PRAGMA

PACIFIC RIM APPLICATIONS AND GRID MIDDLEWARE ASSEMBLY

PRAGMA: An International Model of Collaboration

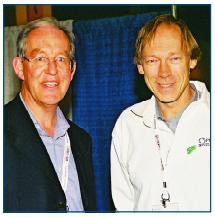
San Diego, December 22, 2003—*Members of the Pacific Rim Applications and Grid Middleware Assembly (PRAGMA), through more than twenty collaborative demonstrations at Supercomputing 2003 (SC2003), highlighted scientific advances both within and utilizing grid technologies. Applications that included climate, quantum chemistry, and structural genomics, among others, employed grid middleware to access resources from across the Pacific Rim. Additionally, two demonstrations pushed the limits of networking at the event, winning two of eight prizes in the High-Performance Bandwidth Challenge sponsored by Qwest Communications. SC2003, the annual international conference on high-performance computing and networking, was held in Phoenix, Arizona from November 15-21.*

All twenty PRAGMA institutions were involved in the collaborative demonstrations including climate simulation using the Grid RPC system Ninf-G; neuroscience using tele-instrumentation, high-performance visualization and collaborative data sharing; bioinformatics, and life sciences activities involving linking heterogeneous database and workflows; simulation of macromolecular systems using distributed parametric tool Nimrod/G; astronomy data distribution using Grid Datafarm; combating SARS using collaborative technologies; lattice QCD using Grid-enabled heterogeneous multi-computer system; and ecology data acquisition and sharing using wireless networks and grid data services. Specific collaborative successes include the following.

Climate Simulation using Ninf-G: Researchers at AIST and NCHC ran a weather prediction system using Ninf-G, developed by AIST, using 22 clusters from 21 institutions and 10 countries (total 853 cpus) spanning PRAGMA and ApGrid sites. The fifteen PRAGMA institutions whose resources were used include Osaka, AIST, TITECH, Tsukuba, KISTI, NCHC, Monash, Hyderabad, KU, BII, USM, NCSA, UCSD/SDSC, TransPAC and APAN. These resources appropriately shared the Grid RPC application layer. The output of the simulation was displayed using tools developed by NCHC on the NCHC's 3D Virtual Reality Equipment. In addition, with a new version Ninf-G Version 2.0.0a a Ninf-G climate simulation was run successfully on the NCSA TeraGrid System, AIST, TITECH, and KISTI, collectively 500 cpus. Other applications were demonstrated using Ninf-G, and Ninf-G, through the PRAGMA collaboration, became part of the software that was automatically installed within a two-hour timeframe for a 128 node cluster using the NPACI Rocks software from UCSD/SDSC.

Grid Based Pseudo-Potential Parameter Search using Nimrod with Applications to Macro Molecular Systems: Researchers at Monash University, the University of California San Diego (UCSD), and the San Diego Supercomputer Center (SDSC) demonstrated Nimrod/G's capabilities by performing an enormous computational chemistry experiment using the grid. Nimrod/G ran some 50,000 instances of the GAMESS chemistry package on as many as 30 super-computers, distributed over 10 countries. It spanned testbeds of PRAGMA, The Australian Grid Forum and the TeraGrid. By harnessing the grid resources so efficiently with grid middleware Nimrod/G, the calculations, a parameter sweep using GAMESS, produced a better understanding of the full parameter space in a few days than could have been gained otherwise over many months. These types of enabling tools will enable much faster analysis procedures and has re-invigorated the approach of using pseudopotential calculations to understand applications in the areas such as drug design or enzymatic reaction processes.

Encyclopedia of Life- Large Scale Grid-enabled Sequence Annotation: Researchers at UCSD/SDSC, the Bioinformatics Institute in Singapore and Tokyo Institute of Technology integrated workflow, portal, grid computing technologies and bioinformatics applications to annotate more than 36,000 proteins, as part of a continuing process to catalog the available proteome of every living species into an electronic reference system, the Encyclopedia of Life (EOL). This demonstration use resources in six countries, the United States, Singapore, Japan, Brazil, Australia and the United Kingdom, and produced the latest annotations (e.g. structural family relationships that give insight to functional activities) for selected proteins from 73 proteomes. All the annotation results from the EOL project are available freely to the global community *(eol.sdsc.edu)*.



Images: PRAGMA participants from SC2003. From the top: 1. Maxine Brown (StarLight) and Radha Nandkumar (NCSA); 2. In the KISTI Booth, Karp Joo Jeong (Konkuk University) and Suntae Hwang (Kookmin University); 3. Donald McMullen (Indiana University); 4. Mason Katz (UCSD/SDSC) and Yoshio Tanaka (AIST); 5. Shingo Takeda (Osaka University) and Richard Russell (Cray Inc.); 6. John O'Callaghan (APAC) and Peter Arzberger (UCSD/SDSC); 7. Shinji Shimojo (CMC/Osaka University)

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During the High-Performance Bandwidth Challenge, a highlight of SC2003, contestants from science and engineering research communities around the world demonstrated the latest technologies and applications for high-performance networking, many of which are so demanding that no ordinary computer network could sustain them. Two demonstrations by PRAGMA members, the "Trans-Pacific Grid Datafarm" team and the "Multi-Continental Telescience" team emphasized that collaborative science applications are a significant force behind the development of high-performance networking by winning awards.

According to Wesley K. Kaplow, chief technology officer for Qwest Government Services, this year's entries focused more on data storage and movement than in years past, and demonstrated significant increases in their capabilities—particularly in the face of problems caused by significant geographic distribution.

PRAGMA winners included:

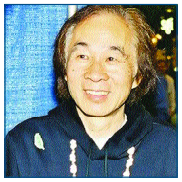
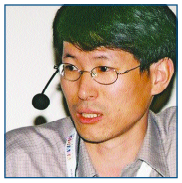
The *"Trans-Pacific Grid Datafarm"* team, which won the Distributed Infrastructure Award for a geographically distributed file system which took advantage of multiple physical paths to achieve high-performance over long distances. For the competition, the National Institute of Advanced Industrial Science and Technology of Japan (AIST) replicated terabyte-scale experimental data between the United States and Japan over several OC-48 links. Five clusters in Japan (AIST, Tokyo Institute of Technology, University of Tsukuba, National Laboratory for High Energy Physics [KEK] in Japan, and APAN Tokyo XP), three in the United States (Indiana University, UCSD/SDSC, and the SC2003 show floor), and one in Thailand (Kasetsart University) constituted a Grid virtual file system of 70 terabytes capacity, federating local file systems on each cluster node. The file transfer rate between the U.S. and Japan—about 10,000 km or 6,000 miles—was 3.57 gigabits per second. The team included members from AIST, Tokyo Institute of Technology, University of Tsukuba, KEK, APAN Tokyo XP, and TransPAC/Indiana University.

The *"Multi-Continental Telescience"* team won the Application Award. The team presented a multidisciplinary entry that showcased technology and partnerships encompassing telescience, microscopy, biomedical informatics, optical networking, next-generation protocols and collaborative research. The demonstration involved globally-distributed resources and users in the United States, Argentina, Japan, Korea, the Netherlands, Sweden and Taiwan. High network bandwidth over IPv6 allowed participants to the control multiple high energy electron microscopes, enabling interactive multi-scale visualization of data pulled from the BIRN Grid and facilitating large-scale grid-enabled computation. The team was the only entrant to use the IPv6 protocols, and sustained an impressive bandwidth of 1.13 gigabits per second. Multi-continental Telescience team included members from UCSD/SDSC, Universidad de Buenos Aires, Karolinska Institute, Osaka University, Center for Ultra High Voltage Microscopy, KDDI R&D Labs, KBSI, KISTI, NCHC, and UCSD/SDSC.

A graphical representation of each team's effort, along with detailed statistics on the data transferred, can be found at *scinet.supercomp.org/2003/bwc/results.*






Images: PRAGMA participants from SC2003. Top Left: Whey-Fone Tsai (NCHC), Peter Arzberger (UCSD), David Abramson (Monash University & APAC), Satoshi Sekiguchi (AIST), Fang-Pang Lin (NCHC);Right-From the top: 1. Philip Papadopoulos (UCSD/SDSC), Teri Simas (UCSD/SDSC), Satoshi Matsuoka (Titech); 2. John Hicks (Indiana University); 3. Nicole Bordes (University of Queensland), Bernard Pailthorpe (University of Queensland); 4. Osamu Tatebe (AIST); 5. Joe Juang (NCHC); 6. Kum-Won Cho (KISTI); 7. Hiroshi Takemiya (AIST); 8. Taisuke Boku (CCP, University of Tsukuba); 9. Hsin-Yen Chen (Academia Sinica Computing Centre)

PRAGMA is an open, institutional-based organization, formed to establish sustained collaborations and to advance the use of grid technologies in applications among a community of investigators working with leading institutions around the Pacific Rim. Applications are the focus of PRAGMA and are used to bring together the key infrastructure and middleware necessary to advance application goals.
PRAGMA is supported by its twenty member institutions and their funding organizations, which include the National Science Foundation's (Grant No. INT-0314015) Office of International Science & Engineering, Division of Shared Cyberinfrastructure & Research, Division of Advanced Networking & Research, and Division of Biological Infrastructure.

For more information on PRAGMA, please visit *www.pragma-grid.net* which includes information about the project, as well as copies of the slide presentations made by PRAGMA partners at SC2003.

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