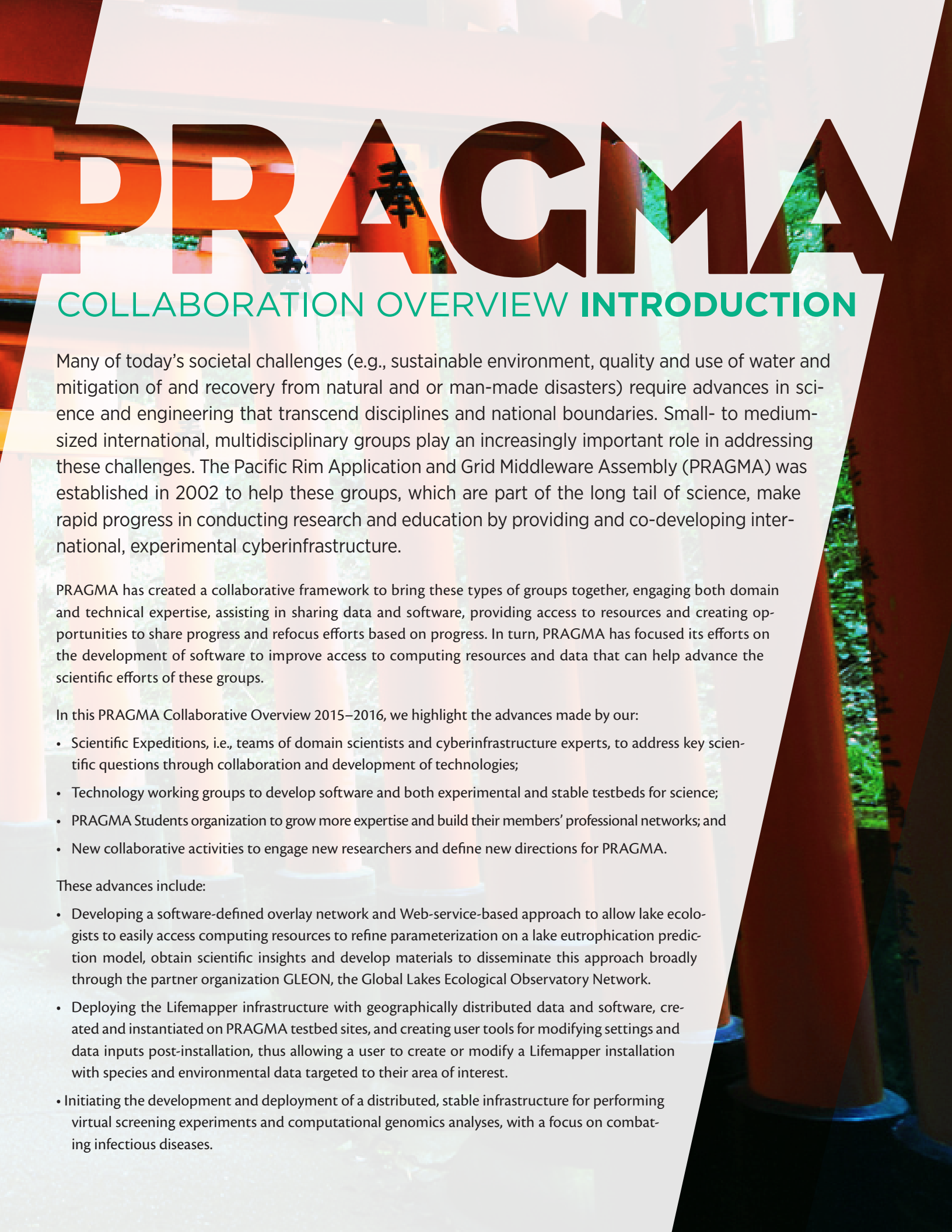
# PACIFIC RIM applications & GRID middleware assembly

2015–2016

# CONTENTS



Background: Fushimi Inari Taisha (Fushimi Inari Shrine) in Kyoto—courtesy of Aimee Stewart, U Kansas



# PRAGMA

## COLLABORATION OVERVIEW **INTRODUCTION**

Many of today's societal challenges (e.g., sustainable environment, quality and use of water and mitigation of and recovery from natural and or man-made disasters) require advances in science and engineering that transcend disciplines and national boundaries. Small- to medium-sized international, multidisciplinary groups play an increasingly important role in addressing these challenges. The Pacific Rim Application and Grid Middleware Assembly (PRAGMA) was established in 2002 to help these groups, which are part of the long tail of science, make rapid progress in conducting research and education by providing and co-developing international, experimental cyberinfrastructure.

PRAGMA has created a collaborative framework to bring these types of groups together, engaging both domain and technical expertise, assisting in sharing data and software, providing access to resources and creating opportunities to share progress and refocus efforts based on progress. In turn, PRAGMA has focused its efforts on the development of software to improve access to computing resources and data that can help advance the scientific efforts of these groups.

In this PRAGMA Collaborative Overview 2015–2016, we highlight the advances made by our:

- Scientific Expeditions, i.e., teams of domain scientists and cyberinfrastructure experts, to address key scientific questions through collaboration and development of technologies;
- Technology working groups to develop software and both experimental and stable testbeds for science;
- PRAGMA Students organization to grow more expertise and build their members' professional networks; and
- New collaborative activities to engage new researchers and define new directions for PRAGMA.

These advances include:

- Developing a software-defined overlay network and Web-service-based approach to allow lake ecologists to easily access computing resources to refine parameterization on a lake eutrophication prediction model, obtain scientific insights and develop materials to disseminate this approach broadly through the partner organization GLEON, the Global Lakes Ecological Observatory Network.
- Deploying the Lifemapper infrastructure with geographically distributed data and software, created and instantiated on PRAGMA testbed sites, and creating user tools for modifying settings and data inputs post-installation, thus allowing a user to create or modify a Lifemapper installation with species and environmental data targeted to their area of interest.
- Initiating the development and deployment of a distributed, stable infrastructure for performing virtual screening experiments and computational genomics analyses, with a focus on combating infectious diseases.

- Extending PRAGMA Experimental Network Testbed (ENT) to new sites to run Trans-Pacific monitoring activities and tests, thereby improving the use of these resources by our expeditions and other small to medium-sized groups working with PRAGMA.
- Migrating a component of the popular simulation software EDISON, developed by the Korea Institute of Science and Technology Information (KISTI), to the National Center for High-performance Computing (NCHC) to help build the computational science community in Taiwan.
- Assisting the launch of the US-East Asia Collaborations to Enable Transnational Cyberinfrastructure Applications (US-EA CENTRA), a multi-site effort launched by the University of Florida, NCHC, and the National Institute of Information and Communication Technology (NICT).

These and other advances can be found in the following pages of this year's PRAGMA Collaborative Overview.

In the coming year, PRAGMA will leverage shared experiences in its community built over the last thirteen years to continue to make advances in each of the areas described above, and it will move forward on two new major efforts:

- Creating a stable computing and data environment for science expeditions and other science groups to access and use to conduct science.
- Testing approaches to ensure access to "persistent" data via software-defined approaches.

The value of resources and data are in their active use. Each of these new major activities has known challenges. The challenge with distributed resources is the ability to easily prepare and securely provide access to the different sites for use by scientific groups. The challenge with the use of data are multifold, including both technical (integration of heterogeneous data, access controls, ability to track data) as well as governance issues (local rules limiting access, migration of data, or citation). Data are often the social bridges of the collaboration, thus underscoring the need to address the social issues of governance. In particular, our expeditions can only succeed when data can be accessed at multiple sites and used to gain improved understanding, that, for example, lead to better predictions of lake water quality or forces on biodiversity.

Image: PRAGMA Co-Investigators Strategic Planning Meeting at UCSD—courtesy of Teri Simas, UCSD

# AT A GLANCE

PRAGMA was established in March 2002, with the mission to *enable the long tail of science through scientific expeditions and infrastructure experimentation for Pacific Rim institutions and researchers*

**MEMBERS:** 29 Institutional Members

**GOVERNANCE:** Steering Committee, and PRAGMA's Operating Principles and Procedures

**WORKSHOPS OF PARTICIPANTS:** Twice a year to share progress and plan future activities; open to all, hosted by PRAGMA members, often in conjunction with other activities

## 2015 WORKSHOPS

- **PRAGMA 28:** April 8–10, 2015, Nara Institute of Science and Technology
- **PRAGMA 29:** October 7–9, 2015, Universitas Indonesia. Held in conjunction with the 7th International Conference on Advanced Computer Science and Information Systems (ICACSIS 2015), PRAGMA Workshop on International Clouds for Data Science (PRAGMA-ICDS'15), and International Workshop on Building Collaborations in Biodiversity Informatics.

## 2016 WORKSHOPS

- **PRAGMA 30:** January 27–29, 2016, Advanced Science and Technology Institute (ASTI). Held in conjunction with the 41st Asia-Pacific Advanced Network (APAN) meeting.
- **PRAGMA 31:** Date TBD, Thammasat University

## SCIENTIFIC EXPEDITIONS

- **BIODIVERSITY:** Understanding biological adaptation in extreme environments
- **LAKE SCIENCE:** Predicting lake eutrophication
- **ENT:** Developing an experimental network testbed for experimenting with software-defined networks and monitoring impacts of choices

## WORKING GROUPS

- **RESOURCES:** Making the distributed resources of PRAGMA useful to diverse applications
- **TELESCIENCE:** Making and improving access to or use of remote equipment (e.g. tiled-display walls or sensors)
- **BIOSCIENCES:** Integrating technologies to create an infrastructure to advance the screening of potential compounds to combat infectious diseases. Creating stable infrastructure to perform computational genomics analyses with a focus on infectious diseases
- **CYBERLEARNING:** Developing simulation-based learning technology

## STUDENTS

- **PRAGMA STUDENTS:** Stimulating international cross-disciplinary collaboration among students and junior researchers

## PARTNER ACTIVITIES

- **GLEON:** Global Lakes Ecological Observatory Network, whose mission is to understand, predict and communicate the role and response of lakes in a changing global environment (gleon.org)
- **US-EA CENTRA:** US–East Asia Collaborations to Enable Transnational Cyberinfrastructure Applications, whose long-term goal is to create an international framework to coordinate research and engage junior researchers in software defined infrastructure, with initial drivers of environmental modeling, disaster management and smart cities (*www.useacentra.org*)
- **SEAIP:** Southeast Asia International Research and Training Program, hosted annually by NCHC, to promote collaborations in cyberinfrastructure among researchers in Southeast Asia and between those researchers and others around the world

## SPONSORS

- Multiple, often associated with members and funded through many different national science foundations

## WEBSITE

- *www.pragma-grid.net*

Background: Great Buddha at Todaiji Temple—courtesy of Teri Simas, UCSD

EXPEDITIONS & HIGHLIGHTS

# PRAGMA LAKE EXPEDITION

## *Understanding and Predicting Degradation of Lake and Reservoir Water Quality around the World*

Scientists in the PRAGMA Lake Expedition are working to better understand and predict the globally pervasive degradation of lake and reservoir water quality. Meaningful advancements require new understanding of how complex biophysical interactions result in extreme growth of phytoplankton (harmful algal blooms) and ensuing production of noxious substances that make water unsuitable for use. While algae blooms can be detected by sensor networks, the real goal is to predict the circumstances in which blooms may occur, thereby providing advanced warning for water managers and the public who may rely on the services provided by lakes and reservoirs.

Technical advancements that span disciplines and national boundaries are helping lake ecologists improve predictions of algal blooms. Large data sets from sensors embedded in lakes and reservoirs, combined with new simulation models and expert knowledge from the global community show promise for making predictions of the future based on patterns from the past. However, many challenges remain due to:

- their nature, extreme events are difficult to predict and tend to be evident only in high-frequency, large data sets, which have an abundance of pattern, as well as noise, at multiple time scales;
- complex models of ecosystems require thousands of model runs and advanced parameterization techniques for proper calibration;
- validation of predicted bloom events requires pattern matching between simulations and the surprises that occur in the data, and
- the cyber-infrastructure and compute resources required to support these activities are out of reach for most lake ecologists.

Scientists in the PRAGMA Lake Expedition are tackling these issues with a three-pronged approach: (1) creative application of pattern detection and classification algorithms adapted from computer science; (2) easy user access to cyberinfrastructure that brings much needed compute resources to the desktops of ecologists and; (3) a community approach to technology systems development that embeds scientists from multiple disciplines in the process.

Background Images: (left) Lake Sunapee—courtesy of June Fichter, Lake Sunapee Protective Association; (right) GLEON researchers—courtesy of Kathleen Weathers, Cary Institute of Ecosystem Studies and Lake Sunapee Protective Association

*1. Applying pattern detection and classification algorithms:* Do sensors and simulations speak the same language? Large volumes of time series data from sensor networks are creating new opportunities to understand time dynamics of lakes. However, the amount of data, the complex patterns in the data and the need for automated pattern discovery and matching demand a highly efficient and flexible representation of the data. Symbolic aggregate approximation (SAX) [1], a symbolic representation of time series, solves many algorithmic problems through dimensionality and numerosity reduction, quantification of similarity between time series and discovery and representation of otherwise difficult to handle data features, such as highly skewed probability densities (Fig. 1). Essentially, SAX converts data to words and uses natural language processing algorithms to discover and classify patterns and collections of patterns in a manner akin to developing a dictionary (i.e., the possible words) and a vocabulary (i.e., the dictionary subset used in a time series). For example, a rare word in sensor data that might represent a surprising algal bloom can be catalogued and easily searched within the collection of words created by the SAX representation of the simulated data.

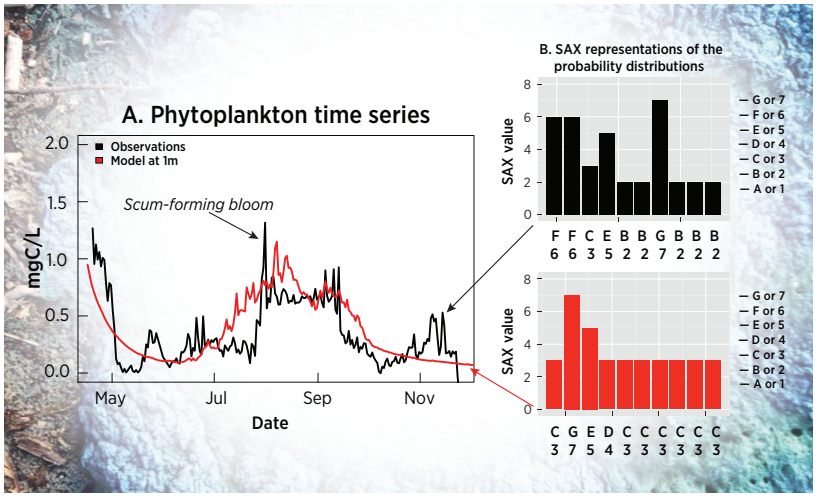
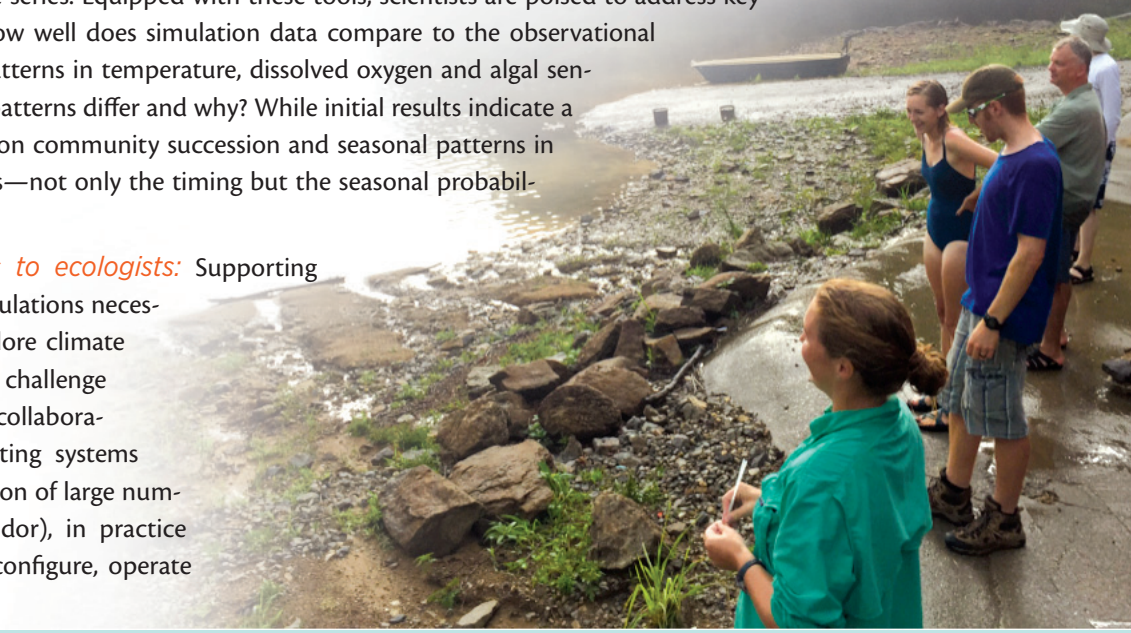



Figure 1. (A) Time series of algae (phytoplankton) from a buoy (black line) plotted with model simulation (red line). The probability densities for these time series are represented as (B) SAX words, with 10 letters per word (x axis) and 7 letters in the alphabet (y axis). The observed data (upper) produce a highly skewed ("F" as the first letter) distribution with rare, but important, events ("G" as the 7th letter). In contrast, the modeled data (lower) conform to a log-normal distribution. The SAX representation allows us to quickly and easily quantify the differences in distributions from thousands of simulations based on a simple distance metric for word comparison. The model has difficulty recreating the algal blooms, as indicated in the observational data and shown in the background image (Aphanizomenon bloom washed up on the shore of Lake Mendota, WI).

Over the past year, the PRAGMA Lake Expedition has developed several SAX algorithmic tools to illuminate time series data features: a similarity metric that quantifies the difference between simulated and observational time series, as well as corresponding probability distributions (Fig. 1); algorithmic motif identification in time series (e.g., most frequent patterns); algorithm anomaly detection in time series; and clustering and classification algorithms to determine the relationship amongst multiple lake time series. Equipped with these tools, scientists are poised to address key research questions, including how well does simulation data compare to the observational data? What are the common patterns in temperature, dissolved oxygen and algal sensor network data? How do the patterns differ and why? While initial results indicate a strong tie between phytoplankton community succession and seasonal patterns in water quality, predicting blooms—not only the timing but the seasonal probability—remains challenging.

*2. Bringing compute resources to ecologists:* Supporting the large numbers of model simulations necessary to calibrate models or explore climate change scenarios raises another challenge that requires interdisciplinary collaboration. While distributed computing systems that support concurrent execution of large numbers of jobs exist (e.g., HTCondor), in practice these systems are complex to configure, operate



and use—especially in collaborations across multiple institutions in different countries and in domains where distributed computing has not been widely adopted. The PRAGMA Lake Expedition has been developing overlay virtual networks that seamlessly aggregate computers across multiple institutions, greatly simplifying the configuration and deployment of geographically distributed HTCondor computing pools (the underlying overlay network, IPOP, is also featured as a technology highlight in this overview). Easy user access to this powerful technology is key to adoption. To this end, the Expedition has focused on augmenting the IPOP-HTCondor back-end distributed system with a Web-services-based middleware that allows users to submit large simulation batches from their own desktops (IPOP is described later in this section). This interdisciplinary work has led to the development of a Web service that supports the distributed execution of General Lake Model (GLM) simulation batches through HTCondor-IPOP pools launched from an intuitive user interface using the R programming language (Fig. 2).

3. *International community development and education:* One of the major goals of the PRAGMA Lake Expedition team is to make these technologies widely accessible to the next generation of interdisciplinary researchers, i.e., enable students from a diversity of backgrounds to gain experience in distributed computing tools and software to enhance their domain-specific research. Thus, approaches for examining the drivers and effects of harmful algal blooms can be broadly applied, both to other lakes by different teams of lake scientists, as well as to other questions, such as climate change effects on lake water quality. The Expedition is growing a user community by training students how to explore lake models that use overlay network and distributed computing technologies to perform thousands of simulations quickly. In June 2015, team members launched this part of the expedition as a lake modeling and software development workshop, and the lessons learned informed the design of a modeling workshop in October for more than thirty graduate students at the 2015 Global Lake Ecological Observatory Network in Chuncheon, South Korea.

While the PRAGMA Lake Expedition team prepares initial water quality research for publication, broader demand grows quickly. Expansion of sensor networks worldwide, along with rapid adoption of the GLM simulation software by the global community, has heightened the urgency for the Expedition to deliver both technological and training support as scientists take on a broad suite of water quality issues.

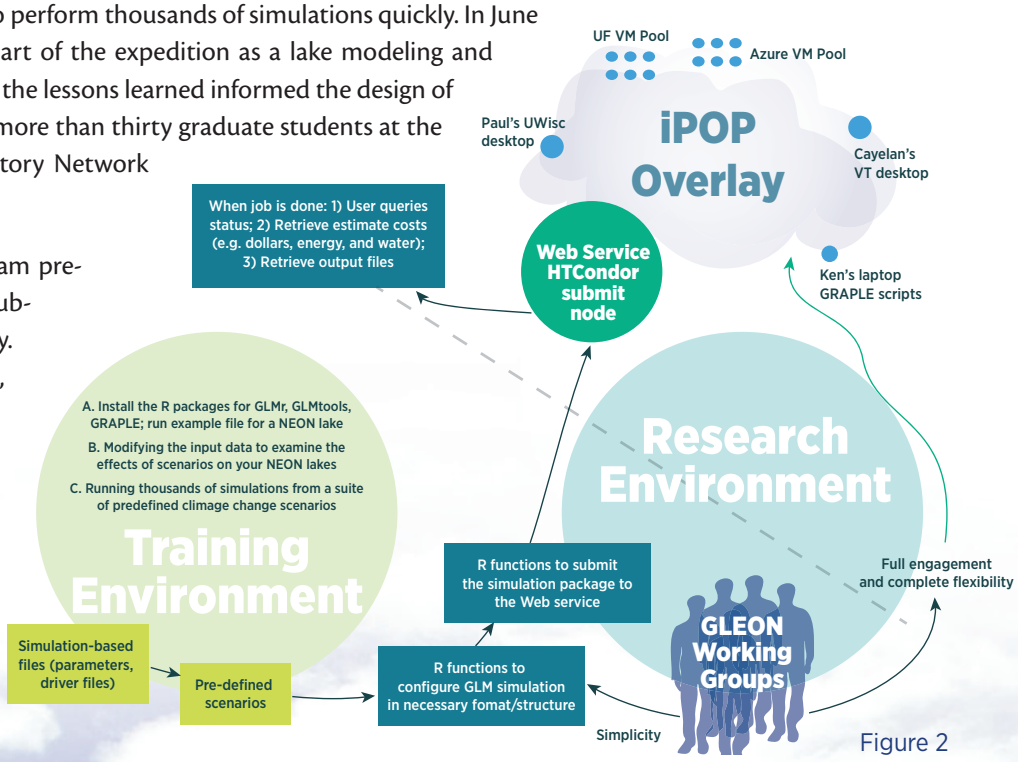



Figure 2

**PARTICIPANTS:** *University of Florida:* Renato Figueiredo, Ken Subratie, Saumitra Aditya; *Virginia Tech:* Cayelan Carey, Jonathan Doubek, Alexandra Gerling, Kate Hamre, Ryan McClure; *University of Wisconsin:* Paul Hanson, Craig Snortheim; *Indiana University:* Guangchen Ruan, Beth Plale

## REFERENCE:


1. Lin J, Keogh E, Lonardi S, Chiu B. 2003. A symbolic representation of time series, with implications for streaming algorithms. Proceedings of the 8th ACM SIGMOD workshop on research issues in data mining and knowledge discovery - DMKD '03:2. http://portal.acm.org/citation.cfm?doid=882082.882086


# VIRTUAL BIODIVERSITY EXPEDITION

## *Developing and Deploying Lifemapper Infrastructure to Understand Forces Driving Biodiversity*

One of the ongoing activities of the PRAGMA is fostering virtual biodiversity expeditions by bringing domain scientists and cyber infrastructure specialists together as a team. Over the past few years, PRAGMA members have been collaborating on virtualizing the Lifemapper software infrastructure. Virtualization and cloud computing have increased scalability, flexibility, efficiency and simplified application deployment on the PRAGMA cloud.

Lifemapper is a complex biological software infrastructure developed by the Biodiversity Institute at The University of Kansas. It creates and maintains an archive of species distribution maps calculated from public specimen data and includes a suite of data and tools for biodiversity researchers that calculate single and multi-species distribution predictions and macro-ecological analyses. Our technical goal is to create a viable virtualization solution that can be easily adopted and reused by scientists at multiple institutions and projects. This solution 1) allows fast deployment of ready-made cluster images; 2) reproduces the complete Lifemapper processing pipeline at different sites and hosting environments; and 3) enables scientists to perform Lifemapper-facilitated data processing on large, sensitive or restricted data.

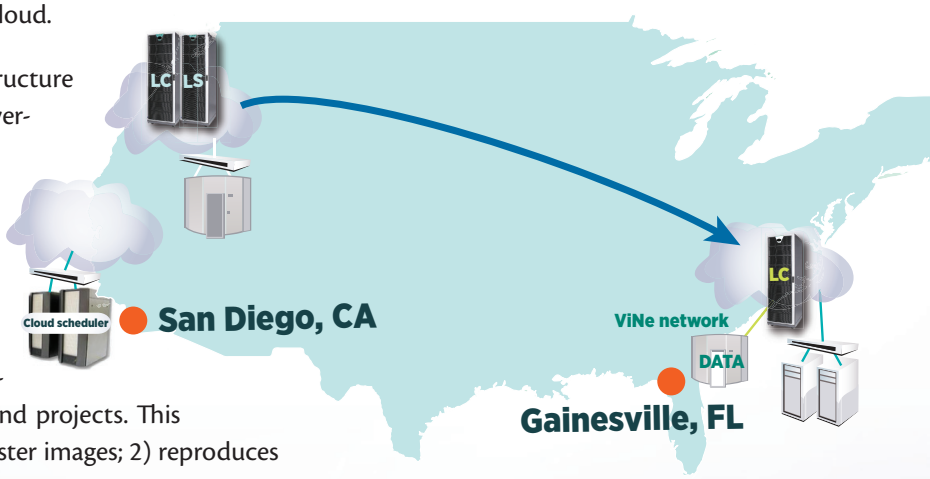



Figure 3. Virtual Lifemapper infrastructure on PRAGMA Testbed with access to private data. Credit: Nadya Williams, UCSD

The inherent complexity of the Lifemapper infrastructure made application installation, management and configuration very challenging. We began by moving the entire Lifemapper infrastructure to the Rocks Cluster Management system, and by packaging the software, dependencies, and configuration scripts into a Rocks "roll". The roll packaging system gave us a robust framework to codify Lifemapper and dependency configurations and requirements. This resulted in a systematic approach to packaging a complex, domain-specific data analysis system for deployment on a variety of system configurations and virtualization softwares.

Background: Mt. Kinabalu, Malaysia—courtesy of Antony van der Ent, U Queensland

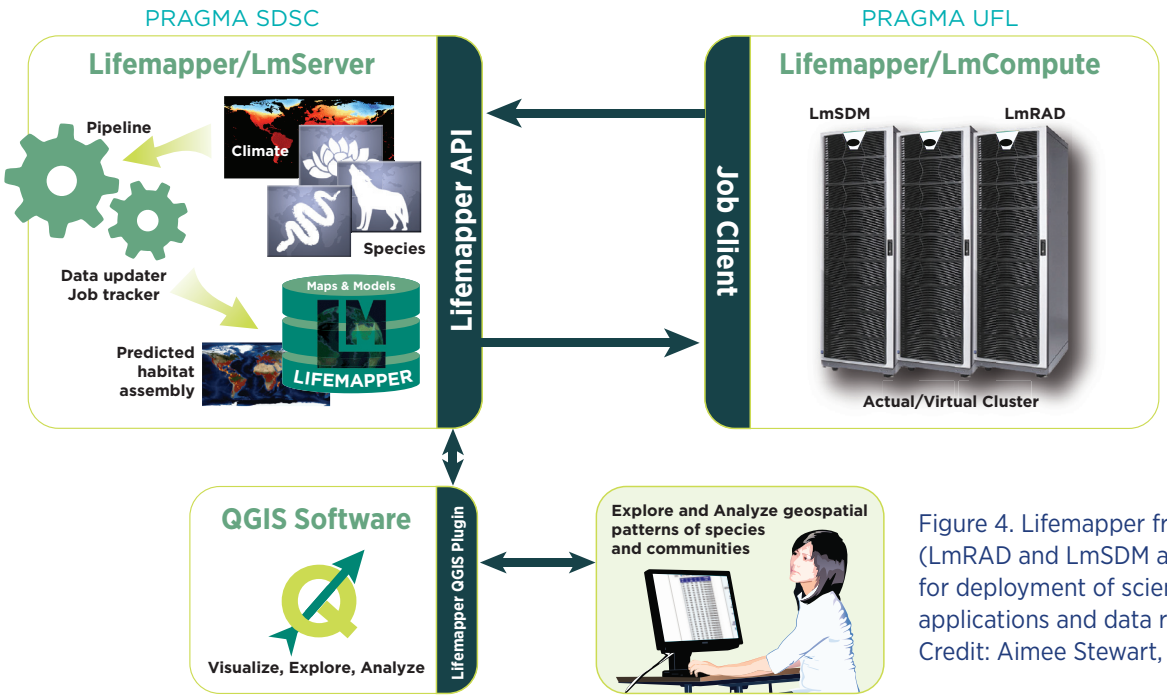



Figure 4. Lifemapper framework (LmRAD and LmSDM analyses) for deployment of scientific applications and data resources. Credit: Aimee Stewart, U Kansas

We use system virtualization to define and make the full application stack portable, including its complex software dependencies. Portability provides advantages ranging from replicating entire clusters to deploying on a single laptop for education or research.

For PRAGMA 28, we addressed both geographically distributed software components and data resources. The PRAGMA Testbed sites were used for instantiating distributed Lifemapper software components: the San Diego Supercomputer Center (SDSC) created virtual images for both Lifemapper components (LmCompute and LmServer) then migrated the LmServer virtual cluster to another site at SDSC and the LmCompute virtual cluster to the University of Florida (UF). Figure 3 illustrates the infrastructure used to distribute Lifemapper components and connect them to the UF data. These data were commercial satellite imagery from Kinabalu (Borneo, Malaysia), licensed only to physically reside at the University of Florida (UF). They were installed on a non-PRAGMA Testbed UF machine then connected to the LmCompute virtual cluster using a ViNe (Tsugawa and Fortes, 2006) private network. We deployed LmCompute at the same location as the input data with usage restricted to UF, with the PRAGMA network simplifying authentication and data permissions. The resulting Lifemapper workflow is illustrated in Figure 4.

For PRAGMA 29, we continued to use our programmatic approach to creating and deploying virtual images on the PRAGMA Testbed, focusing on a reproducible and configurable infrastructure. Automating builds allowed faster and simpler Lifemapper deployment for researcher- or institution-based instances, but the input data population was tied to data and values set in the install package. We generalized data population by adding a site-based configuration file and data population tools that can be edited and executed, respectively, post-installation. This allows site-specific variables to be overridden after installation, directing application tools to download, register and use new data. In addition to modifying installations based on Lifemapper-defined input data, we have simplified and formalized the metadata requirements for user-provided inputs, allowing researchers to process their own species or environmental data once they fully describe its content and location. Our goal with this simplified configuration is wider adoption of the ready built images by collaborators or researchers who wish to run their own instances of Lifemapper. We realized this goal by creating a dedicated LmServer at Universitas Indonesia for new infrastructure bridging Indonesia and other PRAGMA sites.

In addition to installation and configuration improvements, for PRAGMA 29, we also finalized the networking between LmServer and LmCompute components on a single virtual cluster. This simplifies the use of Lifemapper in the classroom as a teaching tool or in the field with newly collected field data.

Our goal in this work is to create a viable virtualization solution that can be easily adopted and reused by scientists at other institutions and projects. A more immediate goal is to garner users (institutional and individual) to use these tools to create and work with their own specialized Lifemapper instance. New tools to modify and re-populate a local installation with new input data was the first and primary step towards achieving that goal. The new Universitas Indonesia Lifemapper installation will be a testing ground for local scientists to suggest improvements to the process. Several additional steps are underway. First, we are extending the data processing pipeline to enable dynamic multi-species pattern analyses of arbitrary subsets of the data archive. The PRAGMA Virtual Biodiversity Expedition will use these new tools in a Lifemapper instance populated with data of Mount Kinabalu, Malaysia for a more complete biodiversity analysis of the region. Second, we will continue modularizing Lifemapper code to adapt data processing steps for unique data needs or to answer a variety of biodiversity researchers' questions. Third, we will incorporate different networking scenarios in the Lifemapper virtual infrastructure facilitated by advances in overlay networks in the PRAGMA Experimental Network Testbed (ENT). Finally, the availability of Lifemapper on the PRAGMA cloud now opens the opportunity to explore additional questions of data sharing. In earlier PRAGMA work, Indiana University (IU) added provenance capture to Lifemapper to capture data lineage (mappings between input data, processes, and outputs) and to contribute to data trustworthiness. As IU prepares to add a data node to the PRAGMA ENT (See ENT later in this section), we will explore how the IU Komadu tool can contribute to data quality and scientific provenance.

**PARTICIPANTS:** *UC San Diego:* Nadya Williams; *University of Kansas:* Aimee Stewart; *University of Florida* and the *National Science Foundation*: Reed Beaman

## REFERENCE:

Tsugawa, M. and J. A. B. Fortes, "A Virtual Network (ViNe) Architecture for Grid Computing," 20th Intl Parallel and Distributed Processing Symposium (IPDPS-2006), 04/06.

**Biodiversity research examines the variation among living things and systems, ranging in scale from molecules, genes, cells, individual organisms, to species through ecosystems. The Pacific Rim, and Southeast Asia in particular, encompasses globally significant areas of biodiversity and is a transition zone between Asia and Australia [Wallace's line], offering unique opportunities to study island effects and geological and tectonic complexity as drivers in adaptation and evolution Also, Southeast Asia is a region of high human and economic growth; biodiversity loss and climate change impacts increase the urgency to use efficient and effective infrastructure methods in research. PRAGMA's interest in Southeast Asia was to bring a focus on an area that is of great importance in understanding biodiversity.**

**To illustrate the value of our overall approach, the virtual biodiversity expedition focuses its scientific questions on Mount Kinabalu (4095 m), in Sabah, Malaysia, which is a biodiversity rich, yet extreme, environment located in the northern part of Borneo. The mountain is marked by numerous ultramafic (serpentine) outcrops where the soil and substrates are high in iron, magnesium, nickel and other metals that create an environment toxic to many plant and animal species. Using a tool such as Lifemapper (described in the text) allows us to understand species distribution and density through use of data collections and images about Mount Kinabalu. This in turn allows us to ask deeper questions, such as how plants, animals and microbes adapt to extreme environments, changing climate and toxic conditions, which is a broad scientific challenge. Finally, such a virtual expedition can only be possible through willing collaboration and support of the researchers "on the ground" at Sabah Parks.**

Background: Mt. Kinabalu, Malaysia—courtesy of Antony van der Ent, U Queensland

# BIOSCIENCES

## *Focusing Infrastructure Efforts to Combat Infectious Diseases*

The Biosciences Working Group has a long history of activity in PRAGMA. Much of this activity has been centered on the use of virtual screening techniques to identify novel chemical compounds with potential therapeutic application for a variety of diseases. This continues to be an area of active interest and collaboration among PRAGMA members. With the increasing amounts of biological data being collected, the Biosciences Working Group is working to redefine its objectives with the goal of developing technologies that will help to create a unified workflow for the processing and analysis of large biologically related datasets. Discussions held at PRAGMA 27 and PRAGMA 28 have identified infectious disease as one particular area of research that is of high importance in the East Asia region. Thus, the focus is to create distributed infrastructure and scientific tools that can be used by biomedical scientists specifically for discoveries in infectious diseases affecting East Asia. These types of experiments could be in proteomics or genomics and would require a stable infrastructure, which PRAGMA is providing.

At PRAGMA 28, a multi-site cloud environment for virtual screening was demonstrated resulting from interactions between the University of Florida (UF), University of California San Diego (UCSD), the Nara Institute of Science and Technology (NAIST) and The National Institute of Advanced Industrial Science and Technology (AIST) Information Technology Research Institute (Figure 5). This environment consisted of public and private cloud resources and utilized Hadoop for mapping tasks during virtual screening. With this stable environment established, members of Biosciences are looking forward to the creation of a unified natural products database with data from Japan, Indonesia, Vietnam, and Malaysia. The invited speaker at PRAGMA 28, Professor Shigehiko Kanaya from NAIST has provided his KNApSAcK Family database, and, through interactions with Universitas Indonesia (UI), this database is being curated so that it may provide a solid starting point for building the larger, unified database.

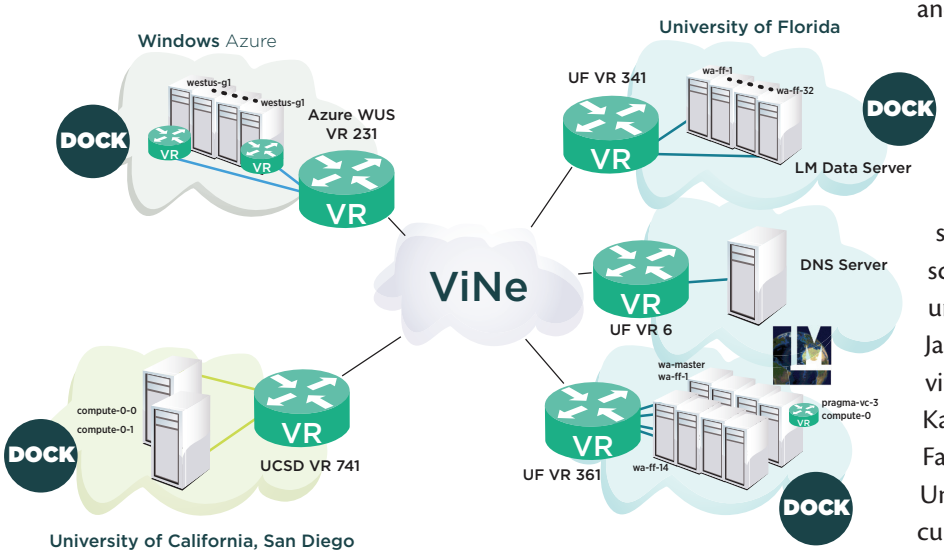



Figure 5. Diagram of multi-cloud environment combining public and private clouds. Credit: Andrea Matsunaga, U Florida

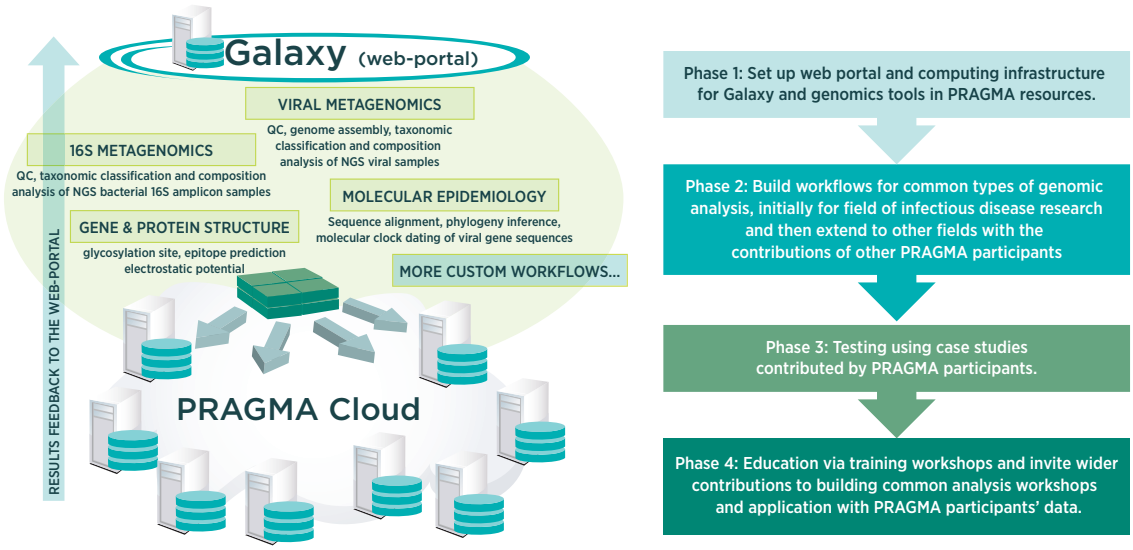
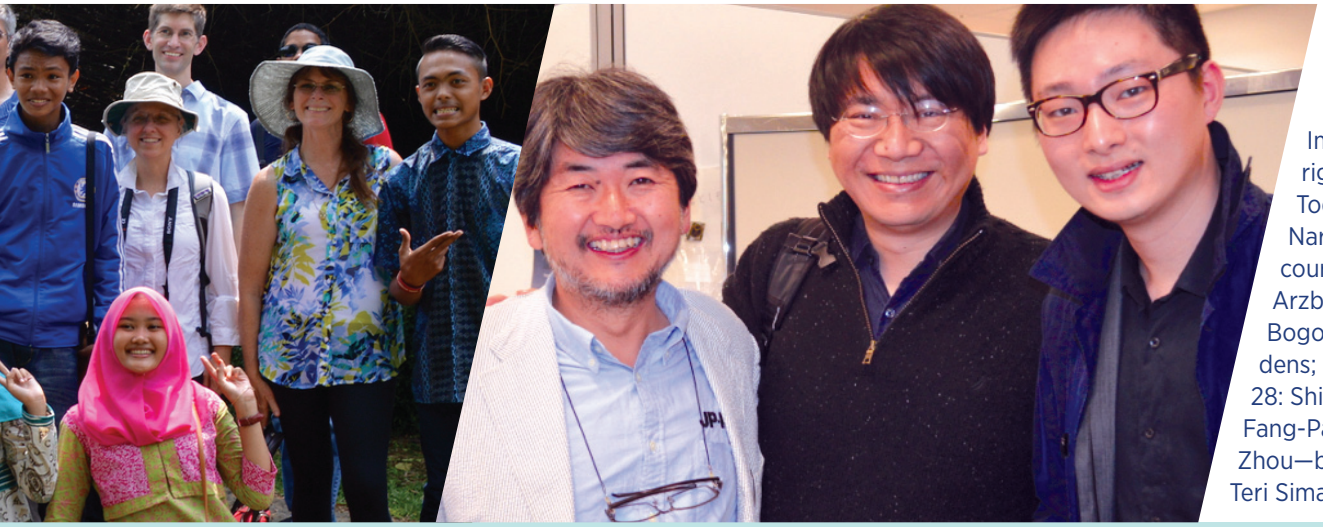



Figure 6. Planned genomics pipline in PRAGMA roadmap. Credit: Tommy Lam. Planned genomics pipline in PRAGMA roadmap. Credit: Tommy Lam.

The Biosciences team will be able to use the resulting database to discover novel chemical products for combating infectious diseases. This has the potential to become a natural products discovery platform that would benefit East Asia countries.

In a complementary activity, the Biosciences Working Group will soon begin genomics studies for infectious diseases. The overall goal is to create a platform for genomics analysis (e.g. genome assembly, sequence alignment, 16s metagenomics, etc.) (Figure 6). Interactions with NAIST, the University of Hong Kong (HKU) UI and Vietnam National University (VNU) have resulted in a preliminary build of a virtual machine (VM) with a package of common genomics analysis tools, including Bio-Linux 8, combined with a user interface and Galaxy, for the creation of reproducible analysis workflows. The VM is being tested, and its requirements are being established in order to better identify the demands these experiments will place on the PRAGMA infrastructure. Small tests will be performed with the functional VM for assembly and annotation. When successfully deployed on the stable PRAGMA infrastructure, there will be a scalable, easy-to-use platform for intensive genomics analyses among PRAGMA bioscientists, which will be easily extendable into other areas beyond infectious disease.

**PARTICIPANTS:** *AIST:* Jason Haga; *USM:* Habibah Wahab; *HKU:* Tommy Lam; *UI:* Arry Yanuar, Heru Suhartanto; *ICST:* Thanh Truong; *VNU:* Ly Le



Images: (left to right) Buddhas, Todai-Ji Temple, Nara, Japan—courtesy of Peter Arzberger, UCSD. Bogor Botanical Gardens; and PRAGMA 28: Shinji Shimojo, Fang-Pang Lin, Quan Zhou—both courtesy of Teri Simas, UCSD

# PRAGMA EXPERIMENTAL NETWORK TESTBED (PRAGMA-ENT)

## *A Resource for the PRAGMA Community*

The PRAGMA-ENT expedition will construct a breakable international software define network (SDN)/OpenFlow testbed for use by PRAGMA researchers and collaborators. PRAGMA-ENT is breakable in the sense that it offers complete freedom for researchers to access network resources in order to develop, experiment and evaluate new ideas without interfering with a production network. PRAGMA-ENT will provide the necessary networking support for the PRAGMA multi-cloud and user-defined trust envelopes. This exposes SDN to the broader PRAGMA community and facilitates the long-tail of eScience by creating new collaborations and new infrastructure among institutes in the Pacific Rim area.

The PRAGMA-ENT team has been connecting resources in the U.S. (University of Florida and University of California, San Diego), Japan (Nara Institute of Science and Technology, National Institute of Advanced Industrial Science and Technology and Osaka University), and Taiwan (National Applied Research Laboratories). The Research Infrastructure for large-Scale network Experiments (RISE) service offered by JGN-X is used as the backbone. Our OpenFlow switches deployed at the participating sites are connected to the backbone through VLANs. RISE is a unique international OpenFlow network service that allows its users to deploy their own OpenFlow controller on the network testbed. Since all OpenFlow switches are interconnected through RISE, it is possible to develop our own controllers to manage the entire network testbed.

We are currently working with Internet2 and Indiana University (IU) researchers to expand the backbone and build an international "trust network" that provides trusted and secure transport of data from data sources to compute resources. Internet2 is also recently beginning a similar service to RISE that allows users to bring their own controller for the testbed by using FlowSpace Firewall (FSFW). Our plan is to interconnect RISE backbone and FSFW service, create a large-scale international SDN testbed and manage the trust network.

As new sources of research data become available worldwide (either through their creation or through enhanced mechanisms for sharing), researchers will be able to analyze data sets that are geographically dispersed, and/or restricted in their use. Restrictions are common for sensitive data, such as data that contain species distribution information, sensitive information about humans, etc.. Access may be restricted to within a university, a state, a region (physical boundaries) or a particular set of users—for instance, "scientific research" (role-based boundaries).

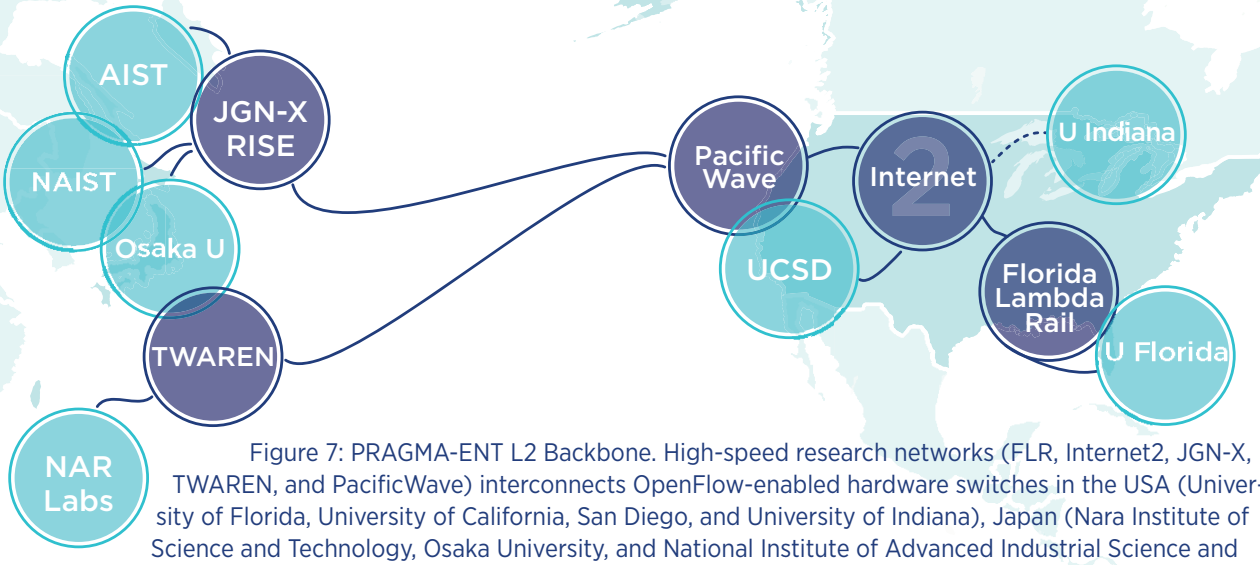



Figure 7: PRAGMA-ENT L2 Backbone. High-speed research networks (FLR, Internet2, JGN-X, TWAREN, and PacificWave) interconnects OpenFlow-enabled hardware switches in the USA (University of Florida, University of California, San Diego, and University of Indiana), Japan (Nara Institute of Science and Technology, Osaka University, and National Institute of Advanced Industrial Science and Technology), and Taiwan (National Applied Research Laboratories).

PRAGMA-ENT combines a network-oriented "trust network" with PRAGMA's strong social trust network to explore what it means to compute with sensitive data. The presence of an encrypted VNC both challenges and blurs the physical boundaries, and creates the trust scenario that allows the defining of role-based boundaries. Thus PRAGMA is uniquely suited to exploring this topic.

IU is entering into the PRAGMA-ENT as the first data node. The IU nodes will host a persistent data repository, a MongoDB datastore. It will initially contain digitized books that were digitized by the Internet Archives, leveraging the HathiTrust Research Center project at Indiana University. While the data from the Internet Archives is open to the public, this data is virtually indistinguishable from similar digitized content that is under copyright, so it is sensitive in nature. The availability of the data store will allow exploration of questions such as authorization and authentication, trust and experimental analysis utilizing distributed sensitive datasets.

**PARTICIPANTS:** *UF:* Matthew Collins (co-lead), Jose Fortes; *NAIST:* Kohei Ichikawa (co-lead), Pongsakorn U-chupala, Chawanat Nakasan, Che Huang, Yasuhiro Watashiba; *NICT:* Hiroaki Yamanaka, Jin Tanaka; *UCSD:* Luca Clementi, Philip Papadopoulos; *Osaka U:* Yoshiyuki Kido, Susumu Date, Shinji Shimojo; *AIST:* Jason Haga, Ryosei Takano, Atsuko Takefusa, Yoshio Tanaka; *NARLabs/NCHC:* Li-Chi Ku, Fang-Pang Lin, JenWei Hu, TeLung Liu; *IU Bloomington:* Quan Zhou, Beth Plale, James Williams, Jennifer Schopf; *Internet2:* John Hicks, Rick McMullen; *CNIC:* Kevin Dong, Yongmao Ren; *JLU:* Xiaohui Wei; *Kasetsart U:* Putchong Uthayopas

# CYBER-LEARNING

## *Propagating EDISON and Computational Science from KISTI to NCHC*

EDISON (EDucation-research Integration through Simulation On the Net) is a simulation-based Cyber-learning system which is based on the EDISON platform v2.0 for computational science and engineering (CSE) students and researchers in Korea. The EDISON system (*www.edison.re.kr*) has been developed over the past four years by Korea Institute of Science and Technology Information (KISTI) under the financial support of Ministry of Science, ICT and Future Planning. Since 2011, the system has become more popular and has been servicing about 28,000 users from more than 150 universities in Korea, with a total of 249 simulation software components or packages from five different CSE disciplines: Computational Fluid Dynamics (CFD), Computational Chemistry (Chem), Nano Physics (Nano), Computational Structural Dynamics (CSD) and Computer-aided Optimal Design (Design). The EDISON portal consists of these five sub-domain sites, in which domain-specific simulation software is found and executed for users. Thanks to its popularity and educational impact in Korea, the international recognition of the EDISON system has been extended to one of the participating institutions in PRAGMA—the National Center for High-performance Computing (NCHC) in Taiwan.

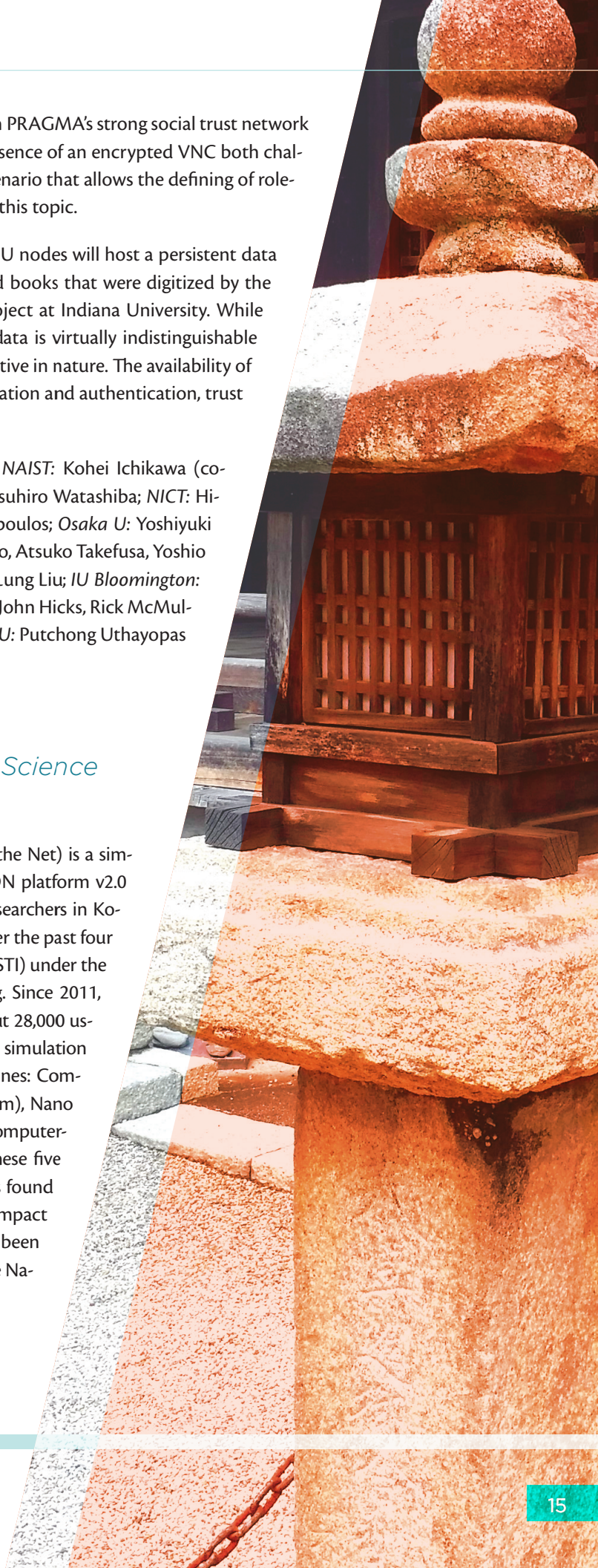
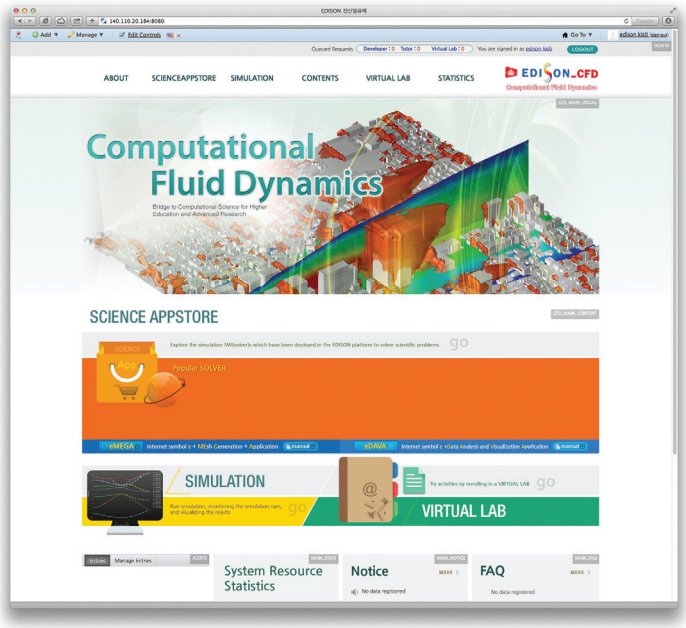


Image: Stone Lantern, Horyuji-temple, Ikaruga, Japan—courtesy of Peter Arzberger

To help boost and expand the high-performance computing (HPC) community in Korea and Taiwan, KISTI and NCHC have been tightly collaborating. In particular, both KISTI and NCHC agreed to deploy the CFD EDISON portals site at NCHC. In the process of deploying the CFD site at NCHC, KISTI encountered technical challenges such as system configurations, firewalls, account management, computing resources and graphic user interface (GUI) in Chinese. Through several months of collaboration, these challenges were overcome, and as a result, KISTI successfully installed the CFD EDISON site at NCHC in the middle of June 2015, as illustrated below.




To better understand the EDISON Portal and its capabilities, KISTI invited NCHC researchers Chien-Heng Wu and Heng-Chuan Kan to KISTI from September 21 to 24, 2015 to meet with EDISON development team members. In addition to developing technical skills, KISTI hopes that the visit will strengthen both parties' collaborations in many other areas. Finally, NCHC plans to complete the localized CFD site at Taiwan in the near future, which it hopes will boost the CFD community by serving Taiwan's domestic CFD users.

In addition to the collaboration with NCHC, KISTI will be continuing to make its international efforts to contribute to the Cyber-Learning community in PRAGMA. This year, KISTI and Vietnam's Institute of Computational Science and Technology (ICST) plan to meet to further discuss the EDISON portal site's installation for Vietnamese CSE users. This collaboration will be under the Official Development Assistance (ODA) project. KISTI is also open to building other collaborations with research institutes and universities throughout the world.

The new release of the EDISON system is based on EDISON Platform v2.0, which was launched at the end of September. To accommodate many new users' requests and further improve the quality of the EDISON system, this release includes many features such as multi-language support, integration of the five different sub-domains, and provision of sample input file associated with each simulation software for running simulation jobs in a convenient way. To see the new release in greater detail, please visit the EDISON web site, *www.edison.re.kr*.

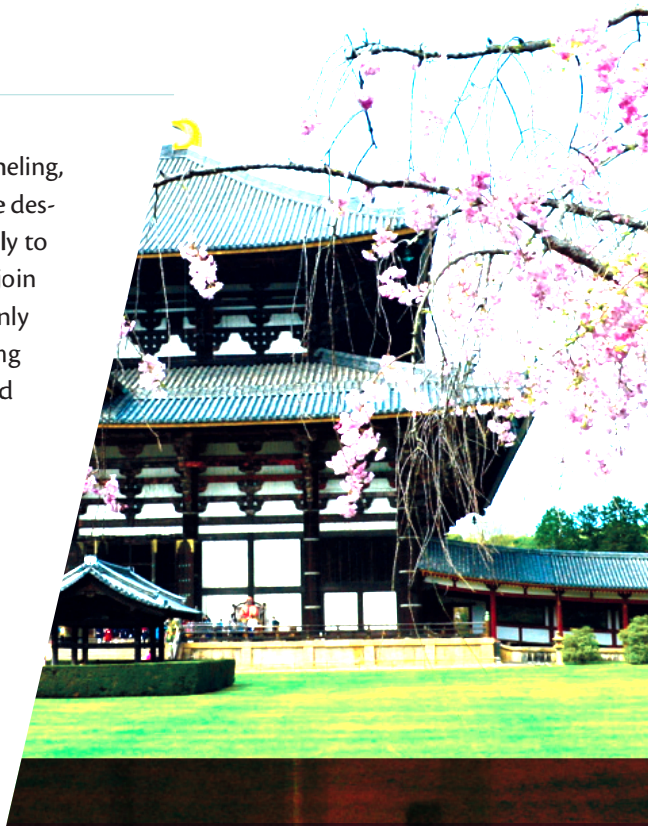
**PARTICIPANTS:** *KISTI:* Ruth Lee (lead); *NCHC:* Hsi-Ching Lin (co-lead)

# IP-OVER-P2P VIRTUAL NETWORK OVERLAY (IPOP)

## *Enabling the Creation of User-Controlled Trust Envelopes*

IPOP is one of the open-source software-defined network technologies used in PRAGMA to enable the creation of user-controlled trust envelopes. IPOP is different from other SDN technologies as it enables user-controlled virtual networks to be defined and managed by end-users themselves, and layered upon the public Internet, without requiring any reconfiguration of network devices, nor any modifications to operating systems, middleware and applications.

IPOP achieves this by running virtualization software—specifically, overlay virtual network routers—on Internet endpoints themselves. The software-defined network exposes an additional, private virtual network interface to computers that join the over-



lay, and is responsible for capturing packets at a source device, encrypting, tunneling, overlay-routing, decrypting and injecting into the virtual network interface at the destination device. The virtual network packet processing is performed transparently to users and applications: users only need to specify which devices are trusted to join the overlay, using Online Social Network (OSN) technologies, and applications only need to use the virtual private network (VPN) interface and communicate using existing network protocols (IPv4, IPv6, and Ethernet). This year's activities focused on three major thrusts.

First, in core IPOP development at the University of Florida, the software has been extended to enable the virtual network to function not only at Layer-3 (with the IPv4 and IPv6 protocols), but also Layer-2 (the Ethernet link-layer network protocol). This allows systems that rely on the use of protocols other than IP (such as ARP, the Address Resolution Protocol) to be supported by IPOP's "switch mode". Furthermore, efforts were applied to refactor the IPOP overlay network's distributed controller framework to support event-driven programming of new VPN features in a modular fashion. The development efforts during this year leveraged contributions from the open-source community through activities including Google Summer of Code.

Second, to facilitate integration with additional PRAGMA middleware, additional PRAGMA sites were involved in the configuration and deployment of a prototype IPOP overlay for private data sharing among PRAGMA members. Currently, this deployment supports physical and virtual machines, which can join the overlay and share files using the Network File System (NFS) protocol. Furthermore, the integration of IPOP with Rocks and Pragma-Cloud has continued, as has exploring the use of IPOP's Layer-2 switch mode.

Third, IPOP has been deployed in applications in support of science and used in conjunction with Web services to provide easy-to-access high-throughput computing services to lake ecology researchers and students (this is described in more detail in the PRAGMA Lake Expedition highlight in this year's Collaborative Overview, earlier in this section).

**PARTICIPANTS:** *IPOP development team* *UF:* Renato Figueiredo, Ken Subratie, Saumitra Aditya, Kyuho Jeong; *Middleware integration* *UCSD:* Philip Papadopoulos, Nadya Williams; *NAIST:* Kohei Ichikawa; *Lake expedition applications* *U Wisconsin:* Paul Hanson; *Virginia Tech:* Cayelan Carey

Image: Tommy T. Y. Lam, Peter Arzberger, and Tomomi Kosaka

# STUDENTS

## ENGAGING CURRENT & FUTURE GENERATIONS OF RESEARCHERS

PRAGMA is committed to engaging new communities of researchers. We focus on two broad efforts: One is to engage students in PRAGMA activities, the other is to work with communities of researchers to broaden the impact of the work we do and to leverage their interests. Both of these activities enrich PRAGMA by infusing ideas, questions, and energy into our workshops and activities between workshops.

In this section we will talk about three specific activities to engage students: PRAGMA Students, PRIME, and MURPA/QURPA.

# PRAGMA STUDENTS

## *Student-Led Activities for Professional Growth*

PRAGMA Students, formed in 2012, aims to help students gain opportunities for professional experiences within PRAGMA's trusted social and technical networks. As a student organization inside PRAGMA, the group is led by the PRAGMA Students steering committee and advised by senior PRAGMA researchers.

To date, activities of PRAGMA Students have included: organizing PRAGMA-affiliated student workshop and poster sessions as part of the PRAGMA Workshops; hosting online seminars with lecturers drawn from the broad PRAGMA community; and developing a unique model to provide multiple opportunities for students to participate in PRAGMA's collaborative scientific research. PRAGMA provides a trusted network and opportunities for leadership that help students gain valuable professional experience.

There are several advantages to joining PRAGMA Students and the PRAGMA community, including but are not limited to:

1. Participating in workshops and conferences in an international setting, which stimulates inspiration, information sharing and collaboration;
2. Strengthening research and ability for scientific exploration through challenging and state-of-the-art projects in collaboration with mentors and advisors throughout PRAGMA;
3. Benefiting from short-term residential research opportunities at other PRAGMA sites, which provides both research and cultural experience.

At the April 2015 PRAGMA 28 workshop in Nara, Japan, PRAGMA Students organized a student workshop. One of the student training opportunities for future professional careers included the organization of poster sessions. Members of PRAGMA Students steering committee reviewed and selected posters from all workshop participants. More than 20 posters were carefully reviewed, and detailed review feedback was provided to the submitters.

Also in the student workshop, we invited three PRAGMA professors and research staff to share their research and experiences. We are very grateful to Beth Plale, Kohei Ichikawa and Nadya Williams for giving us many helpful and informative insights. These fantastic talks not only enlightened students about their research, but also shared with them valuable life experiences. The invited talk session was very successful and we are looking to organize it again in the future.

To encourage students to improve their ability to present and showcase their work, PRAGMA Students once again hosted a lightning talk session during the pre-workshop. They invited around 10 students with innovative and impactful work to give short talks about their respective research posters. Three of the presenters were awarded with prizes for best talk, best technical talk and best talk describing new research.

In addition to poster sessions and lightning talk talks, short-term residential research opportunities are also provided to PRAGMA Students. Jiang Gu, a Ph.D. student from University of Tsukuba, is a visiting scholar from June to November, 2015 at the Data to Insight Center, IU, Bloomington. Gu is working on the SEAD (Sustainable Environment Actionable Data) project. This short-term program serves as an example of a collaboration between PRAGMA institutions that strengthens research by involving mentors and advisors from multiple disciplines and multiple institutions.

Additionally, from June to August 2015, PRAGMA members at Nara Institute of Science and Technology (NAIST) and the National Institute of Information and Communications Technology (NICT) in Japan welcomed three intern students from UCSD under the Pacific Rim Experiences for Undergraduates (PRIME) program. The students worked on various cutting-edge topics, including visualization of human emotions on a 3D screen, a disaster management interface and improving a virtual biochemical screening application (See PRIME Section). The students also had an opportunity to visit many places in Japan and learn about the local culture. In addition to academic and cultural benefits, the students worked closely with host professors and seniors and have built many lasting connections.

At PRAGMA 29 in Depok, Indonesia, PRAGMA Students continued their contributions to the PRAGMA workshop by organizing students' sessions, poster sessions and other activities. In particular, PRAGMA Students invited 13 students to give lightning talks in the pre-workshop. Several students papers were awarded prizes or certificates, and these students had the opportunity to present in the main workshop:

- The Most Innovative Talk: Soetrisno Cahya, Adjacency Hyperedges Matrix, A Hypergraph Model for Constructing Composite Object relationship, Faculty of Computer Science, Universitas Pelita Harapan, Indonesia.
- The Best Technical Talk: Hiroki Ohtsuji, Breaking the Trade-off between Performance and Reliability in Network Storage System, University of Tsukuba, Japan.
- The Most Impactful Talk: Takuya Yamada, Proposal of indoor evacuation system with smartphone, Osaka University, Japan.

Two honorable mentions: Denny Hermawan, Design and Analysis GPU Computing for Molecular Dynamics Simulations with AMBER Applications, Faculty of Computer Science Universitas Indonesia/Informatics Engineering Universitas Al Azhar Indonesia; and Irfan Fadhila, Performance Analysis of Virtual Machine and Container for Cloud Based High Performance Computing Platform, Faculty of Computer Science, Universitas Indonesia

**CURRENT LEADERS OF PRAGMA STUDENTS:** *IU:* Quan Zhou (co-chair); *Konkuk U:* Meilan Jiang (co-chair); *NAIST:* Pongsakorn U-chupala (co-chair), Chawanat Nakasan (co-chair); **PRAGMA STUDENT ADVISORS:** *IU:* Beth Plale; *Konkuk U:* Karpjoo Jeong; *Kasetsart U:* Putchong Uthayopas

# PRIME

## *International Experiential Learning and Collaboration*

The Pacific Rim Experiences for Undergraduates (PRIME) program was created in 2004 to provide a 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 collaboration between UC San Diego and PRAGMA researchers.

PRIME has been a model for providing both life-changing experiences and a rigorous and supportive research environment. This year, the PRIME program was able link students to research because those students were able to earn fellowships at UC San Diego.

## A Browser-based Tool for Virtual Screening Data Visualization

Traditional high-throughput screening uses vast chemical libraries to test thousands of compounds for reactivity with a target protein. Though effective, this process is highly resource-intensive. Virtual screening, which simulates molecular interactions and identifies compounds most likely to react, has therefore been developed to reduce the number of compounds that require physical testing. These programs, however require visualization and inspection of a large number of data files in order to identify favorable compounds and any false positives. Moreover, being able to compare several protein-ligand interactions in a high-throughput manner can enhance the analysis process and help to identify trends in chemical binding motifs. Currently, no tools exist that enable biomedical researchers to do this. Our tool solves this problem by providing a scalable, lightweight, easy-to-use, HTML5/Javascript based platform that has minimal setup requirements to view multiple molecular interactions side-by-side.

The user interface is composed of three different spaces: 1) a left panel with file and model controls, 2) a central workspace containing a grid of 3Dmol.js molecular viewers, and 3) a right panel displaying compound details. The central grid of viewers can be dynamically resized and the number of rows and columns of viewers in it can be easily changed via the left panel. The left panel also has straightforward controls for adding or removing different types of molecular surfaces, changing model display types (e.g.

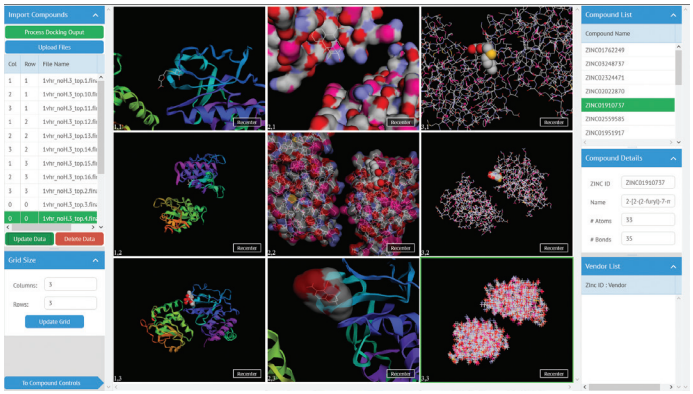


Figure 9. Screen capture of the high-throughput visualization tool. Left side is for grid and file controls and the right side is for chemical metadata. The central viewing grid (3x3 squares) illustrates the different molecular viewing modes that are possible. Credit: Curtis Cera, PRIME 2015

ball-and-stick to cartoon), and synchronizing all models to transformations done in just one viewer. Files may be directly uploaded to the interface and sent to individual viewers via other controls in the left panel. However, the application also possesses a specialized file parser that can filter large sets of files and append ligand model data and metadata to the relevant target compound file. This allows it to work directly with the output of virtual screening programs such as DOCK. The right panel displays key metadata about compounds loaded. Specifically, unique compound identifiers are added to an interactive list in the right panel. Each identifier is clickable, showing information such as the compound IUPAC (International Union of Pure and Applied Chemistry) name, number of atoms, number of bonds, and vendor information. Additional information such as chemical structure, number of H-bonds, pH, etc., are also viewable by clicking the IUPAC name.

Our tool provides a user with a multidimensional viewing space provided that simplifies the manual analysis of virtual screening data. Additionally, it provides the user with a single, streamlined tool for retrieving chemical metadata that is necessary for further investigation.

**PARTICIPANTS:** *PRIME 2015 Student:* Curtis Sera; *AIST*: Jason Haga; *NAIST*: Kohei Ichikawa, Yasuhiro Watashiba



Background: Courtesy of Curtis Sera, PRIME 2015

# Development of a Multi-site Disaster Management Tool

Disasters are sudden events that disrupt the functions of a community—usually beyond that community's ability to cope—and cause human, environmental, economic, or material losses. In preparation for disasters, communities often have disaster management cycles that detail plans to minimize losses and maximize the recovery speed of that community. During the response phase of these cycles, personnel must be able to react to the variable circumstances of the disaster to adequately stabilize the community. The goal of this project was to develop a disaster management application that is able to relay relevant information to decision-makers at multiple locations during a disaster crisis. The tool is harbored in SAGE2 (Scalable Amplified Group Environment 2; LAVA at University of Hawaii, Manoa and EVL at University of Illinois, Chicago), which acts as a platform that allows users to simultaneously interact in a shared collaborative environment. A secondary goal for this project is to expand upon application development in SAGE2.

The requirements for the tool were that it be simple and streamlined, providing enough geographical information to quickly inform decision-makers of disasters and available resources without overloading users with extraneous details. The users need to be able to obtain a quick overview of the regions of interest to help gauge their choices during a response. Because SAGE2 applications are written in JavaScript, the Leaflet Map library was used to generate a geographical map that could be manipulated. The D3 and Heatmap libraries were used to overlay different data types onto the map. Because of the lack of a readily-accessible database that holds relevant data, a data broker utilizing recursive functions was implemented to allow it to parse through different unique JSON (JavaScript Object Notation) datasets. By interacting with the HTML Document Object Model via JavaScript, a user interface was built into the application to allow users to toggle the visualized datasets, giving them access to either coordinate specific datasets (Figure 10) or heatmap type datasets (Figure 11).

Overall, this Disaster Application for Decision-makers (DADm) was able to fulfill the design objectives, being a multi-site application that could display coordinate and area specific JSON data, from different databases, based on the users' specifications. This application is an insightful first step for application development on SAGE2. Future work will include improving DADm to display real-time data in a more streamlined manner using a more universal data broker and more extensive performance testing of the system.

**PARTICIPANTS:** *PRIME 2015 Student UCSD:* Richard Hsiao; *AIST:* Jason Haga; *Osaka U, NICT:* Shinji Shimojo, *Osaka U:* Susumu Date, Hironori Shigeta, Yoshiyuki Kido, Satoru Matsumoto.

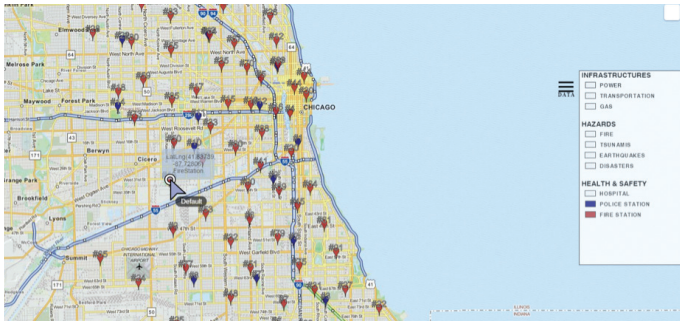



Figure 10. Screen capture of the application running on the SAGE2 interface displaying coordinate specific location data. On the right is a legend that controls different features of interest. Also displayed are two different datasets that show the locations of the local police stations (blue) and fire stations (red) in the city of Chicago, IL. Placing the cursor over an individual marker shows further metadata. Map zoom options are on the top left side. Layer options that control the heatmap layer are in the top right corner. Credit: Richard Hsiao, PRIME 2015

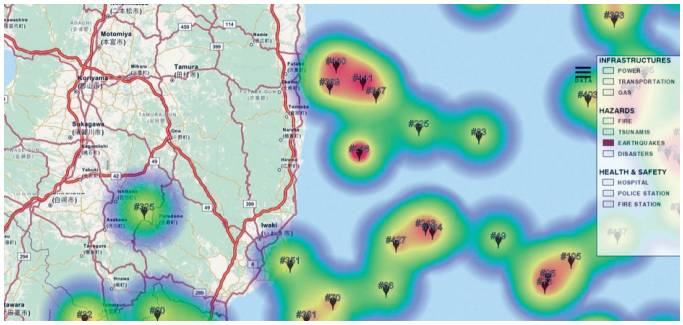



Figure 11: Screen capture of the application running on SAGE2 displaying heatmap data. The data shows JSON earthquake data from 2011 around the East Coast of Japan. The heatmap layer shows the magnitude of each earthquake in that area along with its coordinates (red indicates high magnitude, dark blue indicates low magnitude). Credit: Richard Hsiao, PRIME 2015

# Development of a Virtual Environment for Visualizing Emotions

Research in the field of quantifying the phenomenon of human emotions continues to be an ongoing process. Normally conveyed through speech, text, facial expressions and body language, emotions can also be recognized via a method undetected by the five senses: electrical signals in the brain. As a person's mood changes, so does the brain's activity, and brain-computer interfaces can be powerful tools in translating emotions from an abstract state of mind of one individual to a virtual and auditory environment that multiple people can experience together.

The goal of this project was to develop an interactive virtual reality application that places viewers in an environment comprised of the user's emotions. In order to classify emotions, we utilized the Emotiv EPOC neuroheadset to measure brain activity via EEG (electroencephalography) recordings. The device's 14 EEG channels and two reference channels were used to calculate emotions based on a combination of facial expressions (smiling, furrowing the brow, etc.) and states of mind (frustration, excitement, etc.). The environment was constructed in Unity, a 3D development platform, and demonstrated on a 200-inch auto-stereoscopic 3D high definition wall display provided by the National Institute of Information and Communications Technology (NICT).

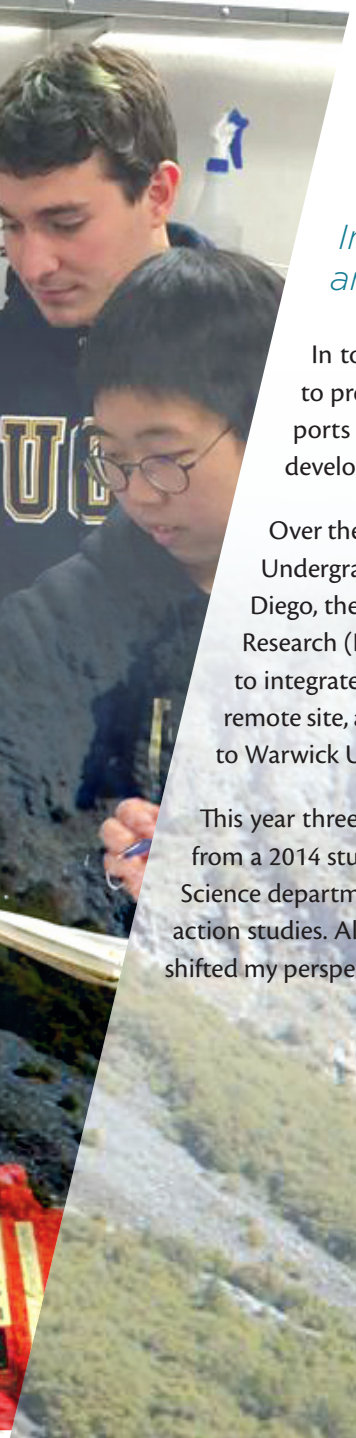
The wall displays 1920 x 1080 images at 60 fps without the need for 3D glasses. As long as viewers remain within 5.5 meters of the screen and look within a 40° angle, they can walk to the left or right in order to peer around the projected images. Once the user puts on the headset, the application calculates his or her emotion and particles then form on screen in varying shades, pulsing to the rhythm of the background music (select Mozart pieces). If the emotion detected is negative, the particles vary in blue hues and pulse slowly; if positive, they vary in orange hues and pulse at an upbeat rate. Calculations are done in real-time and once a change in emotional state is detected, the music and images on screen transition to the alternate state.

This immersive audiovisual experience was demonstrated in the Grand Front Osaka Building and will be showcased in San Diego at Mozart & the Mind, a festival exploring neurotechnology applications.

**PARTICIPANTS:** *PRIME 2015 Student NICT:* Michelle Wu; *Mentor UCSD:* Jurgen Schulze; *Host Mentor Osaka U and NICT:* Shinji Shimojo; *NICT:* Masaki Chikama, Yasushi Naruse, and Naomi Inoue; *Osaka U:* Hideyuki Ando; *XOOMS Co. Ltd.:* Atsuhiko Yasuda

Figure 12. Image of the device displaying emotions on the 3D wall in the Grand Front Osaka. The orange hues indicate positive emotions and blue hues indicate negative emotions. Credit: Michelle Wu, PRIME 2015

Images: (right, from the top) Stone lantern—courtesy of Aimee Stewart, U Kansas; Osaka Aquarium Kaiyukan—courtesy of Curtis Sera; Fushimi Inari Shrine—courtesy of Aimee Stewart, U Kansas



# MURPA AND QURPA

## *International Research Internships at the University of Queensland and Monash University*

In today's educational arena, universities must provide students with opportunities to work and study abroad to prepare them for global citizenship and professional competence in a multi-cultural workplace. Numerous reports have challenged universities to develop educational programs that provide an integrated academic basis for developing students' cultural/global competencies.

Over the past seven years, 34 Monash University students have travelled to international partners under the Monash Undergraduate Research Projects Abroad program (MURPA). They have travelled to the University of California, San Diego, the National Center for Supercomputing Research in Illinois, The Technion in Israel, the Institute for Infocomm Research (I2R) in Singapore and the University of Warwick. Students are placed for a period of 8 weeks, allowing them to integrate into the research groups as team members. Students have a local mentor in Australia as well as one in the remote site, and often bridge international research projects. In 2014/15 one Monash student travelled to UCSD, and one to Warwick University in the UK.

This year three University of Queensland (UQ) students travelled to UCSD. Alexia Lee and Zinta Flodine continued work from a 2014 student, Brian Song, and worked on the iRat project in Professor Andrea Chiba's Rat Lab (in UCSD's Cognitive Science department). Their work focused on giving the iRat social behaviors, making it a more effective tool for social interaction studies. Alex worked on a program that uses computer vision to enable the iRat to follow a rat. He says, "this trip has shifted my perspective on many issues, including why interdisciplinary work is critical, what constitutes a good robot and why

Background: UQ student Troy Smith (back left) and Hayden Razzell (back center) in California's Yosemite National Park with fellow students from the University of California, San Diego International House.

embodied agents are necessary." Zinta worked on tools for analyzing rat-iRat interactions by running experiments and collaboration with the expertise of the Chiba lab.

Troy Smith joined Yifeng Cui at the San Diego Supercomputer Center (SDSC) and worked on earth sciences applications. One project concerned an earthquake forward modeling code developed at SDSC, which uses GPU code and custom IO libraries to predict the effects of earthquakes, then output the data from the model into a strain tensor for use in engineering. The key achievement from this project was in implementing attenuation effects into the existing model to account for changes in energy in the seismic waves propagating through the earth. The second project was to install the Monash-developed geodynamic program Underworld onto the Gordon supercomputer and perform benchmarking tests to evaluate how it performs on larger clusters. The tests were run on up to 128 nodes, or 2048 cores, significantly higher than previous published performance tests. The code was very efficient until more than 64 nodes were used, after which, the performance improvements effectively flattened out.

All MURPA and QURPA projects are listed at *messagelab.monash.edu.au/MURPA/PastProjects*.

MURPA and QURPA involve an advanced seminar scheme, in which students can attend virtual seminars given by world leading experts before they leave. These seminars also allow students to "meet" potential UCSD mentors and get some information about potential projects. In 2015 we sourced the widest range of seminars to date, and covered all time zones of the US.

Seminars were sourced from faculty at Argonne National Labs, UCSD, the National Centre for Supercomputing Applications, the University of Tennessee, the University of Utah, the National Institutes of Health, the University of Iowa, SDSC, Google and the University of Notre Dame, Indiana. As done in the past, seminars were broadcast simultaneously to Monash (in Melbourne) and UQ (in Brisbane), with audiences able to ask questions from either venue. The seminar infrastructure supports a wide range of video conference technologies (both open source and commercial), and is displayed on a 20 MegaPixel OptiPortal.

# BUILDING COMMUNITY

A fundamental component of PRAGMA's activities is to engage new ideas and people, in part through PRAGMA Workshops and PRAGMA Students. In addition, we take intentional steps to co-organize other meetings and new activities that focus on topics of keen interest to PRAGMA and to the individuals and communities we seek to engage. This year we highlight four activities that range from:

- Helping to establish a new organization to enable transnational cyberinfrastructure applications
- Creating a new venue for dissemination of the PRAGMA communities advances in data science
- Building partnerships in Southeast Asia by focusing on big data and applications to disaster management; and
- Building collaborations in biodiversity informatics.

## US-EA CENTRA:

### *US—East Asia Collaborations to Enable Transnational Cyberinfrastructure Applications*

The CENTRA project is a first step towards the vision of a framework to coordinate collaborative research among large research centers or efforts in the US and East Asia on transnational cyberinfrastructure and its applications. In addition to achieving scientific progress, CENTRA aims to engage junior researchers in international activities. Among other topics and applications, CENTRA research focuses on software-defined systems and applications related to environmental modeling, disaster management and smart cities. The two initial partners of CENTRA are the newly created Center of Excellence on Enablement of Cyberinfrastructure Applications at the National Center for High-performance Computing of the National Applied Research Laboratories (NARL) Taiwan and the National Institute of Information and Communication Technologies (NICT) of Japan.

One of the goals of CENTRA and its partners is to educate a new generation of researchers who are technically and culturally competent to engage with international scientific networks. It enables junior Ph.D. candidate researchers working on CENTRA research topics to have short stays at collaborating sites in different countries. At these sites they have direct access to leading-edge facilities, local instances of global problems and top scientists working on these problems, and are immersed in international team activities. Research participants also include senior investigators with experience in international collaborations and broad expertise. Annual workshops help conceptualize, frame, advance and report on collaborative research projects and contribute to establishing the coordination framework. Each partner has committed to hosting one workshop.

The CENTRA project started October 1, 2015. Planning activities are now underway for the first CENTRA workshop at the NCHC Center of Excellence on Enablement of Cyberinfrastructure Applications in Taiwan. CENTRA works closely with PRAGMA to leverage each other's activities and facilitate related research efforts. Towards the long term goal of a collaborative framework for US-East Asia collaboration on cyberinfrastructure research, CENTRA welcomes inquiries and expressions of interest from other potential partners in East Asia. For more information about CENTRA, see *www.useacentra.org*.

## Southeast Asia International Research & Training Program (SEAIP) and PRAGMA Institute

*Taichung and Kaohsiung, Taiwan: December 1–5, 2014*

The SEAIP's ongoing series of workshops, *seaip.narlabs.org.tw* has opened doors for collaborations between researchers in Southeast Asia and the rest of the world, and has formed the basis for growing PRAGMA collaborations in Southeast Asia. The theme of this 10th SEAIP was "Cloud Computing and the Internet of Things." The informal atmosphere is conducive to learning and to developing collaborations. The workshop, held December 1–5, 2014, was organized by the National Center for High-performance Computing (NCHC), with funding from the Ministry of Science and Technology in Taiwan as well as from the National Applied Research Laboratory. In addition to sessions at NCHC's Taichung branch, there was a session held at the National Sun Yat-sen University in Kaohsiung. This year's workshop also was used to plan other activities, including laying the groundwork for US-EA CENTRA. The next SEAIP meeting will be held in Keelung, December 7–11, 2015.

## International Workshop on Building Collaboration in Biodiversity Informatics *Bogor, Indonesia: October 5–6, 2015; Depok, Indonesia: October 7*

This two-and-a-half-day workshop was to help build collaborations among users and developers in biodiversity informatics. The first day consisted of presentations about biodiversity research in the region, along with some technology approaches and developments to facilitate biodiversity research. The second day consisted of general "data carpentry" tutorials, allowing participants to get an overview of tools useful in geospatial modeling (specifically on the Lifemapper infrastructure). The third day provided opportunities for participants with deeper interest in species distribution modeling, GIS, range and diversity modeling and those who wish to build skills in scripting, data management, and analysis methods used in Biodiversity Informatics. More than 50 students participated in the workshop. For more information, see *cs.ipb.ac.id/pragma*.

## Inaugural PRAGMA Workshop on International Clouds for Data Science *Depok, Indonesia: October 7, 2015*

The first PRAGMA Workshop on International Clouds for Data Science (PRAGMA ICDS'15) is a new research-oriented workshop drawing from the broad PRAGMA community. In particular, PRAGMA ICDS'15 leverages the long history of experimentation in PRAGMA to showcase the latest research on the design, implementation, evaluation and the use of cloud technology, networking and data management, which enable new forms of research that span international boundaries. PRAGMA ICDS'15 was held on October 7, 2015 and co-located with the PRAGMA 29 conference.

The inaugural PRAGMA ICSD'15 workshop consisted of 10 presentations from cutting-edge fields, including fields traditionally of interest to PRAGMA, such as cloud technologies, virtualization and application areas of these technologies. A number of these presentations were associated with PRAGMA projects. The final workshop papers will be archived at a reliable online storage service.

Additionally, high-quality workshop papers will be included in a special issue of the CC&PE journal (Concurrency and Computation: Practice Experience). The journal opportunity gives workshop authors an opportunity to publish their work in an archival venue, which further expands the impact of PRAGMA. The local logistics were supported by the Universitas Indonesia. For more information see *d2i.indiana.edu/pragma/index.html*.

**GENERAL CHAIR:** Beth Plale, *Indiana University*; **LOCAL ARRANGEMENTS CHAIR:** Heru Suhartanto, *Universitas Indonesia*; **PROGRAM COMMITTEE:** *Co-Chair:* Renato Figueiredo, *University of Florida*, Miao Chen, *Indiana University*; David Abramson, *The University of Queensland*; Peter Arzberger, *UCSD*; Huah Yong Chan, *USM*; Kevin Dong, *CNIC*; Suntae Hwang, *Kookmin University*; Kohei Ichikawa, *NAIST*; Jysoo Lee, *KISTI*; Frances Lee, Nanyang Technical University; Prapaporn Rattanatamrong, Thammasat University; Heru Suhartanto, *Universitas Indonesia*; Mauricio Tsugawa, *University of Florida*; Putchong Uthayopas, *Kasetsart University*

# WORKSHOPS & WORKING GROUPS

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. New participants bring new perspectives, applications, technologies, students, and resources. These workshops are critical for demonstrating progress between meetings and to plan for actions prior to the subsequent workshop.

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.

The workshops are organized to allow for the activities of 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. Co-leaders: Yoshio Tanaka (AIST) and Phil Papadopoulos (SDSC/UC San Diego).
- **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. Co-leaders: Shinji Shimojo (NICT and Osaka U) and Fang-Pang Lin (NCHC). This group also includes activities from an earlier working group on Global Earth Observing (GEO), and their focus on disaster management.
- **BIOSCIENCES WORKING GROUP:** Focusing much of its efforts over the last several years on infrastructure development that allows performing virtual screening experiments and computational genomics analyses, with an emphasis on combating infectious diseases. Leader: Jason Haga (AIST).
- **CYBER-LEARNING:** Focusing on use of technologies to improve understanding in several areas of computational science, through use and improvement of EDISON. Leaders: Ruth Lee (KISTI), Hsi-ching Lin (NCHC).

# PRAGMA WORKSHOPS

In 2015, two PRAGMA Workshops were held:

- PRAGMA 28: April 8–10, 2015, Nara, Japan, hosted by the Nara Institute of Science and Technology.
- PRAGMA 29: October 7–9, 2015 Depok, Indonesia, hosted by Universitas Indonesia. This was held in conjunction with three other activities:
  - International Workshop on Building Collaborations in Biodiversity Informatics, October 5–7, Bogor and Depok, Indonesia, hosted by Bogor Agricultural University and Universitas Indonesia (See Building Community)
  - PRAGMA Workshop on International Clouds for Data Science (PRAGMA-ICDS'15), hosted by Universitas Indonesia (See Building Community)
- 7th International Conference on Advanced Computer Science and Information Systems (ICACSIS 2015), October 10–11, 2015, Jakarta, Indonesia

In addition, training programs such as SEAIP (Southeast Asia International Joint Research and Training Program (*seaip.narlabs.org.tw*) provided PRAGMA with new members (See Building Community)

Looking to the future, we will continue to employ these strategies to engage new researchers. In addition, we will work with our members to identify strategic partners and engage them through focused scientific or technical workshops. Listed below are our planned workshops:

- PRAGMA 30: January 27–29, 2016, Advanced Science and Technology Institute (ASTI). Held in conjunction with the 41st Asia-Pacific Advanced Network (APAN) meeting
- PRAGMA 31: Date TBD, Thammasat University

We acknowledge the contributions for hosting PRAGMA workshops and thank the organizers and host institutions for their efforts to ensure PRAGMA's continued success.

Images: (right, from the top): Kazutoshi Fujikawa, PRAGMA 28 General Chair; Shinji Shimojo in Nara Park; Penny Hutabarat performs at PRAGMA 29—all courtesy of Teri Simas, UCSD

# PARTNERS & SPONSORS, INSTITUTIONS

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 listing below) may be found at *www.pragma-grid.net/people.php*.

## INSTITUTIONS

### 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.

**ADVANCED SCIENCE AND TECHNOLOGY INSTITUTE** (ASTI): Denis Villorente, *denis@asti.dost.gov.ph*; Jelina Tanya H. Tetangco*; *jeng@asti.dost.gov.ph*

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

**CYBERMEDIA CENTER** (CMC), **OSAKA UNIVERSITY**: Shinji Shimojo*, *shimojo@cmc.osaka-u.ac.jp*; Susumu Date*, *date@ais.cmc.osaka-u.ac.jp*

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**NATIONAL ELECTRONICS AND COMPUTER TECHNOLOGY CENTER** (NECTEC): 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* ; Jason Haga, *jh.haga@aist.go.jp*

**NATIONAL INSTITUTE OF SUPERCOMPUTING AND NETWORKING** (NISN), **KOREA INSTITUTE OF SCIENCE AND TECHNOLOGY INFORMATION** (KISTI): Kum Won Cho*, *ckw@kisti.re.kr*; Jong-Suk Ruth Lee, *jsruthlee@kisti.re.kr*

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**UNIVERSITAS INDONESIA** (UI), in particular Faculty of Computer Science: Heru Suhartanto*, *heru@cs.ui.ac.id*; Wisnu Jatmiko, *wisnuj@cs.ui.ac.id*

**UNIVERSITY OF CALIFORNIA, SAN DIEGO** (UCSD): *including the California Institute for Telecommunications and Information Technology (Calit2), San Diego Supercomputer Center (SDSC), National Biomedical Computation Resource (NBCR)*; Peter Arzberger*, *parzberg@ucsd.edu*; Philip Papadopoulos*, *phil@sdsc.edu*; Teri Simas, *simast@sdsc.edu*

**UNIVERSITY OF FLORIDA** (UF), in particular the Advanced Computing and Information Systems Laboratory and the Florida Museum of Natural History: Jose Fortes, *fortes@acis.ufl.edu;* Renato Figueiredo, *renato@acis.ufl.edu*; Matthew Collins, *mcollins@acis.ufl.edu*; Reed Beaman, *rbeaman@gmail.com* (now at the National Science Foundation)

**UNIVERSITY OF HONG KONG** (HKU): W.K. Kwan*, *hcxckwk@hku.hk*; P.T. Ho, *hcxchpt@hku.hk*; Lilian Y.L. Chan, *lilianyl@hku.hk*

**UNIVERSITY OF WISCONSIN** (UW), in particular the Center for Limnology: Paul Hanson, *pchanson@wisc.edu*

## 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): Markus Buchhorn, *markus@apan.net*

**PACIFIC WAVE:** John Silvester, *jsilvest@usc.edu*

**STARLIGHT:** Maxine Brown, *maxine@uic.edu*

**TRANSPAC3, INDIANA UNIVERSITY**: Jennifer Schopf, *jmschopf@indiana.edu;* Andrew Lee, *leea@indiana.edu*

## Other Members

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**UNIVERSITI SAINS MALAYSIA** (USM): Habibah A. Wahab*, *habibahw@usm.my;* Chan Huah Yong, *hychan@cs.usm.my;* Mohd Azam Osman; *azam@cs.usm.my*

**UNIVERSITY OF HYDERABAD** (UoH): Rajeev Wankar, *wankarcs@uohyd.ernet.in, rajeev.wankar@gmail.com*

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

# Additional Organizations Active in PRAGMA

**BIODIVERSITY INSTITUTE, UNIVERSITY OF KANSAS** (*biodiversity.ku.edu*), and its researchers and students conduct research on seven continents in areas such as biodiversity informatics, systematics and ecology and evolutionary biology. They have contributed to the biodiversity expedition through participation in workshops and in the use and extension of the Lifemapper software.

**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 Research and Development 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 can bring to bear several other laboratories at NARL for PRAGMA collaborations.

**NATIONAL INSTITUTE FOR INFORMATION AND COMMUNICATION TECHNOLOGY** (NICT; *www.nict.go.jp*), 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 from 2009 through 2015 and has participated in the activities of the Telescience Working Group through support of the high speed networking and SDN (Software Defined Network).

**UNIVERSITY OF QUEENSLAND** (*www.uq.edu.au*) has recently become involved in PRAGMA through David Abramson's move there. David remains actively involved in PRAGMA and PRIME, supporting two students from UCSD from June to August 2013 (see Section on PRIME) and sending students to PRAGMA sites (see MURPA QURPA section).

**VIRGINIA TECH:** Cayelan Carey and colleagues in Project EDDIE (Environmental Data-Driven Inquiry and Exploration; *projecteddie.org*, an NSF-funded project) have developed sensor-based and time series data analysis activities that can be integrated into classrooms to improve quantitative skills, reasoning, and increase student engagement. Prof. Carey is expanding this effort by

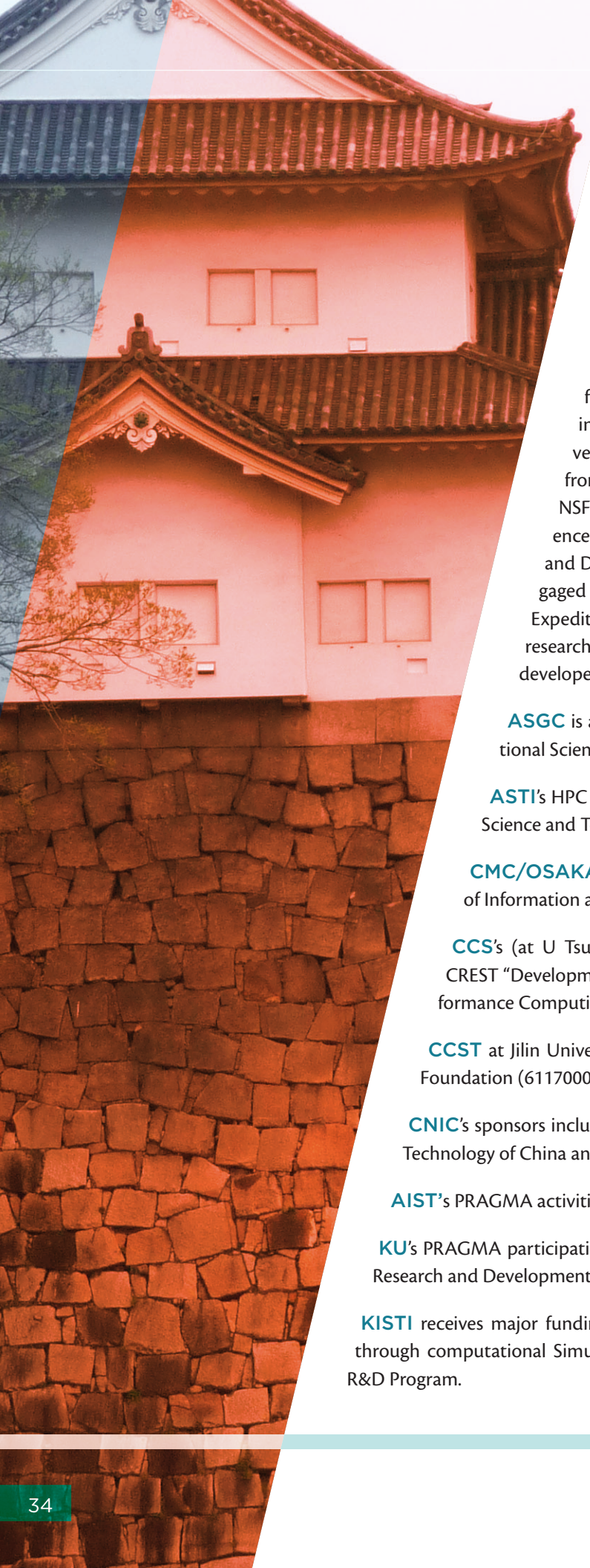

Background: Group Photo from PRAGMA 28 Meeting in Nara, Japan

developing additional teaching modules that use the overlay network developed as part of PRAGMA to run lake simulations of climate change scenarios. The modules will be piloted at eight universities in the 2015-2016 academic year before becoming publicly available and will be assessed to determine how participation in the module activities alters student reasoning about climate change and computing.

# PARTNERS

The **GLOBAL LAKES ECOLOGICAL OBSERVATORY NETWORK** (GLEON), is a grassroots network of limnologists, ecologists, information technology experts, and engineers who uses the network of people, sensors, and data to understand issues such as eutrophication or climate change at regional to global scales. GLEON, established based on an early PRAGMA expedition to place sensors on a lake in Taiwan in 2004, GLEON has grown to a network of more than 300 members, has developed new knowledge and insights, created new data products and developed a very successful Graduate Student Association. There are several ties between GLEON and PRAGMA, including shared personnel, learning from the GLEON GSA to develop PRAGMA Student group, the shared Scientific Expedition on Lake Eutrophication, and the joint hosting of a workshop on Big Data in Taiwan in December 2012. For more about GLEON, see *gleon.org*.

**NETWORK STARTUP RESEARCH CENTER** (NSRC, *www.nsrc.org*) has longstanding experience in running hands-on networking training workshops and providing engineering assistance at both the campus and national network levels. They have worked in more than one hundred countries throughout the world over the past 20+ years. NSRC has been working with PRAGMA recently in the area of Southeast Asia, supporting researchers from Myanmar to attend PRAGMA 24 and collaborating with PRAGMA and IU on the Lower Mekong Initiative to help enable more international science education. In addition they have been able to encourage participation in PRAGMA workshops.



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

**ASTI**'s HPC and cloud computing activities are funded by the Department of Science and Technology (DOST), Philippines.

**CMC/OSAKA UNIVERSITY** is supported by JGN-X of the National Institute of Information and Communications Technology (NiCT), Japan.

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**KISTI** receives major funding from MSIP through EDISON (EDucation-industry Integration through computational SimulatiOn and Net) Project and KISTI through its Supercomputing R&D Program.

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**TRANSPAC** receives major funding from NSF and collaborates closely with PacificWave, Japan's National Institute of Information and Communications Technology, APAN ,TEIN, and other Asian networking groups.

**UNIVERSITAS INDONESIA**'s PRAGMA participation has been partly funded by Faculty of Computer Science, and research grants from The Ministry of Research Technology and Higher Education, Republic Indonesia.

**USM**'s grid activities in Malaysia are funded mainly through E-science and USM Central Funding.

**PRIME** has support from a variety of sources: PRIME Alumni Haley Hunter-Zinck, given in tribute to her mother; and partner sites. The Revelli Family's contributions have helped support students in the PRIME program

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PRAGMA
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