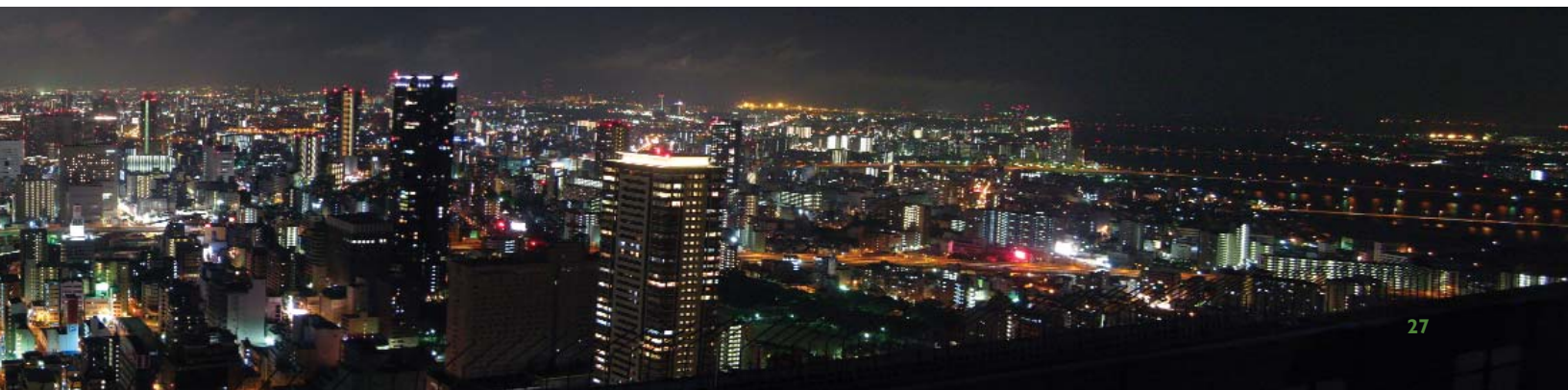


Image: Meiji Shrine, Tokyo—courtesy of Peter Arzberger

Konkuk University (Konkuk U.)

Konkuk University (Konkuk U.) has been participating in PRAGMA since the 3rd PRAGMA workshop in Fukuoka, Japan in 2003 and officially joined PRAGMA as an institute member during PRAGMA 12. Through both the participation in workshops and a number of collaborative efforts together with other members, Konkuk U. has been developing its experiences and strength in interdisciplinary research and global collaboration. Based on experiences and lessons from Working Group (WG) activities in PRAGMA, Konkuk U. established an interdisciplinary graduate program called the Department of Advanced Technology Fusion in 2006, which addresses a wide range of scientific disciplines: information technology, environment technology, biotechnology and intelligent microsystems. The program was selected as one of eleven graduate programs of excellence in interdisciplinary science and engineering in 2006 and has been financially and administratively supported by the Ministry of Education and Science. Largely due to this graduate program, Konkuk U. is now considered as one of a few universities leading interdisciplinary research and education.

In 2008, based on the Department of Advanced Technology Fusion, Konkuk U. founded a research institute focused on information technology-based interdisciplinary research: the Institute for Ubiquitous Information Technology and Applications (UBITA). UBITA has been doing large-scale interdisciplinary research projects.

Through activities with the Biosciences WG, Konkuk U. and KISTI have jointly developed a grid computing system for molecular simulation called MGrid which is considered one of the few successful grid computing projects in Korea. The system is now available in the Korea shared supercomputing infrastructure called PLSI. PLSI consists of twelve high performance computing centers in Korea and currently provides three computing services; MGrid is one of these services.

In 2011, an interdisciplinary research collaboration network for ecology, meteorology, and information technology, the Korea Ecological Observation Network (KEON) was founded in Korea. KEON consists of government and university research institutes, as well as individual members in Korea. UBITA is one of the founding institute members. The vision and organization of KEON is largely inspired by PRAGMA and the Global Lake Ecological Observatory Network (GLEON). GLEON is a grassroots organization of more than 300 members that draws its origins to the NCHC Ecogrid projects. One specific component of KEON is the Korean Lake Ecological Observatory Network (KLEON, see next story).

For the last decade, PRAGMA has given Konkuk U. opportunities for global collaboration with excellent research groups in the world. Due to such opportunities, Konkuk U. has become one of the leading institutes in interdisciplinary education and research in Korea.

ADDITIONAL INFORMATION: Department of Advanced Technology Fusion: **atf.konkuk.ac.kr**; Institute for Ubiquitous Information Technology and Applications (UBITA): **www.ubita.org**; PLSI: **www.plsi.or.kr** and **mgrid.plsi.or.kr/portal**; Korea Ecological Observation Network (KEON): **www.keon.kr**; GLEON: **www.gleon.org**

> For the last decade, PRAGMA has given Konkuk U. opportunities for global collaboration with excellent research groups in the world and due to such opportunities, Konkuk U. has become one of the leading institutes in interdisciplinary education and research in Korea. **Konkuk University**

Partnerships

Korean Lake Ecological Observatory Network (KLEON)

In 2011, the KLEON group developed a robust, maintenance-free wireless communication service between water quality sensors in the field and the KLEON data server, with the technical collaboration of SK Telecom (the largest mobile network operator in Korea). We have used an innovative CDMA-based M2M (machine-to-machine) communication service from SK Telecom. In this commercial service, a small M2M device (a kind of embedded system with the CDMA communication capability) is connected to a sensor, reads data from the sensor, and delivers sensor data to any server process with the TCP/IP connection over CDMA wireless networks. In addition, the device can receive an SMS message (text message) and we can use such messages to change the configuration of the M2M device and sensors.

We have also integrated this M2M service into the Data Turbine system to filter, multicast, and store sensor data in databases (DBs). We have found the integration of the M2M service and the Data Turbine system enables the easy development of a very robust, flexible, extensible, and customizable monitoring infrastructure.

The main advantages of this approach are little maintenance overhead and cost-effectiveness. In this approach, we do not have to worry about the maintenance of wireless communication networks and communication software (a major maintenance overhead). Also, we do not have to build our own expensive communication system in the field, using instead an already-available, nation-wide commercial wireless communication service, for a small charge. We have been using the technology for monitoring the Soyang Lake since March of this year and plan to extend the application of this technology to other lakes in the future.

In addition, the KLEON group has extended the KLEON cyberinfrastructure to increase compatibility with the GLEON system. Currently, we are working towards the management of KLEON sensor data in the GLEON cyberinfrastructure by using Ziggy Stardust and Vader.

ADDITIONAL INFORMATION: Founding Members of KLEON include Konkuk University, Kookmin University, Kangwon National University, and KISTI. For more about KLEON see the PRAGMA Collaborative Overview 2010-2011. GLEON: **www.gleon.org**

WORKING GROUPS, WORKSHOPS AND, INSTITUTES

PRAGMA workshops are meetings of all members of the PRAGMA community. They are the major vehicle for information exchange between working groups, researchers, and institutions; they also provide excellent opportunities to engage new researchers and students at the host sites.

Workshops are hosted by different organizations to provide a platform for PRAGMA members to meet and discuss research interests, and ideally develop new collaborations, with members of the hosting institutions. This was the case during PRAGMA 18 (March 2010, San Diego) when the plan to add the Racha Island to the CREON network was launched. Similarly at PRAGMA 20 (March 2011, Hong Kong) there were conversations of new research areas in the Biosciences Working Group to utilize the CADD software pipeline.

PRAGMA Workshops are also used to host other targeted activities, such as the case at PRAGMA 21 (October 2011, Sapporo), where a GEO Grid workshop was held the day before the PRAGMA Workshop. This allows more dialog between participants of the two activities.

The workshops are organized by the four working groups in PRAGMA, which are as follows:

- RESOURCES WORKING GROUP: Working to make the distributed resources of PRAGMA useful to diverse applications. Coleaders: Yoshio Tanaka (AIST) and Cindy Zheng (SDSC/UCSD).
- TELESCIENCE WORKING GROUP: Focusing on a variety of activities that require access to, or use of, remote equipment, such as tiled-display walls (TDW) and sensors. Coleaders: Shinji Shimojo (NICT and Osaka U) and Fang-Pang Lin (NCHC).
- GEO WORKING GROUP: Creating an infrastructure to share and integrate data on global earth observations, including remote sensing data and data from land-, lake-, and ocean-based sensors. Coleaders: Sornthep Vannarat (NECTEC), Ryosuke Nakamura (AIST), and Franz Cheng (NARL).
- BIOSCIENCES WORKING GROUP: Focusing much of its efforts over the last several years on integrating technologies to create an infrastructure to advance the screening of potential compounds to combat infectious diseases. Coleaders: Wilfred Li (NBCR/UCSD) and Habibah Wahab (USM).

In 2011, two PRAGMA Workshops were held:

- PRAGMA 20, hosted by the University of Hong Kong, March 2011, in Hong Kong
- PRAGMA 21, hosted by the National Institute for Advanced Industrial Science and Technology (AIST), Osaka University, Tokyo Institute of Technology, and the University of Tsukuba, 17-19 October, in Sapporo

Background image: Kiyomizu-Dera, one of Kyoto's wooden temples in the Higashiyama district—courtesy of Wesley Hsu

In addition to workshops, PRAGMA has a tradition of disseminating information and tools to a broader community through member training activities. The two most recent training activities are: 1) NCHC organized and hosted the Southeast Asia International Joint Research and Training Program in High-performance Computing Applications and Networking Technology (SEAIP, 6-10 December 2010, in Hsinchu) and 2) the National Biomedical Computation Resource (NBCR) Summer Institute (1-5 August 2011, at UCSD in La Jolla, CA). The SEAIP has been a wonderful opportunity for introducing PRAGMA to researchers from Southeast Asia and for interactions between them and the PRAGMA community. Each year there have been new contacts made. This year there was interaction between researchers at the University of Indonesia and the Biosciences Working Group that resulted in one of the Indonesian researchers attending the NBCR Summer Institute to learn more about the CADD pipeline.

Future Meetings:

- Southeast Asia International Program, 29 November-3 December 2011, hosted by NCHC (**event.nchc.org.tw/2011/southeast_asia/index.php**)
- PRAGMA 22, hosted by Monash University, April 2012 in Melbourne
- NBCR Summer Institute, hosted at UCSD, 30 July 2012 - 3 August 2012

INSTITUTIONS AND THEIR SPONSORS

Active Members

A key component of PRAGMA is active involvement, by participation in workshops, contributing resources, hosting workshops, and/or promoting and supporting student and researcher exchanges. The following institutions have contributed to PRAGMA activities in the past year.

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

ADVANCED SCIENCE AND TECHNOLOGY INSTITUTE (ASTI): Denis Villorente, *denis@asti.dost.gov.ph*; Grace Dy Jongco, *gracedj@asti.dost.gov.ph*

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

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

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

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

KASETSART UNIVERSITY (KU): Putchong Uthayopas*, *pu@ku.ac.th*

KONKUK UNIVERSITY (Konkuk U.): Karpjoo Jeong, *jeongk@konkuk.ac.kr*

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

MIMOS: Thillai Raj T. Ramanathan, *thillairaj@mimos.my*; Ng Kwang-Ming, *kwang.ming@mimos.my*; Luke Jing Yuan, *jyluke@mimos.my*

MONASH UNIVERSITY (Monash): David Abramson*, *david.abramson@infotech.monash.edu.au*

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

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

NATIONAL INSTITUTE OF ADVANCED INDUSTRIAL SCIENCE AND TECHNOLOGY (AIST): Satoshi Sekiguchi*, *s.sekiguchi@aist.go.jp*; Yoshio Tanaka*, *yoshio.tanaka@aist.go.jp*

UNIVERSITI SAINS MALAYSIA (USM): Habibah A. Wahab*, *habibahw@usm.my*

UNIVERSITY OF CALIFORNIA, SAN DIEGO (UCSD): including the CALIFORNIA INSTITUTE FOR TELECOMMUNICATIONS AND INFORMATION TECHNOLOGY (Calit2), SAN DIEGO SUPERCOMPUTER CENTER (SDSC), CENTER FOR RESEARCH IN BIOLOGICAL SYSTEMS (CRBS), NATIONAL CENTER FOR MICROSCOPY AND IMAGING RESEARCH (NCMIR), NATIONAL BIOMEDICAL COMPUTATION RESOURCE; Peter Arzberger*, *parzberg@ucsd.edu*; Philip Papadopoulos*, *phil@sdsc.edu*; Teri Simas, *simast@sdsc.edu*

UNIVERSITY OF HONG KONG (HKU): W.K. Kwan*, *kwk@cc.hku.hk*; P.T. Ho, *hpt@cc.hku.hk*

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

Networking Members

Networking partners provide access to expertise to improve the efficiency of the resources groups in running distributed experiments and applications.

ASIA-PACIFIC ADVANCED NETWORK: (APAN): Seishi Ninomiya, *snino@isas.a.u-tokyo.ac.jp*; Kento Aida, *aida@nii.ac.jp*

PACIFIC WAVE: Jacqueline Brown, jbrown@ms.uw.edu

STARLIGHT AND TRANSLIGHT/STARLIGHT INITIATIVES: Maxine Brown, maxine@uic.edu

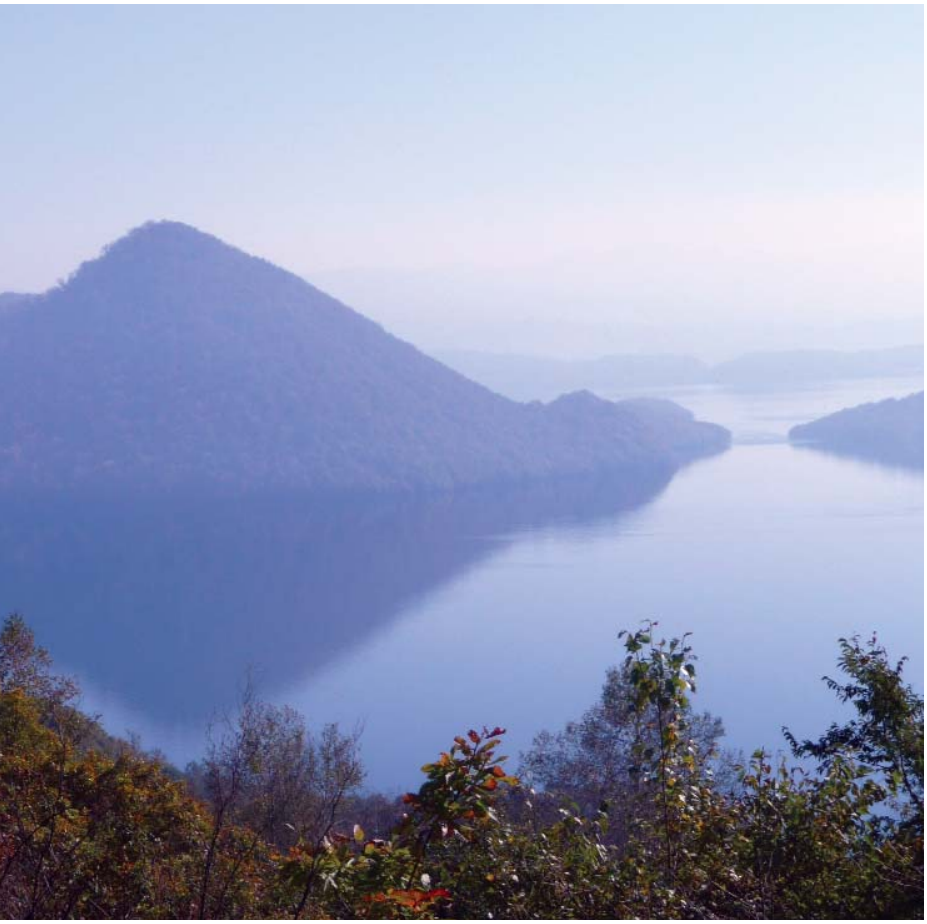
TRANSPAC2, INDIANA UNIVERSITY: James Williams*, *william@indiana.edu*; John Hicks, *jhicks@iupui.edu*

Industry Member

We gratefully acknowledge the contribution & support of our industrial partner.

CRAY INC.: Andrew Wyatt, *andrew.wyatt@cray.com*

PRAGMA is an institution- and people-based organization governed by a Steering Committee that invites new members, determines locations of workshops, and sets overall direction. More information about Steering Committee members (denoted with an asterisk * in the listings here) may be found at **www.pragma-grid.net/about/committee**.



Images, above: Lake Toya from Mount Usu—courtesy of Peter Arzberger; below left to right: PRAGMA PI Philip Papadopoulos leads the way during a PRAGMA 21 visit to Mt. Usu in Shikotsu Toya National Park—courtesy of Teri Simas; Red berries decorate a mountain ash tree in Shin-Sapporo—courtesy of Teri Simas

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

Additional Organizations Active in PRAGMA

Instituto Tecnológico de Costa Rica (ITCR) is a national autonomous institution of higher education, dedicated to the teaching, research and extension of technology and associated sciences aimed at the development of Costa Rica. Researchers there have been steadily building the cyberinfrastructure of Costa Rica and building ties with PRAGMA partners in particular regarding cloud computing . Recent efforts aimed to create a massively distributed PRAGMA Grid/PRAMA Cloud workflow for volcanic ash-dispersion simulation and risk management, named NG-TEPHRA, in close collaboration with the MeSsAGE Lab at Monash University.

LanZhou University (LZU; **www.lzu.edu.cn**) has contributed resources to the PRAGMA Grid, attended the PRAGMA 12, 13, 17, 18, and 19 workshops. They are currently providing resources and will participate in the PRAGMA Cloud.

National Applied Research Laboratory (NARL; **www.narl.org.tw/en**) was established in 2003 to consolidate nine national laboratories into a single nonprofit organization to construct, operate, and maintain the large-scale R&D facility and platform in support of 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.

National Institute for Information and Communication Technology (NICT; **www.nict.go.jp/index.html**), is an incorporated administrative agency that conducts general research and development on information technology supporting the ubiquitous society of the future. NICT supported students in the PRIME program in 2009, 2010, and 2011, and has participated in the activities of the Telescience Working Group through support of the high-definition video conferencing testing.

PRAGMA Sponsors

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ASGC is an e-Science center funded by both the Academia Sinica and National Science Council of Taiwan.

ASTI's grid activities are funded by the Department of Science and Technology (DOST), Philippines.

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Background Image: View from the ferry ride from Mainland Malaysia to Penang Island, George Town—courtesy of Peter Arzberger

AIST's sponsors include the Special Coordination Funds for Promoting Science and Technology (MEXT, Japan) and the Core Research of Evolutional Science and Technology Program (JST, Japan).

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NCHC receives major funding support from the National Science Council, Taiwan.

NCSA is a high-end computing center funded by NSF, the state of Illinois, the University of Illinois, industrial partners, and additional U.S. federal agencies.

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