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A reflection on the origins, evolution, and future of PRAGMA

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A Reflection on the Origins, Evolution, and Future of PRAGMA

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SUMMARY

All of the papers in this special collection have been shaped by and/or have helped shape PRAGMA. This paper, a reflection on PRAGMA, will provide additional technical, scientific and human context to many of these papers. We hope to illustrate that it is the people who set directions by following their interests or posing questions, who make progress by honoring their commitments, and who build community by establishing open communications and trust.

1. SETTING THE STAGE

As with any research organization, there are factors leading to its origins, there are the critical first steps, the establishments a framework for growth, and the need to evolve, especially when technology and science are evolving rapidly.

1.1. Origin (1998 to 2002): PRAGMA's origins resulted from persistent and intentional encouragement (from Bill Chang of the National Science Foundation (NSF)) and fortuitous human interactions (a spontaneous meeting with Sangsan Lee of Korea Institute of Science and Technology Information (KISTI) in 2001) and from observing, gauging and anticipating technical trends (interaction among computational centers in Korea, Japan, and Taiwan, and the growth of the grid concept and the investment by the community in venues such as the Global Grid Forum).

Based on interactions with and commitments from KISTI and the National Institute of Advanced Industrial Science and Technology (AIST), two of us at the University of California San Diego (UCSD) proposed to NSF a series of three workshops (San Diego, Seoul, and Fukuoka) to establish a community of researchers to advance science by accelerating the daily use of the grid; and to build sustained collaborations of stakeholders from around the Pacific Rim. The intent was to identify common challenge areas where we could work together to make progress.

These first three workshops were successful as observed by progress through collaborations between workshops, by interest of others in the community to join, by sharing software and experience openly, and by using PRAGMA to leverage other activities. The success focused us on the longer-term issue of creating a framework for the

In designing the logo, there were three guidelines for the graphic designer, Jennifer Matthews. The logo should convey Pacific Rim, collaboration, and Grid Computing. In retrospect, the first two sufficed!

Logo Design: Jennifer Matthews, IGPP/UCSD

Figure 1

collaboration, in terms of Operating Principles and Practices[1] (what a steering committee would be, how decisions were to be made, what membership meant); how we could productively work together (working groups); and growing an identity, with the first step a logo (Figure 1).

1.2. Early Stage (2003-2004): This was a period where PRAGMA was still exploring what it could do while learning its limits. A defining moment is the PRAGMA community response to the SARS epidemic that affected many PRAGMA sites [1]. At PRAGMA site National Center for High-performance Computing (NCHC), Fang-Pang Lin asked what could we, with our technologies do, to help those affected. The community responded with sharing of a technology to allow doctors, patients and families to interact, remotely. A second defining moment came at PRAGMA 5 (October 2003) with a focus by the Steering Committee to make the grid usable for application researchers.

Yuan Yang Lake, Taiwan 2004

An early PRAGMA Expedition in Taiwan, Yuan Yang Lake [2]

Photo: Dong Kun Liao

Figure 2

During this time two other activities were initiated, using the PRAGMA framework. For the first case PRAGMA brought together technologies and application scientists to deploy new technologies to address scientific needs. The early "expedition" deployed a wireless sensor network to stream data from a lake in Taiwan (it took nine months from conception to implementation), and created a team of researchers to gain understanding of the impact of typhoons on lakes (Figure 2) [2].

The second activity leveraged the collaborations in PRAGMA to send UCSD undergraduate students to PRAGMA sites for research internships. The Pacific Rim Experiences for Undergraduates (PRIME) program sent its first students in 2004 [3]. This program launched two other activities, in Osaka University [4] and in Monash University [5]. These programs helped strengthen collaborations, built future PRAGMA leaders[2], and explore new areas, e.g., in technologies useful for museums [6].

1.3. Growth and Technology Challenge (2004 – 2009): Through twice a year workshops and interactive activities between workshops, the PRAGMA organization grew in membership and results. The driving focus of one of working group was "how to make the grid usable". This group made progress by attacking specific scientific problems through the use of middleware on distributed resources, some in PRAGMA and some in other groups. Three examples include:

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[1] PRAGMA's Operating Principles and Procedures (http://www.pragma-grid.net/images/operating-principles.pdf) were motivated by documents establishing the Global Biodiversity Information Facility (GBIF)

[2] For example Kohei Ichikawa was a graduate student at Osaka University – and is now faculty at Nara Institute of Science and Technology and lead of PRAGMA's ENT; Kevin Dong was a graduate student at the Chinese Academy of Sciences Graduate School, and is now a researcher at CNIC, and key developer of Duckling, a collaboration platform used by PRAGMA workshops. Both are now members of the PRAGMA Steering Committee.

- Savannah Burn simulations, using Nimrod middleware to understand the complex interactions between burning of a savannah and Monsoon rain patterns in Australia [7] [8].
- Grid Interoperation Experiment with Open Science Grid, which used AIST's Ninf-G grid implementation of the Fragment Molecular Orbital for first-principle calculations of macromolecules [9] [10].
- Grid Interoperations Now, and the PRAGMA led effort of the Open Grid Forum to harness six grids, using Nimrod-G to apply the technique of molecular replacement to test protein structures in the Protein Data Bank [11] [12].

In each of these cases science was advanced, software was improved, and much was learned about the infrastructure.

Even with these successes, by 2009, many in PRAGMA came to the realization that using the grid was "just too hard to use" and that we could not "make the grid usable" for the scientific community. In part, the heterogeneity of the resources led to long "set up" times, by experts, a barrier most application scientist would not tolerate and could not afford.

1.4. Switch Technologies: Virtualization of Computing (2009 – 2012): Given the realization that the approach used by the grid was too hard for scientists and many technologies, PRAGMA made a deliberate effort to explore other technologies and then learn about them by focused efforts. Two early focused efforts included

- Taking advantage of the PRAGMA Grid and Amazon EC2 cloud, simulating the ash distribution after a volcano eruption, based on the NG-TEPHRA code, with Nimrod middleware [13] [14]
- Looking at migration of virtual machines across several different hosting environments [15] [16].

Tohoku Earthquake

Ground motion map [17]

Credit: AIST, Japan

Figure 3

At subsequent meetings we extended our results of virtual machine / virtual cluster migration. This proved to be very timely and useful in the case of migrating services after the Tohoku Pacific Ocean Earthquake and tsunami, when key services at PRAGMA member AIST were disabled. Within a few days after the earthquake, services including QuickQuake, Hot Spot and World Map Service Server were migrated onto the virtual machine cluster at NCHC. In addition, UCSD (via SDSC's Triton resource) generated the ground motion map covering all of Japan to observe and analyze the March 2011 earthquake (Figure 3) [17] [18].

1.5. Contributions of Many to the Collaborative Framework: PRAGMA's advances have been made possible by multiple types of contributions: collaborative efforts and expertise as described throughout this paper; shared software and resources; leveraged project; organized and hosted workshops full of work, food, and cultural experiences; and active engagement of people and communities.

- Shared Software: One of PRAGMA's values is its members' ability to share, experiment with, and improve software. This was the case in the "grid days" and remains the case today. It is the use of the software that leads to improvements [19] [20] [21] [22] [23]. In fact, since 2010 we have used the Duckling[3] software, developed by Computer Network Information Center (CNIC), for PRAGMA's workshop meetings.

- Leveraged Projects: The early expedition on the lake leveraged the NCHC Ecogrid Project. Efforts on disaster mitigation leveraged the NCHC Floodgrid, and the AIST GEOGrid activities. These in turn have helped PRAGMA, in particular the Geoscience / Telescience working group efforts. Moreover, it has allowed us to create new activities, for example the Cyberlearning activities of KISTI.
- Hosted Workshop[4]: Members of PRAGMA agree to host workshop as part of being a member. This allows greater involvement of the host site's researchers in PRAGMA, which is mutually beneficial to all involved. It also allows PRAGMA members to experience local culture, such as traditional performances of hand puppet in Taiwan (Figure 4), the electrifying Saman dance in Indonesia, the water puppetry in Vietnam, face mask changing in China, as well as modern performances of song, often by PRAGMA participants.

PRAGMA 3 banner, integrating technology and culture. Note the hand puppets.

More artwork developed by PRAGMA sites can be seen at http://www.pragma-grid.net/workshops.php

Design: Yu-Wen Chai, NCHC, Taiwan

Figure 4

- Engagement of Communities: PRAGMA has often held pre-workshop meetings on topics of interest to local hosts and PRAGMA members (e.g. Biodiversity, Disaster Management) to engage a broader community in the topic. In addition there have been additional workshops and activities. There are two notable examples.
  - The first is the Shonan meeting in July 2014 on Water Disaster Management and Big Data, sponsored by Japan's National Institute of Information, organized by NCHC, AIST, Osaka and UCSD. This brought together members of the GEO/Telescience working group and leveraged activities of NCHC [24] and AIST.
  - The second example is the long standing Southeast Asia International Joint-Research and Training Program (SEAIP), supported by Taiwan's Ministry of Science and Technology, with the goal of strengthen the connections around the Pacific Rim, in particular Southeast Asia, and develop collaborations through the exchange of research results and ideas. This workshop series has led to additional membership in PRAGMA: Vietnam Academy of Science and Technology, Institute of Information Technology (hosting PRAGMA 17), the Universitas Indonesia (hosting PRAGMA 29), the Advanced Science and Technology Institute (hosting PRAGMA 30). This series has led to a focus in PRAGMA on Biodiversity, and on a new activity, US-EA (described later).
- Individuals: Finally, participants contribute their own expertise, time, and funds to attend PRAGMA workshops, both for themselves and for their students.

[3] A collaborative software developed by CNIC, https://en.wikipedia.org/wiki/Duckling_(software)

[4] For a list of workshops and locations, see http://www.pragma-grid.net/workshops.php

PRAGMA's collaborative framework enables and encourages multiple types of contributions. In many ways, this is akin to the making stone soup, the folk story in which many individual contributions to a common "pot" allow for the creation of a community resource, benefiting the contributors.

Real expeditions can be dangerous, when ascending a mountain in Taiwan in a typhoon.

For the song capturing this expedition see https://youtu.be/WGlWBb6eaD8

Photo: Peter Arzberger

Figure 5

1.6. Global Lake Ecological Observatory Network (GLEON) A Partner Global Organization: Growth and Contribution to PRAGMA (2004 – present)

The very early expedition (Figure 5) on a lake in Taiwan (2003-2004) led to the questions: Could we deploy sensors on other lakes around the world? What could we learn if we did that? Through a series of preliminary discussions, the Global Lakes Ecological Observatory Network was launched in a workshop in March 2005[5], to conduct science by harnessing the power of combining data from sensors from multiple lakes, and ultimately to understand larger questions and to revise existing ecological models [2].

Because there were several members in PRAGMA who helped launch GLEON, GLEON borrowed from PRAGMA (e.g., regular meetings, Operating Principles and Procedures). But it also developed its own practices, in particular with the establishment of a strong Graduate Student Association, new project tracker mechanisms to allow for open collaborations at the beginning of a project but focus at the end, and by having constructive mechanisms for and assessment of engaging new members [25] [26] [27].

Currently GLEON has more than 500 individual members and collectively GLEON members have been able to integrate data from multiple lakes to gain new understanding about processes in lakes [28], by teams often led by graduate students, which make up between 35% and 40% of participants at their meetings.

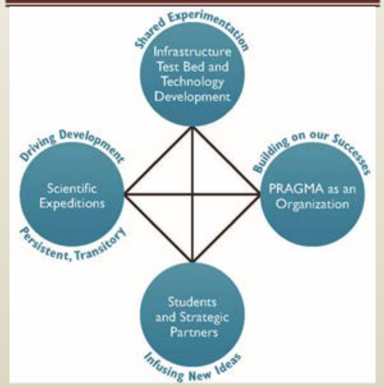
GLEON has a rich set of questions, a strong network, and mechanisms that they have evolved. As noted in the next section, PRAGMA learned from GLEON, and its partnership is one that is mutually beneficial, bringing together complementary strengths.

2. FRAMEWORK FOR COLLABORATION: APPLICATION, TECHNOLOGY, IDEAS, PEOPLE (2012 – present; PRAGMA 23 – 30 and beyond)

In PRAGMA's first ten years, it had evolved with the technology and has refined its approach to the collaboration framework. PRAGMA's past successes often resulted from concerted efforts, bringing together application, software, and resources, to accomplish a specific objective.

[5] For a summary of GLEON's 10 years, see http://blog.gleon.org/reflections-on-gleons-10th-birthday/

Our continued goal is to make resources useable to the community. We have restated this desire as enabling small- to medium-sized international groups to make rapid progress in conducting research and education by providing and developing international, experimental cyberinfrastructure.



Four interdependent activities essential to PRAGMA

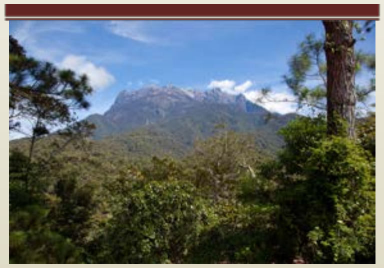
Credit: Jennifer Matthews, IGPP/UCSD

Figure 6

PRAGMA's experiences have shaped its current activities[6], which include (Figure 6):

- Fostering international "scientific expeditions" by forging teams of domain scientists and cyberinfrastructure researchers who develop and test information technologies that are needed to solve specific scientific questions and create usable, international-scale, cyber environments;
- Developing and improving a grassroots, international cyberinfrastructure for testing, computer science insight and advancing scientific applications by sharing resources, expertise and software;
- Infusing new ideas by developing young researchers who gain experience in cross-border science and by extending engagements with strategic partners; and
- Building and enhancing the essential people-to-people trust and organization developed through regular, face-to-face meetings – a core foundation of PRAGMA's success.

These activities are interdependent. Infrastructure that has impact must be built to meet the specific needs of users and applications, while scientific expeditions and sharing of data require organizational support to succeed. New ideas are generated by experimentation and engagement of additional people and communities.



Mt Kinabalu, Sabah Parks, Sabah, Malaysia.

Photo: Antony Van der Ent, U. Queensland

Figure 7

In 2012 we launched two persistent scientific expeditions. One seeks to understand biological adaption in extreme environments, while researching the specific biotic, abiotic and evolutionary factors that affect patterns of diversity, distribution and endemism in ultramafic (high magnesium- and iron-oxide concentration) regions in Southeast Asia (Figure 7). The choice of this expedition was based on the desire by a researcher to use technologies to understand this scientific question. It was also based on a series of workshops, starting in 2011, including a special session at SEAIP 2011, to engage a broader community.

[6] PRAGMA has retained working groups as a source of additional activities and the source of new expeditions. The current working groups include Resources including Data, Telescience and Geoscience which are working together, Biosciences, and the recently develop Cyberlearning led by KISTI and NCHC, which is building on KISTI's investment in Edison (https://www.edison.re.kr/)

Currently, a key technology accomplishment to date has been the refactoring of Lifemapper[7], a software for predicting species distribution, to allow it be to migrated to various sites [29].

A second expedition addresses the societal issues inherent in predicting lake eutrophication (i.e., excessive plant, algal and bacterial growth in lakes due to nutrient enrichment) – one of the greatest water-quality challenges facing freshwater ecosystems throughout the world. Currently there is a working software environment, GLEON Research and PRAGMA Lake Expedition (GRAPLE). GRAPLE makes available the well-known General Lake Model through a deployment of an IPOP[8] overlay virtual network and the HTCondor[9] batch job scheduler across participating GLEON/PRAGMA institutions. This environment enables aggregation and sharing of computational resources and models by a distributed group of collaborators [30]. The choice of this expedition came from the ongoing dialog between PRAGMA and GLEON since the deployment of sensors in the early expedition in 2003 – 2004.

We note that both of these expeditions are leveraging existing software and through the use are improving it, and making them useful for others. For example, the Lake Expedition is taking advantage of IPOP (IP over P2P) (U Florida), open-source user-centric software virtual network allowing end users to define and create their own virtual private networks (VPNs). The Biodiversity Expedition is virtualizing Lifemapper (U Kansas). Also, both expeditions require developing tools that track usage of data and protect sensitive data by using virtual private networks. In both cases, we will work with existing scientific networks (e.g., GLEON) or grow nascent networks of researchers to ensure that our projects have a broad impact. In particular, members of the Lake Expedition have funds to build that user base, which if successful, has the potential to transform the research environment for an entire community.

Since 2012 PRAGMA has been building on its successes in migrating virtual machines to become a cloud testbed. Our approach uses software-defined networks (SDN) to simplify application design by solving various connectivity issues among cooperating, virtualized resources. The SDNs also form trust envelopes (Figure 8) so that PRAGMA can practically address fundamental issues in selective data sharing, provenance and raw data acquisition. Furthermore, the PRAGMA resources require development [31] and can be used as a resource to evaluate cyberinfrastructure components, gain insights into long-term data use, and advance science.

A Trust Envelop for Expeditions to share resources

Credit: Jennifer Matthews, IGPP/UCSD

Figure 8

A third expedition grew out of PRAGMA 25 (October 2013, Beijing), where it was proposed that PRAGMA should have an experimental networking testbed (ENT) to test new SDN software and approaches, using a very wide area network, distributed across some of the

[7] Lifemapper is developed by the Biodiversity Institute of the University of Kansas, http://lifemapper.org/
[8] IPOP creates a virtual private network, is developed by PRAGMA member U Florida, http://ipop-project.org/
[9] HTCondor is a high throughput computing software, developed by U Wisconsin, https://research.cs.wisc.edu/htcondor/

PRAGMA sites. In the PRAGMA spirit, there was sufficient interest among members and key individuals to lead this effort that has moved ENT from concept to utilization and testing [32]. At a systems level, the value of the PRAGMA Grid and more recently the PRAGMA ENT is that is provides a testbed for approaches and can be intentionally disrupted to understand how the software and system responds [33] [34].

PRAGMA Students, a relatively new student activity in PRAGMA, was first discussed at PRAGMA 22 (Melbourne, 2012) and launched at PRAGMA 23 (Seoul, 2012). This effort was motivated by the GLEON Student Association, with the goal of providing professional leadership opportunities in a global network of researchers. Since then students have had an opportunity to organized student-focused workshop, organize the poster sessions for PRAGMA and share their work with PRAGMA members.

The founders of CECEA, IVO, and US CENTRA, together with the individual who motivated PRAGMA's start (far left)

Photo: Anna Fortes

Figure 9

PRAGMA will continue to experiment and whenever possible help grow new collaborations. A recent activity has grown out of multi-year efforts of PRAGMA and its members, leveraging meetings at SEAIP and at Shonan. Out of these discussions, efforts in the United States, Taiwan and Japan led to the conceptualization and funding of the Collaborations to Enable Transnational Cyberinfrastructure Applications (CENTRA)[10]. The coordinated activities, US CENTRA at U Florida in the United States, a Center of Excellence in Cyber-Enabled Applications (CECEA) at NCHC in Taiwan, and the International Virtual Organization (IVO) at National Institute of Information and Telecommunication Technology (NICT) in Japan (Figure 9). These activities started simultaneously, and have two major goals: advance the science to harness software defined technologies to address societal issues[11] and to educate a new generation of researchers who are technically and culturally competent to engage with international scientific networks, through short and medium term international stays, working with senior researchers.

3. FINAL THOUGHTS

Looking back the fourteen years since PRAGMA started, **who would have thought a simple idea would have led to a long standing activity**, where we are continuing to learn, develop collaborations and contribute to advancing knowledge. While our collective, previous experiences helped to shape what we did, PRAGMA was new for all of us. The existence of GLEON indicates that global networks are viable mechanisms for conducting global research, the research no single group can do.

What have been some key ingredients of the success of PRAGMA and GLEON? Since we started these activities, more research focus has been aimed at the question of what makes groups

[10] The website is http://www.globalcentra.org/

[11] The initial application areas are disaster management, environmental modeling, and smart and connected communities

work well. We provide a few observations based on experience, although we do not try to quantify the impact of any of these. We suspect that each new group will likely evolved to a mixture of the following, based on its internal organizational culture (admittedly an unsubstantiated claim, although reflected in the difference between PRAGMA and GLEON).

- A shared vision of what is possible and a shared mission for the participants
- Flexible governance structures, that allows participants the ability to follow ideas collaboratively
- People willing to share, lead, pose questions, collaborate, and commit to the effort, during start up and growth, always looking for ways to stay relevant to participants
- Openness, trust, and communication among members
- Experimenting with new ideas, approaches, and partners
- Opportunities to interact outside of the research setting
- Clear benefit to participants from investing time and money.

Key challenges for both groups are the funds to continue the interactions and maintaining the sense of community. This in turn depends on the ongoing need to articulate the value of this approach to science, and the understanding of the funding agencies that the conduct of science and education are changing, and need new models of funding.

Another key challenge for science in general will be the ability of the groups to identify ways to share data. The challenges 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 an improved understanding. We need to remember that the value of data are in their active use[12].

Strong, Interdisciplinary Teams learn from each other . Paul Hanson (modeler), Renato Figueiredo (virtual networking), Cayelan Carey (fresh water ecologist).

Photo: Carey Lab, Virginia Tech

Figure 10

Looking forward, we are very excited by the new opportunities that the new CENTRA / CECEA / IVO offers, both for research but in particular for the students who will be involved. In a certain sense, hopefully some of the lessons learned from PRAGMA and GLEON will help guide this new activity.

From a personal perspective it has been rewarding to see the power of a network of engaged people and the evolution of the organization. Because both PRAGMA and GLEON have existed for multiple years, one can see the growth of people, advancing from graduate students to active researcher who are contributing to their communities through their leadership and work with students and collaborators. Furthermore, there are opportunities to learn more across

[12] The concept is motived by the statement "The value of data lies in their use." From Bits of Power. NAP. 1997.

disciplines, as evidenced in the PRAGMA-GLEON Lake Expedition, where an ecologist is reading about software-defined networks, and a computer scientist is learning about limnology (Figure 10).

Finally, we have benefited tremendously from the wisdom, partnerships, and friendships of all of those who have made these organizations and all of the successes possible.

ACKNOWLEDGEMENTS

It is impossible to thank everyone who has contributed, in large ways and small, in this journey, from pre-idea to current day. Thanks goes to all who have contributed ideas, energy, and enthusiasm, and have chosen to walk together on some or all of this journey.

One individual does deserve acknowledgement for his steadfast vision, support, and action. Dr. William Chang, a Program Officer at the US National Science Foundation since 1988, has been instrumental in planting the seed, and then financially investing in the idea, that has resulting in 15 years of funding for the US participation and leadership in PRAGMA (INT-0216895; INT - 0314015; OCI-0627026; OCI 1234983). In many cases PRAGMA was supported by several programs in NSF, including in the Biological Sciences, Computer and Information Sciences and Engineering, the Office of (and later Division of Advanced) Cyberinfrastructure and the Office of International Science and Engineering.

In addition, there have been many other supporters across the world of PRAGMA members, of the PRIME program, and of GLEON. Let me thank Phil Papadopoulos, who has helped engineer the PRAGMA system, from the very beginning; Teri Simas, who provided the heart and welcoming spirit to PRAGMA; Gabriele Wienhausen for her vision and leadership to put together the PRIME opportunity for students; and Tim Kratz, for being willing to take a leap of faith to travel to Taiwan in 2003, leading to GLEON. And of course my thanks to all of the PRAGMA members who have contributed to PRAGMA and from whom I have learned a great deal.

Finally, I wish to acknowledge the support of the US National Science Foundation (NSF), both as a researcher at UCSD and during times of service at NSF. This material is based upon work supported by the NSF, through awards noted above, and in part while I have served there. The thoughts in this paper are mine, and do not necessarily reflect the views of NSF.

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