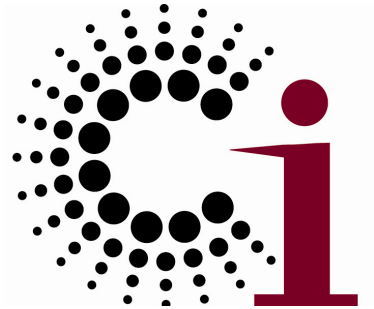
Looking to the Future

Ian Foster



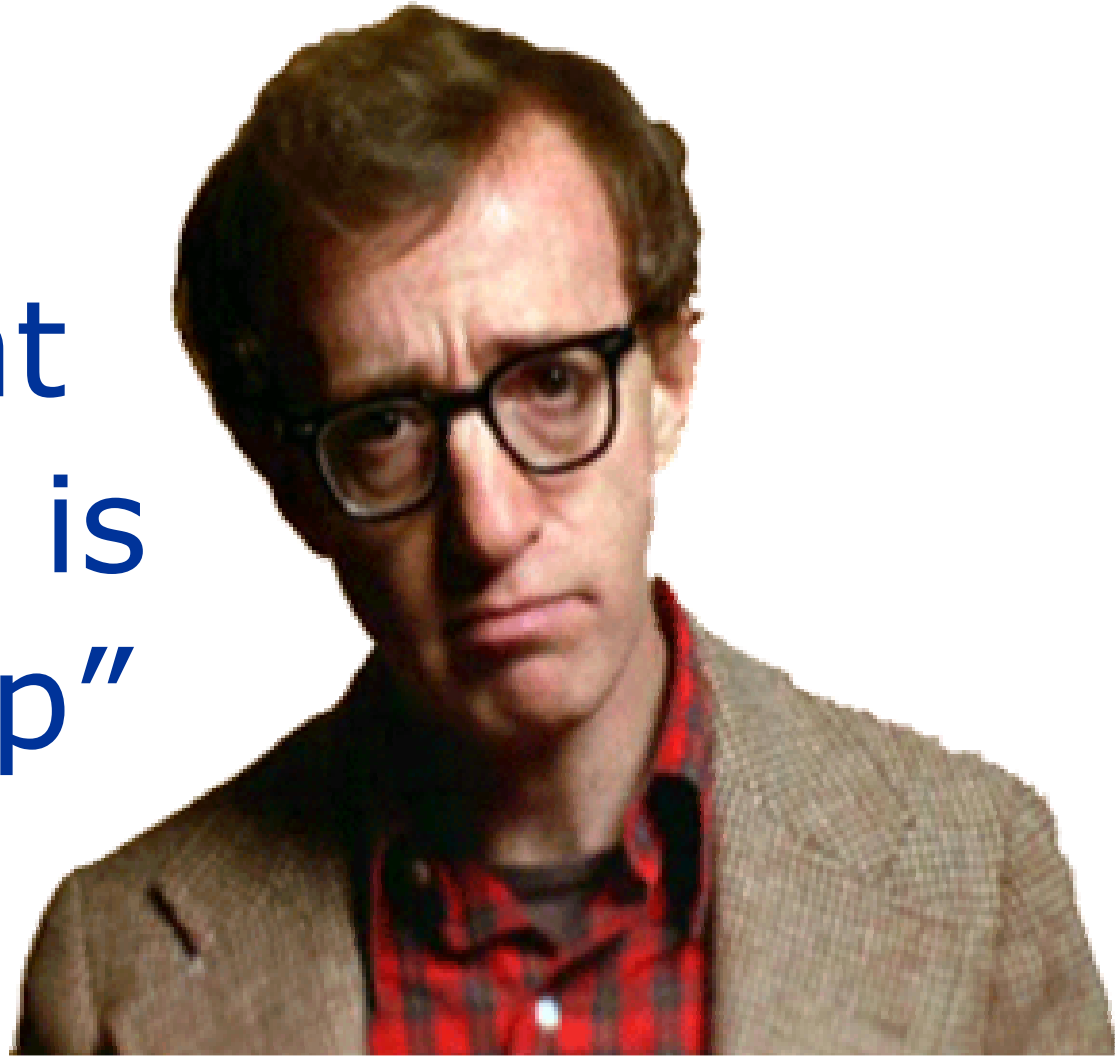
Computation Institute

Argonne National Lab & University of Chicago

http://ianfoster.typepad.com

An American Philosopher Speaks on the Value of KAREN

"80 percent of success is showing up"



Woody Allen

J.C.R. Licklider Reflecting in 1960 on Where His Time Went

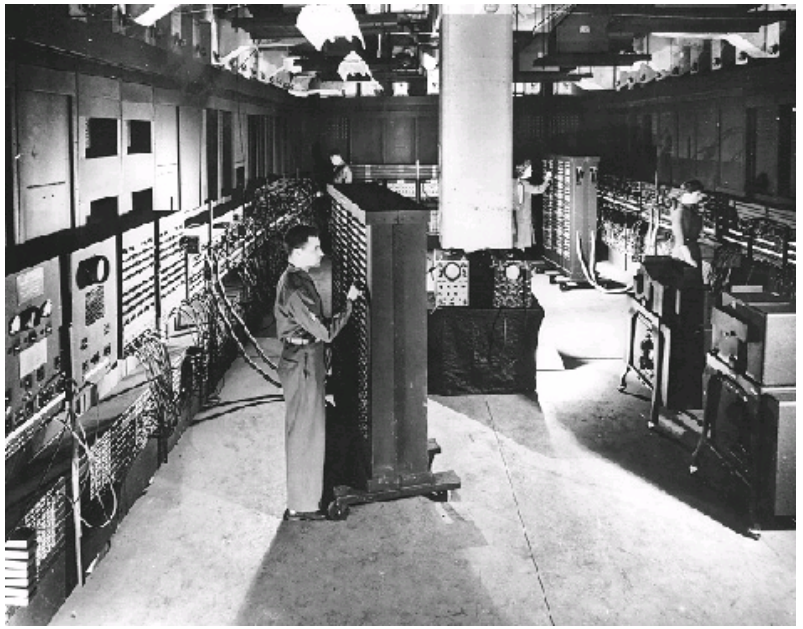
About 85 per cent of my "thinking" time was spent getting into a position to think, to make a decision, to learn something I needed to know

For Example …

"At one point, it was necessary to compare six experimental determinations of a function relating speech-intelligibility to speech-to-noise ratio. No two experimenters had used the same definition or measure of speech-to-noise ratio. Several hours of calculating were required to get the data into comparable form. When they were in comparable form, it took only a few seconds to determine what I needed to know."

Man-Computer Symbiosis

"… will involve very close coupling between the human and the electronic members of the partnership … Preliminary analyses indicate that the symbiotic partnership will perform intellectual operations much more effectively than man alone can perform them."



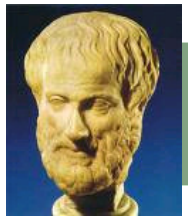
Licklider's Vision

- He imagined
  - Low-cost personal computers
  - Organized, easily searchable data stores
  - Intuitive user interfaces
  - Computer aided reasoning
  - Interactive numerical simulation
- He didn't mention (at least in CMS paper)
  - Standard representations of knowledge
  - Collaborative problem solving among people

Fast Forward to 2007

"Compare six experimental determinations of a function relating speech-intelligibility to speech-to-noise ratio"

Emergence of New Problem Solving Methodologies

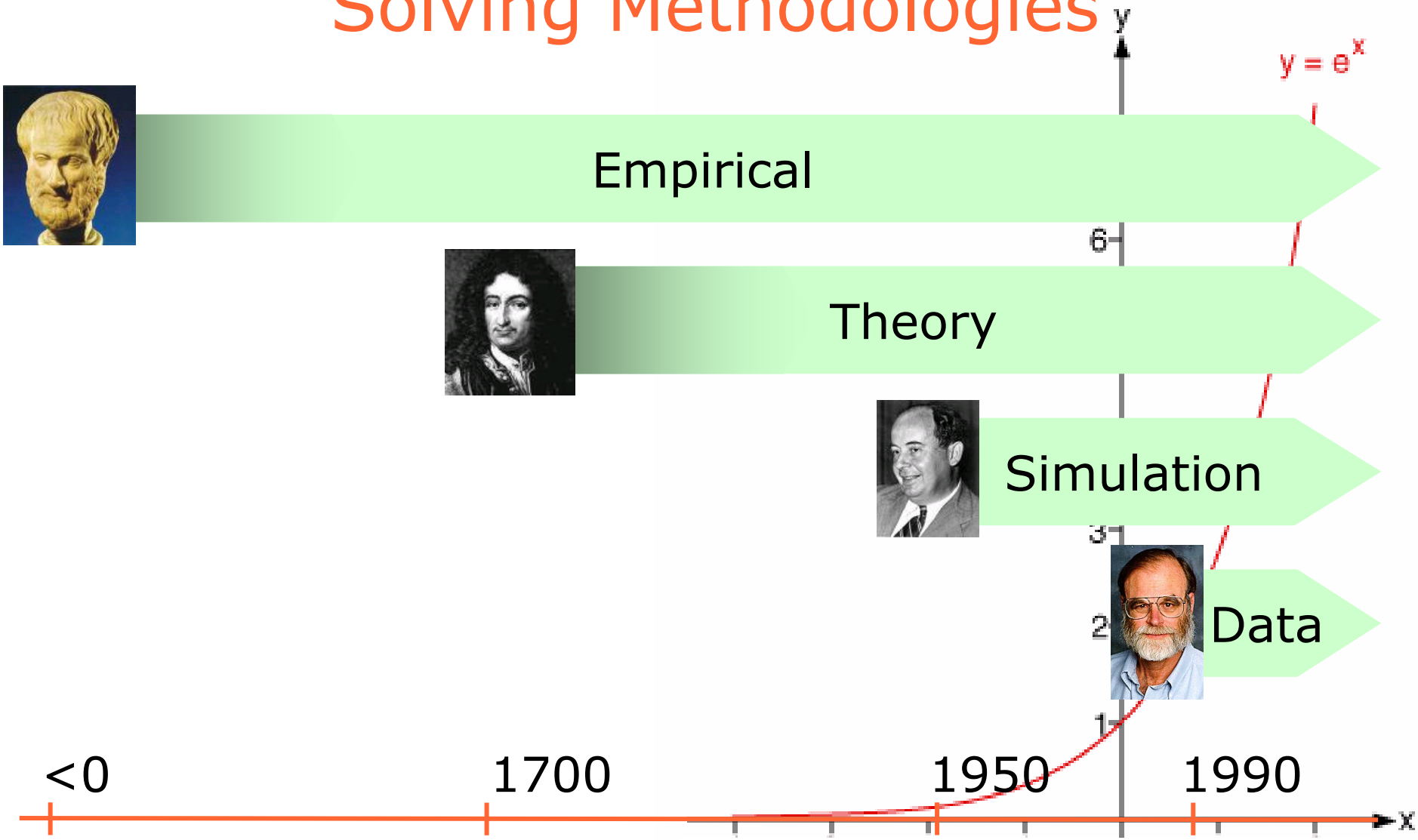


Empirical

Theory

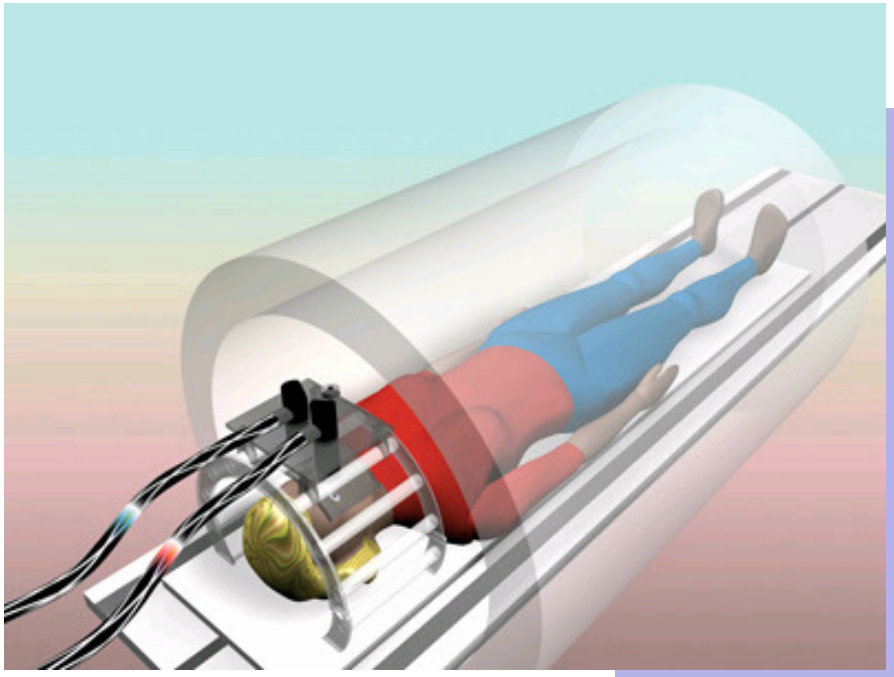
Simulation

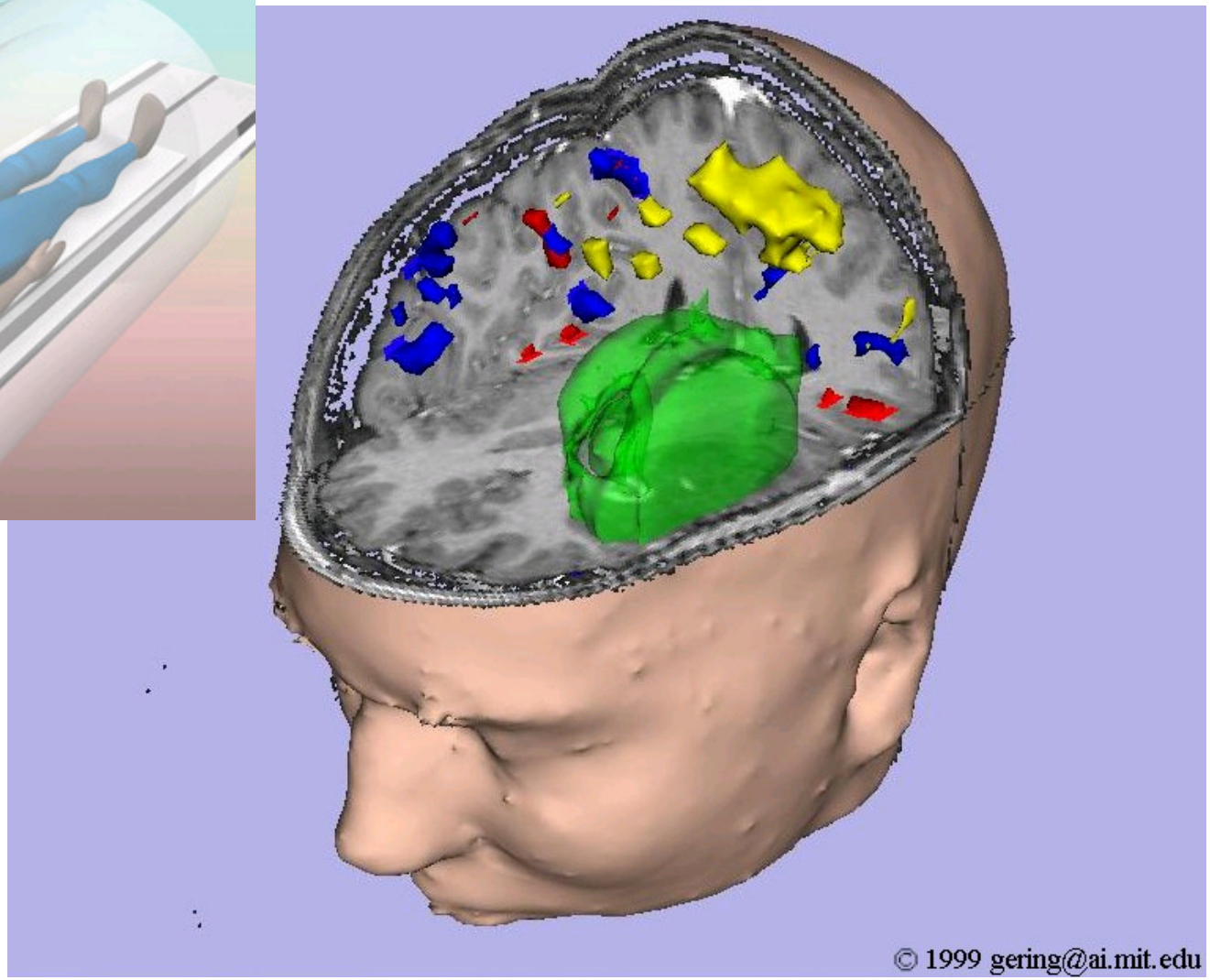
Data

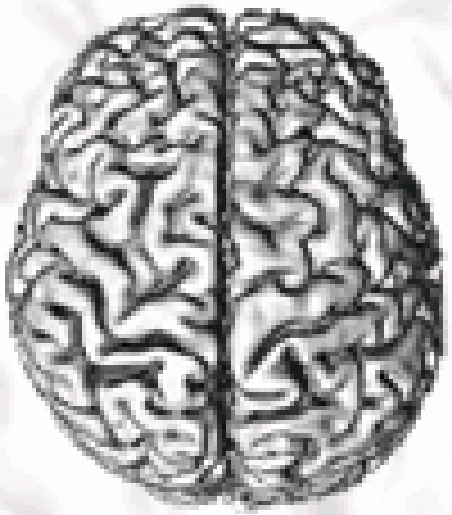


eScience: When brute force doesn't work anymore (Szalay)

Functional Magnetic Resonance Imaging (fMRI)







A public repository of peer-reviewed fMRI studies and their underlying data.

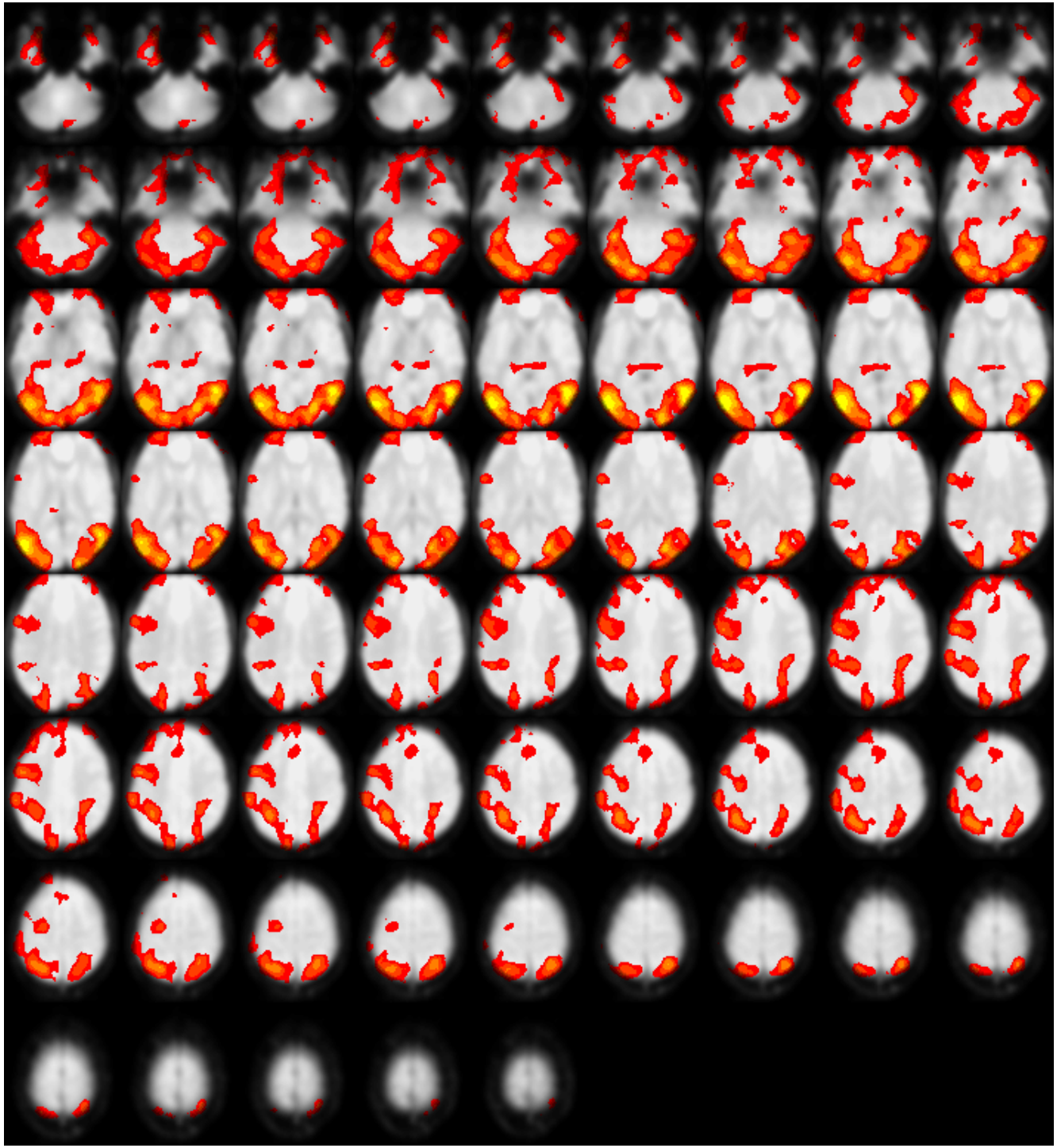
The fMRI Data Center (www.fmridc.org)

- A typical study comprises
  - 3 groups,
  - 20 subjects/group,
  - 5 runs/subject,
  - 300 volumes/run

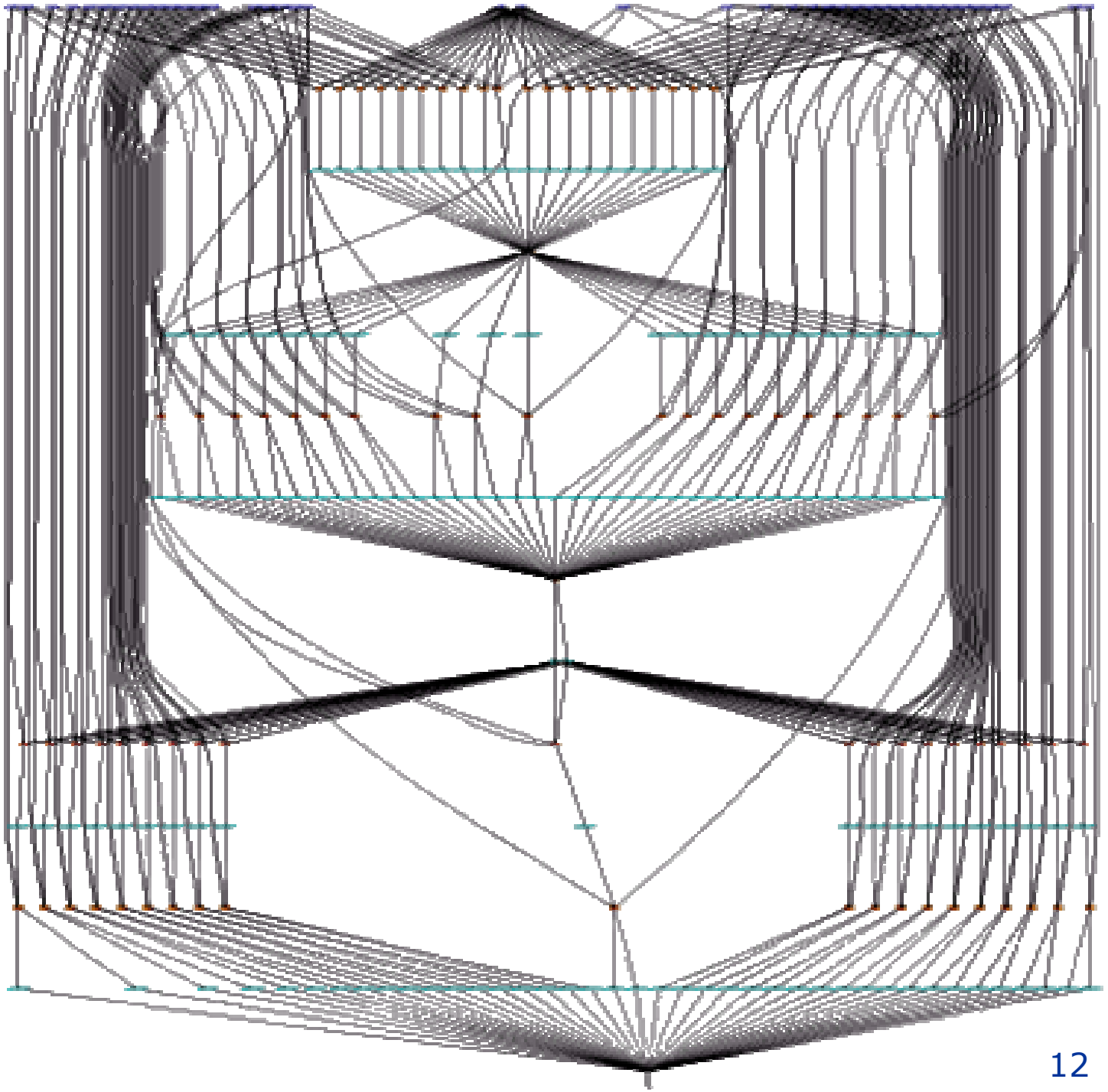
  → 90,000 volumes, 60 GB raw

  → 1.2 million files processed
- 100s of such studies in total

Functional MRI Analysis

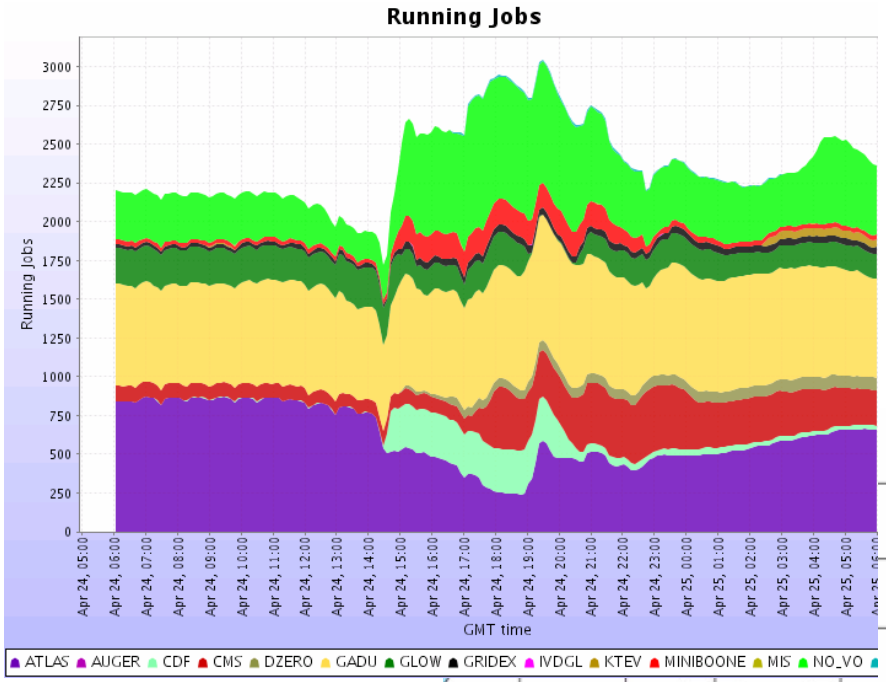


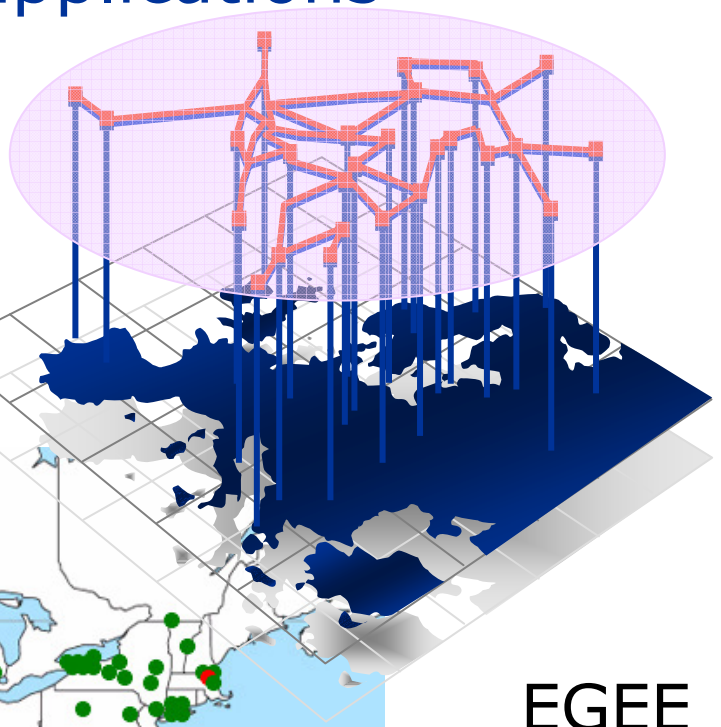
A Simple Analysis

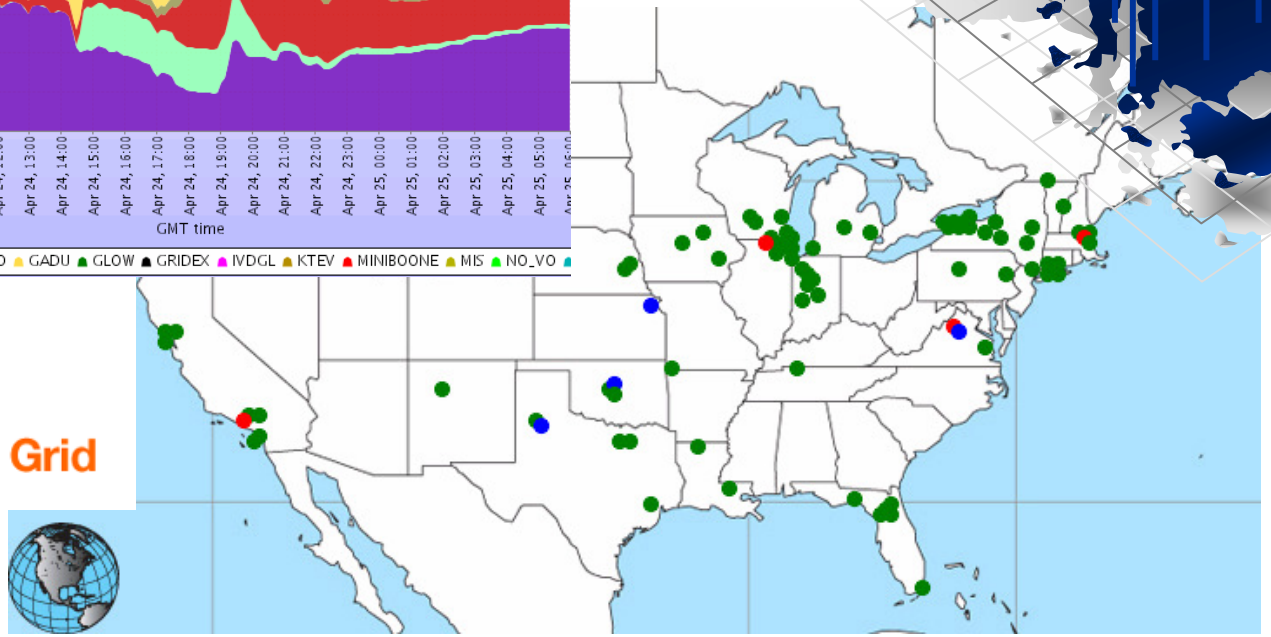


First Generation Grids: On-Demand/Batch Computing

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



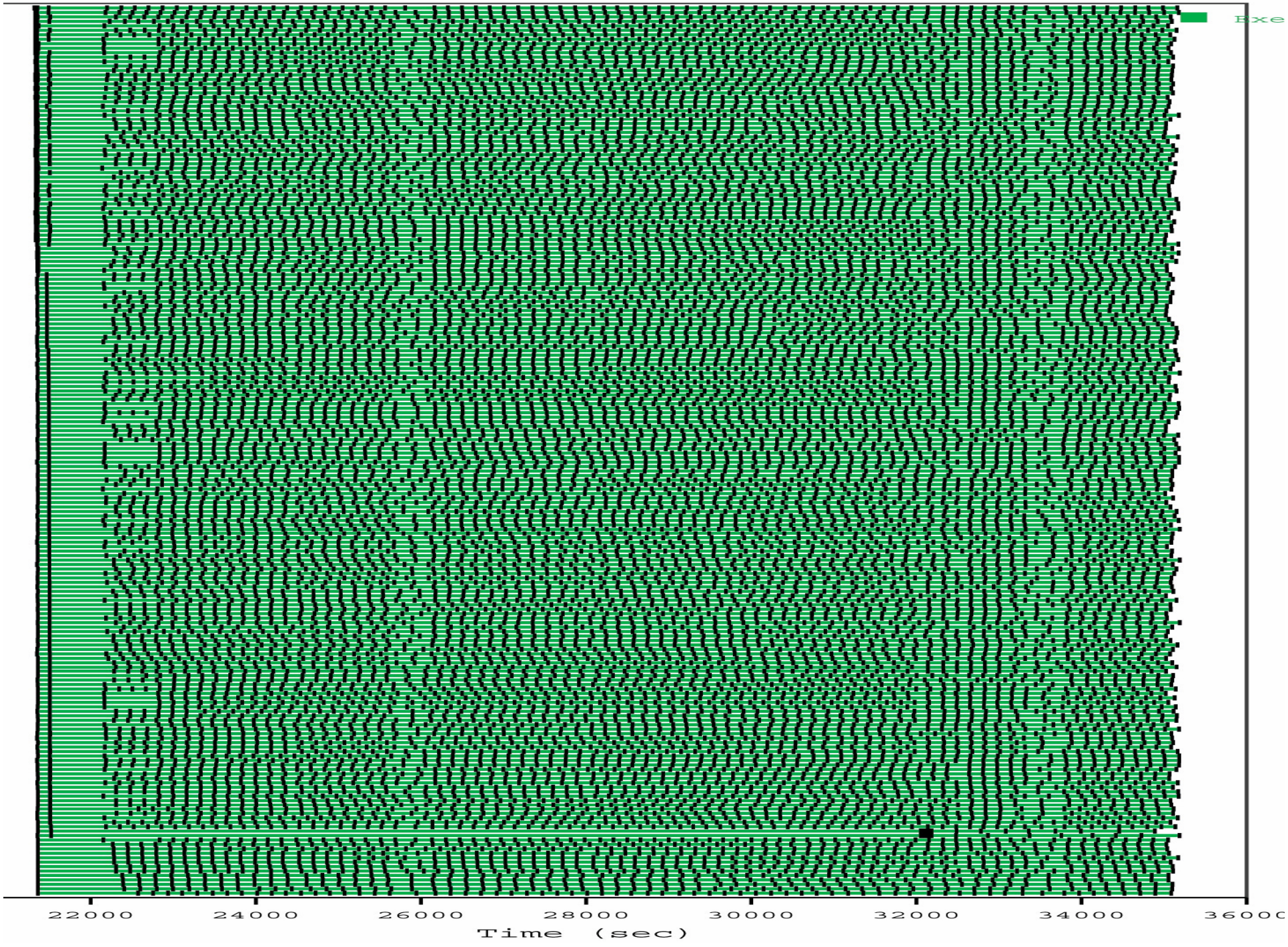




Open Science Grid

EGEE

Globus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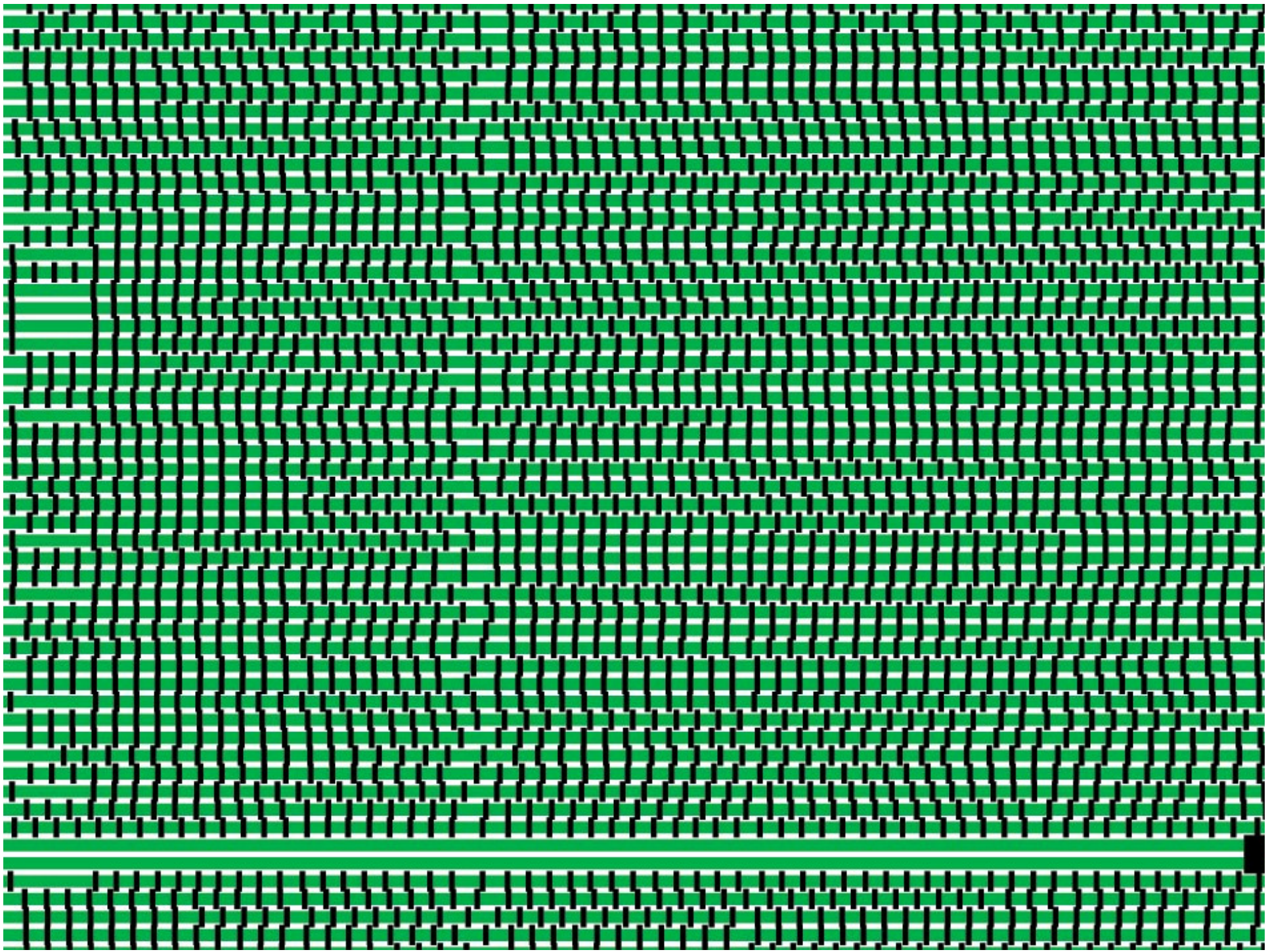
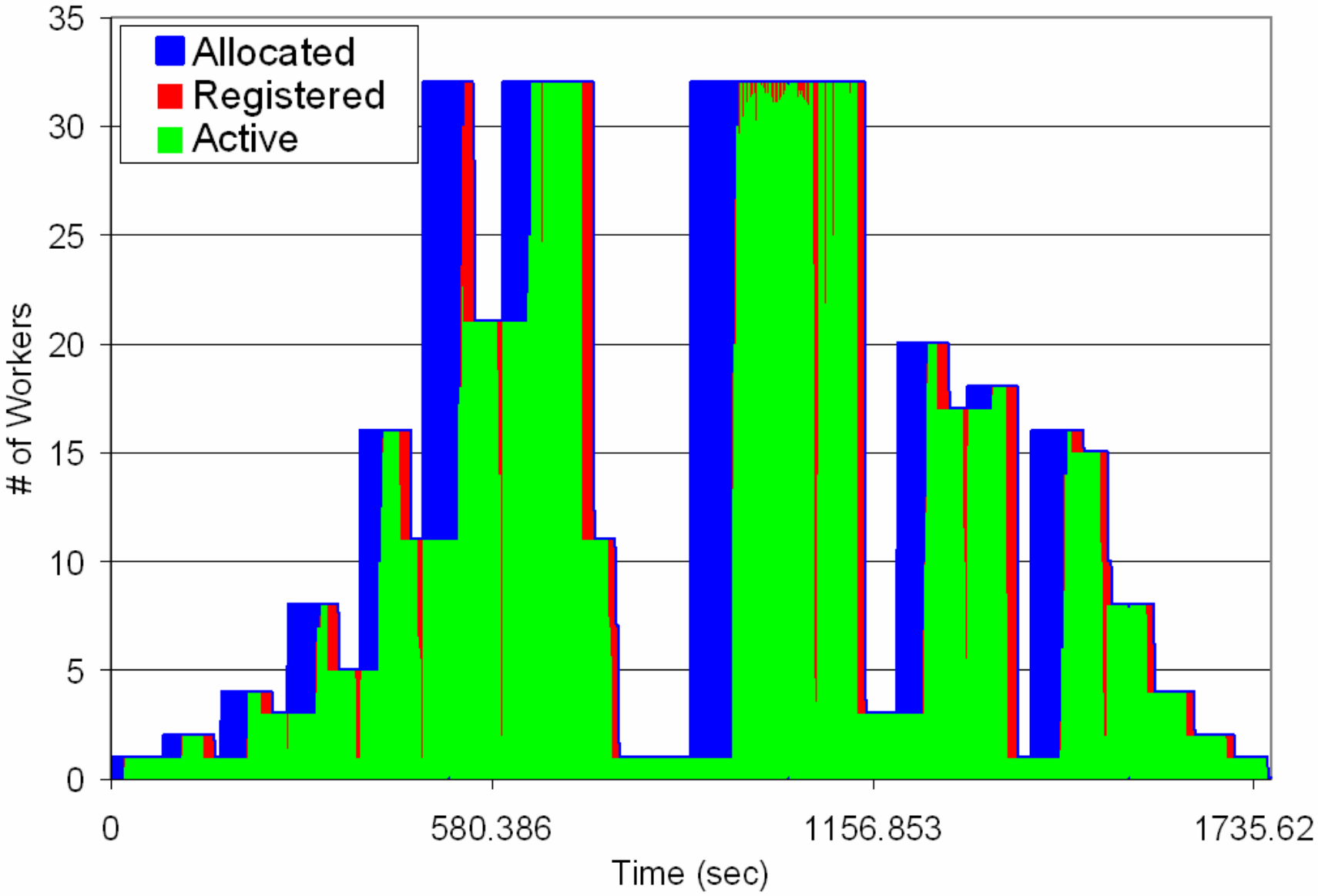
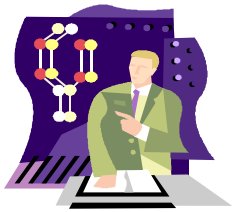
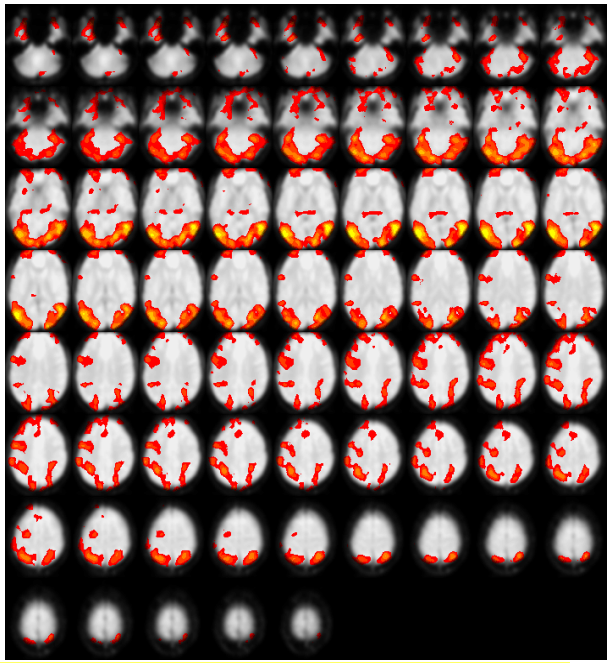


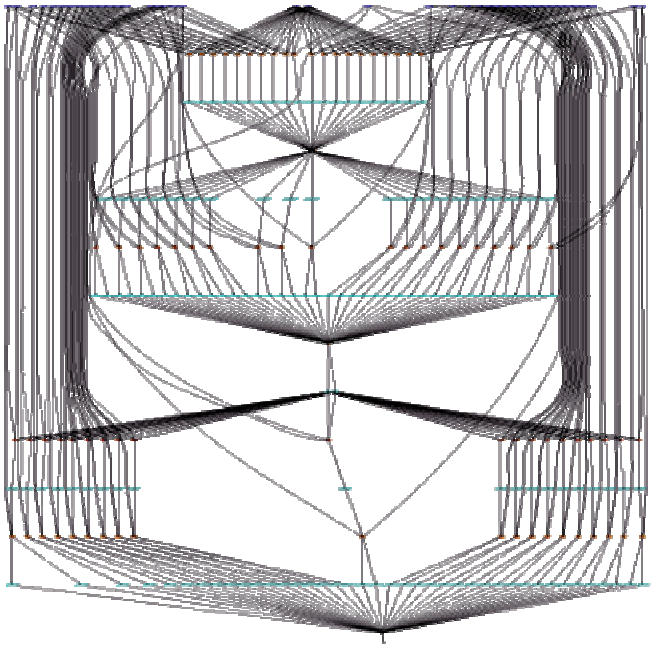
Dynamic Allocation for Dynamic Workloads

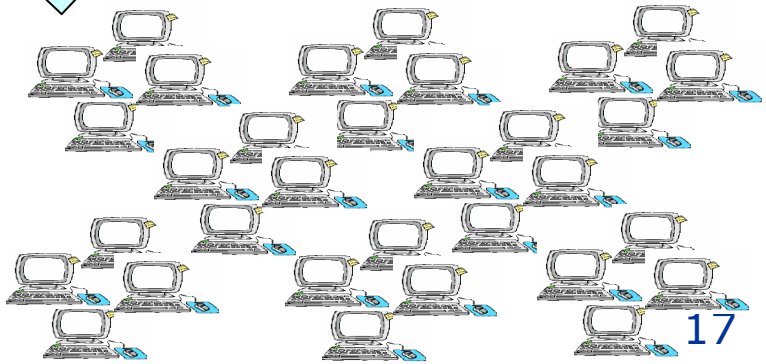


Many Users Analyze fMRI Data in Many Different Ways









- Wide range of analyses
  - Testing, interactive analysis, production runs
  - Data mining
  - Parameter studies

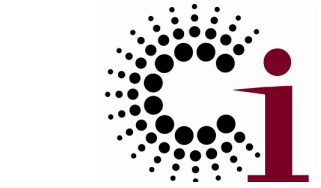
Second Generation Grids: **Service-Oriented Science**

- 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

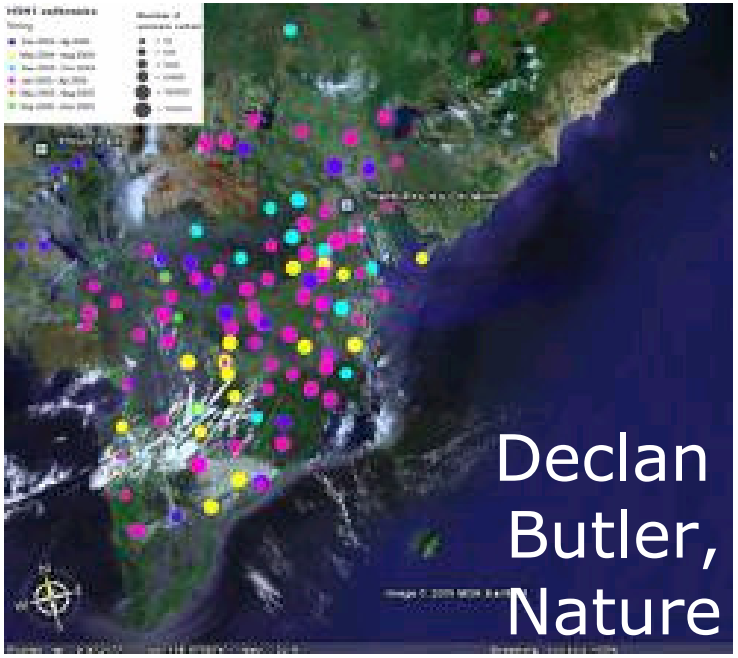
Science Gateways

TeraGrid™
EMPOWERING DISCOVERY

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

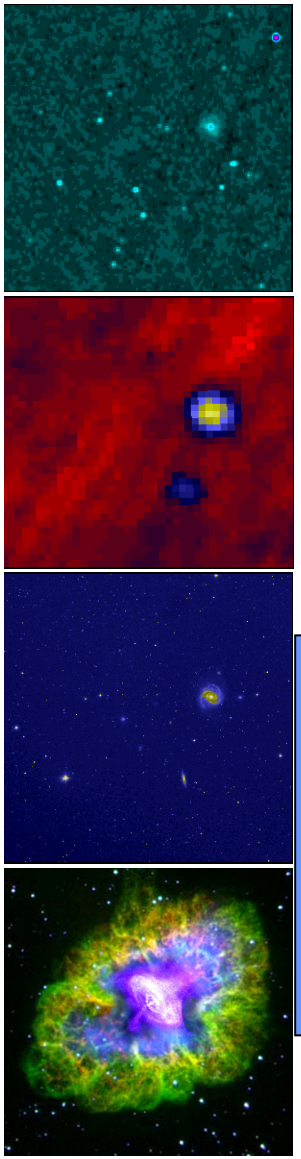


"Web 2.0"



- 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



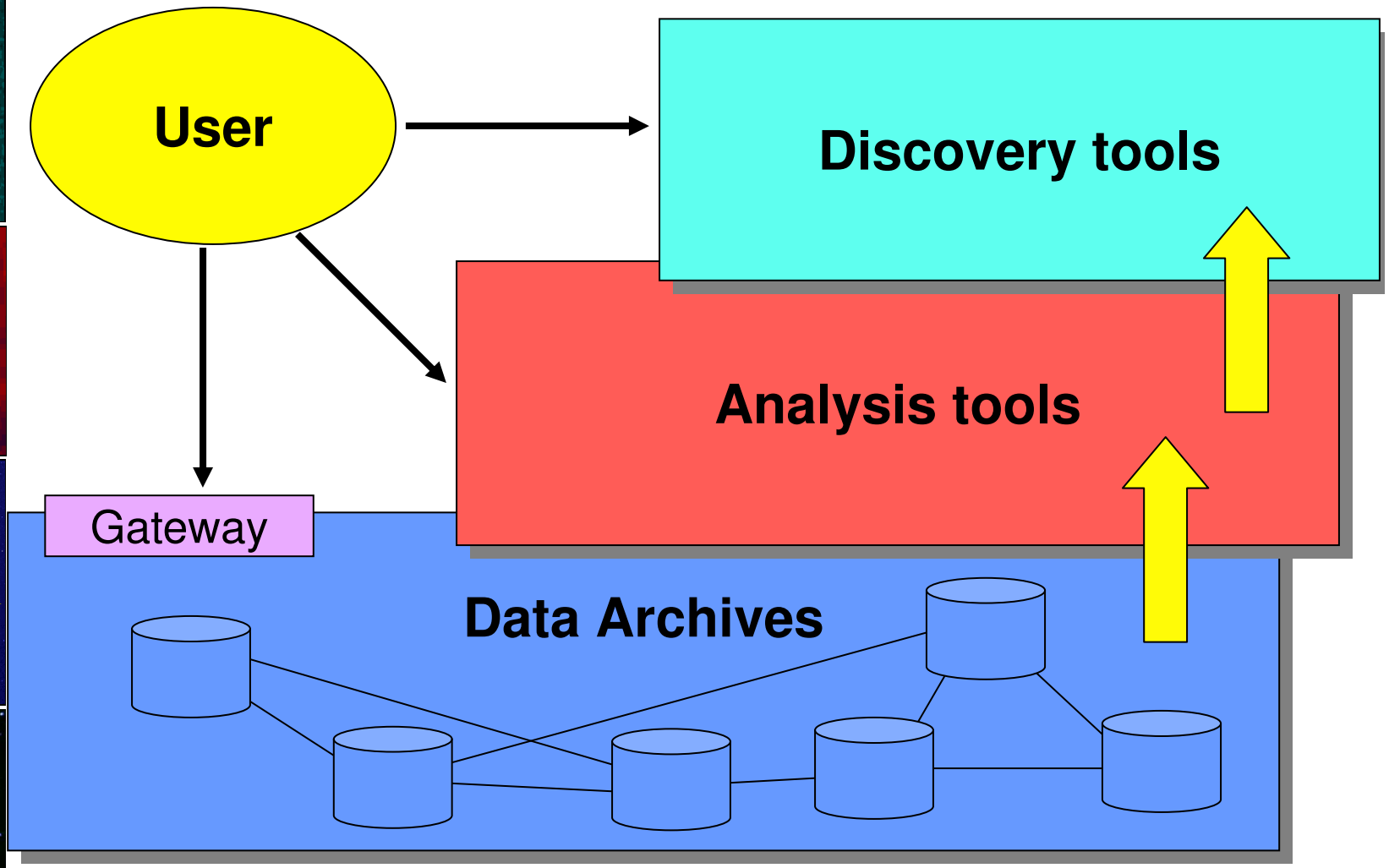
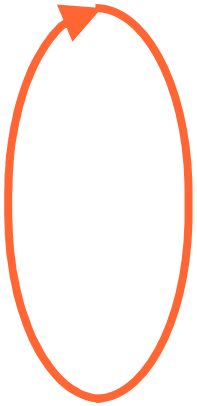


Figure: S. G. Djorgovski

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, …*

!!

BeSTGRID

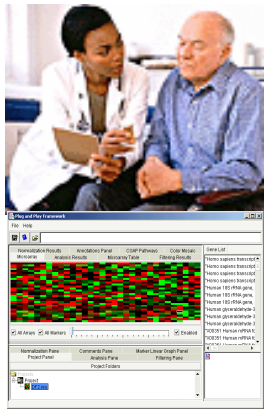
TeraGrid™ EMPOWERING DISCOVERY

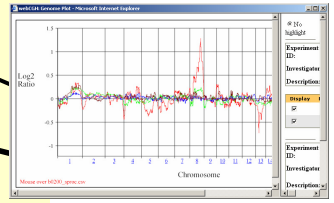
amazon web services™

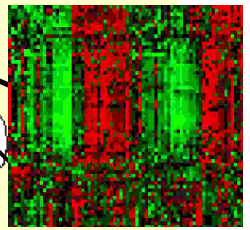
"Service-Oriented Science", *Science*, 2005

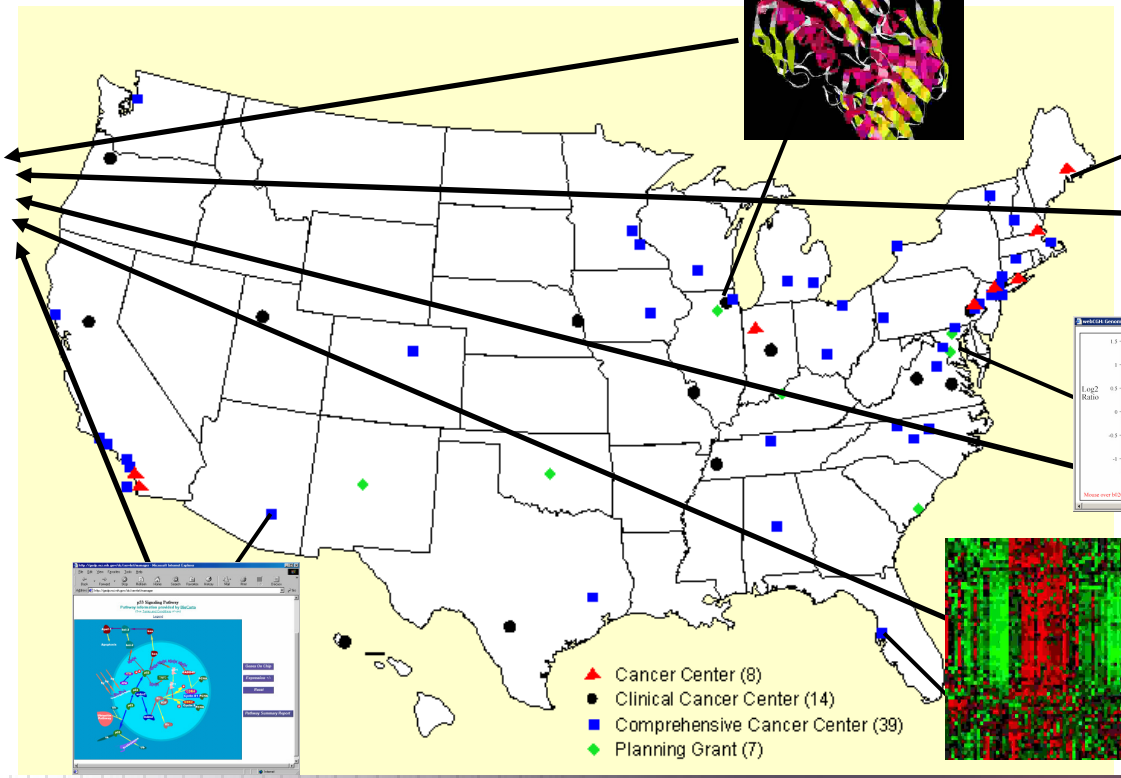
Service-Oriented Science & Cancer Biology

caBIG: sharing of infrastructure, applications, and data.





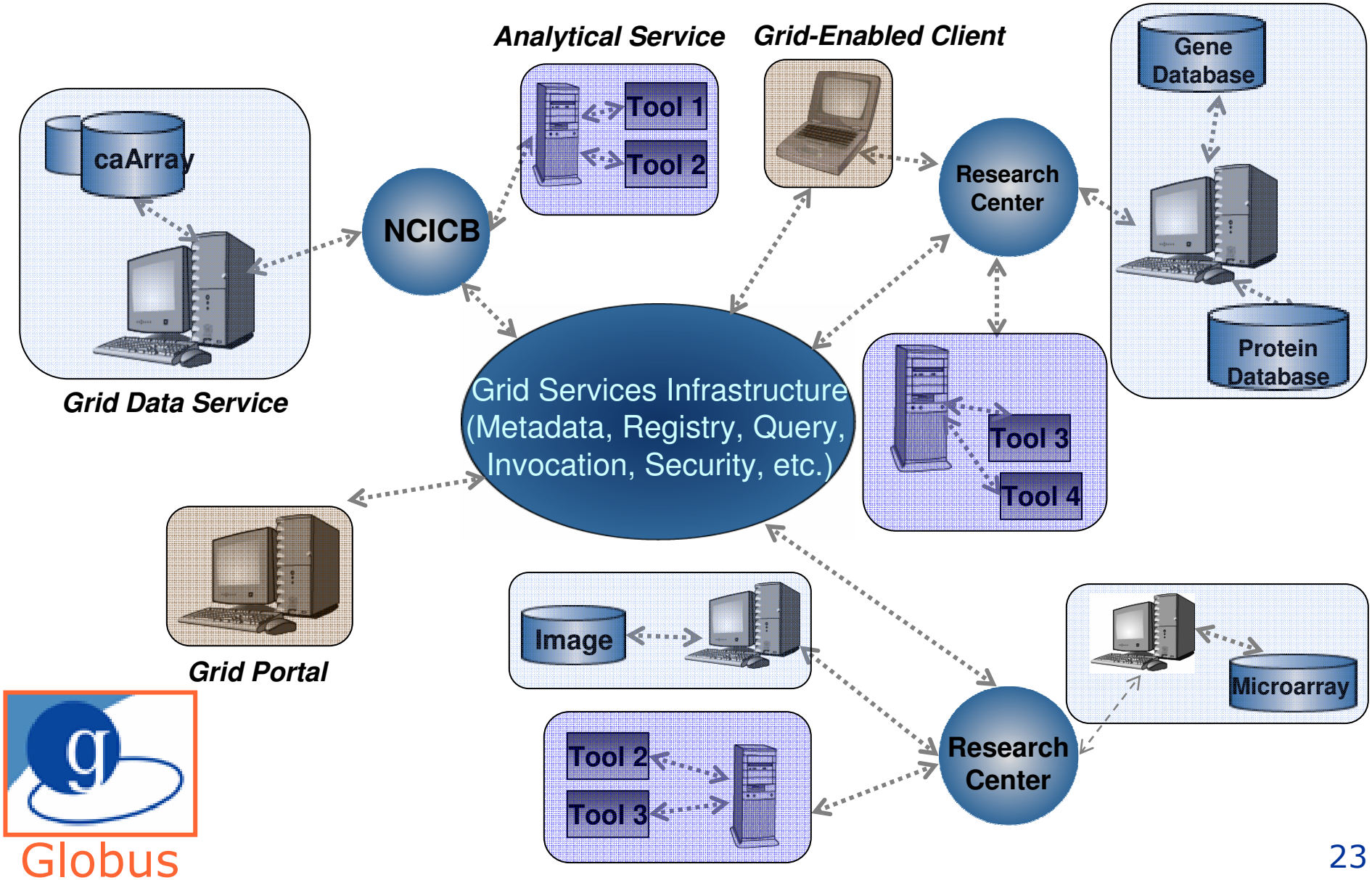




Data Integration!

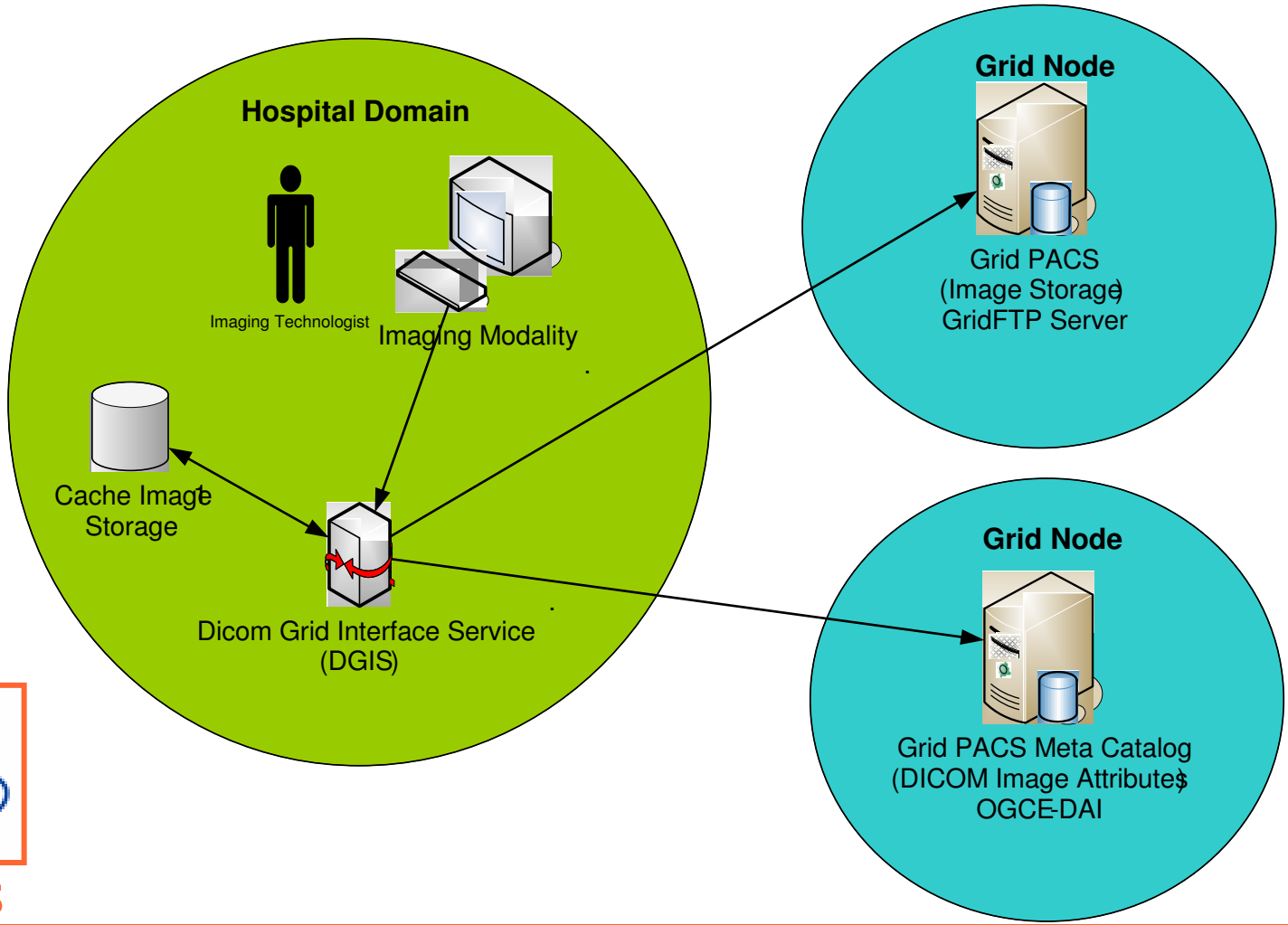
caBIG cancer Biomedical Informatics Grid

Cancer Bioinformatics Grid



Globus

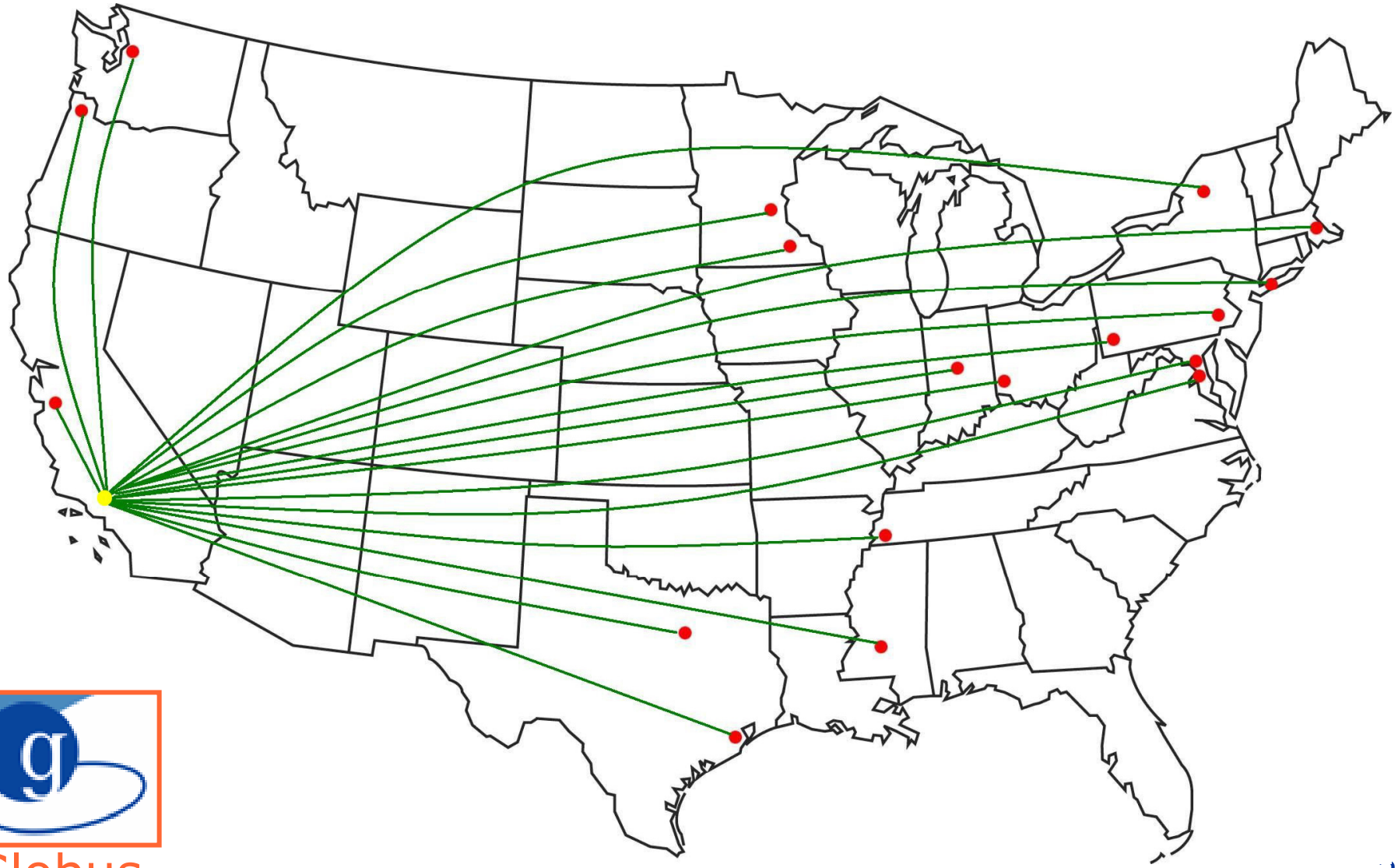
MEDICUS: Management of DICOM Images



Globus

Stephan Erberich, Manasee Bhandekar, Ann Chervenak, et al.

Children's Oncology Grid: A MEDICUS Deployment

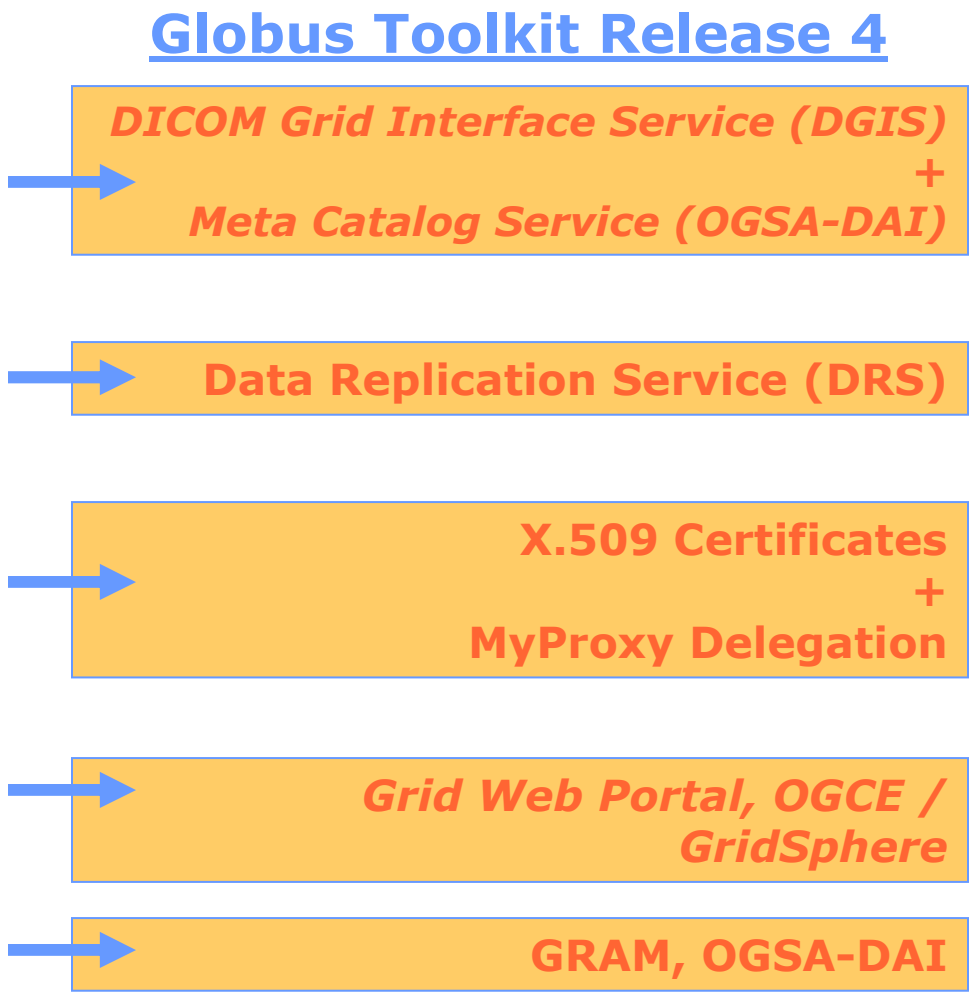


Globus

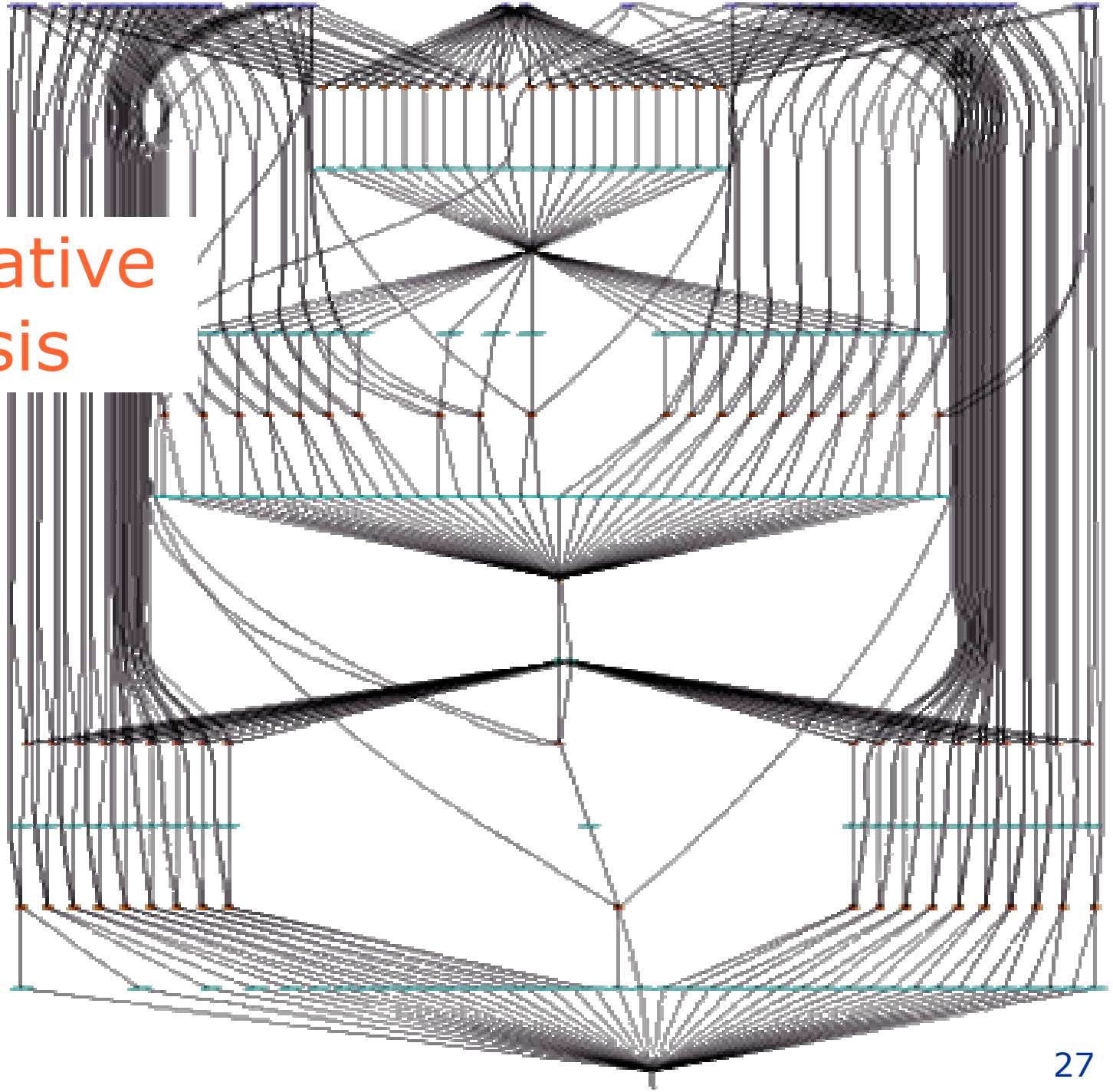
MEDICUS Under the Covers

Globus

- DICOM images
  - Send (publish)
  - Query/Retrieve (discover)
- Grid Archive
  - Fault tolerant
  - Bandwidth
- Security
  - Authentication
  - Authorization
  - Cryptography
- Access
  - Web portal
- Applications
  - Computing
  - Data Mining

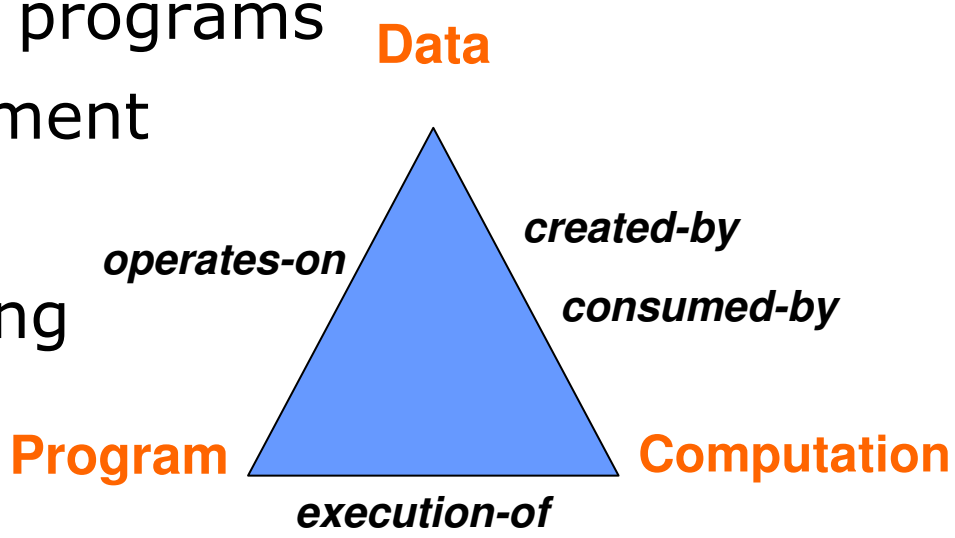


Collaborative Analysis



The Virtual Data Concept

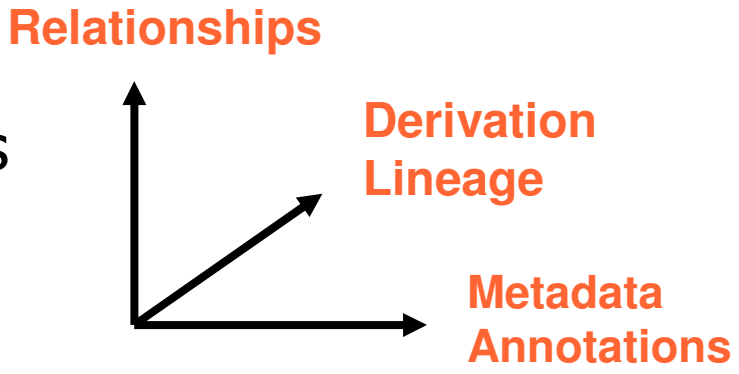
- Capture information about relationships among
  - Data (varying locations and representations)
  - Programs (& inputs, outputs, constraints)
  - Computations (& execution environments)
- Apply this information to:
  - Discovery of data and programs
  - Computation management
  - Provenance
  - Planning and scheduling
  - Performance optimization



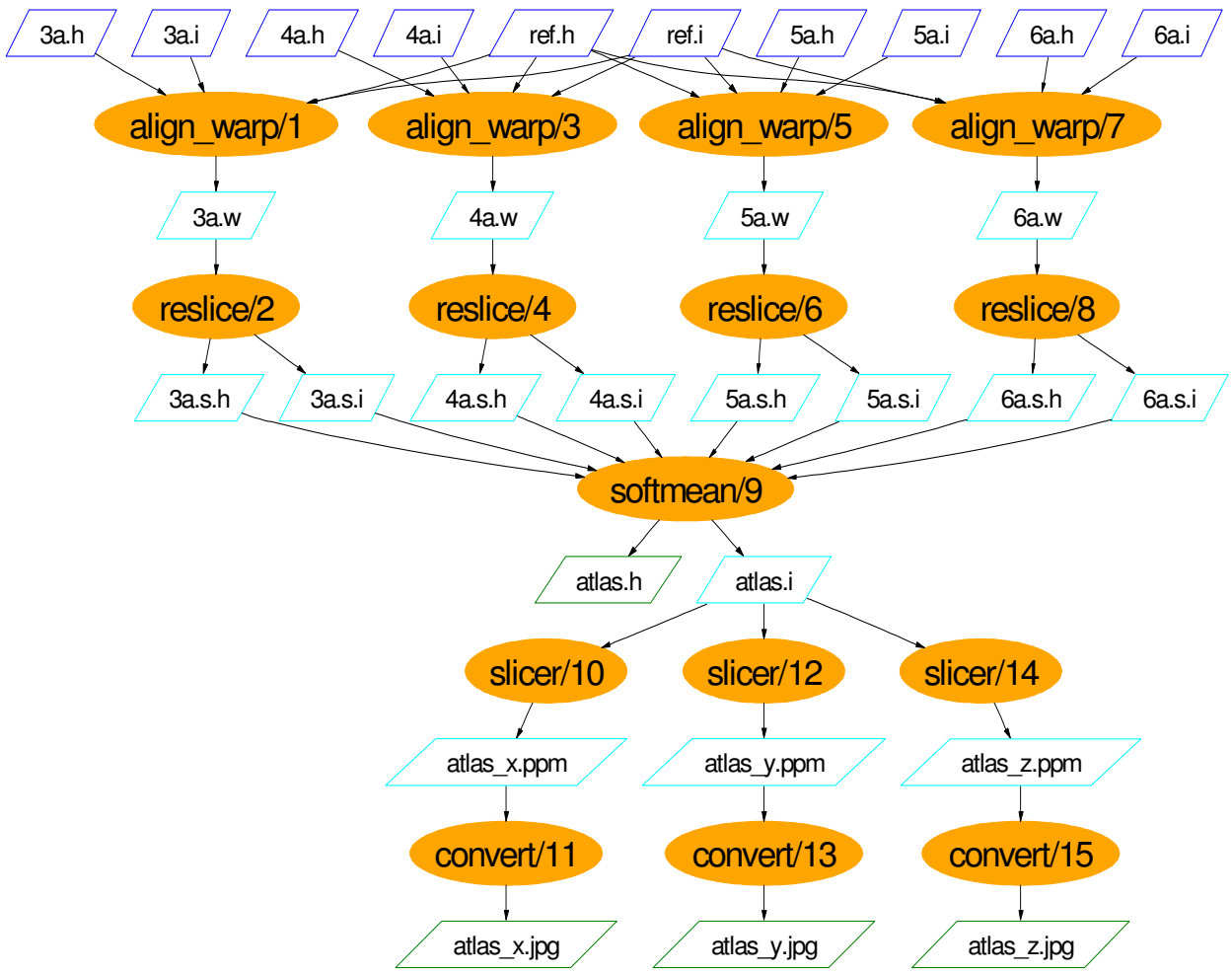
Provenance Model

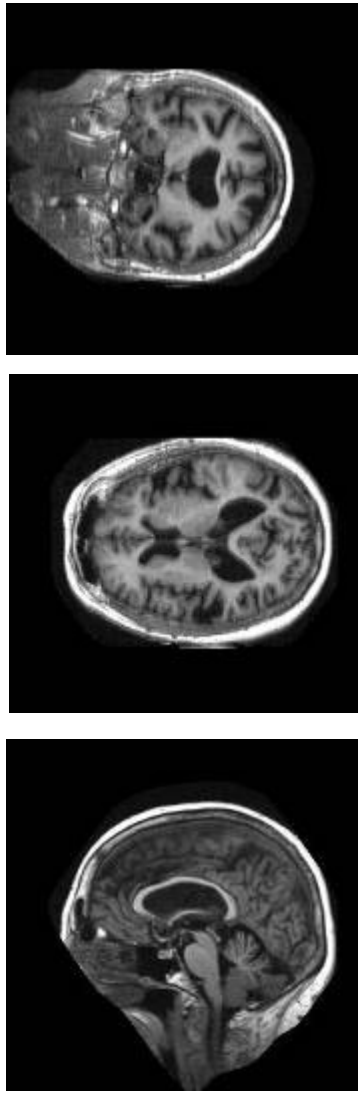
- Temporal aspect
  - **Prospective** provenance
    - Recipes for how to produce data
    - Metadata annotations about procedures and data
  - **Retrospective** provenance
    - Invocation records of run time environments and resources used: site, host, executable, execution time, file stats ...

- Dimensional aspect
  - **Virtual data** relationships
  - **Derivation** lineage
  - **Metadata** annotations



Query Context: fMRI Analysis





First Provenance Challenge, http://twiki.ipaw.info/

Query Examples

- Query by procedure signature
  - Show procedures that have inputs of type *subjectImage* and output types of *warp*
- Query by actual arguments
  - Show *align_warp* calls (including all arguments), with argument *model=rigid*
- Query by annotation
  - List anonymized subject images for young subjects:
    - Find datasets of type *subjectImage* , annotated with *privacy=anonymized* and *subjectType=young*
- Basic lineage graph queries
  - Find all datasets derived from dataset '5a'
- Graph pattern matching
  - Show me all output datasets of *softmean* calls that were aligned with *model=affine*
- Multi-dimensional query

Thailand joins the grid

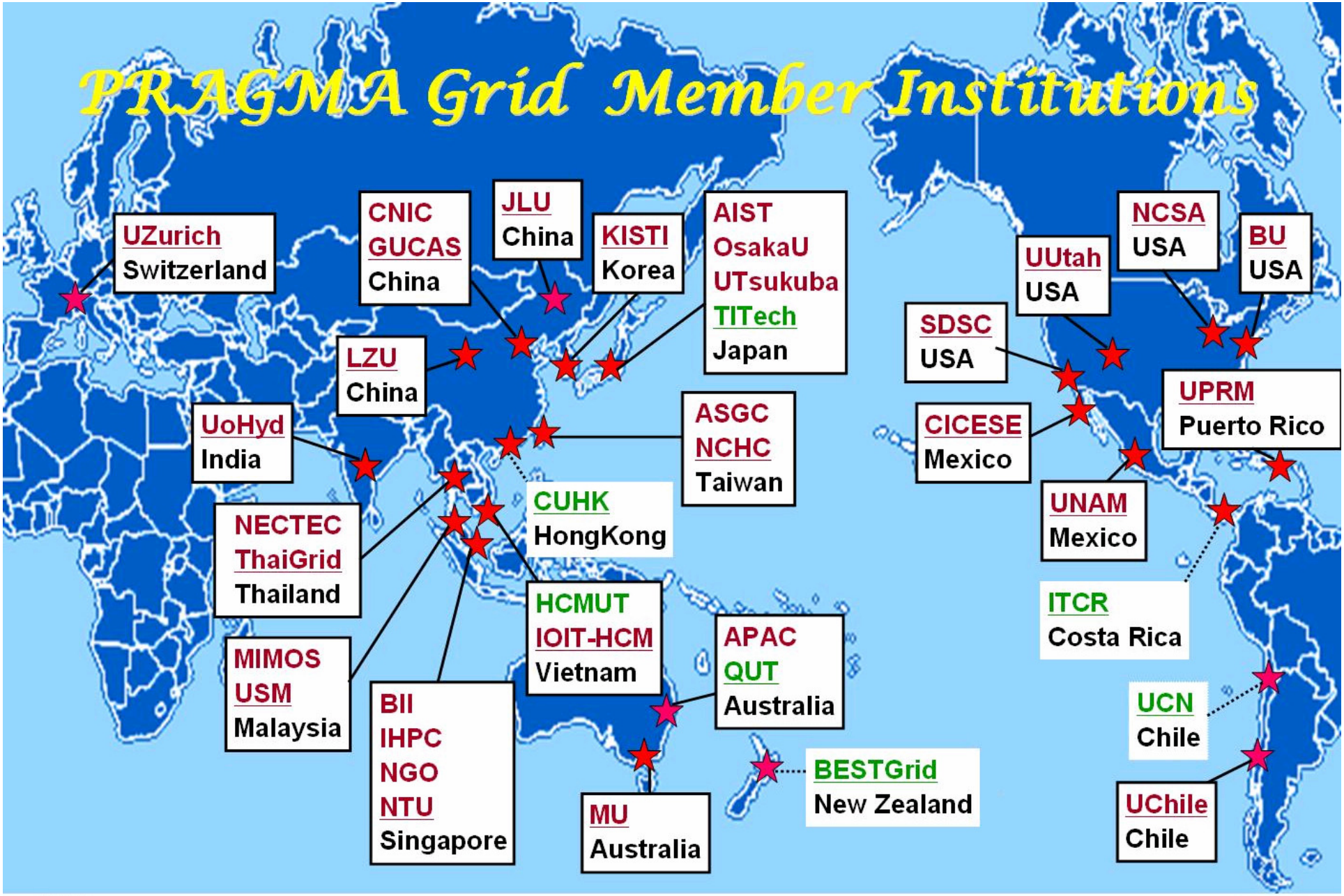
By Don Sambandaraksa, Bangkok Post
Wednesday, May 16 2007 11:34 AM

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

Globus Downloads Last Month

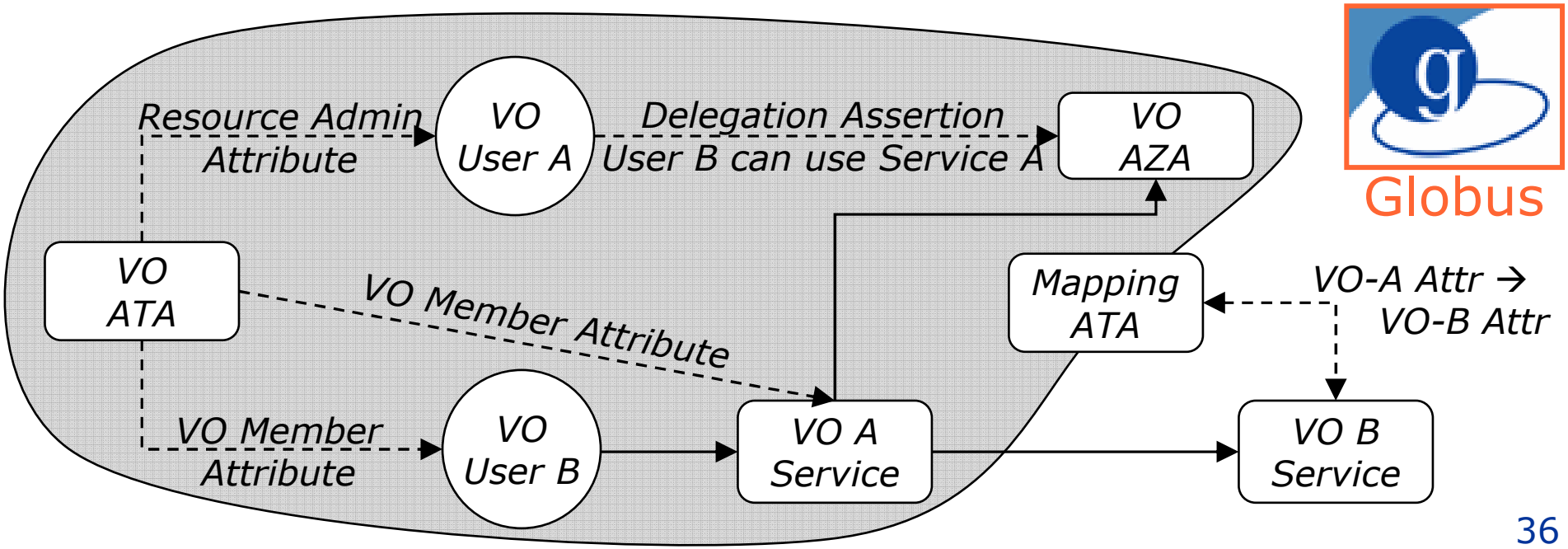
Grids are Communities of **People** as well as Computers

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

- Supported by software, standards, infrastructure

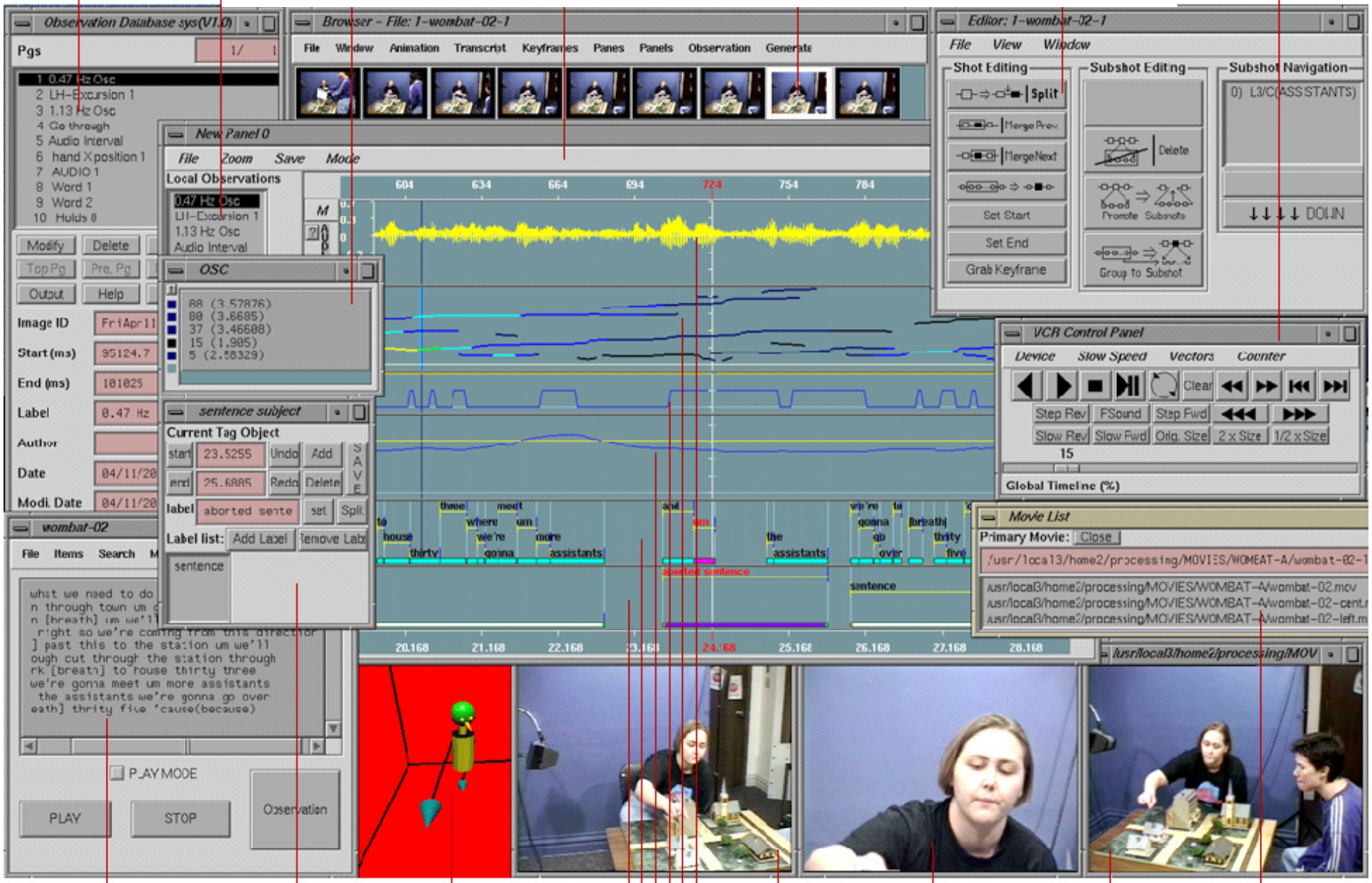
Security Services for Virtual Organization Policy

- Attribute Authority (ATA)
  - Issue signed attribute assertions (incl. identity, delegation & mapping)
- Authorization Authority (AZA)
  - Decisions based on assertions & policy
- Use with message- or transport-level security



Globus

Social Informatics Data Grid



Bennett Berthenthal et al., www.sidgrid.org

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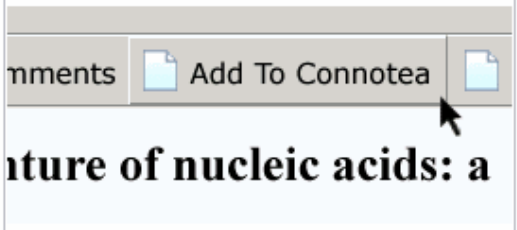
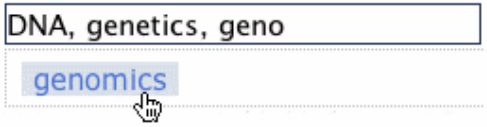


3 Add your own keywords for easy retrieval



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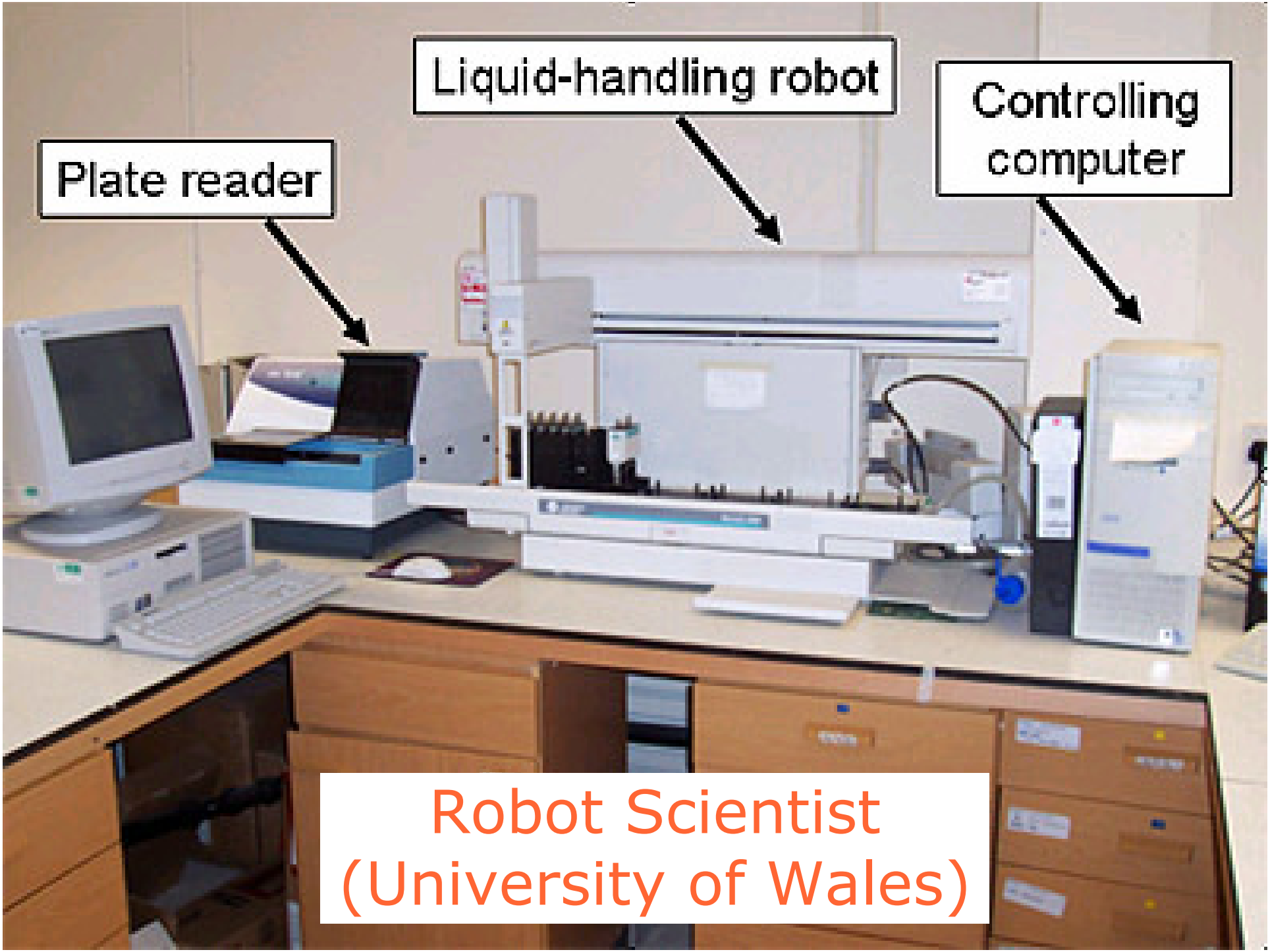
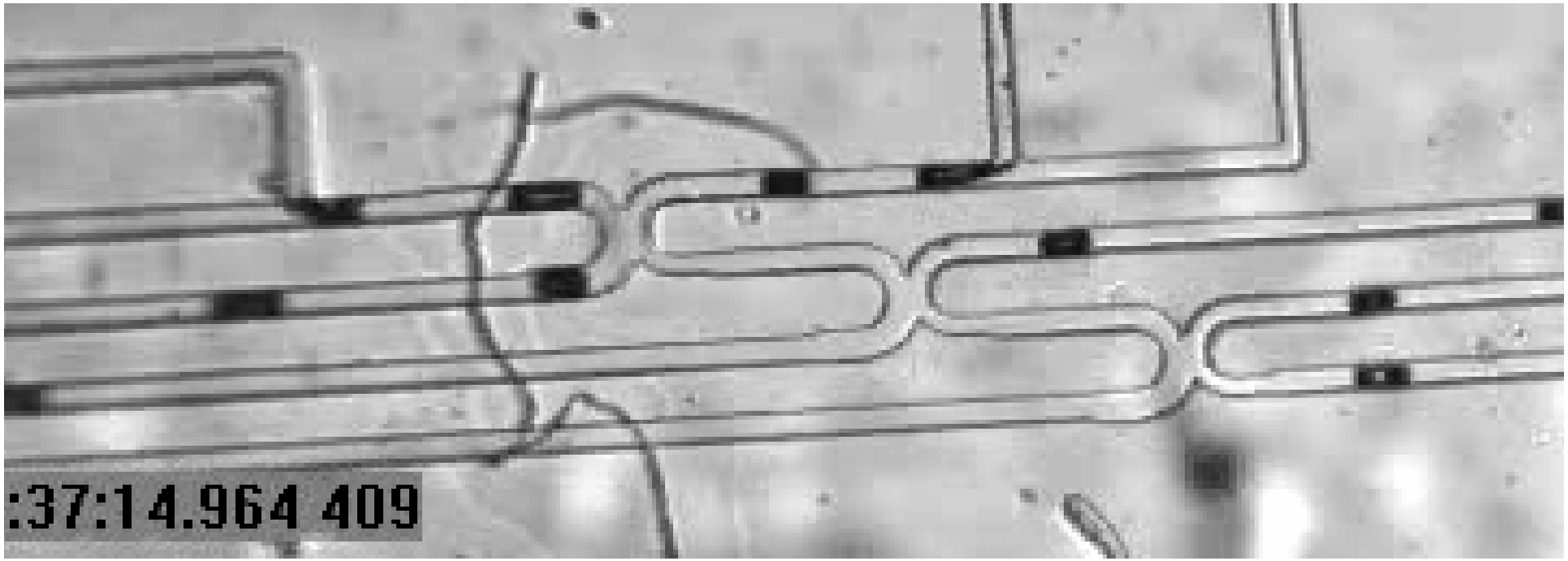
Automating Science Protocols

Protocol: "a predefined written procedural method in the design and implementation of experiments. This should establish standards that can be adequately assessed by peer review and provide for successful replication of results by others in the field."

(Wikipedia)


Liquid-handling robot
Plate reader
Controlling computer
Robot Scientist
(University of Wales)

Microfluidic Bubble Logic (Prakash and Gershenfeld)

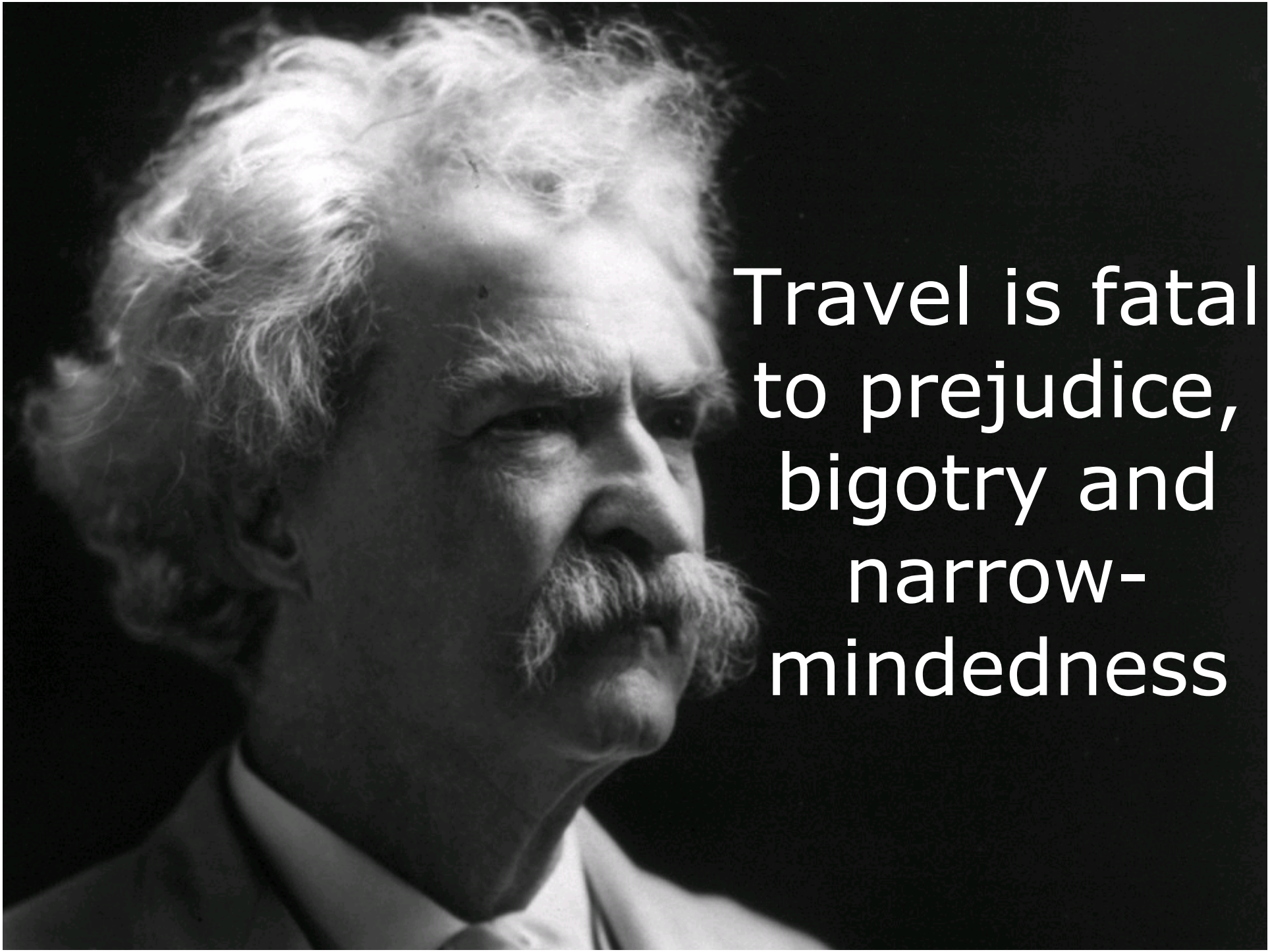


Man-Computer Symbiosis: 50 Years On

- Service oriented science
- Provenance
- Virtual organizations
- Automating science protocols

Concluding Thoughts

- Networks are necessary but not sufficient
- There is only global software
- We build communities by doing experiments
- Persistent infrastructure is needed
- Persistent workers are needed
- Showing up
- Team New Zealand?
- Where are the students?


Travel is fatal
to prejudice,
bigotry and
narrow-
mindedness