



Grid

Ian Foster

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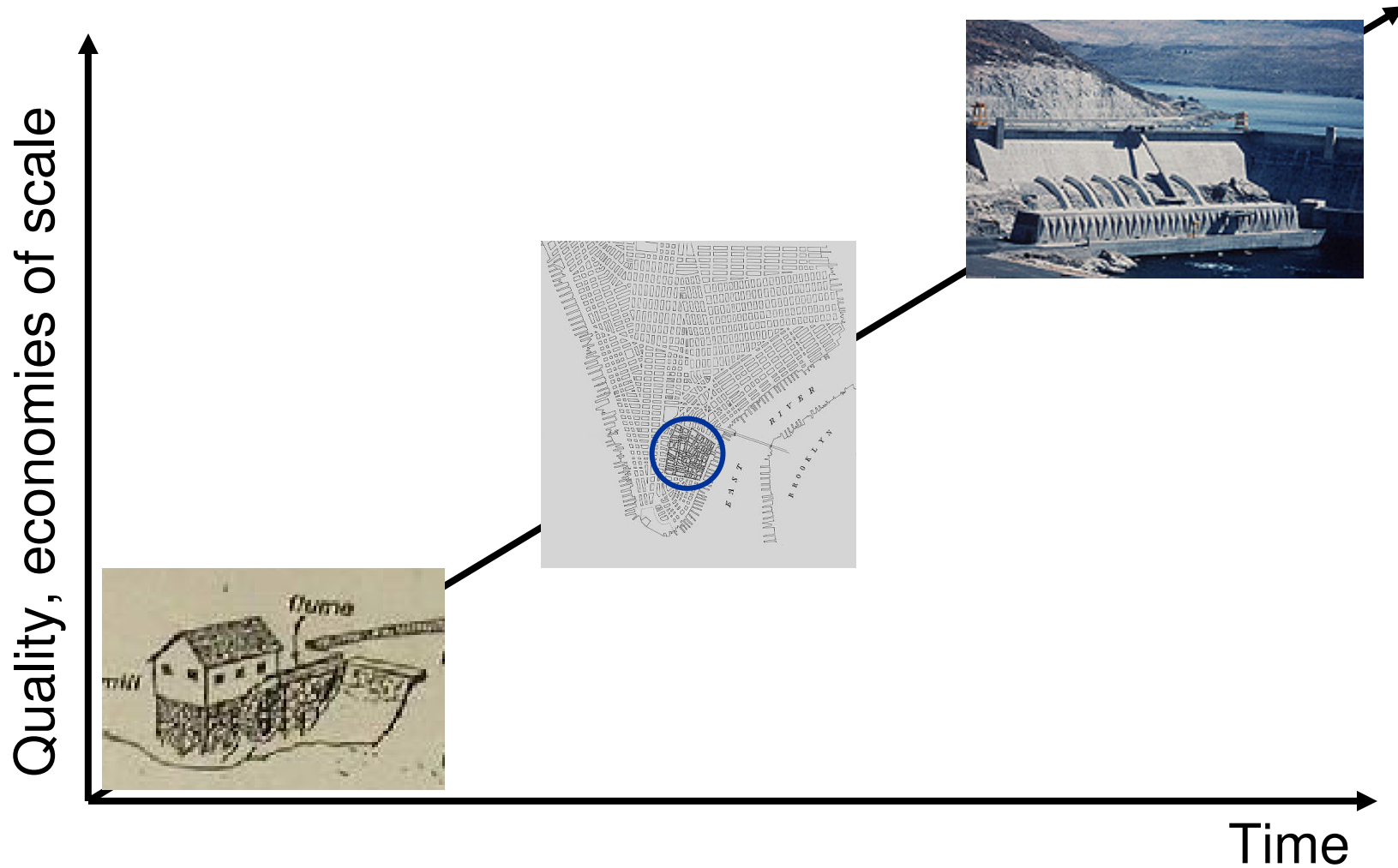




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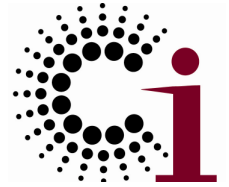


The (Power) Grid: On-Demand Access to Electricity



An Old Idea ...

- “The time-sharing computer system can unite a group of investigators one can conceive of such a facility as an ... intellectual public utility.”
 - ◆ Fernando Corbato and Robert Fano, 1966
- “We will perhaps see the spread of ‘computer utilities’, which, like present electric and telephone utilities, will service individual homes and offices across the country.”
 - ◆ Len Kleinrock, 1967



Why Grid? — The Changing Nature of Work

Collaborative & Dynamic

Project focused, globally distributed teams, spanning organizations within and beyond company boundaries

Distributed & Heterogeneous

Each team member/group brings own data, compute, & other resources into the project

Data & Computation Intensive

Access to computing and data resources must be coordinated across the collaboration

Concurrent Innovation Cycles

Resources must be available to projects with strong QoS, & also reflect enterprise-wide biz priorities

IT must adapt to this new reality

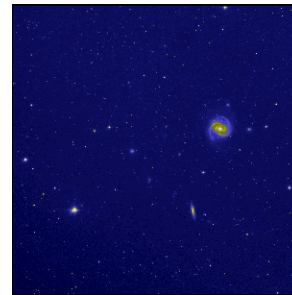
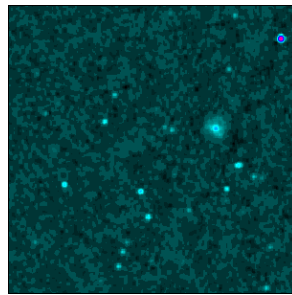
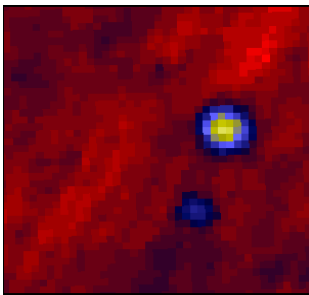


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For Example: Digital Astronomy



- Digital observatories provide online archives of data at different wavelengths



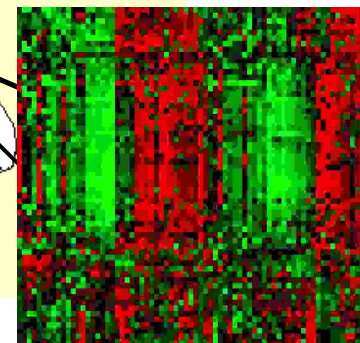
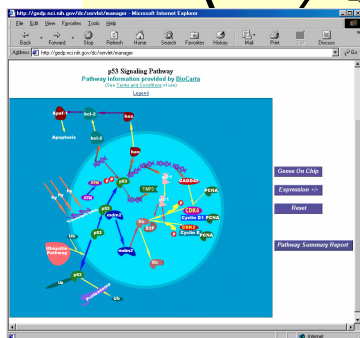
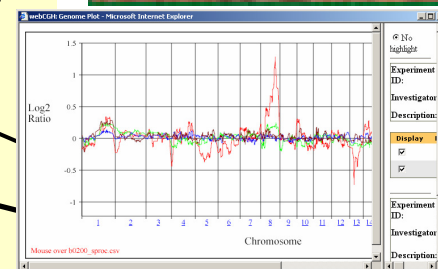
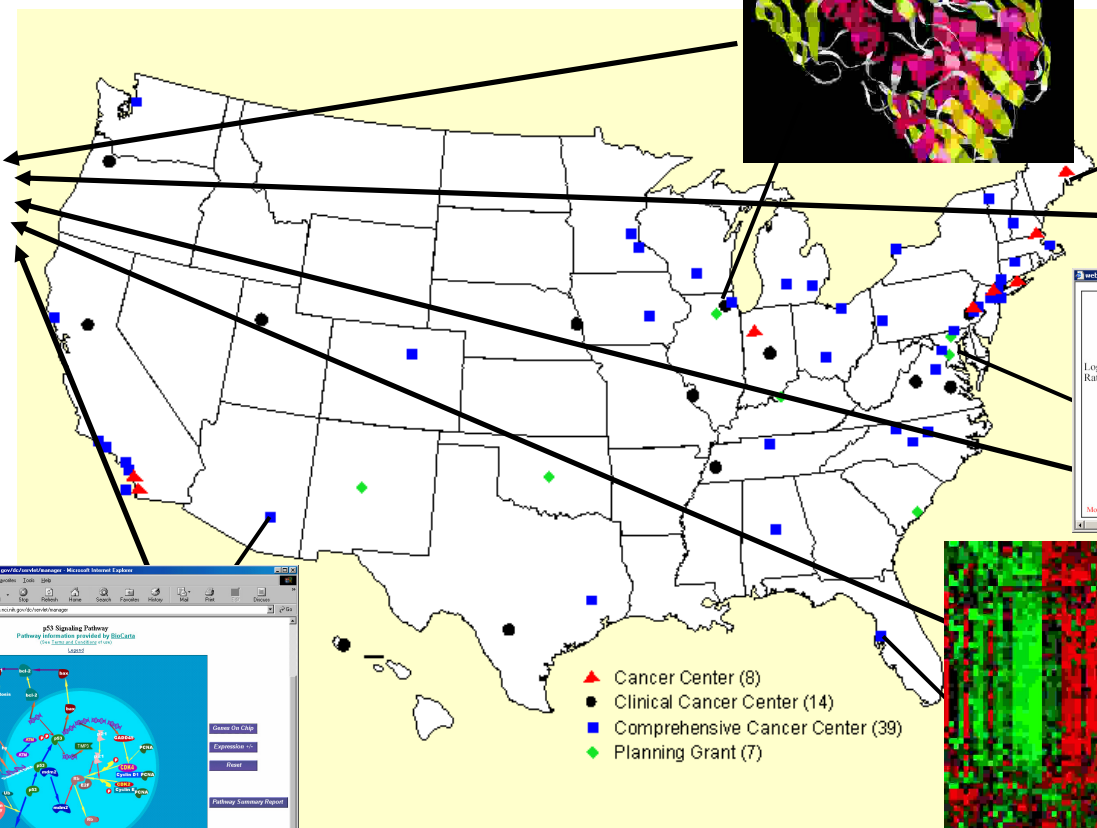
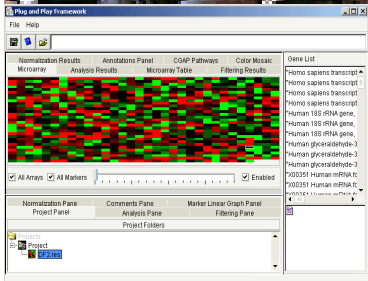
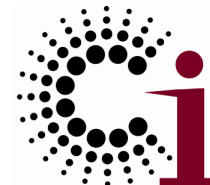
- Ask questions such as: what objects are visible in infrared but not visible spectrum?



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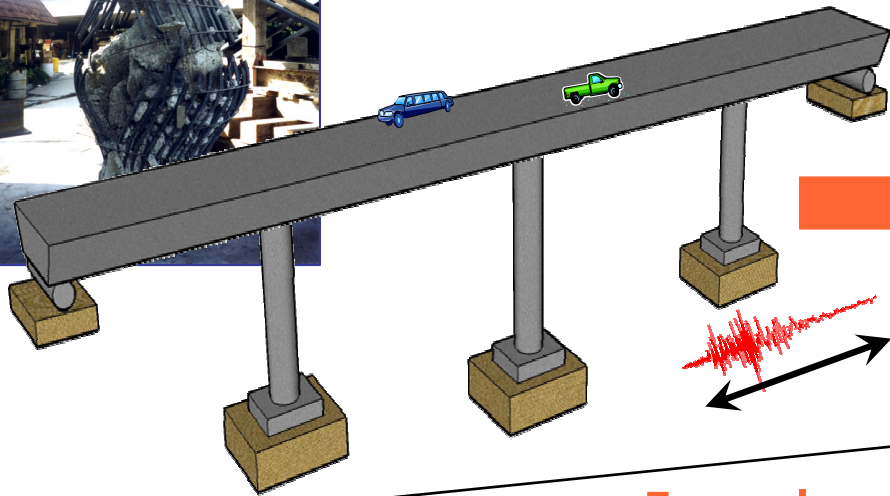
For Example: Cancer Biology



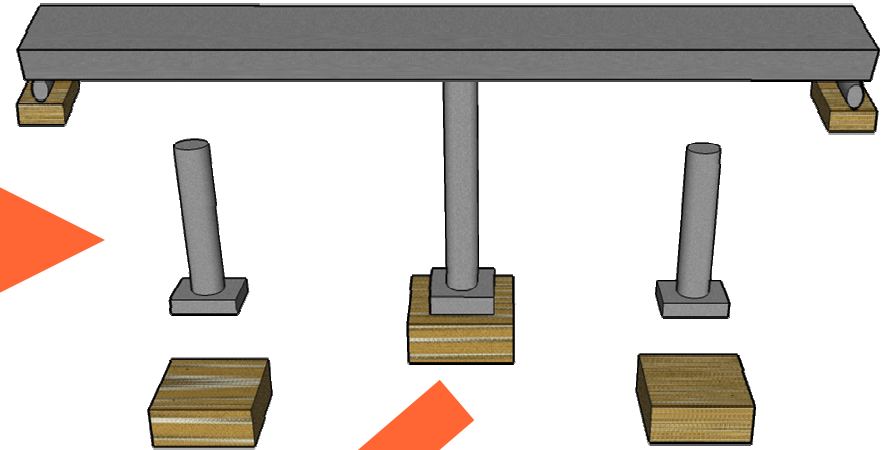
- ▲ Cancer Center (8)
- Clinical Cancer Center (14)
- Comprehensive Cancer Center (39)
- ◆ Planning Grant (7)



System-Level Problem

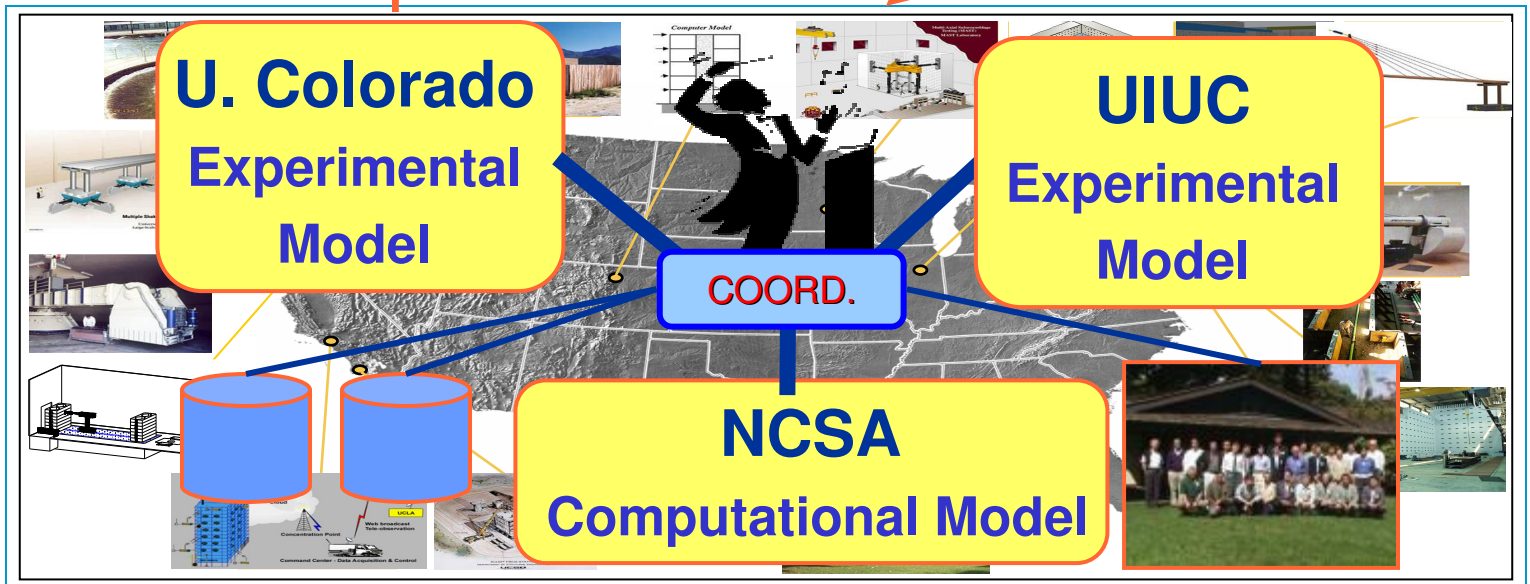


Decomposition



Implementation

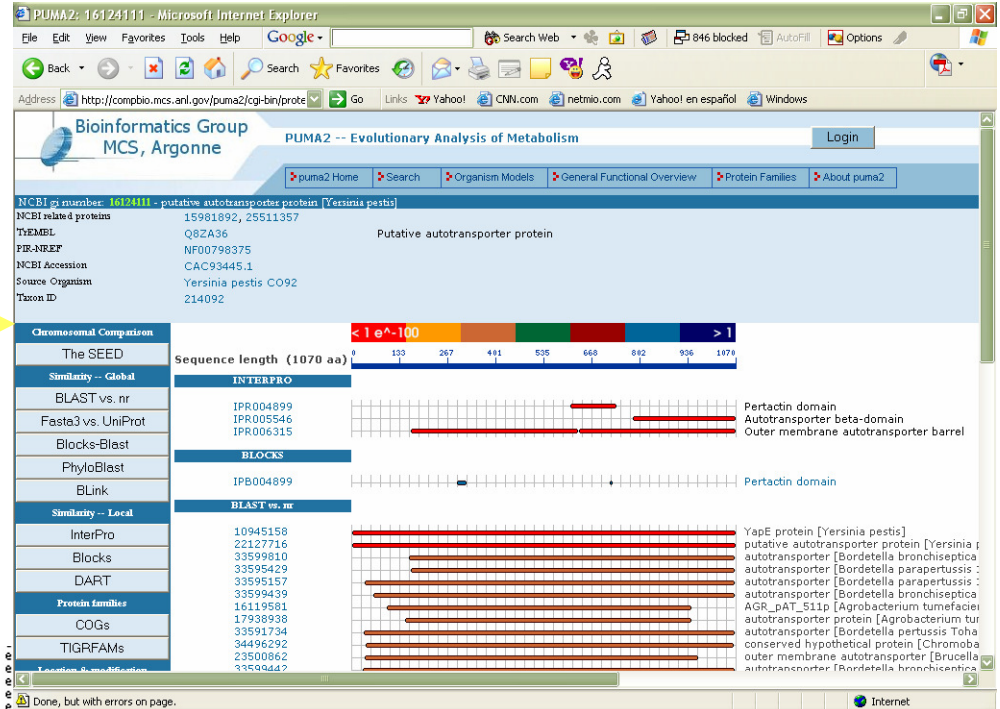
Facilities
Computers
Storage
Networks
Services
Software
People



For Example: Bioinformatics



Public PUMA Knowledge Base
Information about proteins analyzed against ~2 million gene sequences



gi 23499780 gn REF_tigr BRA0013	gi 16080253 ref NP_391080.1	44.27	253	131	1	15	257	8	2603.7	e-33	142.9
gi 23499780 gn REF_tigr BRA0013	gi 23098409 ref NP_691875.1	43.48	253	133	2	16	258	5	2573.8	e-32	141.4
gi 23499780 gn REF_tigr BRA0013	gi 48637187 ref ZP_00294182.1	44.92	256	125	2	14	256	7	2591.1	e-32	140.2
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gi 23499780 gn REF_tigr BRA0013	gi 30348891 gb AA028934.1	39.53	253	138	3	18	257	5	2552.0	e-31	137.9
gi 23499780 gn REF_tigr BRA0013	gi 19655222 gb AF93939.1	40.64	251	138	1	17	256	10	2602.7	e-30	134.8
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gi 23499780 gn REF_tigr BRA0013	gi 46363318 ref ZP_0026079.1	39.58	240	135	2	14	253	6	2361.8	e-30	134.4
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REF_tigr BRA0013	gi 48782600 ref ZP_00279106.1	35.92	245								
REF_tigr BRA0013	gi 41407534 ref NP_960370.1	36.09	266								
REF_tigr BRA0013	gi 48851585 ref ZP_00305793.1	32.39	247								
REF_tigr BRA0013	gi 15966306 ref NP_386659.1	36.50	263								
REF_tigr BRA0013	gi 17548526 ref NP_521866.1	36.36	264								
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gi 23499780 gn REF_tigr BRA0013	gi 25029334 ref NP_739388.1	35.20	250	147	4	15	256	6	2485.7	e-30	132.9
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gi 23499780 gn REF_tigr BRA0013	gi 46314029 ref ZP_00214635.1	33.86	254	153	2	12	259	3	2485.7	e-30	132.9
gi 23499780 gn REF_tigr BRA0013	gi 41406852 ref NP_959688.1	35.61	238	149	2	16	253	2	2309.8	e-30	132.1
gi 23499780 gn REF_tigr BRA0013	gi 11564471 ref NP_229523.1	35.69	255	144	5	12	256	2	2469.8	e-30	132.1
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gi 23499780 gn REF_tigr BRA0013	gi 3328306 ref NP_232830.1	34.20	241	143	5	18	256	6	2363.7	e-29	130.2

Back Office Analysis

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

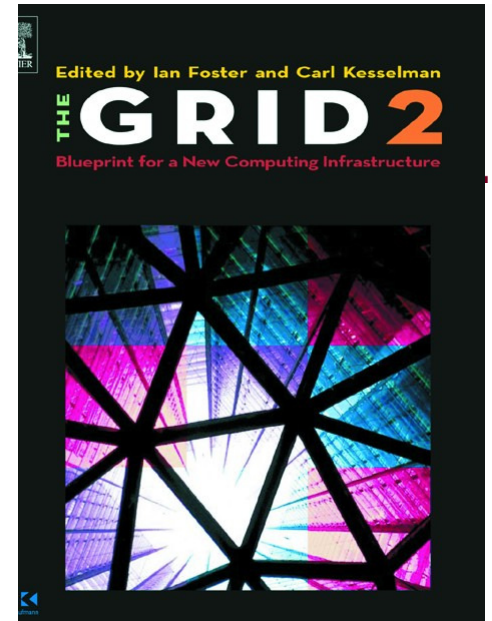


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The Grid

Enable "*coordinated resource sharing & problem solving in dynamic, multi-institutional virtual organizations.*"

(Source: "**The Anatomy of the Grid**")



- Access to shared resources
 - Virtualization, allocation, management
- With predictable behaviors
 - Provisioning, quality of service
- In dynamic, heterogeneous environments
 - Standards-based interfaces and protocols

More Specifically, I May Want To ...



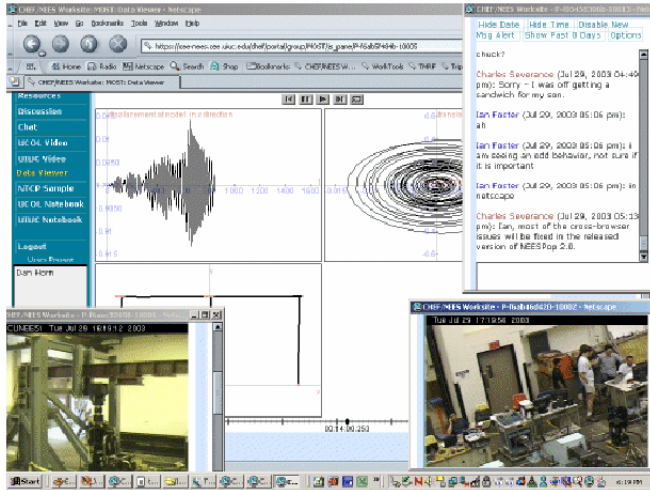
- Create a service for use by my colleagues
- Manage who is allowed to access my service (or my experimental data or ...)
- Ensure reliable & secure distribution of data from my lab to my partners
- Run 10,000 jobs on whatever computers I can get hold of
- Monitor the status of the different resources to which I have access



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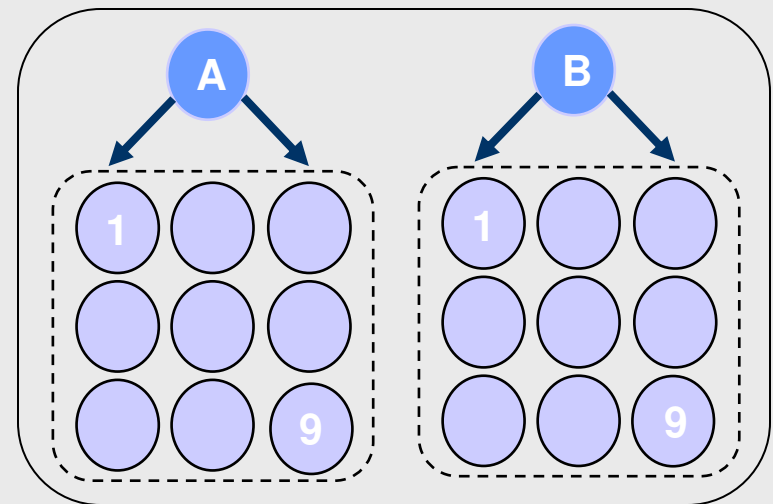
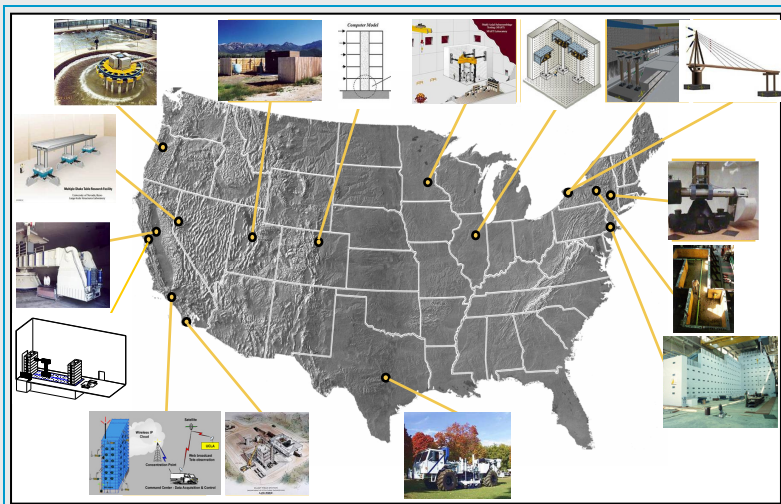
Underlying Problem: The Application-Infrastructure Gap



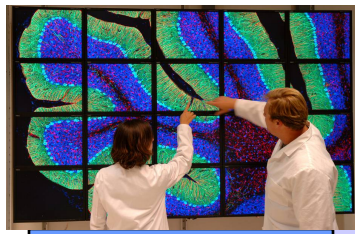
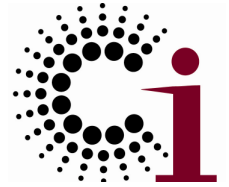
**Dynamic
and/or
Distributed
Applications**



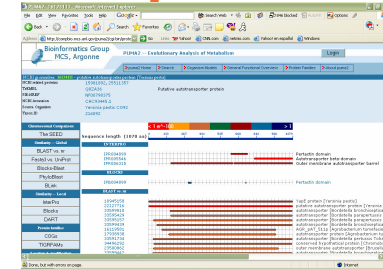
Shared Distributed Infrastructure



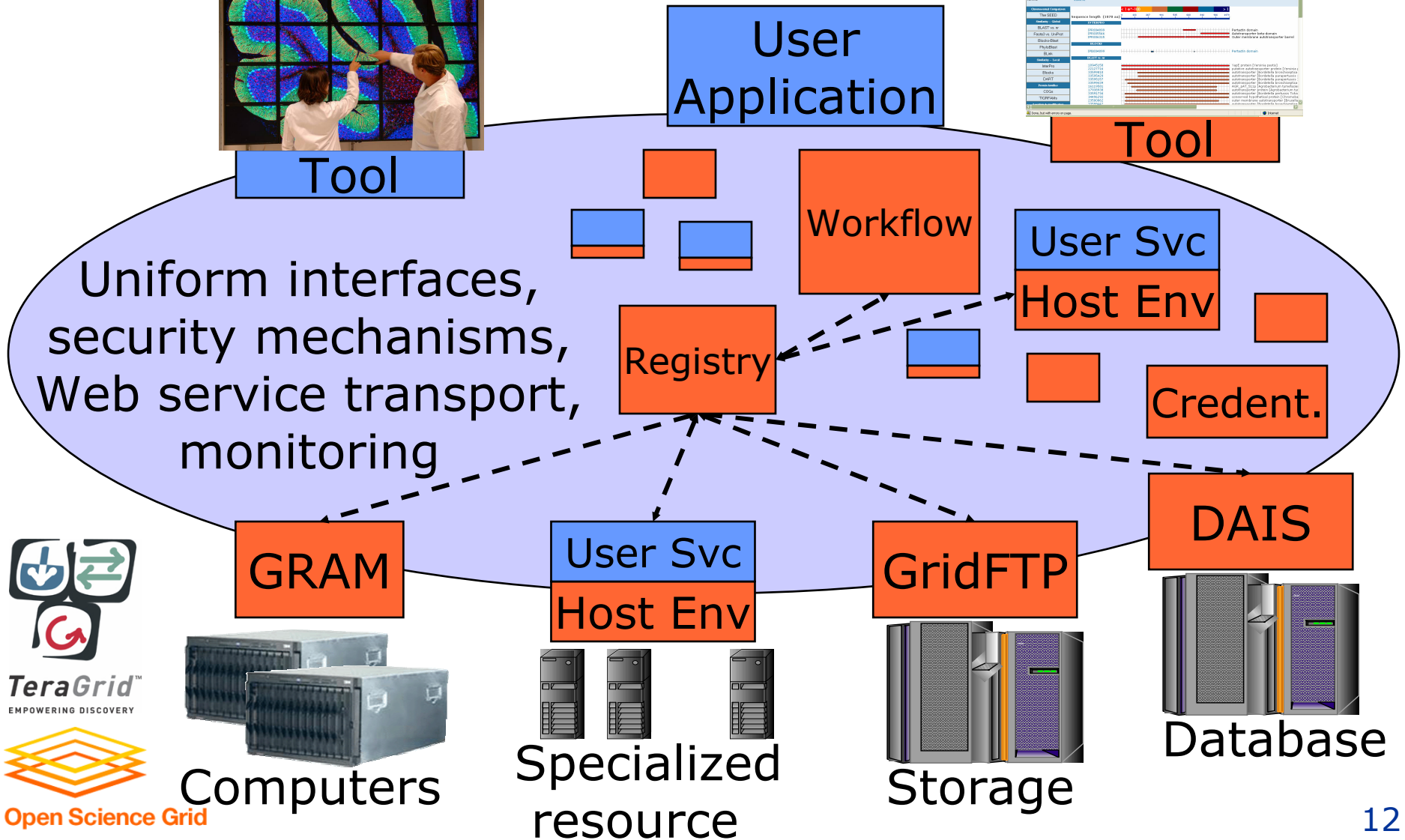
Bridging the Application-Resource Gap



Tool



Tool



TeraGrid™
EMPOWERING DISCOVERY

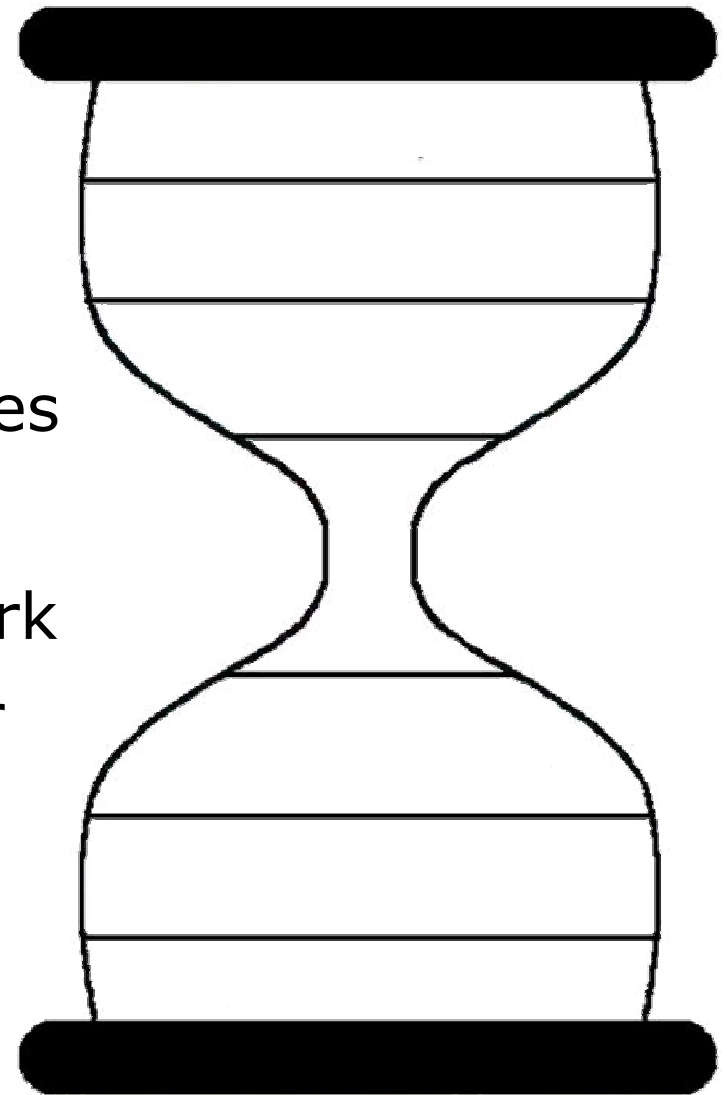


Open Science Grid



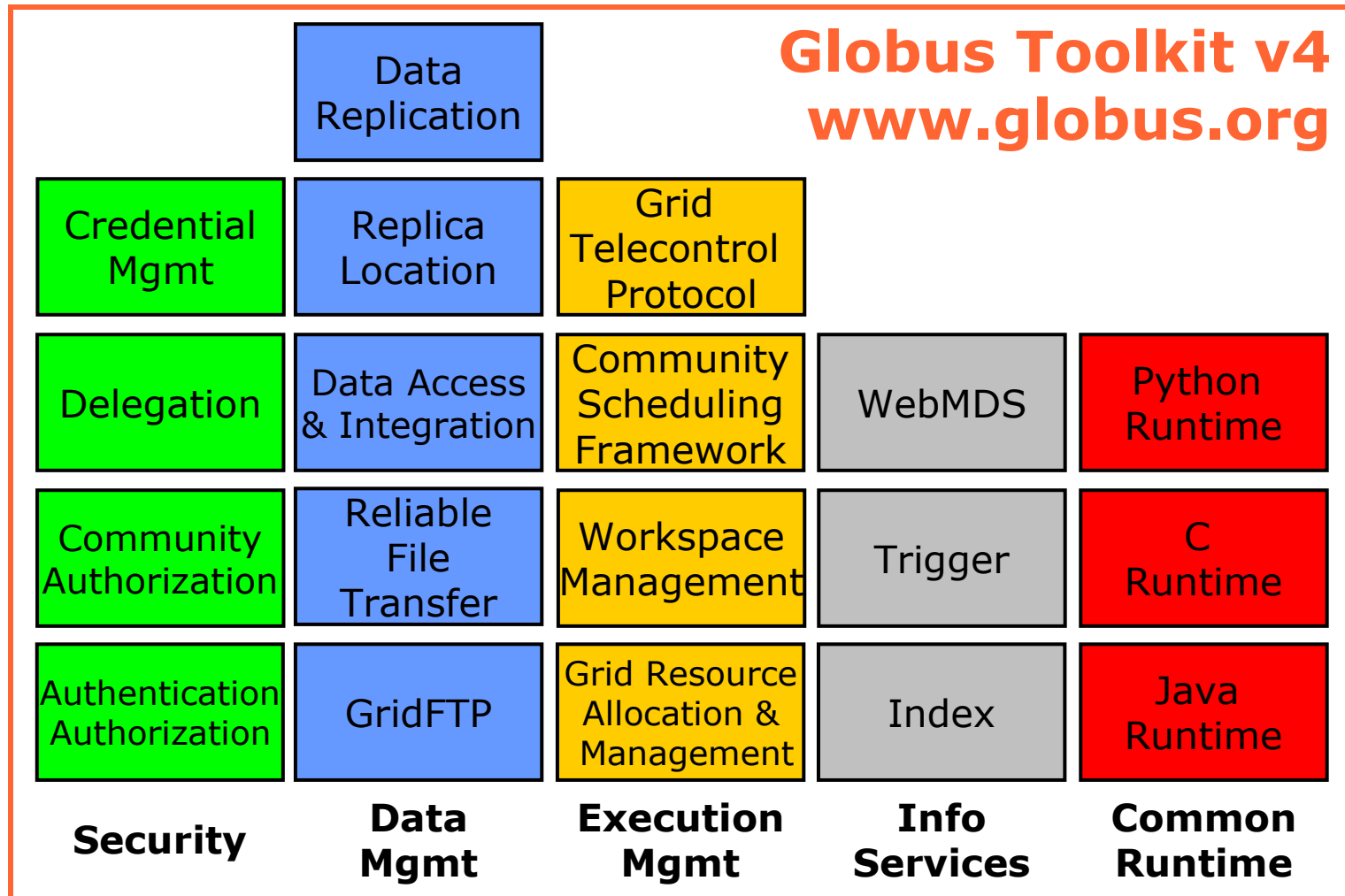
Grid Infrastructure

- Distributed management
 - ◆ Of physical resources
 - ◆ Of software services
 - ◆ Of communities and their policies
- Unified treatment
 - ◆ Build on Web services framework
 - ◆ Use WS-RF, WS-Notification (or WS-Transfer/Man) to represent/access state
 - ◆ Common management abstractions & interfaces





Globus Toolkit: Open Source Grid Infrastructure



More Specifically, I May Want To ...

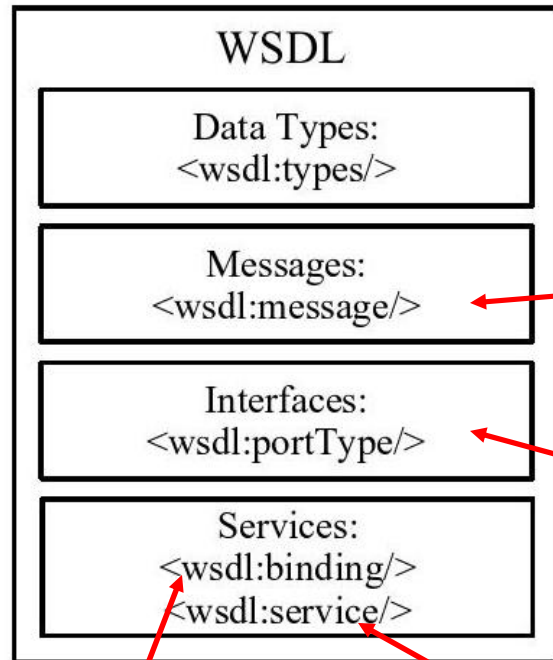


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Web Services

- Standards for defining & accessing services
 - ◆ WSDL: Web Services Description Language
 - ◆ SOAP: Simple Object Access Protocol
 - ◆ Also other standards for security, state access, etc., etc.
- Technology for hosting services, e.g.:
 - ◆ Apache Axis (Java)
 - ◆ Microsoft (C#)
 - ◆ Others in other languages (C, Python, etc.)

WSDL: Web Services Description Language



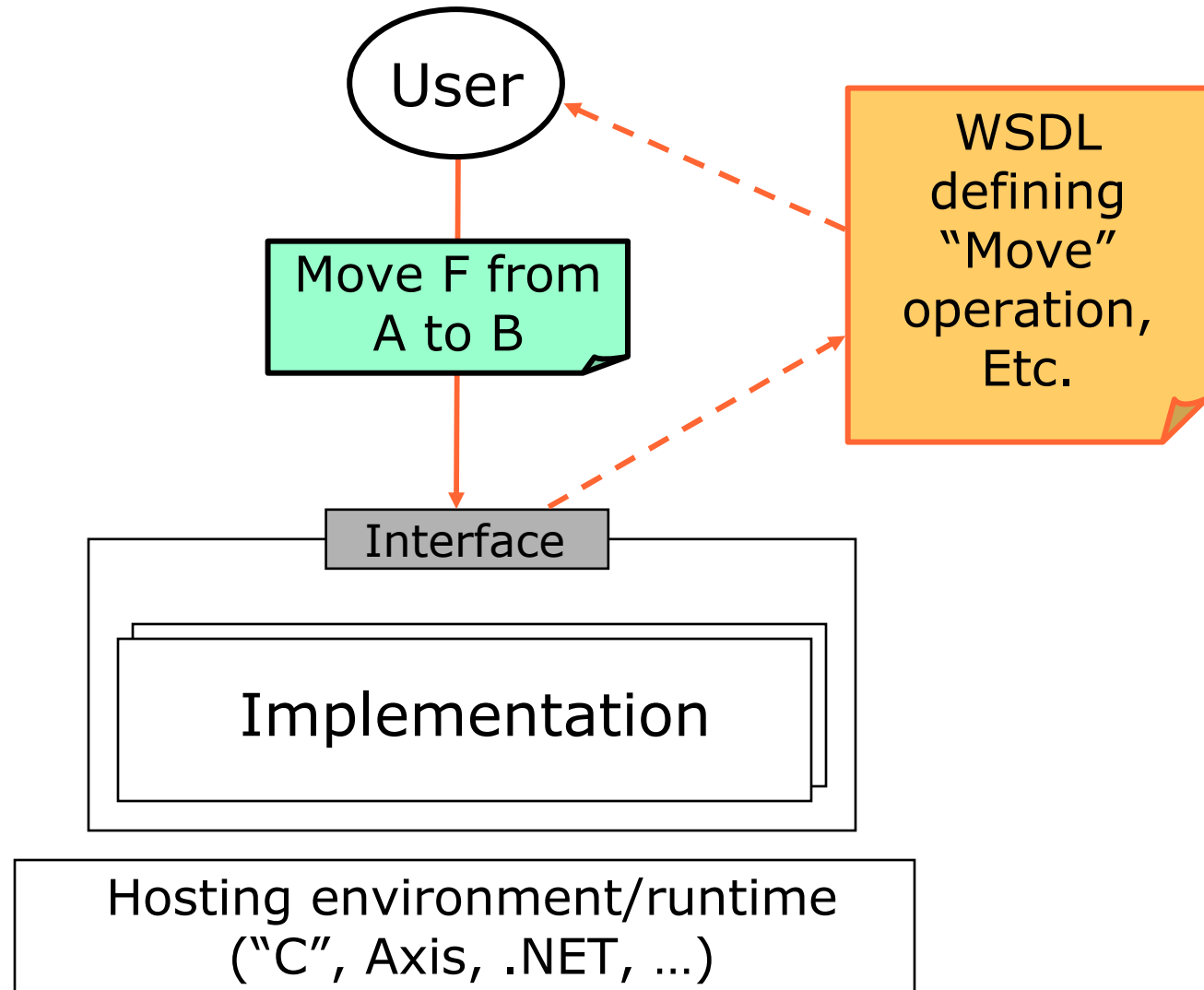
Define expected messages for a service, and their (input or output parameters)

An interface groups together a number of messages (operations)

Bind an Interface via a definition to a specific transport (e.g. HTTP) and messaging (e.g. SOAP) protocol

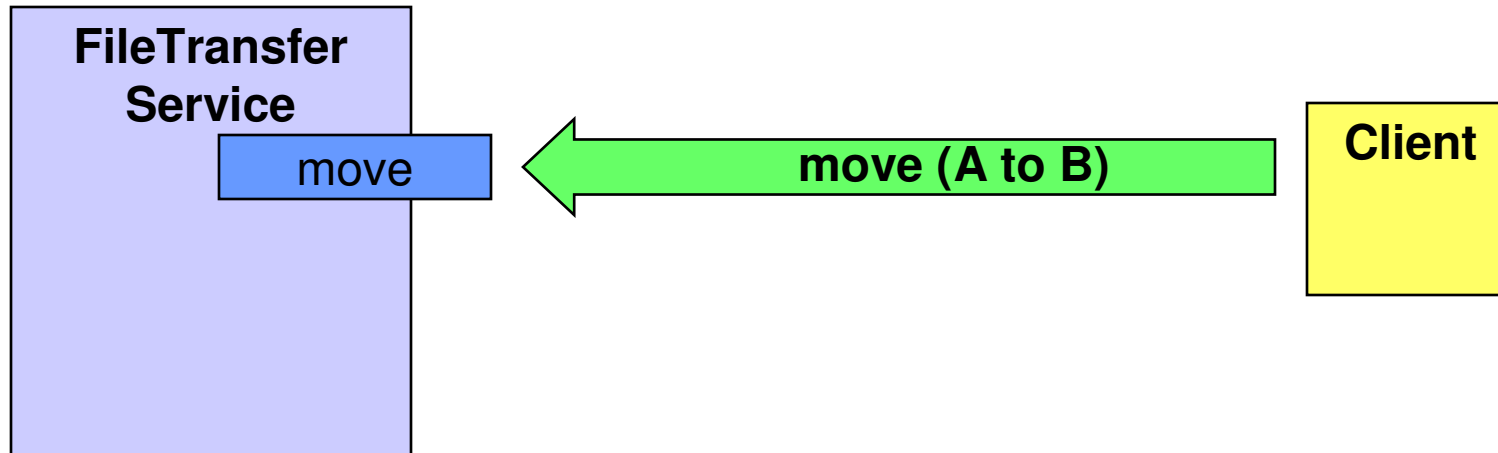
The network location where the service is implemented , e.g. <http://localhost:8080>

Web Services: E.g., File Transfer Service



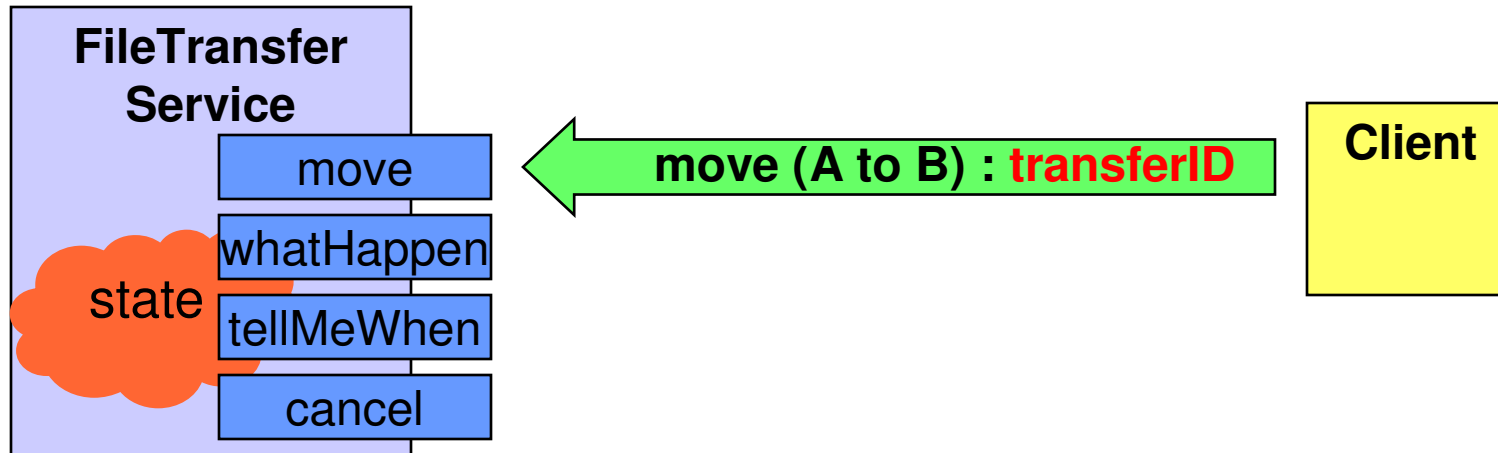


"Stateless" vs. "Stateful" Services



- Without state, how does client:
 - ◆ Determine what happened (success/failure)?
 - ◆ Find out how many files completed?
 - ◆ Receive updates when interesting events arise?
 - ◆ Terminate a request?
- Few useful services are truly "stateless", but WS interfaces alone do not provide built-in support for state

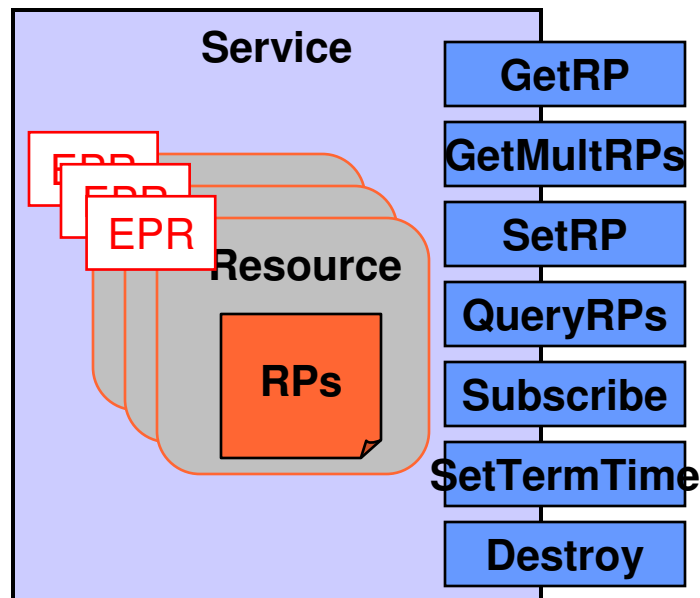
FileTransferService (without WSRF)



- Developer reinvents wheel for each new service
 - ◆ Custom management and identification of state: **transferID**
 - ◆ Custom operations to inspect state synchronously (**whatHappen**) and asynchronously (**tellMeWhen**)
 - ◆ Custom lifetime operation (**cancel**)



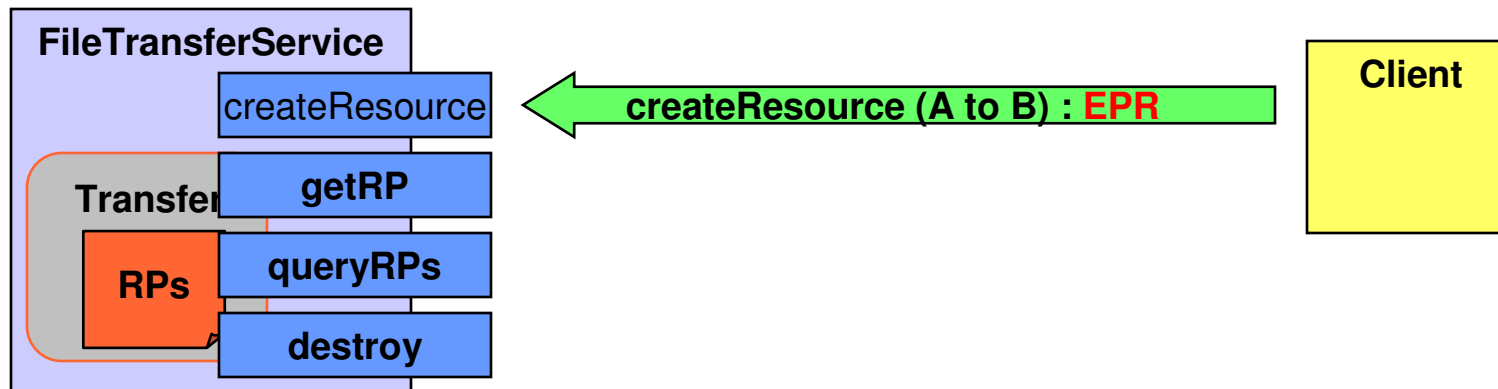
WSRF in a Nutshell



- 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



FileTransferService (w/ WSRF)

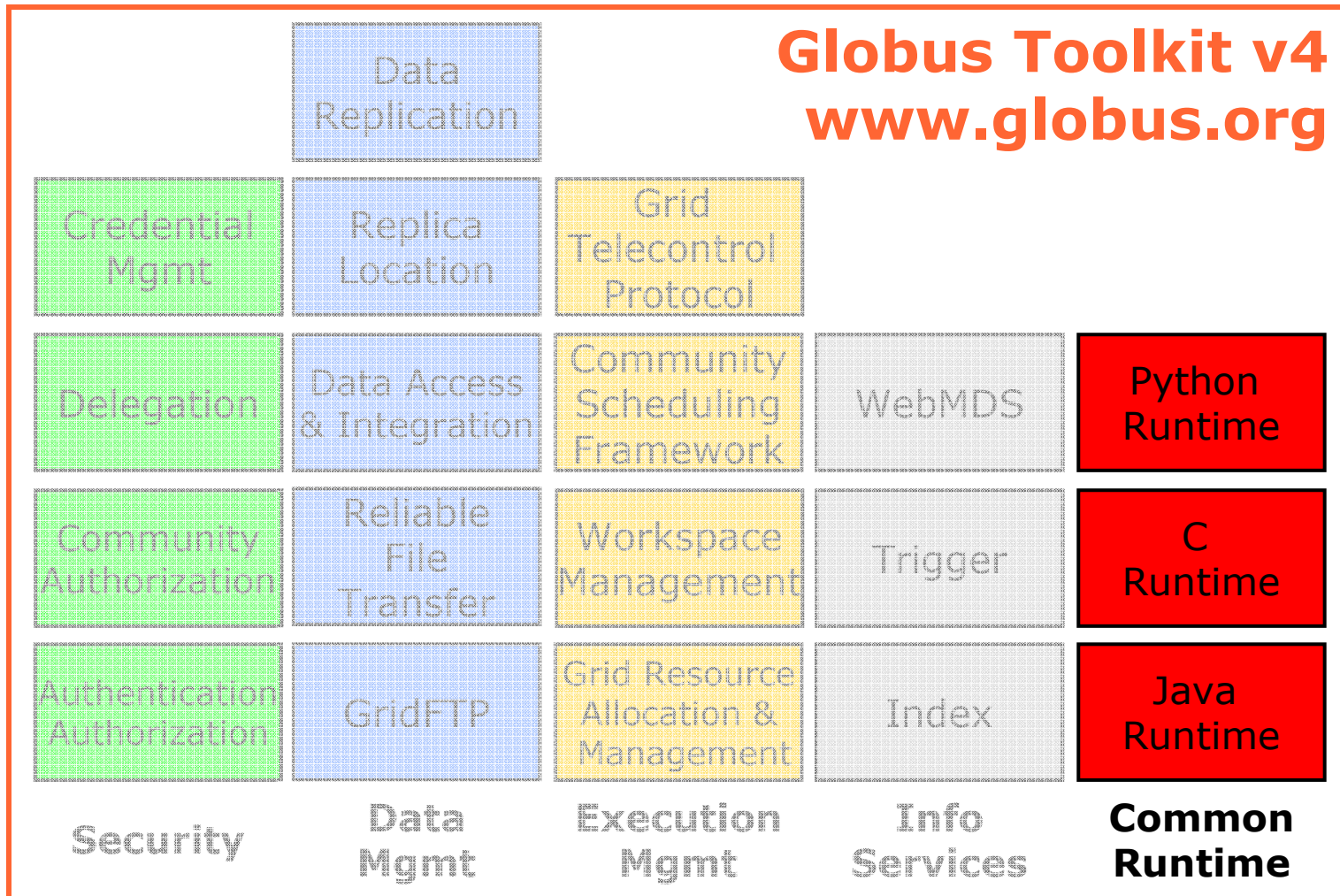


- Developer specifies custom method to createResource and leaves the rest to WSRF standards:
 - ◆ State exposed as Resource + Resource Properties and identified by Endpoint Reference (EPR)
 - ◆ State inspected by standard interfaces (GetRP, QueryRPs)
 - ◆ Lifetime management by standard interfaces (Destroy)

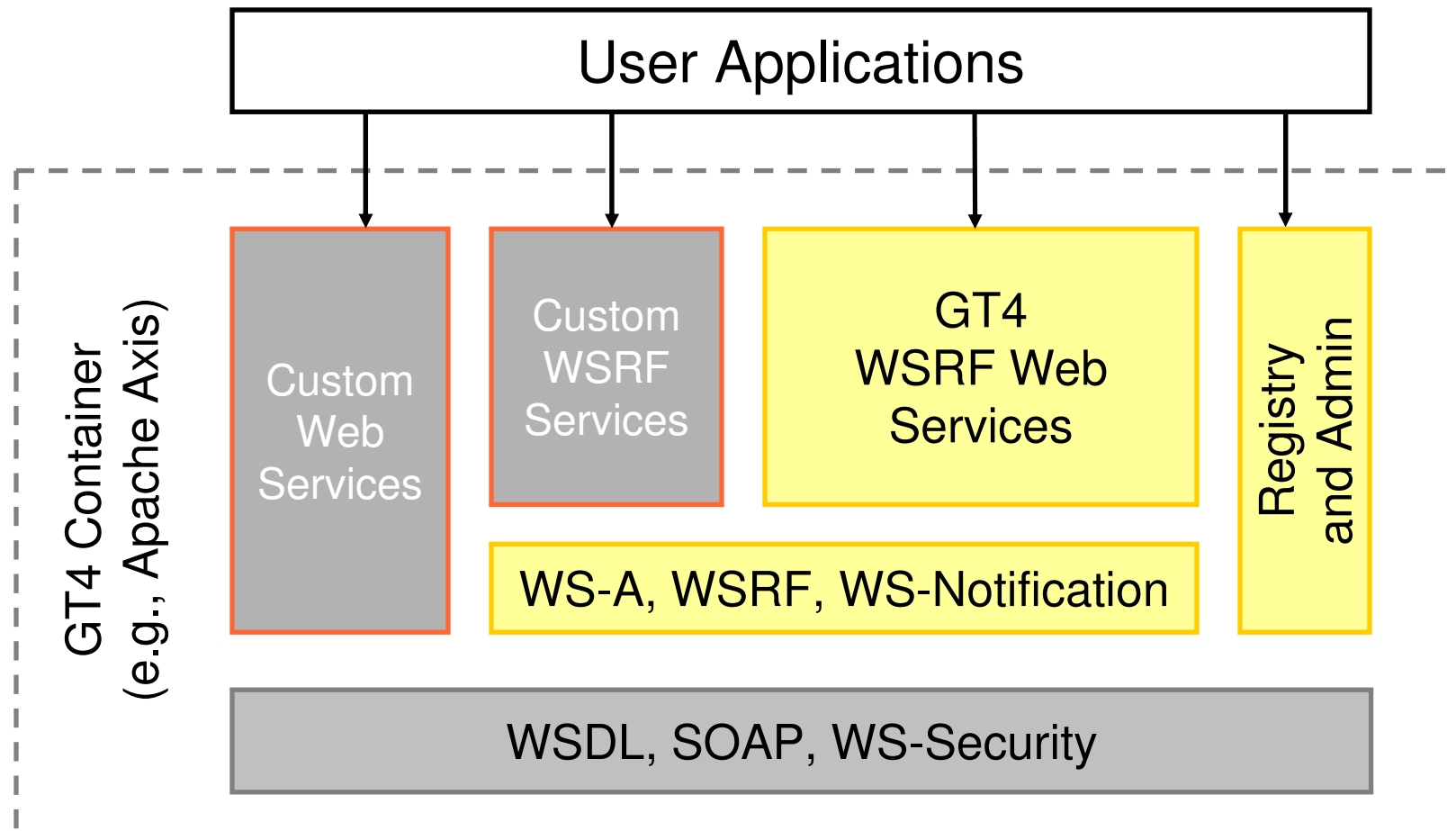


Globus Toolkit: Open Source Grid Infrastructure

Globus Toolkit v4
www.globus.org



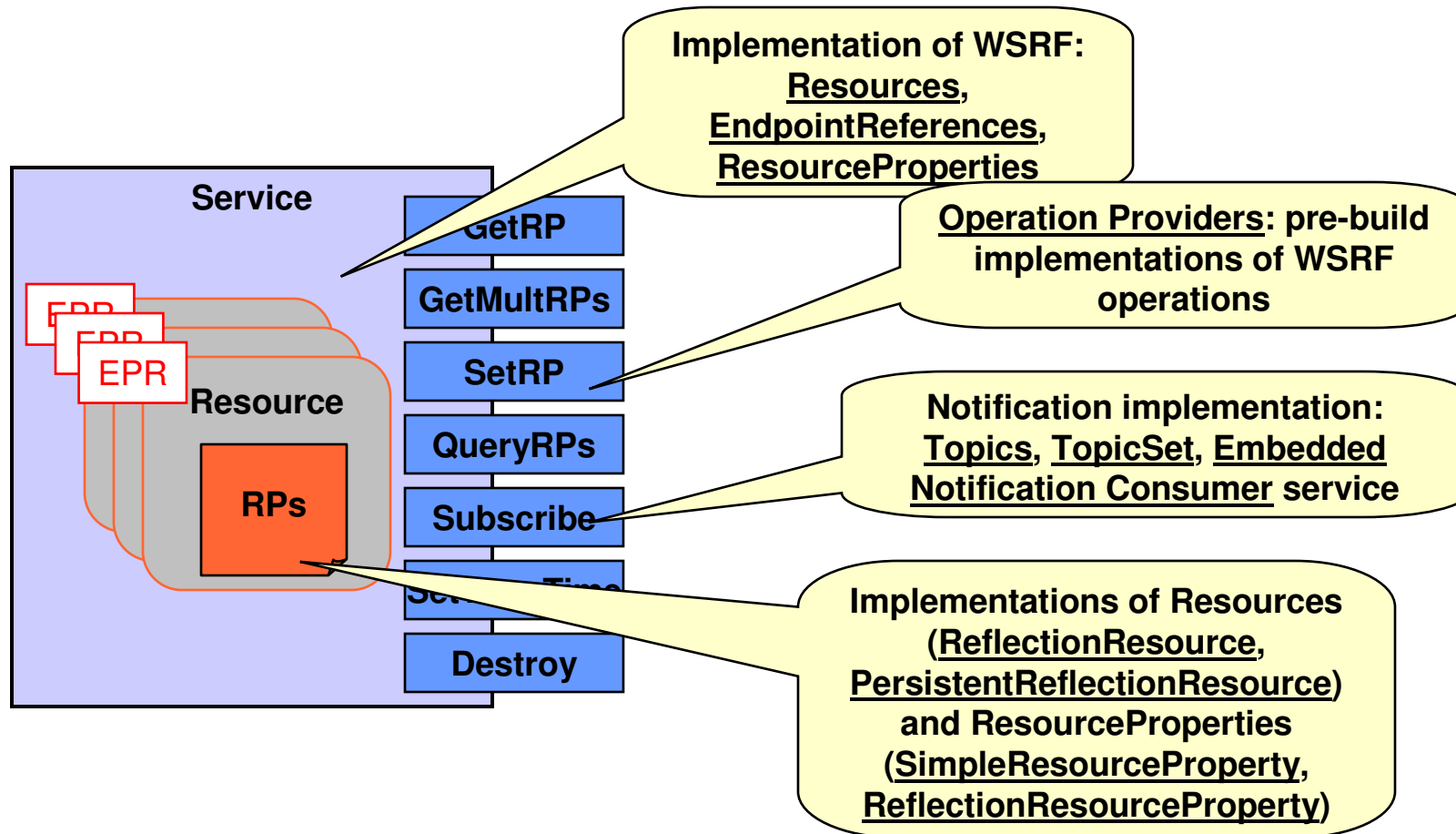
GT4 and Web Services



Java (standard Apache Axis), C (fast, small footprint), Python

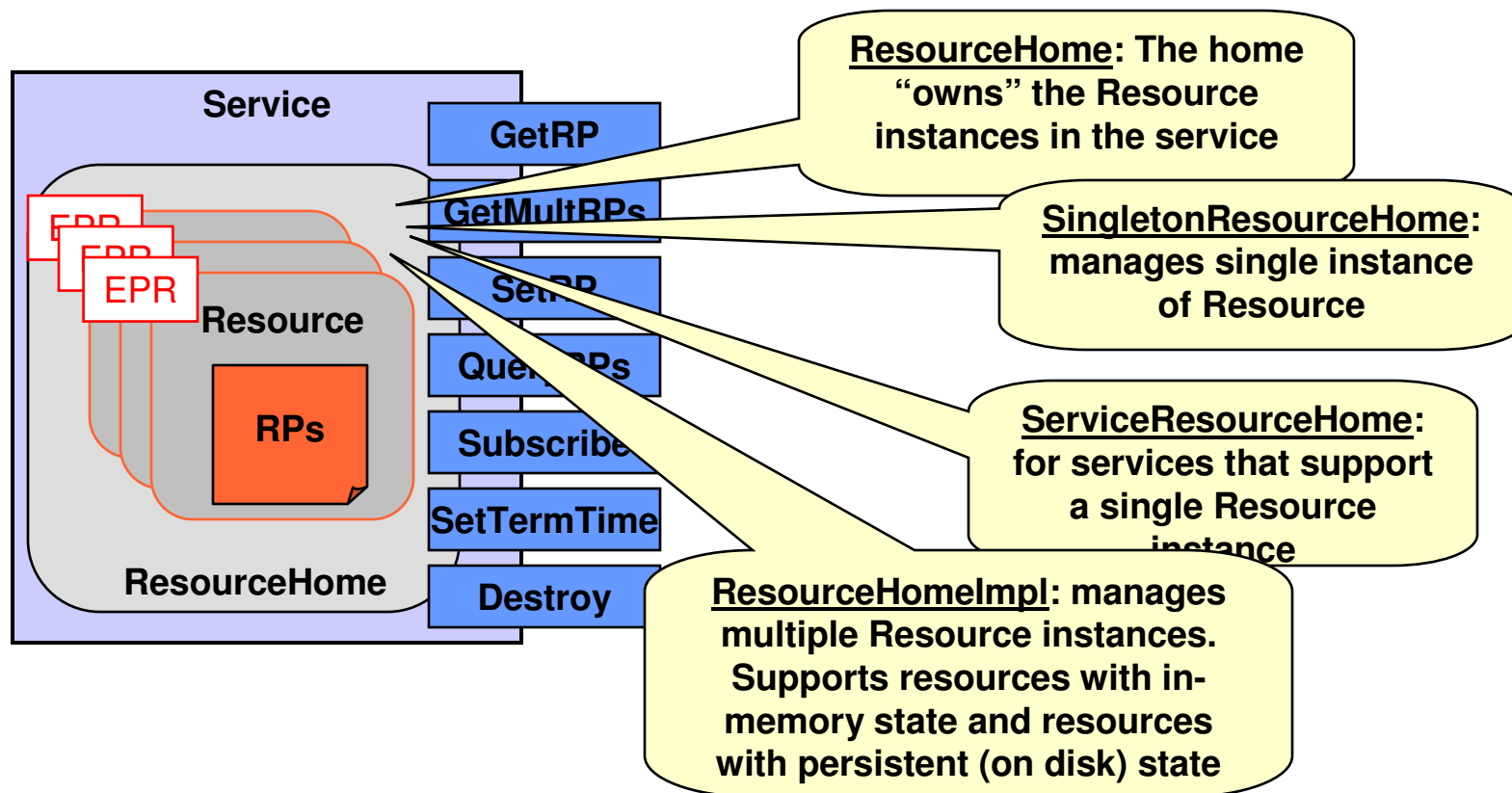


GT4 WS Core in a Nutshell



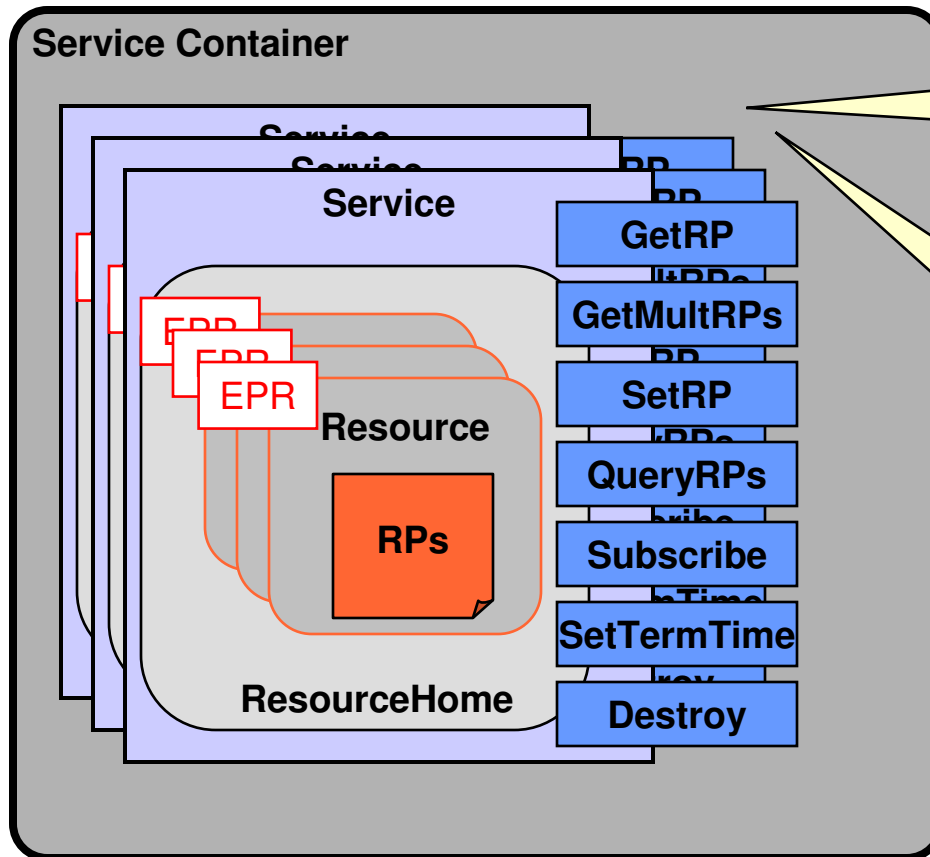


GT4 WS Core in a Nutshell



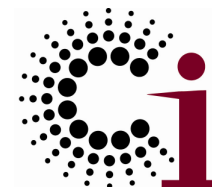


GT4 WS Core in a Nutshell

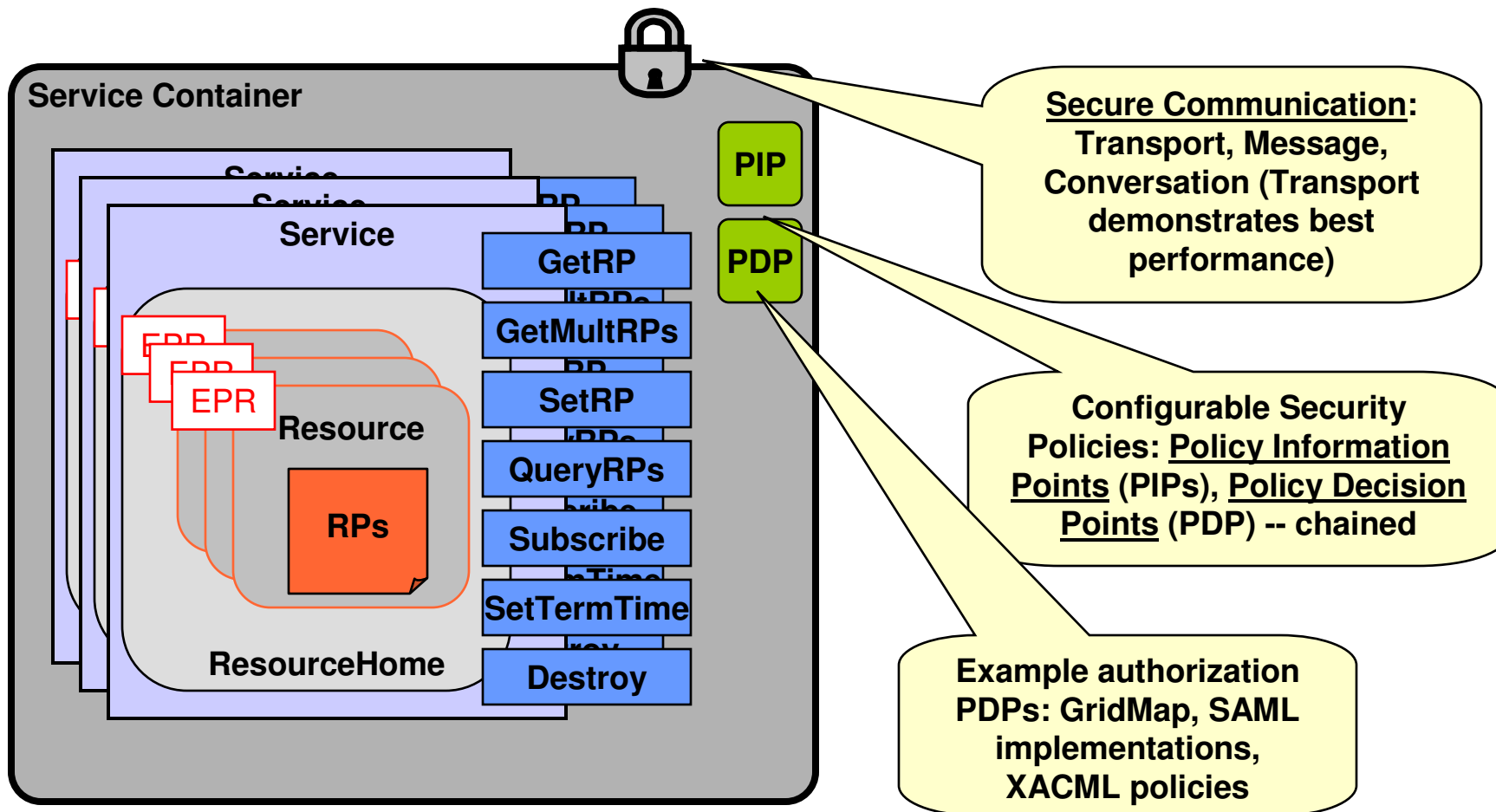


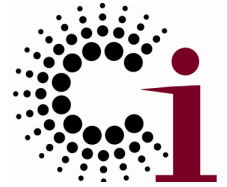
Service Container: host multiple services in container; one JVM process

...more details: based on AXIS service container, processes SOAP messages, ResourceContext extension.

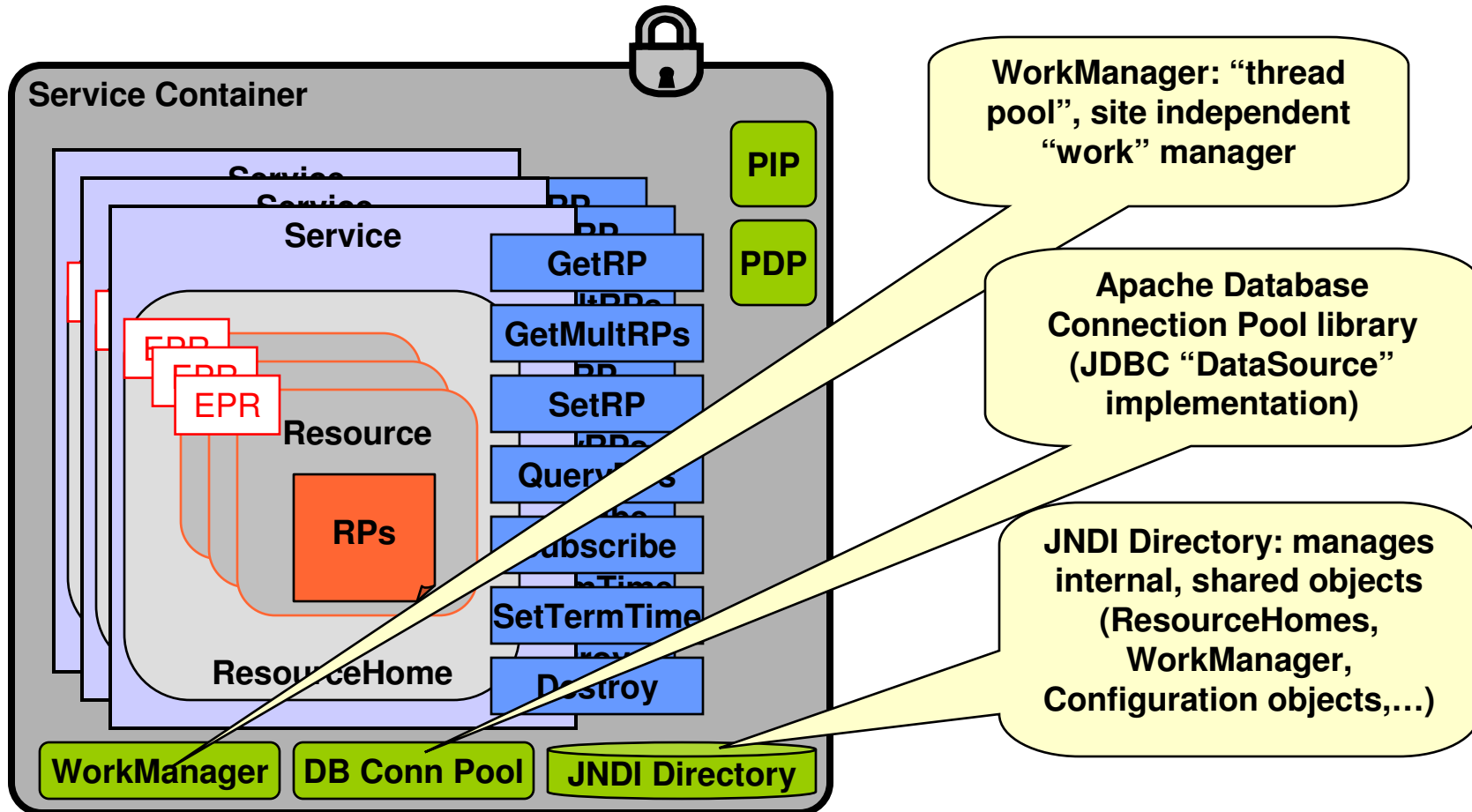


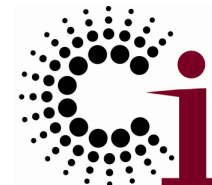
GT4 WS Core in a Nutshell



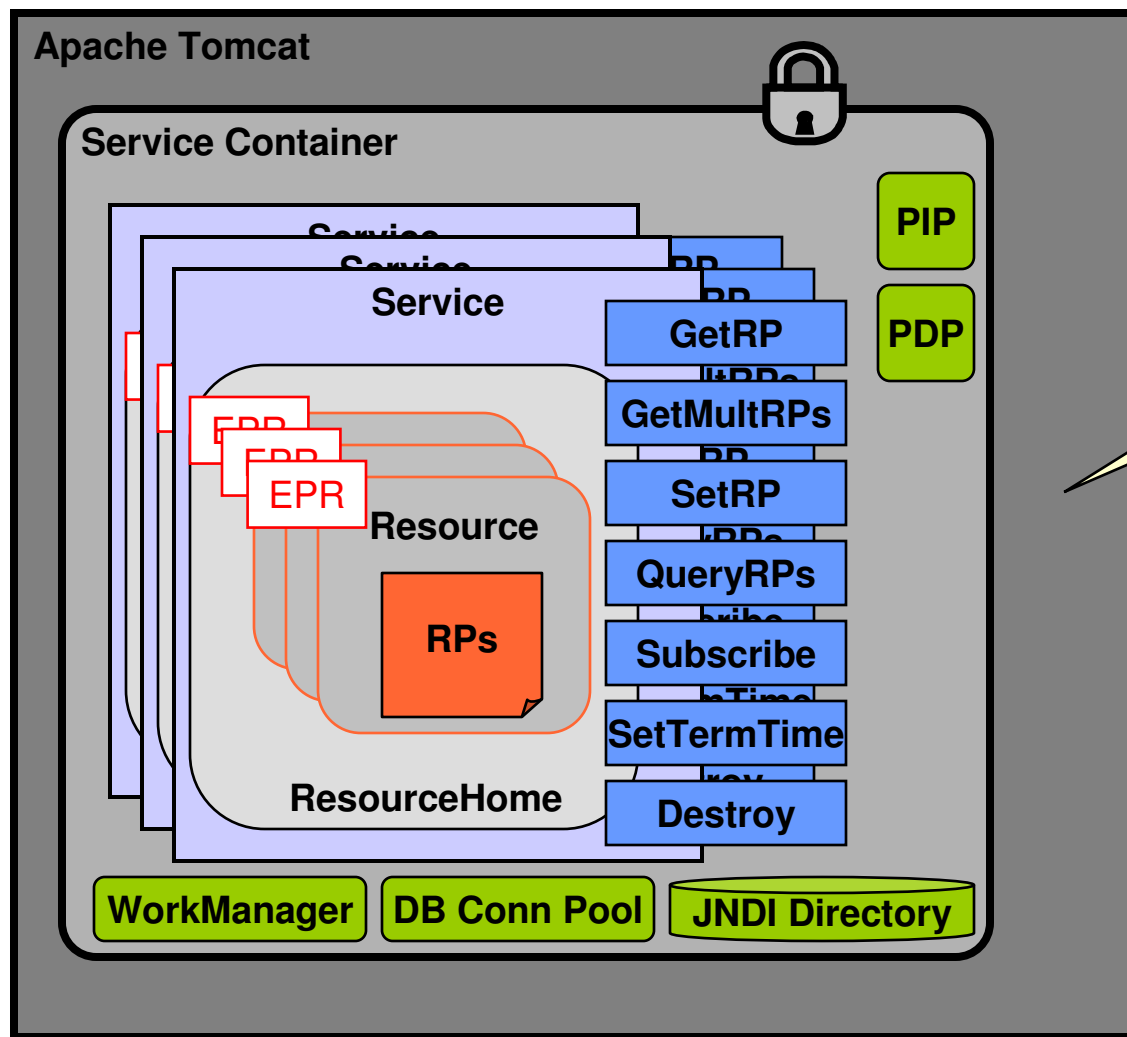


GT4 WS Core in a Nutshell





GT4 WS Core in a Nutshell



Deploy Service Container "standalone" or within Apache Tomcat



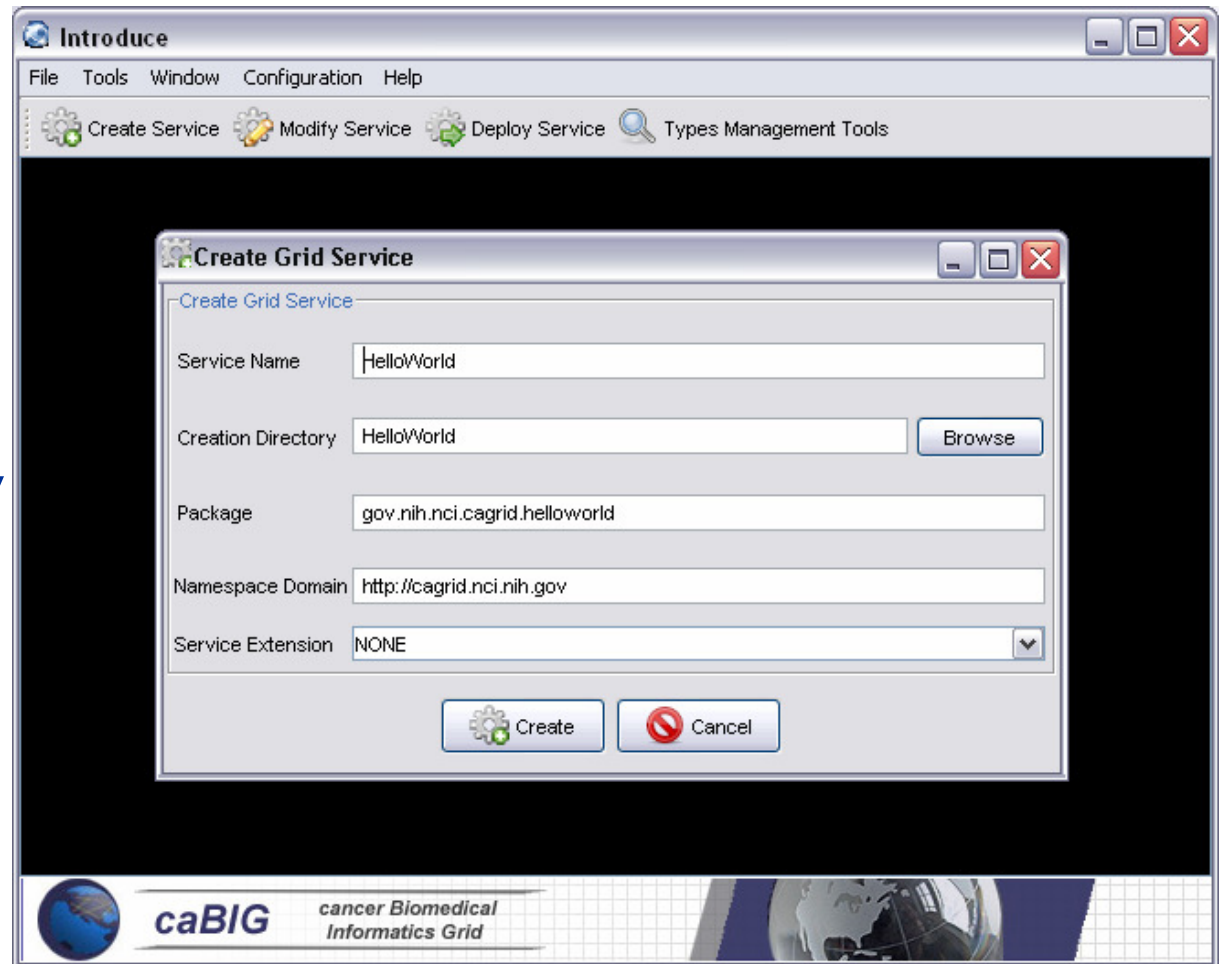
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The Introduce Authoring Tool

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

See also: SOAPLab,
OPAL, pyGlobus,
Gannon, etc.

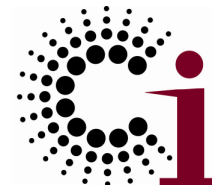


Introduce: Hastings, Saltz, et al., Ohio State University

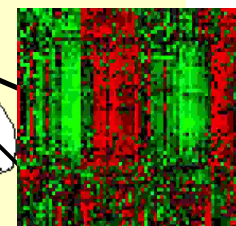
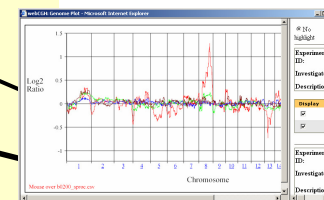
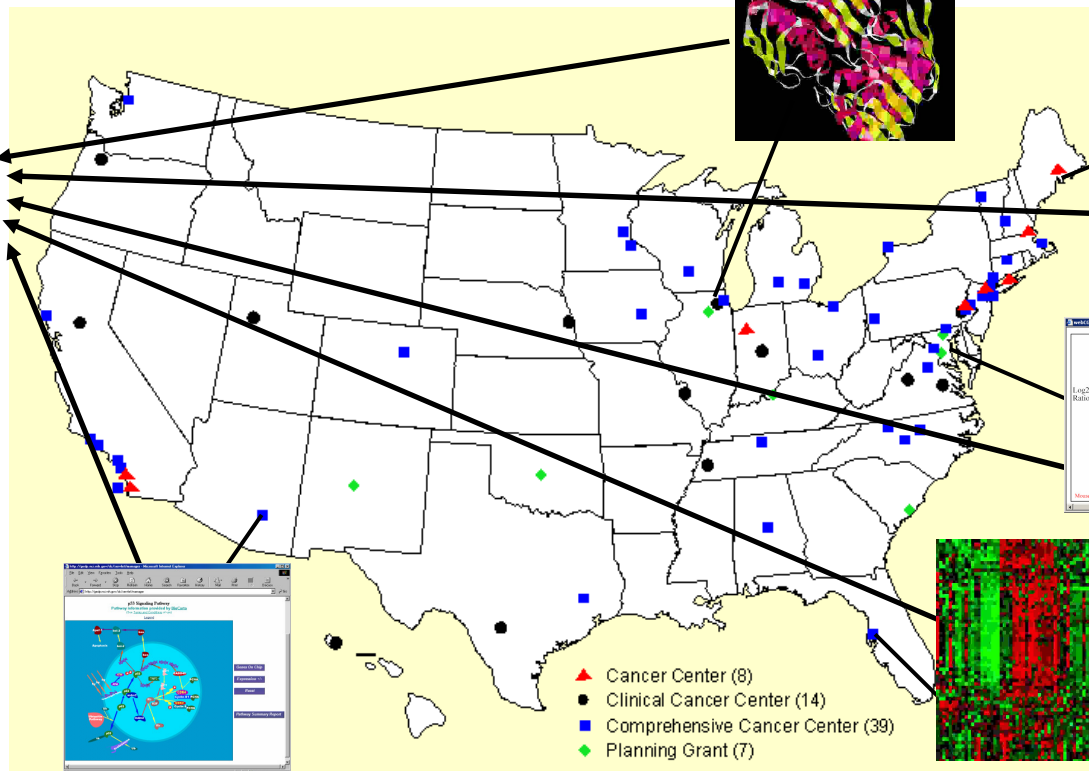
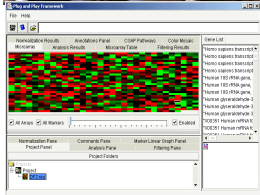


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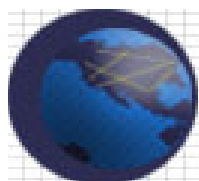
For Example: Cancer Biology



caBIG: sharing of infrastructure, applications, and data.

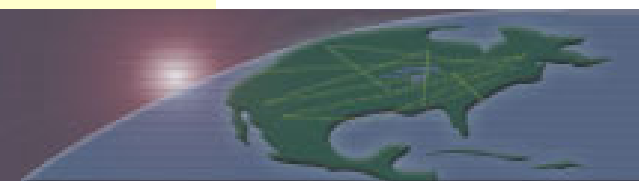


**Data
Integration!**



caBIG

cancer Biomedical
Informatics Grid

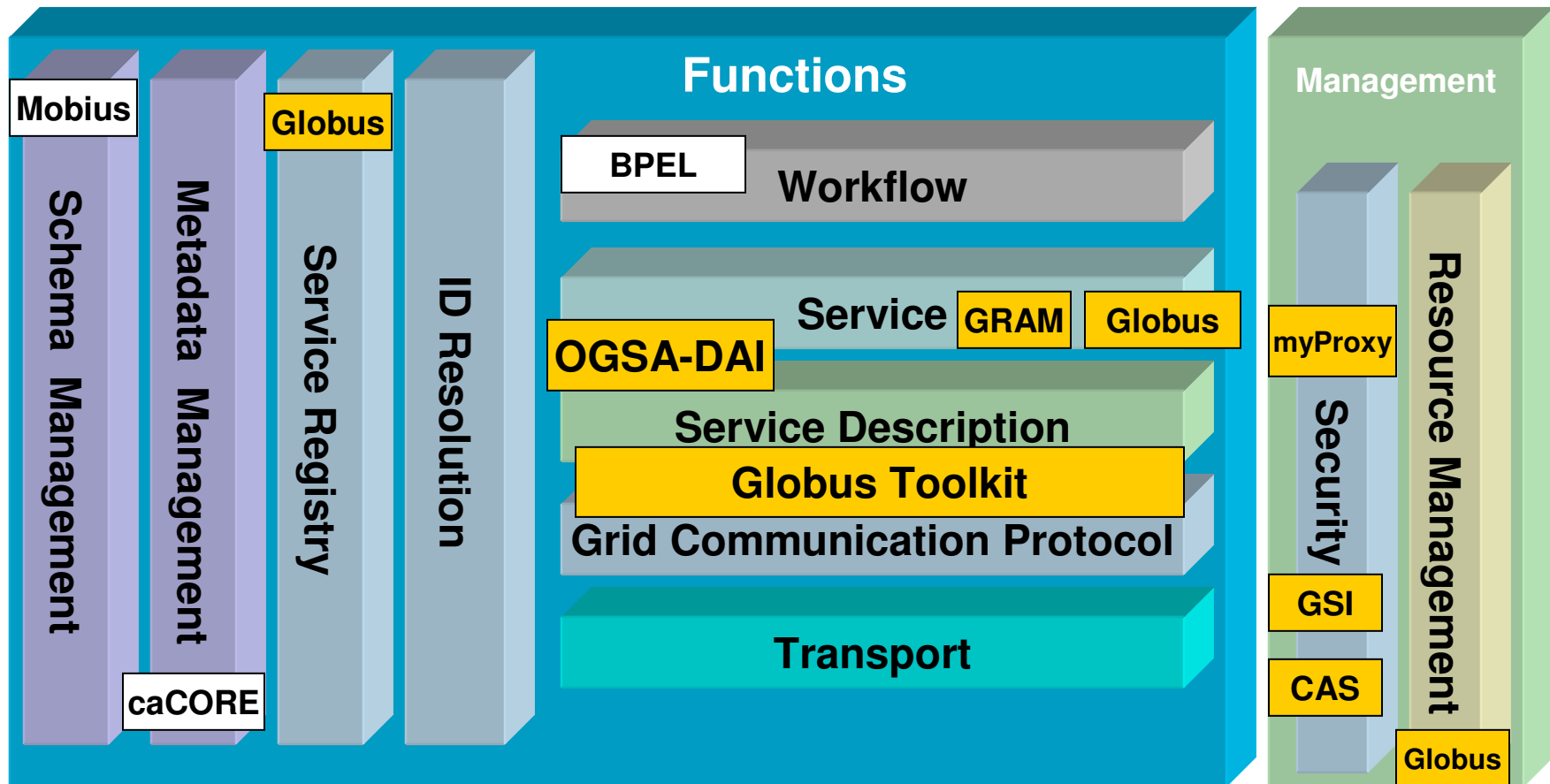




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Cancer Biomedical Informatics Grid



Spans 60 NIH cancer centers across the U.S.



caBIG™ cancer Biomedical Informatics Grid™

an initiative of the National Cancer Institute

Slide credit: Peter Covitz, National Institutes of Health

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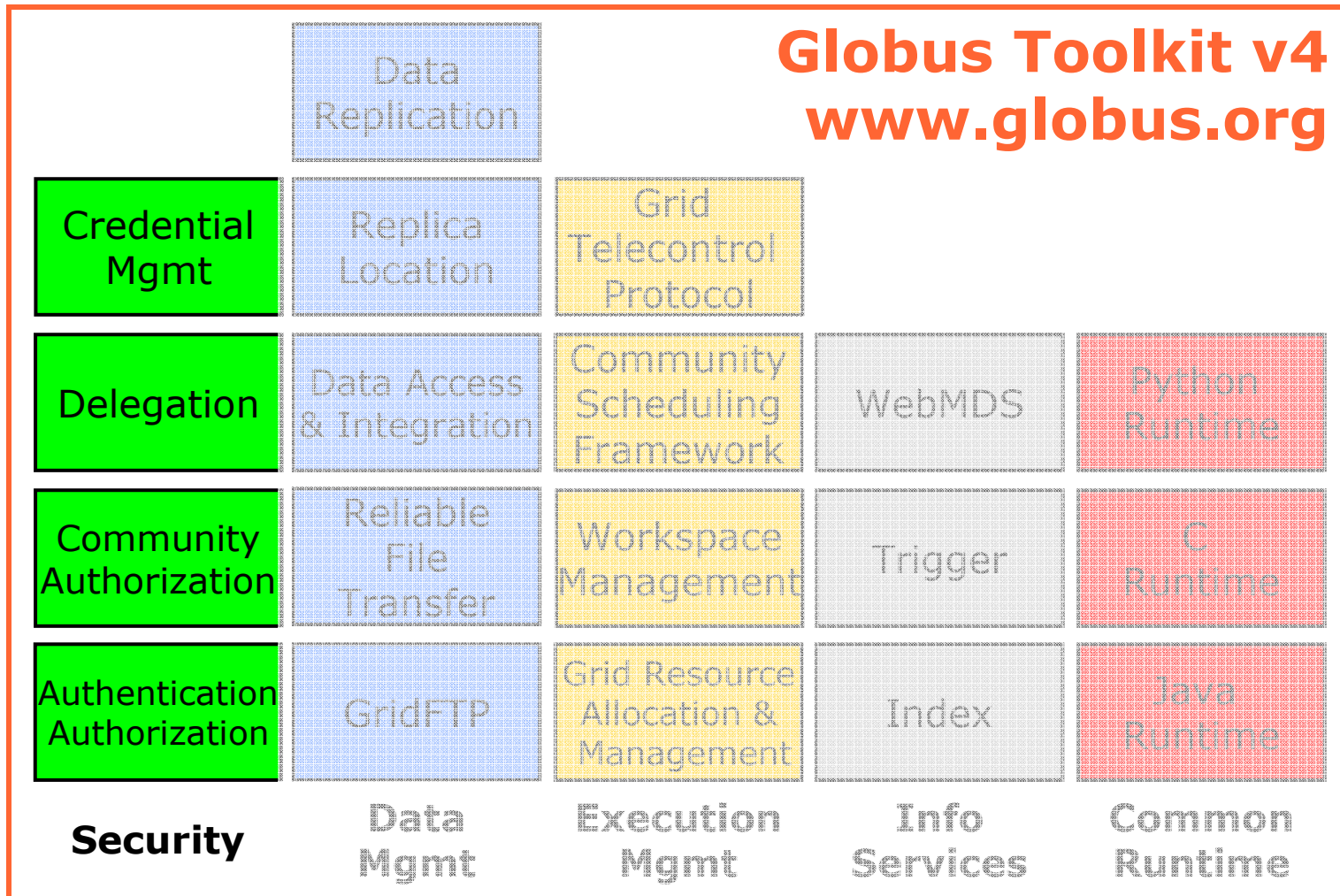
Grid Security Concerns

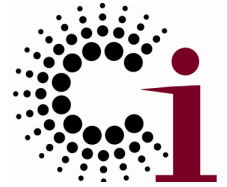
- Control access to shared services
 - ◆ Address autonomous management, e.g., different policy in different work groups
- Support multi-user collaborations
 - ◆ Federate through mutually trusted services
 - ◆ Local policy authorities rule
- Allow users and application communities to set up dynamic trust domains
 - ◆ Personal/VO collection of resources working together based on trust of user/VO



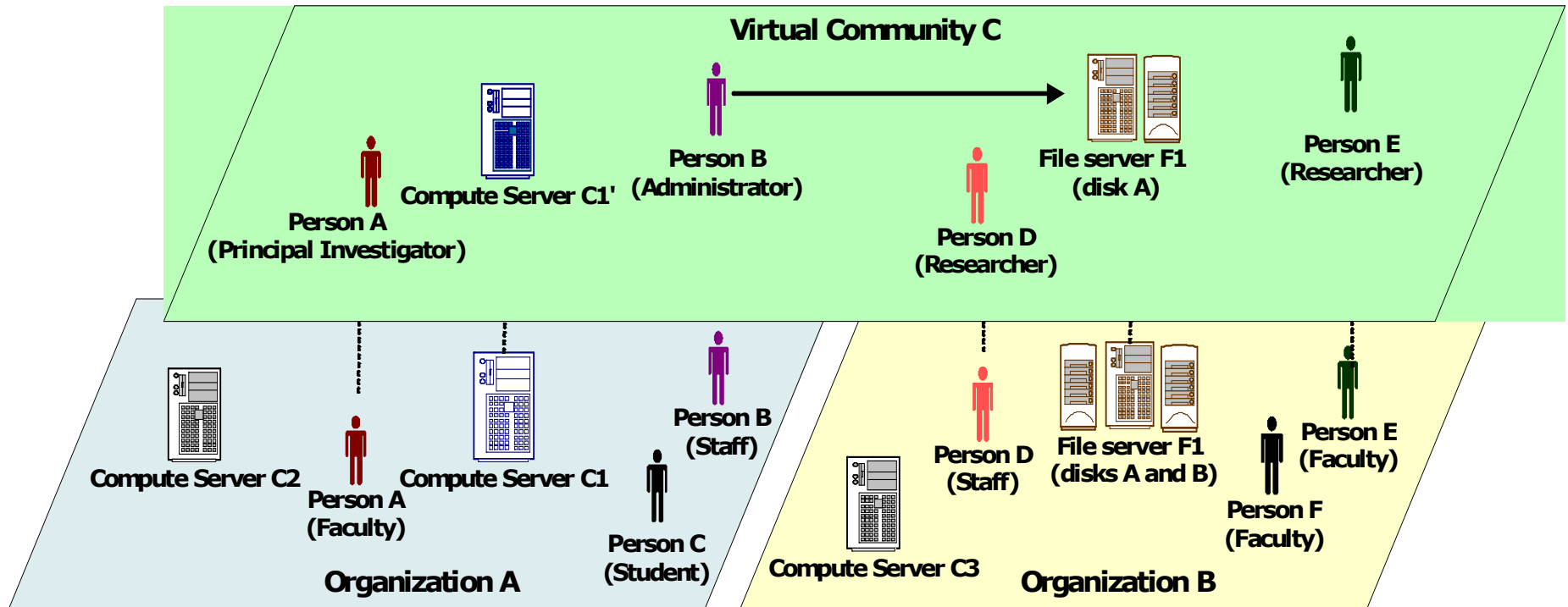
Globus Toolkit: Open Source Grid Infrastructure

Globus Toolkit v4
www.globus.org

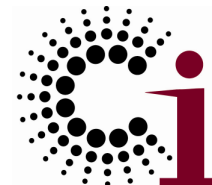




Virtual Organization (VO) Concept



- VO for each application or workload
- Carve out and configure resources for a particular use and set of users



Equipment:
Must have X-Ray training

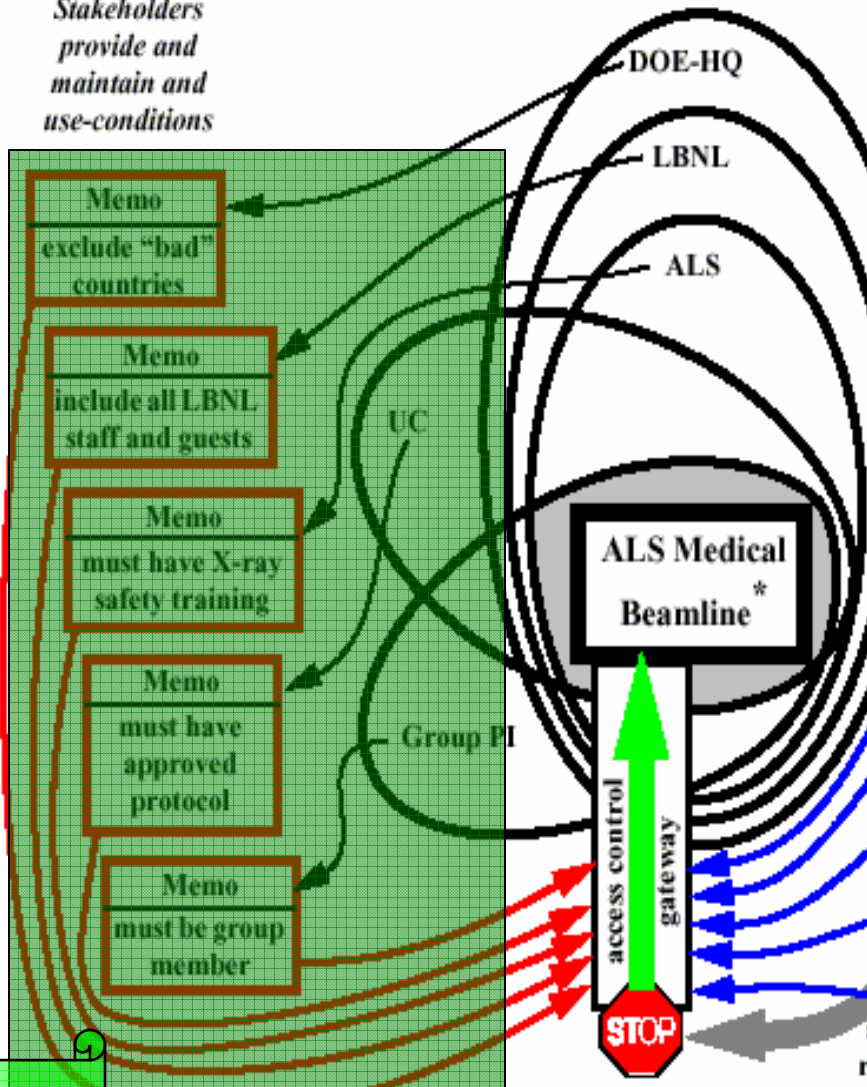
LAB:
Exclude "bad" countries
Include all LBNL staff and guests

R&D Group:
Must be a group member

Effective permission

(1) Use-conditions are Imposed by Independent Stakeholders

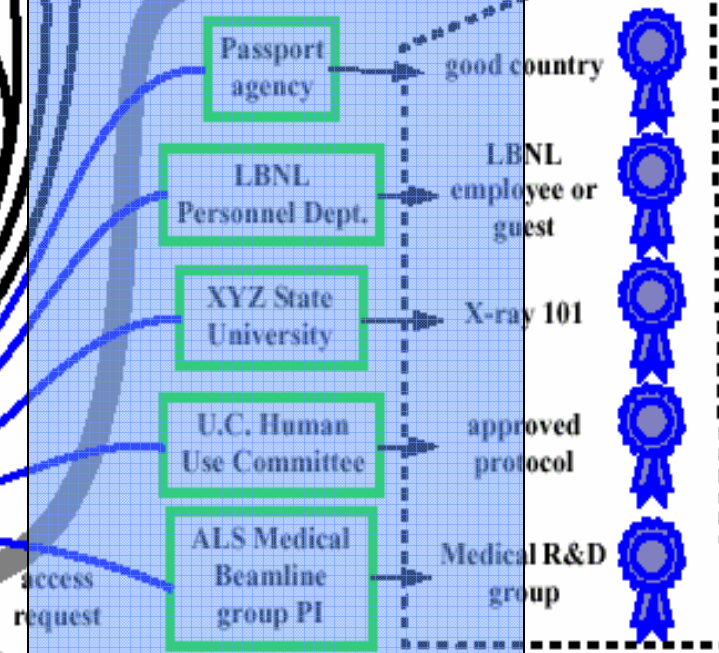
Stakeholders provide and maintain and use-conditions



SAML

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

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



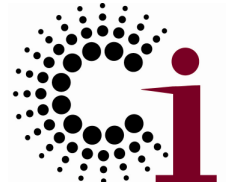
GT4 Security

- Public-key-based authentication
- Extensible authorization framework based on Web services standards
 - ◆ SAML-based authorization callout
 - As specified in GGF OGSA-Authz WG
 - ◆ Integrated policy decision engine
 - XACML (eXtensible Access Control Markup Language) policy language, per-operation policies, pluggable
- Credential management service
 - ◆ MyProxy (One time password support)
- Community Authorization Service
- Standalone delegation service



GT4's Use of Security Standards

	Message-level Security w/X.509 Credentials	Message-level Security w/Usernames and Passwords	Transport-level Security w/X.509 Credentials
Authorization	SAML and grid-mapfile	grid-mapfile	SAML and grid-mapfile
Delegation	X.509 Proxy Certificates/ WS-Trust		X.509 Proxy Certificates/ WS-Trust
Authentication	X.509 End Entity Certificates	Username/ Password	X.509 End Entity Certificates
Message Protection	WS-Security WS-SecureConversation	WS-Security	TLS
Message format	SOAP	SOAP	SOAP
	Supported, but slow	Supported, but insecure	Fastest, so default

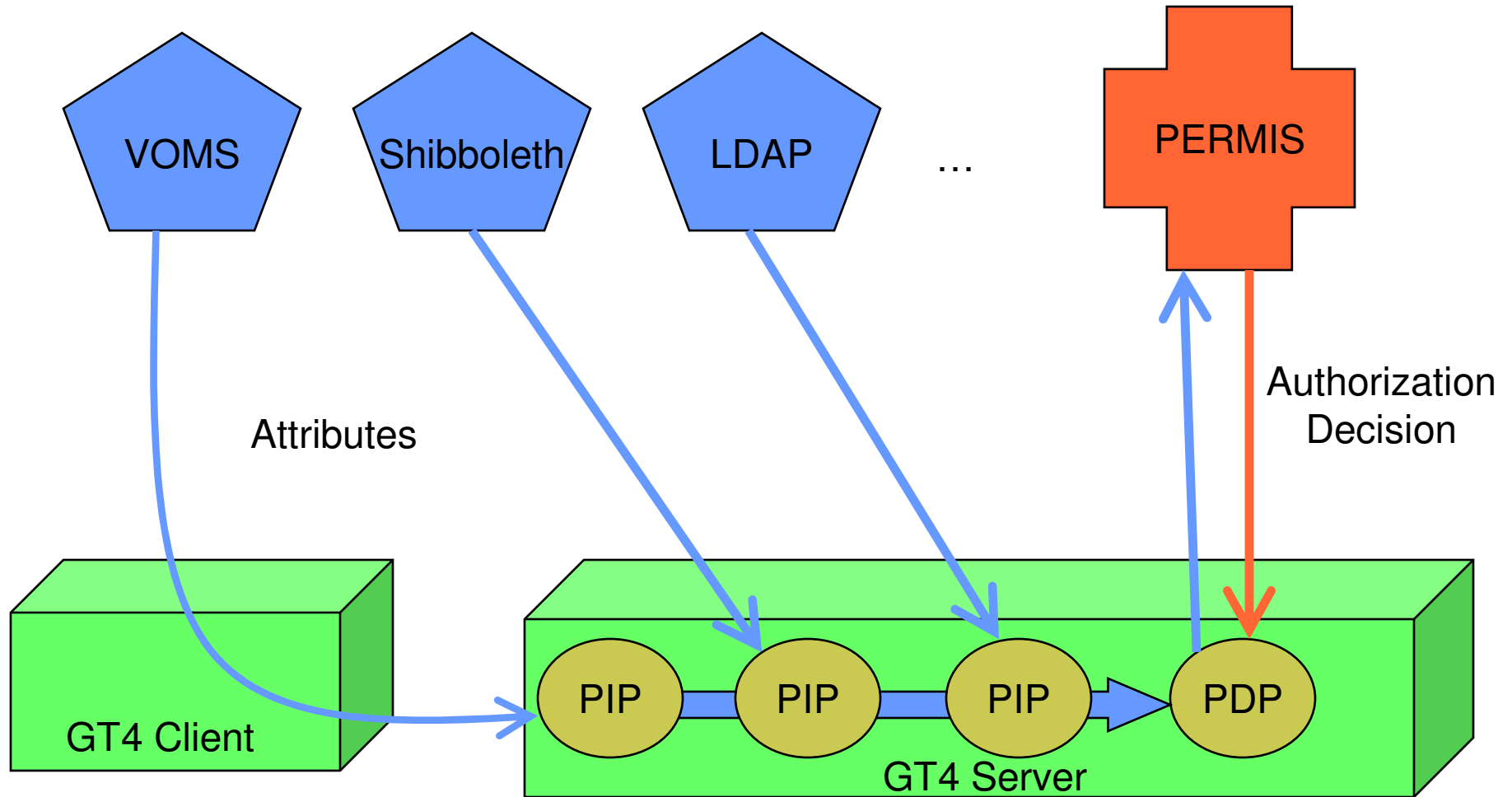


GT-XACML Integration

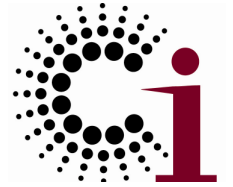
- eXtensible Access Control Markup Language
 - ◆ OASIS standard, open source implementations
- XACML: sophisticated policy language
- Globus Toolkit ships with XACML runtime
 - ◆ Included in every client and server built on GT
 - ◆ Turned-on through configuration
- ... that can be called transparently from runtime and/or explicitly from application ...
- ... and we use the XACML-“model” for our Authz Processing Framework



GT Authorization Framework



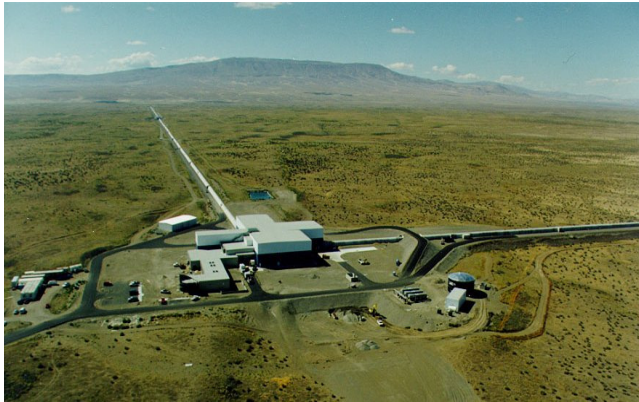
More Specifically, I May Want To ...



- Create a service for use by my colleagues
- Manage who is allowed to access my service (or my experimental data or ...)
- Ensure reliable & secure distribution of data from my lab to my partners
- Run 10,000 jobs on whatever computers I can get hold of
- Monitor the status of the different resources to which I have access

Use Case: Distribution of a New Data Set

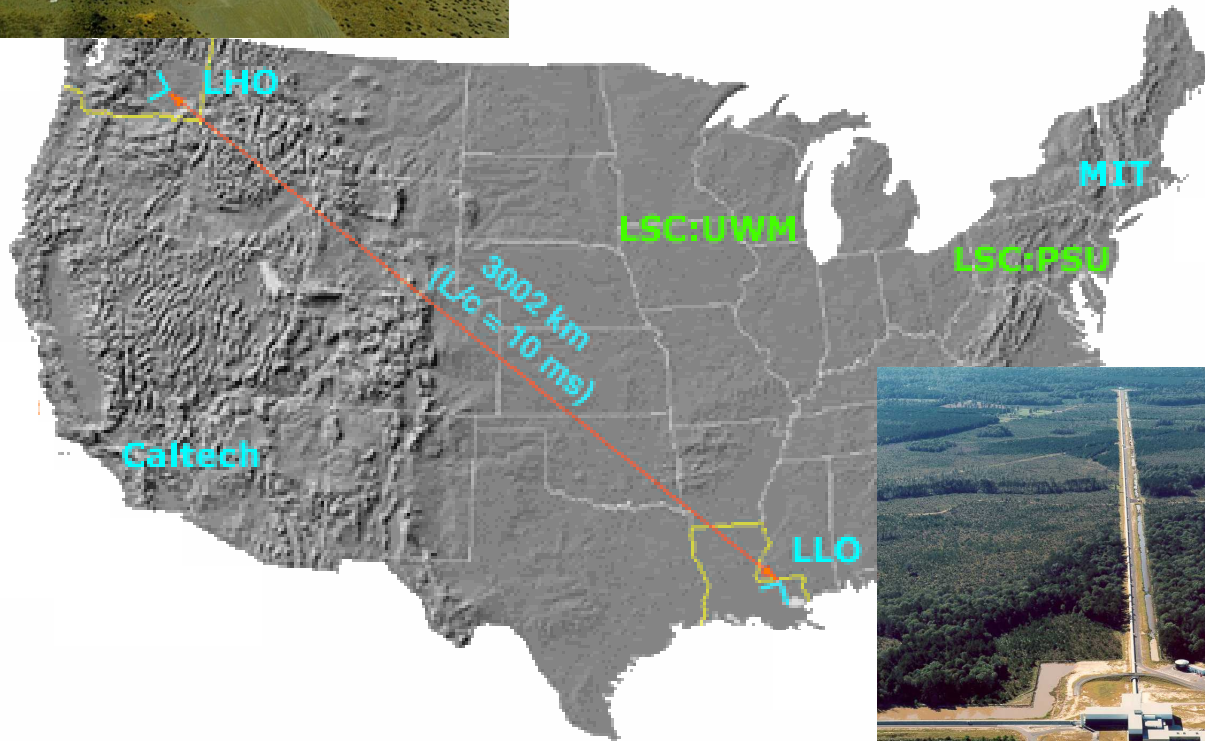
- Typical requirement for a distributed team performing iterative design tasks
- Data set is logically defined
 - ◆ Domain-specific name: 'System Design V1.32'
 - ◆ Map to physical files: directories, catalog, etc.
- Users, applications, workflows request latest data
 - ◆ Scripted or through a web service interface.
 - ◆ Requests are recorded and failures are retried.
- Global policies are applied
 - ◆ Bandwidth usage is managed
 - ◆ Access policies are enforced
- Replicas at each site are tracked
 - ◆ Redundant transfers are avoided
 - ◆ Files are copied from cheapest up-to-date source



Reliable Wide Area Data Replication



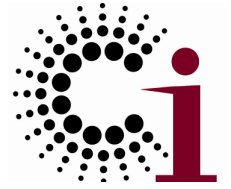
LIGO Gravitational Wave Observatory



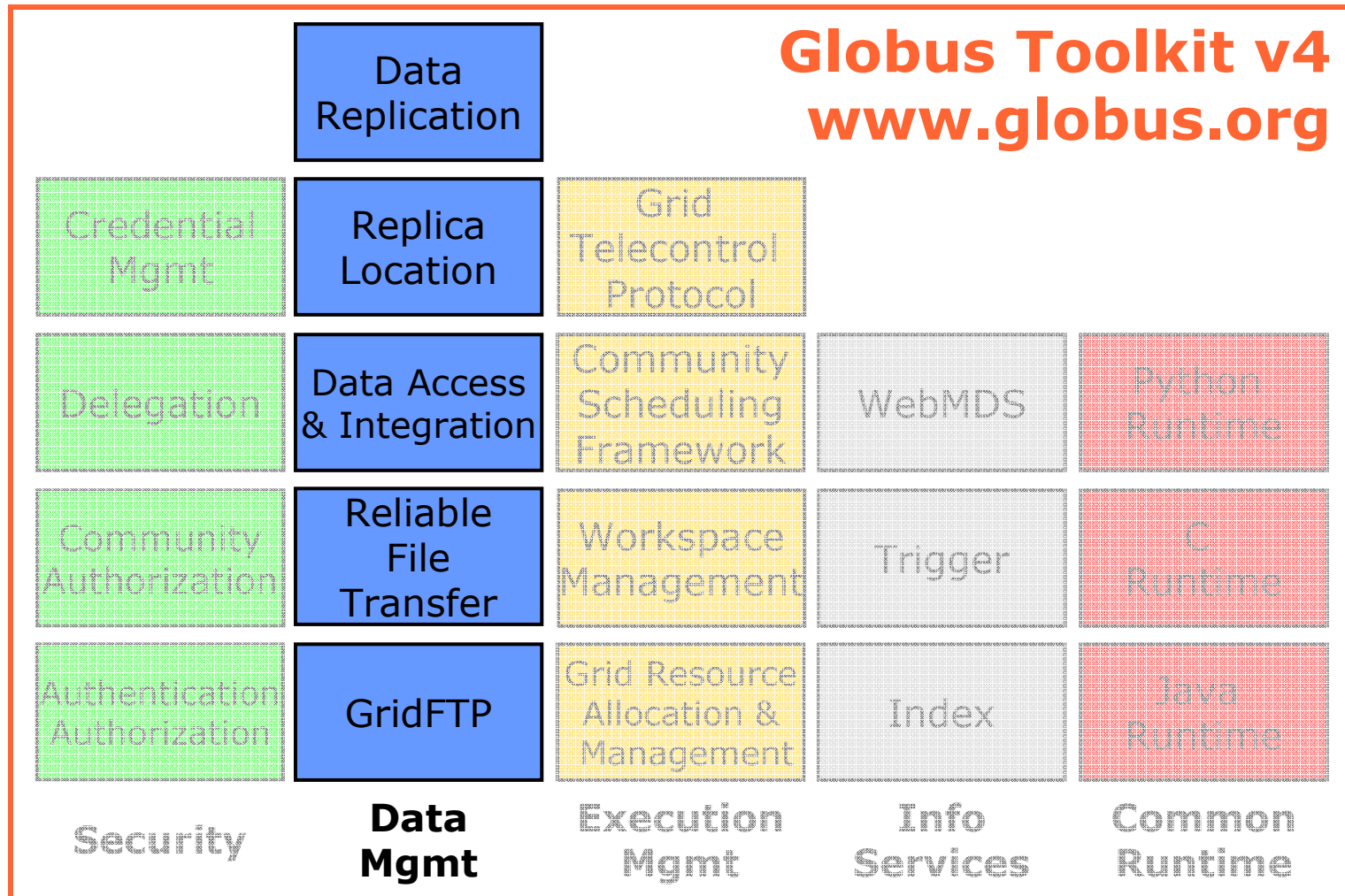
Replicating >1 Terabyte/day to 8 sites
>30 million replicas so far

MTBF = 1 month www.globus.org/solutions



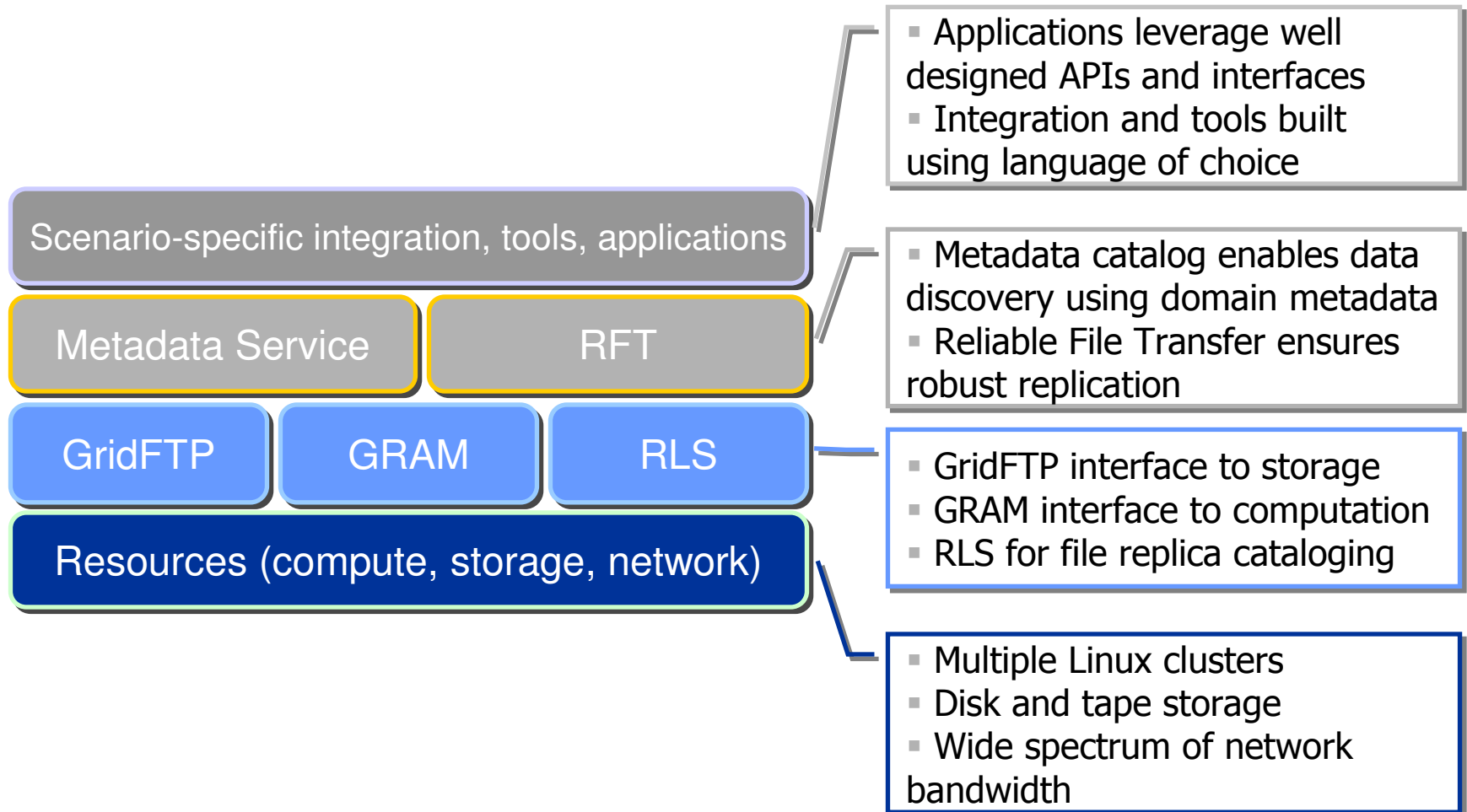


Globus Toolkit: Open Source Grid Infrastructure





Data Services Foundation





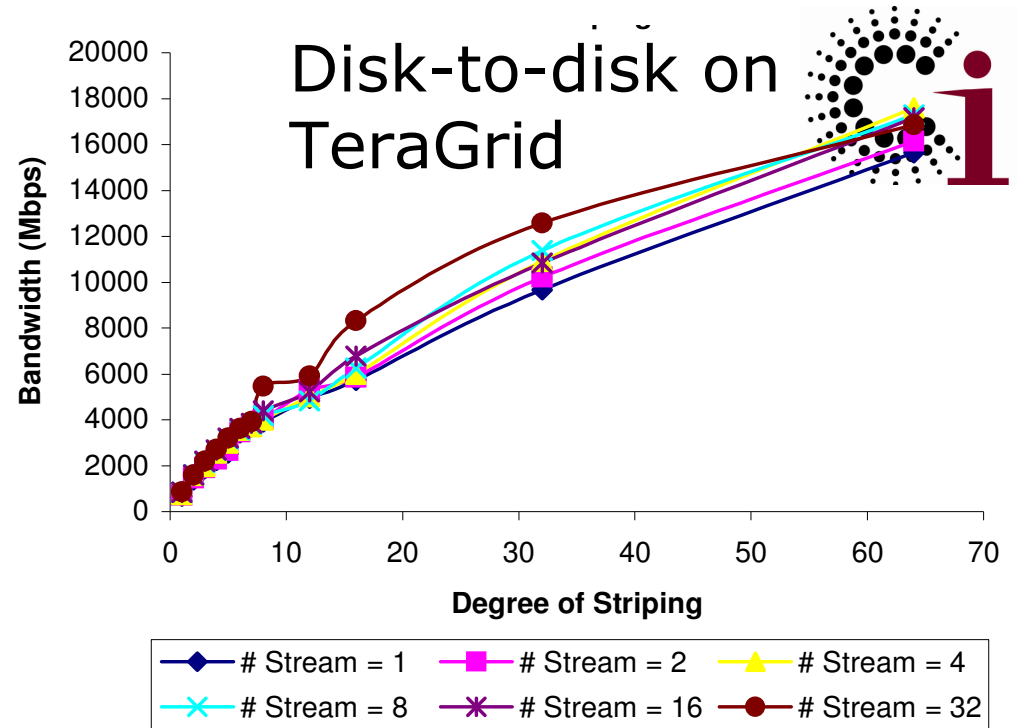
GT4 Data Management

- **Stage/move** large data to/from nodes
 - ◆ GridFTP, Reliable File Transfer (RFT)
 - ◆ Alone, and integrated with GRAM
- **Locate** data of interest
 - ◆ Replica Location Service (RLS)
- **Replicate** data for performance/reliability
 - ◆ Distributed Replication Service (DRS)
- Provide **access** to diverse data sources
 - ◆ File systems, parallel file systems, hierarchical storage: GridFTP
 - ◆ Databases: OGSA DAI



GridFTP in GT4

- 100% Globus code
 - ◆ No licensing issues
 - ◆ Stable, extensible
- IPv6 Support
- XIO for different transports
- Striping → multi-Gb/sec wide area transport
 - ◆ 27 Gbit/s on 30 Gbit/s link
- Pluggable
 - ◆ Front-end: e.g., future WS control channel
 - ◆ Back-end: e.g., HPSS, cluster file systems
 - ◆ Transfer: e.g., UDP, NetBLT transport





GridFTP: Secure, High Performance Data Transport

- Integrated instrumentation: Developers can use client API and plug-in mechanism to leverage different instrumentation
 - ◆ Performance markers
 - ◆ Restart markers
 - ◆ Throughput performance
 - ◆ Netlogger style performance
- Logging/audit trail: Extensive logging in the server
 - ◆ Multiple log levels: ERROR, WARN, INFO, DUMP, ALL
 - ◆ Log to stdio, syslog, file, ...
 - ◆ Log all connections/transfers to single file or unique files
 - ◆ Netlogger style logging
 - ◆ Control permissions on log files

GridFTP: Secure, High Performance Data Transport

- Parallel data streams
 - ◆ Multiple TCP streams between sender and receiver
 - ◆ Sender pushes multiple blocks in parallel streams
 - ◆ Blocks reassembled at receiving side and put into correct order
 - ◆ Protection against dropped packets for each stream
- TCP buffer size control
 - ◆ Tune buffers to latency of network
 - ◆ Regular FTP optimized for low latency networks, not tunable
- Dramatic improvements for high latency WAN transfers
 - ◆ 90% of network utilization possible
 - ◆ 27 GB/s achieved with commodity hardware



GridFTP: Secure, High Performance Data Transport

- Server-side computation
 - ◆ Extended retrieve (ERET), Extended store (ESTO)
 - ◆ Simple pre-processing (partial get, sub-sampling)
 - ◆ Can greatly reduce network load
 - ◆ Client must also support ESTO/ERET functionality
- Striped server configurations
 - ◆ Multiple server back ends act as single server
 - ◆ Underlying parallel file system accessible to all nodes
 - ◆ High performance requires capable parallel file system
 - ◆ Each node must read/write its blocks of file
 - ◆ Allows multiple levels of parallelism (CPU, bus, NIC, disk, etc.)
 - ◆ Client sees a single logical server

GridFTP: Secure, High Performance Data Transport

- Data Storage Interface (DSI)
 - ◆ Interfaces to various storage types
 - ◆ Implement simple functions such as send, receive, mkdir,...
 - ◆ DSI modules available for HPSS and SRB
- Globus FTP client library (API):
 - ◆ Integration of data transport capabilities directly into applications
 - ◆ Plug-in architecture for installing fault recovery and performance tuning algorithms
 - ◆ Asynchronous programming model



GridFTP: Client API

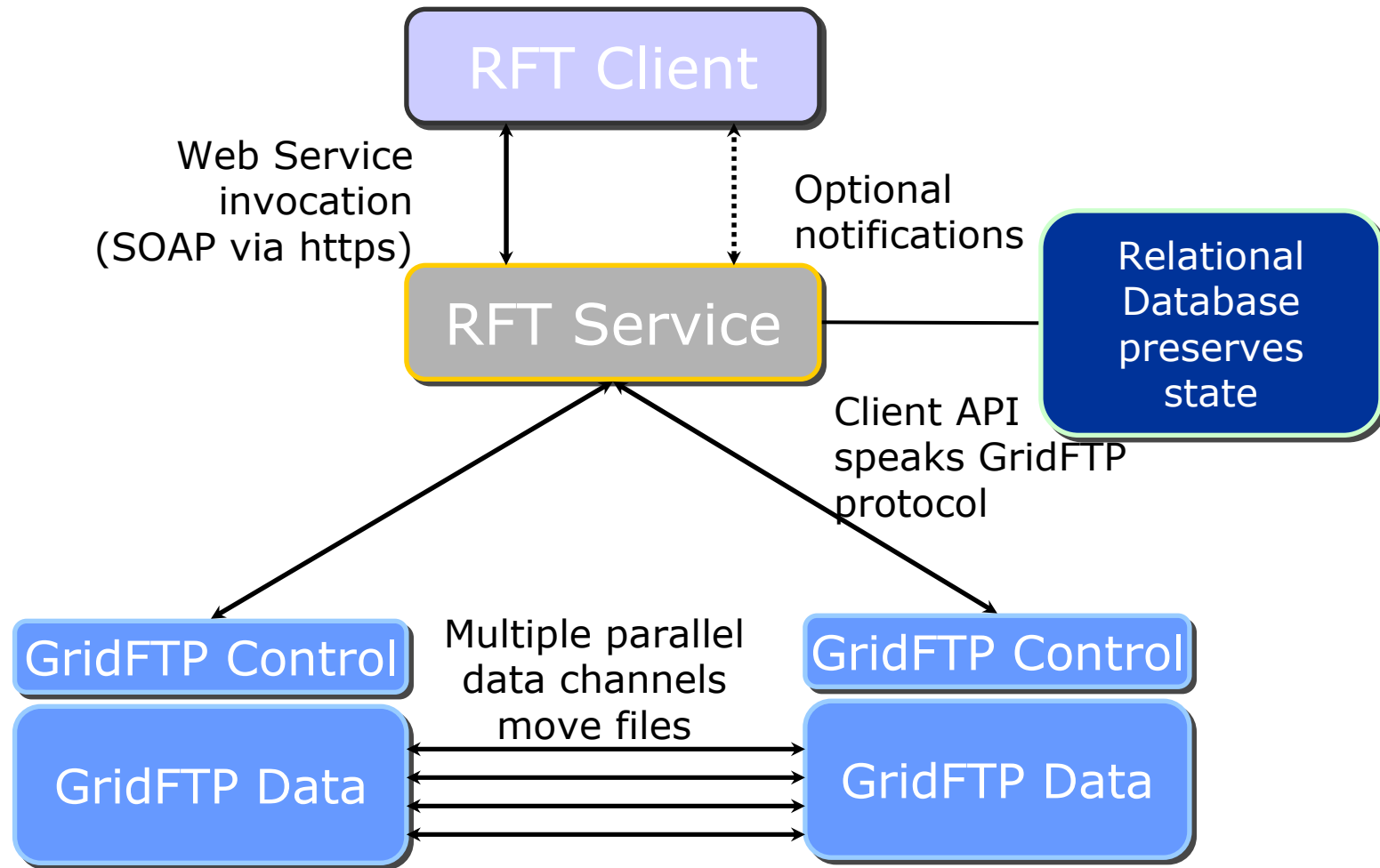
- Simple client flow comprises:
 1. Setup transfer details including number of parallel data channels, TCP buffer size, local buffer number and size
 2. Open connection to server URL and provide a "completion callback" function to be called when transfer complete
 3. Setup local buffers to hold read/write
 4. Register "data callback" function to be called for filling/flushing buffers
 5. Set "not done flag"
 6. Loop/wait until "completion callback" clears not done flag
- Work is done inside the "data callback" function
 - ◆ Local buffer filled with data (receiver) & ready to be flushed
 - ◆ Receive the offset into the file and any error code
 - ◆ fseek() to the correct place and fwrite() to file
 - ◆ Register another empty buffer/callback combination



GridFTP: Tool Mechanics

- **Server mechanics**
 - ◆ `globus-gridftp-server`
 - ◆ Usually runs as root
 - ◆ Usually run as a daemon; connections fork new process and `setuid`
 - ◆ Can run `inetd/xinetd` if so desired
 - ◆ Port 2811 is standard but is configurable
 - ◆ Logging and security highly configurable
- **Client mechanics**
 - ◆ `globus-url-copy`
 - ◆ Options for parallel channels, TCP buffer size, data buffer size, debugging, recursive directory transfers, etc.

Reliable File Transfer (RFT)



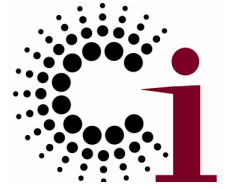
Has transferred >900,000 files.



the globus alliance

www.globus.org

Globus RFT for Robust Data Management



- Supports concurrency
 - ◆ Multiple files in transit at any given time
 - ◆ Useful when transferring many small files
- Restart markers saved by service in database
 - ◆ Failed transfers restarted from where left off
- Client need not stay connected during transfers
 - ◆ Submit RFT transfer then grab laptop and go
- Clients check status in two ways
 - ◆ Subscribe to notifications from RFT service
 - ◆ Poll service to find status of transfers



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Globus RFT

for Robust Data Management



- Exposes WSRF compliant interface
 - ◆ Code RFT client using favorite Web services tools
- Single RFT service fronts multiple RFT resources
 - ◆ Each “user” can have separate resource
 - ◆ Each resource maintains own queue, notifications, lifetime
- Delete sets of files/directories on a GridFTP server
- Configurable exponential back off before retrying failed transfer
- Transfer all or none option
- Configurable # of concurrent transfers per container, request
- Configurable number of retries for failed transfers per request



RFT: Tool Mechanics

- RFT Service
 - ◆ Runs in Globus Java WS container/Tomcat
 - ◆ Uses JDBC capable database; PostgreSQL and MySQL most widely tested and used
- RFT clients
 - ◆ rft and rft-delete: simple clients, not intended for production use
 - ◆ Recommend application-specific Web Services clients developed against the service WSDL

Globus RLS for File Replica Management



- Why replicate files?
 - ◆ Fault tolerance: avoid single points of failure
 - ◆ Reduce latency: use "nearest" copy
- Use GridFTP and RFT to move the files
 - ◆ Fast, robust transfer but no replica management
- Globus Replica Location Service (RLS)
 - ◆ Registry recording file locations
 - ◆ Enables discovery of replicas
 - ◆ Distributed catalog for scalability/fault tolerance
 - ◆ Capable of tracking tens of millions of files across distributed sites



Globus RLS for File Replica Management

- Maintains mappings between logical identifiers and target names
- Logical identifier or Logical File Name (LFN)
 - ◆ Location-independent identifier (name)
 - ◆ Example: `foo`
- Target name or Physical File Name (PFN)
 - ◆ Specific file identifier such as a URL
 - ◆ E.g.: `gsiftp://myserver.mycompany.com/foo`
- RLS maps between LFNs and PFNs
 - ◆ `foo` \Rightarrow `gsiftp://myserver.mycompany.com/foo`

Globus RLS for File Replica Management

- LFN to PFN mappings are often many-to-one
- Multiple PFNs may indicate different access to a file





Globus RLS for File Replica Management



- Local replica catalog (LRC): Catalog of LFN to PFN mappings
- LRCs contain consistent information about local to target mappings

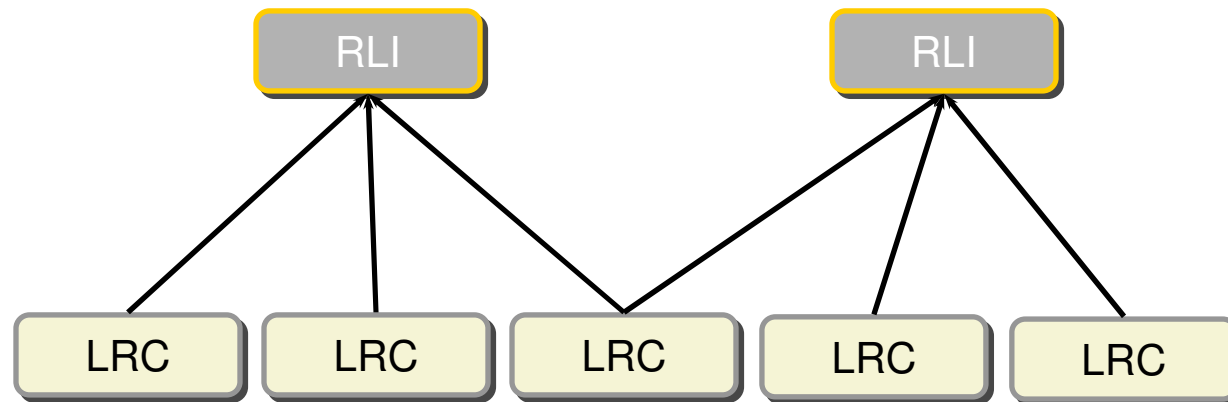
Local Replica Catalog (LRC)

```
fee ⇒ gsiftp://dataserver.mycompany.com/fee  
fii ⇒ file://nodeA.mycompany.com/fii  
foo ⇒ file://nodeB.mycompany.com/foo  
fum ⇒ https://www.mycompany.com/fum
```



Globus RLS for File Replica Management

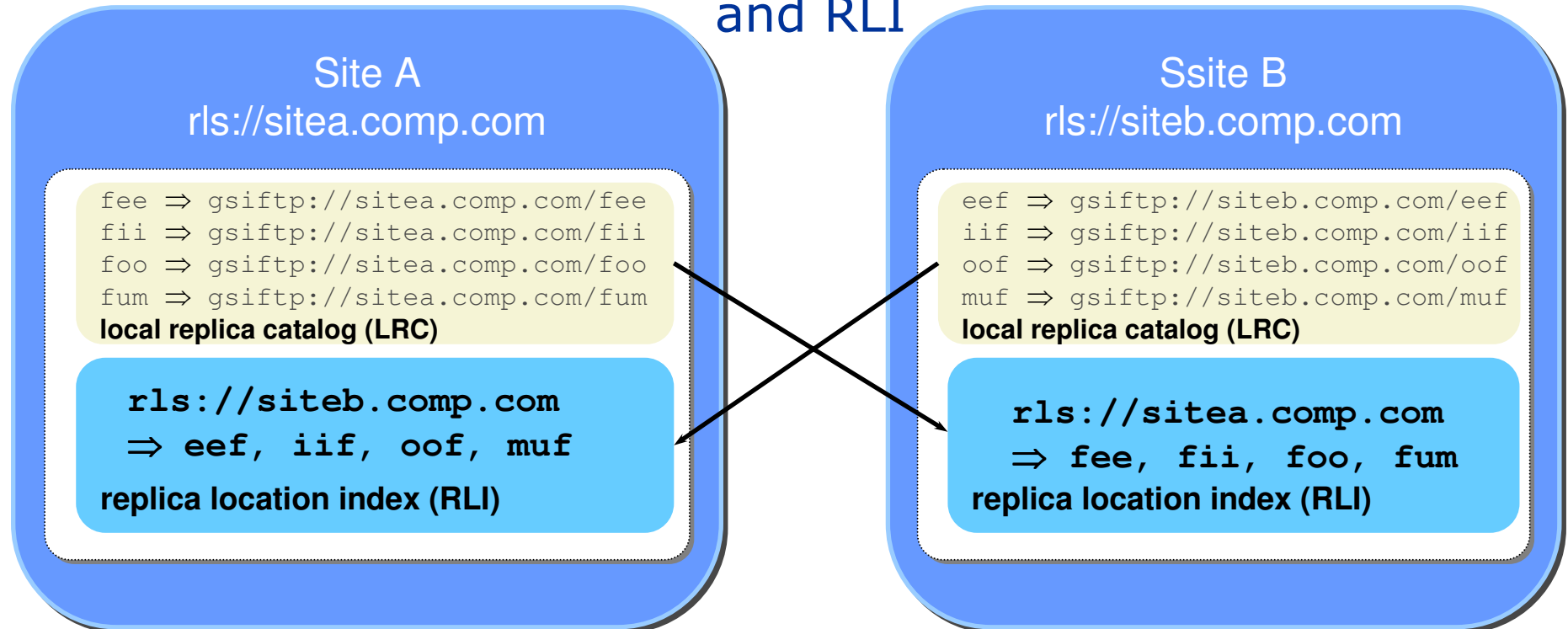
- Replica Location Index (RLI): Aggregate information about one or more LRCs
- Only the LFN content for LRC is aggregated
 - ◆ Each configured LRC sends list of LFNs to LRCs
 - ◆ PFNs and mappings **not** aggregated





Globus RLS for File Replica Management

Each *site* represented by a RLS
server instance with both LRC
and RLI





Finding Files Across the Grid

File `foo` is available at
`gsiftp://sitea.comp.com/foo`

site A

`rls://sitea.comp.com`

```
fee => gsiftp://sitea.comp.com/fee
fii => gsiftp://sitea.comp.com/fii
foo => gsiftp://sitea.comp.com/foo
fum => gsiftp://sitea.comp.com/fum
```

local replica catalog (LRC)

```
rls://siteb.comp.com
=> eef, iif, oof, muf
```

replica location index (RLI)

site B

`rls://siteb.comp.com`

```
fee => gsiftp://siteb.comp.com/eef
fii => gsiftp://siteb.comp.com/iif
foo => gsiftp://siteb.comp.com/oof
fum => gsiftp://siteb.comp.com/muf
```

local replica catalog (LRC)

```
rls://sitea.comp.com
=> fee, fii, foo, fum
```

replica location index (RLI)

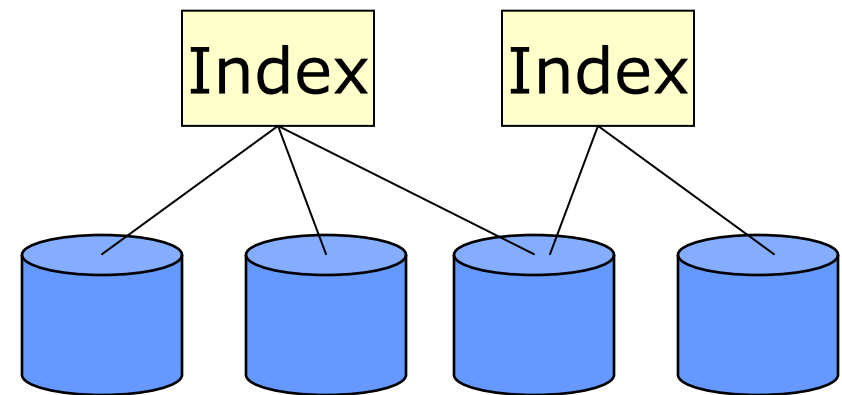
Globus RLS for File Replica Management



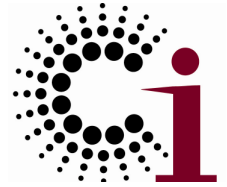
- **Soft state update** from LRCs to RLIs
 - ◆ Relaxed consistency of index
 - ◆ Tunable depending on desired load
- **Two alternative update methods supported**
 - ◆ Full list updates send entire list of LFNs periodically, partial updates in between
 - Complete list means always accurate
 - Large lists put drain on network, CPU, storage
 - ◆ Optional compressed bloom filter or hash
 - Compression relieves load on network, CPU, storage
 - False positives are possible (tunable rate)

Replica Location Service

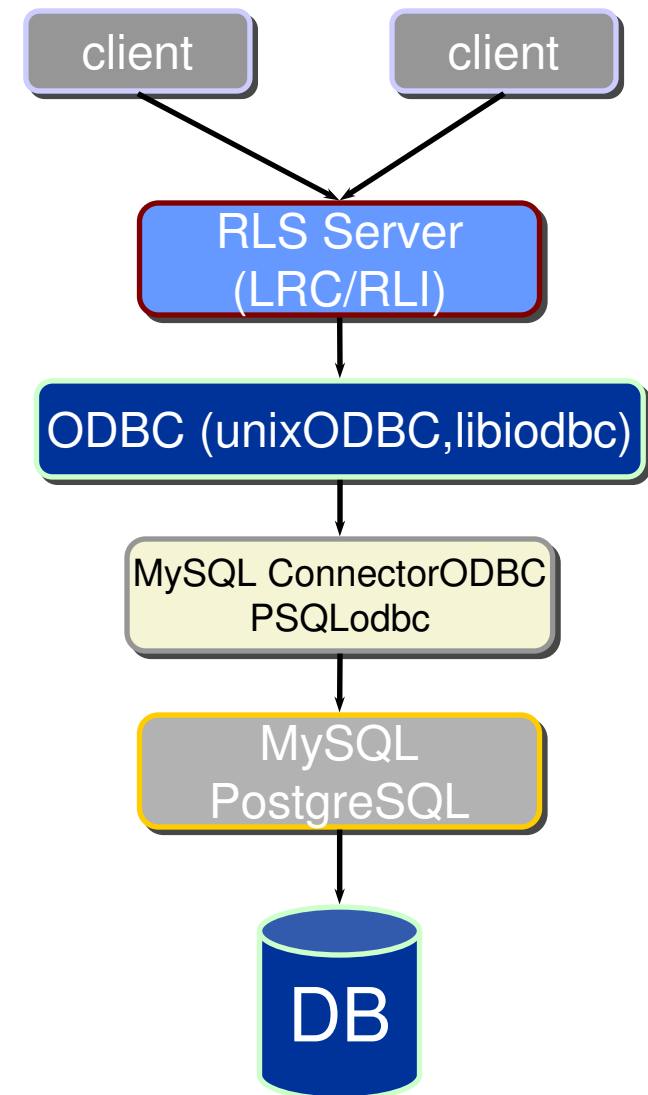
- Identify location of files via logical to physical name map
- Distributed indexing of names, fault tolerant update protocols
- GT4 version scalable & stable
- Managing ~40 million files across ~10 sites



Local DB	Update send (secs)	Bloom filter (secs)	Bloom filter (bits)
10K	<1	2	1 M
1 M	2	24	10 M
5 M	7	175	50 M



- Server runs as daemon
- Usually not run as root
- Use with any ODBC RDBMS
 - ◆ MySQL, PostgreSQL, Oracle most tested
- Multi-threaded, written in C
- GSI socket server
 - ◆ Single interface for both LRC and RLI
 - ◆ Differentiated by API calls
- ACL for types of access (admin, update, query, write, all)



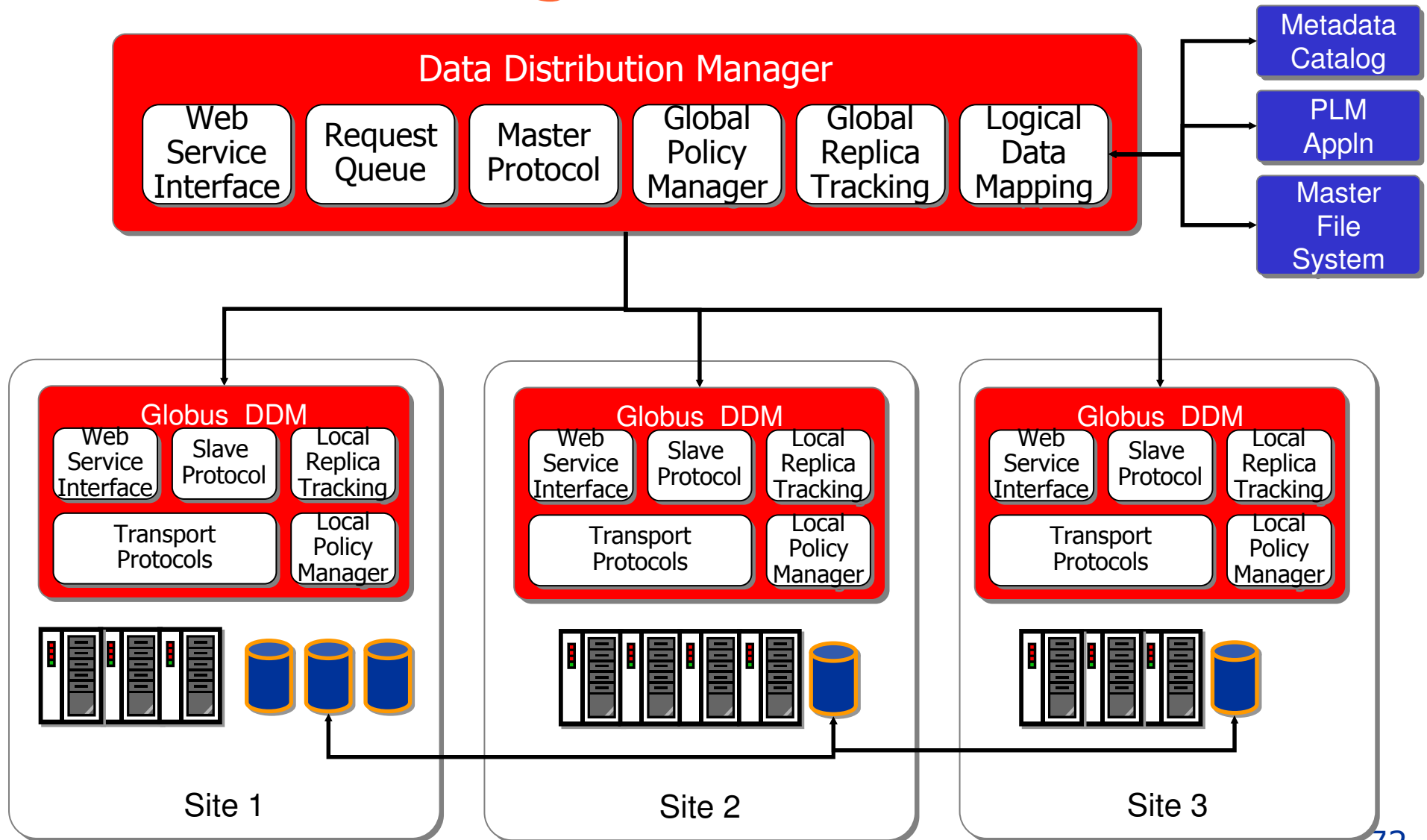


RLS Mechanics

- **Command line tools**
 - ◆ `globus-rls-admin`: administration and on the fly configuration changes
 - ◆ `globus-rls-cli`: simple command line client for interacting with both LRC and RLI part of server
- **Client APIs**
 - ◆ C and Java APIs available
 - ◆ Functions to publish mappings, query, wildcard queries, administration tasks
 - ◆ “Bulk” versions of functions for publishing and queries on many objects



Data Management Architecture





LIGO Data Grid: Before & After

Before:

- Data replication via “FedEx” Grid
- Ad-hoc site-by-site idioms for finding data in storage
- Ad-hoc error prone mapping from metadata to file names
- Workflow limited to a single compute resource site

After:

- 24 x 7 x 365 continuous fault tolerant data streaming
- Single client tool for scientists and applications to find data
- Scientists concentrate on metadata and forget file names
- Multi-site planning of workflows across LIGO Data Grid

LIGO scientists searching for signals from neutron stars and black holes run **more jobs** across **more resources** and access **more data** using the LIGO Data Grid built on Globus.

Papers are published faster due to Globus and the LIGO Data Grid.



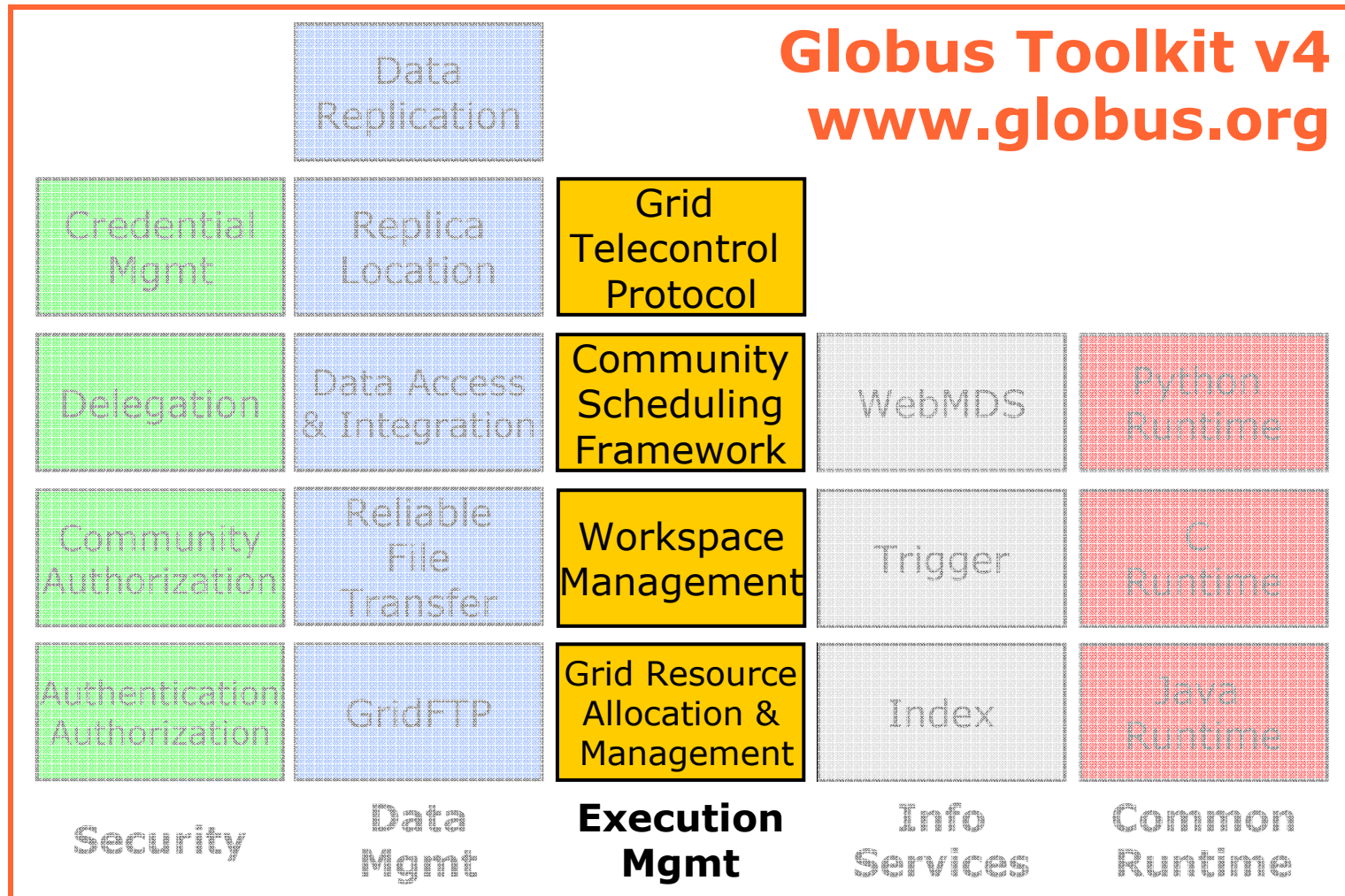
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- Run 10,000 jobs on whatever computers I can get hold of
- Monitor the status of the different resources to which I have access



Globus Toolkit: Open Source Grid Infrastructure

Globus Toolkit v4
www.globus.org





Execution Management (GRAM)

- Common WS interface to schedulers
 - ◆ Unix, Condor, LSF, PBS, SGE, ...
- More generally: interface for process execution management
 - ◆ Lay down execution environment
 - ◆ Stage data
 - ◆ Monitor & manage lifecycle
 - ◆ Kill it, clean up
- A basis for application-driven provisioning

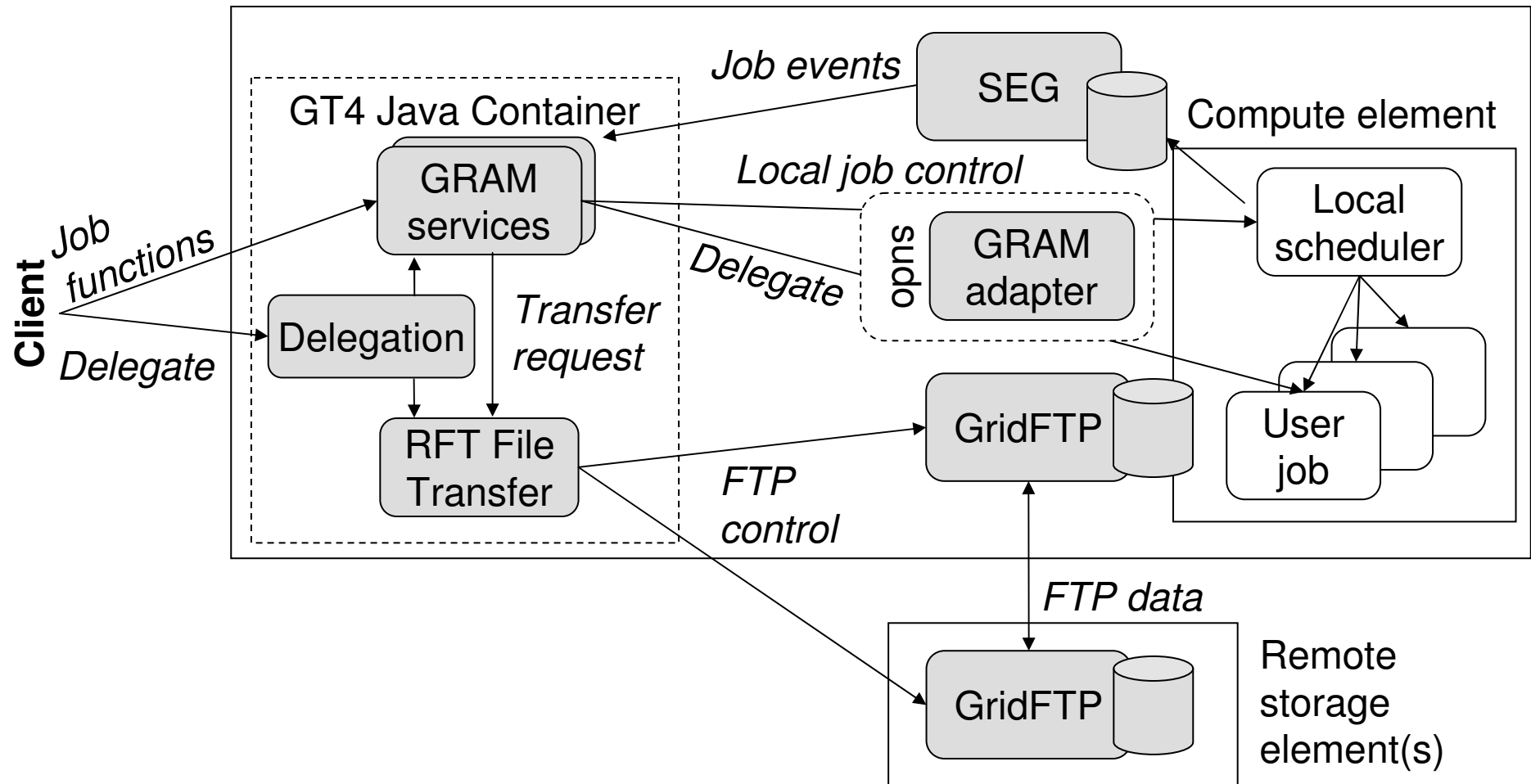


GRAM4: A Big Advance over GRAM2

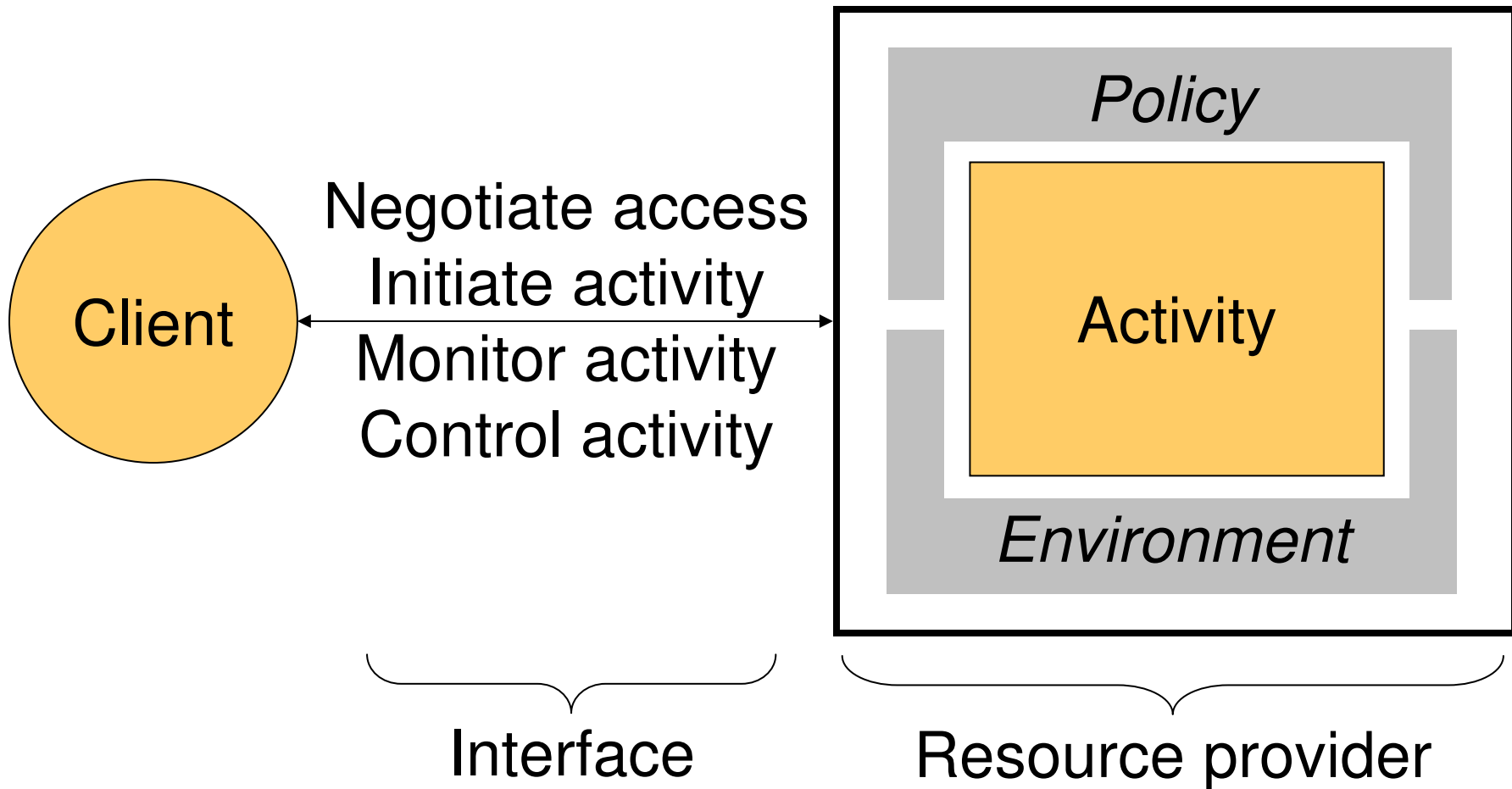
- Big scalability/performance improvements
 - ◆ 32,000 active jobs (GRAM2 max ~100)
 - ◆ Ability to manage load on control node
 - ◆ Reuse delegated credentials
- New functionality
 - ◆ Flexible authorization
 - ◆ Modular LRM interface
 - ◆ Notifications
 - ◆ JSDL support
 - ◆ Advance reservation, BES support (soon)

GT4 WS GRAM Architecture

Service host(s) and compute element(s)

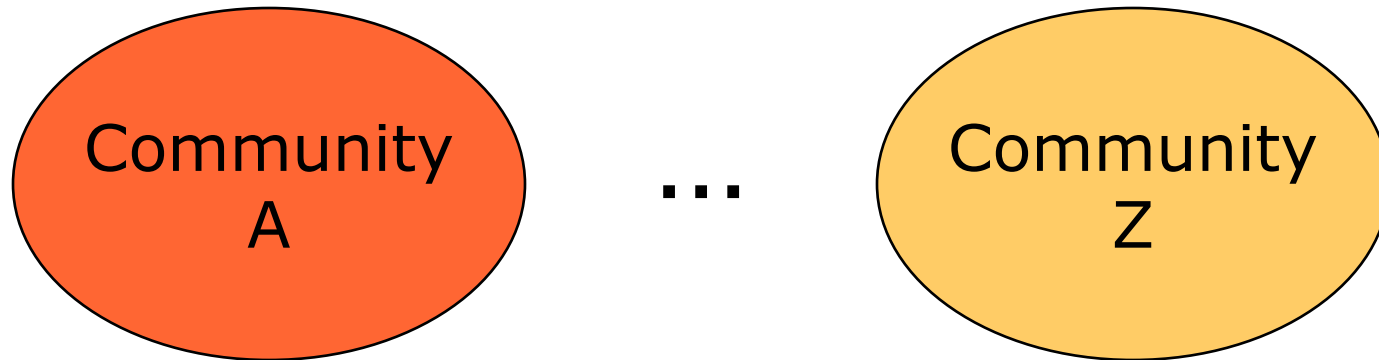


Workspace Service: The Hosted Activity





Dynamic Service Deployment



- Community scheduling logic
- Data distribution
- Community management
- Science services
- ...

Requirements:

- Community control
- Persistence
- Resource guarantees
- Non-interference



Case Study: Functional MRI (fMRI) Data Center

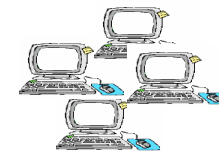
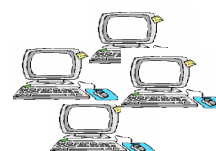
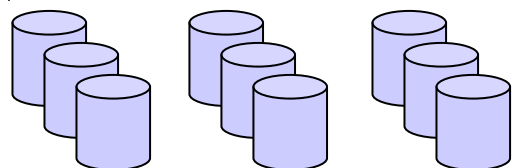
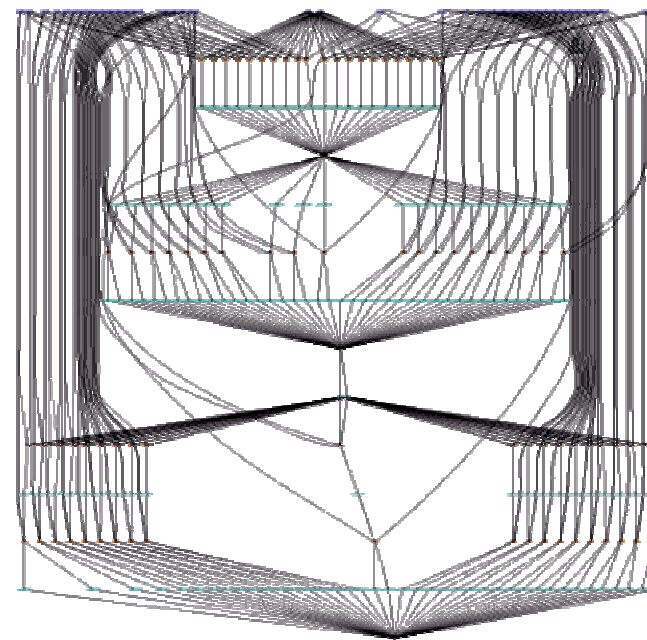
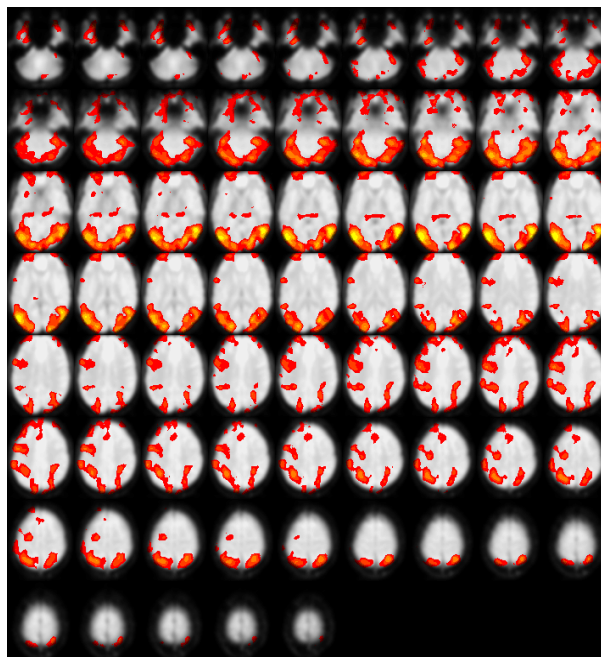
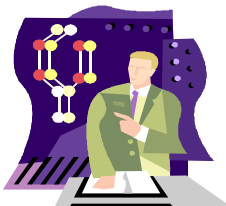
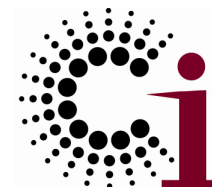
- An online repository of neuroimaging data
 - ◆ A typical study comprises 3 groups, 20 subjects/gp, 5 runs/sub, 300 volumes/run
 - 90,000 volumes, 60 GB raw data
 - 1.2 million files processed data
 - ◆ 100s of such studies in total
- Many users analyze this data
 - ◆ Wide range of complex analysis procedures
 - ◆ Testing → production
 - ◆ Ensemble: a set of data analyses by parameters, datasets



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fMRI: A Broad Picture





Challenges

- Deluge of data: instrumentation, simulation
- Data analysis turns into data integration
- Community-wide collaboration
- Provenance: tracking, query, application
- Scalability: desktop to Grid
- Productivity: throughput, performance



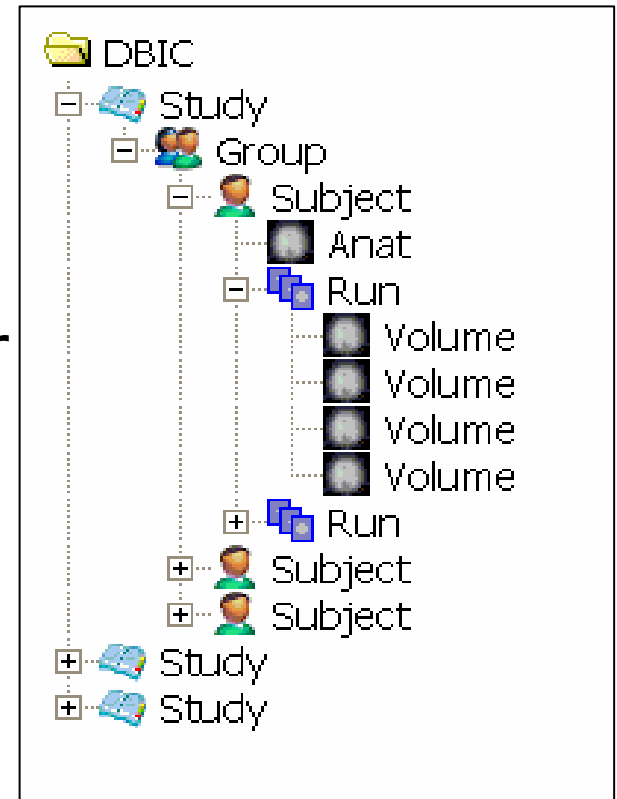
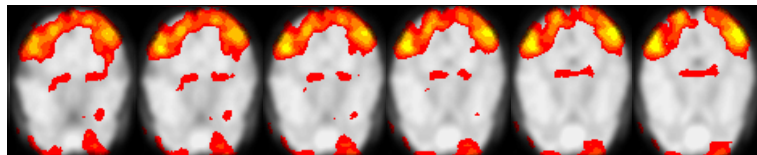
Swift System

- Clean separation of logical/physical concerns
 - ◆ **XDTM** specification of logical data structures
- + Concise specification of parallel programs
 - ◆ **SwiftScript**, with iteration, etc.
- + Efficient execution on distributed resources
 - ◆ Lightweight threading, dynamic provisioning, Grid interfaces, pipelining, load balancing
- + Rigorous provenance tracking and query
 - ◆ Virtual data schema & automated recording
- **Improved usability and productivity**
 - ◆ Demonstrated in numerous applications



The Messy Data Problem (1)

- Scientific data is often logically structured
 - ◆ E.g., hierarchical structure
 - ◆ Common to map functions over dataset members
 - ◆ Nested map operations can scale to millions of objects





The Messy Data Problem (2)

- But physically “messy”
- Heterogeneous storage format and access protocol
 - ◆ Logically identical dataset can be stored in textual File (e.g. CSV), spreadsheet, database, ...
 - ◆ Data available from filesystem, DBMS, HTTP, WebDAV, ...
- Metadata encoded in directory and file names
- Hinders program development, composition, execution

```
./knottastic
total 58
drwxr-xr-x 4 yongzh users 2048 Nov 12 14:15 AA
drwxr-xr-x 4 yongzh users 2048 Nov 11 21:13 CH
drwxr-xr-x 4 yongzh users 2048 Nov 11 16:32 EC

./knottastic/AA:
total 4
drwxr-xr-x 5 yongzh users 2048 Nov  5 12:41 04nov06aa
drwxr-xr-x 4 yongzh users 2048 Dec  6 12:24 11nov06aa

./knottastic//AA/04nov06aa:
total 54
drwxr-xr-x 2 yongzh users 2048 Nov  5 12:52 ANATOMY
drwxr-xr-x 2 yongzh users 49152 Dec  5 11:40 FUNCTIONAL

./knottastic/AA/04nov06aa/ANATOMY:
total 58500
-rw-r--r-- 1 yongzh users  348 Nov  5 12:29 coplanar.hdr
-rw-r--r-- 1 yongzh users 16777216 Nov  5 12:29 coplanar.img

./knottastic/AA/04nov06aa/FUNCTIONAL:
total 196739
-rw-r--r-- 1 yongzh users  348 Nov  5 12:32 bold1_0001.hdr
-rw-r--r-- 1 yongzh users 409600 Nov  5 12:32 bold1_0001.img
-rw-r--r-- 1 yongzh users  348 Nov  5 12:32 bold1_0002.hdr
-rw-r--r-- 1 yongzh users 409600 Nov  5 12:32 bold1_0002.img
-rw-r--r-- 1 yongzh users  496 Nov 15 20:44 bold1_0002.mat
-rw-r--r-- 1 yongzh users  348 Nov  5 12:32 bold1_0003.hdr
-rw-r--r-- 1 yongzh users 409600 Nov  5 12:32 bold1_0003.img
```

XML Dataset Typing & Mapping (XDTM)

- Describe logical structure by **XML Schema**
 - ◆ Primitive scalar types: int, float, string, date, ...
 - ◆ Complex types (structs and arrays)
- Use **mapping descriptors** for mappings
 - ◆ How dataset elements are mapped to physical representations
 - ◆ External parameters (e. g. location)
- Use **XPath** for dataset selection

XDTM: Related Work

- Data format standardization
 - ◆ FITS, CDF, HDF-5, DICOM
- Data format description
 - ◆ DFDL [Beckerle,Westhead04] embeds annotations with XML Schema
 - ◆ PADS [Fisher,Gruber05], PADX [Fernandez,Fisher06], declarative specs of physical layout and semantic properties
- Logical object
 - ◆ ADO [Microsoft01], in memory relational model
 - ◆ SDO [Beatty,Brodsky03], logical data model for J2EE programming



XDTM: Implementation

- Virtual integration
 - ◆ Each data source treated as virtual XML source
 - ◆ Data structure defined as XML schema
 - ◆ Mapper responsible for accessing source and translating to/from XML representation
 - ◆ Bi-directional
- Common mapping interface
 - ◆ Data providers implement the interface
 - Responsible for data access details
 - ◆ Standard mapper implementations provided
 - String, file system, CSV, ...



SwiftScript

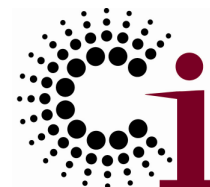
- **Typed parallel programm** [SIGMOD05, Springer06]
 - ◆ XDTM as data model and type system
 - ◆ Typed dataset and procedure definitions
- **Scripting language**
 - ◆ Implicit data parallelism
 - ◆ Program composition from procedures
 - ◆ Control constructs (foreach, if, while, ...)

Clean application logic
Type checking
Dataset selection, iteration
Discovery by types
Type conversion

A Notation & System for Expressing and Executing Cleanly Typed Workflows on Messy Scientific Data [SIGMOD05]

SwiftScript: Related Work

- Coordination language
 - ◆ Linda[Ahuja,Carriero86], Strand[Foster,Taylor90], PCN[Foster92]
 - ◆ Durra[Barbacci,Wing86], MANIFOLD[Papadopoulos98]
 - ◆ Components programmed in specific language (C, FORTRAN) and linked with system
- “Workflow” languages and systems
 - ◆ Taverna[Oinn,Addis04], Kepler[Ludäscher,Altintas05], Triana [Churches,Gombas05], Vistrail[Callahan,Freire06], DAGMan, Star-P
 - ◆ XPDL[WfMC02], BPEL[Andrews,Curbera03], and BPML[BPML02], YAWL[van de Aalst,Hofstede05], Windows Workflow Foundation [Microsoft05]



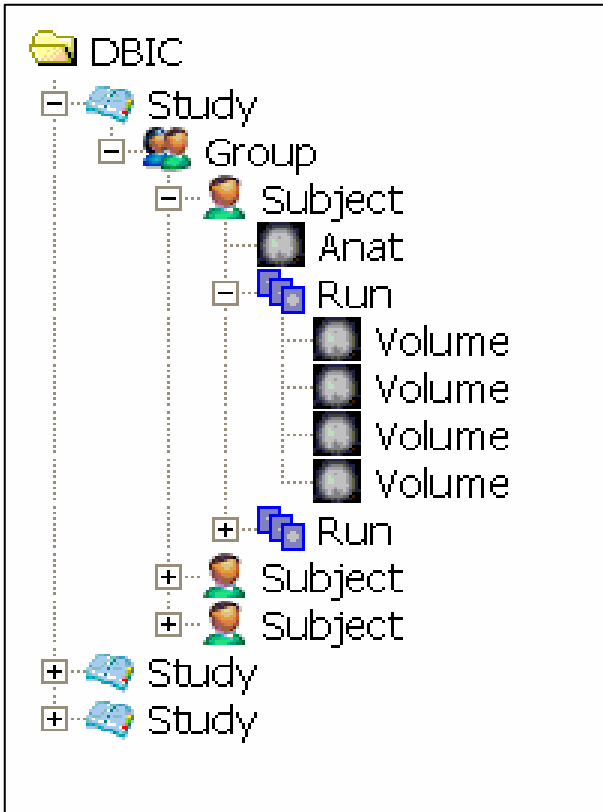
Related Work

	SwiftScript	BPEL	XPDL	MW Wflow	DAGMan	Tavana	Triana	Kepler	Vistrail	Star-P
Scales to Grids	++	-	-	-	++	-	-	-	-	+
Typing	++	++	++	++	-	-	-	+	-	+
Iteration	++	-/+	-	+	-	-	-	+	-	+
Scripting	++	-	-	+	+	+	-	-	+	++
Dataset Mapping	+	-	-	-	-	-	-	-	-	-
Service Interop	+	-	+	-	-	-	-	+	-	-
Subflow/comp.	+	-	+	+	-	-	+	+	-	+
Provenance	+	-	-	+	-	+	-	+	+	-
Open source	+	+	+	-	+	+	+	+	+	-

“A 4x200 flow leads to a 5 MB BPEL file ... chemists were not able to write in BPEL” [Emmerich,Buchart06]



fMRI Type Definitions in SwiftScript



Simplified version of
fMRI AIRSN Program
(Spatial Normalization)

```

type Study {
    Group g[ ];
}

```

```

type Group {
    Subject s[ ];
}

```

```

type Subject {
    Volume anat;
    Run run[ ];
}

```

```

type Run {
    Volume v[ ];
}

```

```

type Volume {
    Image img;
    Header hdr;
}

```

```

type Image {};

```

```

type Header {};

```

```

type Warp {};

```

```

type Air {};

```

```

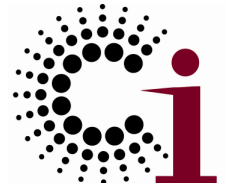
type AirVec {
    Air a[ ];
}

```

```

type NormAnat {
    Volume anat;
    Warp aWarp;
    Volume nHires;
}

```



Type Definitions in XML Schema

```
<xs:schema targetNamespace="http://www.fmri.org/schema/airsn.xsd"
  xmlns="http://www.fmri.org/schema/airsn.xsd"
  xmlns:xs="http://www.w3.org/2001/XMLSchema">
  <xs:simpleType name="Image">
    <xs:restriction base="xs:string"/>
  </xs:simpleType>
  <xs:simpleType name="Header">
    <xs:restriction base="xs:string"/>
  </xs:simpleType>
  <xs:complexType name="Volume">
    <xs:sequence>
      <xs:element name="img" type="Image"/>
      <xs:element name="hdr" type="Header"/>
    </xs:sequence>
  </xs:complexType>
  <xs:complexType name="Run">
    <xs:sequence minOccurs="0" maxOccurs="unbounded">
      <xs:element name="v" type="Volume"/>
    </xs:sequence>
  </xs:complexType>
</xs:schema>
```



AIRSN Program Definition

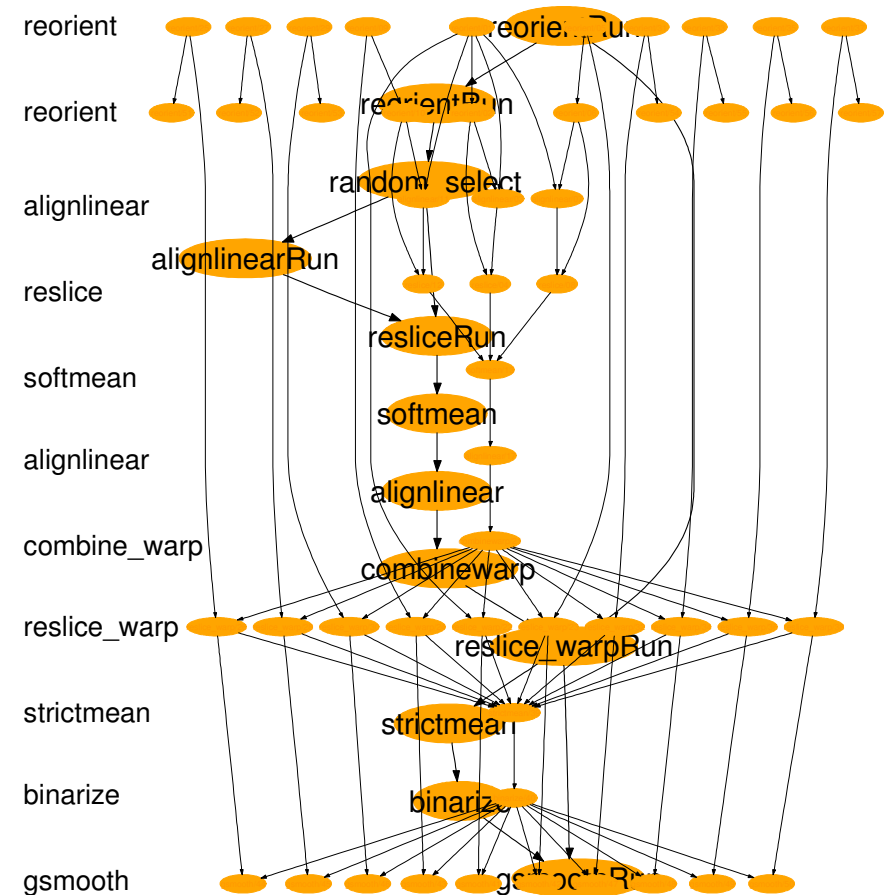
```
(Run snr) functional ( Run r, NormAnat a,  
                      Air shrink ) {  
  Run yroRun = reorientRun( r , "y" );  
  Run roRun = reorientRun( yroRun , "x" );  
  Volume std = roRun[0];  
  Run rndr = random_select( roRun, 0.1 );  
  AirVector rndAirVec = align_linearRun( rndr, std, 12, 1000, 1000, "81 3 3" );  
  Run reslicedRndr = resliceRun( rndr, rndAirVec, "o", "k" );  
  Volume meanRand = softmean( reslicedRndr, "y", "null" );  
  Air mnQAAir = alignlinear( a.nHires, meanRand, 6, 1000, 4, "81 3 3" );  
  Warp boldNormWarp = combinewarp( shrink, a.aWarp, mnQAAir );  
  Run nr = reslice_warp_run( boldNormWarp, roRun );  
  Volume meanAll = strictmean( nr, "y", "null" )  
  Volume boldMask = binarize( meanAll, "y" );  
  snr = gsmoothRun( nr, boldMask, "6 6 6" );
```

```
(Run or) reorientRun (Run ir,  
                      string direction) {  
  foreach Volume iv, i in ir.v {  
    or.v[i] = reorient(iv, direction);  
  }  
}
```

Expressiveness

Lines of code with different encodings

Appln	Script	Generator	Swift Script
ATLAS1	49	72	6
ATLAS2	97	135	10
FILM1	63	134	17
FEAT	84	191	13
AIRSN	215	~400	34

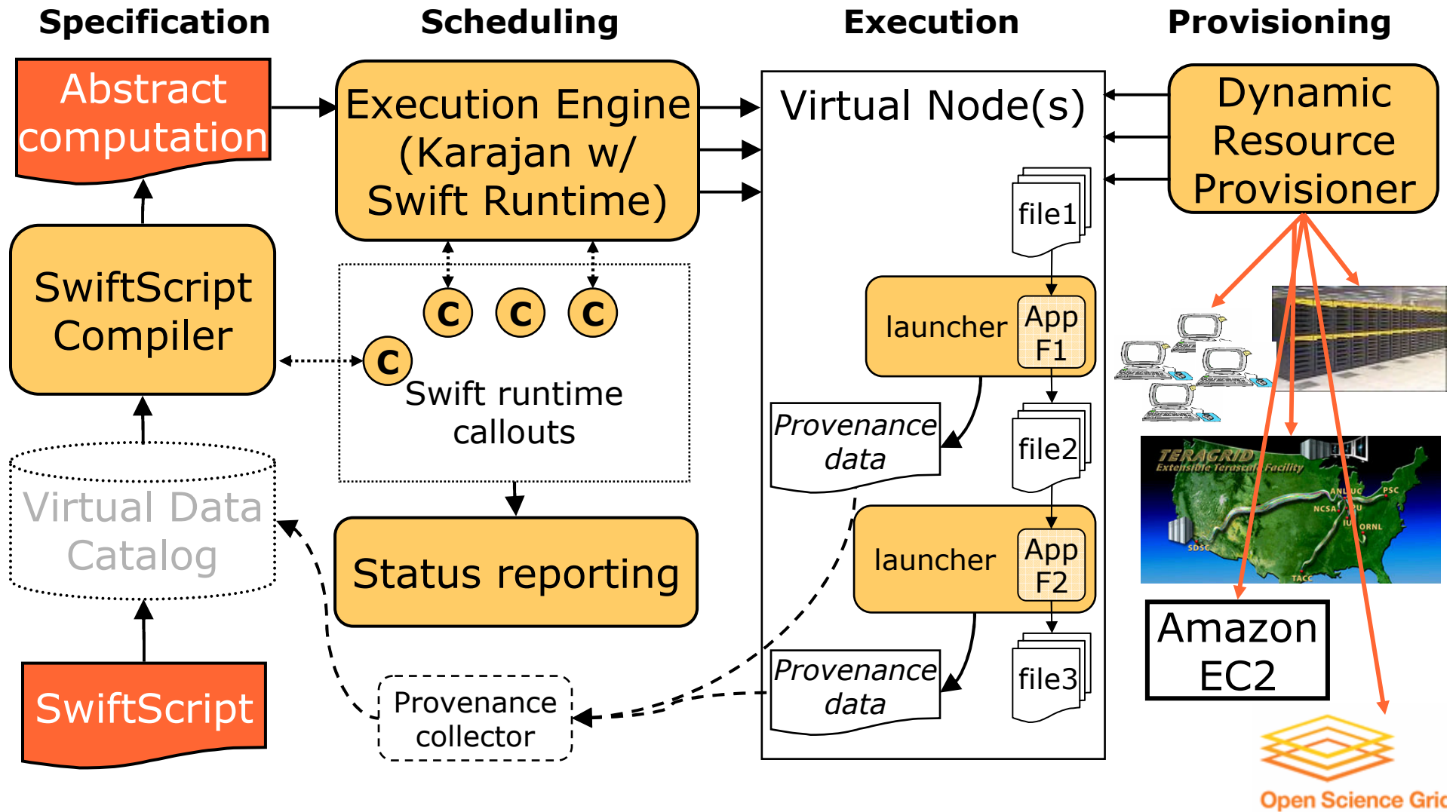




Swift Runtime System

- Runtime system for SwiftScript [SSDBM02,CIDR03,Springer06]
 - ◆ Populate, update, query virtual data products
 - ◆ Schedule, monitor, execute resulting computation on distributed Grid resources
 - ◆ Annotate virtual data products with customized metadata
 - ◆ Trace provenance of virtual data products
- Grid scheduling and optimization
 - ◆ Lightweight execution engine: Karajan
 - ◆ Dynamic resource provisioning
 - ◆ Site selection, data movement, caching
 - ◆ Pipelining, clustering, load balancing
 - ◆ Fault tolerance, exception handling

Swift Architecture





Swift uses Karajan Workflow Engine

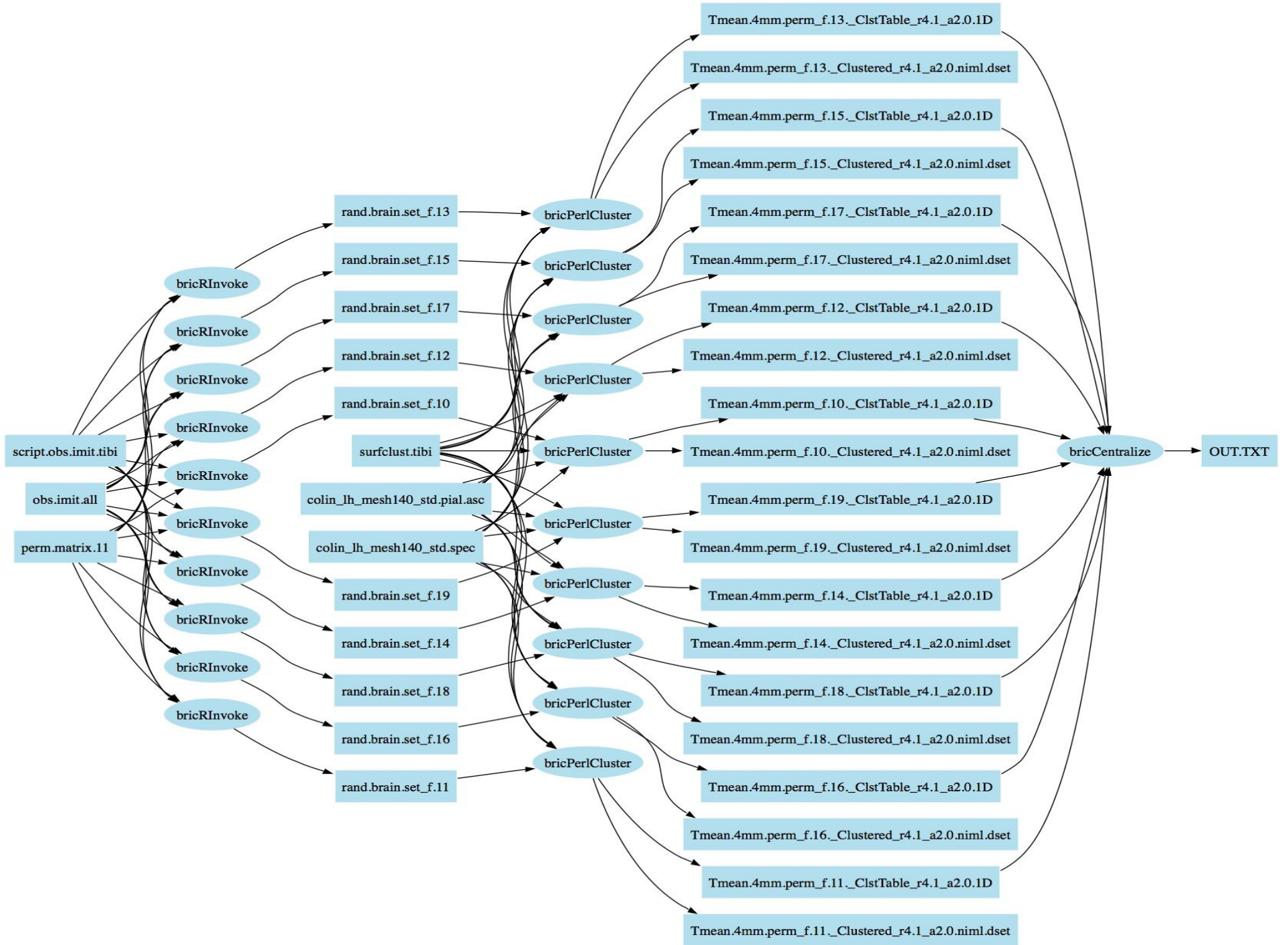
- Fast, scalable threading model
- Suitable constructs for control flow
- Flexible task dependency model
 - ◆ “Futures” enable pipelining
- Flexible provider model allows for use of different run time environments
 - ◆ Job execution and data transfer
 - ◆ Flow controlled to avoid resource overload
- Workflow client runs from a Java container



Application Example

ACTIVAL: Neural Activation Validation

- Identifies clusters of neural activity not likely to be active by chance:
 - ◆ switch labels of conditions for 1+ participants;
 - ◆ calculate delta values in each voxel;
 - ◆ re-calculate reliability of delta in each voxel; &
 - ◆ evaluate clusters found
- If clusters in data $>$ majority of clusters found in permutations, then null hypothesis is refuted, indicating that clusters of activity found in experiment are not likely to be found by chance



SwiftScript Program ACTIVAL – Datatypes & Utilities

```
type script {}
type brainMeasurements{}
type precomputedPermutations{}
type brainClusterTable {}
type brainDatasets{ brainDataset b[]; }
type brainClusters{ brainClusterTable c[]; }

type fullBrainData {}
type fullBrainSpecs {}
type brainDataset {}
```

// Procedure to run "R" statistical package

```
(brainDataset t) bricRInvoke (script permutationScript, int iterationNo,
    brainMeasurements dataAll, precomputedPermutations dataPerm) {
    app { bricRInvoke @filename(permutationScript) iterationNo
        @filename(dataAll) @filename(dataPerm); }
}
```

// Procedure to run AFNI Clustering tool

```
(brainClusterTable v, brainDataset t) bricCluster (script clusterScript,
    int iterationNo, brainDataset randBrain, fullBrainData brainFile,
    fullBrainSpecs specFile) {
    app { bricPerlCluster @filename(clusterScript) iterationNo
        @filename(randBrain) @filename(brainFile)
        @filename(specFile); }
}
```

// Procedure to merge results based on statistical likelihoods

```
(brainClusterTable t) bricCentralize ( brainClusterTable bc[]) {
    app { bricCentralize @filenames(bc); }
}
```

ACTIVAL: Dataset Iteration Procedures

// Procedure to iterate over the data collection

```
(brainClusters randCluster, brainDatasets dsetReturn)
  brain_cluster(fullBrainData brainFile, fullBrainSpecs specFile)
{
  int sequence[]=[1:2000];

  brainMeasurements      dataAll<fixed_mapper; file="obs.imit.all">;
  precomputedPermutations dataPerm<fixed_mapper; file="perm.matrix.11">;
  script                 randScript<fixed_mapper; file="script.obs.imit.tibi">;
  script                 clusterScript<fixed_mapper; file="surfclust.tibi">;
  brainDatasets          randBrains<simple_mapper; prefix="rand.brain.set">;

  foreach int i in sequence {
    randBrains.b[i] = bricRInvoke(randScript, i, dataAll, dataPerm);
    brainDataset rBrain=randBrains.b[i];
    (randCluster.c[i], dsetReturn.b[i]) =
      bricCluster(clusterScript, i, rBrain, brainFile,specFile);
  }
}
```

ACTIVAL: Main Program

// Declare datasets

```
fullBrainData      brainFile<fixed_mapper; file="colin_lh_mesh140_std.pial.asc">;
fullBrainSpecs    specFile<fixed_mapper; file="colin_lh_mesh140_std.spec">;

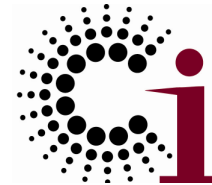
brainDatasets     randBrain<simple_mapper; prefix="rand.brain.set">;
brainClusters     randCluster<simple_mapper; prefix="Tmean.4mm.perm",
                  suffix="_ClstTable_r4.1_a2.0.1D">;
brainDatasets     dsetReturn<simple_mapper; prefix="Tmean.4mm.perm",
                  suffix="_Clustered_r4.1_a2.0.niml.dset">;
brainClusterTable clusterThresholdsTable<fixed_mapper; file="thresholds.table">;
brainDataset      brainResult<fixed_mapper; file="brain.final.dset">;
brainDataset      origBrain<fixed_mapper; file="brain.permutation.1">;
```

// Main program – executes the entire application

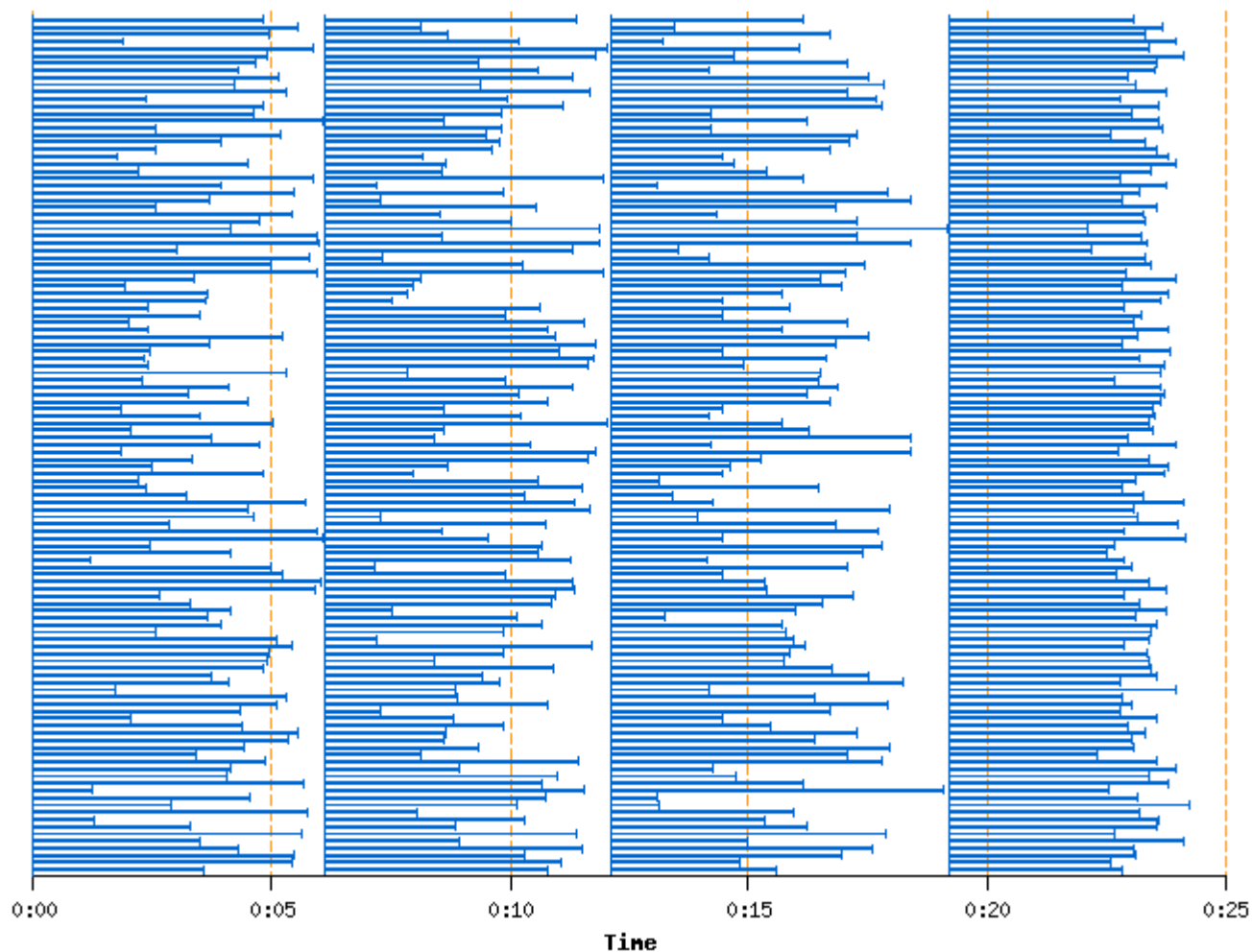
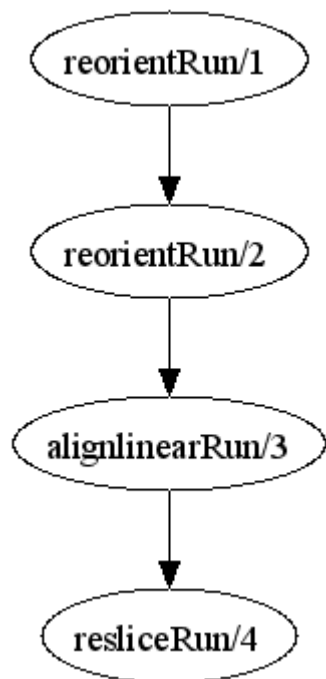
```
(randCluster, dsetReturn) = brain_cluster(brainFile, specFile);
```

```
clusterThresholdsTable = bricCentralize(randCluster.c);
```

```
brainResult = makebrain(origBrain, clusterThresholdsTable, brainFile, specFile);
```

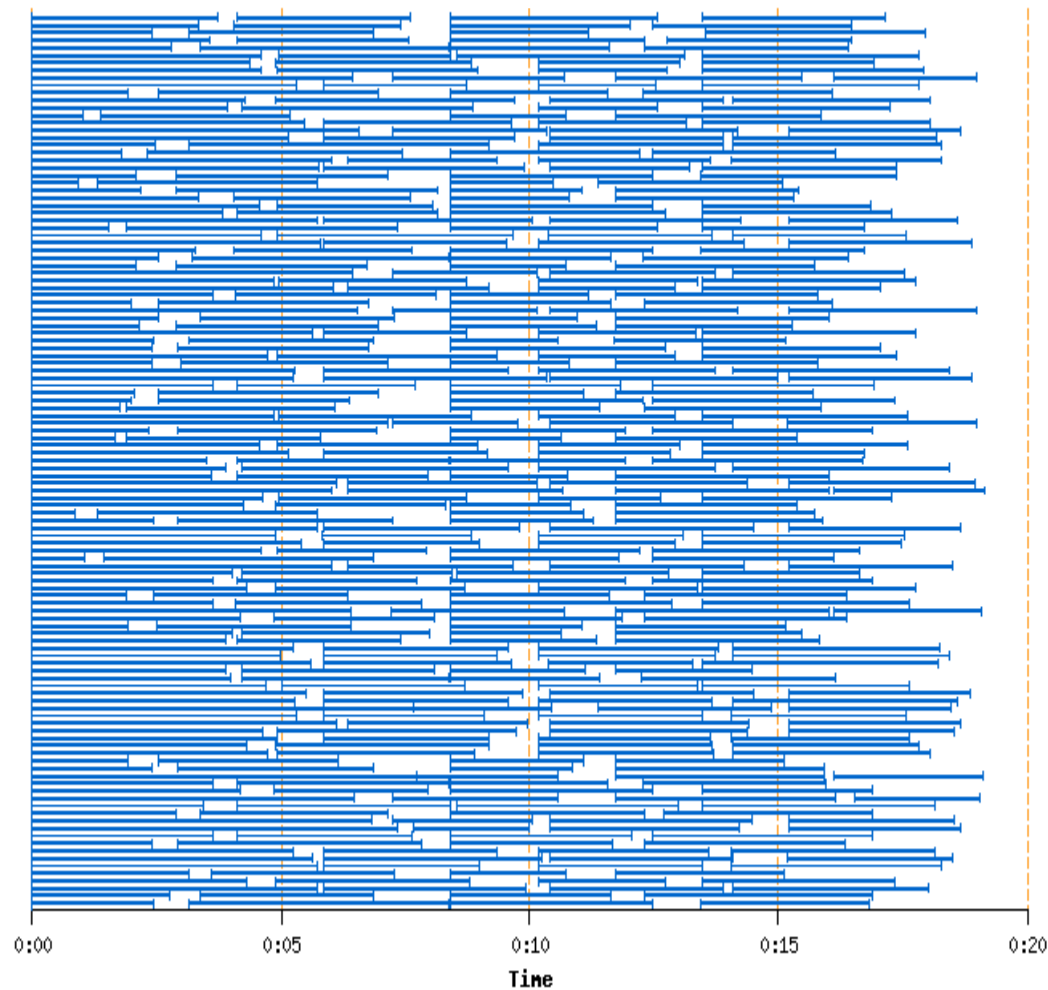
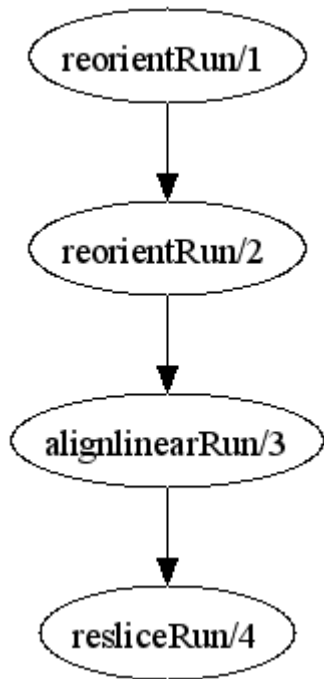


Example Performance Optimizations





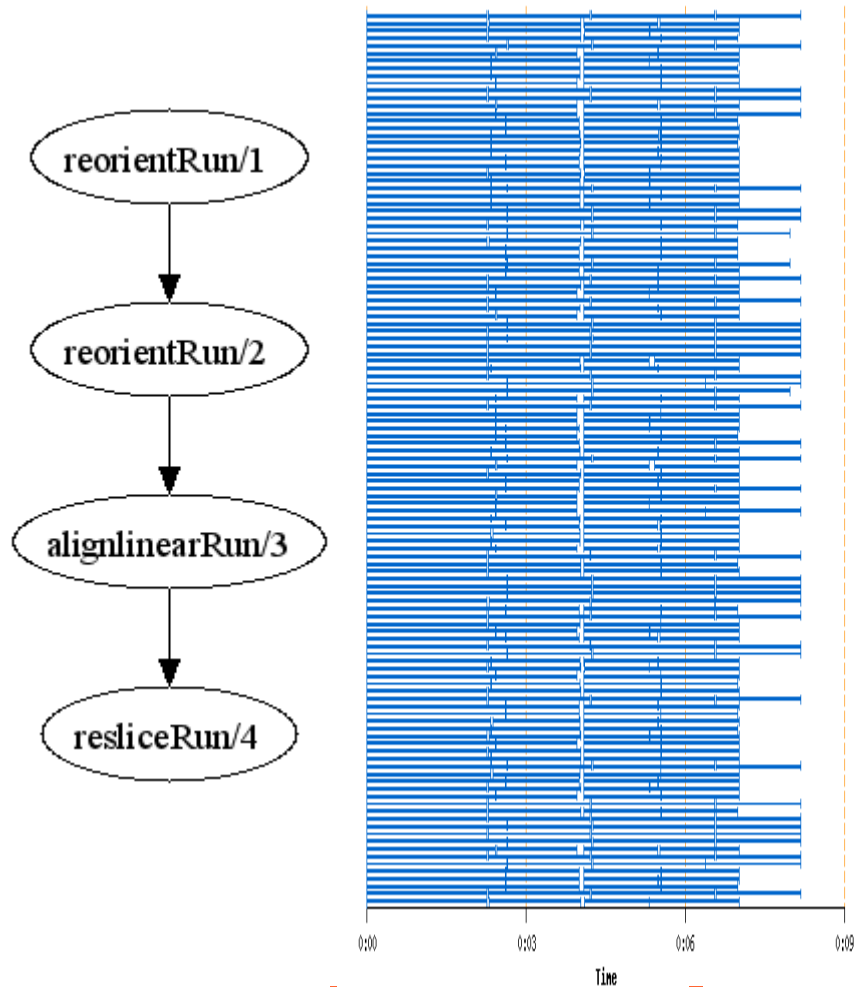
Example Performance Optimizations



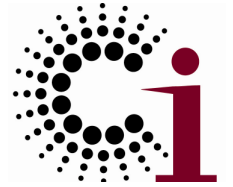
Pipelining



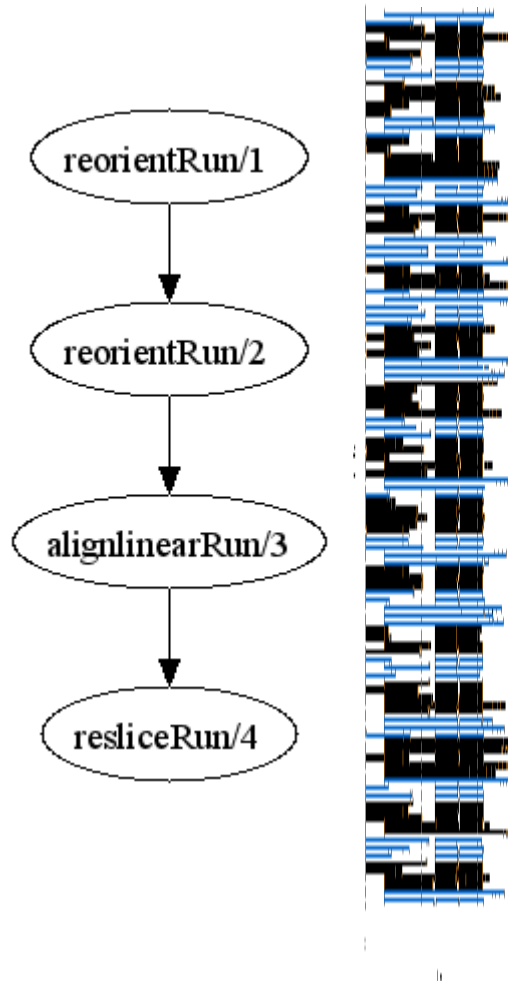
Example Performance Optimizations



Pipelining + **clustering**



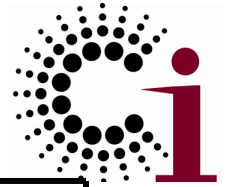
Example Performance Optimizations



Pipelining + provisioning



Other Applications



Application	#Jobs/computation	Levels
ATLAS* HEP Event Simulation	500K	1
fMRI DBIC* AIRSN Image Processing	100s	12
FOAM Ocean/Atmosphere Model	2000 (core app runs 250 8-CPU jobs)	3
GADU* Genomics: (14 million seq. analyzed)	40K	4
HNL fMRI Aphasia Study	500	4
NVO/NASA* Photorealistic Montage/Morphology	1000s	16
QuarkNet/I2U2* Physics Science Education	10s	3-6
RadCAD* Radiology Classifier Training	1000s	5
SIDGrid EEG Wavelet Proc, Gaze Analysis, ...	100s	20
SDSS* Coadd, Cluster Search	40K, 500K	2, 8

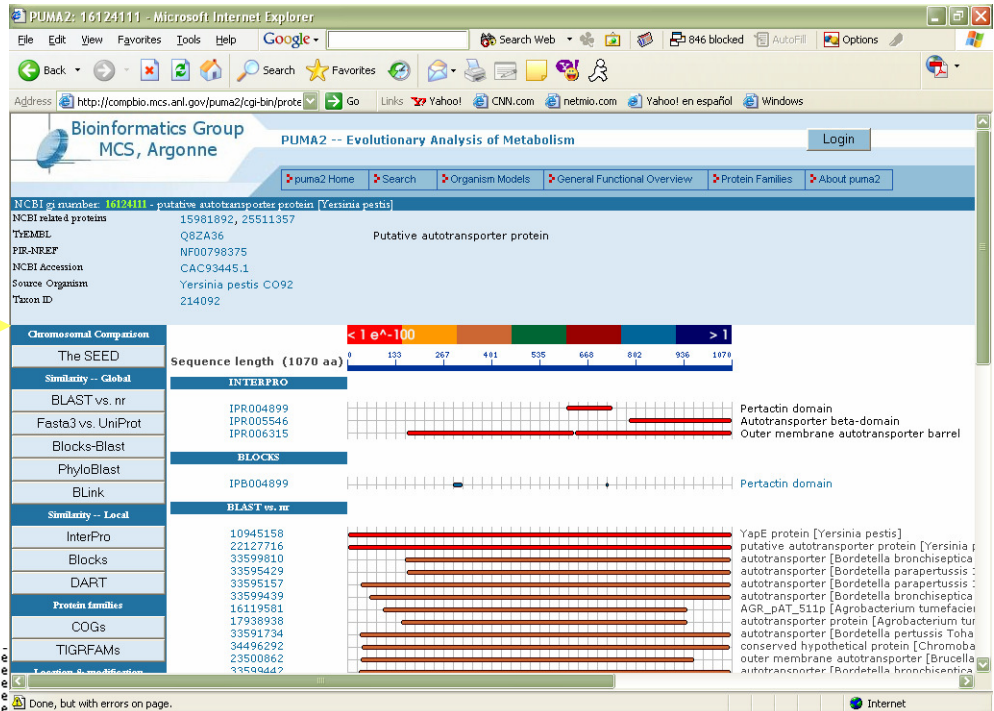


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www.globus.org

Production Science: Biology



Public PUMA Knowledge Base
Information about proteins analyzed against ~2 million gene sequences



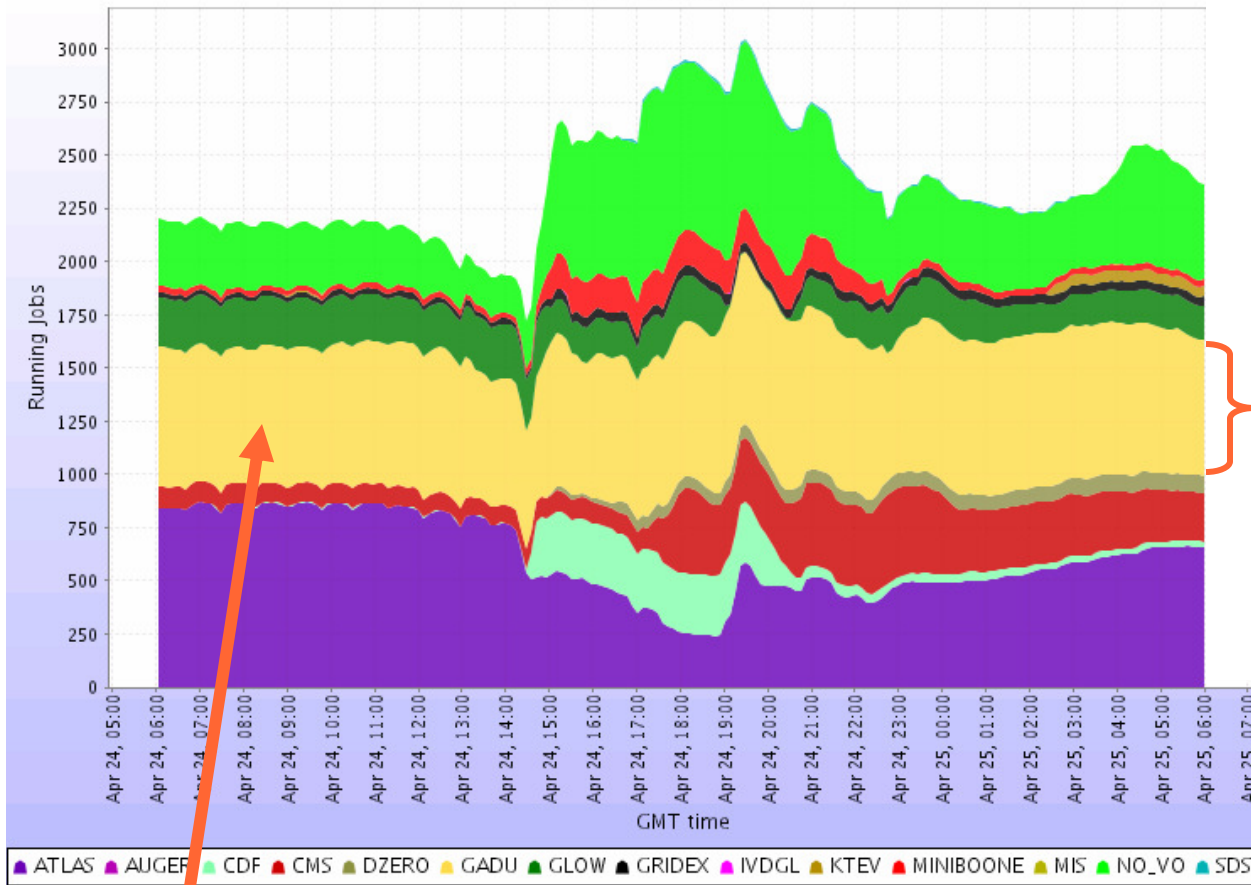
gi 23499780 gn REF_tigr BRA00013 gi 16080253 ref NP_391080.1 44.27 253 131 1 15 257 8 2603.7 e	gi 23499780 gn REF_tigr BRA00013 gi 123098409 ref NP_691875.1 43.48 253 133 2 16 258 5 2573.8 e
gi 23499780 gn REF_tigr BRA00013 gi 48637187 ref ZP_00294182.1 44.92 256 125 2 14 256 7 2591.1 e	gi 23499780 gn REF_tigr BRA00013 gi 52005400 gb IAWN2942.1 44.75 257 126 2 15 258 3 2561.9 e
gi 23499780 gn REF_tigr BRA00013 gi 48684015 ref ZP_00317908.1 44.49 245 134 1 13 257 5 2476.1 e	gi 23499780 gn REF_tigr BRA00013 gi 30348891 gb IAWN28934.1 39.53 253 138 3 18 257 5 2552.0 e
gi 23499780 gn REF_tigr BRA00013 gi 19655222 gb IAF93939.1 40.64 251 138 1 17 256 10 2602.7 e	gi 23499780 gn REF_tigr BRA00013 gi 12735806 gb IAA007757.1 43.03 251 130 4 18 256 11 2602.5 e
gi 23499780 gn REF_tigr BRA00013 gi 112597924 gb IAA185899.2 46.70 162 96 1 62 243 5 1856.8 e	gi 23499780 gn REF_tigr BRA00013 gi 46363318 ref ZP_0026079.1 39.58 240 136 2 14 253 6 2361.8 e
REF_tigr BRA00013 gi 39933731 ref NP_946007.1 34.90 255	REF_tigr BRA00013 gi 48782600 ref ZP_00279106.1 35.92 245
REF_tigr BRA00013 gi 41407534 ref NP_960370.1 36.09 266	REF_tigr BRA00013 gi 48851585 ref ZP_00305793.1 32.39 247
REF_tigr BRA00013 gi 15966306 ref NP_386659.1 36.50 263	REF_tigr BRA00013 gi 17548526 ref NP_521866.1 36.36 264
gi 23499780 gn REF_tigr BRA00013 gi 51891730 ref WP_074421.1 38.87 247 136 7 18 256 1 2403.4 e	gi 23499780 gn REF_tigr BRA00013 gi 1145881 gb IAA23739.1 33.87 246 147 3 13 253 3 2404.4 e
gi 23499780 gn REF_tigr BRA00013 gi 25029334 ref NP_739388.1 35.20 250 147 4 15 256 6 2485.7 e	gi 23499780 gn REF_tigr BRA00013 gi 21220953 ref NP_536732.1 36.52 257 138 6 12 255 5 2545.7 e
gi 23499780 gn REF_tigr BRA00013 gi 46314029 ref ZP_00214635.1 33.86 254 153 2 12 259 3 2485.7 e	gi 23499780 gn REF_tigr BRA00013 gi 41406852 ref NP_959683.1 35.61 238 149 2 16 253 2 2309.8 e
gi 23499780 gn REF_tigr BRA00013 gi 115644471 ref NP_229523.1 35.69 255 144 5 12 256 2 2469.8 e	gi 23499780 gn REF_tigr BRA00013 gi 23470090 ref ZP_00125423.1 35.20 250 145 4 12 253 3 2439.8 e
gi 23499780 gn REF_tigr BRA00013 gi 24935279 gb IAA64237.1 34.63 257 146 4 12 257 4 2499.8 e	gi 23499780 gn REF_tigr BRA00013 gi 48647655 ref ZP_00303815.1 36.05 258 145 9 12 257 4 2531.3 e
gi 23499780 gn REF_tigr BRA00013 gi 28851510 gb IAA054587.1 36.40 250 142 4 12 253 3 2431.3 e	gi 23499780 gn REF_tigr BRA00013 gi 127378783 ref NP_770312.1 36.25 251 143 3 14 255 7 2491.3 e
gi 23499780 gn REF_tigr BRA00013 gi 11708836 sp I50198 [LINC_PSEPA 34.23 260 143 4 12 257 4 2491.7 e	gi 23499780 gn REF_tigr BRA00013 gi 33594148 ref NP_381792.1 34.17 240 148 5 18 256 6 2363.7 e
gi 23499780 gn REF_tigr BRA00013 gi 33598116 ref NP_381750.1 34.17 240 148 5 18 256 6 2363.7 e	gi 23499780 gn REF_tigr BRA00013 gi 3328306 ref NP_232827.1 34.23 260 143 4 12 257 4 2491.7 e

Back Office Analysis on Grid
Millions of BLAST, BLOCKS, etc., on OSG and TeraGrid

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

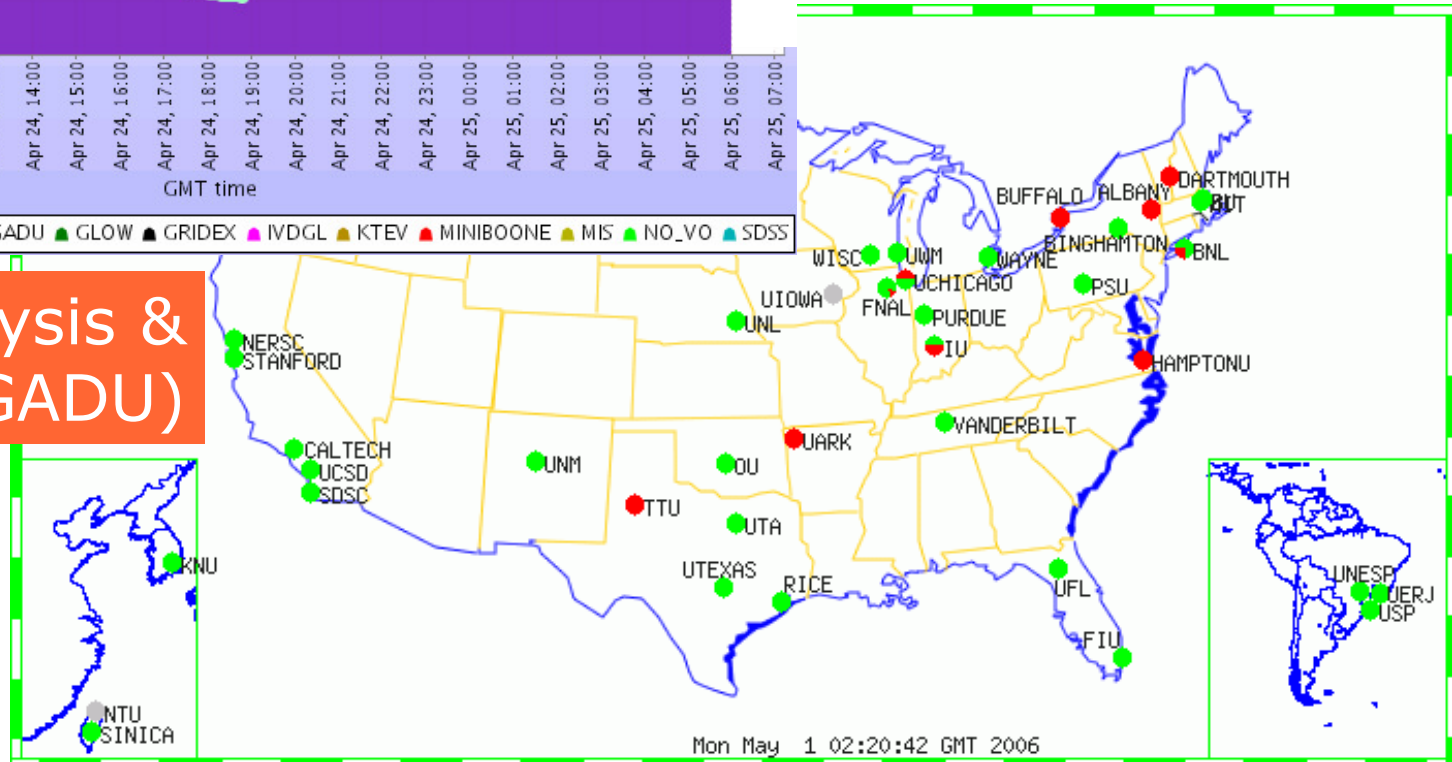


Running Jobs



600-1000+ CPUs

Genome Analysis & DB Update (GADU)





the globus alliance
www.globus.org



Swift Summary

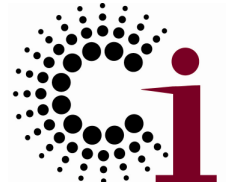
- Clean separation of logical/physical concerns
 - ◆ XDTM specification of logical data structures
- + Concise specification of parallel programs
 - ◆ SwiftScript, with iteration, etc.
- + Efficient execution on distributed resources
 - ◆ Grid interface, pipelining, clustering, load balancing
- + Rigorous provenance tracking and query
 - ◆ Virtual data schema & automated recording
- **Improved usability and productivity**
 - ◆ Demonstrated in numerous applications

<http://www.ci.uchicago.edu/swift>



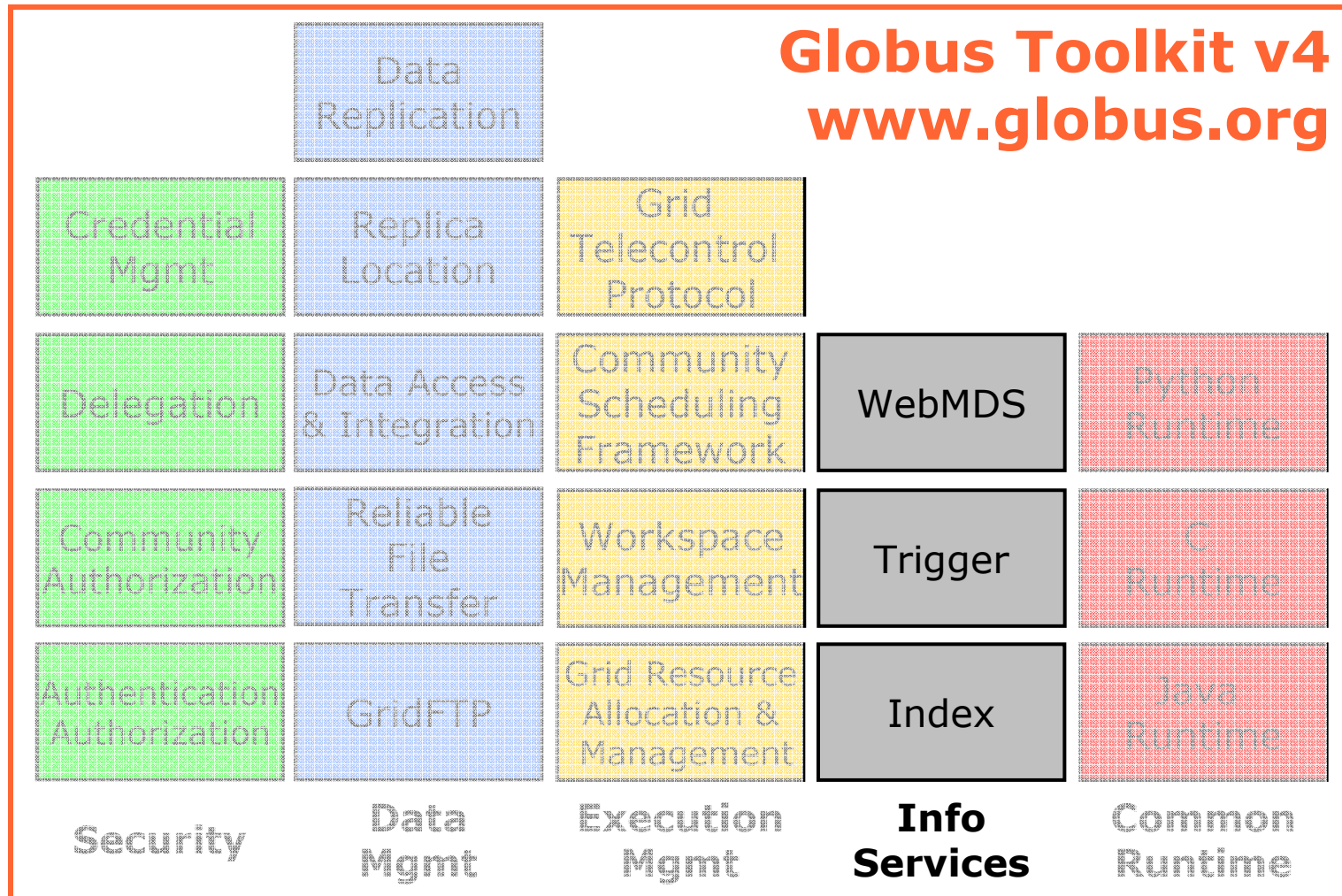
More Specifically, I May Want To ...

- Create a service for use by my colleagues
- Manage who is allowed to access my service (or my experimental data or ...)
- Ensure reliable & secure distribution of data from my lab to my partners
- Run 10,000 jobs on whatever computers I can get hold of
- Monitor the status of the different resources to which I have access



Globus Toolkit: Open Source Grid Infrastructure

Globus Toolkit v4
www.globus.org



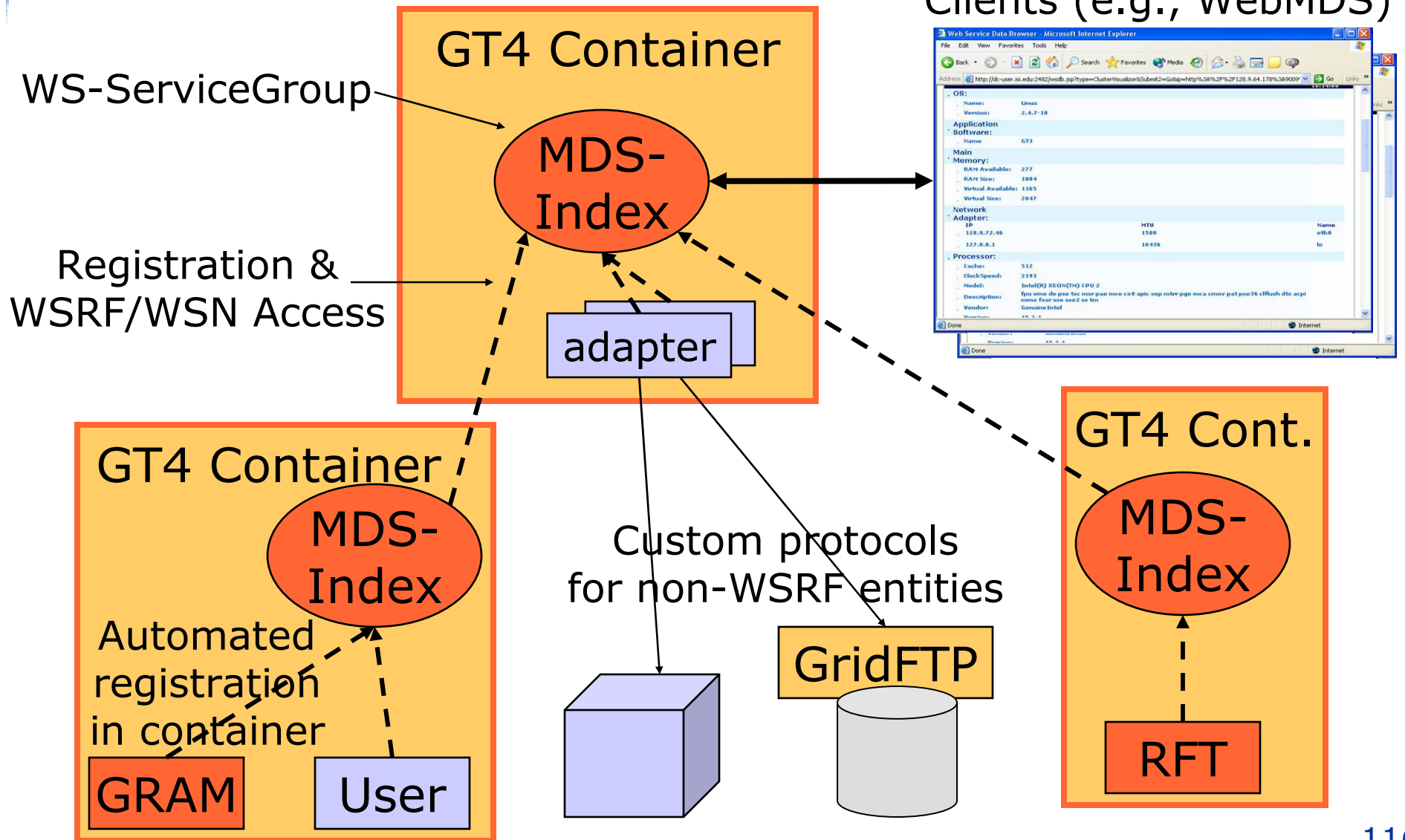


Monitoring and Discovery

- “Every service should be monitorable and discoverable using common mechanisms”
 - ◆ WSRF/WSN provides those mechanisms
- A common **aggregator** framework for collecting information from services, thus:
 - ◆ MDS-Index: Xpath queries, with caching
 - ◆ MDS-Trigger: perform action on condition
 - ◆ (MDS-Archiver: Xpath on historical data)
- Deep integration with Globus containers & services: every GT4 service is discoverable
 - ◆ GRAM, RFT, GridFTP, CAS, ...



Clients (e.g., WebMDS)





Information Providers

- **GT4 information providers** collect information from some system and make it accessible as WSRF resource properties
- Growing number of information providers
 - ◆ Nagios, SGE, LSF, PBS
- Many opportunities to build additional ones
 - ◆ E.g., network monitoring, storage systems, various sensors



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Earth System Grid

DOE Earth System Grid



Goal: Enable sharing & analysis of high-volume data from advanced earth system models

Live Access to Climate Data - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <http://dataportal.ucar.edu/esg-las/main.pl?>

Home Help Options

THE EARTH SYSTEM GRID

ESG

Scientific Discovery through Advanced Computing

b20.007.cam1.h0.0500-01.nc

Average of TREFHT daily maximum

Select view: xy (lat/lon) slice

Select: single variable comparison

Get Data

Full Region

87.86379883

180.0 W 180.0 E

87.86379883

Zoom In Zoom Out

Select time: 01-Feb-0500 01-Feb-0500

Select product: Shaded plot (GIF) in 800x600 window

Internet

www.earthsystemgrid.org



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ESG Facts and Figures



Earth System Grid

ESG Portal at NCAR

130 TB of data at four locations

- 840,331 files
- Includes the past 6 years of joint DOE/NSF climate modeling experiments

3,200 registered users

Downloads to date

- 25 TB
- 91,000 files



Worldwide ESG user base

IPCC AR4 ESG Portal

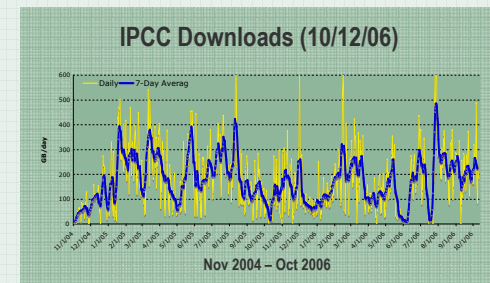
28 TB of data at one location

- 68,400 files
- Generated by a modeling campaign coordinated by the Intergovernmental Panel on Climate Change
- Model data from 11 countries

818 registered analysis projects

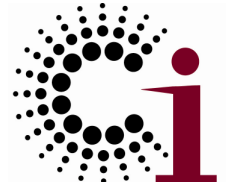
Downloads to date

- 123 TB
- 543,500 files
- 300 GB/day (average)

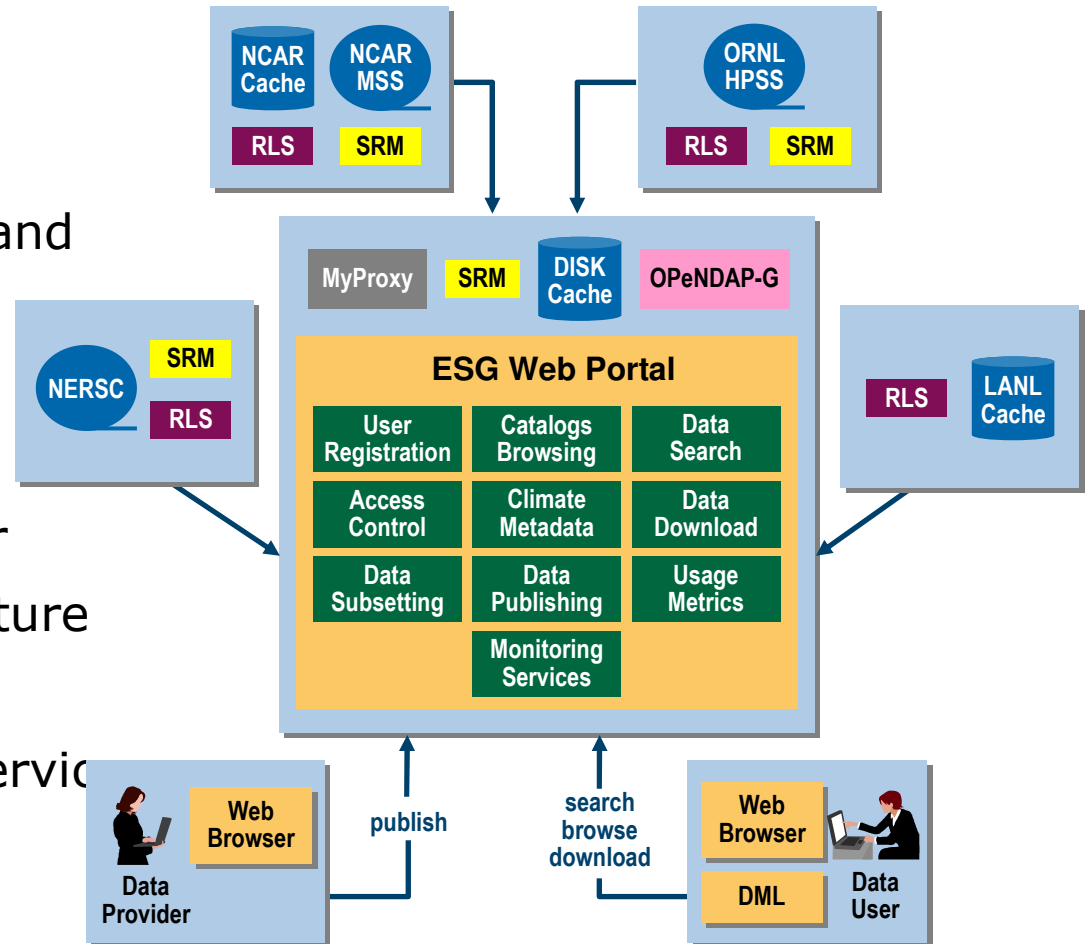


300 scientific papers published to date based on analysis of IPCC AR4 data

ESG Architecture and Technologies



- Climate data
 - ◆ Metadata catalog
 - ◆ OPeNDAP-G (aggregation and subsetting)
- Data management
 - ◆ Data Mover Lite
 - ◆ Storage Resource Manager
 - ◆ Globus Security Infrastructure
 - ◆ GridFTP
 - ◆ Globus Replica Location Service
- Security services
 - ◆ Access control
 - ◆ MyProxy
 - ◆ PURSE User registration



MSS, HPSS: Tertiary data storage systems



Monitoring Overall System Status

- Monitored data are collected in MDS4 Index service
- Information providers check resource status at a configured frequency
 - ◆ Currently, every 10 minutes
- Report status to Index Service
- Information in Index Service is queried by ESG Web portal
- Used to generate overall picture of state of ESG resources
- Displayed on ESG Web portal page

ESG Current Status
Updated: Tue Jun 27 16:52:32 MDT
2006 MDT

	LANL	LBNL	NCAR	ORNL
MSS/HPSS		☹	☹	☹
SRM	☹	☹	☹	☹
RLS		☹	☹	☹
OpenDAPg			☹	
GridFTP server			☹	
HTTP server	☹		☹	

(Explanation of current status)



Example Monitoring Information

Total error messages for May 2006	47
Messages related to certificate and configuration problems at LANL	38
Failure messages due to brief interruption in network service at ORNL on 5/13	2
HTTP data server failure at NCAR 5/17	1
RLS failure at LLNL 5/22	1
Simultaneous error messages for SRM services at NCAR, ORNL, LBNL on 5/23	3
RLS failure at ORNL 5/24	1
RLS failure at LBNL 5/31	1

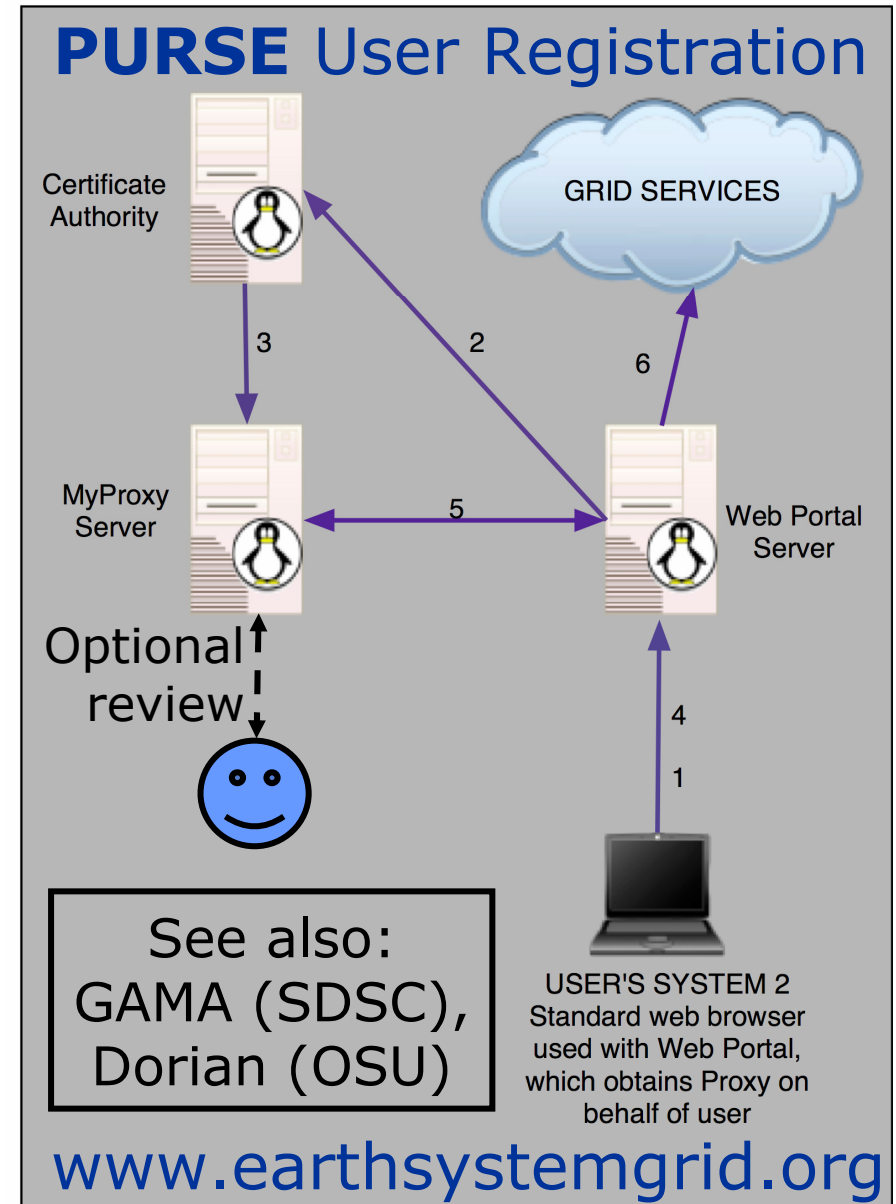


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Security Needn't Be Hard: PURSe & Earth System Grid



- Purpose
 - ◆ Access to large data
- Policies
 - ◆ Per-collection control
 - ◆ Different user classes
- Implementation (GT)
 - ◆ PURSe
 - ◆ PKI, SAML assertions
- Experience
 - ◆ >4000 users
 - ◆ >100 TB downloaded





Guidelines
(Apache
Jakarta)

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](#)
- [CAS/SAML Utilities](#)
- [Delegation Service](#)

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.
- Information about Globus community events.
- [The conventions and guidelines that apply to contributions](#)

dev.globus

- Globus software is organized as several dozen “Globus Projects”
 - ◆ Projects release products
- Each project has its own “Committers”
 - ◆ Committers are responsible for governance on matters relating to their products
- A “Globus Management Committee”
 - ◆ provides overall guidance and conflict resolution
 - ◆ approves the creation of new Globus projects

Initial Globus Projects

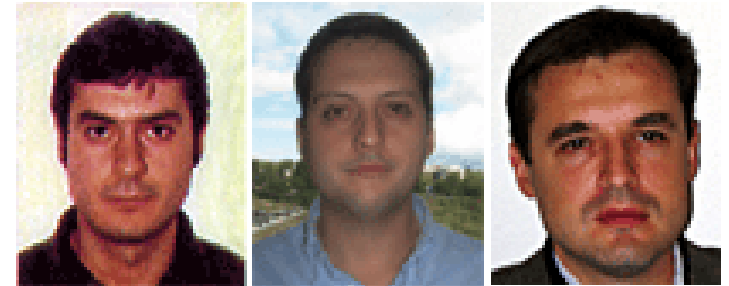
- **Runtime**
 - ◆ C Core Utilities
 - ◆ C WS Core
 - ◆ CoG jglobus
 - ◆ Core WS Schema
 - ◆ Java WS Core
 - ◆ Python Core
 - ◆ XIO
- **Execution**
 - ◆ GRAM
 - ◆ MPICH-G
- **Data**
 - ◆ GridFTP
 - ◆ OGSA-DAI
 - ◆ Reliable Transfer
 - ◆ Replica Location
 - ◆ Replication
- **Distribution**
 - ◆ Globus Toolkit
- **Documentation**
 - ◆ Build a Service Tutorial
 - ◆ GT Release Manuals
 - ◆ GT Programmer's Tutorial
- **Security**
 - ◆ C Security
 - ◆ CAS/SAML Utilities
 - ◆ Delegation
 - ◆ GSI-OpenSSH
 - ◆ MyProxy
- **Information**
 - ◆ MDS4

Globus Incubator Projects (Partial List)



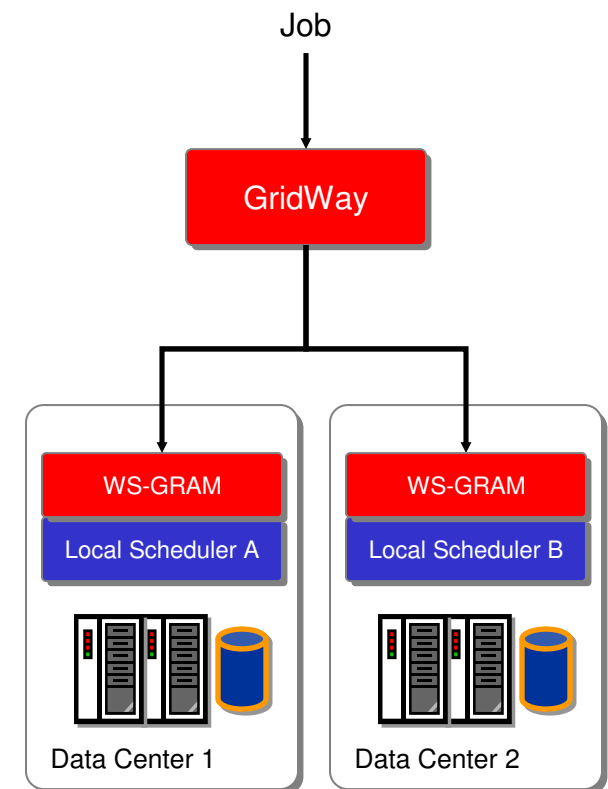
- **CoG Workflow** — Fine-grained workflow system
- **Dynamic Accounts** — UNIX account allocation
- **GridShib** — Integration with Shibboleth
- **GridWay** — Metascheduler
- **gt-hs** — Integration of Handle System
- **MEDICUS** — Medical image management
- **Metrics** — Infrastructure for usage reporting
- **OGCE** — Portal toolkit
- **PURSe** — Portal-based user registration service
- **ServMark** — Grid service performance tester
- **Virtual Workspaces** — Virtual machine mgmt 127

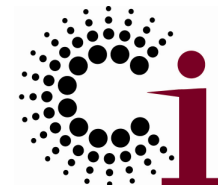
GridWay



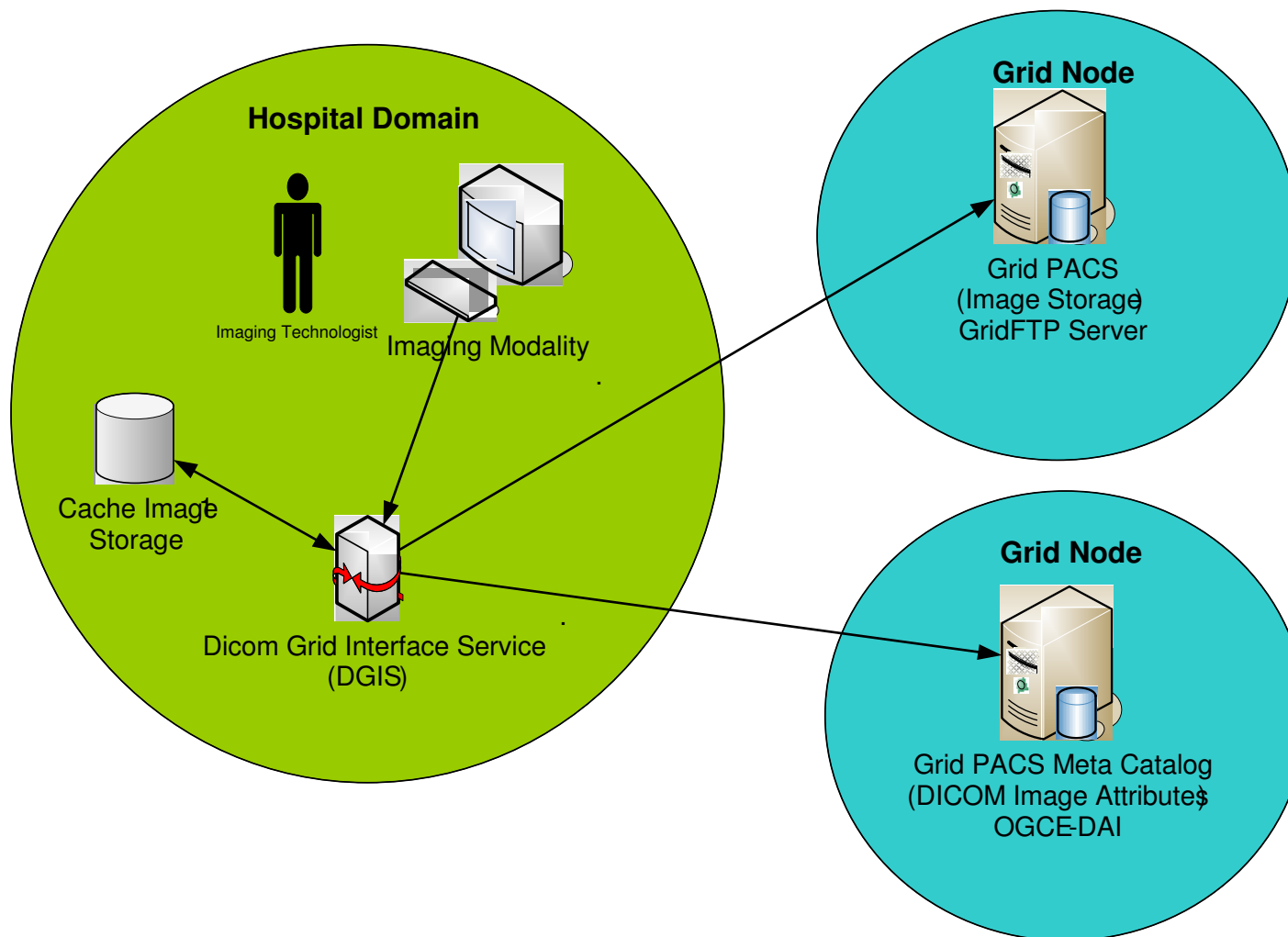
Ignacio M. Llorente,
Ruben S. Montero,
Eduardo Huedo

- Open source meta-scheduler
- dev.globus incubator project
 - ◆ Started in 2002, now on v5
- Talks to local scheduler via WS-GRAM
- WS-GRAMs can interface to heterogeneous local schedulers





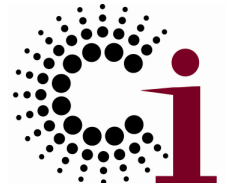
MEDICUS: Management of DICOM Images



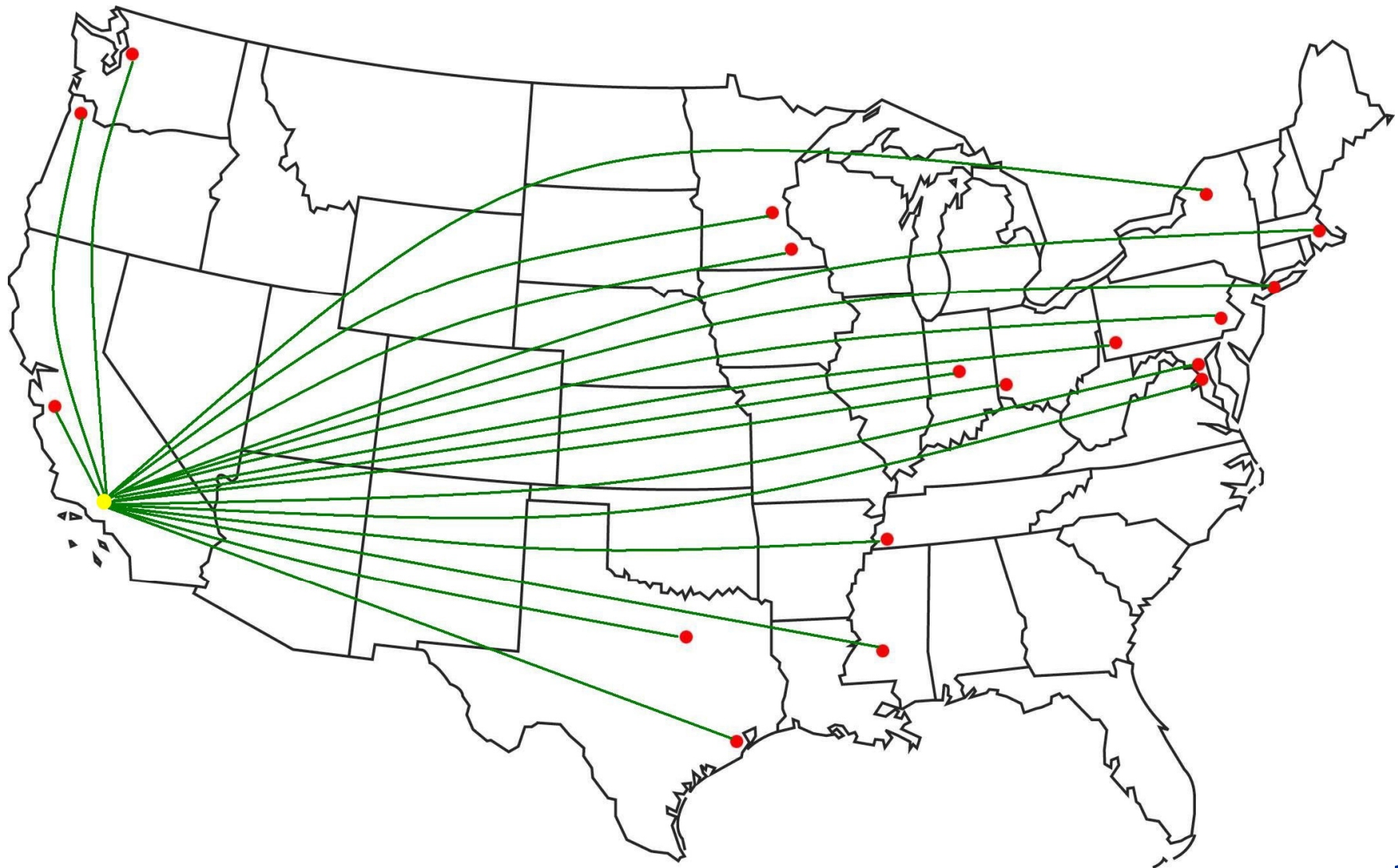


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Children's Oncology Grid: A MEDICUS Deployment





MEDICUS Under the Covers

Globus Toolkit Release 4

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

DICOM Grid Interface Service (DGIS)
+
Meta Catalog Service (OGSA-DAI)

Data Replication Service (DRS)

X.509 Certificates
+
MyProxy Delegation

Grid Web Portal, OGCE / GridSphere

GRAM, OGSA-DAI

- Provider of commercial support, services, & products around open source Globus
 - ◆ Commercial distribution of GT4 & beyond
 - ◆ Integration with enterprise systems
 - ◆ Committed to open source & open standards
- Univa is contributing to Globus open source
 - ◆ Big contributions to GT4 development, testing
 - ◆ New functionality: install shields, security configurator, GridFTP extensions
 - ◆ Additional contributions expected



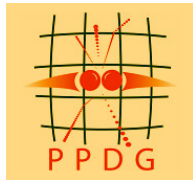
Globus User Community

- Large & diverse
 - ◆ 10s of national Grids, 100s of applications, 1000s of users; probably much more
 - ◆ Every continent except Antarctica
 - ◆ Applications ranging across many sciences
 - ◆ Dozens (at least) of commercial deployments
- Successful
 - ◆ Many production systems doing real work
 - ◆ Many applications producing real results
- Smart, energetic, demanding
 - ◆ Constant stream of new use cases & tools

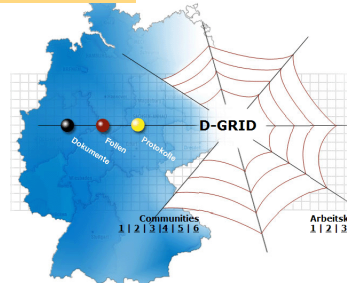
Global Community



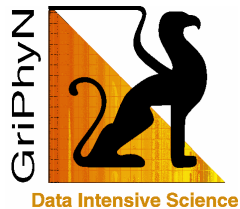
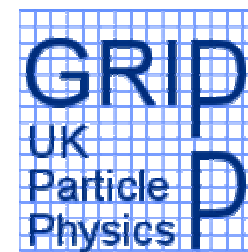
GRID.it
project



K*GRID



National Grid
NG
SINGAPORE



- tota la informació sobre el projecte
- presentació
 - descripció tècnica
 - els serveis oferts
 - participants
 - documentació pública
 - com puc participar?
 - accés al Portal
 - Intranet per a investigadors
 - estat dels serveis actius



国立情報学研究所グリッド研究開発推進拠点 NII -The National Institute of Informatics



Examples of Production Scientific Grids

- APAC (Australia)
- China Grid
- China National Grid
- DGrid (Germany)
- EGEE
- NAREGI (Japan)
- Open Science Grid
- Taiwan Grid
- TeraGrid
- ThaiGrid
- UK Natl Grid Service

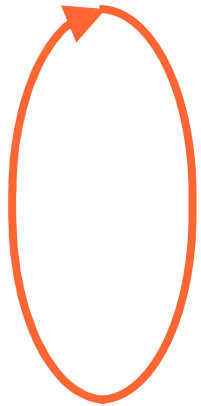




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Future Directions: Service Oriented Science



People **create** services (data or functions) ...
which I **discover** ...
& maybe **compose** to create a new function ...
and 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, ...



TeraGrid™
EMPOWERING DISCOVERY

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



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For Example: Virtual Observatories

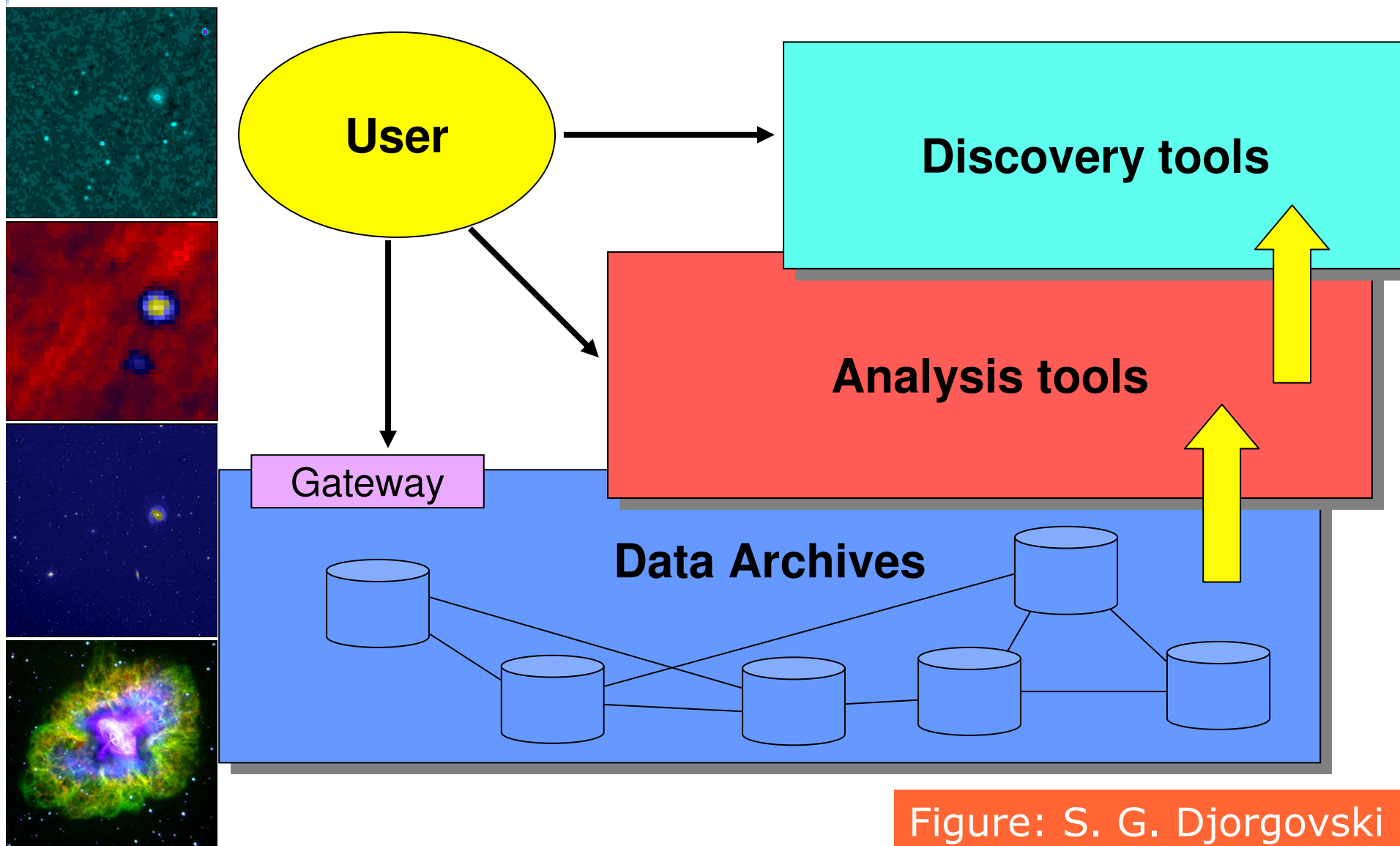
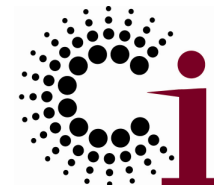
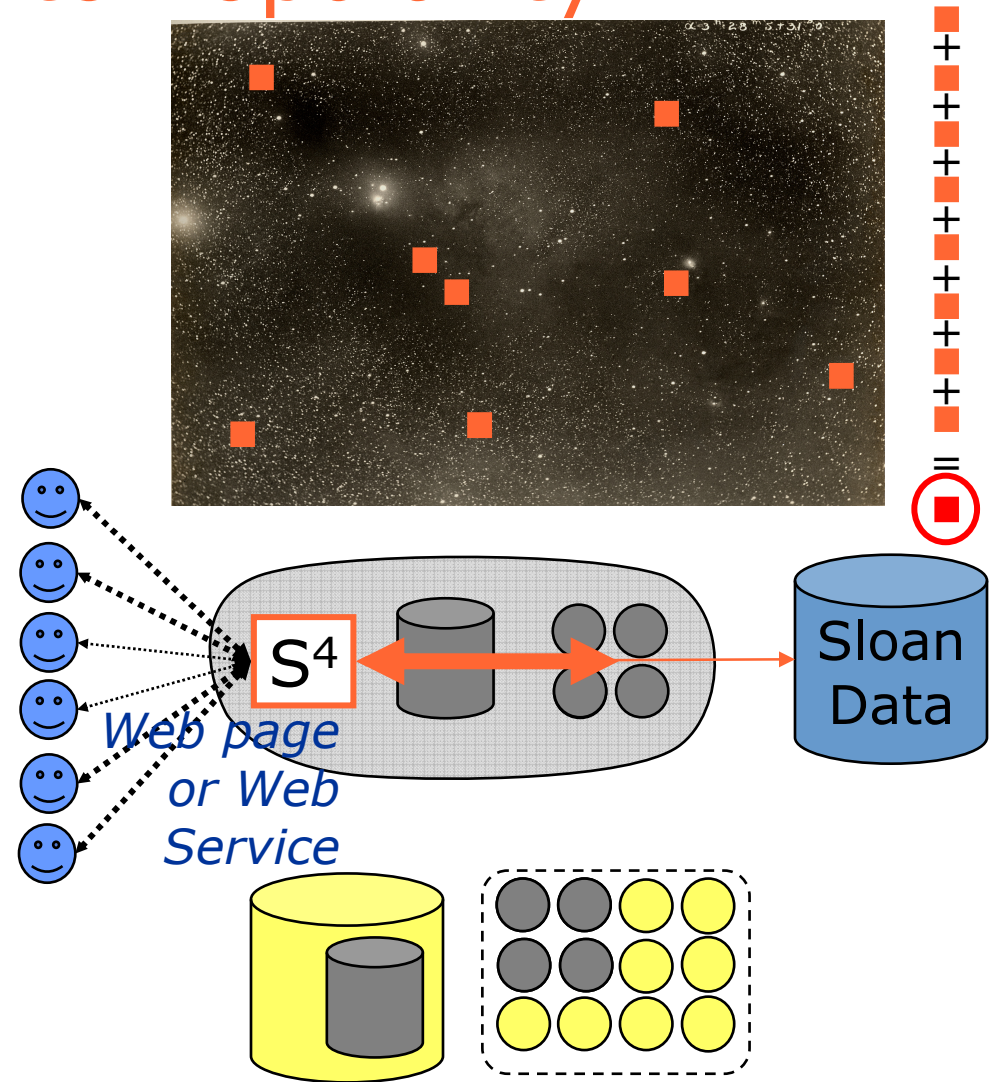


Figure: S. G. Djorgovski

Using Grid Infrastructure to Respond to Popularity



- 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





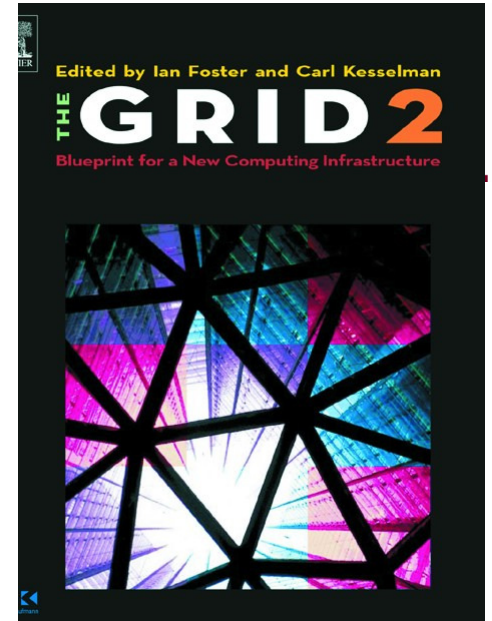
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Summary: Grid is About ...

Enabling *"coordinated resource sharing & problem solving in dynamic, multi-institutional virtual organizations."*

(Source: **"The Anatomy of the Grid"**)

- Access to shared resources
 - Virtualization, allocation, management
- With predictable behaviors
 - Provisioning, quality of service
- In dynamic, heterogeneous environments
 - Standards-based interfaces and protocols



More Specifically, Making it Possible to ...



- Create a service for use by my colleagues
- Manage who is allowed to access my service (or my experimental data or ...)
- Ensure reliable & secure distribution of data from my lab to my partners
- Run 10,000 jobs on whatever computers I can get hold of
- Monitor the status of the different resources to which I have access
- And so on ...

... By Providing Open Infrastructure



- Web services standards
 - ◆ State, notification, security, ...
- Services that enable access to resources
 - ◆ Service-enable new & existing resources
 - ◆ E.g., GRAM on computer, GridFTP on storage system, custom application services
 - ◆ Uniform abstractions & mechanisms
- Tools to build applications that exploit this infrastructure
 - ◆ Registries, security, data management, ...
- A rich tool & service ecosystem

For More Information

- Globus
 - ◆ www.globus.org: software, documentation
 - ◆ dev.globus.org: community development
- Swift
 - ◆ www.ci.uchicago.edu/swift
- TeraGrid, Open Science Grid
 - ◆ www.teragrid.org, www.opensciencegrid.org
- Random ramblings
 - ◆ ianfoster.typepad.com