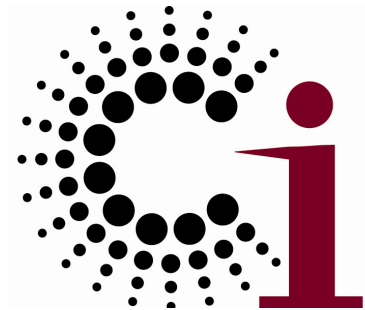


Scaling eScience Impact

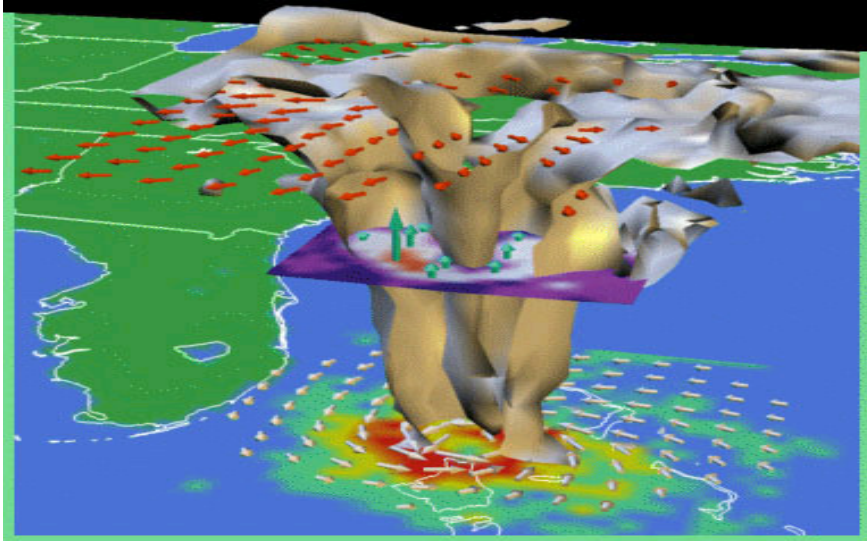
Ian Foster



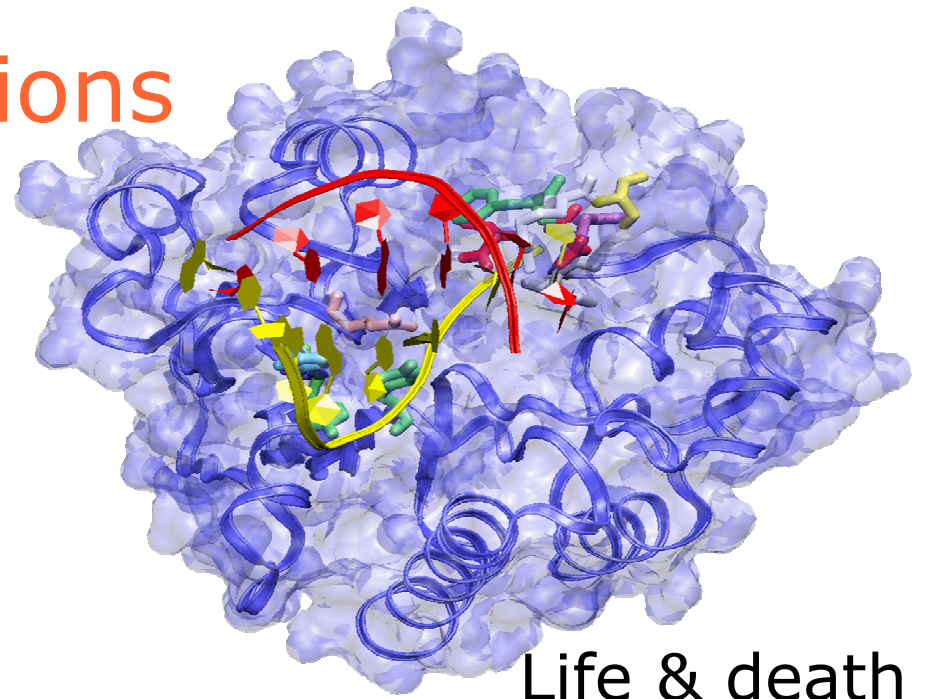
Computation Institute

Argonne National Lab & University of Chicago

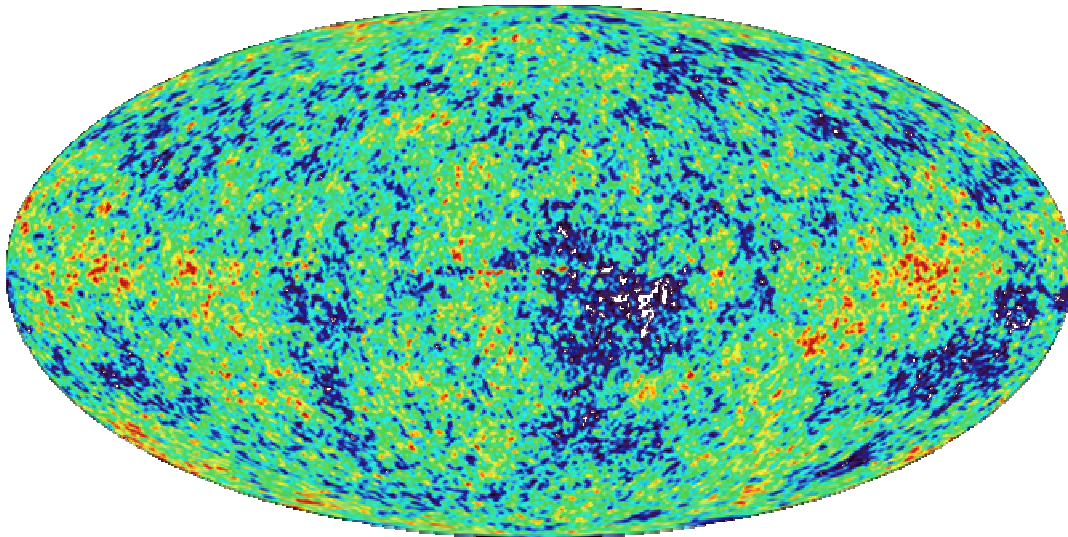
The Big Questions



Future of the planet



Life & death



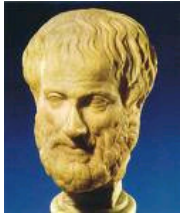
Nature of the universe



Consciousness



How Do We Answer Them?



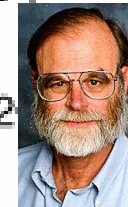
Empirical



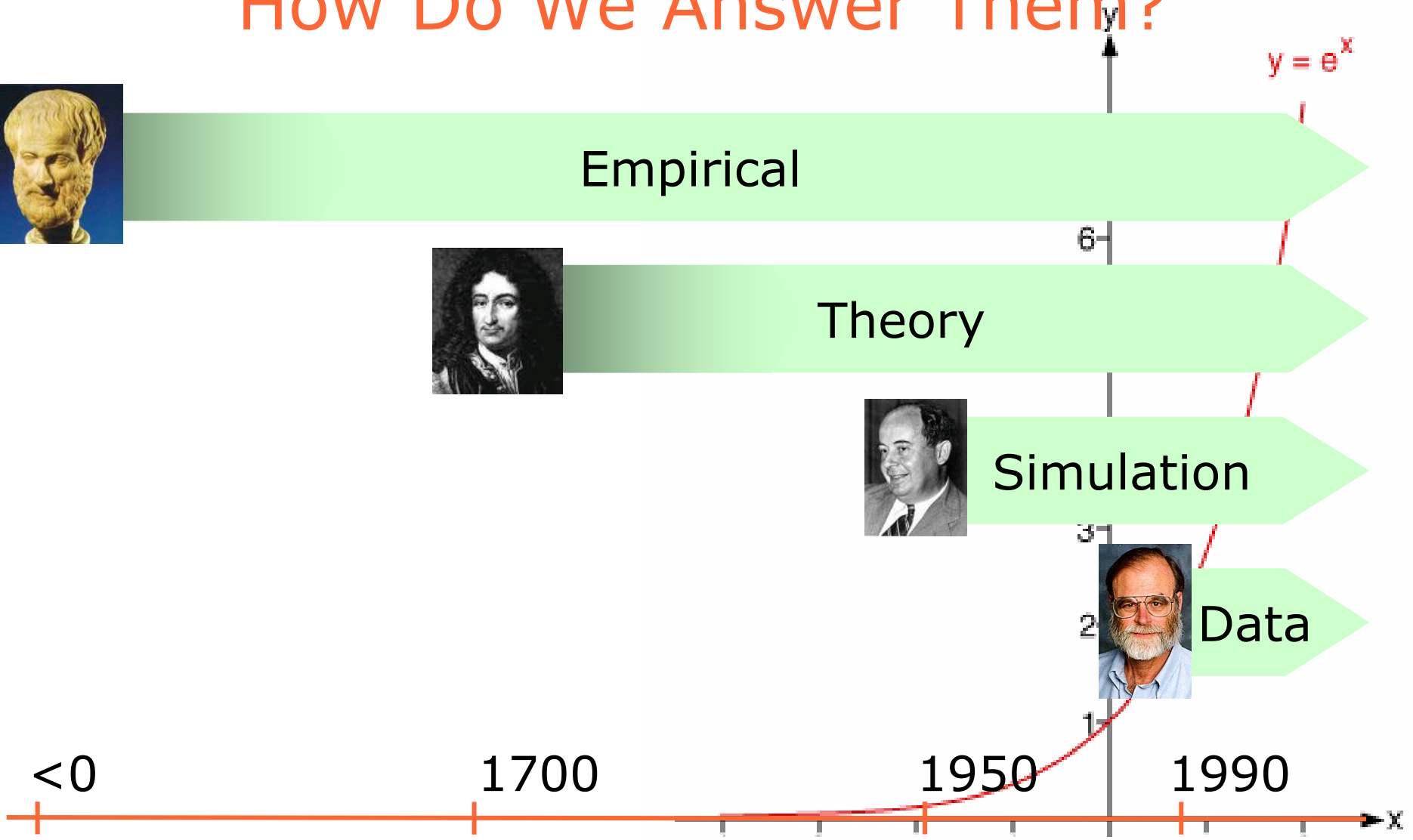
Theory



Simulation



Data



The Same is True of Smaller Questions

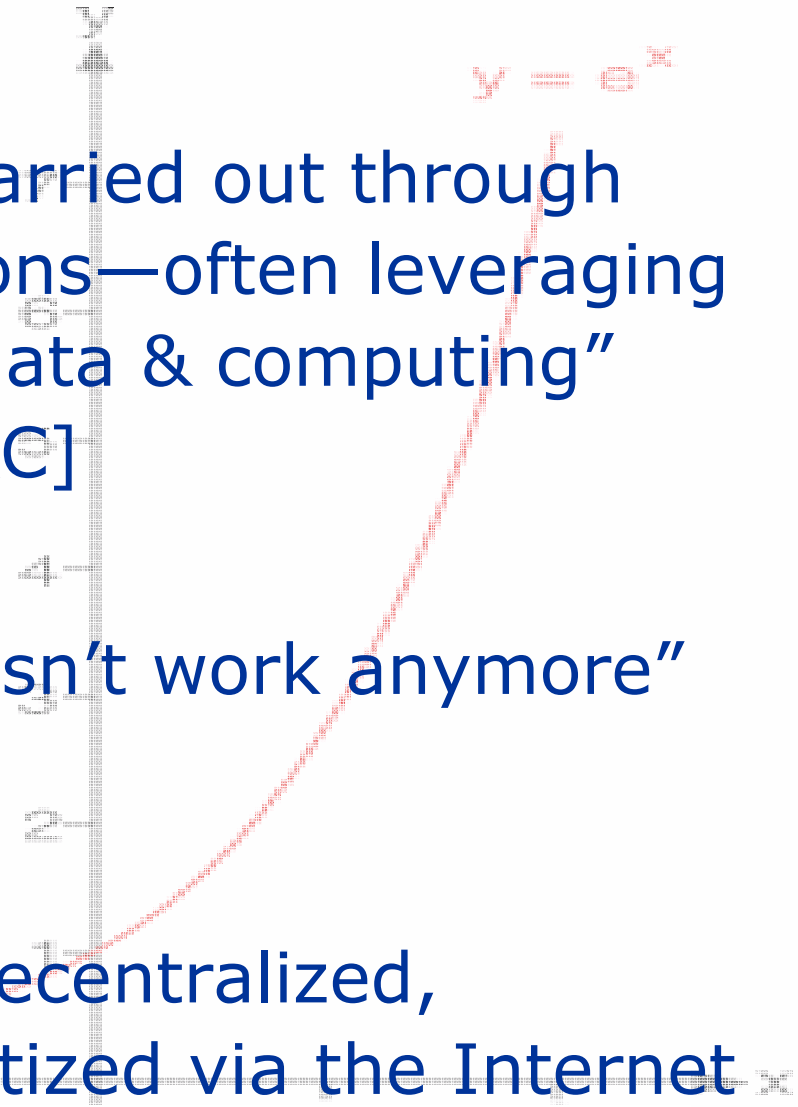


- Designing new chemical catalysts
- Selling advertising
- Creating entertainment
- Finding parking



eScience: Science in an Exponential World

- “Large-scale science carried out through distributed collaborations—often leveraging access to large-scale data & computing”
[John Taylor, UK EPSRC]
- “When brute force doesn’t work anymore”
[Alex Szalay]
- Science accelerated, decentralized, integrated, & democratized via the Internet



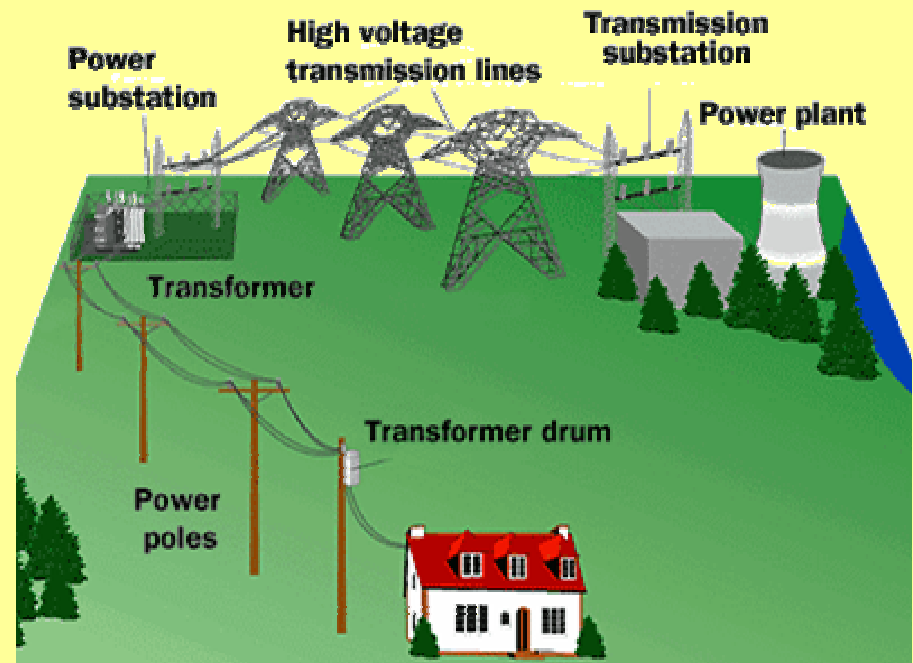
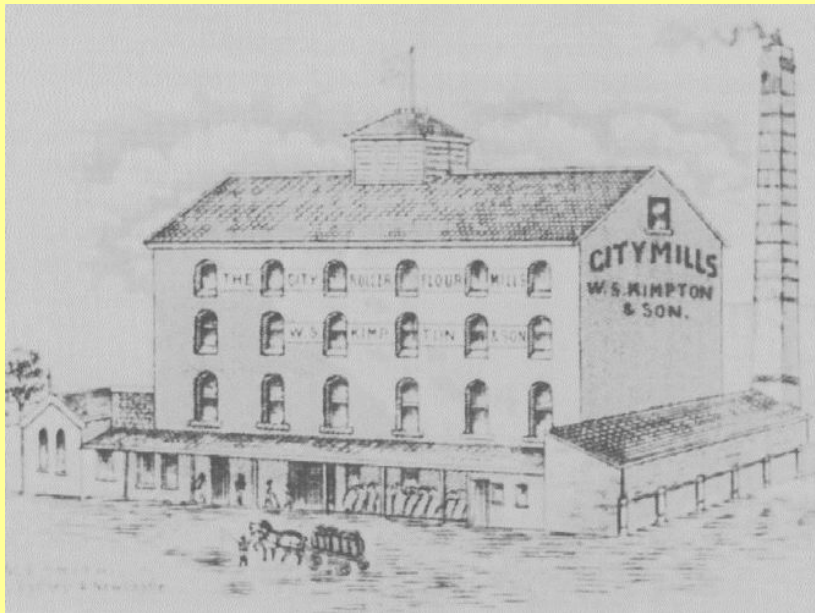


Grid: An Enabler of eScience



The dubious electrical power grid analogy

Must we buy (or travel to) a power source?



Or can we ship power to where we want to work?

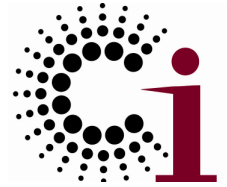
Enable on-demand access to, and integration of, diverse resources & services, regardless of location



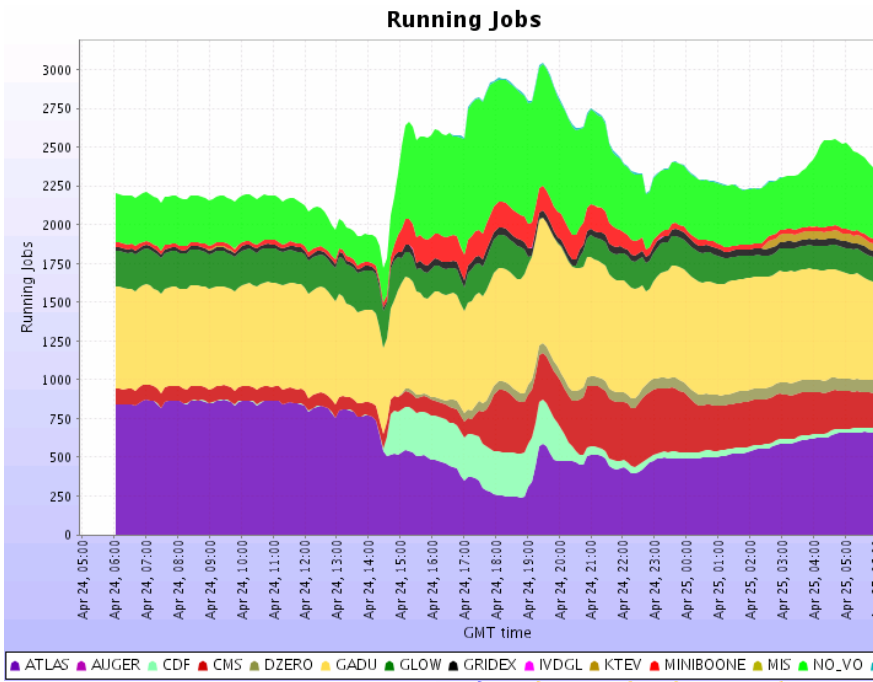
the globus alliance

www.globus.org

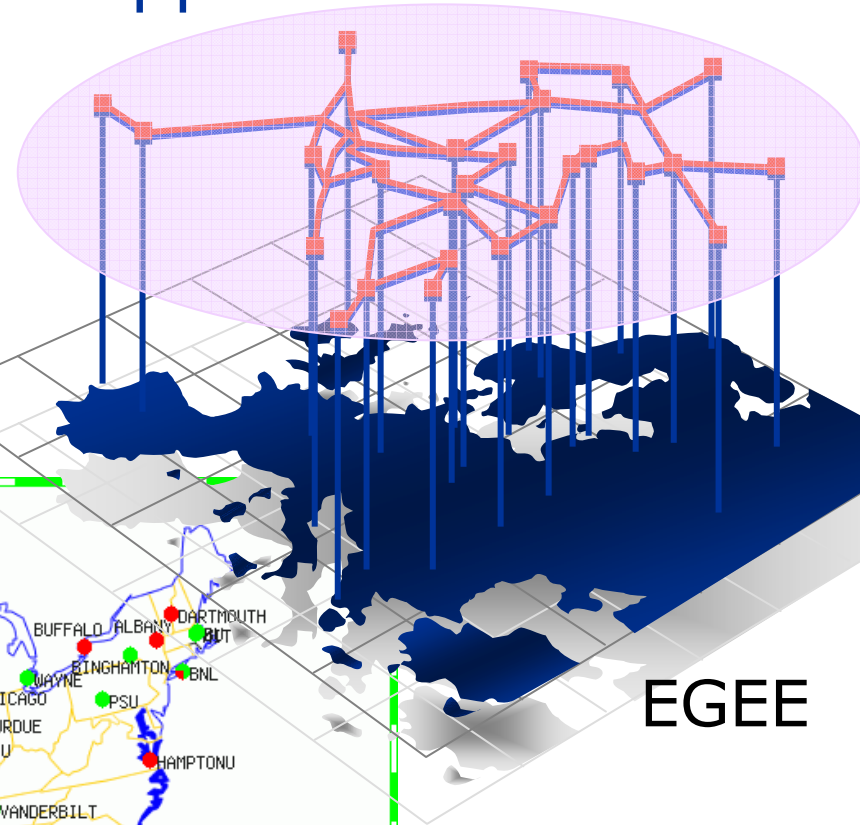
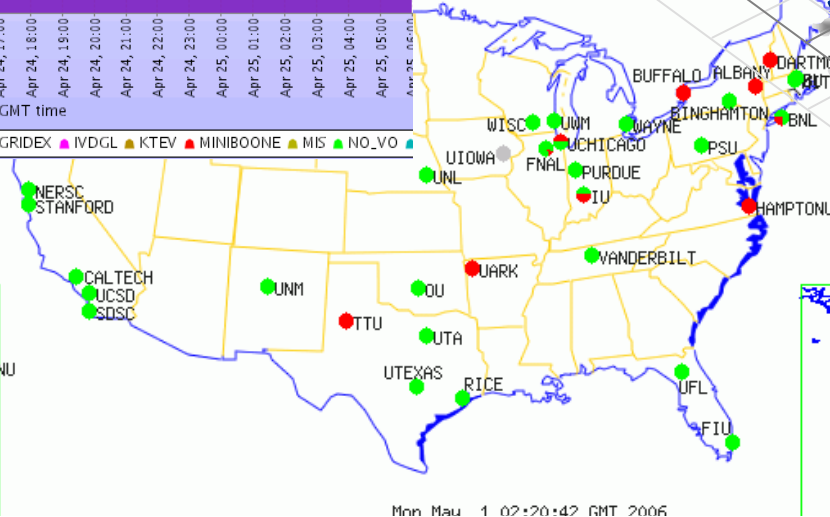
1st Generation Grids



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



Open Science Grid



Second-Generation Grids

- Empower many more users by enabling on-demand access to **services**
- Science gateways (TeraGrid)
- Service oriented science
- Or, "Science 2.0"



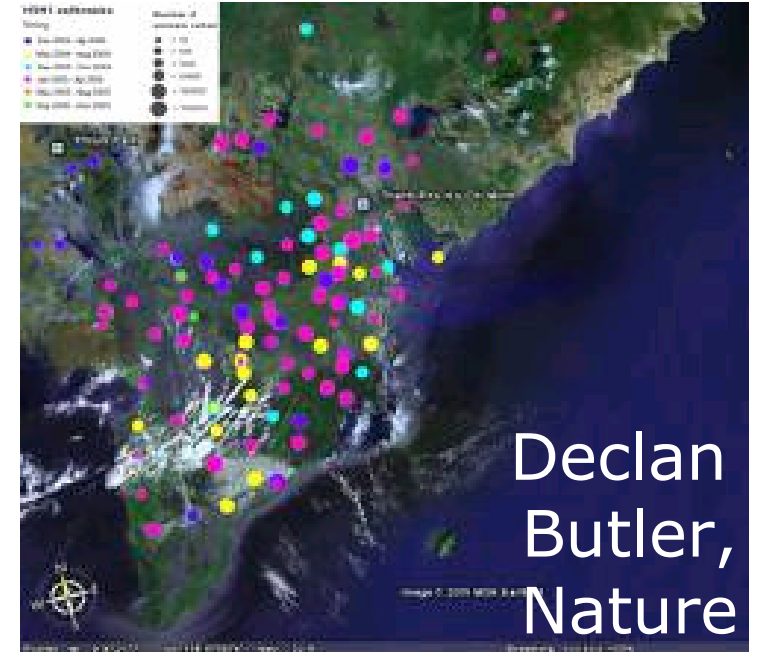


the globus alliance

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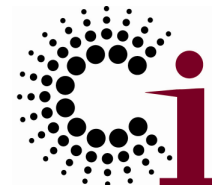
"Web 2.0"

- 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





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www.globus.org



Science 2.0: E.g., Virtual Observatories

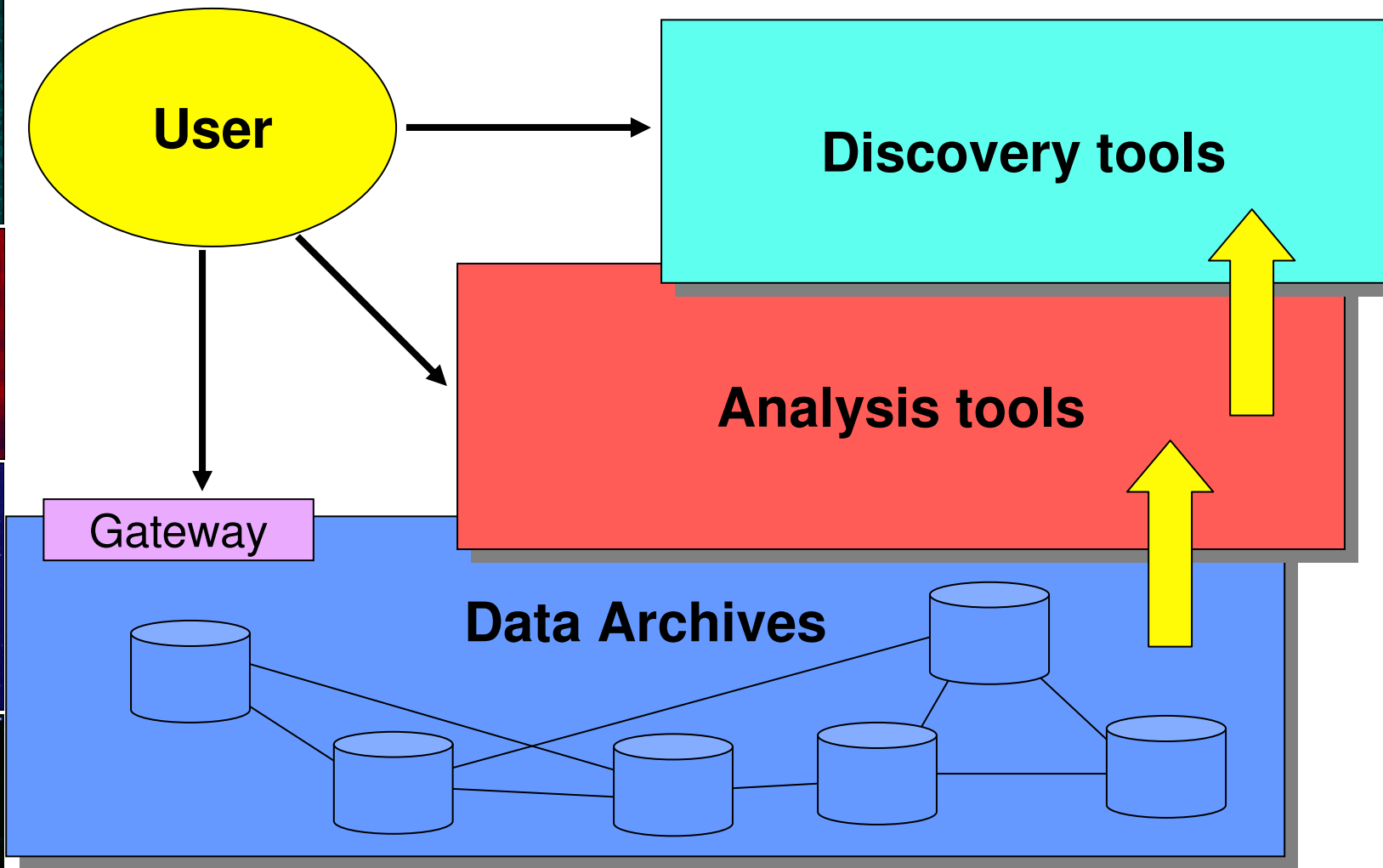
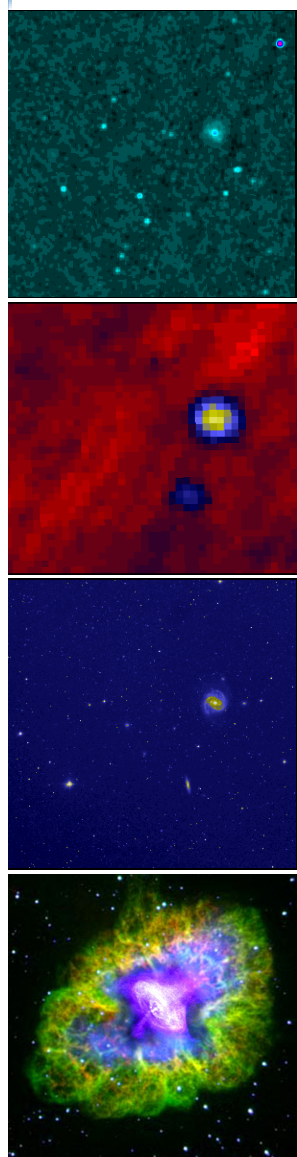


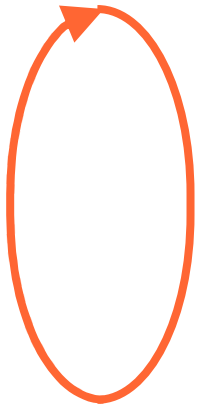
Figure: S. G. Djorgovski



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www.globus.org



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!



TeraGrid™
EMPOWERING DISCOVERY



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

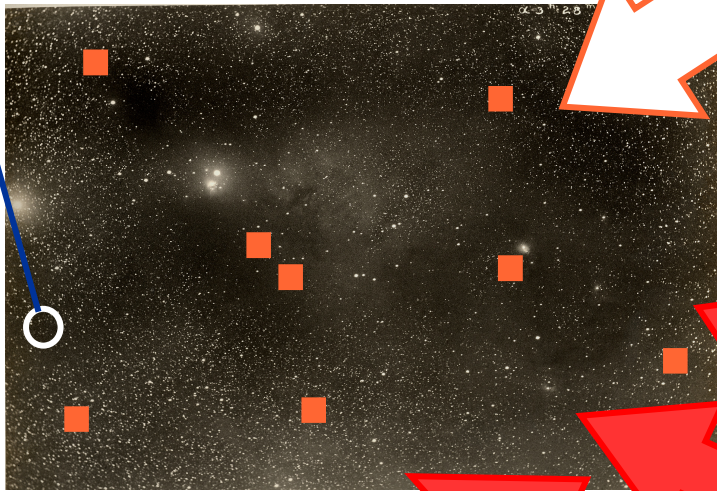


"Service-Oriented Science", *Science*, 2005

The Importance of "Hosting" and "Management"

Tell me about this star

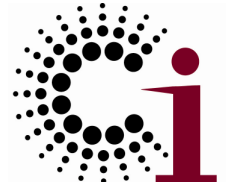
Tell me about these 20K stars



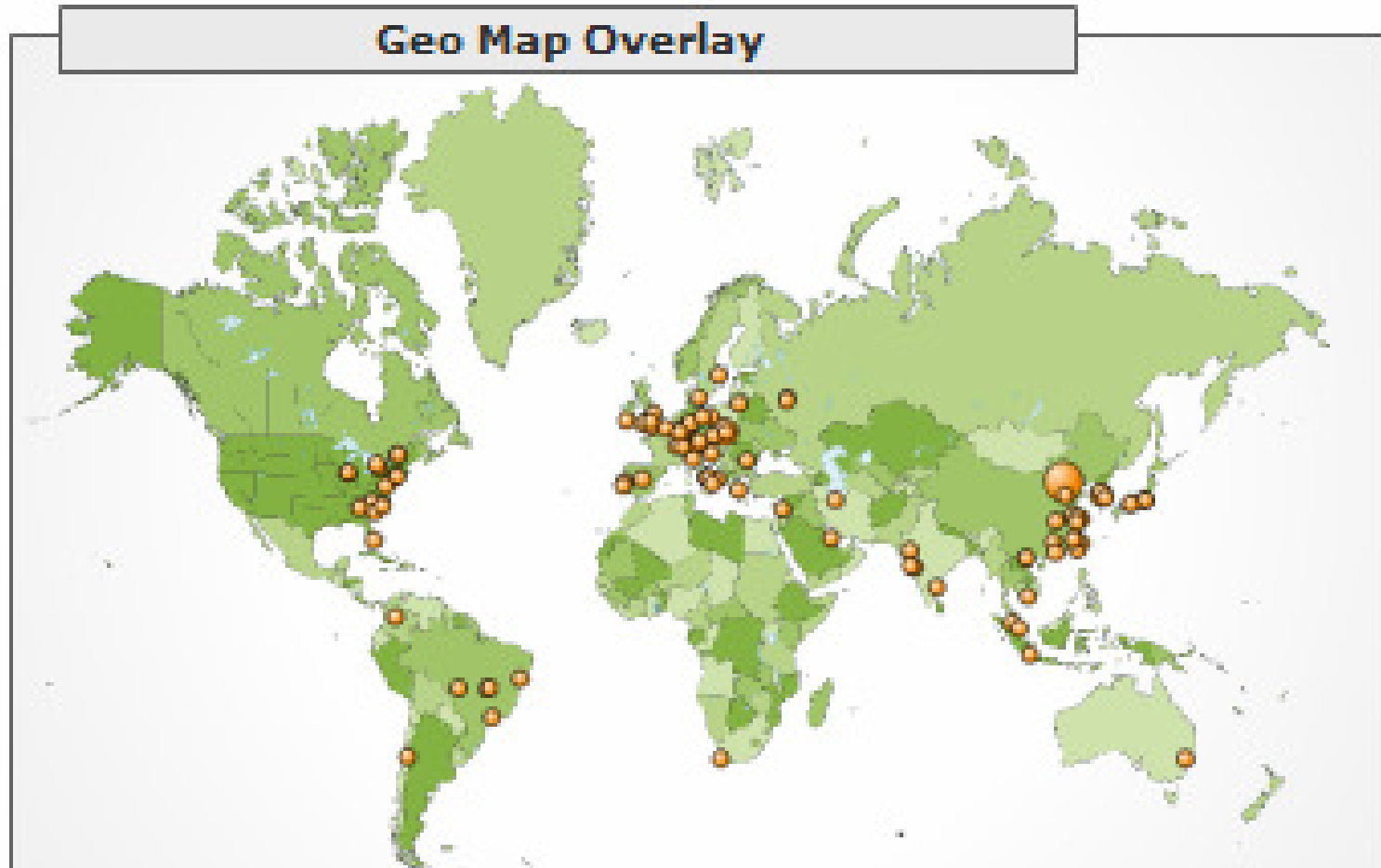
Support 1000s of users

E.g., Sloan Digital Sky Survey, ~10 TB; others much bigger



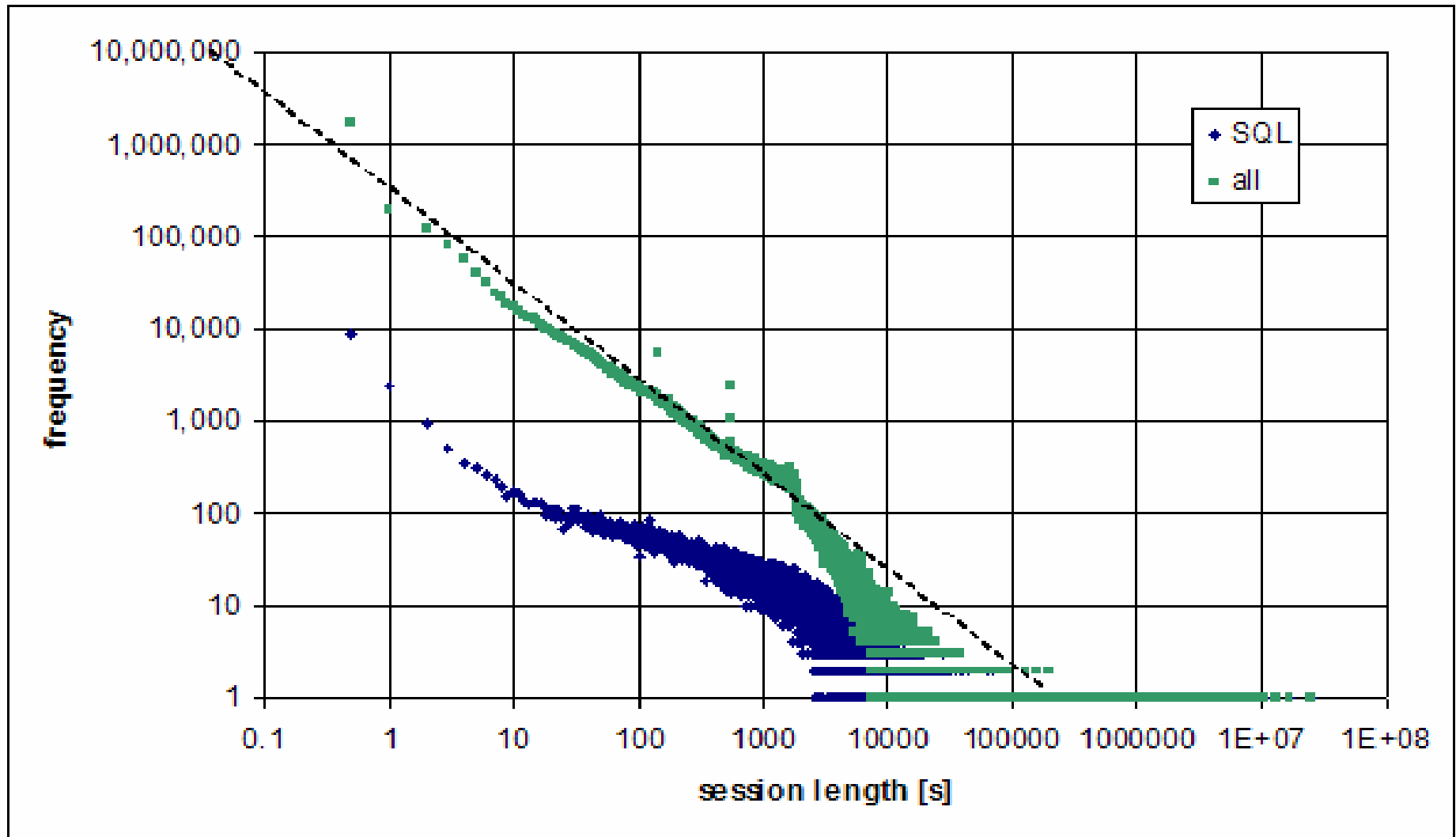


Load Comes from All Over ...

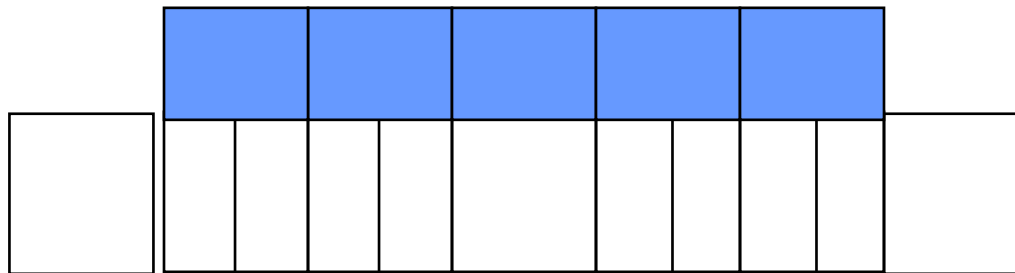


A few hours of Globus.org access, early one morning ...¹³

Skyserver Sessions (Thanks to Alex Szalay)



The Two Dimensions of Service Oriented Science

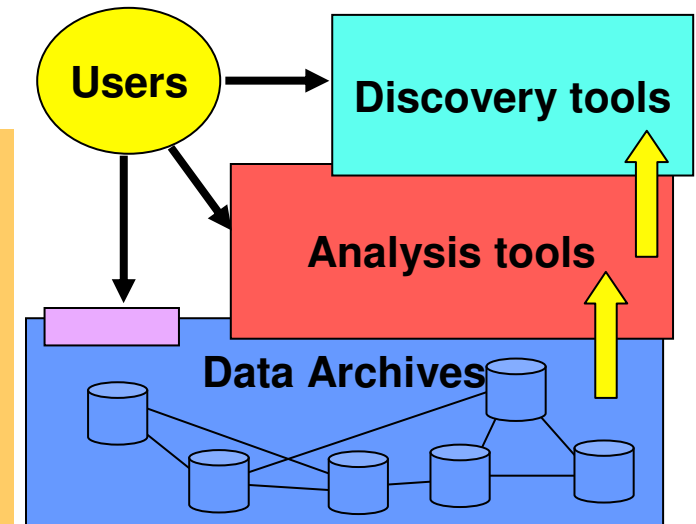


Function
Resource

- **Decompose** across network

Clients **integrate** dynamically

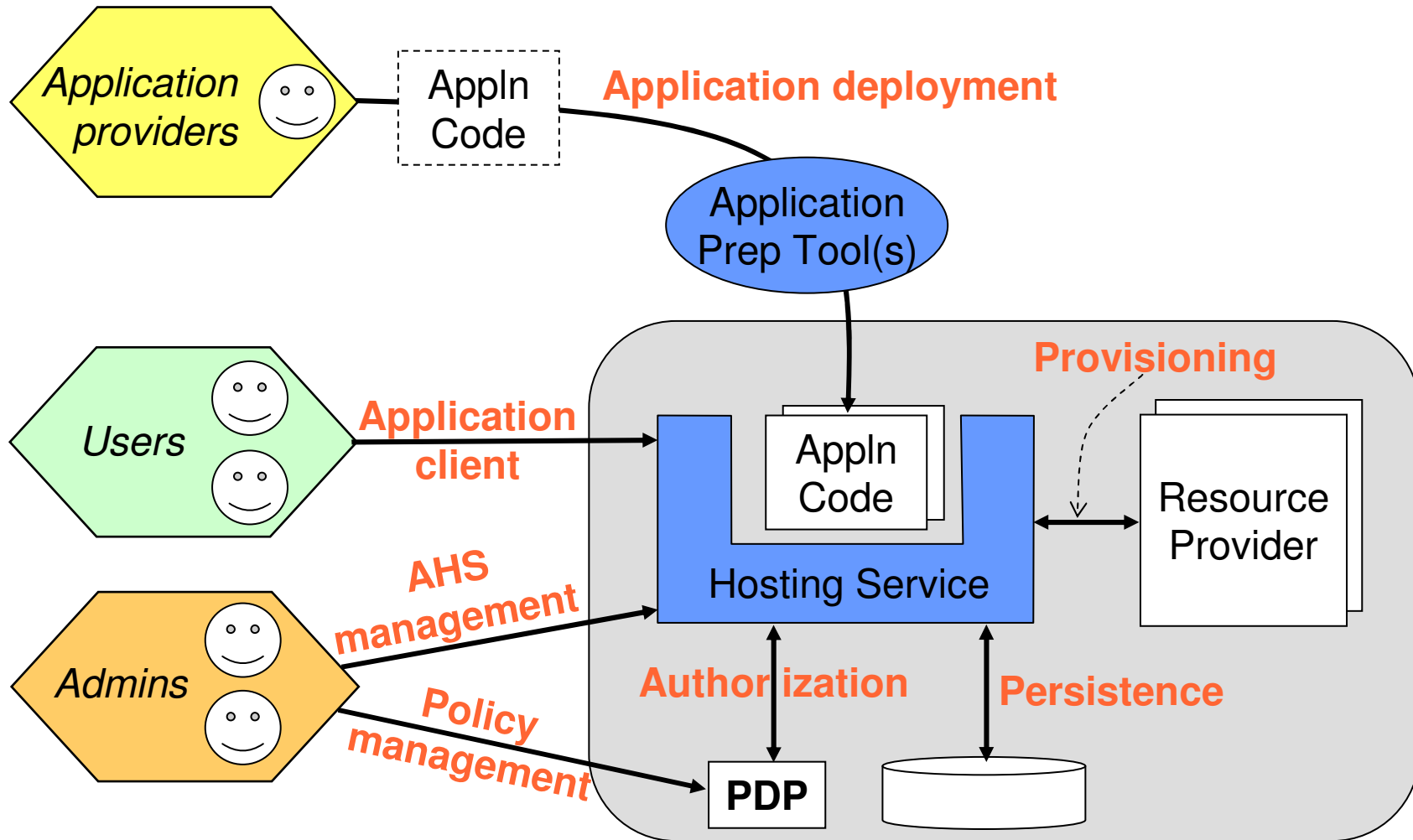
- ◆ Select & compose services
- ◆ Select "best of breed" providers
- ◆ Publish result as new services



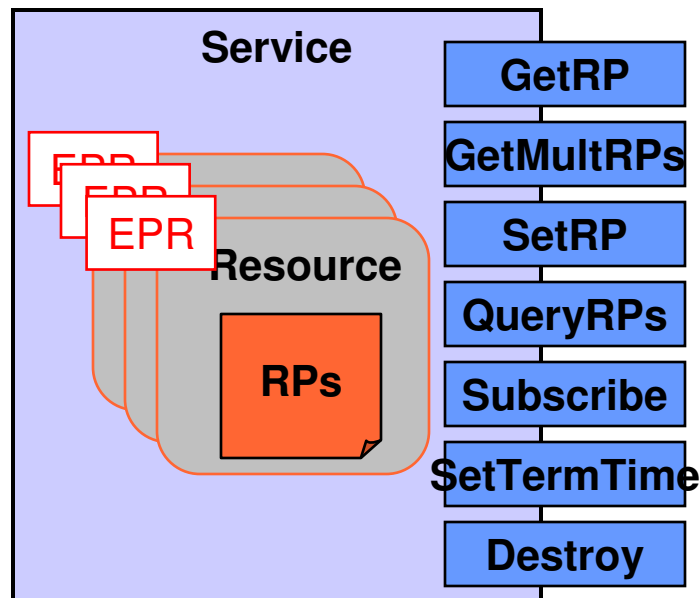
- Decouple **resource** & **service** providers

Fig: S. G. Djorgovski

Hosting & Management: Application Hosting Services



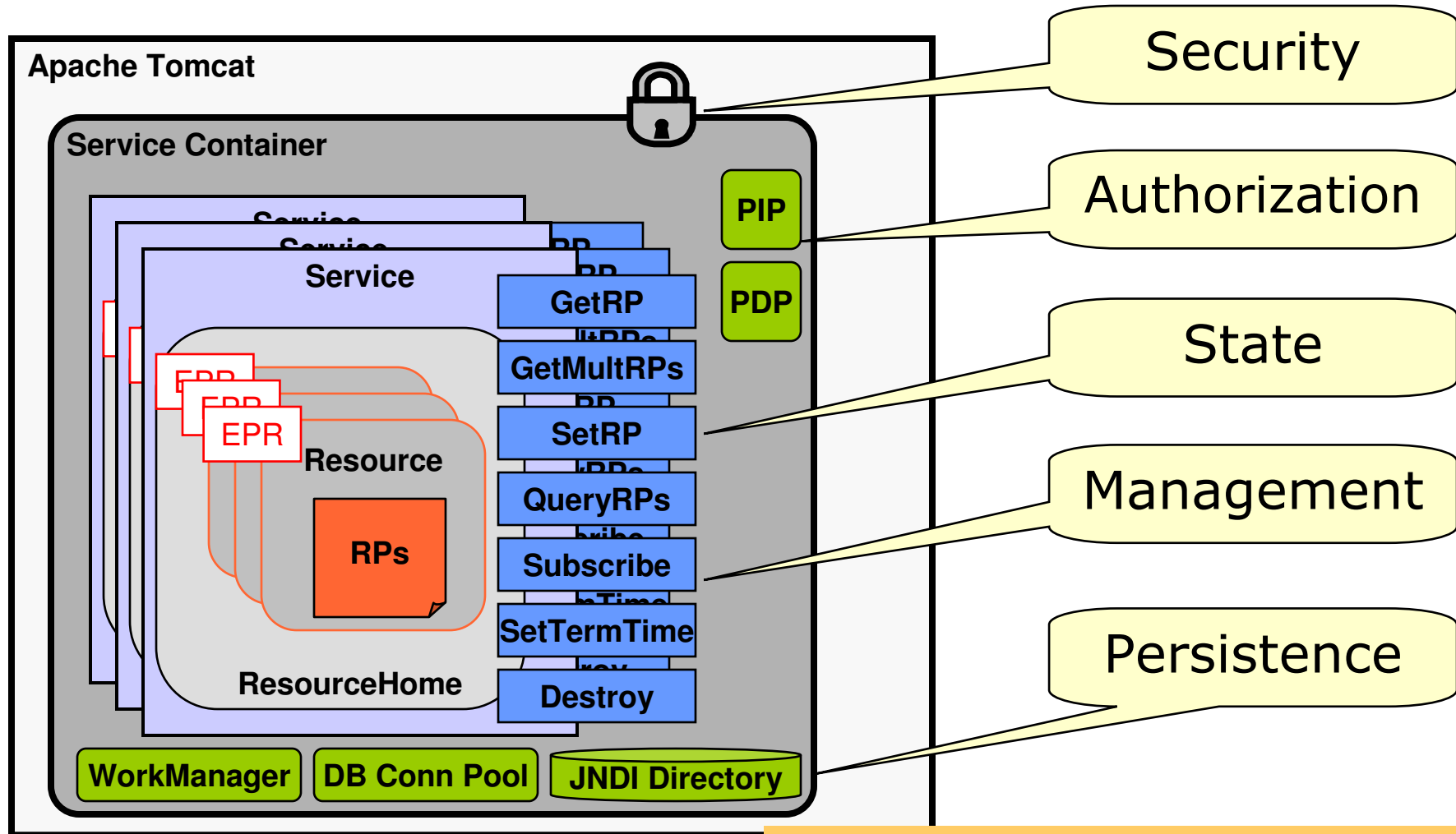
Web Services Resource Framework in a Nutshell



- Service
- State representation
 - ◆ Resource
 - ◆ Resource Property
- State identification
 - ◆ Endpoint Reference
- State Interfaces
 - ◆ GetRP, QueryRPs, GetMultipleRPs, SetRP
- Lifetime Interfaces
 - ◆ SetTerminationTime
 - ◆ ImmediateDestruction
- Notification Interfaces
 - ◆ Subscribe
 - ◆ Notify
- ServiceGroups



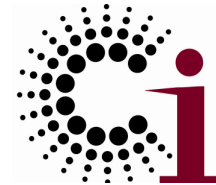
Globus Toolkit Web Services Container



GT4 Web Services Container



RAVE

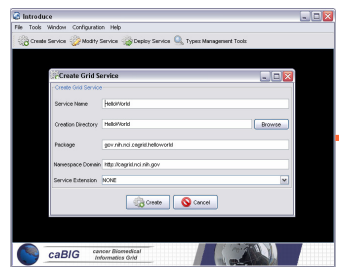


- **Remote Application Virtualization Environment**

- **Builds on Introduce**

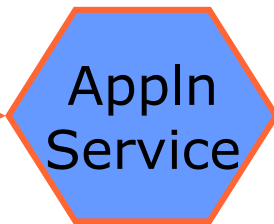
- ◆ Define service
- ◆ Create skeleton
- ◆ Discover types
- ◆ Add operations
- ◆ Configure security

- **Wrap arbitrary executables**

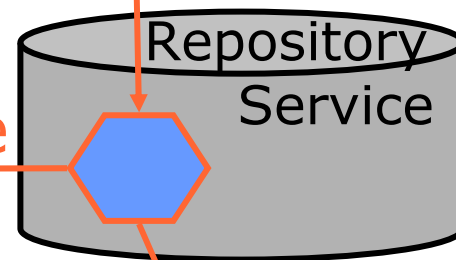


Introduce

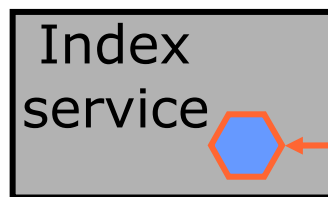
Create



Store



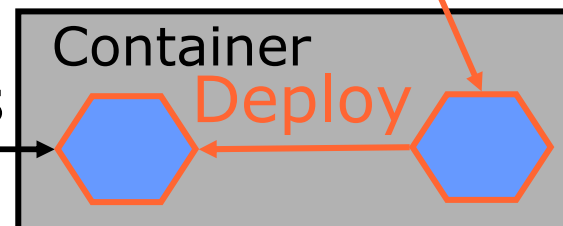
Advertize



Discover



Invoke;
get results



Transfer
GAR

Deploy

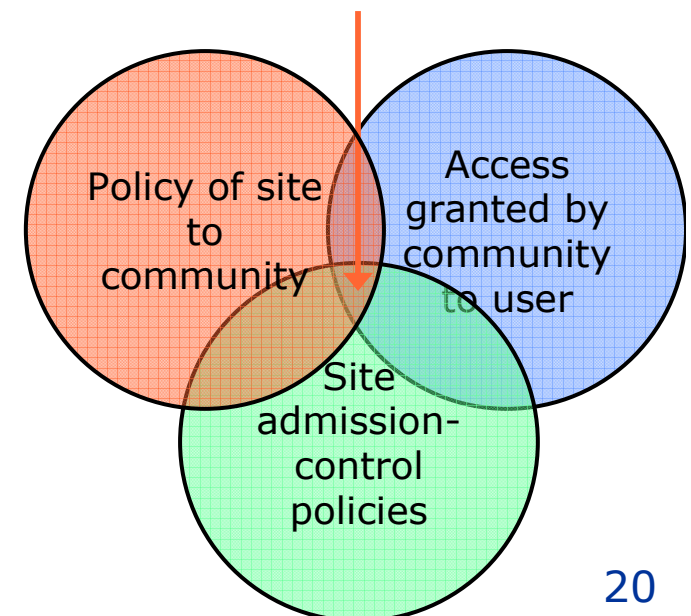
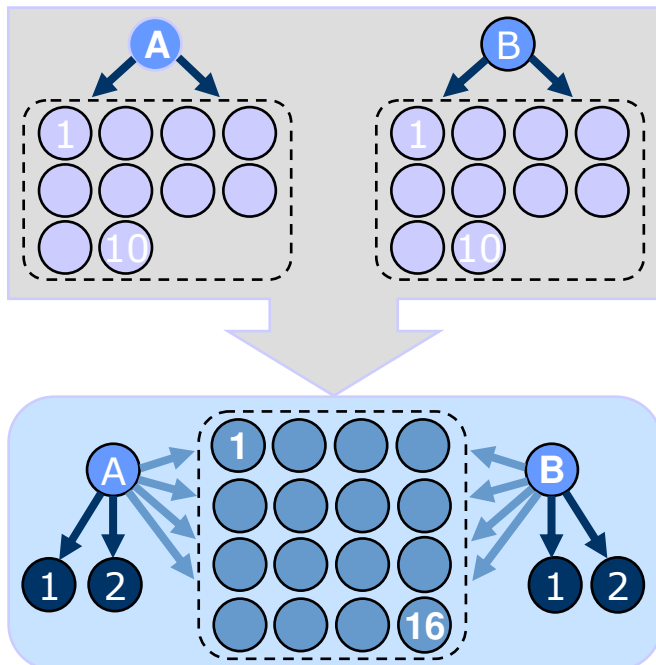


Defining Community: Membership and Laws



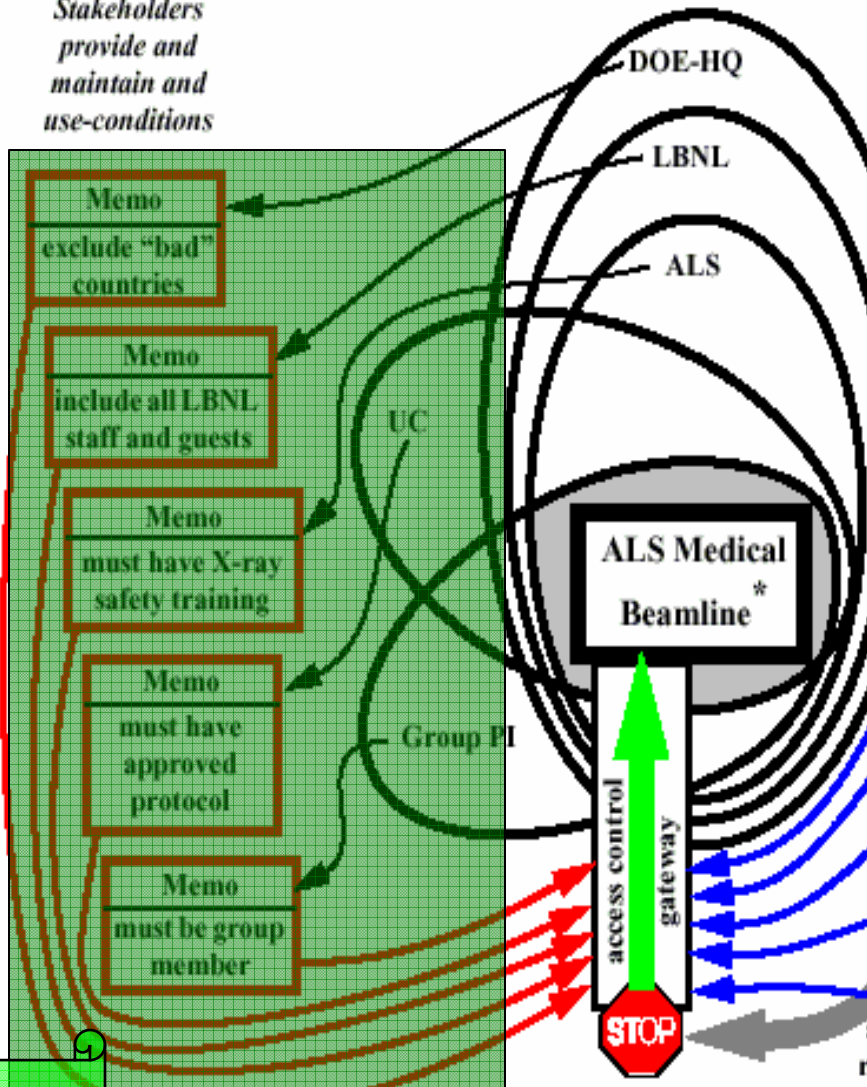
- Identify VO participants and roles
 - ◆ For people and services
- Specify and control actions of members
 - ◆ Empower members → delegation
 - ◆ Enforce restrictions → federate policy

Effective
Access



(1) Use-conditions are Imposed by Independent Stakeholders

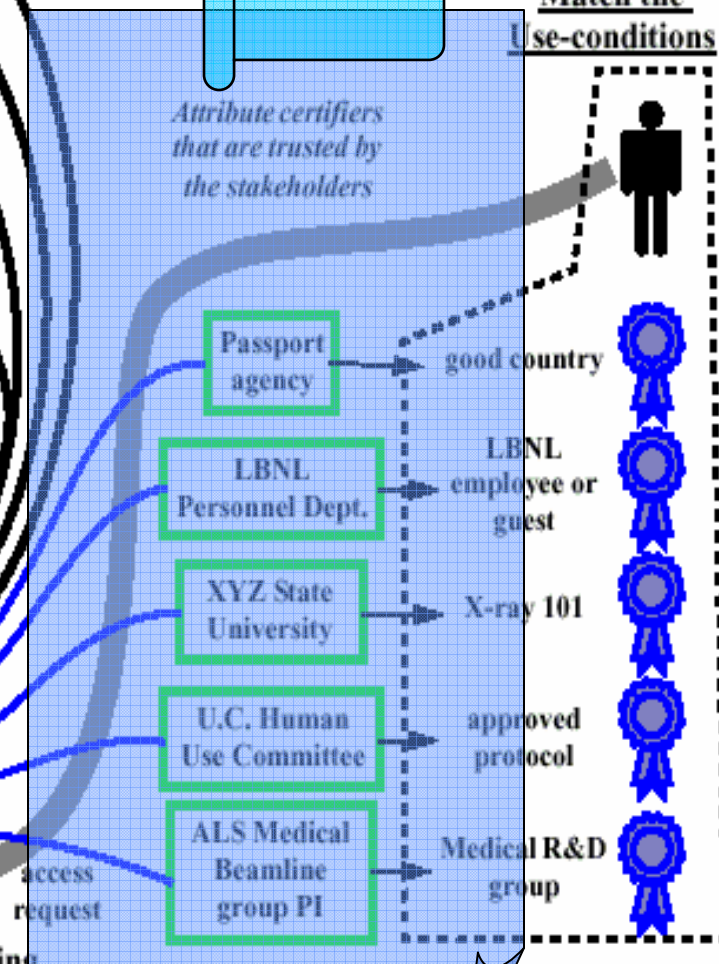
Stakeholders provide and maintain and use-conditions



(2) Users have Attributes that Match the Use-conditions

SAML

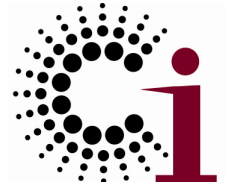
Attribute certifiers that are trusted by the stakeholders



(3) Access is Granted after Verifying that User Attributes Match the Required Use-Conditions

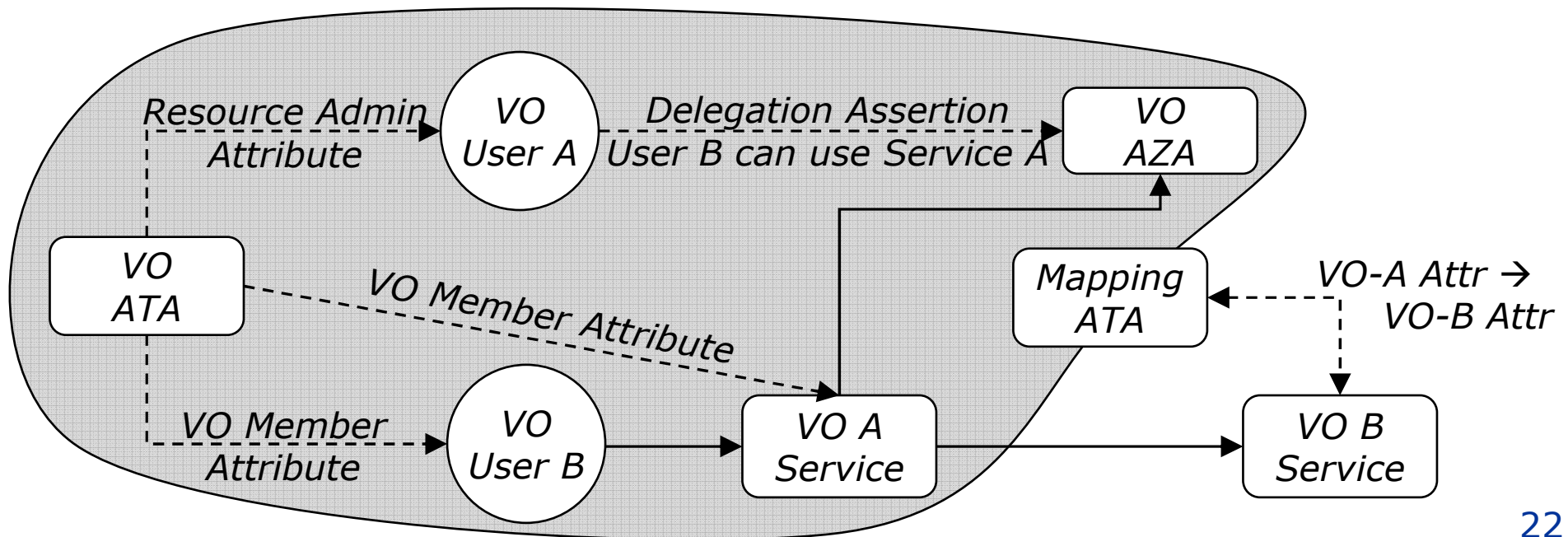
XACML

1 Societal Access Control Model

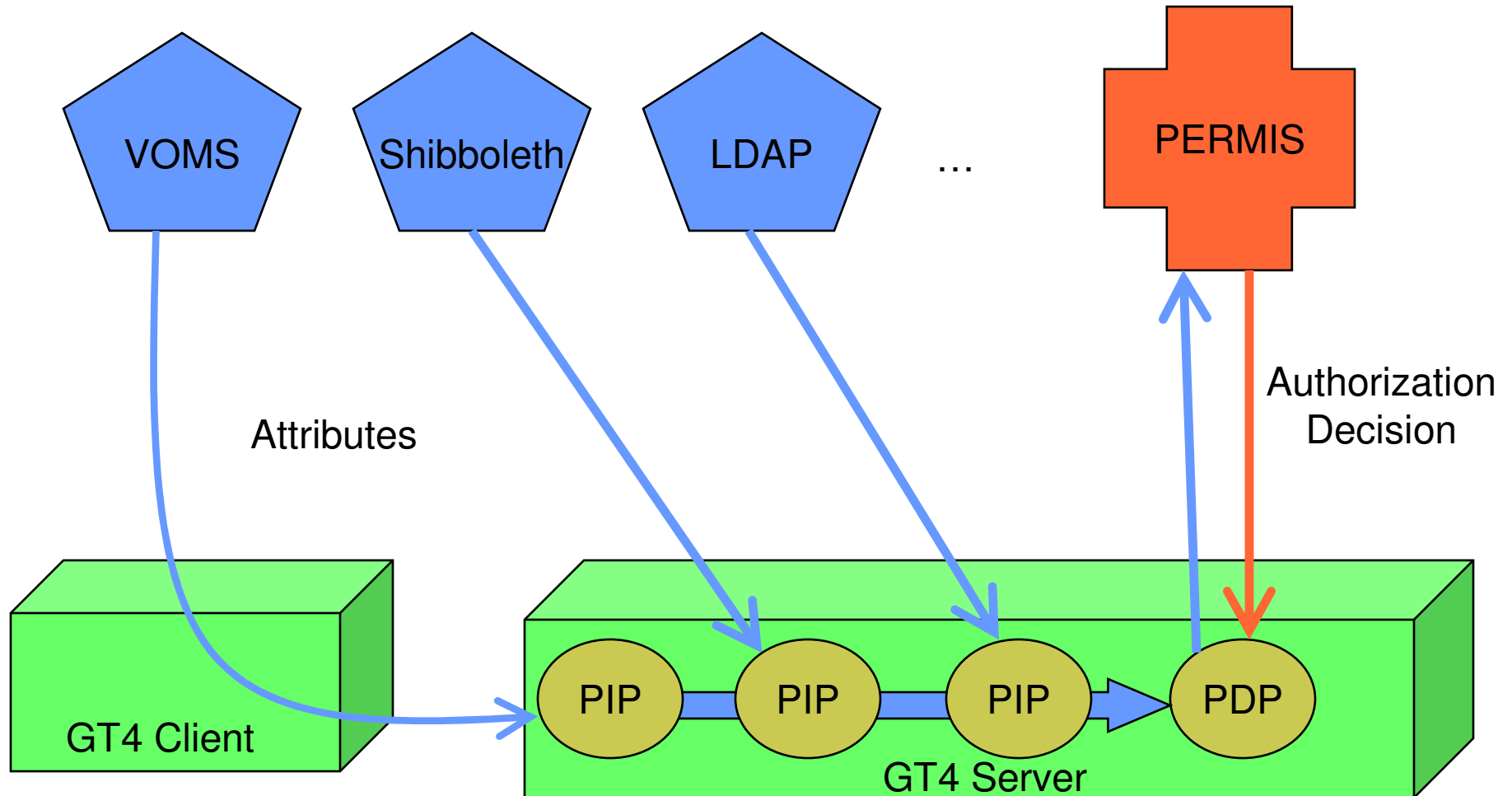


Security Services for VO Policy

- 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 Authorization Framework

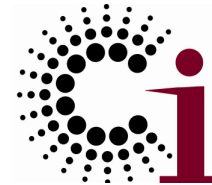




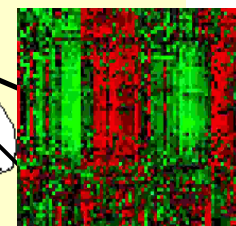
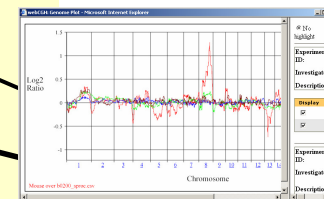
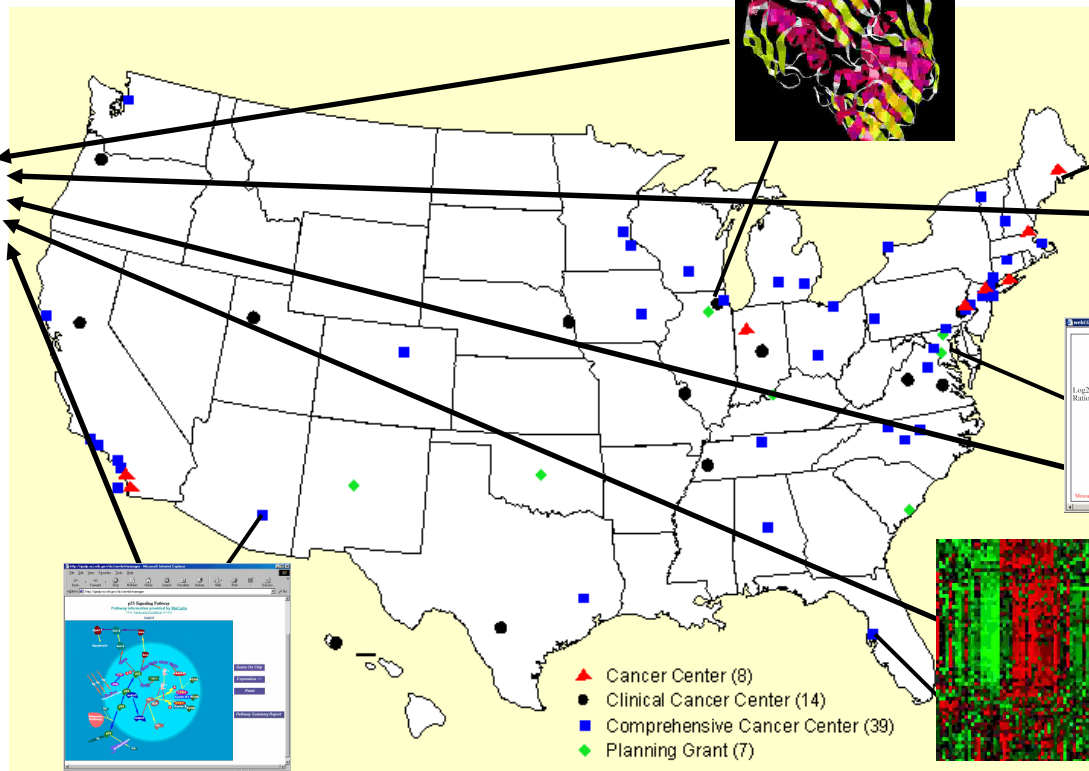
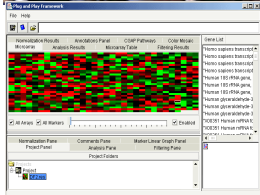
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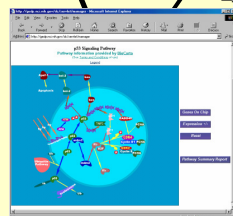
Service-Oriented Science & Cancer Biology



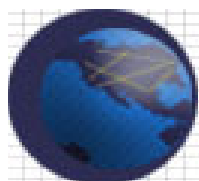
caBIG: sharing of infrastructure, applications, and data.



**Data
Integration!**

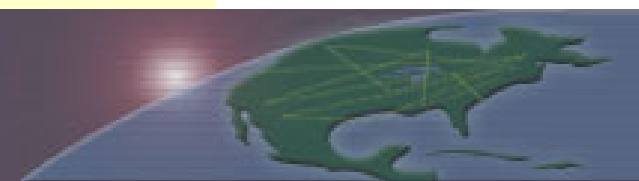


- ▲ Cancer Center (8)
- Clinical Cancer Center (14)
- Comprehensive Cancer Center (39)
- ◆ Planning Grant (7)



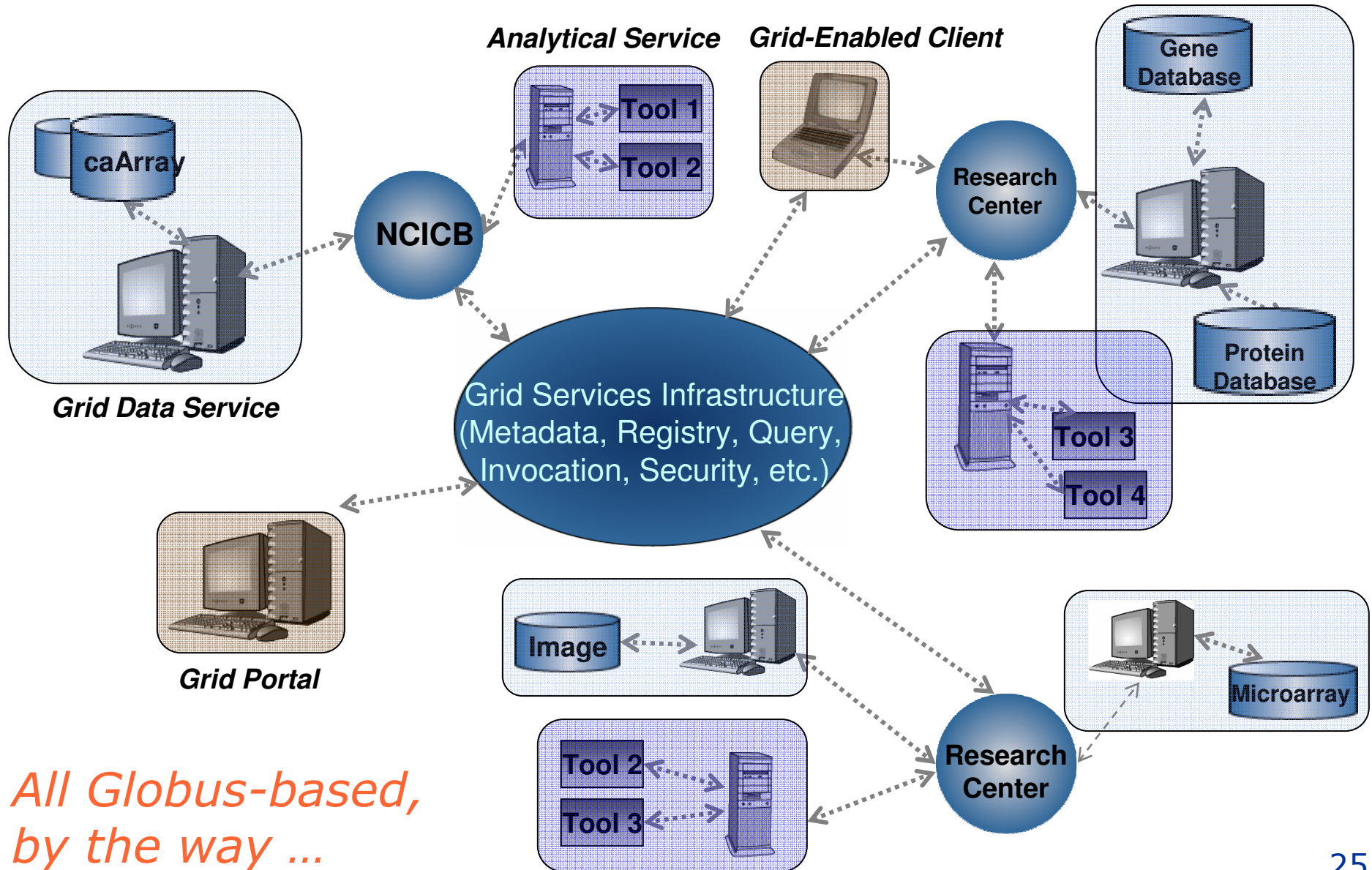
caBIG

cancer Biomedical
Informatics Grid



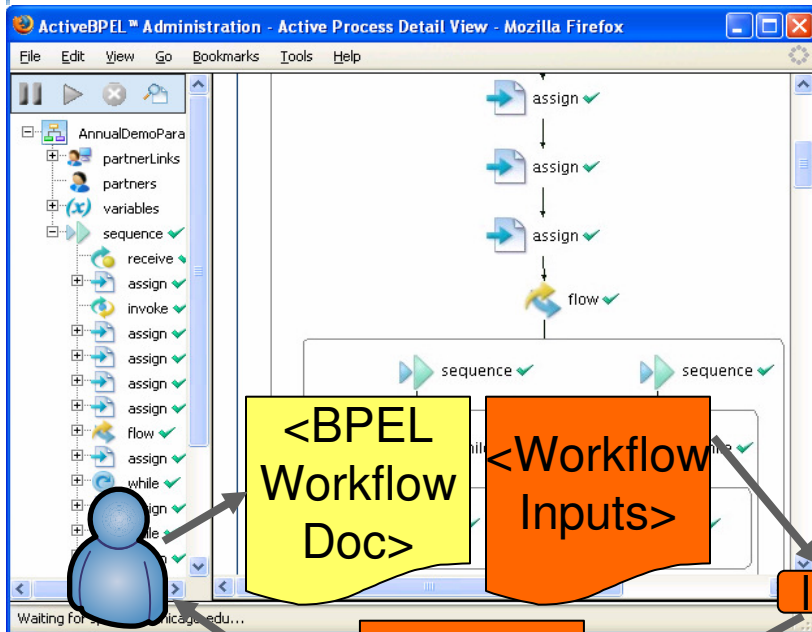


Cancer Bioinformatics Grid



*All Globus-based,
by the way ...*

Composing Services: E.g., BPEL Workflow System



Researcher
Or Client App

<BPEL
Workflow
Doc>

<Workflow
Inputs>

<Workflow
Results>

BPEL
Engine

Data Service
@ uchicago.edu

Analytic service
@ duke.edu

Analytic service
@ osu.edu

See also Kepler & Taverna



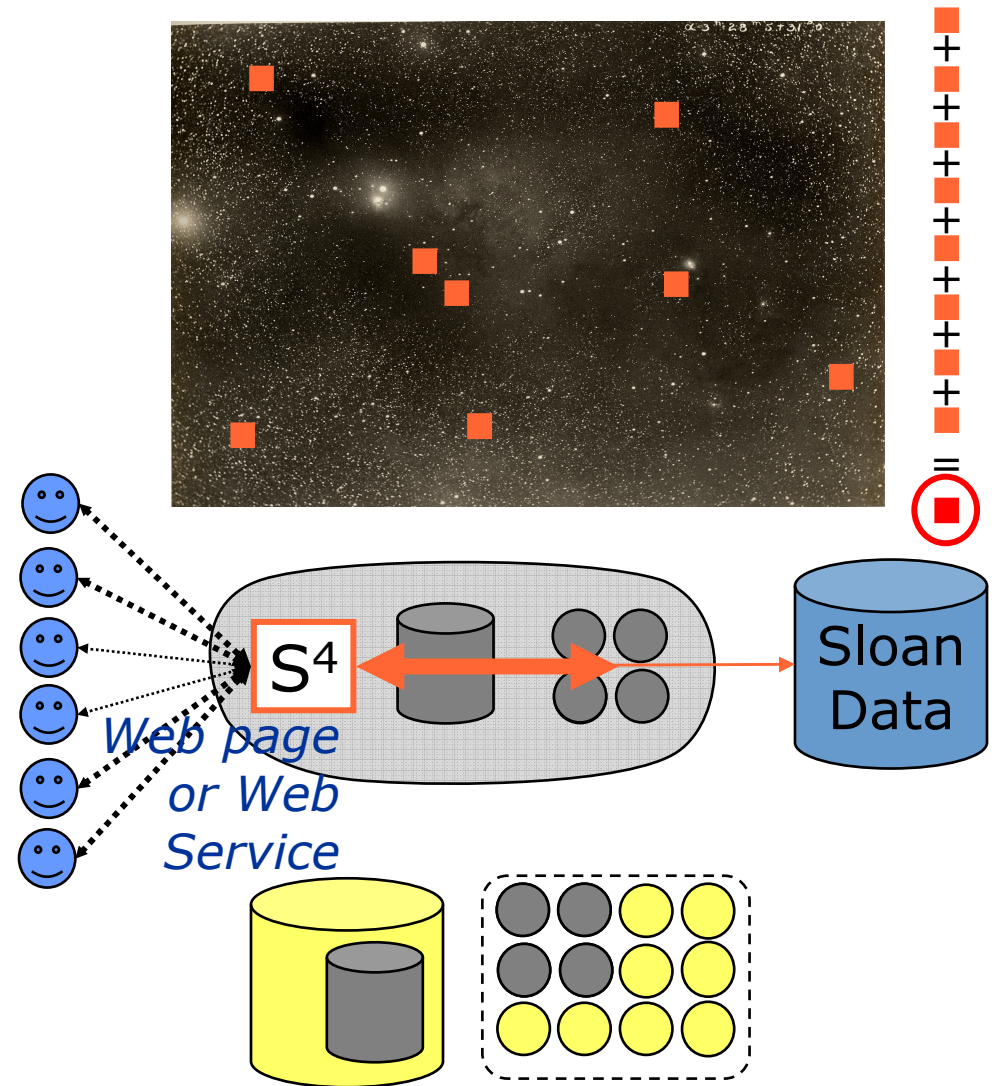
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Provisioning: Astro Portal Stacking Service



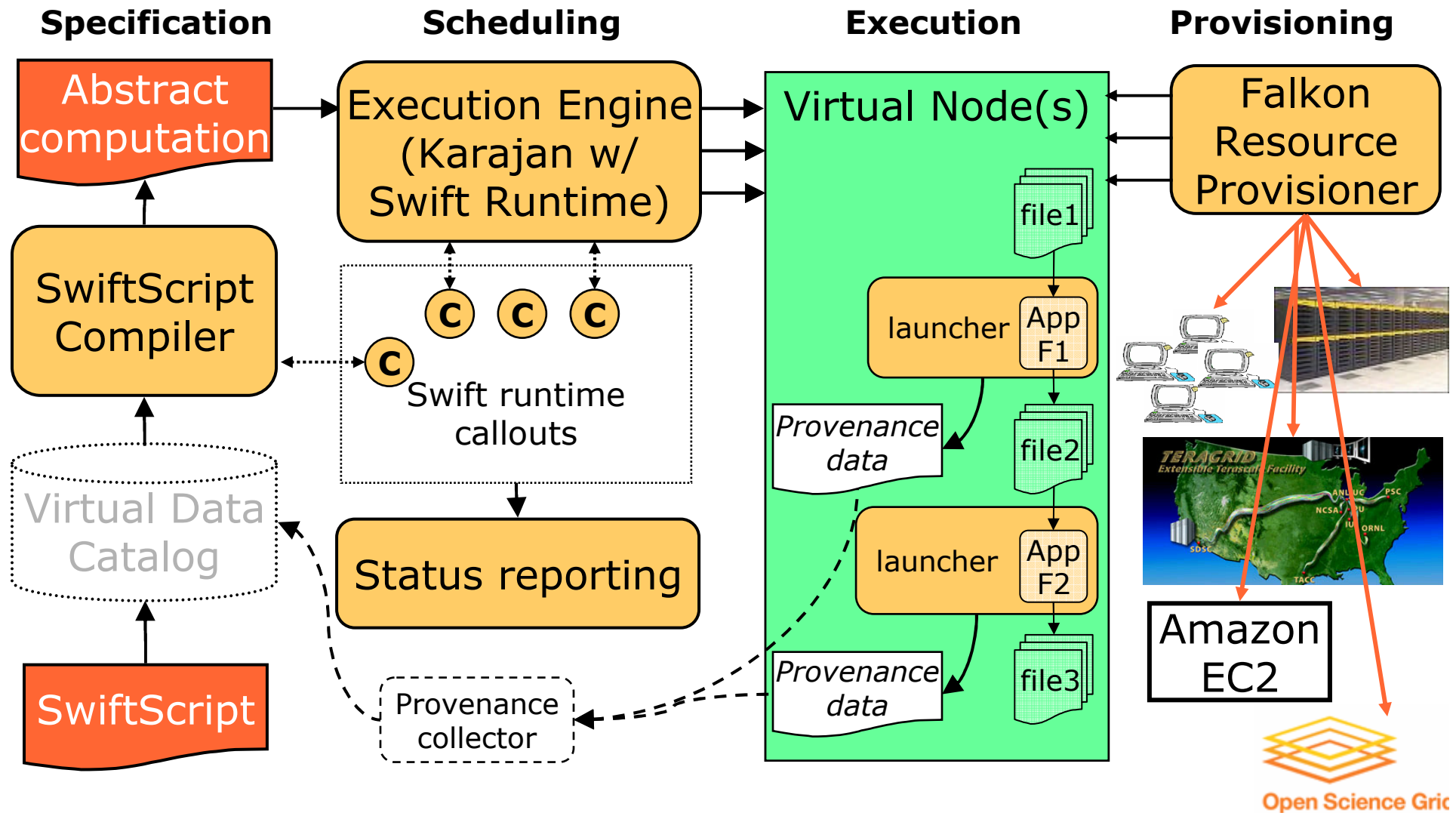
- Purpose
 - ◆ On-demand “stacks” of random locations within ~10TB dataset
- Challenge
 - ◆ Rapid access to 10-10K “random” files
 - ◆ Time-varying load
- Solution
 - ◆ Dynamic acquisition of compute, storage



Joint work with Ioan Raicu & Alex Szalay



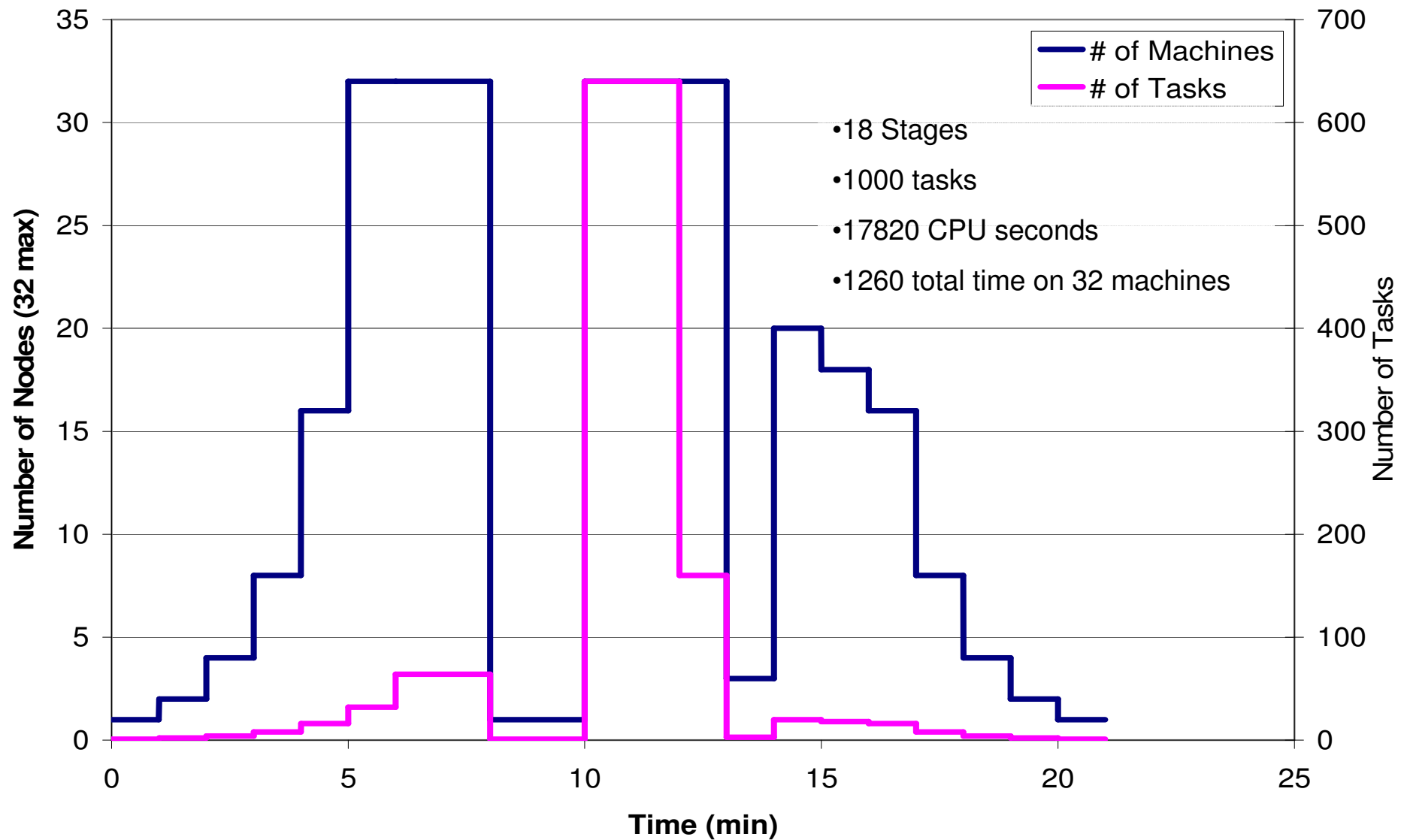
Dynamic Provisioning: Swift Architecture



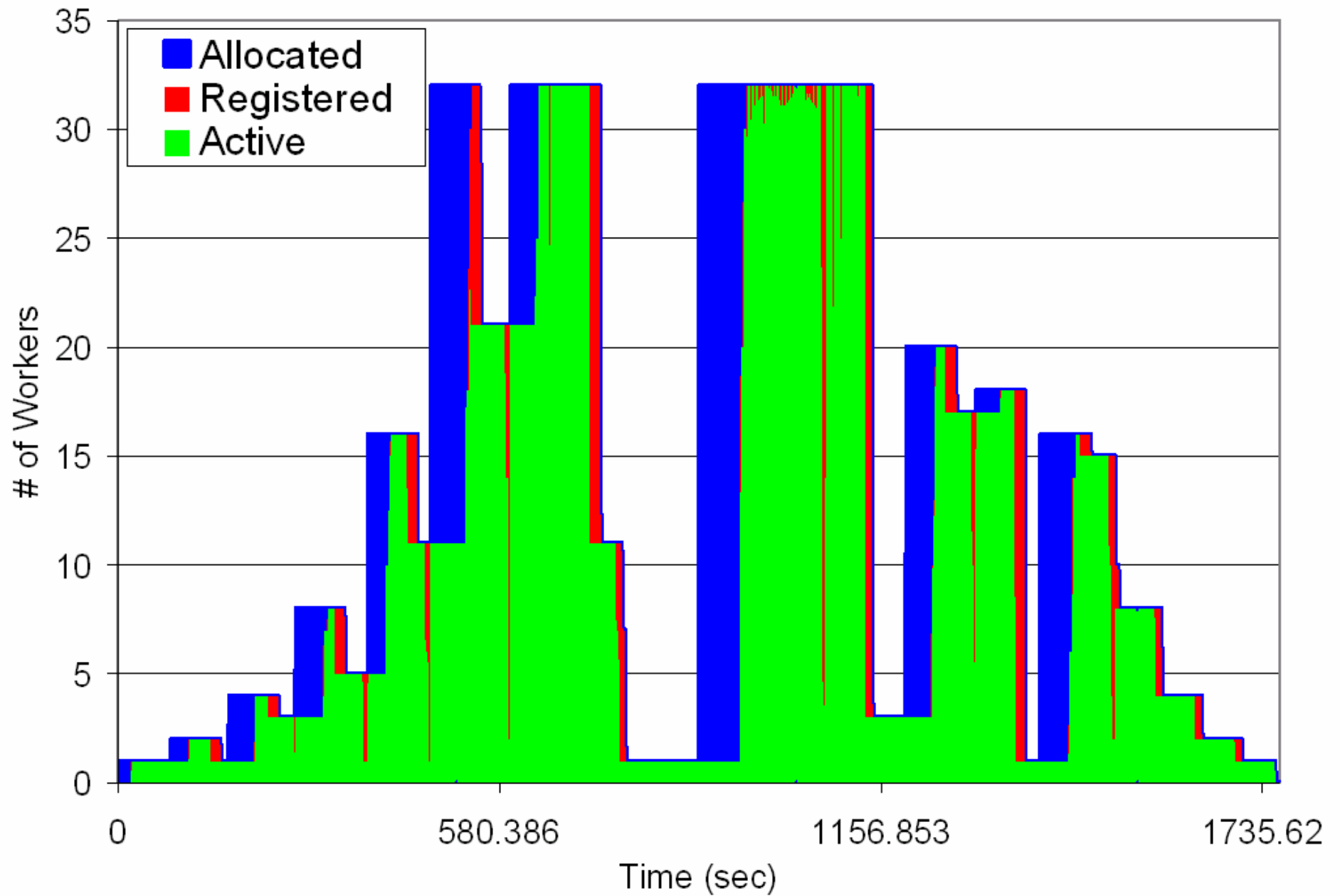
Open Science Grid



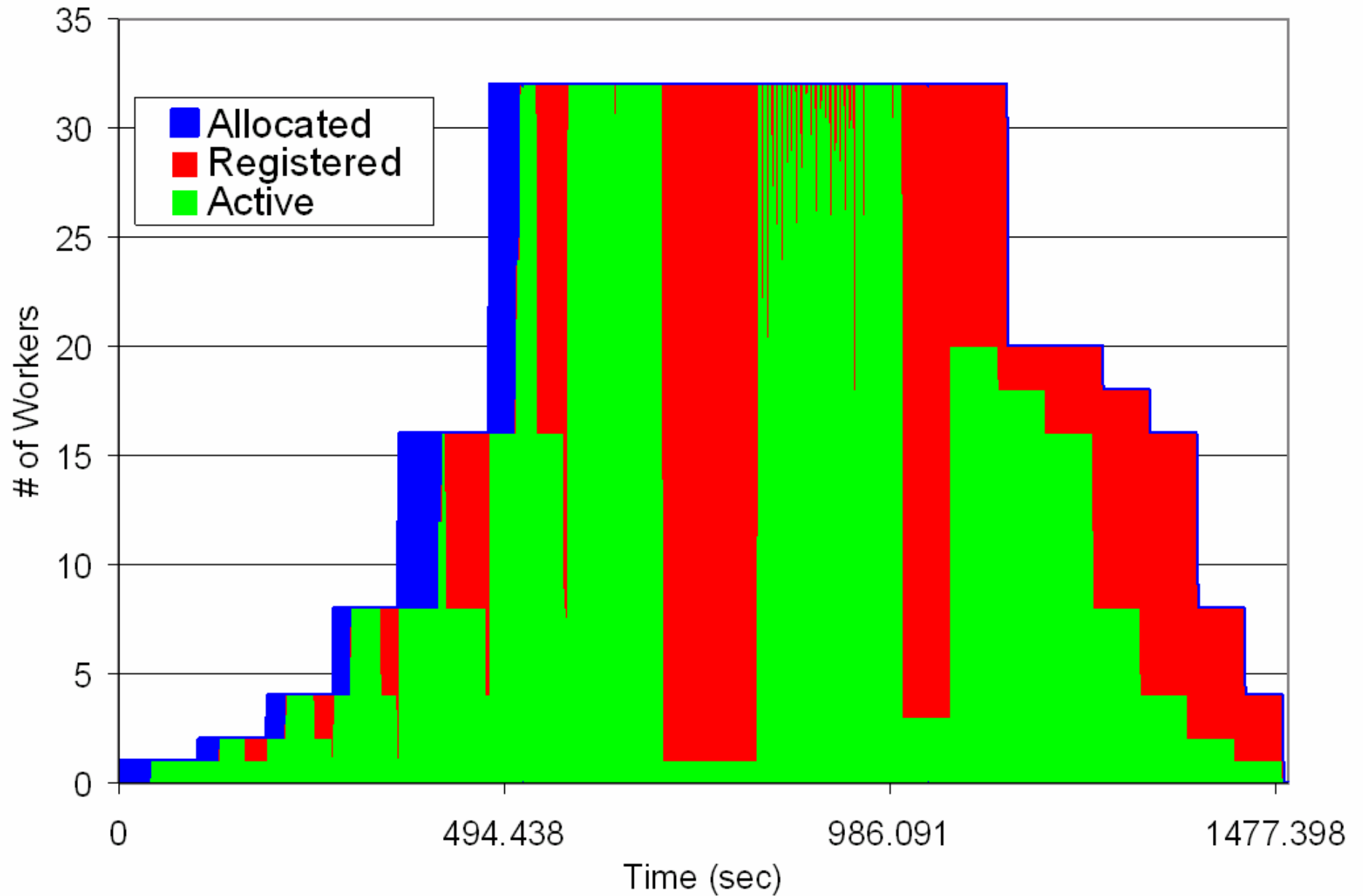
Synthetic Benchmark



Release after 15 Seconds Idle

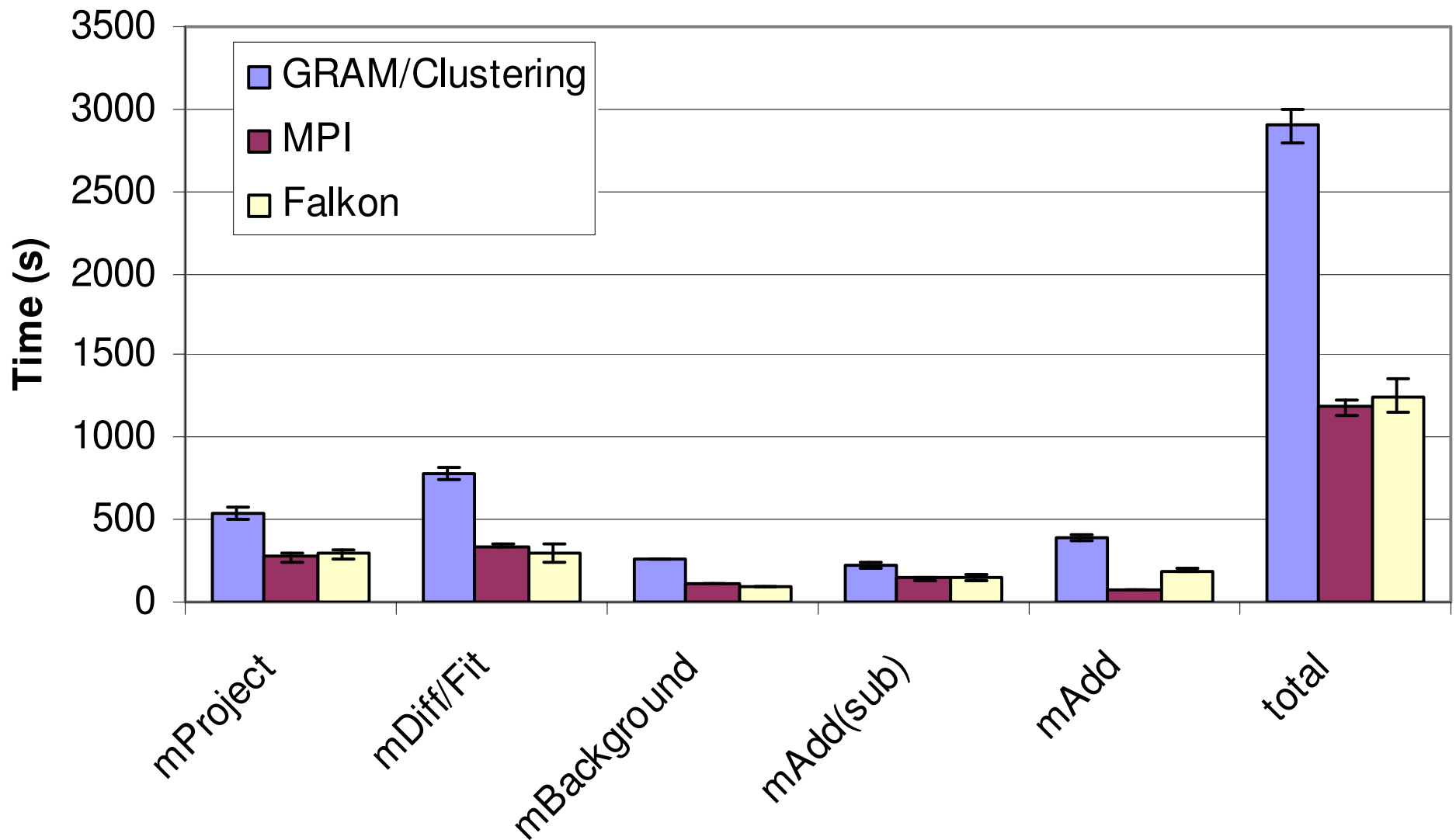


Release after 180 Seconds Idle

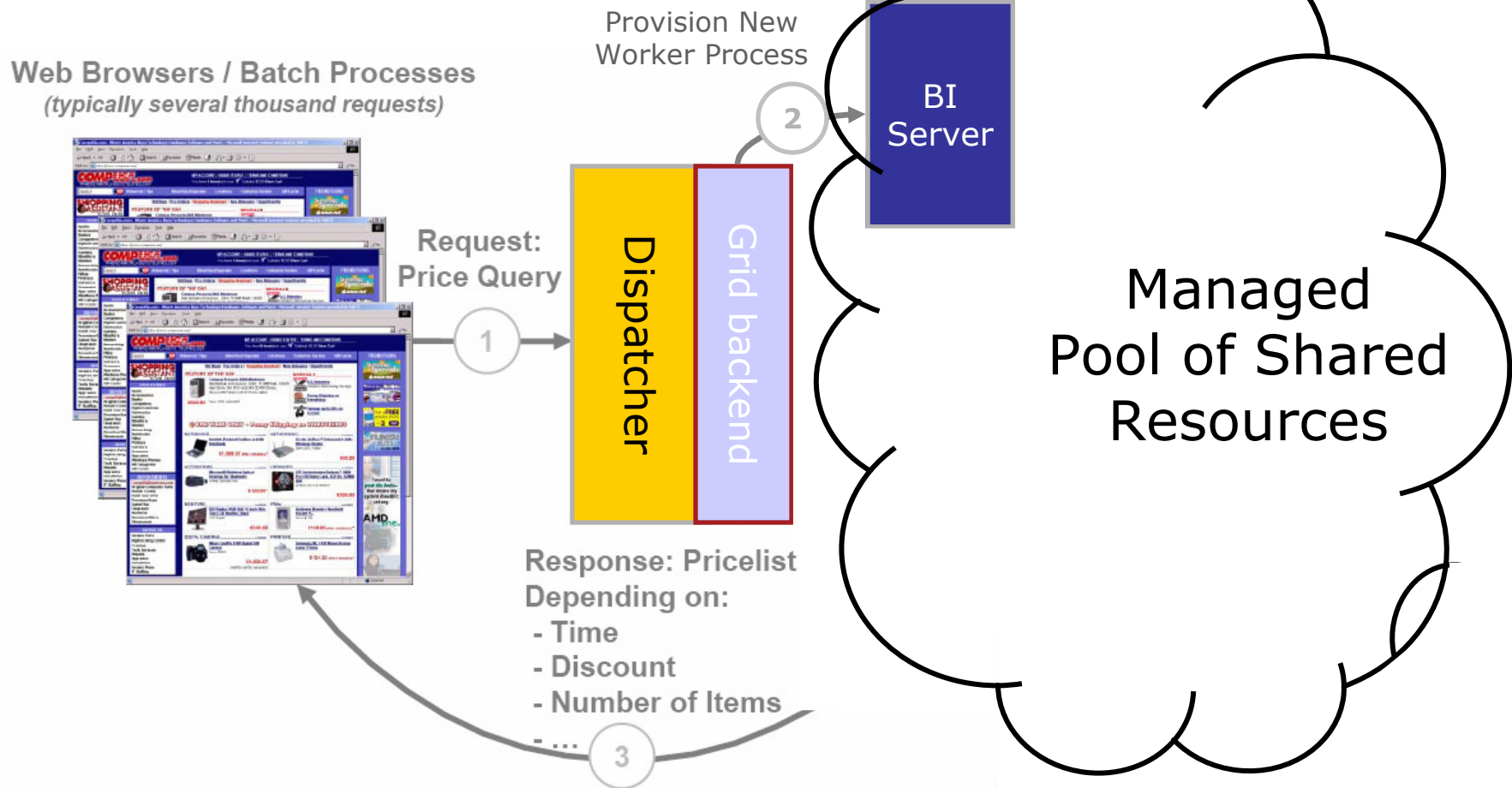




Montage



Grid-enabled Business Intelligence (BI) Application



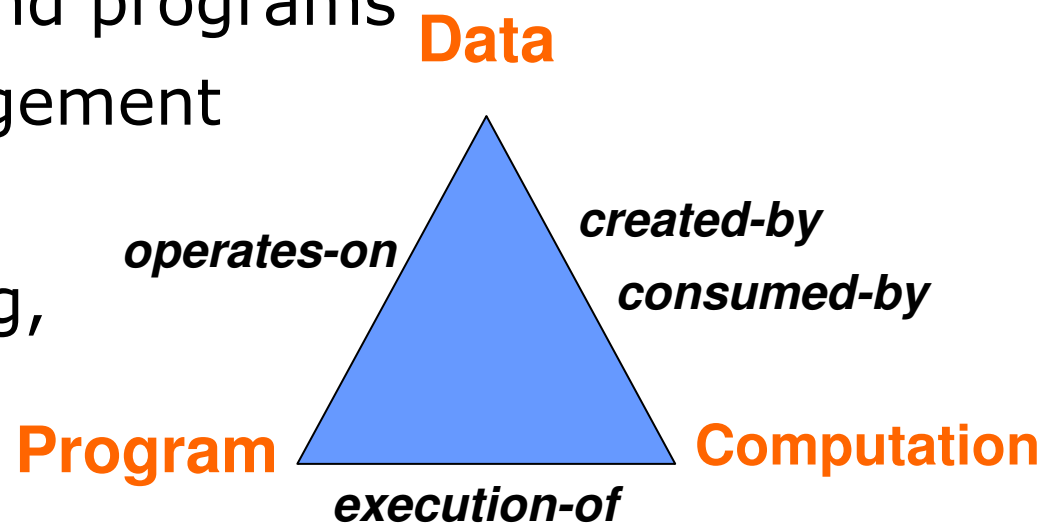
BI server applications started and decommissioned by a Grid-enabled dispatcher



Computation as a First-Class Entity



- 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, scheduling, performance optimization

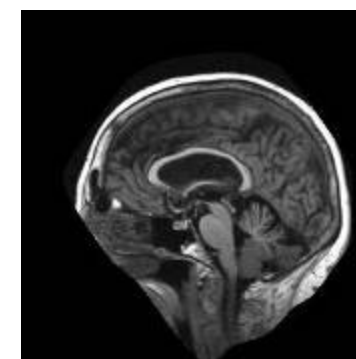
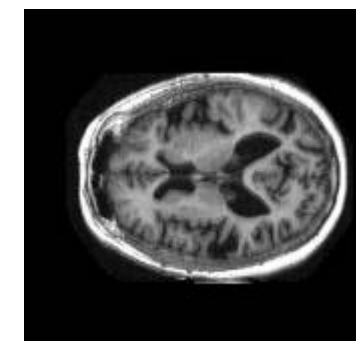
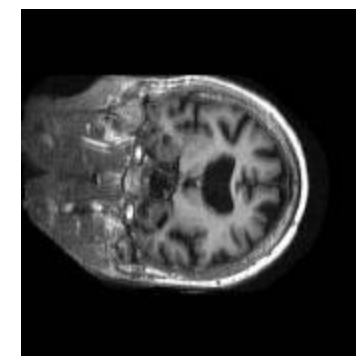
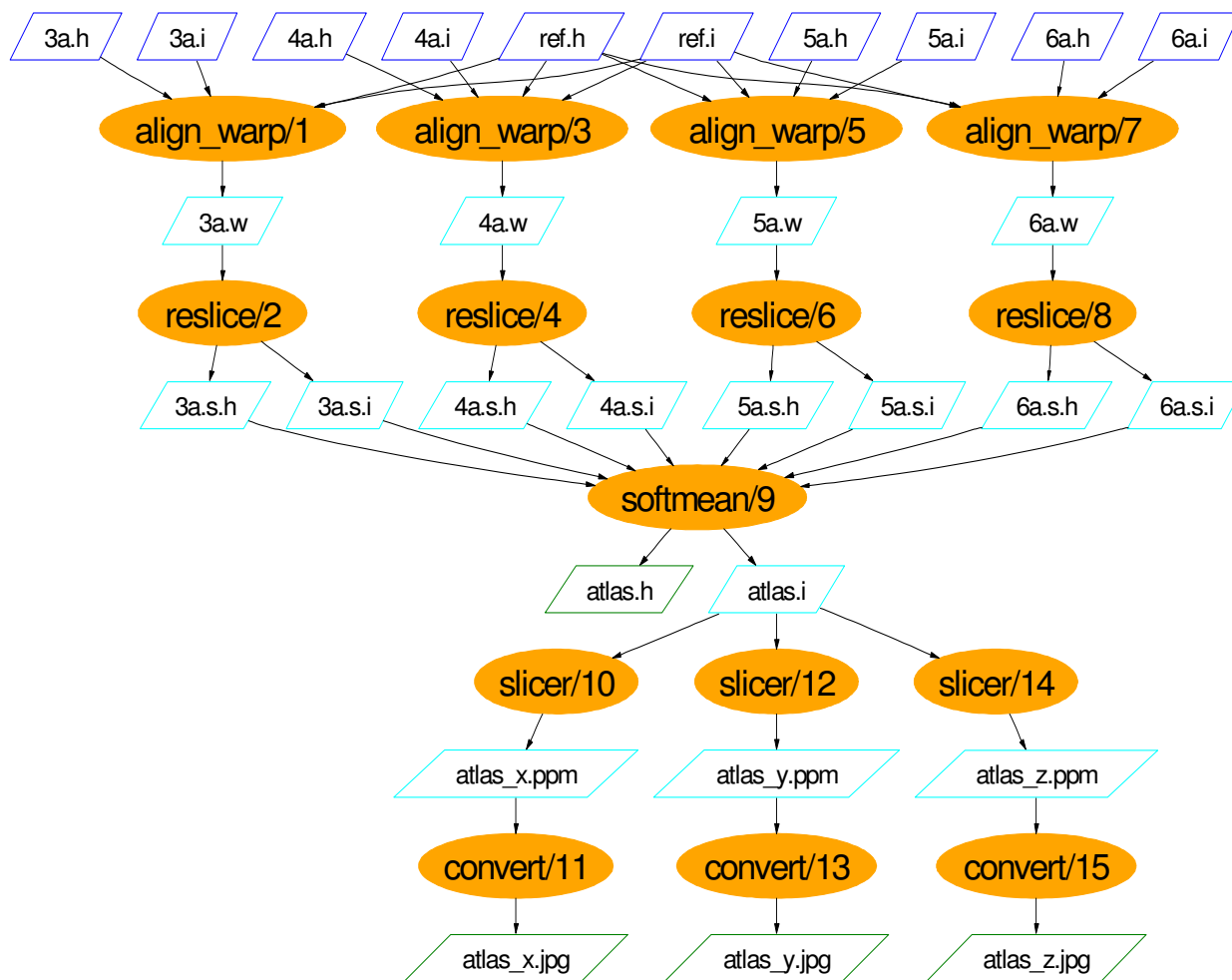
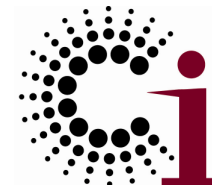




the globus alliance

www.globus.org

Example: fMRI Analysis





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*



Guidelines
(Apache)

Infrastructure
(CVS, email,
bugzilla, Wiki)

Projects
Include

...

- Welcome
- List of projects
- Guidelines
- Infrastructure
- How to contribute
- GlobDev events
- Recent changes
- GlobDev FAQ

common runtime projects

- C Core Utilities
- C WS Core
- CoG jglobus
- Core WS Schema
- Java WS Core
- Python Core
- XIO

data projects

- GridFTP
- OGSA-DAI
- Reliable File Transfer
- Replica Location

execution projects

- GRAM

information projects

- MDS4

security projects

- C Security

Welcome

This is the new home Globus software development; it is still under construction. The current status of our efforts to build this environment can be found [on this page](#). Comments regarding this site can be sent to info@globus.org. Thank you for your interest in Globus development!

Globus was first established as an open source software project in 1996. Since that time, the Globus development team has expanded from a few individuals to a distributed, international community. In response to this growth, the Globus community (the "Globus Alliance") established in October 2005 a new source code development *infrastructure* and meritocratic *governance model*, which together make the process by which a developer joins the Globus community both easier and more transparent.

The Globus governance model and infrastructure are based on those of [Apache Jakarta](#). In brief, the governance model places control over each individual software component (*project*) in the hands of its most active and respected *contributors* (*committers*), with a *Globus Management Committee* (GMC) providing overall guidance and conflict resolution. The infrastructure comprises *repositories*, *email lists*, Wikis, and *bug trackers* configured to support per-project community access and management.

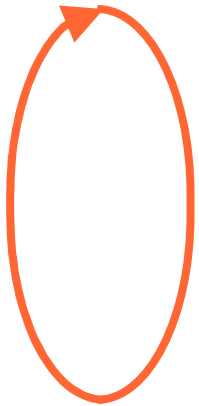
For more information, see:

- The [Globus Alliance Guidelines](#), which address various aspects of the Globus governance model and the Globus community.
- A description of the Globus Alliance [Infrastructure](#).
- A list of current Globus projects.



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Summary: 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!*



TeraGrid™
EMPOWERING DISCOVERY



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

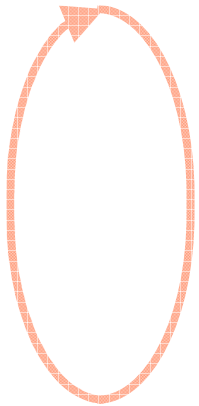
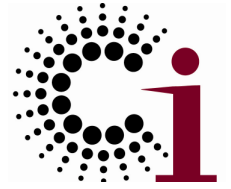


"Service-Oriented Science", *Science*, 2005



the globus alliance
www.globus.org

Summary: 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.

Profoundly revolutionary:

- **Accelerates the pace of enquiry**
- **Introduces a new notion of “result”**
- **Requires new reward structures, training, infrastructure**

“Service-Oriented Science”, *Science*, 2005



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 scientists
- 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

Service-Oriented Science Challenges

- A need for new **technologies, skills, & roles**
 - ◆ Creating, publishing, hosting, discovering, composing, archiving, explaining ... services
- A need for substantial **software development**
 - ◆ “30-80% of modern astronomy projects is software”—S. G. Djorgovski, Caltech
- A need for more & different **infrastructure**
 - ◆ Computers & networks to host services
- And certainly profound **research challenges**
 - ◆ In every part of the service & science lifecycle

For more information: <http://ianfoster.typepad.com>