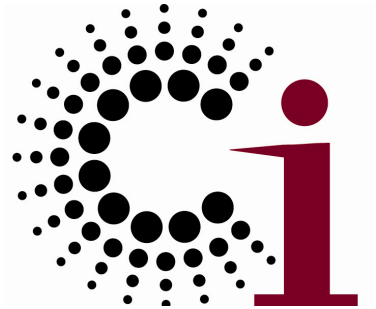
Grid
Enabling Open Science

Ian Foster



Computation Institute

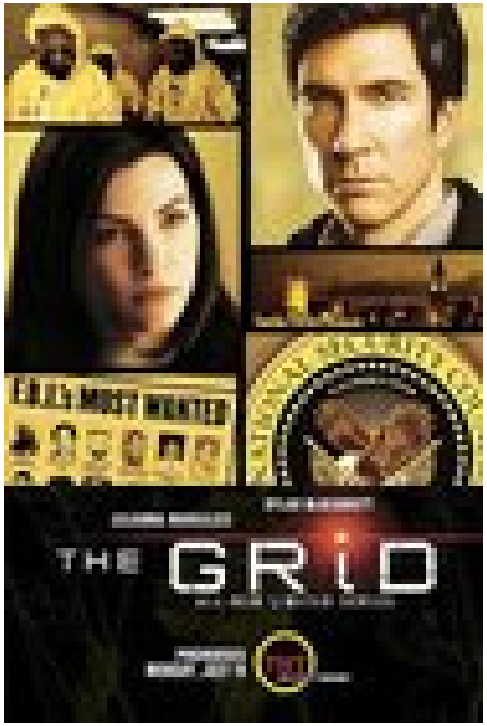
Argonne National Lab & University of Chicago

Abstract

Rapid advances in both science and information technology are driving the emergence of "eScience.” Grid technologies play a crucial role in eScience by enabling resource and service federation across organizational boundaries, supporting on-demand access to computing resources, and allowing the formation and operation of distributed, multi-organizational collaborations. eScience and Grid also require new tools, infrastructure, and policies. I will discuss opportunities, achievements, and challenges in these related areas.

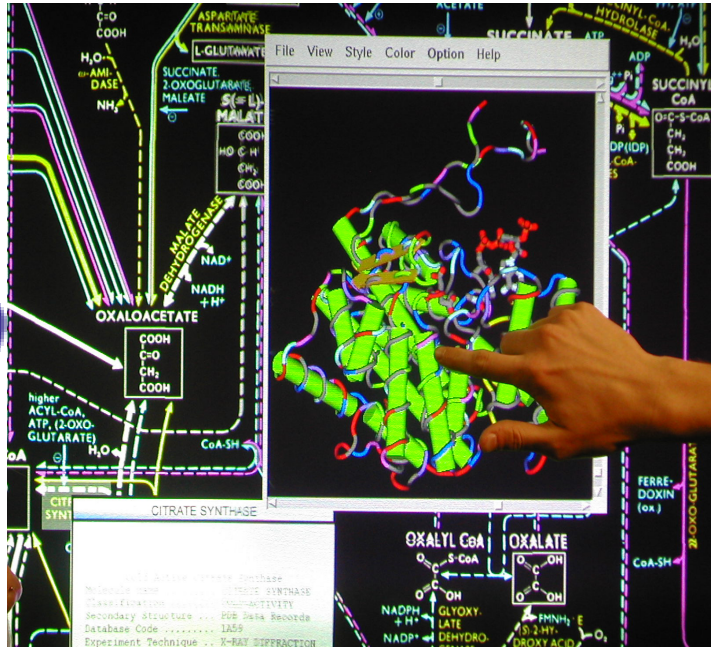
What is the Grid?

"**The Grid** is an international project that looks in detail at a terrorist cell operating on a global level and a team of American and British counter-terrorists who are tasked to stop it"

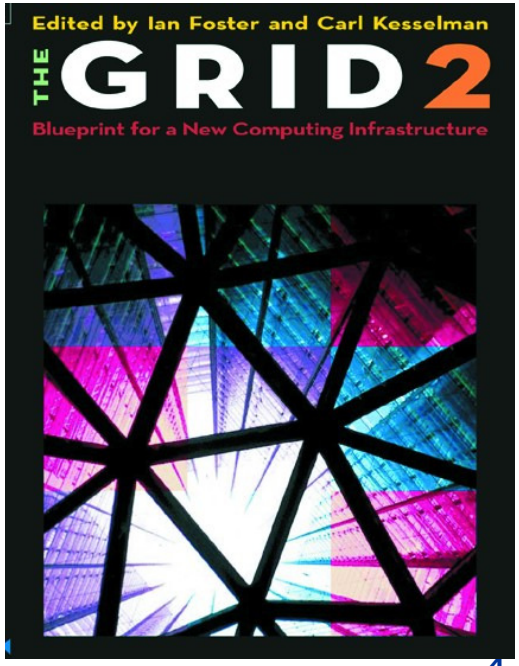


Gareth Neame, BBC's head of drama

Well, Not Exactly!

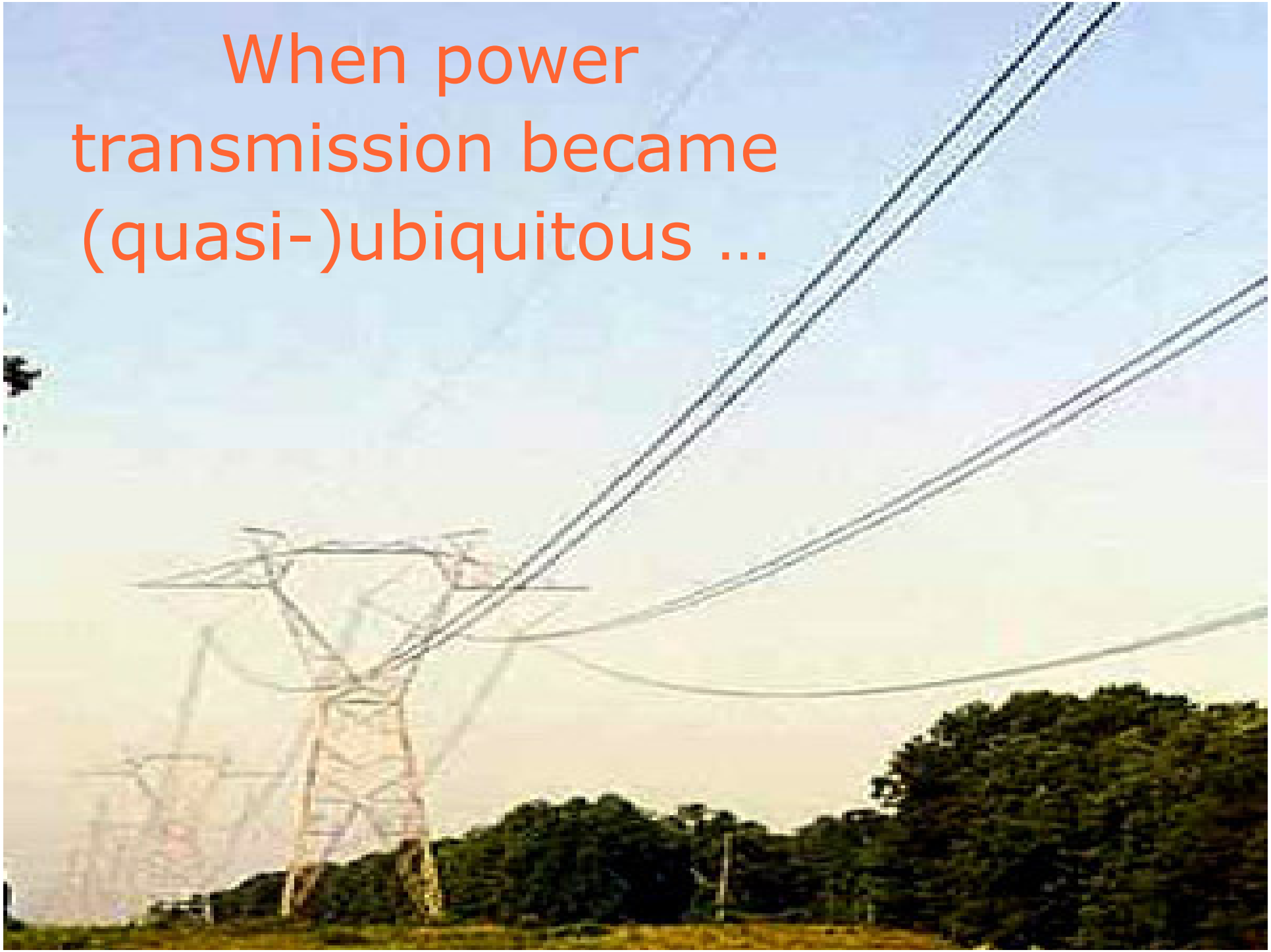


"**The Grid** is an international project that looks in detail at scientific collaborations operating on a global level and a team of computer scientists who are tasked to enable it"

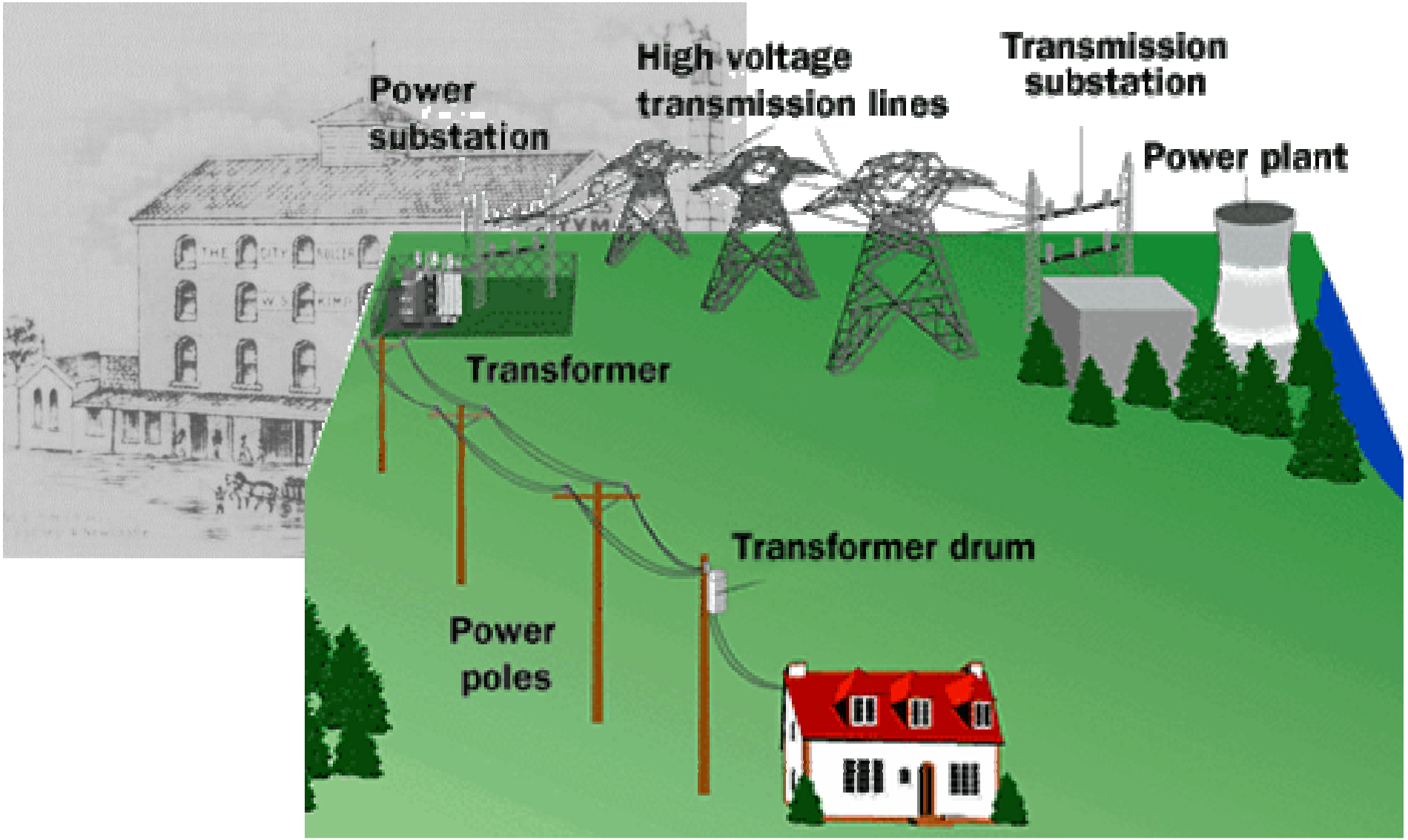


At least, that's where it started …

When power transmission became (quasi-)ubiquitous …

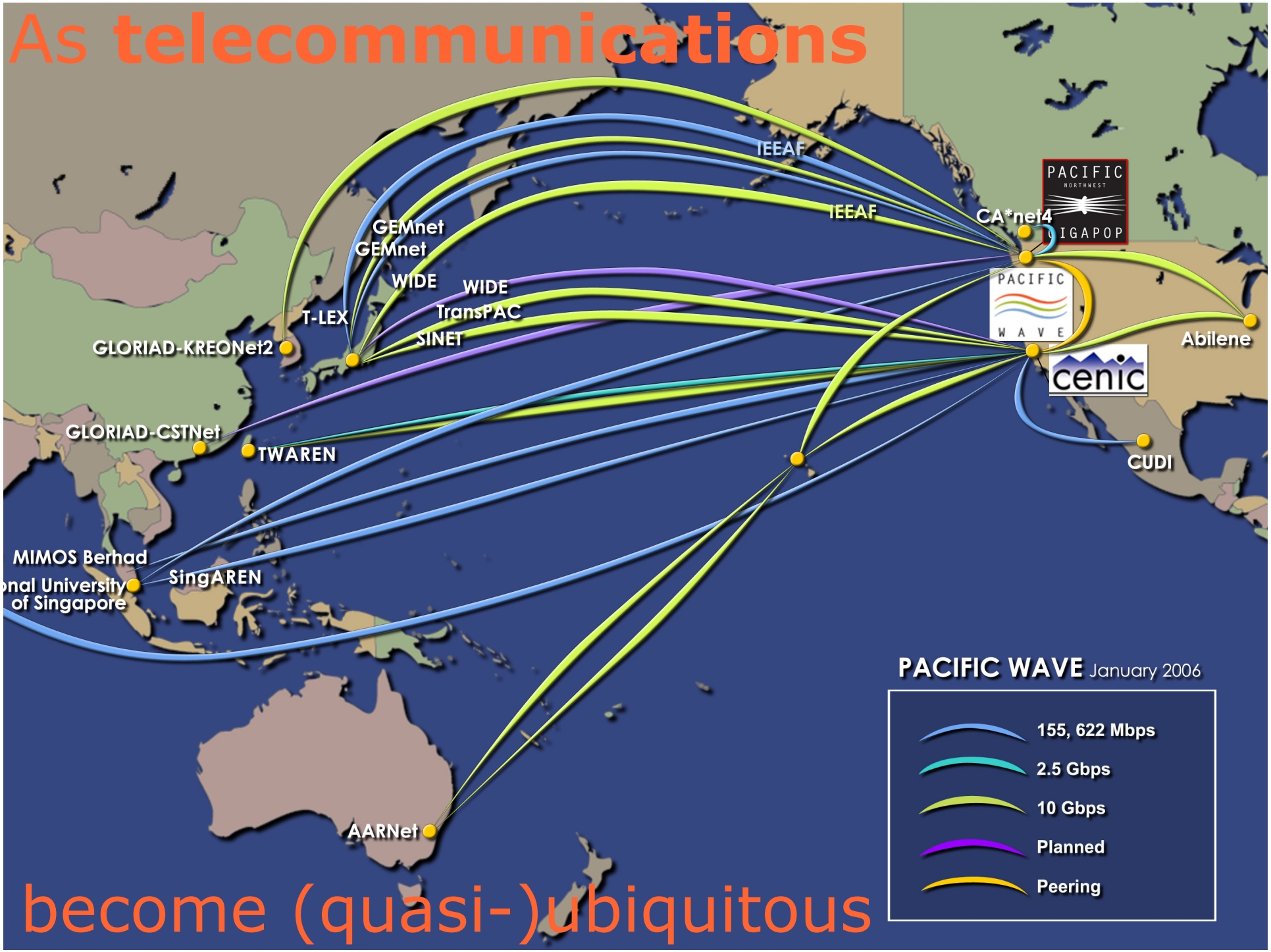


We No Longer Had to Travel to Power Plants



We Invented New Tools

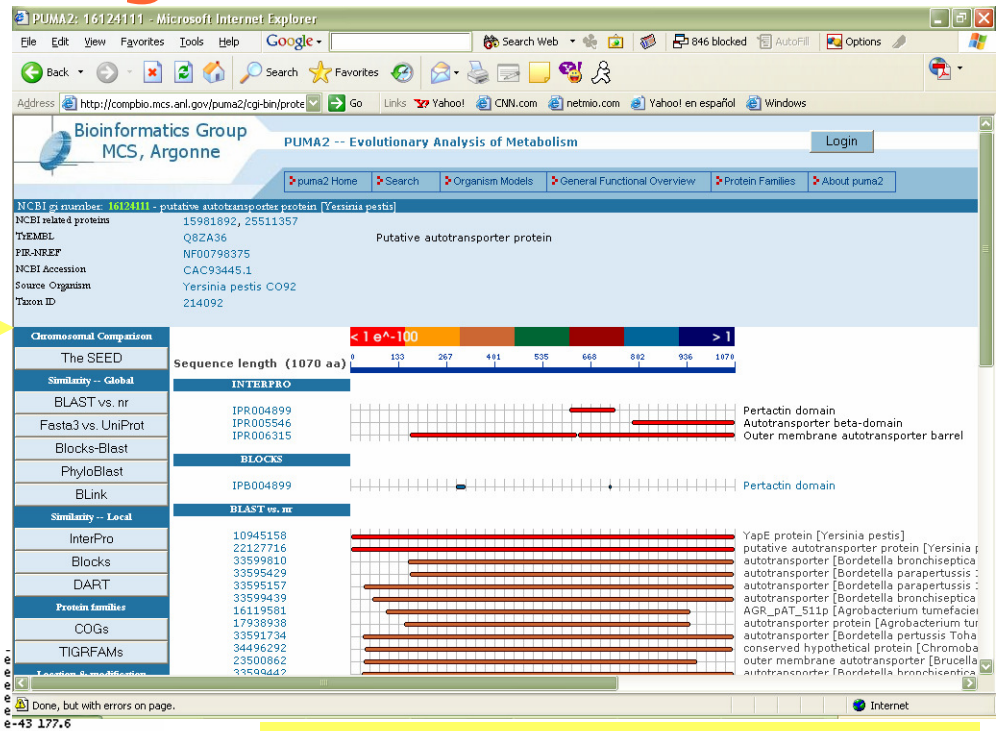
We Worked in New Ways

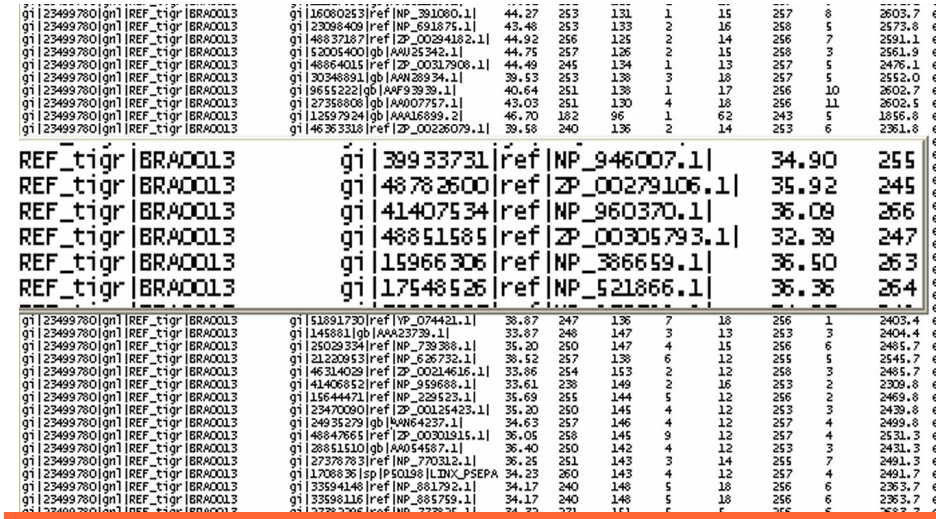

As telecommunications
become (quasi-)ubiquitous
IEEAF
IEEAF
GEMnet
GEMnet
WIDE
WIDE
TransPAC
SINET
T-LEX
GLORIAD-KREONet2
GLORIAD-CSTNet
TWAREN
MIMOS Berhad
SingAREN
of Singapore
AARNet
CA*net4
PACIFIC
NORTHWEST
GIGAPOP
PACIFIC
WAVE
cenic
Abilene
CUDI
PACIFIC WAVE January 2006
155, 622 Mbps
2.5 Gbps
10 Gbps
Planned
Peering

We Can Access Computing on Demand

Public PUMA Knowledge Base

Information about proteins analyzed against ~2 million gene sequences





Back Office Analysis on Grid

Millions of BLAST, BLOCKS, etc., on OSG and TeraGrid

Natalia Maltsev et al., http://compbio.mcs.anl.gov/puma2

We Can Invent New Tools

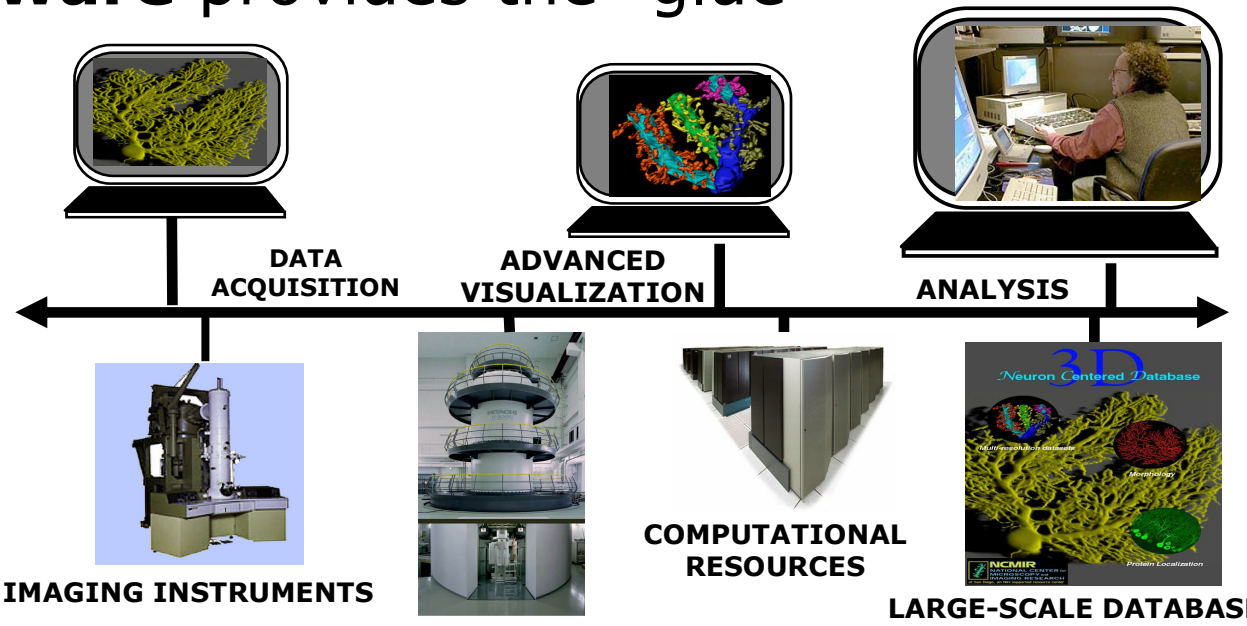
Bennett Berthenthal et al., www.sidgrid.org

We Can Work in New Ways: Access Grid and SARS

Grid:
Unifying Concept & Technology

Enable **on-demand access** to, and **federation** of, diverse resources

- Computers, storage, data, people, …
- Resources can be distributed, heterogeneous
- **Networks & protocols** provide the connectivity
- **Software** provides the "glue"

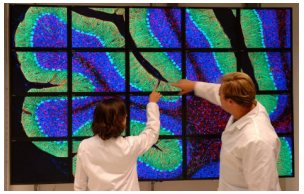


Technology, Infrastructure, & Standards

interoperability

integration

Applications



User-level Middleware and Tools

Ninf

System-level Common Infrastructure

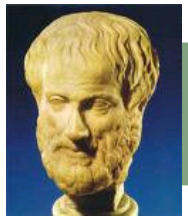
the globus toolkit
www.globustoolkit.org

Resources

TeraGrid
EMPOWERING DISCOVERY

For example

Emergence of New Problem Solving Methodologies

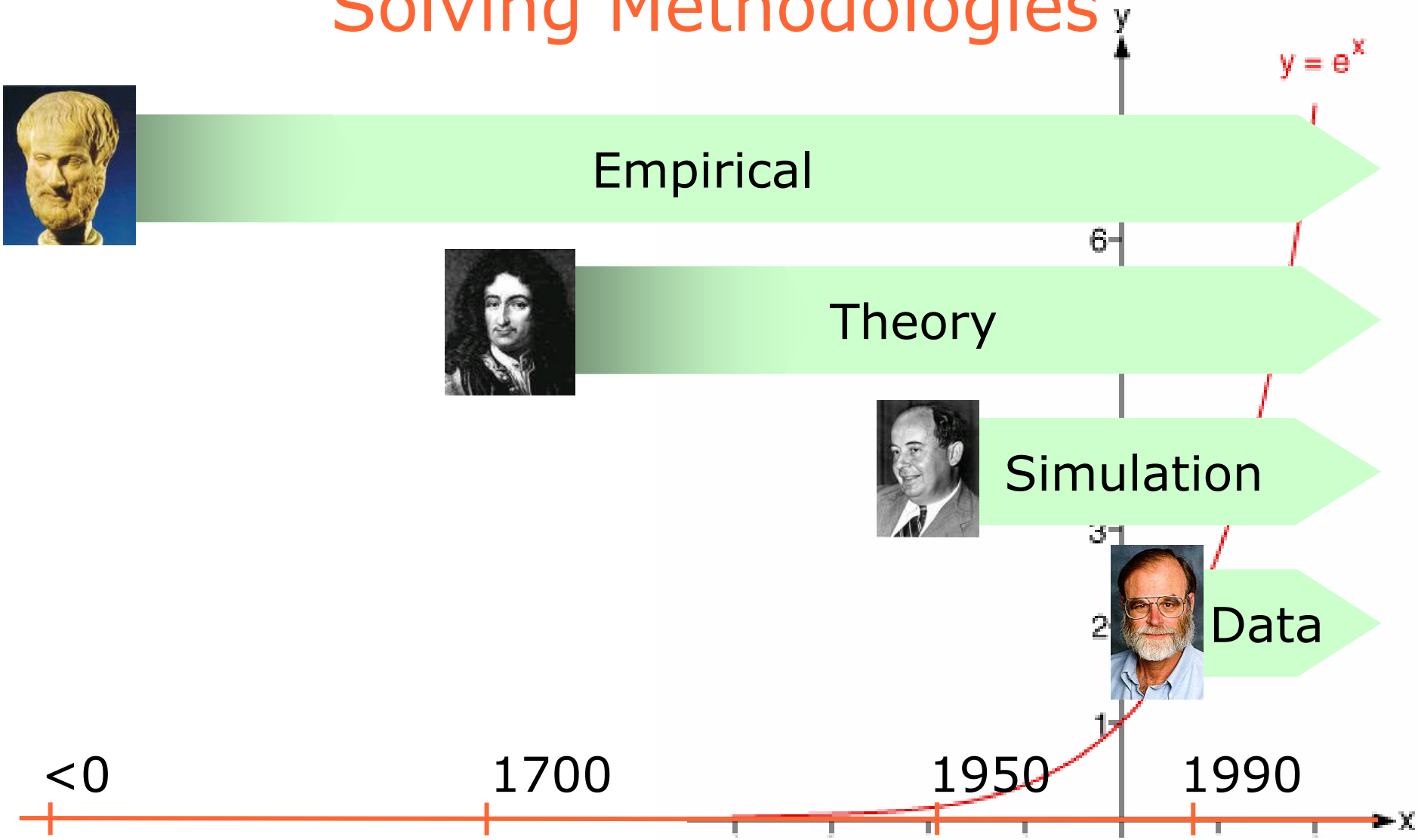


Empirical

Theory

Simulation

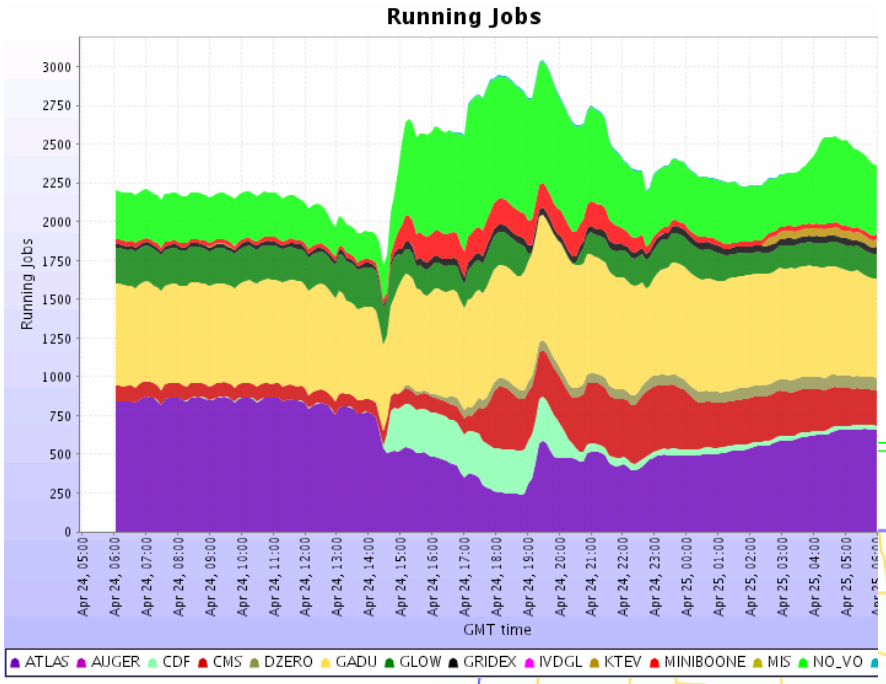
Data

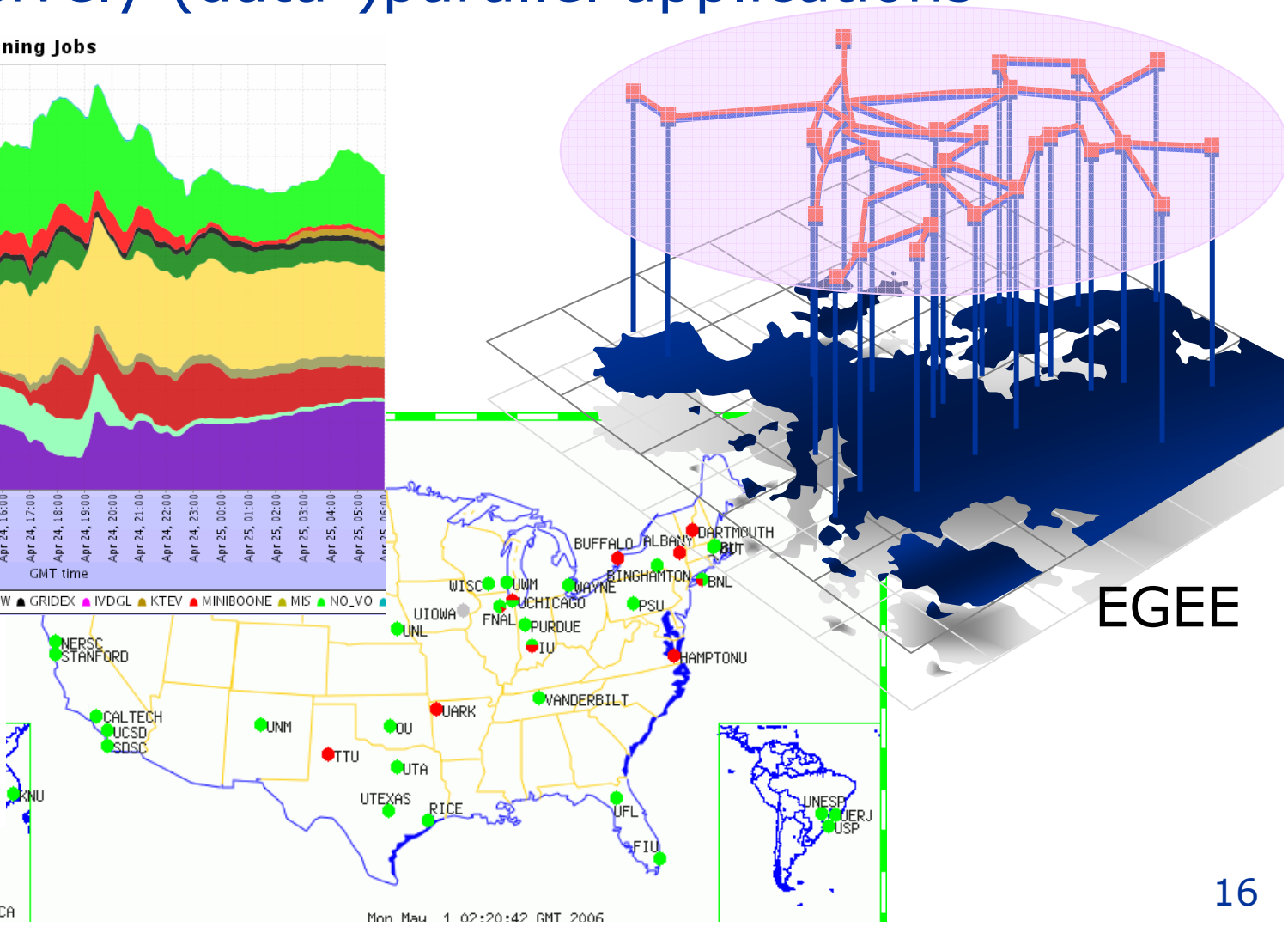


eScience: When brute force doesn't work anymore (Szalay)

First Generation Grids:
Batch Computing

Focus on aggregation of many resources for massively (data-)parallel applications





EGEE

Open Science Grid

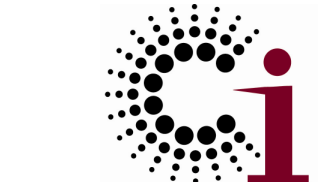
Second Generation Grids: **Service-Oriented Science**

- Empower many more users by enabling on-demand access to **services**
- Grids become an enabling technology for **service oriented science** (or business)
  - Grid infrastructures host services
  - Grid technologies used to build services

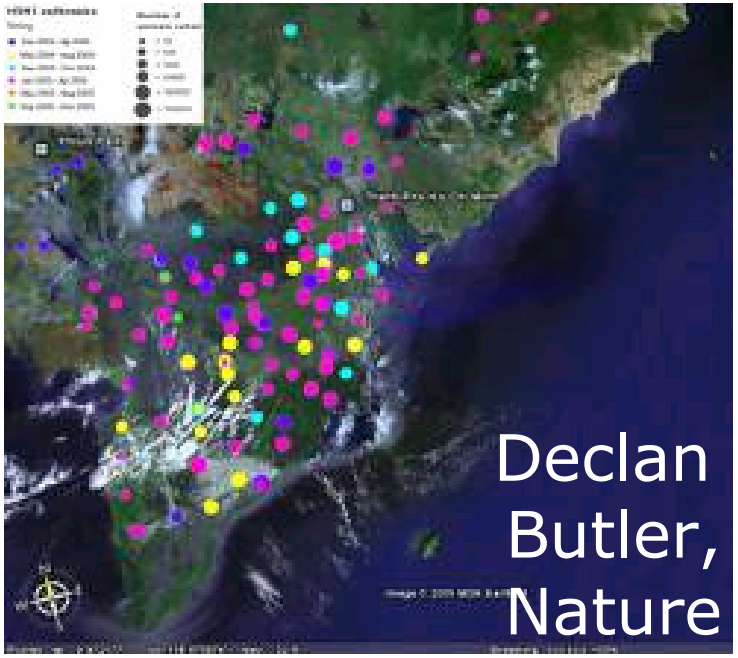
Science Gateways

TeraGrid™
EMPOWERING DISCOVERY

"Service-Oriented Science", *Science*, 2005

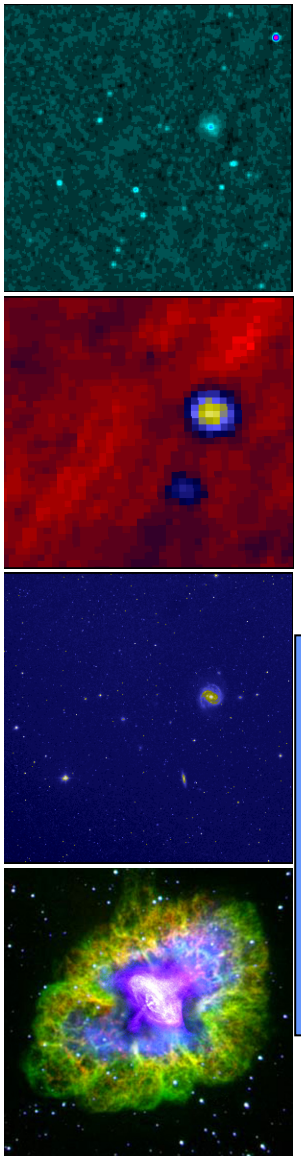


"Web 2.0"



- Software as services
  - Data- & computation-rich network services
- Services as platforms
  - Easy composition of services to create new capabilities ("mashups")—that themselves may be made accessible as new services
- Enabled by massive infrastructure buildout
  - Google projected to spend $1.5B on computers, networks, and real estate in 2006
  - Many others are spending substantially
- Paid for by advertising

Service-Oriented Science: E.g., Virtual Observatories



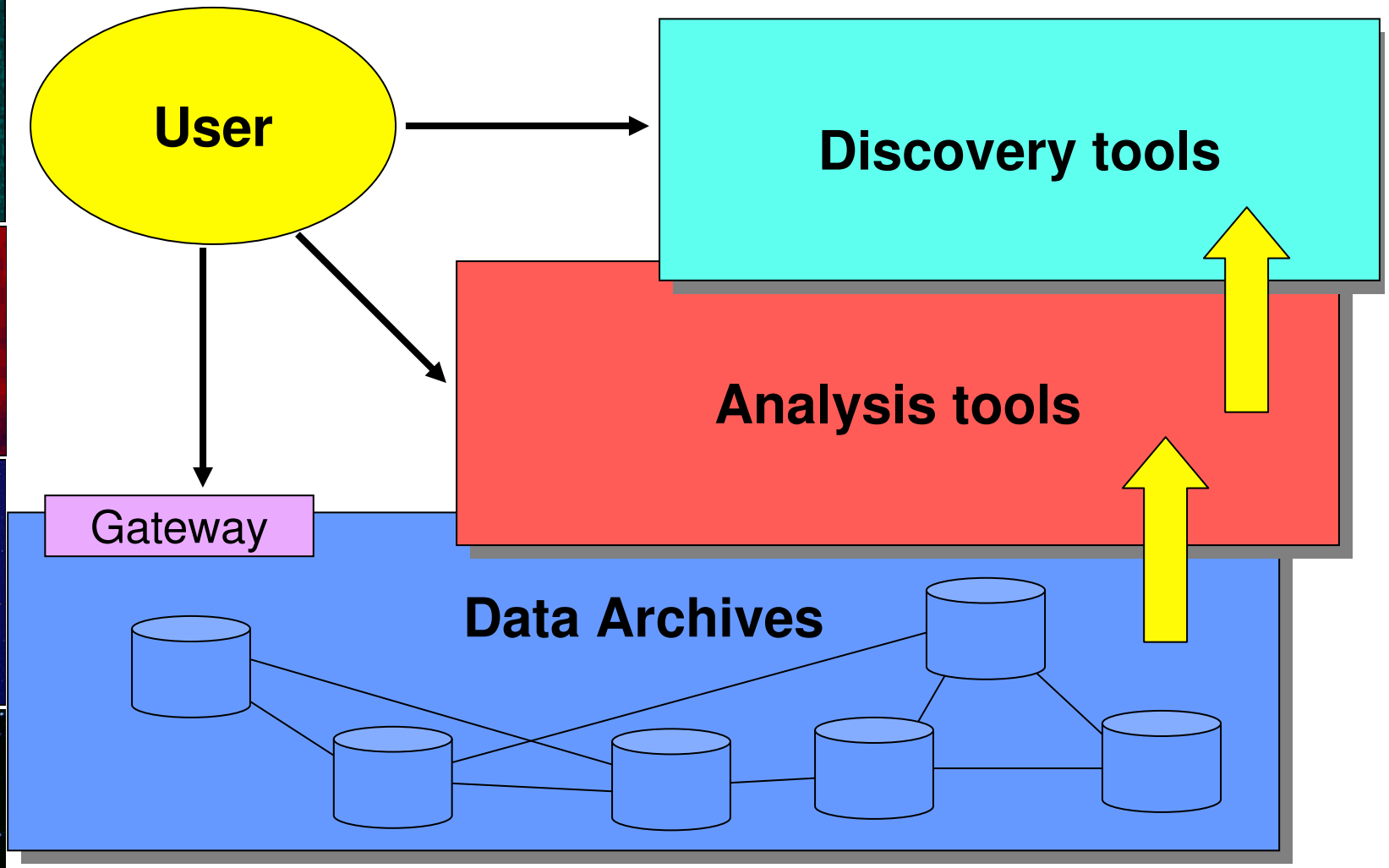
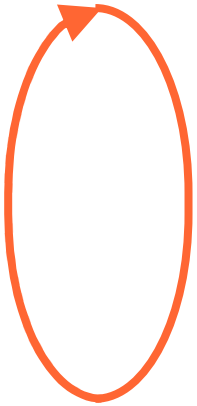


Figure: S. G. Djorgovski

Service-Oriented Science



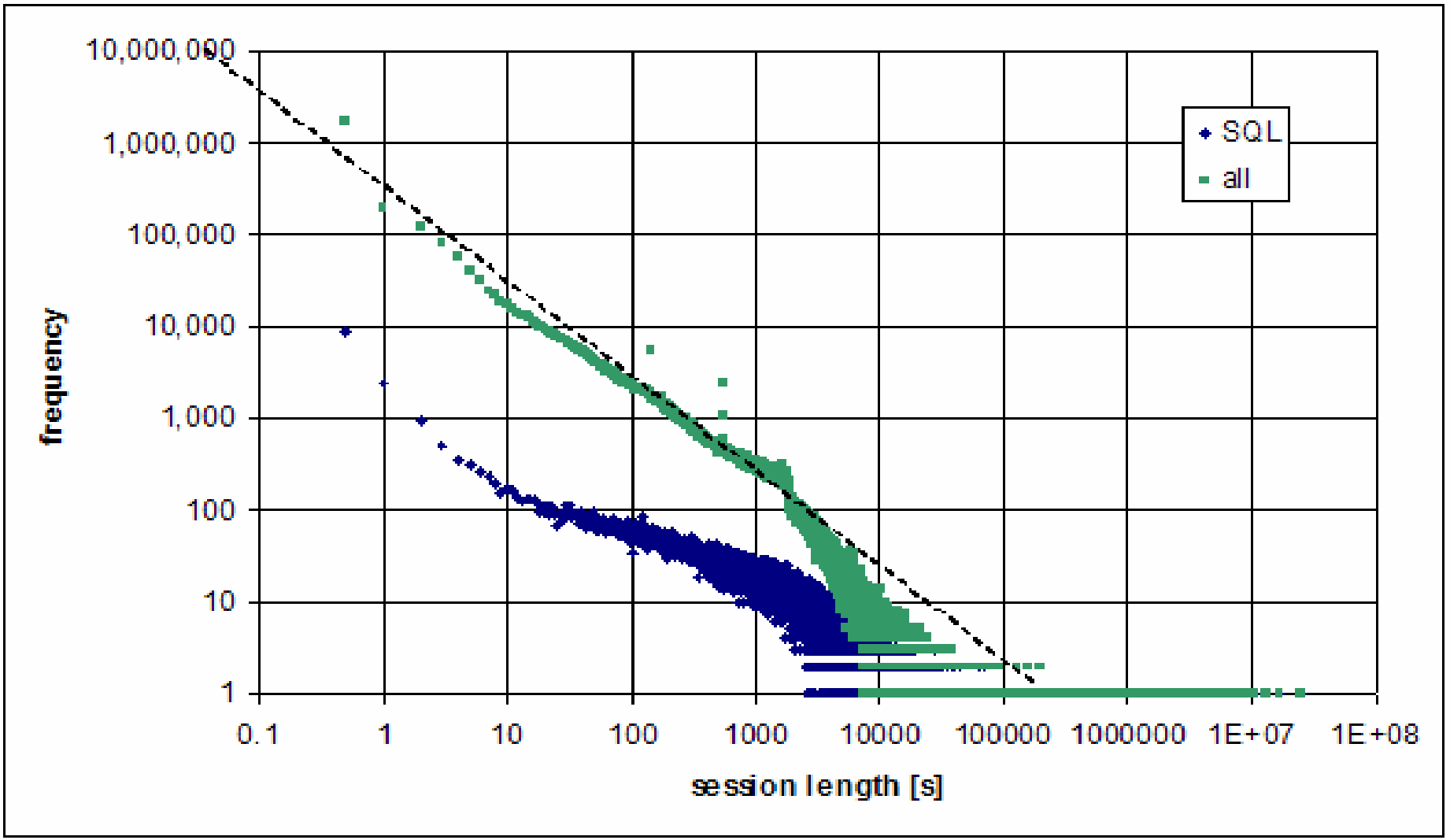
People **create** services (data or functions) …
which I **discover** (& decide whether to use) …
& **compose** to create a new function ...
& then **publish** as a new service.

→ *I find "someone else" to **host** services, so I don't have to become an expert in operating services & computers!*

→ *I hope that this "someone else" can **manage** security, reliability, scalability, …*

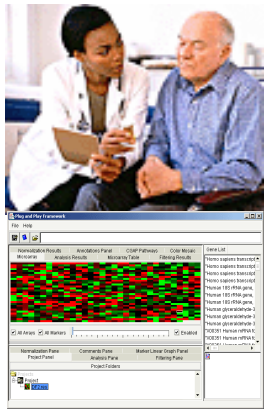
"Service-Oriented Science", *Science*, 2005

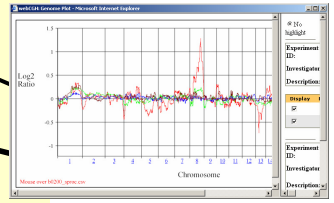
Skyserver Sessions (Thanks to Alex Szalay)

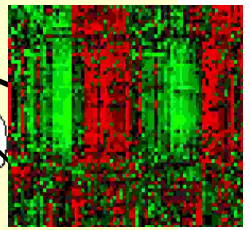


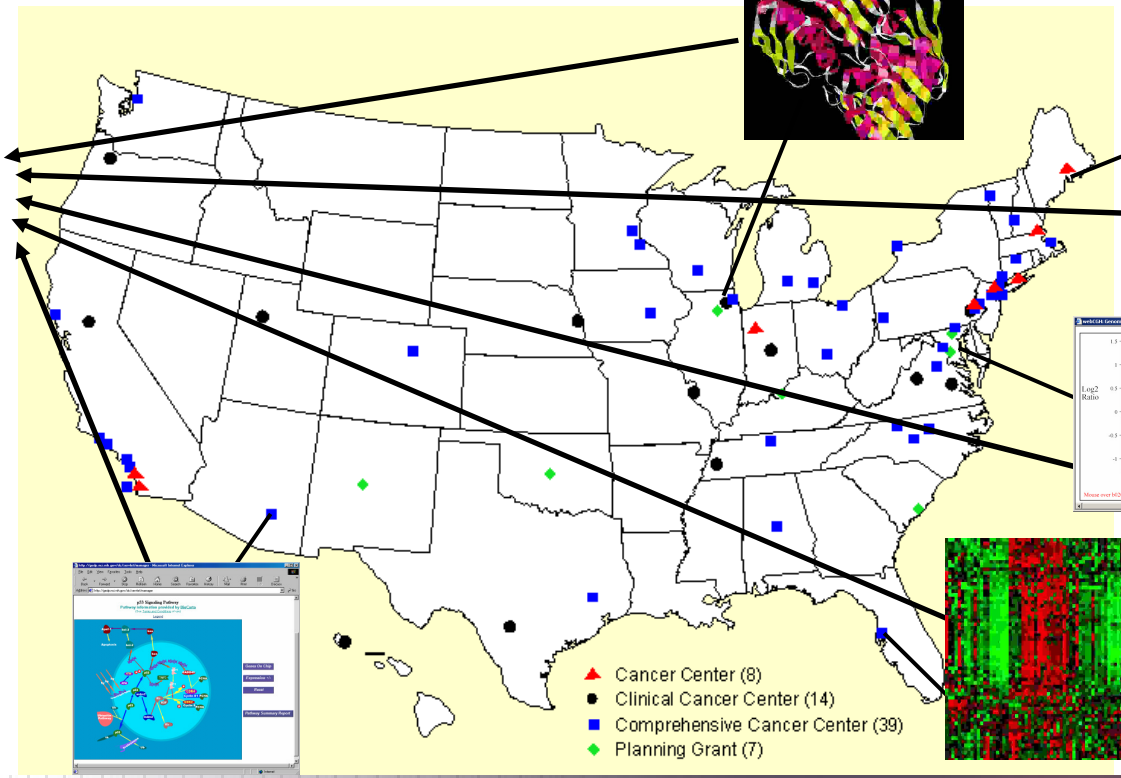
Service-Oriented Science & Cancer Biology

caBIG: sharing of infrastructure, applications, and data.





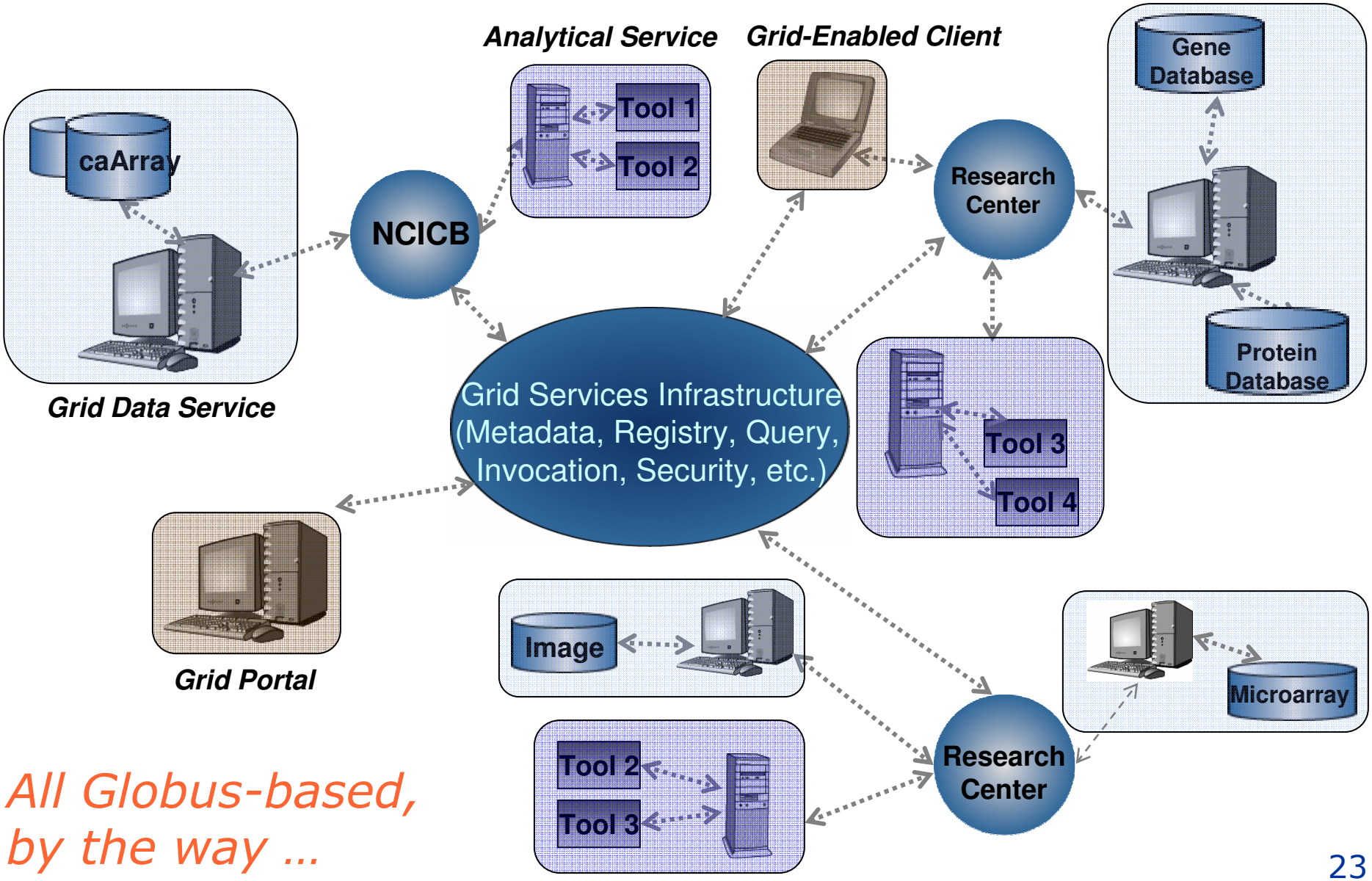




Data Integration!

caBIG cancer Biomedical Informatics Grid

Cancer Bioinformatics Grid



All Globus-based, by the way …

Thailand joins the grid

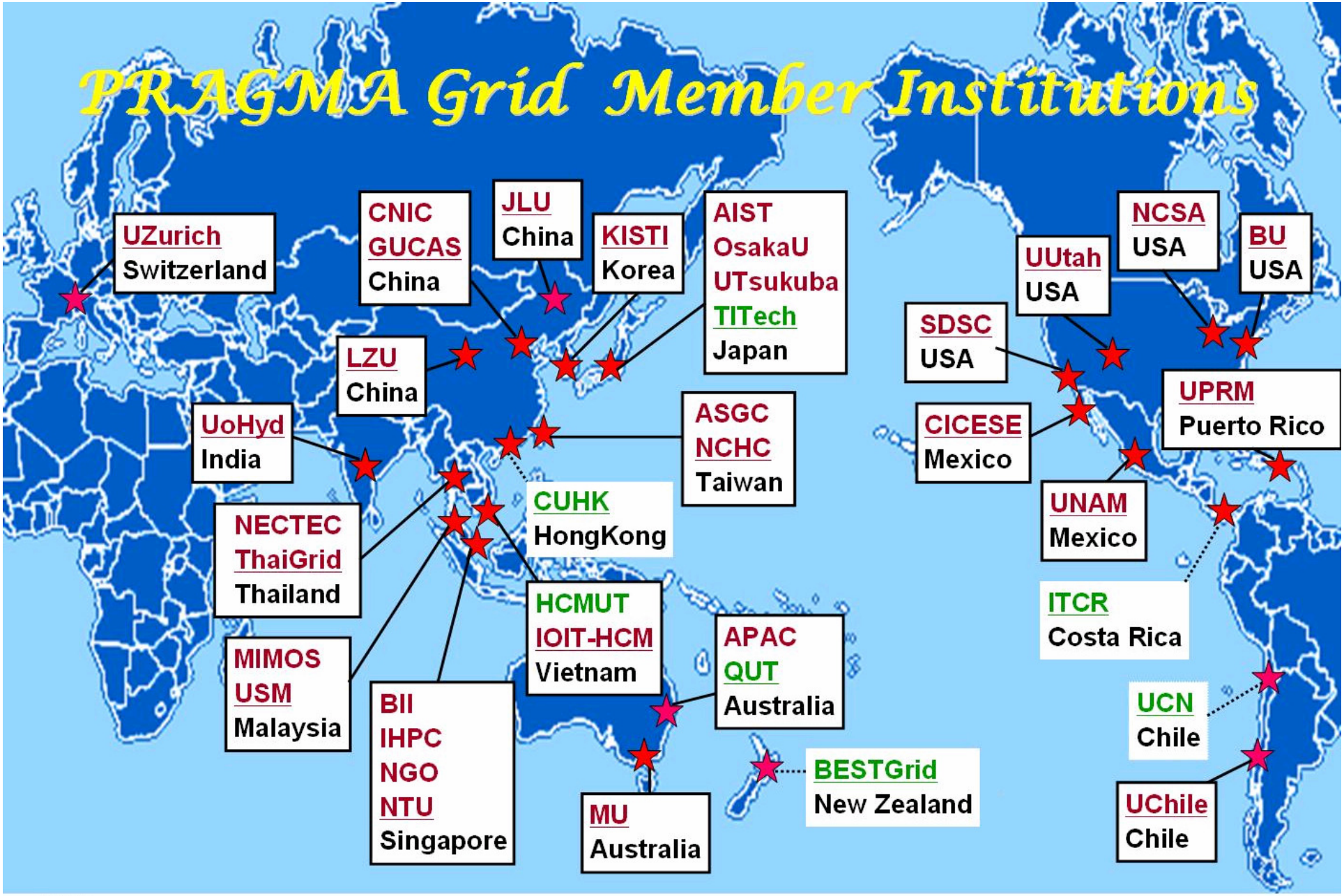
By Don Sambandaraksa, Bangkok Post
Wednesday, May 16 2007 11:34 AM

TALKBACK
PRINT STORY
EMAIL STORY

Bangkok Post

Grid computing is no longer just about universities getting together to pool and share their computing power, but increasingly it is about grids of sensors, information and of experts that are shared and leveraged across the world. And now Thailand is playing a major part in this new wave, having recently hosted the 12th meeting of the Pacific Rim Application and Middleware Assembly (Pragma).

"Grids are not just communities of computers, but communities of researchers, of people."
— Peter Arzberger



31 institutions in 15 countries/regions (+ 7 in preparation)

Last update: 5/30/2007

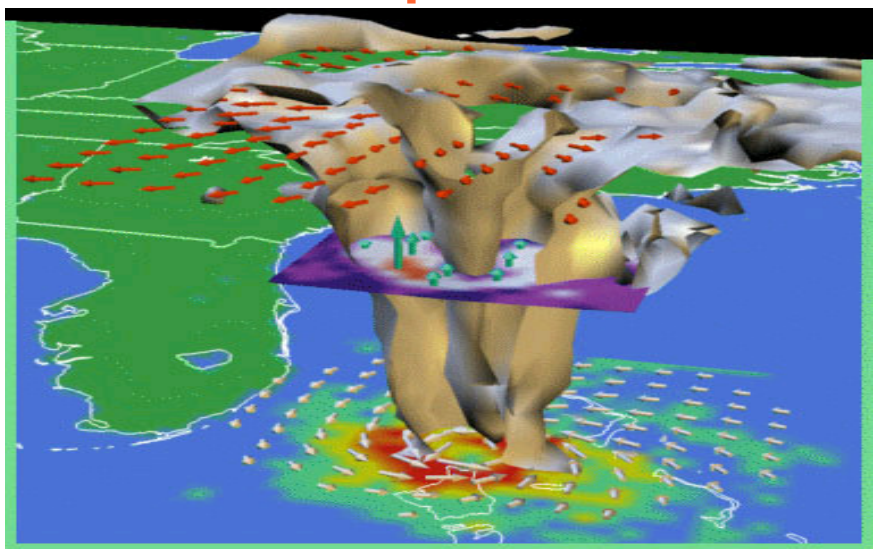
Grids are Communities …

- Based on (technology-mediated) trust
  - Common goals
  - Processes and policies
  - Reward systems
- That share resources
  - Computers
  - Data
  - Sensor networks
  - Services
- Supported by software and standards

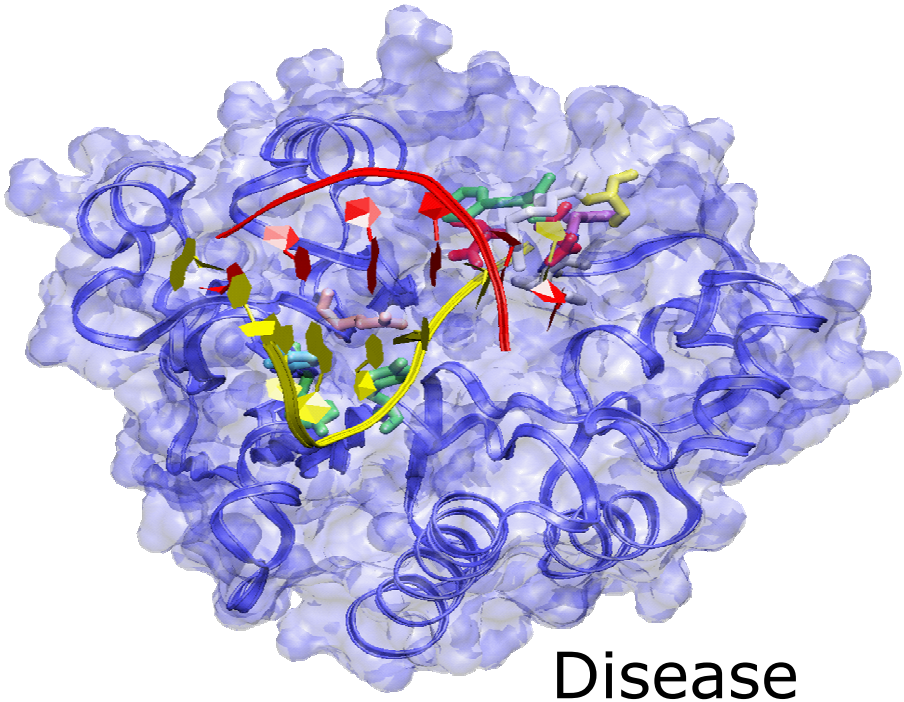
Global Community

Globus Downloads Last 24 Hours

Towards Open eScience



Climate change



Disease

Natural disasters

Sustainable energy

Science 1.0 → Science 2.0

Megabytes & gigabytes	→ Terabytes & petabytes
Tarballs	→ Services
Journals	→ Wikis
Individuals	→ Communities
Community codes	→ Science gateways
Supercomputer centers	→ Campus & national grids …
Makefile	→ Workflow
Computational science	→ Science as computation
Mostly physical sciences	→ All sciences (& humanities)
1000s of computationalists	→ Millions of researchers
Government funded	→ Government funded

Thanks!

- DOE Office of Science

- NSF Office of Cyberinfrastructure
- Colleagues at Argonne, U.Chicago, USC/ISI, and elsewhere
- Many members of the German DGrid community

Summary

- Technology exponentials are transforming the nature of research
  - Data-, compute-, & communication-intensive approaches are increasingly influential
- Grid is a unifying concept & technology
  - Federation & on-demand access to resources
- An enabler of "service-oriented science"
  - Transforms how we conduct research & communicate results
  - Demands new reward structures, training, & infrastructure

For more information: **http://ianfoster.typepad.com**