Pacific Rim Application and Grid Middleware Assembly (PRAGMA)[1]:

PRAGMA Overview, Software, Virtualization and Resource sharing

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Research Scientist, Calit2

University of California San Diego

[1] US Participation funded by NSF Award OCI-1234983

Agenda

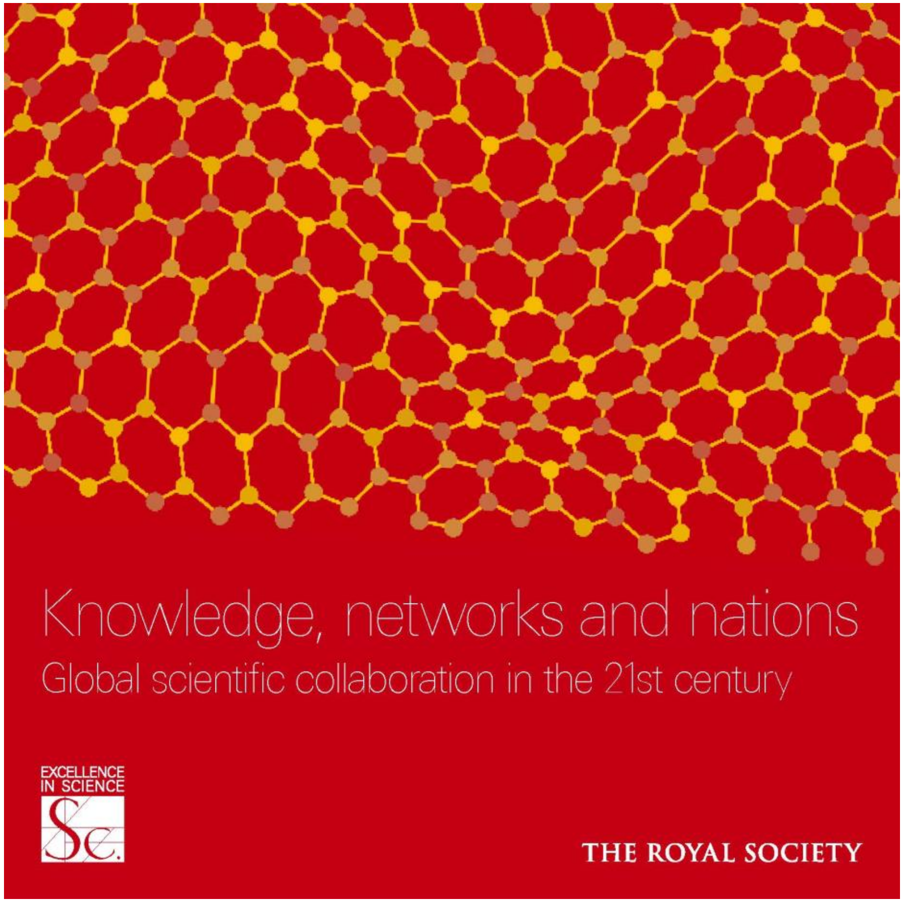
- Introduction to PRAGMA as an organization
- Scientific Expeditions
  - Lake Ecology
  - Biodiversity
  - Experimental Networking Testbed (Not discussed today)
- Technical Developments
  - Virtual Machines → Virtual Cluster
  - Overlay Networks
  - System Software Packaging
  - Better/easier control of distributed resources

Global Investments and Nature of Collaboration Why are these important?

- Global problems require global, collaborative responses: investment and collaborations
- Working across disciplines, cultures requires new skill sets
- Working in the *marketplace of ideas* improves quality and helps transfer knowledge more rapidly

We need to articulate the "value proposition" of collaboration

Trends in Collaboration



- The scientific world is becoming increasingly interconnected, with international collaboration on the rise.
- Science in 2011 is increasingly global, occurring in more and more places than ever before.

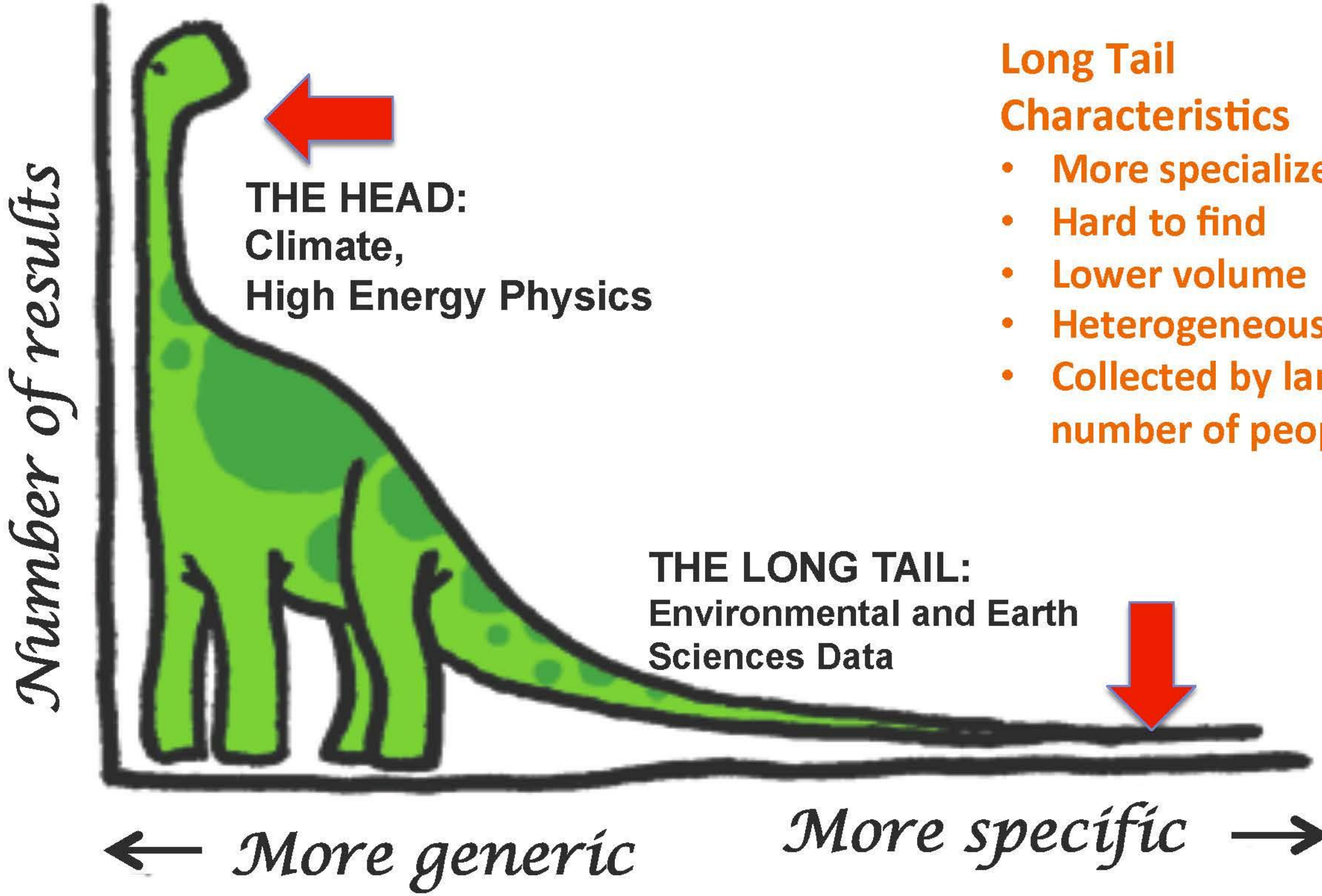
Knowledge, Networks and Nations:
Global scientific collaboration in the 21st century.
The Royal Society. March 2011

"intellectual power [is] becoming increasingly evenly distributed"
N. Birdsall, F Fukuyama

Future Human Capital
Why do we need to worry?

- Solving problems, developing technology, making investments and collaborating are done by people
- Are we creating the next generation to face the global challenges, and work in multidisciplinary, multicultural teams?

Environmental and Earth Sciences Data have Characteristics of a Long Tail



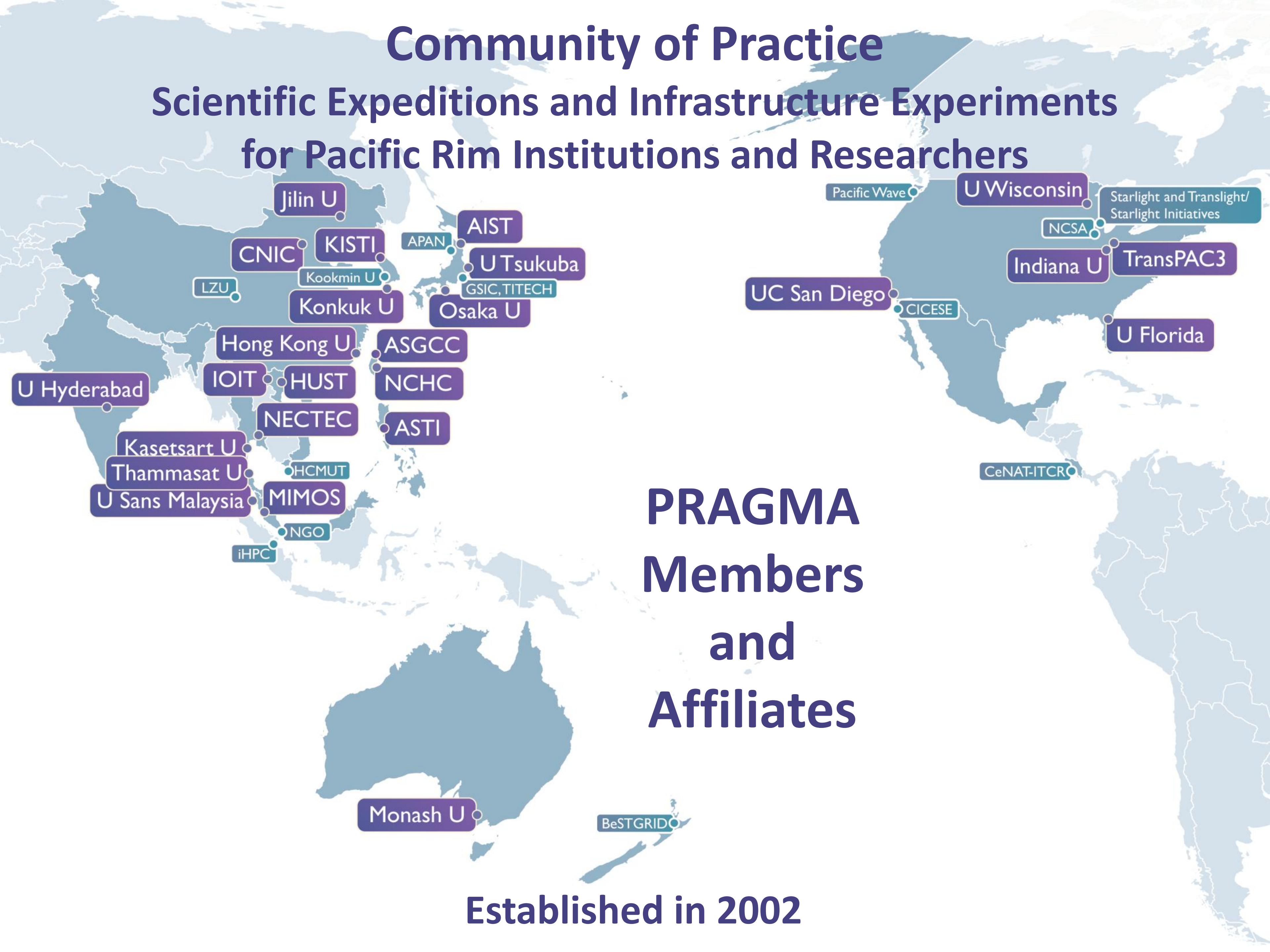
Long Tail Characteristics

- More specialized
- Hard to find
- Lower volume
- Heterogeneous
- Collected by large number of people

Wyborn 2013

Community of Practice

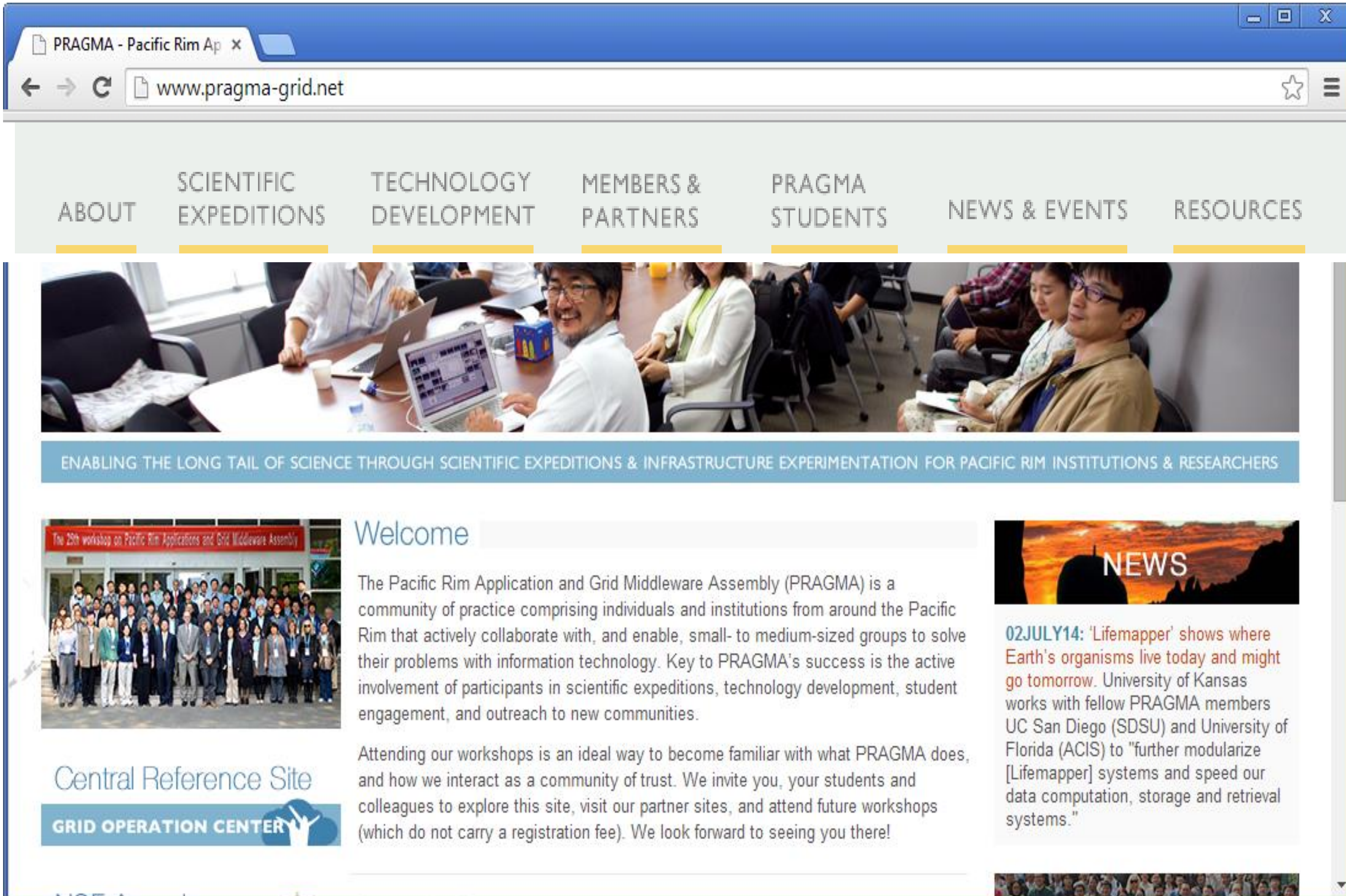
Scientific Expeditions and Infrastructure Experiments for Pacific Rim Institutions and Researchers



PRAGMA Members and Affiliates

Established in 2002

On the Web – Key Activities



Broad Organization

- Scientific Expeditions (focal activity)
- Cooperative technology development
  - Open Source
- Student Engagement
  - Student's Association
  - Undergraduate summer exchanges via PRIME (US), MURPA/QURPA (Australia)
  - Graduate student visits
- International testbed resources
  - Applications
  - Systems/integration Software
- Steering Committee

Began in 2002 as a small workshop series to better understand "grid" technologies.

PRAGMA Involves People

- Twice a year workshops
- Working groups
  - Resources
  - GEO Sciences and Telescience (Disaster Mitigation)
  - Life Sciences
- Expeditions
  - Lake Eutrophication
  - Biodiversity

- Future Meetings
  - PRAGMA 27, Bloomington Indiana October 15 – 17, 2014
  - PRAGMA 28 Nara Japan April 8-10 2015

PRAGMA Actively Engages New Communities via PRAGMA Institutes and Mini-PRAGMA Workshops

- Water Disaster Management and Big Data
  - NII Shonan Meeting, 7 – 10 July 2014
- Mini-PRAGMA Indonesia, June 2013
- Lower Mekong Initiative Workshop
  - Hanoi August 18 – 22

Why 2X/year in-person working meetings

- Hosts highlight activities within their country
  - Chance to learn about research and activities that might otherwise go unnoticed
- Critical time for “shoulder-to-shoulder” collaborative work
- Recurring structure is a natural “clock” to keep distributed activity focused and moving forward
- Participation is open, but is based upon the ***desire to work with others.***
- Virtual meetings, email, shared code repository are all practical methods for time between meetings

PRAGMA 26 – Theme Living with Big Data

Grad Students with Faculty Mentor

Interviewing Students during Lightning talks

Poster Session

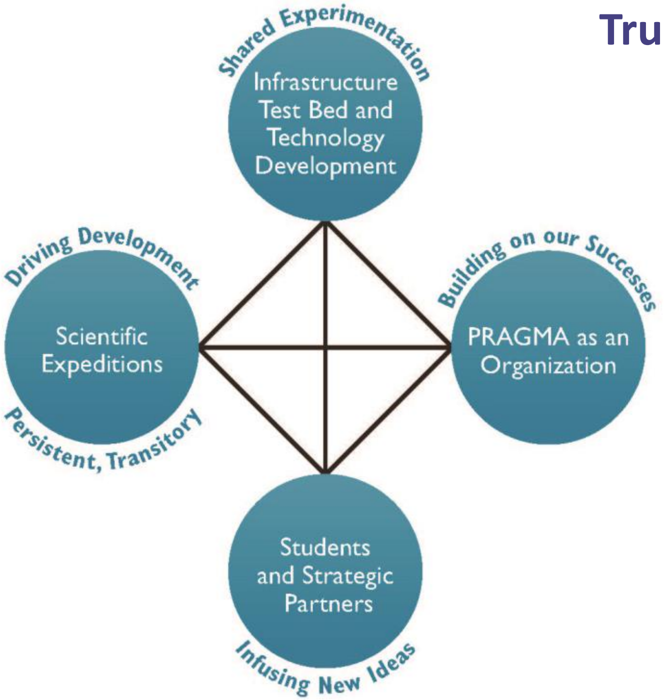
Working Together

The Gap Between Technology Capability and Practice

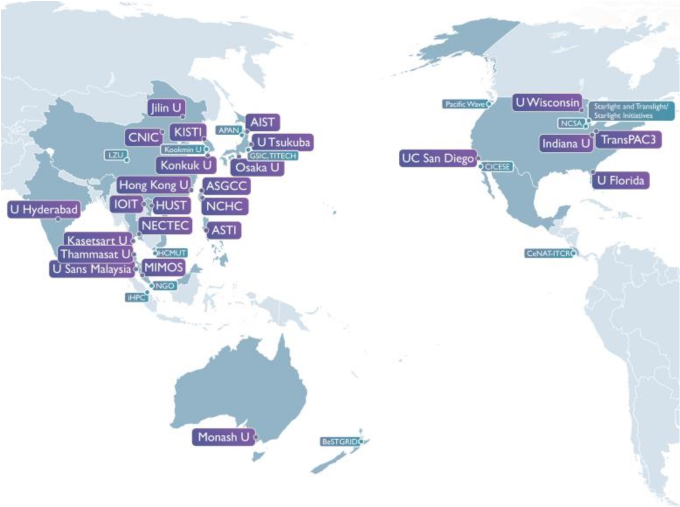
- Technology developers are not always focused on the specific needs of domain scientists
- The pace of change can be dizzying
  - Vector Supers (1990) → Massively Parallel (1995) → Grid (2000) → Clusters (2005) → Cloud (2010) → ??
- Smaller groups of scientists are often left to fend for themselves
- PRAGMA focuses on bringing technologists and scientists together to make technology work in an international setting → Enable collaborative science

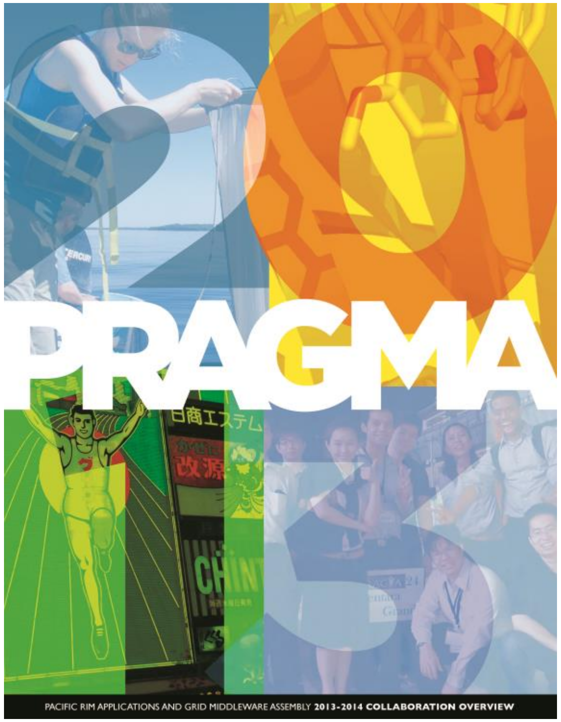
Enabling the Long Tail of *Team* Science

Virtual Scientific Expeditions



Trust Envelope (network overlay)





PRAGMA Students

PRAGMA Member Sites

PRAGMA Community

Key Organizing Principle: Scientific Expeditions

Savannah Burn 2006

Addressing Science Needs & Developing/ Improving Tools

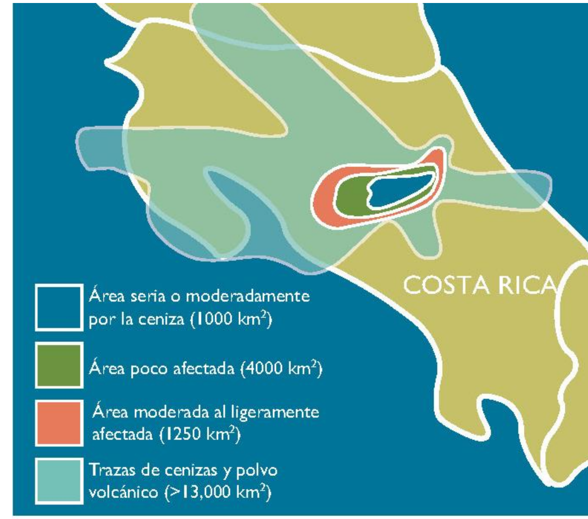
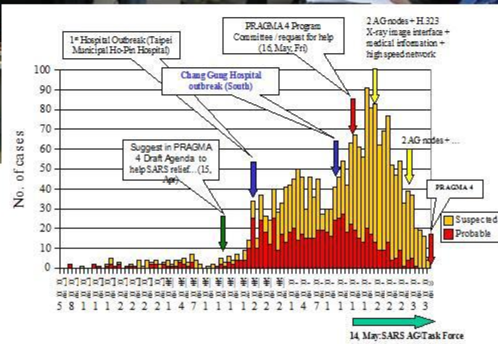


Fig. 1. Irazú volcano location and ash distribution during 1963-1965

Distribution of ash from

NCHC SARS Task Force

Developers at the NCHC Access Grid node test the SARS Grid network links



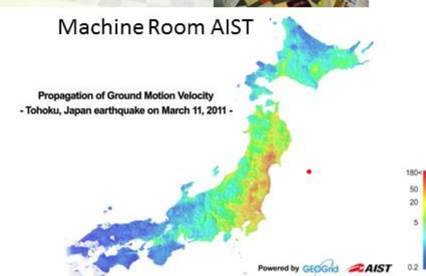
http://antisars.nchc.gov.tw/

Source: Fang-Pang Lin

March 2011:Tohoku Earthquake and Tsunami

Machine Room AIST

- GEO Grid Disaster Task Force migrated services to other sites, including
  - NARL|NCHC|NSPO
  - UCSD|SDSC
  - OCC, Orkney, ERSDAC, NTT-data-CCS, CTC, Univ. Lille, and ITT
- Used aspects of virtualization porting and distributed resources at NCHC and SDSC



GEO Grid Disaster Response Task Force
http://disaster-e.geogrid.org

A "Resource" view of collaborative science

- Researchers want to work together
  - Identify essential data sets (what, where, how big? Allowable use models, …)
    - Not all data is open
    - Not all data can be shared
  - Identify the types of resource(s) needed to accomplish analysis
    - Computing cluster, Visualization System, data handling,..
    - If you are "lucky" these are all in one place
      - Most scientists are not so fortunate

Scientific Expeditions

- Information technology specialists + domain science application == Scientific Expeditions
- Domain scientists benefit from deep technical expertise
- Information technology specialists benefit from seeing how their tools/techniques can be used and improved.

Use "Overlay" Networks to provide a trusted environment for focused sharing of resources

Some Specific PRAGMA Activities

Enabled International Collaboration

Applications

- LifeMapper Biodiveristy
- Lake Ecology
- Network Experiment
- Cyber Learning

Technologies

- Data Provenance
- Overlay Networks
- Virtual Cluster Migration
- Application Integration

PACIFIC RIM APPLICATIONS AND GRID MIDDLEWARE ASSEMBLY
PRAGMA

Students

Researchers

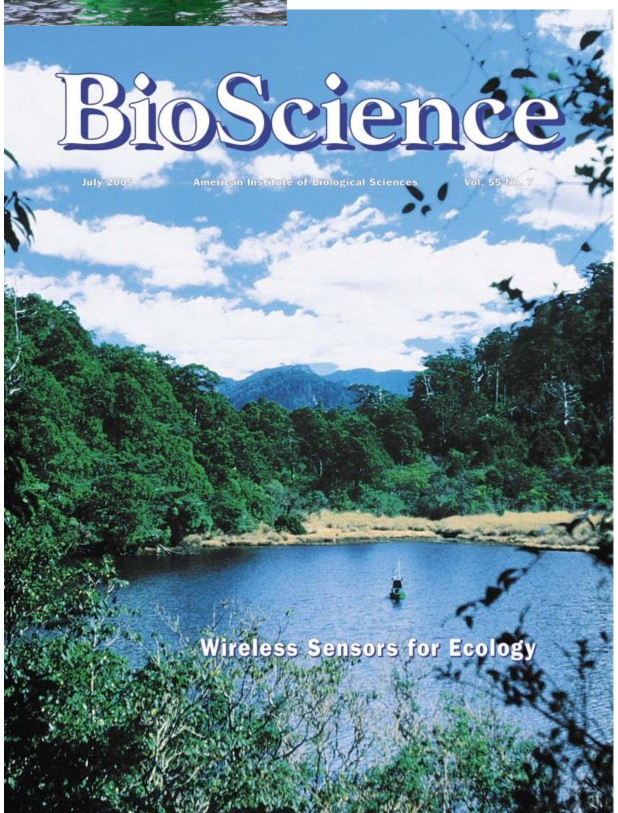
PRAGMA Helps Establish GLEON

PACIFIC RIM APPLICATIONS AND GRID MIDDLEWARE ASSEMBLY
PRAGMA

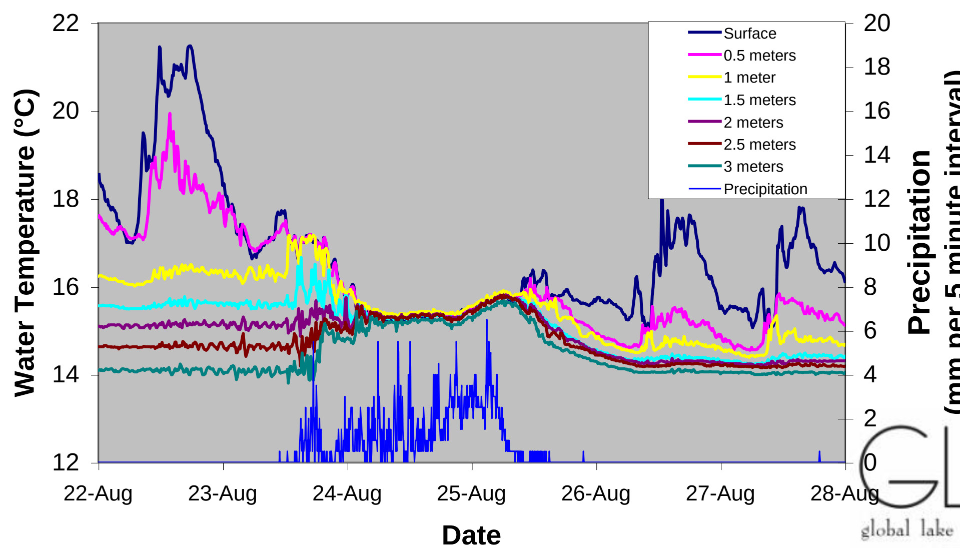
GLEON
global lake ecological observatory network

From Scientific Expedition to Community

Building on NCHC Ecogrid in Taiwan
8 Months: Concept to Deployment



- Wireless Infrastructure (2004)
- Science
- Need more than one lake to understand processes



GLEON

Networked lake science

Global Lake Ecological Observatory Network

P.C. Hanson and K.C. Weathers
GLEON Steering Committee co-Chairs

Mission: *GLEON conducts innovative science by sharing and interpreting high-resolution sensor data to understand, predict and communicate the role and response of lakes in a changing global environment*




Argentina
Australia
Austria
Brazil
Canada
Chile
China
Colombia
Denmark
Estonia
Finland
Germany
Hungary
India
Ireland
Israel
Italy
Kenya
Netherlands
New Zealand
Nigeria
Pakistan
Poland
Puerto Rico
Russia
South Korea
Spain
Sweden
Switzerland
Taiwan
Turkey
United Kingdom
United States

GLEON, a network of >100 lakes and ~10^7 data

Technological challenges in sensing and information management

Analytical challenges in interpreting and modeling very large data sets

Scientific challenges in interpreting broad spatio-temporal gradients from many ecosystems

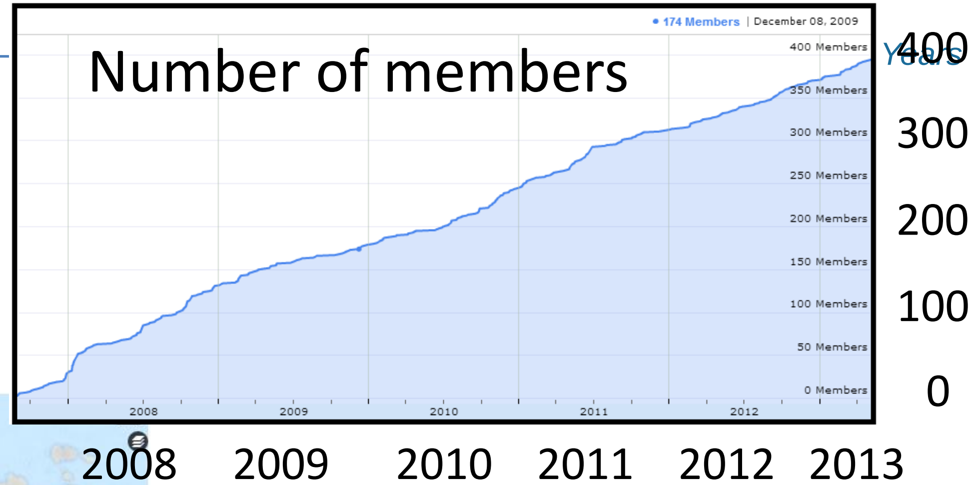
Social and cultural challenges in diverse teams with diverse and distributed resources

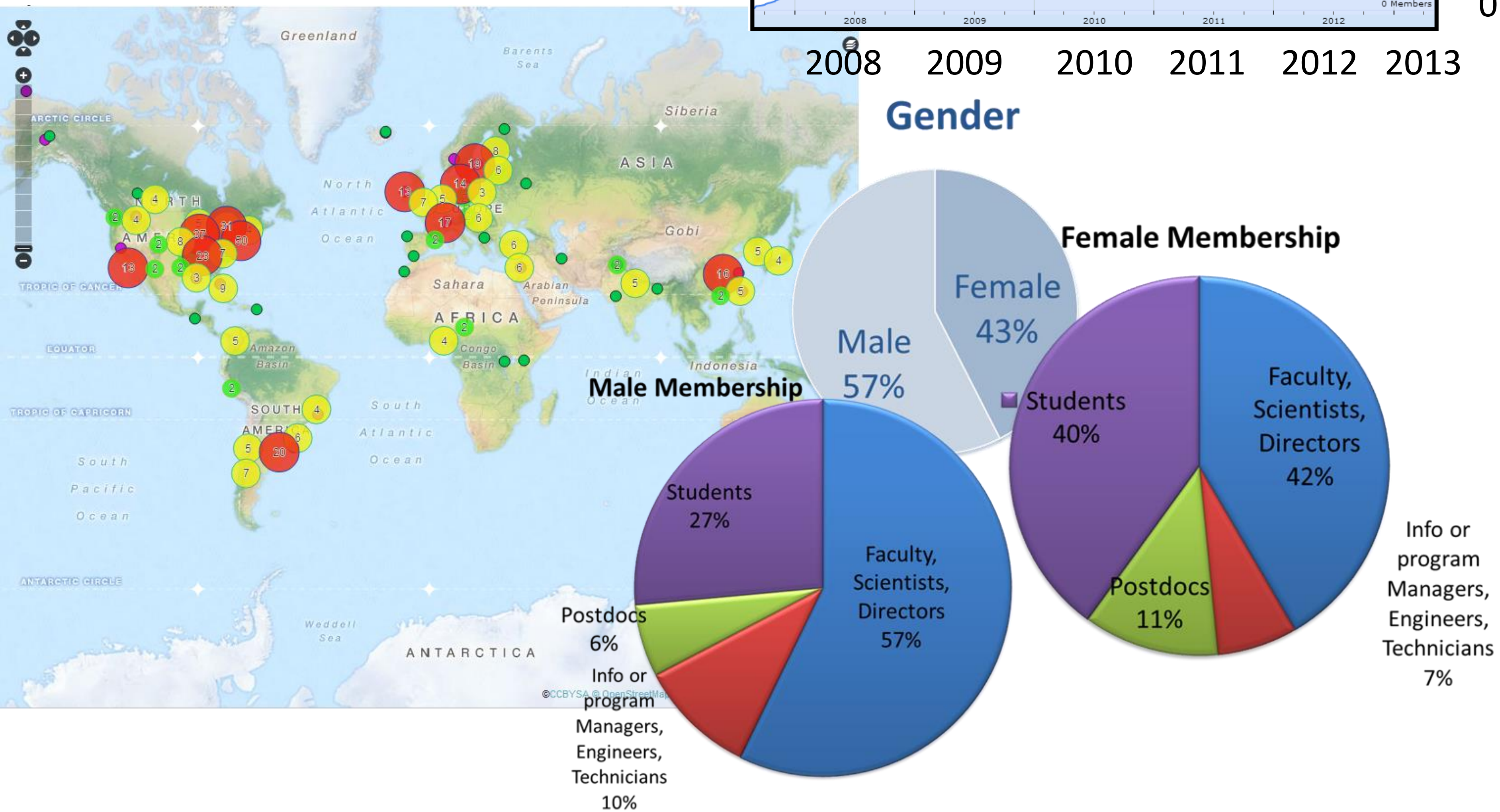
A rich and productive research, education and outreach environment!

But most importantly a network of people

~ 450 individual members

~ 45 countries





Metabolic changes and the resistance and resilience of a subtropical heterotrophic lake to typhoon disturbance

Jeng-Wei Tsai, Timothy K. Kratz, Paul C. Hanson, Nobuaki Kimura, Wen-Cheng Liu, Fang-Pan Lin, Hsiu-Mei Chou, Jiunn-Tzong Wu, and Chih-Yu Chiu

Can. J. Fish. Aquat. Sci. 68: 768–780 (2011) doi:10.1139/F2011-024

Lake-size dependency of wind shear and convection as controls on gas exchange

Jordan S. Read,[1] David P. Hamilton,[2] Ankur R. Desai,[3] Kevin C. Rose,[4,5] Sally MacIntyre,[6] John D. Lenters,[7] Robyn L. Smyth,[5] Paul C. Hanson,[8] Jonathan J. Cole,[9] Peter A. Staehr,[10] James A. Rusak,[11] Donald C. Pierson,[12] Justin D. Brookes,[13] Alo Laas,[14] and Chin H. Wu[1]

GEOPHYSICAL RESEARCH LETTERS, VOL. 39, L09405, doi:10.1029/2012GL051886, 2012

Large gradients of ecosystems enable new insights

Reconciling the temperature dependence of respiration across timescales and ecosystem types

Gabriel Yvon-Durocher, Jane M. Caffrey, Alessandro Cescatti, Matteo Dossena, Paul del Giorgio, Josep M. Gasol, José M. Montoya, Jukka Pumpanen, Peter A. Staehr, Mark Trimmer, Guy Woodward & Andrew P. Allen

Nature **487**, 472–476 (26 July 2012) | doi:10.1038/nature11205

Lakes help us understand fundamental principles of ecology.

MACROSYSTEMS ECOLOGY

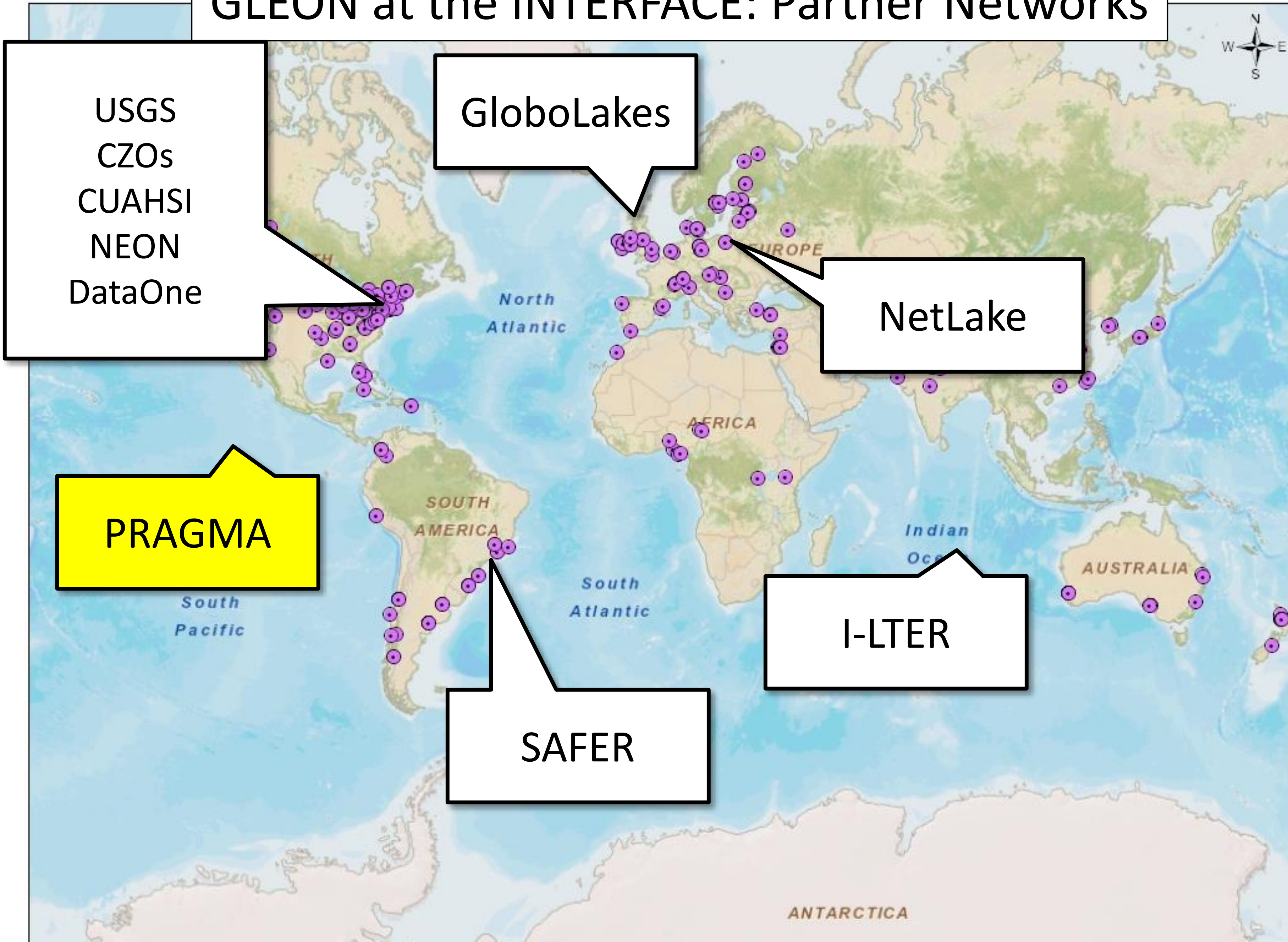
Creating and maintaining high-performing collaborative research teams: the importance of diversity and interpersonal skills

Kendra S Cheruvelil[1,2*], Patricia A Soranno[2], Kathleen C Weathers[3], Paul C Hanson[4], Simon J Goring[5], Christopher T Filstrup[6], and Emily K Read[3,4]

Front Ecol Environ 2014; 12(1): 31–38, doi:10.1890/130001

How you form and manage collaborations matters!

GLEON at the INTERFACE: Partner Networks



PRAGMA EXPEDITION

Lake eutrophication

GLEON

PRAGMA-GLEON Expedition Goals

- Create a collaborative human and technological infrastructure that supports distributed team
- Apply a new hydrodynamic-water quality model, GLM-FABM-AED, to GLEON lakes.
- Consider a different set of rules that govern biological communities in lakes
- Expand research to additional lakes and broader research community

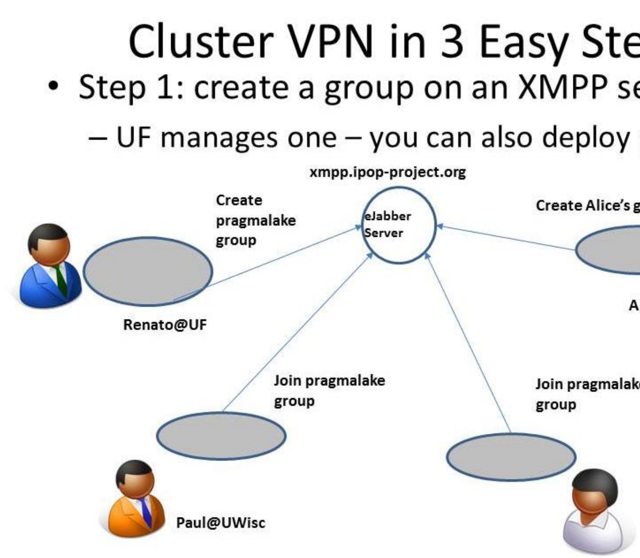
Leverage and expand science momentum…

Predicting Water Quality in Lakes

Developing Predictive Models using IPOP Overlay

- Lake eutrophication is global issue, results in degraded water quality
- Calibrate new hydro-dynamic model, check model against data
- Using IP-over-P2P (IPOP) to **<u>interconnect resources</u>** (and Virtual Machines) across multiple institutions, creating "**<u>trust envelope</u>**"

Collecting light, temperature data



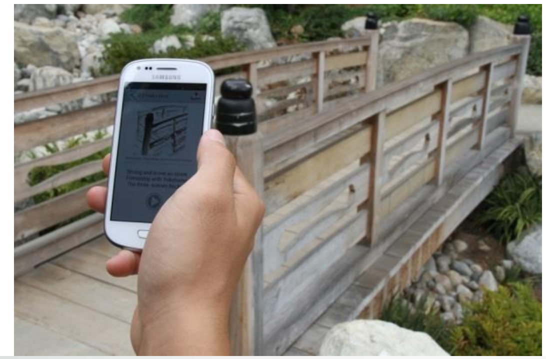
global lake ecological observatory network

<u>Paul Hanson</u><u>, Craig Snortheim, Luke Winslow (U. Wisconsin),</u>
<u>Cayelan Carey (Virginia Tech); Renato Figueiredo, Pierre St. Juste, Ken Subratie (U. Florida)</u>

Biodiversity Expedition

Technology Trends Affecting Biodiversity

- Digitization of Collections
- Mobile Technologies
- Sensors – aquatic, terrestrial, and airborne
- Software Defined Networks



2 M wingspan, 4.9 kg

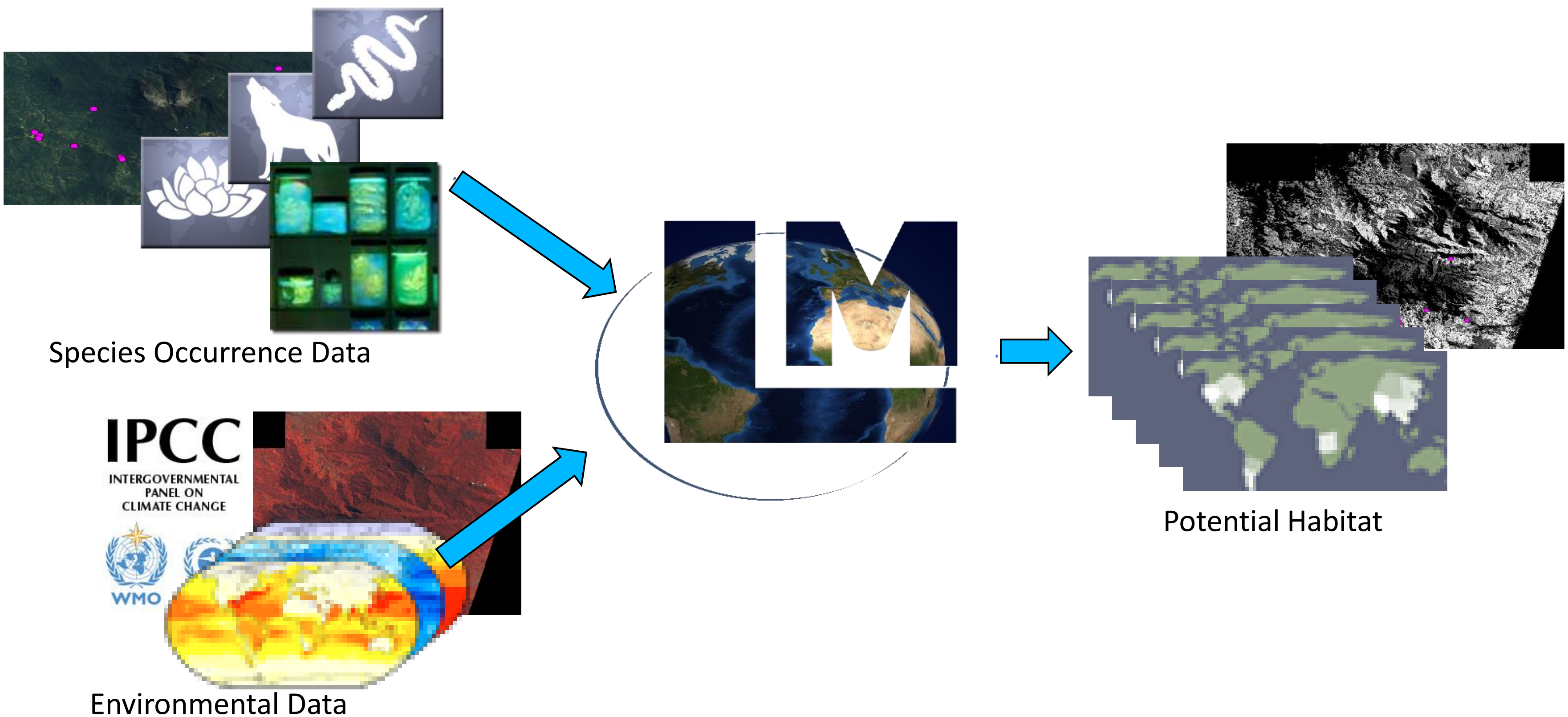
Lots of Data, Lots of Opportunities to Share

Lifemapper – A Key Domain Science Tool

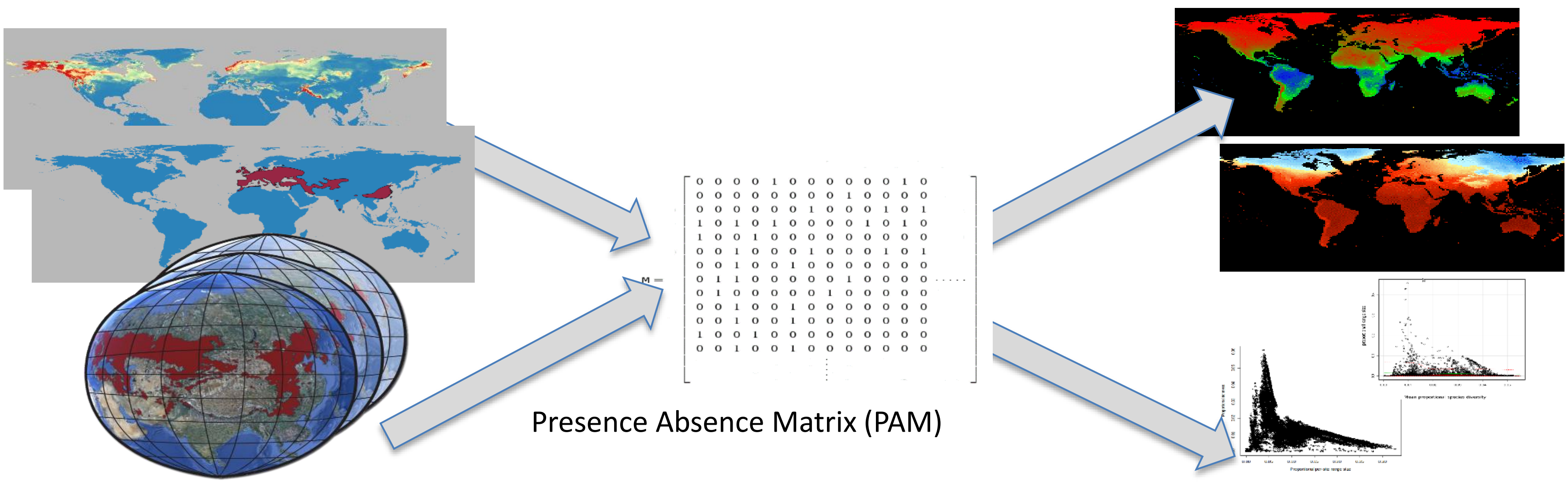
- Data library
  - Climate
    - Observed
    - IPCC Predicted Future Climate
  - Species
    - Occurrence Points
    - Potential habitat maps
- Tools
  - LmSDM: Species Distribution Modeling
  - LmRAD: Range and Diversity

GBIF

LmSDM:
Species Distribution Modeling



LmRAD:
Range and Diversity



Species Habitat Data

Presence Absence Matrix (PAM)

Multi-species analyses

Range and Diversity Quantifications

Biodiversity in Extreme Environments

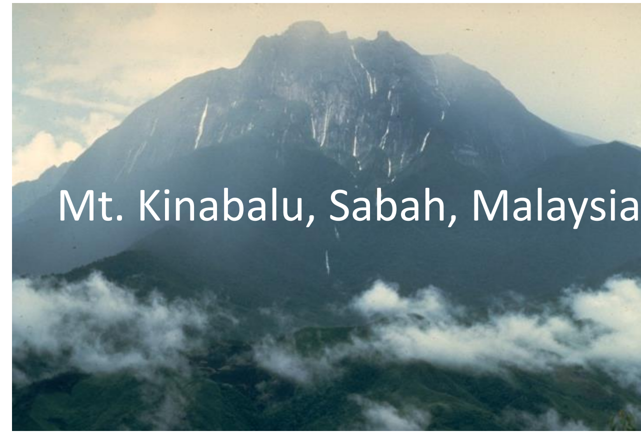
Distribution Prediction by Sharing CI and Provenance Capture

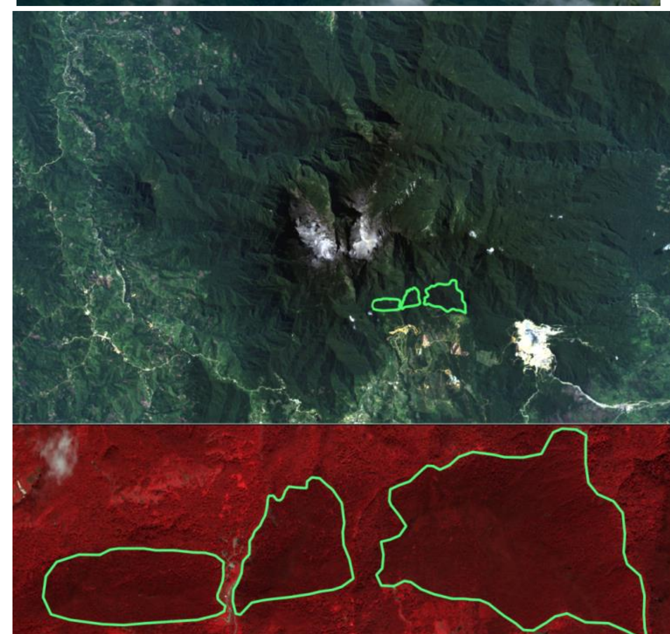
Approach: Improve Lifemapper (LM)

- Extend previous LM work to enable data management and portability of software
- Increase the availability and flexibility of LM to enable scientists to
  - Assemble multi-species macro-ecology experiments
  - Perform other LM-facilitated data processing on:

    Unique datasets; Restricted use data

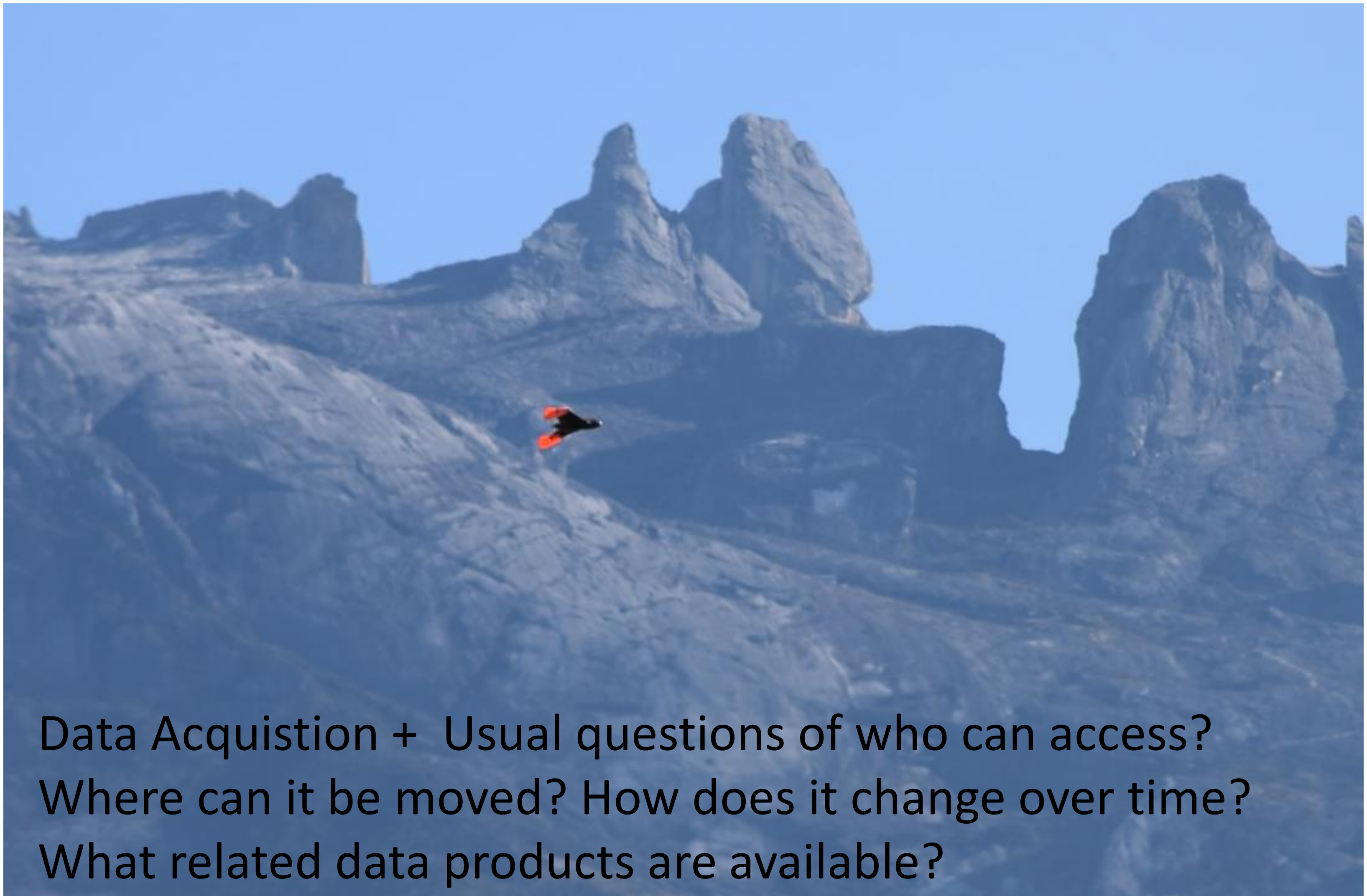
    Very large datasets





Aimee Stewart (Kansas), Nadya Williams, Philip Papadopoulos (UCSD), Reed Beaman (U Florida)
Antony van der Ent, Peter Erskinge (U Queensland) Rimi Pepin (Sabah Parks)

UAV Flight (Kinabalu Donkey Ears)



Data Acquistion + Usual questions of who can access?
Where can it be moved? How does it change over time?
What related data products are available?

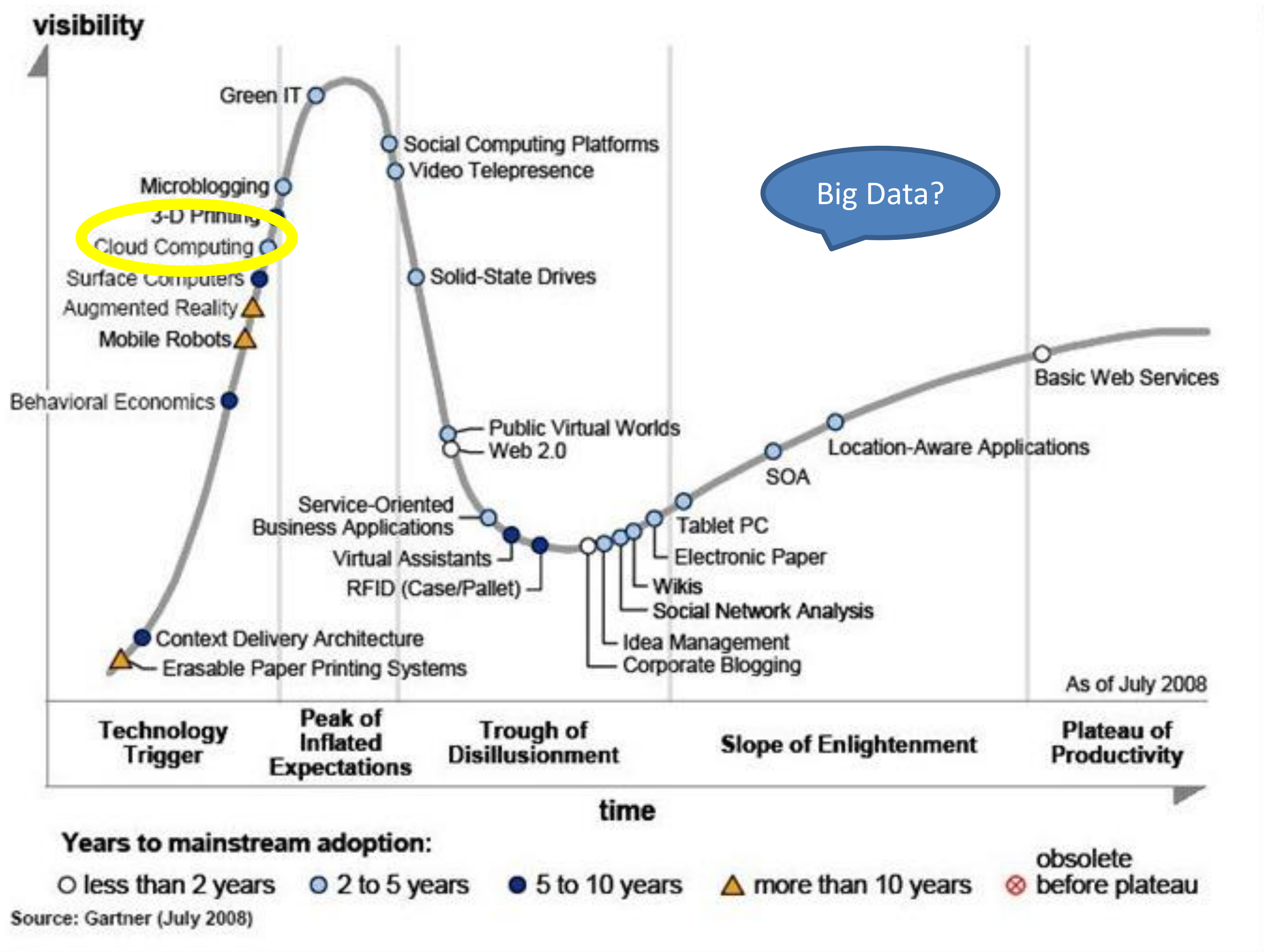
Expedition → Infrastructure

- What are some of the key technologies and trends?
- How do we construct the systems needed without being restricted to a physical site?

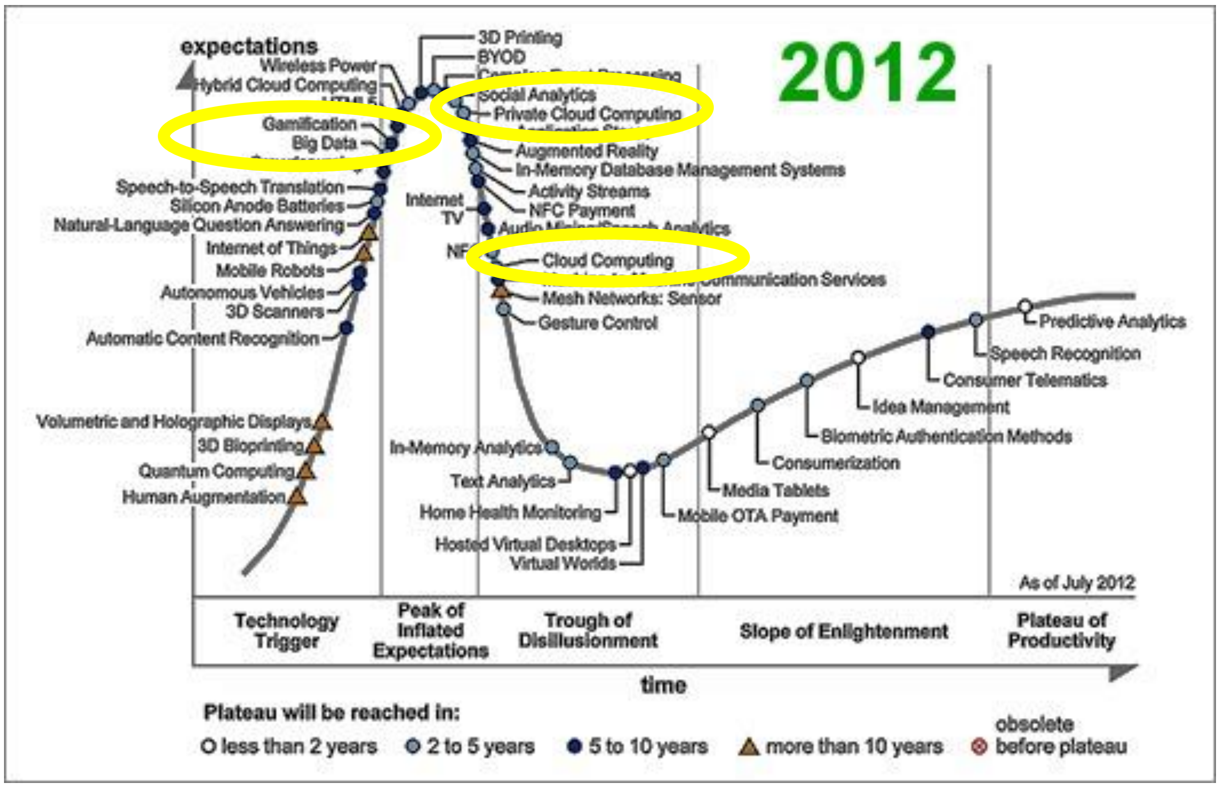
Some Things that Happened on the Way to Cloud Computing

- Web Version 1.0 (1995)
- 1 Cluster on Top 500 (June 1998)
- Dot Com Bust (2000)
- Clusters > 50% of Top 500 (June 2004)
- Web Version 2.0 (2004)
- **Cloud Computing (EC2 Beta - 2006)**
- Clusters > 80% of Top 500 (Nov. 2008)

Gartner Emerging Tech - 2008

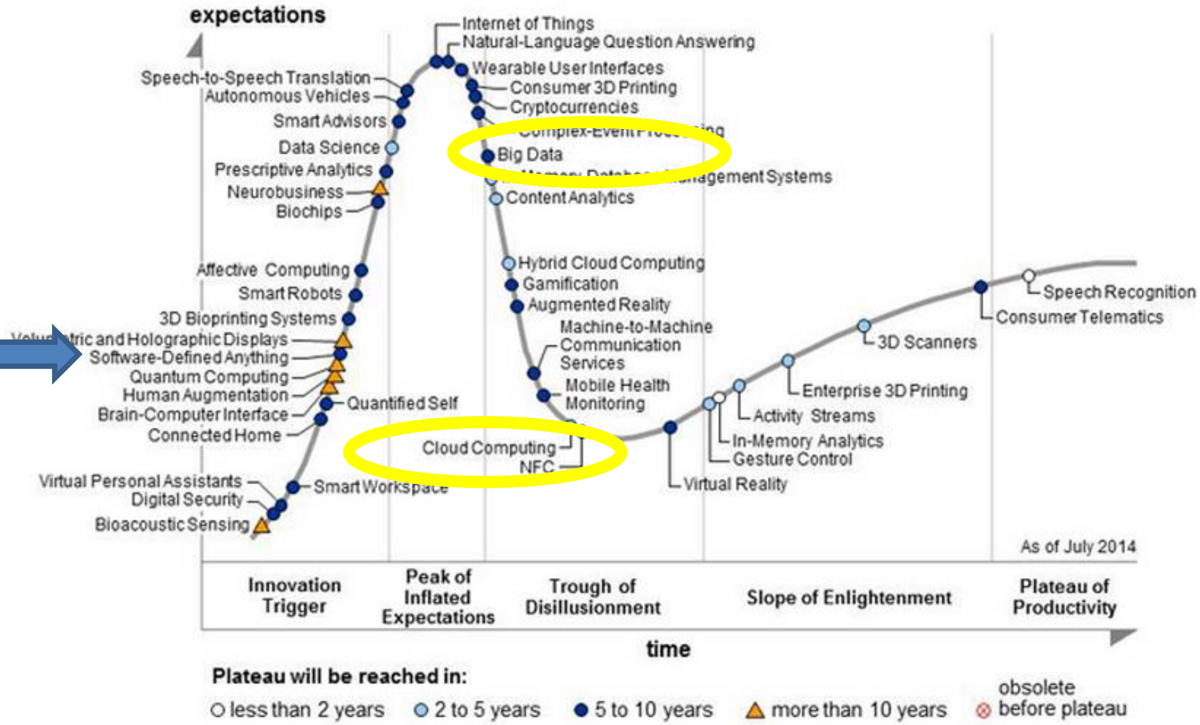


Gartner Emerging Tech 2012



Gartner 2014

Figure 1. Hype Cycle for Emerging Technologies, 2014

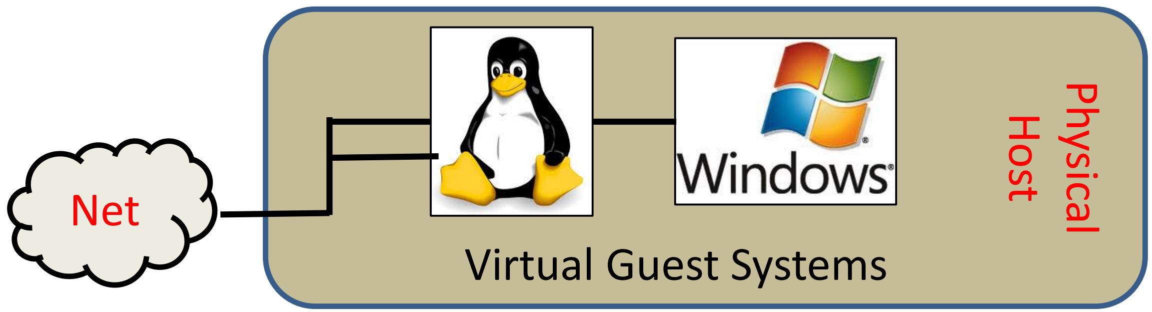


What is fundamentally different about Cloud computing vs. Grid Computing

- Cloud computing – You **adapt the infrastructure** to your application
  - Should be less time consuming
- Grid computing – you **adapt your application** to the infrastructure
  - Generally is more time consuming
- Cloud computing has a financial model that seems to work – grid *never* had a financial model

System Virtualization – Underlying Technology for cloud computing

- Software the allows you to run a virtualized computer inside of a physical one



- Different systems create this software illusion
  – VMWare, Virtualbox, Xen, KVM,
- Different cloud systems give users a web-services interface to virtual systems
  – Amazon EC2, OpenStack, CloudStack, Eucalyptus, OpenNebula, …

Physical Clusters → Virtual Clusters

- Beowulf and HPC Clusters are today the most common architectures for delivering scientific computing
- Specific Scientific Software can be quite complex to configure and maintain properly
  - This makes it difficult to move infrastructure from place to place
  - "Cloud computing" by itself doesn't solve the underlying system issues.
- HPC Clouds are very close to reality

An HPC (cloud) for the 99%
(Production Date: 1 Jan 2015)

The next-generation of HPC will support high-performance virtual clusters @SDSC

(One reason why PRAGMA doesn’t focus running resources)

SDSC
SAN DIEGO SUPERCOMPUTER CENTER

UCSD

Comet Will Serve the Long Tail of Science

CHALLENGES OUR PROPOSAL ADDRESSES

- ✓ Attract new users and communities
- ✓ Support diverse applications with complex workflows
- ✓ Ensure responsiveness for thousands of users
- ✓ Transfer, store, analyze, and share massive data sets
- ✓ Integrate with XSEDE

COMET COMPUTE SYSTEM

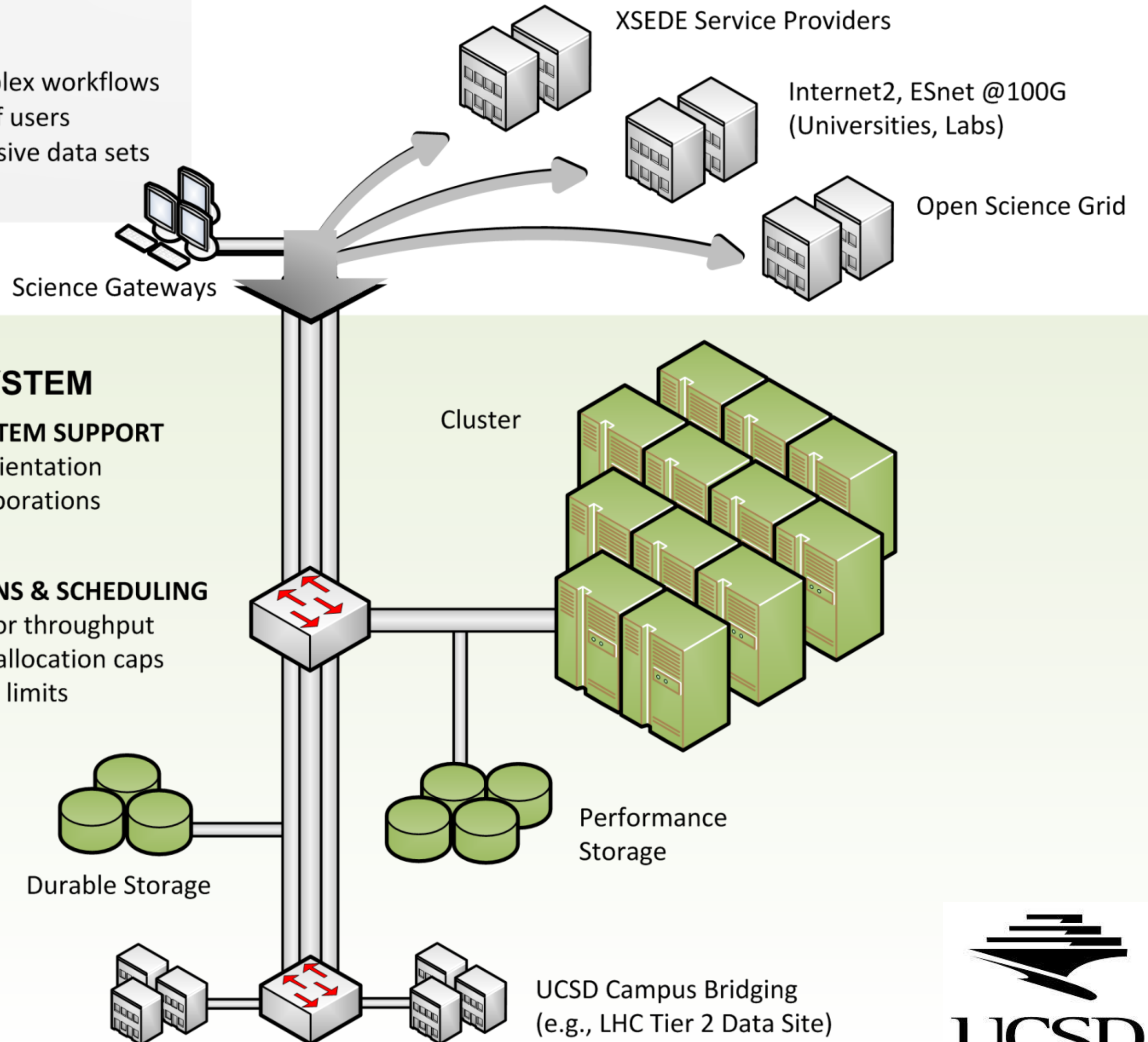
Cluster architecture
Fast standard nodes
Large-memory nodes
GPU-accelerated nodes
FDR InfiniBand

Storage architecture
Performance Storage
Durable Storage

Software
Science Gateways
Rich base of installed apps
Virtualization

USER & SYSTEM SUPPORT
New user orientation
XSEDE collaborations
FutureGrid

ALLOCATIONS & SCHEDULING
Optimized for throughput
Per-project allocation caps
Per-job core limits



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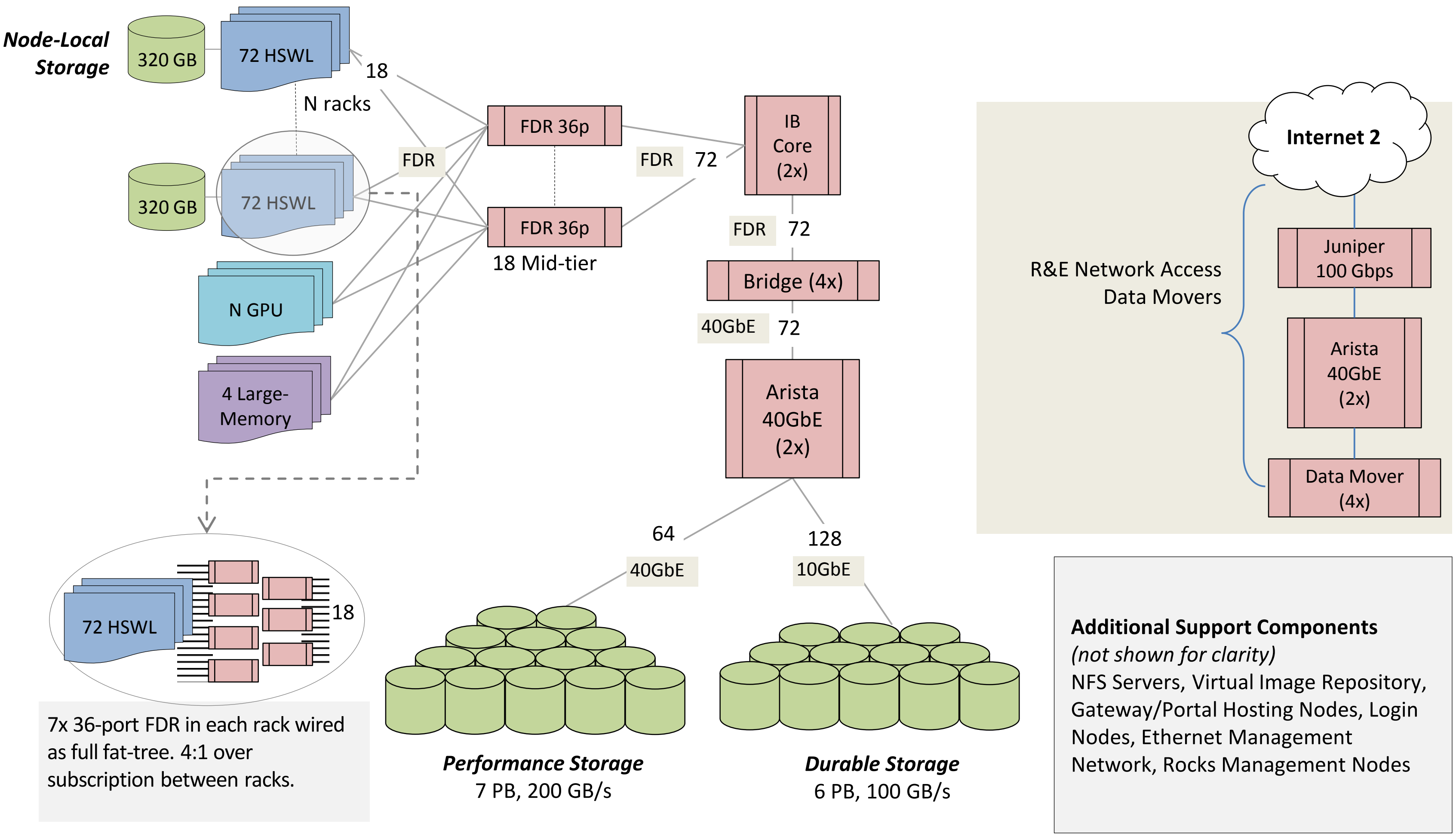
Comet Architecture



> 45K Cores

SDSC SAN DIEGO SUPERCOMPUTER CENTER

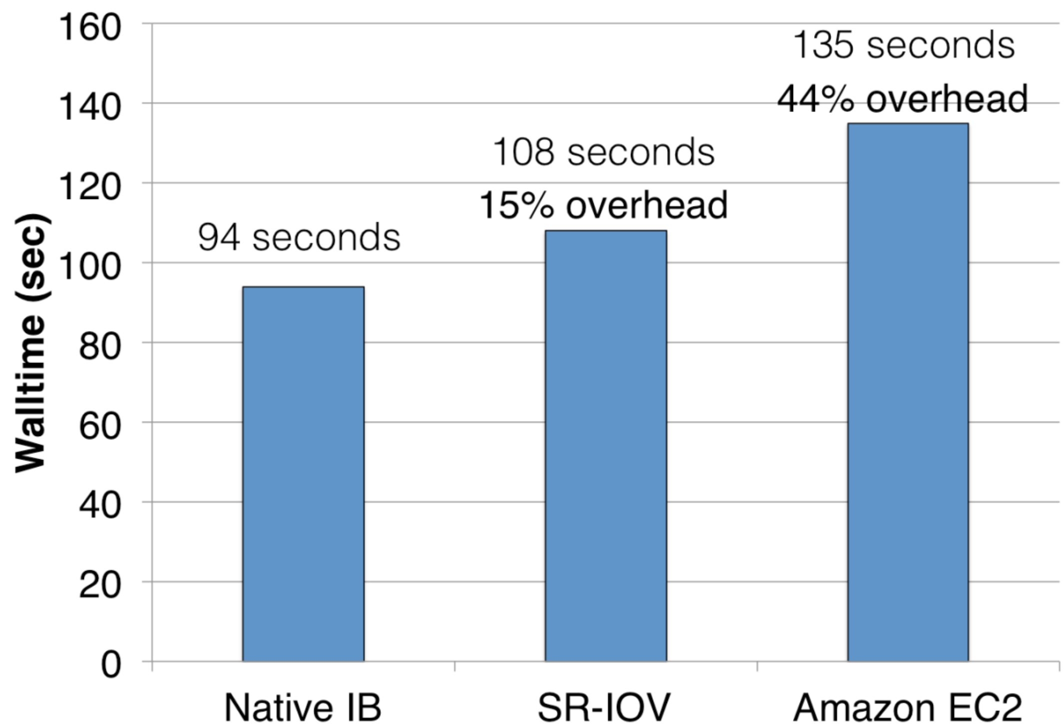
UCSD

High-Performance Virtualization on Comet

- Mellanox FDR InfiniBand HCAs with SR-IOV (Single Root IO Virtualization)
- Rocks and OpenStack Nova to manage VMs
- Flexibility to support complex science gateways and web-based workflow engines
  - Custom compute appliances and virtual clusters developed with FutureGrid and their existing expertise
  - Backed by virtualized Storage running over virtualized InfiniBand

Virtualization performance modest impact : Weather Modeling – 15% Overhead

- 96-core (6-node) calculation
- Nearest-neighbor communication
- Scalable algorithms
- SR-IOV incurs modest (15%) performance hit
- ...but still still 20% faster*** than Amazon



WRF 3.4.1 – 3hr forecast

*** 20% faster despite SR-IOV cluster having 20% slower CPUs

Back to the Biodiversity Expedition …

… What do we need to do run Lifemapper in this type of environment?

Lifemapper Server Virtualization

Aimee Stewart (KU) astewart@ku.edu
Nadya Williams (UCSD) nadya@sdsc.edu

Lifemapper Server Virtualization

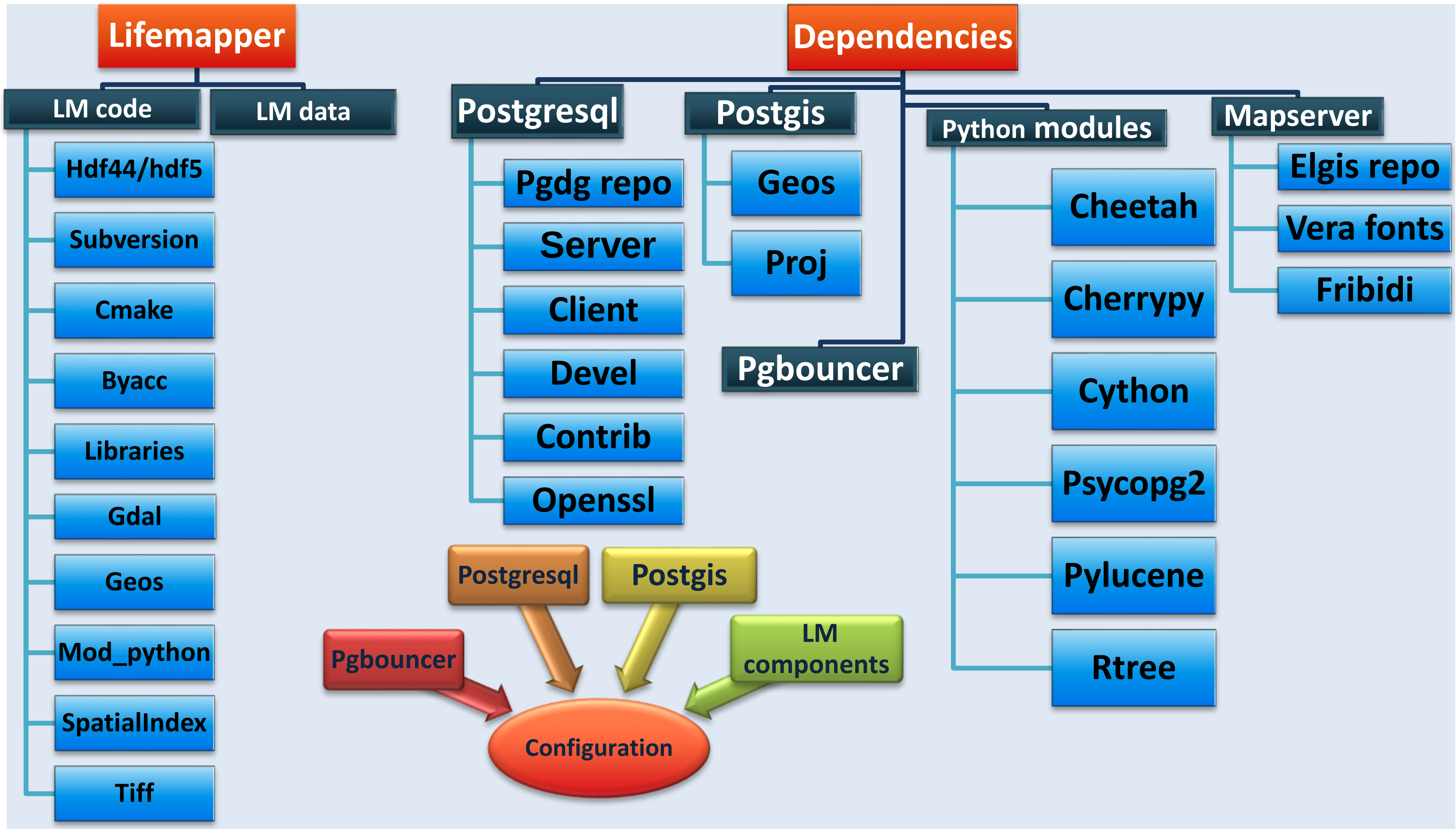
Domain scientist's viewpoint:

1. Extend previous Lifemapper work to enable data management (LmDBServer) and web services (LmWebServer) components virtualization
2. Increase the availability and flexibility of Lifemapper to enable scientists to
   - *Assemble multi-species macro-ecology experiments*
   - *Perform other LM-facilitated data processing on:*
     Unique datasets
     Restricted use data
     Very large datasets

Cyber-infrastructure viewpoint:

1. Continue practical use of PRAGMA cloud infrastructure
2. Encapsulate the complexity of software build/configure in ROCKS rolls
3. Create a complete system as an end-to-end solution
4. Reduce cost of installing/configuring/replicating

Complexity of Scientific Applications
Lifemapper Server Roll – More than 20 Software components

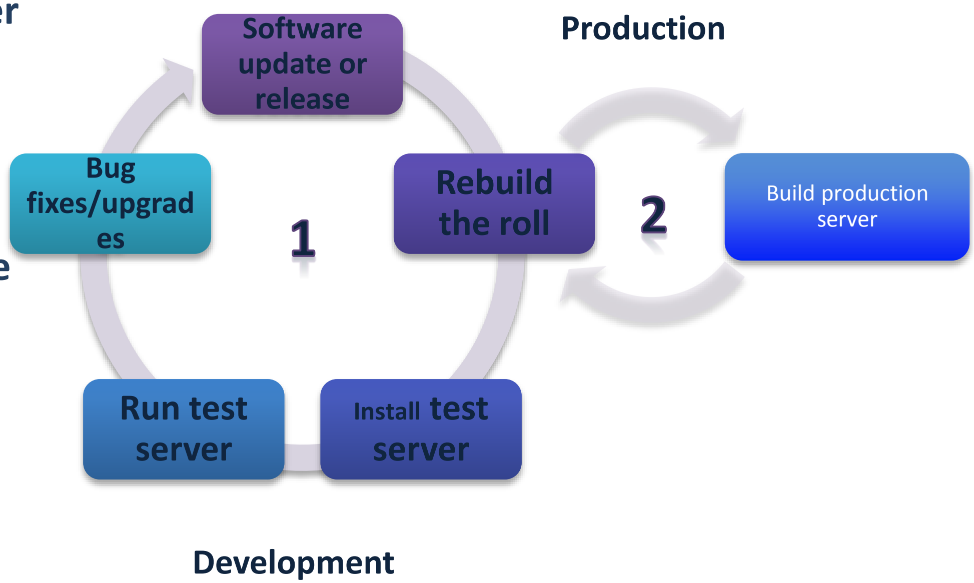


Total: 56 RPMS (packages)

What we are trying to do

- **Increase availability and flexibility of Lifemapper Server as a complete system**
  - reduce cost of installing/configuring/replicating and ease burden of integrating hardware and software
- **Enable a fast "workflow" from software update to server availability:**
  - Minimize time spent on software build and configuration
  - Automate most hands-on tasks.
  - Essential: have test cases for all installed components and their configuration
- **Prepare for greater quantity and quality of data and complexity of operations**
  - From low resolution climate data to high resolution satellite imagery for Mt. Kinabalu
  - From simple single-species SDM experiments to multi-species macro-ecology experiments with more species

This work is a part of PRAGMA's "Resources and Data" working group



Lifemapper

http://lifemapper.org

https://github.com/lifemapper/

Rocks

http://www.rocksclusters.org

Pragmagrid GitHub

https://github.com/pragmagrid/lifemapper

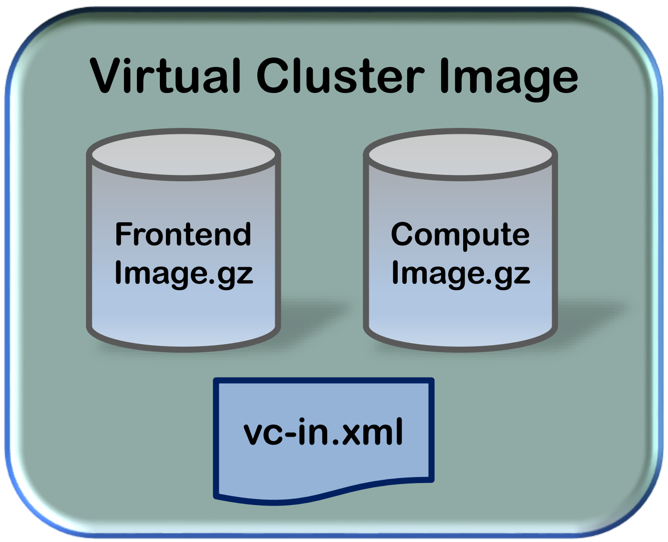
https://github.com/pragmagrid/lifemapper-server

PRAGMA-Developed Tech

- You have a Virtual Cluster with your scientific software properly configured, What's the next step?
- PRAGMA_boot
  - Practically solve the problem of moving a virtualized cluster from one cloud hosting system to another

Virtual Cluster Image

- Define a standard way to share cluster images
  - E.g. frontend: LmDbServer, compute: LmCompute



Deployment

- Different hosting environments:
  - UCSD uses Rocks Clusters
  - AIST (Japan) uses OpenNebula
  - …

- How can deploy the Virtual Cluster Image?

pragma_boot:
https://github.com/pragmagrid/pragma_boot

The pragma_boot script

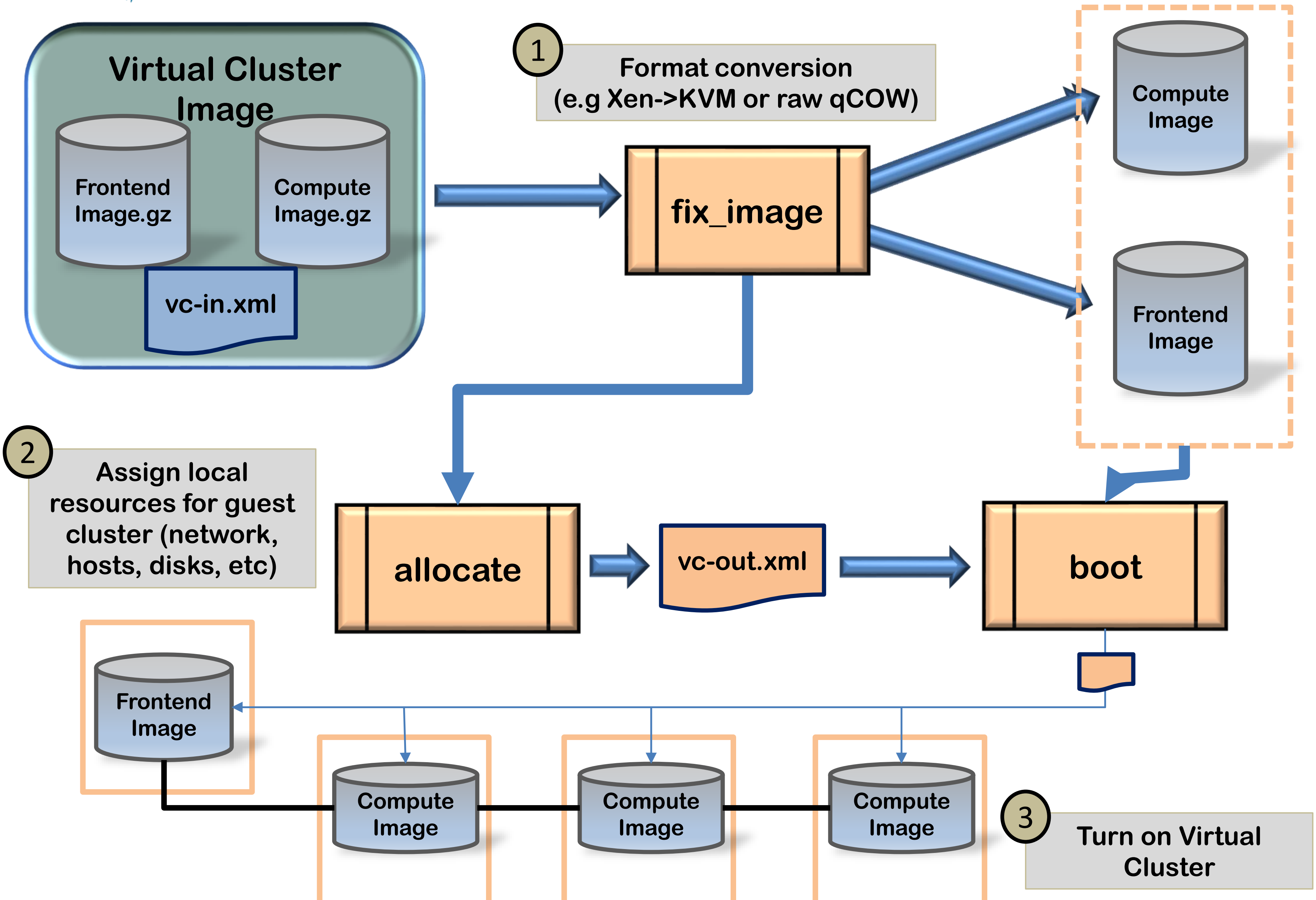
pragma_boot is the main program to instantiate Virtual Machine in Pragma. It accepts the following agruments:

- **--list** list the available images
- **--num_cpus N** the number of compute node to start up (default to 0)
- **--vcname vcname** the name of the virtual clutster to start up (the name must be in the database)
- **--base_path path** the base path of the VM database
- **--key path** The ssh key that will be authorized on the frontned of the cluster (default is /root/.ssh/id_rsa.pub)

pragma_boot ivokes the follwing subscripts which will be invoked in the order described below. In the commands below the ve_dirver will be replaced with the local Virtual Engine (VE) driver (the base path used to find all the VE drivers can be configured in the file site_conf.conf) site_conf.conf should be used also to set the path for the temporary_directory used for staging all VM images

- **ve_driver/fix_images** prepare the given VC images to be run on the current system (fix kernel, drivers, boot options, for current platform, etc.). It's input argumets are (in the following order):
  1. **vc_in_file** the path to the vc-in.xml file of the virtual machine we have to convert
  2. **temp_directory** the temporary directory used to place all the temporary virtual
  3. **node_type** a command separated list of node type to be prepared (e.g. "frontend,compute")
- **ve_driver/allocate** this script takes care of verifying that there are enough resoureces to satisfy the user request, if so it will also allocate public IP, private IPs, MAC addresses, and computing resources. If the system can create SMP nodes it can allocate less compute node with multiple cpus in each node. If successful it will write a /root/vc-out.xml file inside the various virtual machines images (see below for more info)
  1. **num_cpus** it specifies the number of CPU requested by the user.
  2. **vc_in_path** it points to the vc-in.xml of the selected cluster
  3. **vc_out_path** this should point to the path where the frontend vc-out.xml will be saved

Rocks Implementation

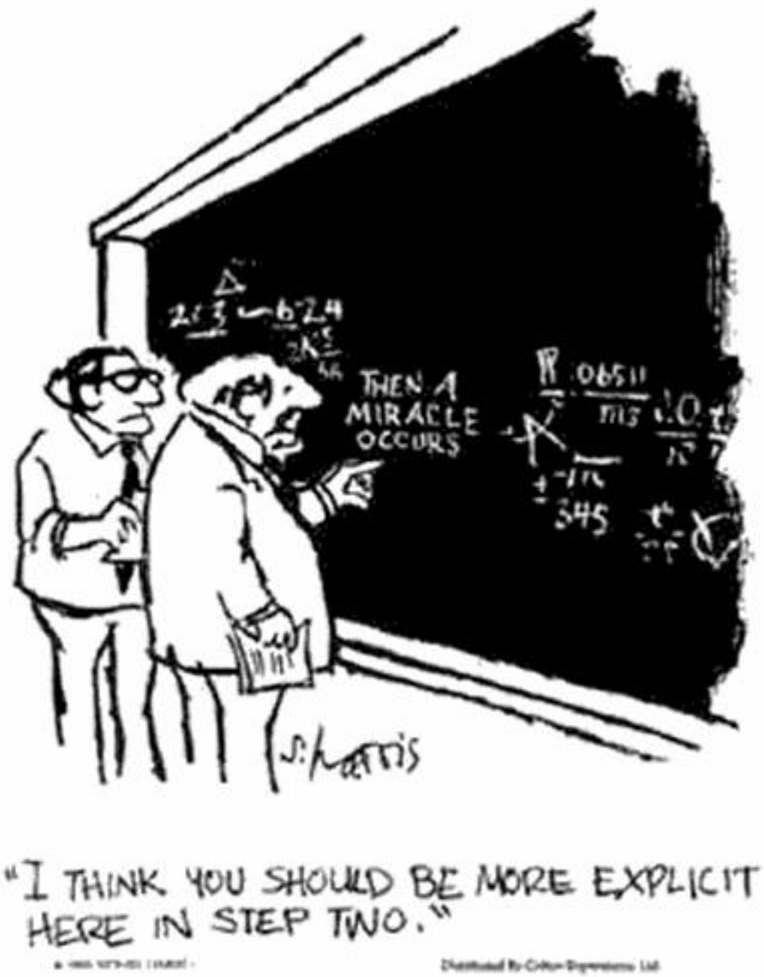


Next logical Step

1. Scientific Software Installed in Virtual Cluster (VC)
2. Can boot boot virtual cluster on a variety of hosting resources (without redefining your VC)
3. How do you get to protected/sensitive/unpublished data?

We Can move VCs between different clouds, can we get controlled access to remote data?

VC + Pragma_boot + Overlay network + Data Source: This is a lot to put together



Is there something we can do to make it simpler for the end-user?

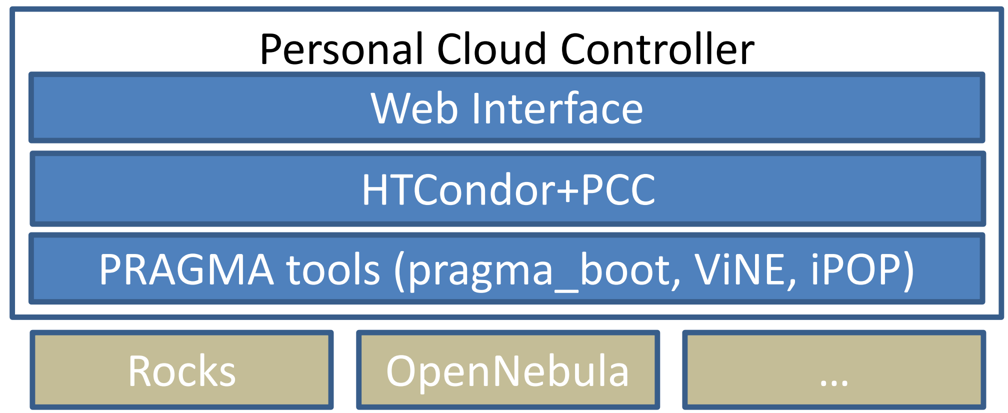
Personal Cloud Controller (PCC)

(Yuan Luo (IU), Shava Smallen (UCSD), Beth Plale (IU), Philip Papadopoulos(UCSD))

- Goals:
  - Enable **lab/group** to easily **manage** application **virtual clusters** on available resources
  - Leverage PRAGMA Cloud tools: pragma_bootstrap, IPOP, ViNE.
  - Lightweight, extends HTCondor from U Wisc.
  - Provide command-line and Web interfaces
- Working Group: Resources

Personal Cloud Controller (PCC) - cont.

- Current status
  - Start and monitor virtual cluster using pragma_bootstrap via HTCondor (VM GAHP)
  - Web interface prototype (PHP)
- Near-term goals
  - Add increased controllability and robustness (April – June)
  - Multi-site clusters (July – Sept)



- Longer-term goals
  - Data-aware scheduling
  - Fault tolerance
  - Provenance

A Prototype Web Interface

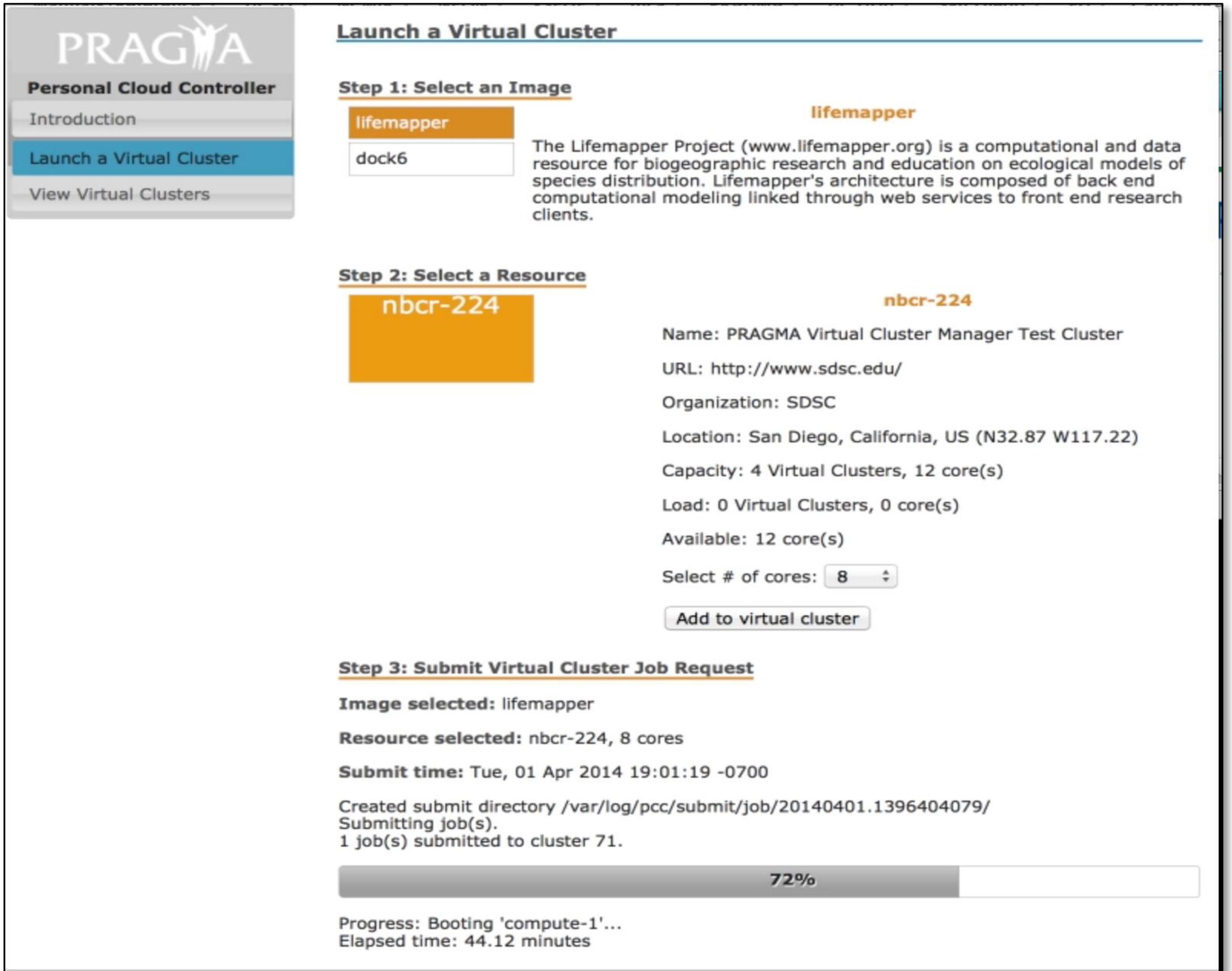
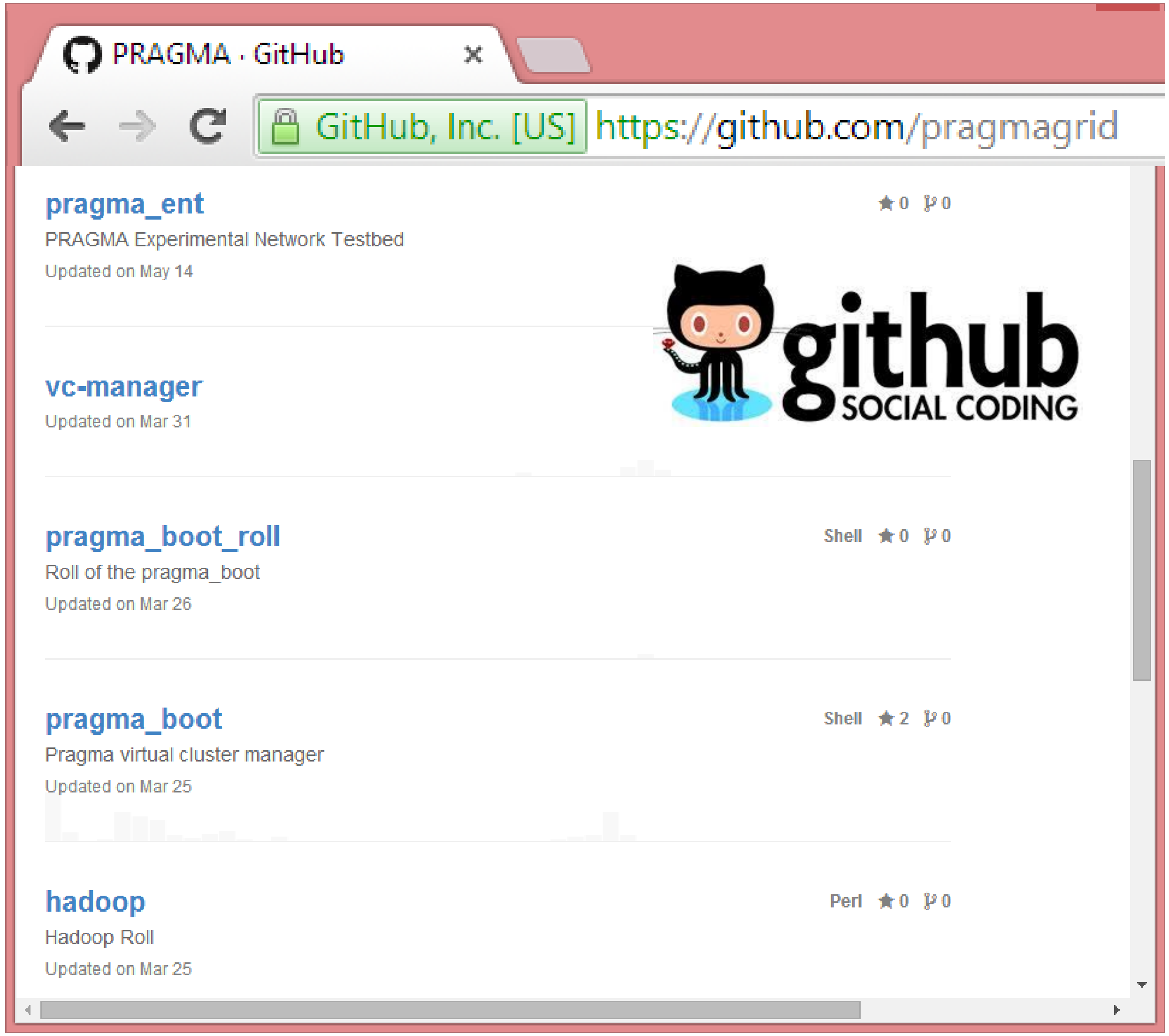


Figure 2: Frontend web interface of PCC showing the launch of a virtual cluster.

Shared Software Development

- Experimental Network Testbed
- Virtual Cluster Migration
- Network Overlays
- LifeMapper in a virtual machine



PRAGMA Works Because of a Culture of Sharing and Trust

- Mutual technology interests – Some shared development.
- Mutual scientific interests
- Bridging the gap between technology capabilities and domain science needs
- Open to experiments in science and technology
- Next Meeting: Bloomington, Indiana Oct 15-17