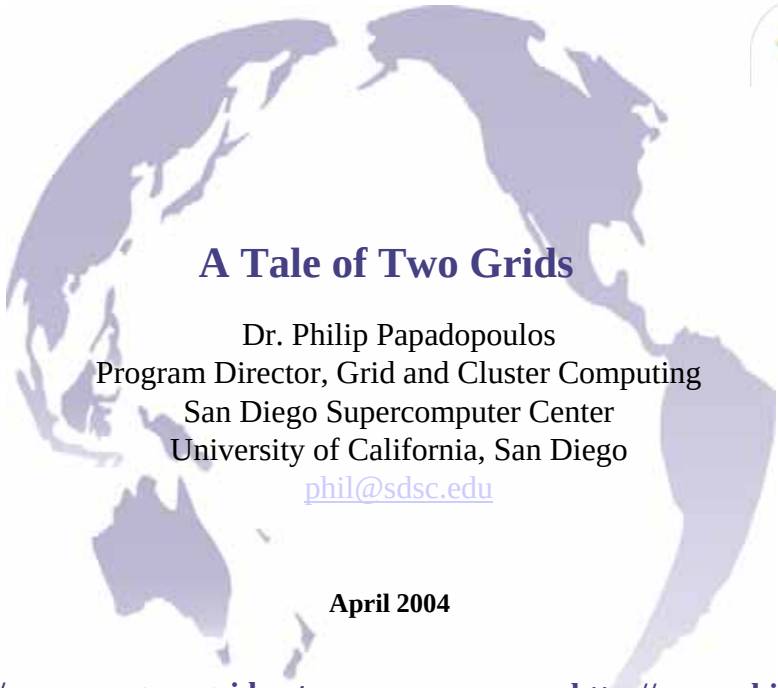


# A Tale of Two Grids

Dr. Philip Papadopoulos
Program Director, Grid and Cluster Computing
San Diego Supercomputer Center
University of California, San Diego
phil@sdsc.edu

**April 2004**

**http://www.pragma-grid.net** **http://www.nbirn.net**

## Two Very Successful Grids

- PRAGMA – Pacific Rim Applications and Grid Middleware Assembly
  - Focused on making grid infrastructure usable by scientists
  - Cooperating administrators
- BIRN – Biomedical Informatics Research Network
  - Focused on neuro-imaging scientists as a test bed
  - Highly prescribed software infrastructure

## Agenda

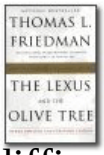
- Overview of PRAGMA
- Overview of BIRN
- High-level comparisons
- What have we learned?

## PRAGMA Founding Motivations

- Science is an intrinsically global activity

***IVOA***

- The grid is transforming computing and collaboration




e-Science Core Programme

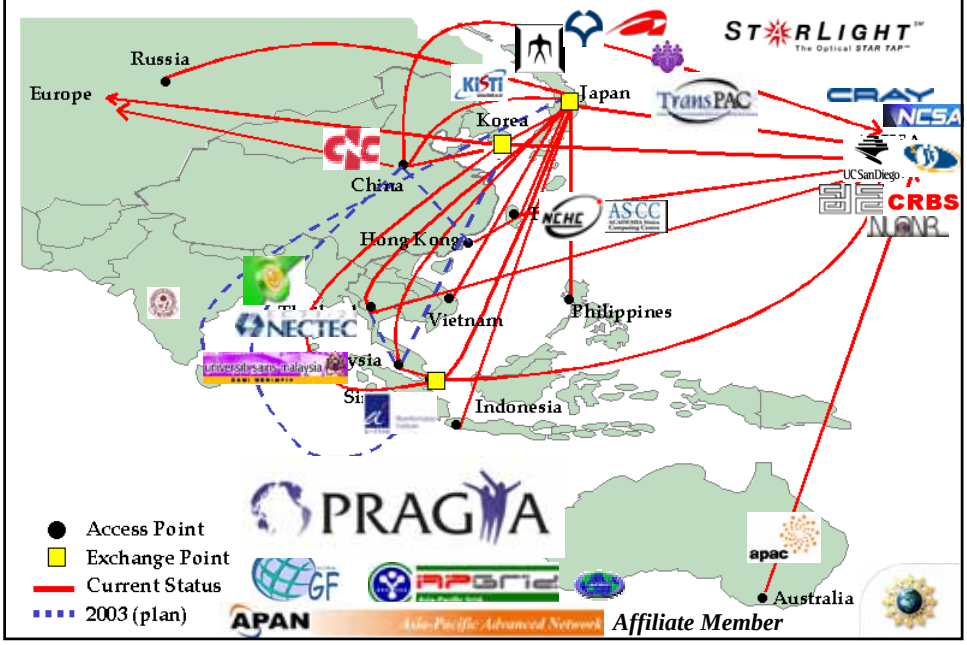
The UK Research Councils

- The grid is too difficult to use

- Middleware software needs to interoperate

NSF MIDDLEWARE INITIATIVE

# PRAGMA PARTNERS




# PRAGMA

## Key Goals

Establish sustained collaborations

and

Advance the use of the grid technologies for applications

among a community of investigators working with leading institutions around the Pacific Rim

Working closely with established activities that promote grid activities or the underlying infrastructure, both in the Pacific Rim and globally.

PACIFIC RIM APPLICATIONS AND GRID MIDDLEWARE ASSEMBLY

## Series of Meetings

- **PRAGMA 4: 4-5 June 2003, Melbourne, Australia**
  - **ICCS2003: 3-4 June**
  - **David Abramson (APAC): Chair; Co-chair: Fang-Pang Lin (NCHC)**

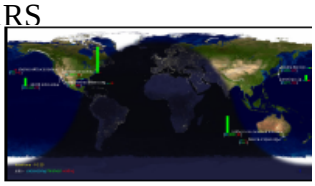
- **PRAGMA 5: 22-23 October 2003, Hsinchu/Fushan, Taiwan**
  - **Fang-Pang Lin (NCHC): Chair; Co-chair: Kai Nan (CNI**

- **PRAGMA 6: 16 – 18 May 2004, Beijing, China**
  - **Baoping Yan (CNIC): Chair; Co-chairs: Mason Katz (UCSD), Jim Williams (TransPAC)**

- **PRAGMA 7: 15-17 September 2004, San Diego, USA**
  - **Chairs: Mason Katz (UCSD), Jim Williams (TransPAC)**

## PRAGMA Success Stories

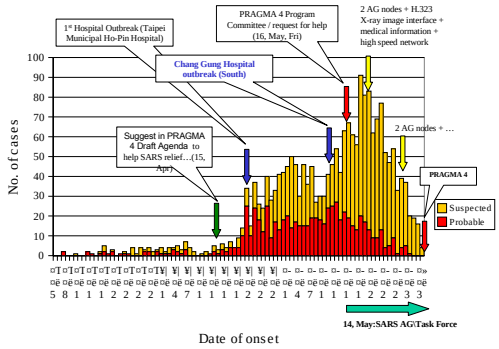
- Grid Community Pulls together to Battle SARS



- Merging Grid Technology and Computational Chemistry
- Telescience Marshals Rich Network of Technologies at iGRID2002

- Grid Demo Sets US to Japan Data Speed Records
- EcoGrids
- Encyclopedia of Life

## NCHC SARS Task Force




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

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

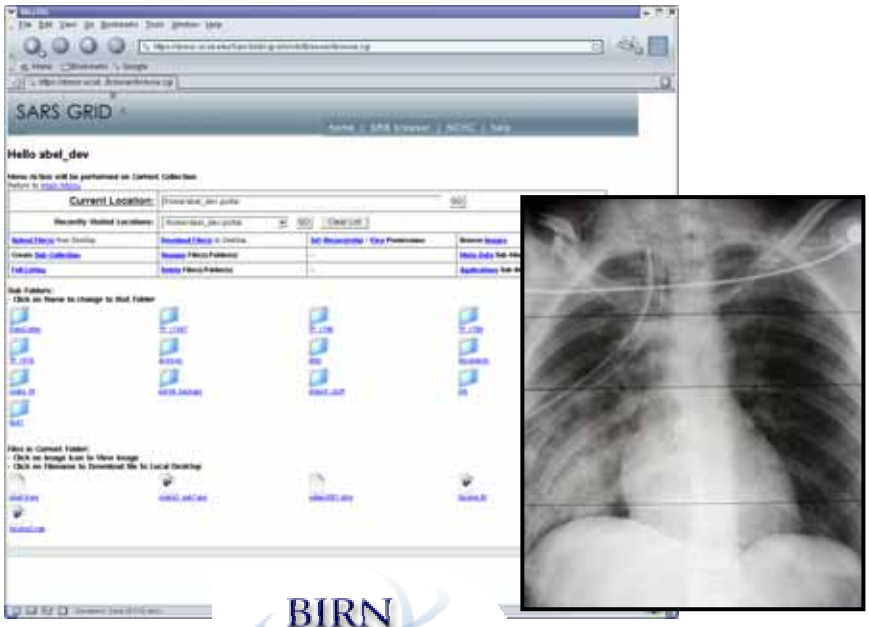
***Source: Fang-Pang Lin***

## Using Grids to Battle SARS


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

***Source: Fang-Pang Lin***

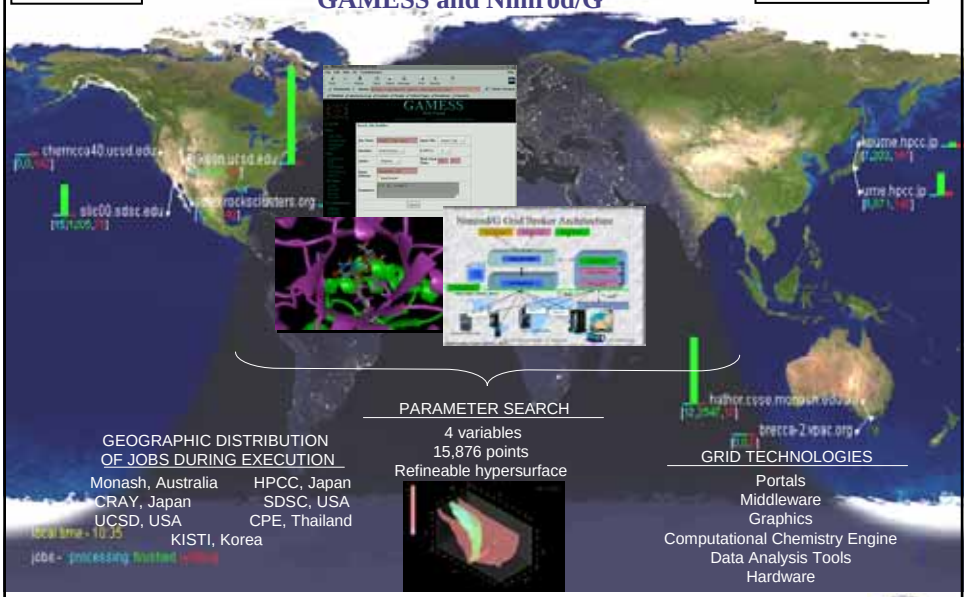
## Telescience/BIRN Portal was Quickly Adapted to a SARS Portal for Taiwan




## ENABLING NEW SCIENCE
### GAMESS and Nimrod/G

ICCS'03

PRAGMA 4




PARAMETER SEARCH
4 variables
15,876 points
Refineable hypersurface

GEOGRAPHIC DISTRIBUTION OF JOBS DURING EXECUTION
Monash, Australia
CRAY, Japan
UCSD, USA
KISTI, Korea
HPCC, Japan
SDSC, USA
CPE, Thailand

GRID TECHNOLOGIES
Portals
Middleware
Graphics
Computational Chemistry Engine
Data Analysis Tools
Hardware

Exploiting grid technology & hybrid computational methods

***Source: Wibke Sudholt, Kim Baldridge, David Abramson, Colin Enticott, Slavisa Garic***

# PRAGMA Telescience at iGRID 2002


Demonstrate advanced features of the Telescience Portal:

1. Perform Telemicroscopy controlling the IVEM at NCMIR
   - Digital Video is encapsulated in IPv6 and transmitted at 30fps over native IPv6 networks (SDSC, Abeline, SURFnet) between San Diego and Amsterdam
2. Data will be computed with heterogeneous, distributed resources within NCMIR, NPACI, NCHC and Osaka University
3. Render and visualize data in Amsterdam using distributed resources in NCHC

***Courtesy: Abel Lin, Steve Peltier, Mark Ellisman, Shinji Shimojo, Toyokazu Akiyama, Fang-Pang Lin***

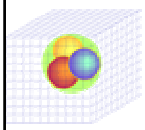
## File replication performance between Japan and US (total)

GRID DATA FARM

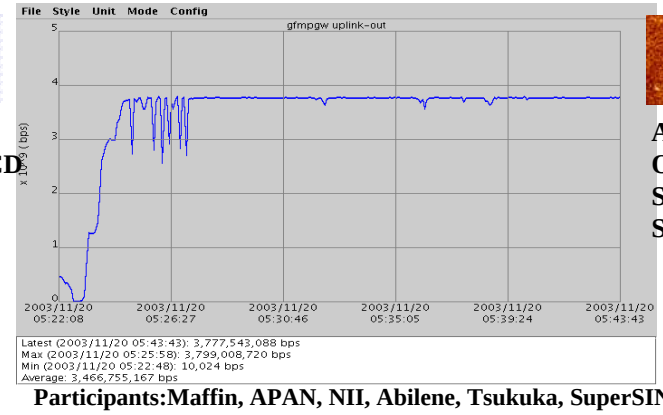
**Stable transfer rate of 3.79Gbps**

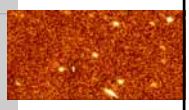
**out of theoretical peak 3.9 Gbps (97%)**

using 11 node pairs (MTU 6000B) **1.5TB data was transferred in an hour**



**Lattice QCD [CCP, U Tsukuba]**



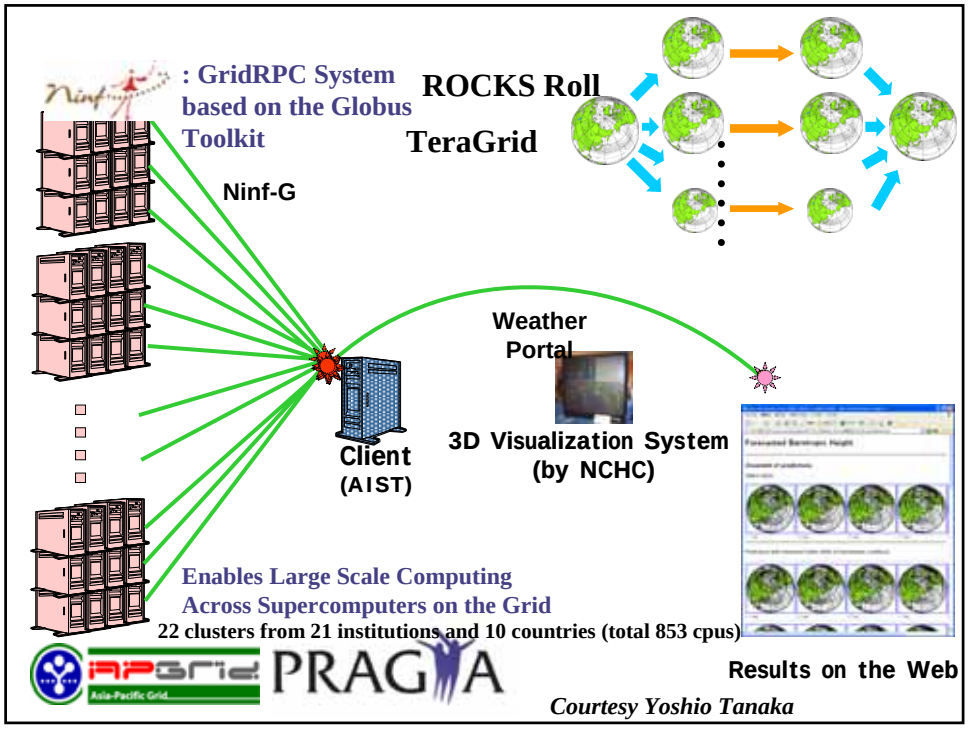
**Astronomical Object Survey Subaru Tele-Scope** [AIST]

**Participants:Maffin, APAN, NII, Abilene, Tsukuka, SuperSINET, Force10 Networks, PRAGMA, APGrid, SDSC, TransPAC/Indiana U, Kasetsart U**

***Source: Osamu Tatebe***

AIST

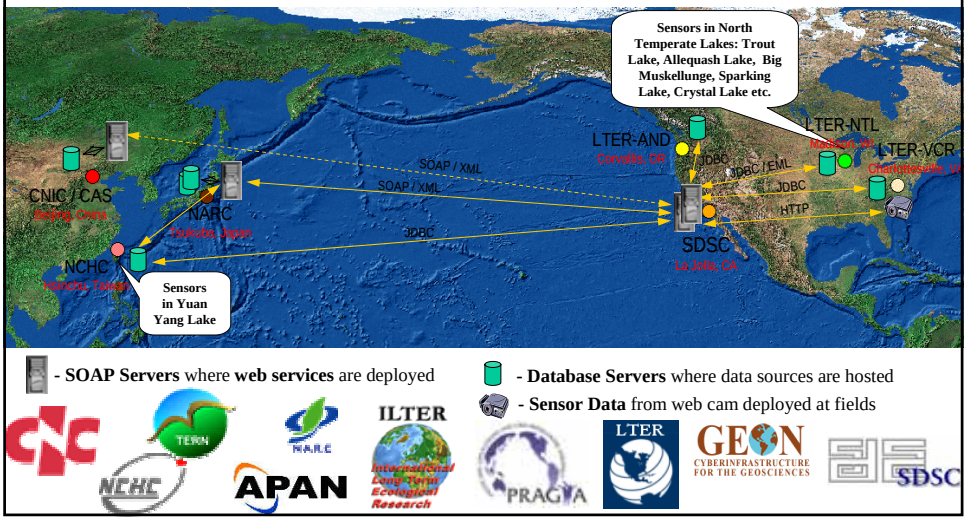
National Institute of Advanced Industrial Science and Technology


: GridRPC System based on the Globus Toolkit
ROCKS Roll
TeraGrid
Ninf-G
Weather Portal
3D Visualization System (by NCHC)
Client (AIST)
Enables Large Scale Computing Across Supercomputers on the Grid
22 clusters from 21 institutions and 10 countries (total 853 cpus)
Results on the Web
PRAGMA
Courtesy Yoshio Tanaka


EcoGrid: Fushan
United Daily 2003 March 09
Liberty Time 2003 March 09
Research Sites
Scenario for Ecogrid
NCHC
TERN
Wireless

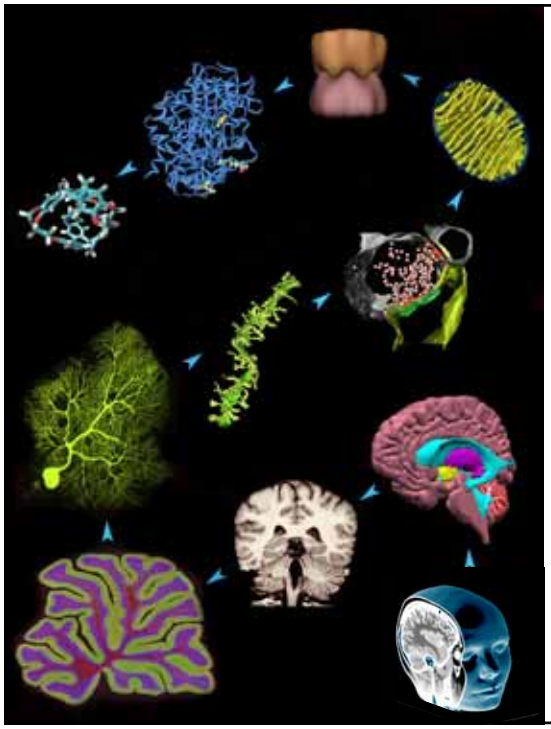
# I2G Web Services Infrastructure and Sensor-based Lake Monitoring and Analysis

Understanding Impacts of Episodic Events in Lake Metabolism




# PRAGMA Testbed Details
# Resources/Middleware Working Group

- **Bottom-up approach on hardware**
  - Most systems are linux-based, but other types are available
  - More than 240 nodes across 15 (or more) sites
  - Work with APGrid (http://www.apgrid.org)
- **Agreement to Participate:**
  - Minimum software requirement to join (e.g. Globus 2.2)
  - Need to exchange certificates with all other sites
- **Technical and Policy Issues**
  - Compatibility of basic middleware (versions of Globus)
  - What other software to have at all sites
    - Using Software that others have developed
    - Eg. PRAGMA Cluster at SDSC Runs Rocks (SDSC) and SCE (Thailand)
- **Challenges**
  - Run applications on grid on routine basis (only a few at first)
  - Capture rough measure of usage (international resource)
  - What does it mean to dedicate a resource to an international group (with national funding supporting the resource)?



## BIRN is Team Science Applied to Stretch Goals

***A Big Challenge or Vision:***

**"Enable new understanding of the healthy and diseased brain by linking data about macroscopic brain function to its molecular and cellular underpinnings"**

***Taking practical steps toward a grand goal using cyberinfrastructure:***

- **Federate geographically distributed brain data of the same & different types**
- **Accommodate requirements to collaboratively interact with shared databases of large-scale data, share methods, and computational resources**

## BIRN Network


**IT Infrastructure to hasten the derivation of new understanding and treatment of disease through use of distributed knowledge**

## BIRN Today is …

- Three neuroscience test beds building on research projects:
  - Mouse BIRN- Morph BIRN
  - Functional BIRN - BIRN Coordinating Center
- Integrating the activities of the advanced biomedical imaging and clinical research centers in the US.
- Developing hardware and software infrastructure for managing distributed data: creation of data grids.
- Exploring data using “intelligent” query engines that can make inferences upon locating “interesting” data.
- Building bridges across tools and data formats.
- Changing the use pattern for research data from the individual laboratory/project to shared use

## BIRN Project Coordination

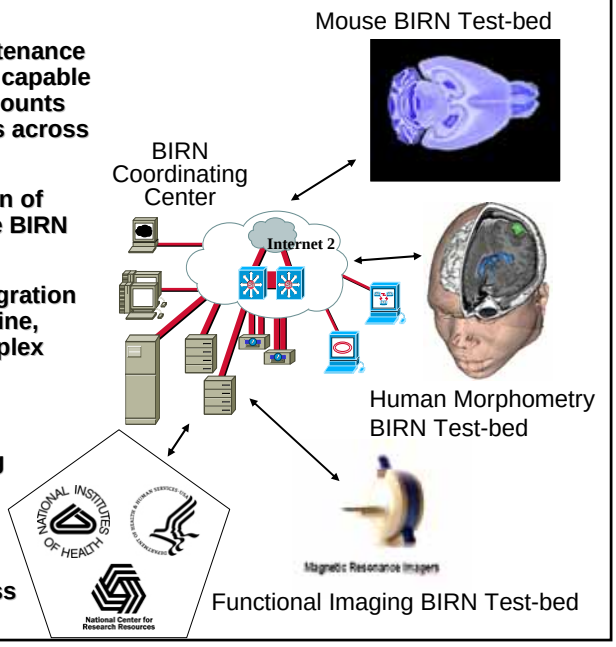
**The BIRN-CC leads…**

**• the deployment and maintenance of a network infrastructure capable of quickly moving large amounts of data between BIRN sites across the country.**

**• the creation of a federation of databases pertaining to the BIRN scientific projects.**

**• the development and integration of software to refine, combine, compare, and analyze complex biomedical data.**

**• and cultivates group activities to overcome cultural barriers to building a forum for collaborative research, co-authoring research papers, and sharing methods/tools/codes across institutions.**



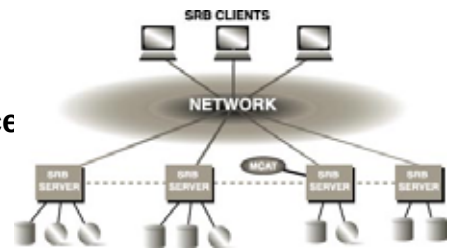
## Each BIRN Site Has Standard Hardware

- Controlled Software and Hardware configuration
- Software managed from the BIRN Coordinating Center
- OS and BIRN tool integration enabled by Rocks Cluster management
- Software Stack Components
  - Globus
  - Storage Resource Broker
  - Test bed application tools
  - Portal Technologies
  - Oracle Database
  - Data Mediation SW

## BIRN Forms a Virtual Data Grid

- **Defines a Distributed Data Handling System**
- **Integrates Storage Resources in the BIRN network**
- **Integrates Access to Data, to Computational and Visualization Resources**

- **Acts as a Virtual Platform for Knowledge-based Data Integration Activities**
- **Provides a Uniform Interface to Users**



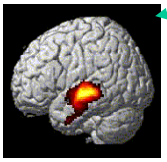
## Function BIRN: Integrated Data Query

**Are chronic, but not first-onset patients, associated with superior temporal gyrus dysfunction (MMN)?**

**Integrated View**

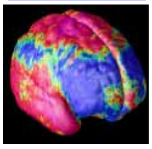
**Mediator**

Wrapper



**fMRI**

Wrapper

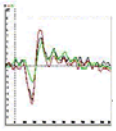


**Structure**

Wrapper

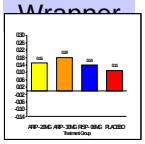
**Receptor Density**

Wrapper



**ERP**

Wrapper



**Clinical**

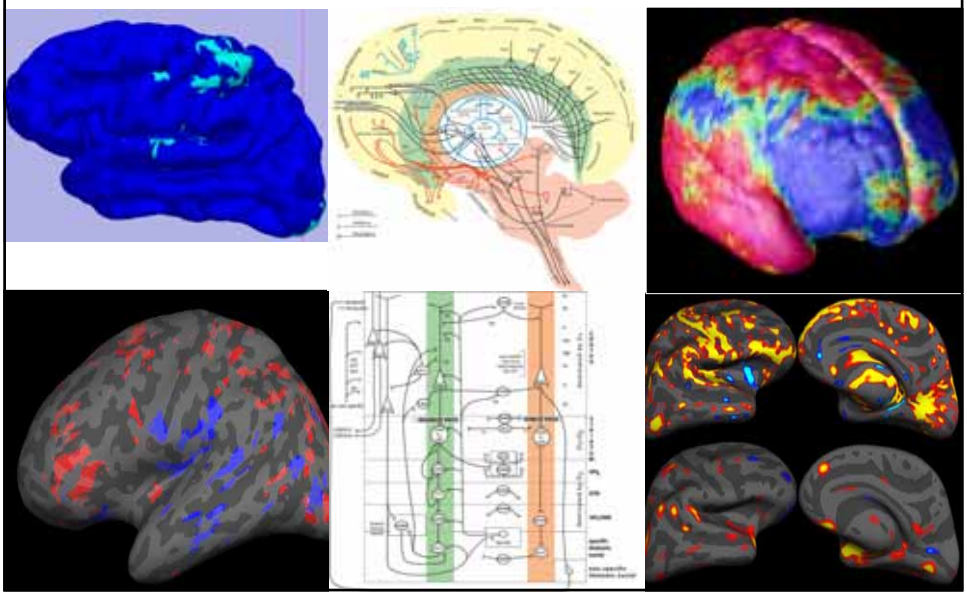
Wrapper

**Web**

**PubMed, Expasy**

## Function BIRN: Federated Imaging Databases

**Calibration, Integration from ½ dozen sites**



## Morphometry BIRN

- Overall Goal:

  Develop capability to analyze and mine data acquired at multiple sites using processing and visualization tools developed at multiple sites
- Context:

  – Human Brain MR Based Morphometry
- Initial Application:

  –Alzheimer's, Depression, Aging Brain
- Participants:

  –BWH, MGH, Duke, UC Los Angeles, UC San Diego, Johns Hopkins, UC Irvine, Washington University

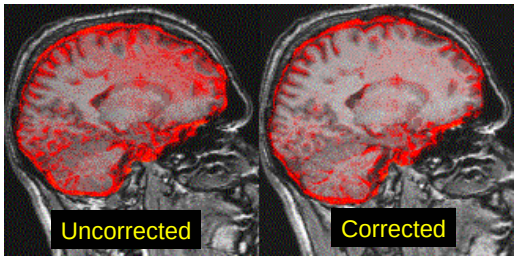
## Morphometry BIRN: **Solving Issues in Distributed Data Acquisition**

Multi-site Structural MRI Data Acquisition & Calibration

**Accomplishment:** develop acquisition & calibration protocols that improve reproducibility, within- and across-sites

**Methods:** common acquisition protocol, distortion correction, evaluation by scanning human phantoms multiple times at all sites

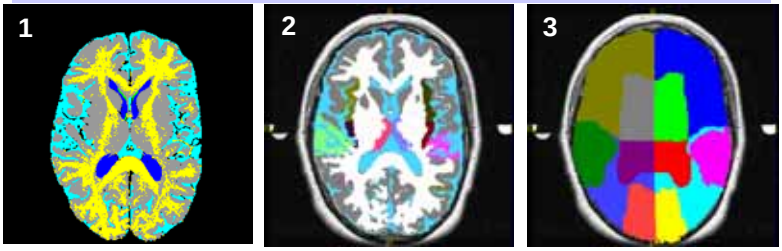
- GH (NMR): J. Jovicich, A. Dale, D. Greve, E. Haley
- WH (SPL): S. Pieper
- CI: D. Keator
- CSD (fMRI): G. Brown
- uke University (NIRL): J. MacFall



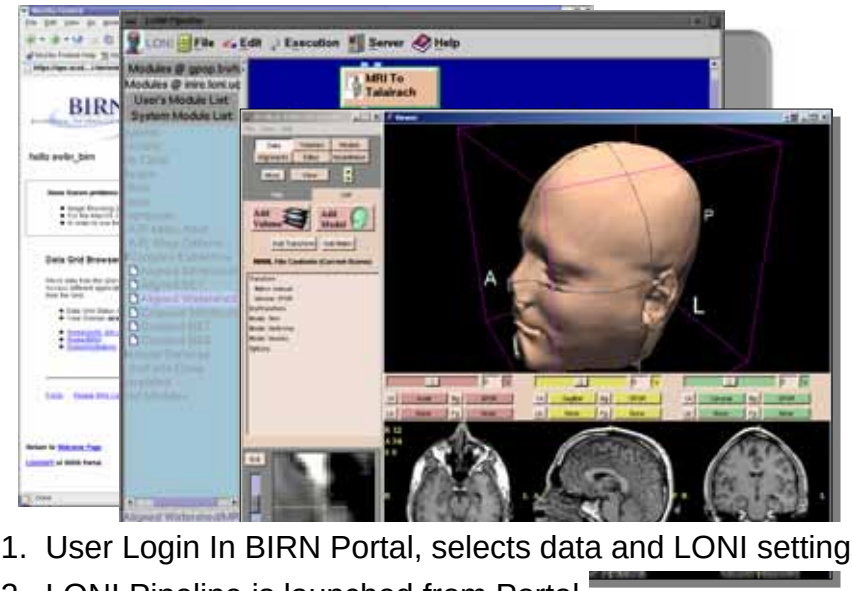
## MIRIAD Project: Improving throughput

### Improved computational capabilities

| Segmentation Item | Duke (semi-automated) | BIRN-MIRIAD (fully-automated) |
|---|---|---|
| # of tissue classes | 3 (Fig1) | 23 (Fig2) |
| Time for 200 brains | 400 hours | 1 hour |
| Time for 200 lobe & | 250 hours | all lobes (Fig3) and 27 regional analysis regions included above |

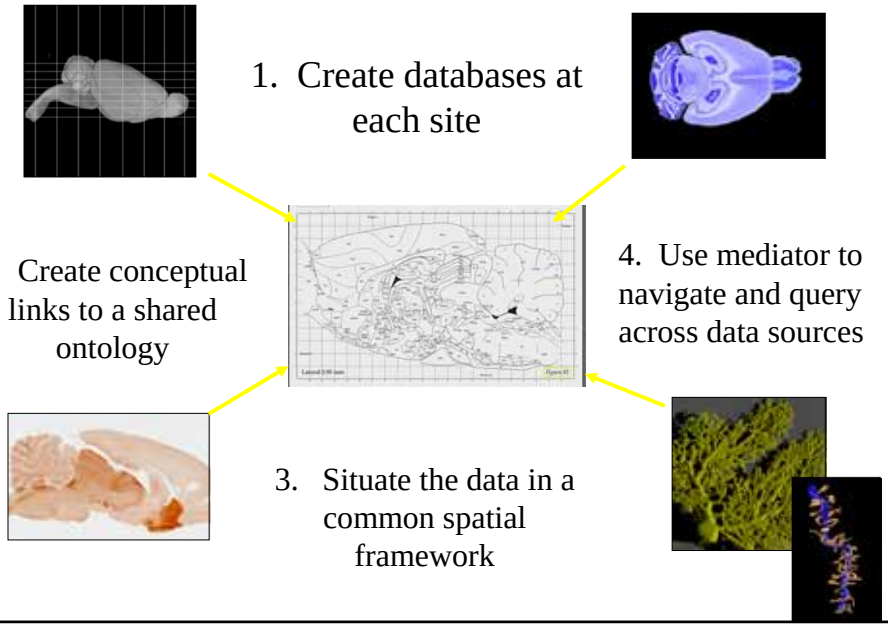



## BIRN Portal: Launches Scientific Workflow




1. User Login In BIRN Portal, selects data and LONI settings
2. LONI Pipeline is launched from Portal
3. Results are automatically displayed in Slicer 3D

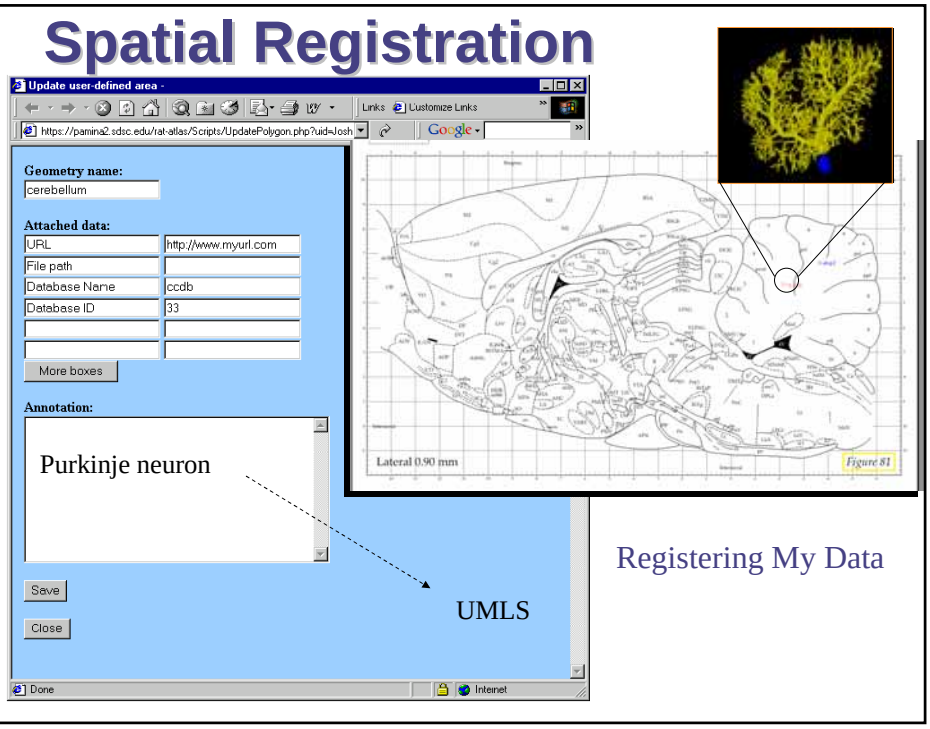
## Mouse BIRN: Multiscale Data Mediation




## Accomplishments of Mouse BIRN

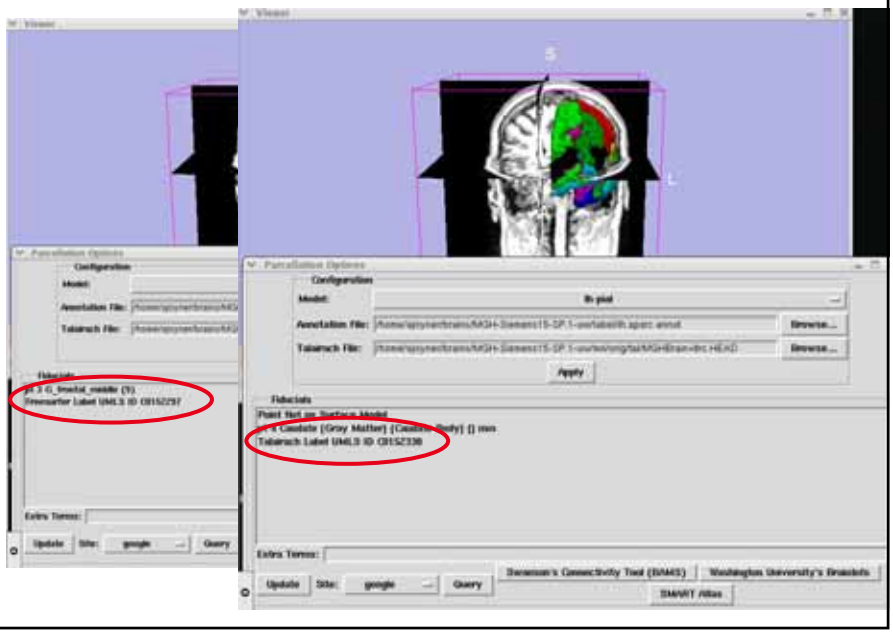
1) Established a data sharing infrastructure using the BIRN for multiscale investigations of animal models of human neurological disease
   - Shared file collections using the Storage Resource Broker
   - Developed common specimen preparation protocols
   - Developed a set of shared analysis and visualization tools working through the BIRN portal
2) Developed a database federation as a data sharing mechanism and a persistent data archive
   - Established independent databases at each site and populated them with mouse imaging data
   - Mapped data to shared knowledge sources like the UMLS and atlas coordinate systems
   - Created a virtual data federation through semantic and spatial mediation tools

# Spatial Registration




Registering My Data

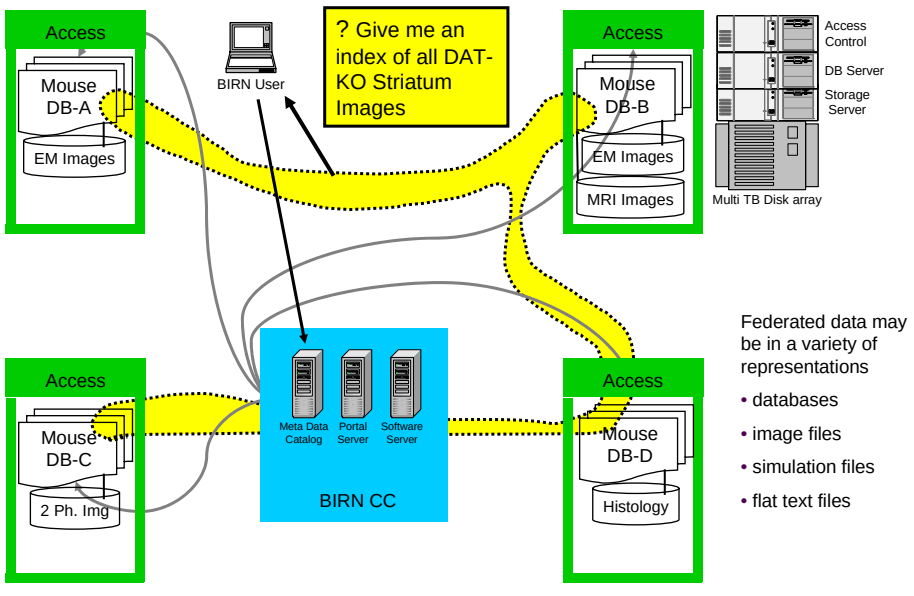
# Human-Mouse Data Integration



## Key Systems Challenges

- Large-scale data is distributed on a National Scale
  - How do you easily locate what you want?
  - How do you translate it to what your SW tools understand?
  - Where do you analyze it?
  - How do you move it efficiently?
  - How do you secure it to properly limit and log access?
- The underlying software systems are complex
  - How effectively can this complexity be hidden?
    - Software technology continually evolves and BIRN must adapt
- Goal: provide a systems "cookie-cutter" for adding new, secured, resources to form a federation

## A View on BIRN Federated Data



http://www.nbirn.net


## High-Level Comparisons

| BIRN | PRAGMA |
|---|---|
| 3 well-defined biomedical testbeds | A variety of scientific discplines |
| Integration across scales and federation of data | How to make the grid work |
| Security of information is a key driver | How to share resources and software across the PacRim |
| Well-controlled hardware and software environment | Agreed-upon minimal software at each site |
| Dedicated Resources | Some dedicated, most shared |

## Key Software Systems Being Deployed

**BIRN**

- Rocks Cluster Mgmt
- BIRN Certificate Authority
- Globus
- Storage Resource Broker
- Oracle
- Data Mediator
- ½ dozen specific applications
- Netscout Monitoring
- BIRN Portal

**PRAGMA**

- Globus
- Accept Certs from Many Authorities

- Rocks
- SCE
- Ninf-G
- gFarm
- NIMROD
- ½ dozen specific applications
- SARS portal
- Telescience Portal

## What have we learned

- Top-down (BIRN) and Bottom-up (PRAGMA) can both work
  - These work because of committed collaborators
  - Application drivers are critical to keeping focus
- Both grids deployed and used the infrastructure even when all SW was not available.
  - Hands on experience has taught us a great deal
  - A large fraction of grid software is still “fragile”
- Software packaging and availability is critical to making things practical
- Integration of networked resources and people have enabled new ways of doing research