14th International Symposium on Parallel and Distributed Computing

A Web-Based Platform for Publication and Distributed Execution of Computing Applications

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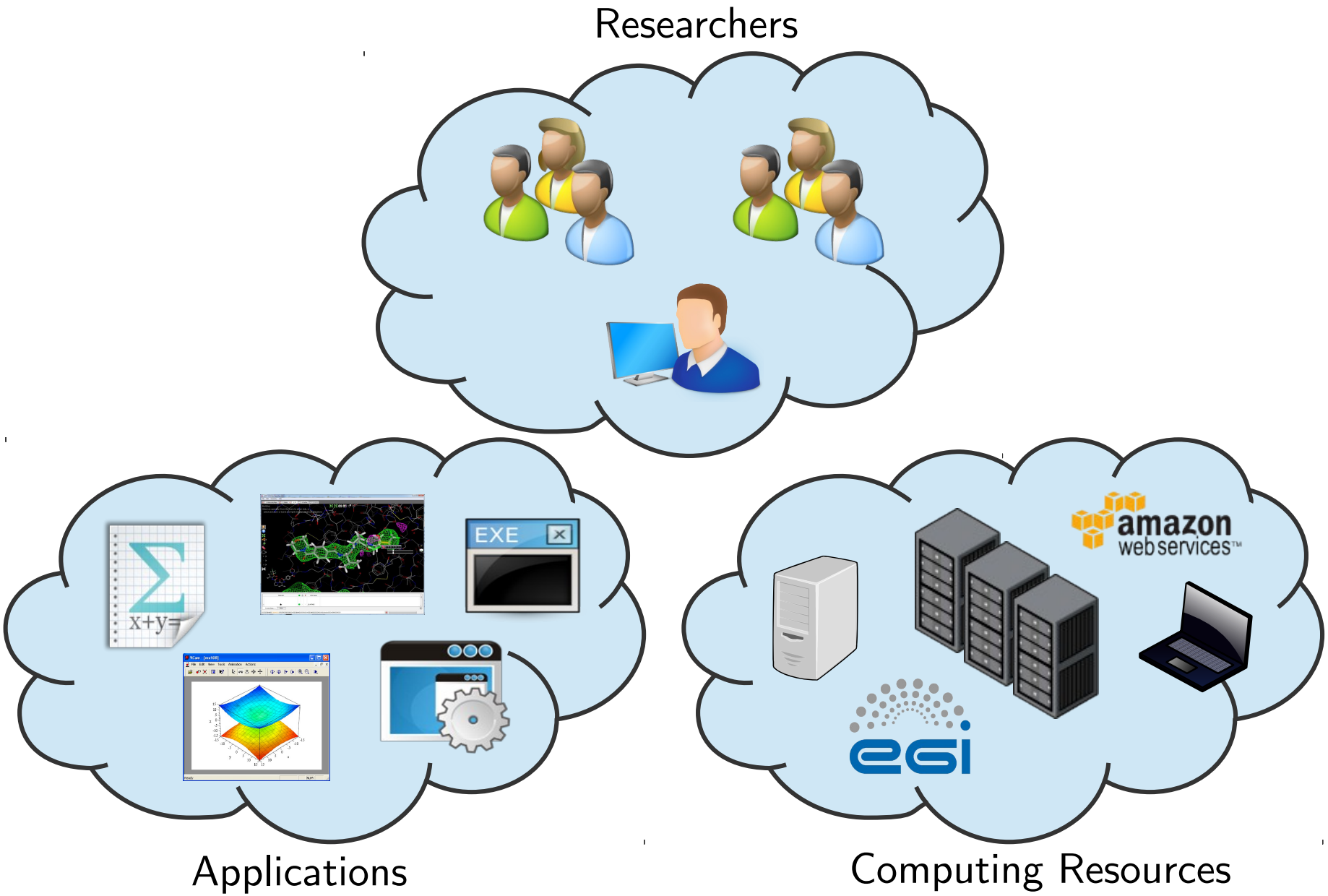
Motivation


Researchers
EXE
amazon
web services
egi
Applications
Computing Resources

Challenges

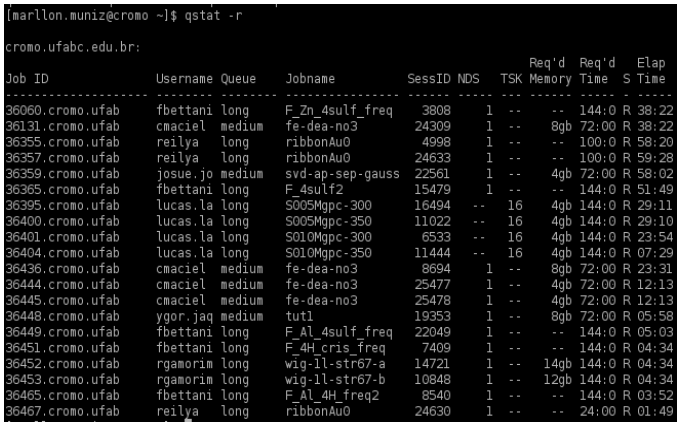
- Convenient access to computational applications
- Execution of applications on heterogeneous distributed computing resources
- Automation of workflows involving multiple applications
- Sharing applications/workflows with colleagues

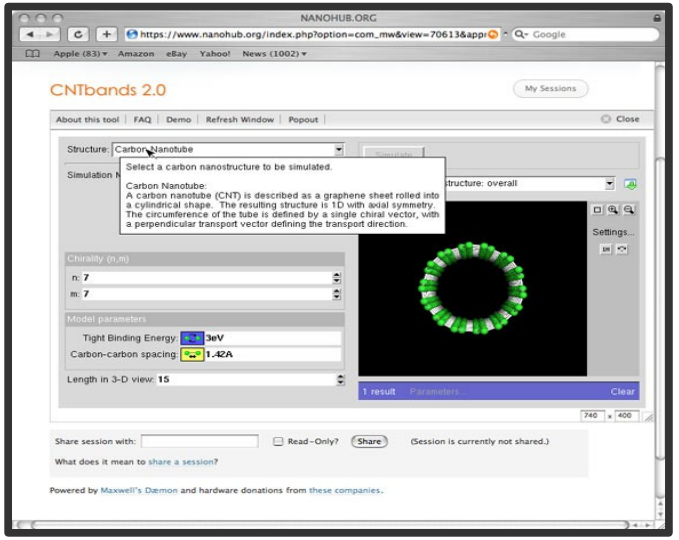
Current Solutions

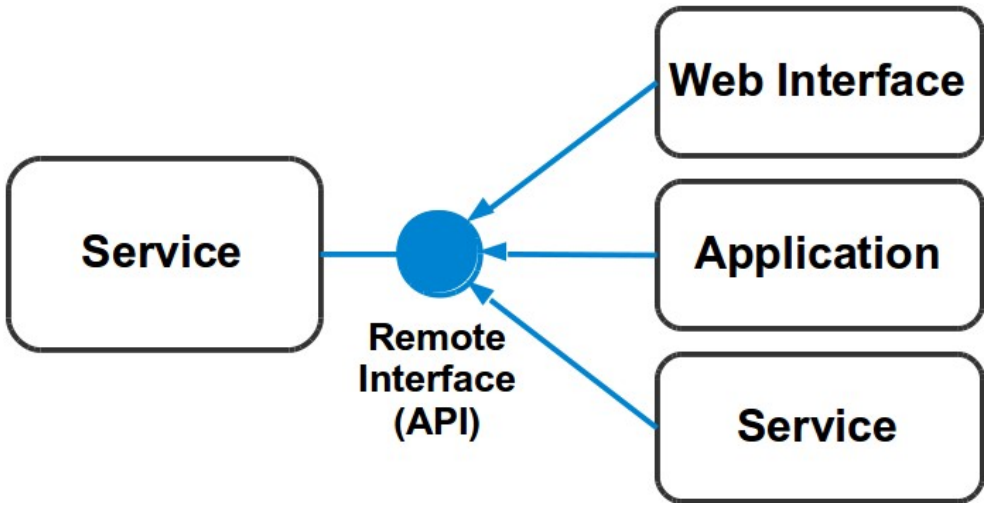
	Hosted vs Standalone	Arbitrary Resources	Application Sharing	Application Composition	Remote API
Grid Middleware					
User-level Toolkits / Workflow Systems					
Scientific Gateways					
Web Service Toolkits					

Sharing a Scientific Application

- Publish a source code
- Send an executable
- Create a web-based interface
- Run a web service







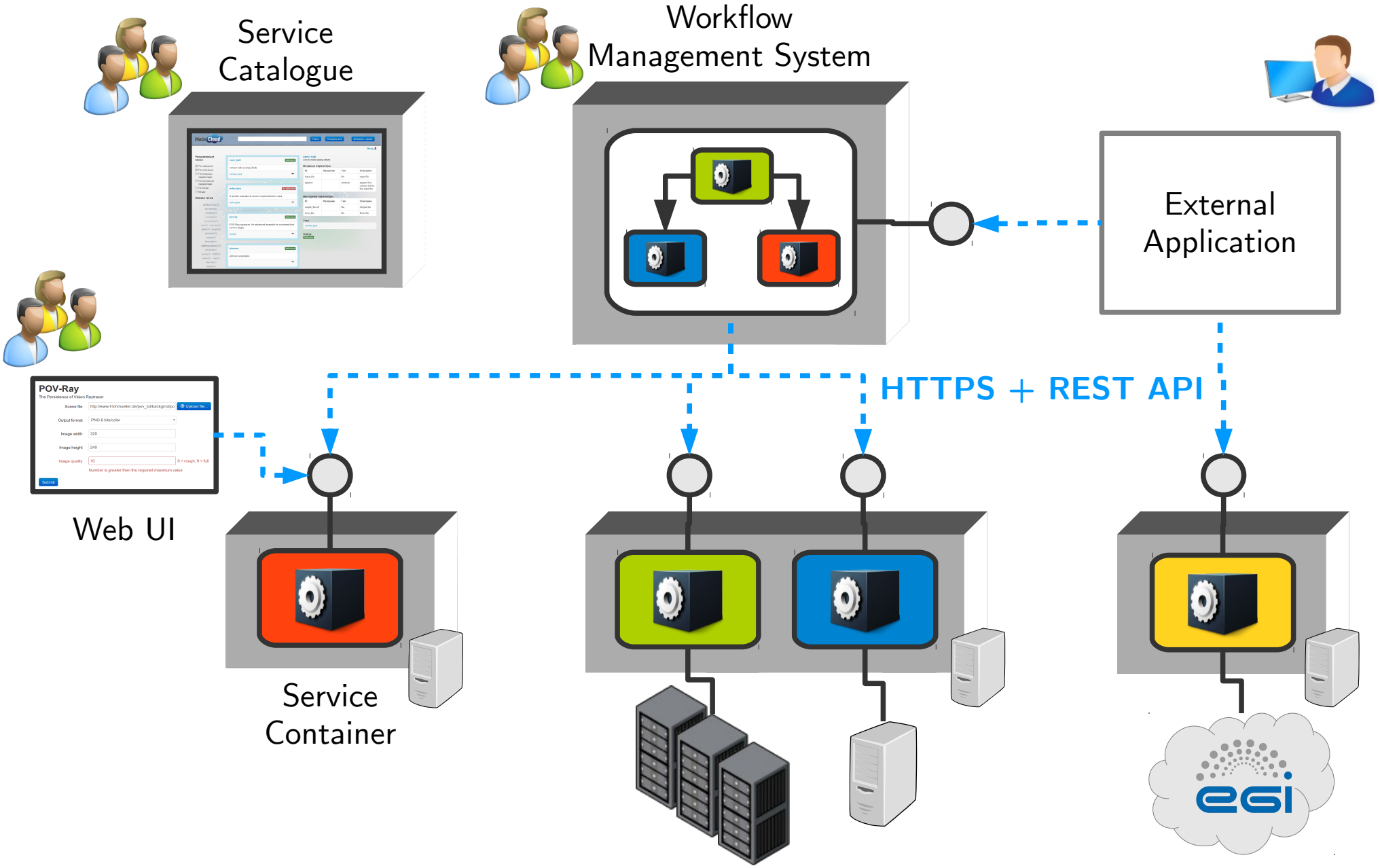
Scientific Application as a Service

- Software as a Service (SaaS)
- No need to install software and deal with computing resources
- Centralized maintenance and accelerated feature delivery
- Application composition and integration with third-party tools
- Collaboration
- Publication and reproducibility

MathCloud (2009-2013)

- Software toolkit for building, deployment, discovery and composition of computational web services
- Based on the unified web service interface
  - Follows REST (Representational state transfer) architectural style
- Main components
  - Service Runtime Environment (Container)
  - Service Catalogue
  - Workflow Management System (WfMS)
  - Security Mechanism
  - Client Interfaces

MathCloud Architecture



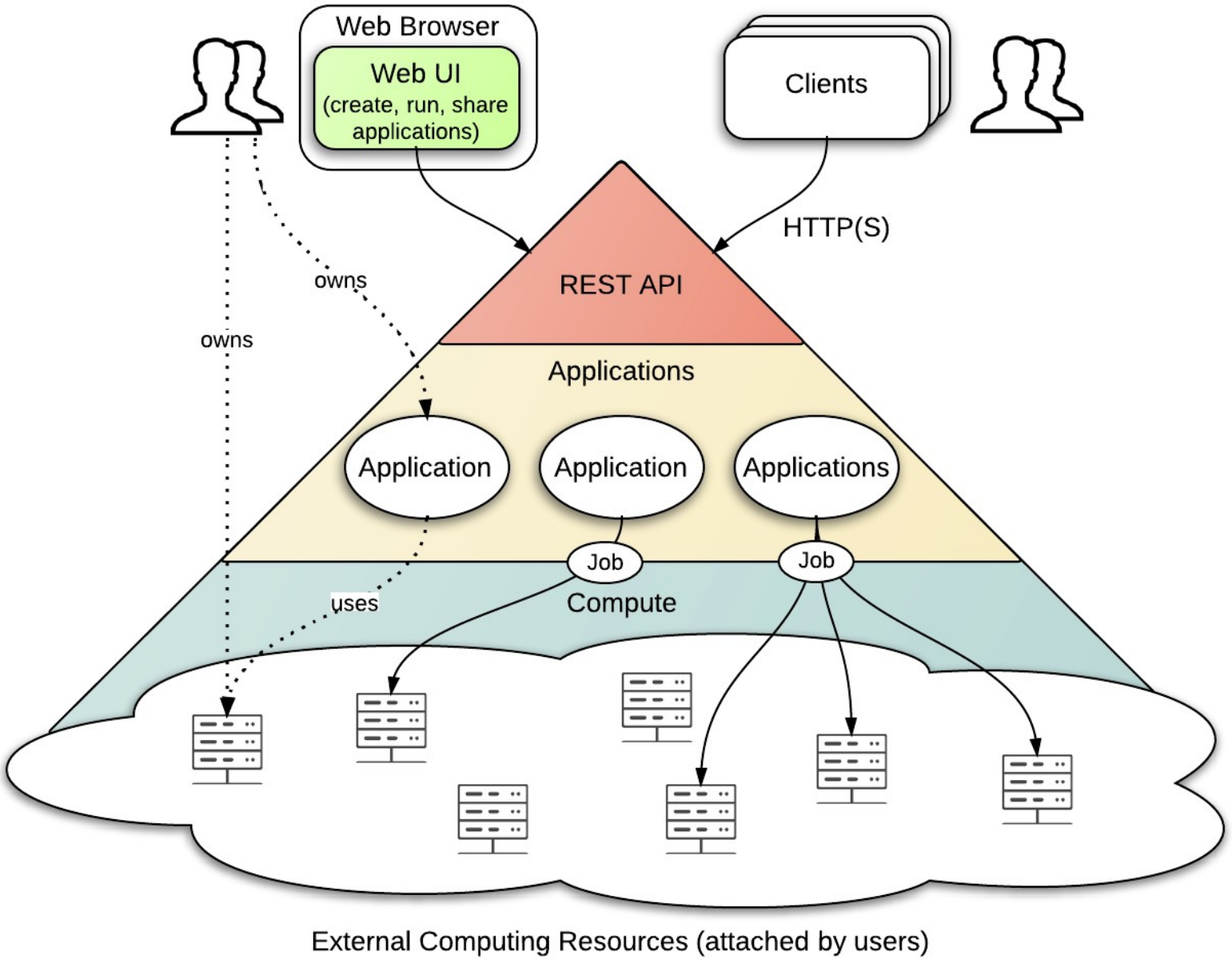
Problems

- Lack of convenient infrastructure to host services
- Sharing an application implies sharing a resource
- Service user cannot override the resource

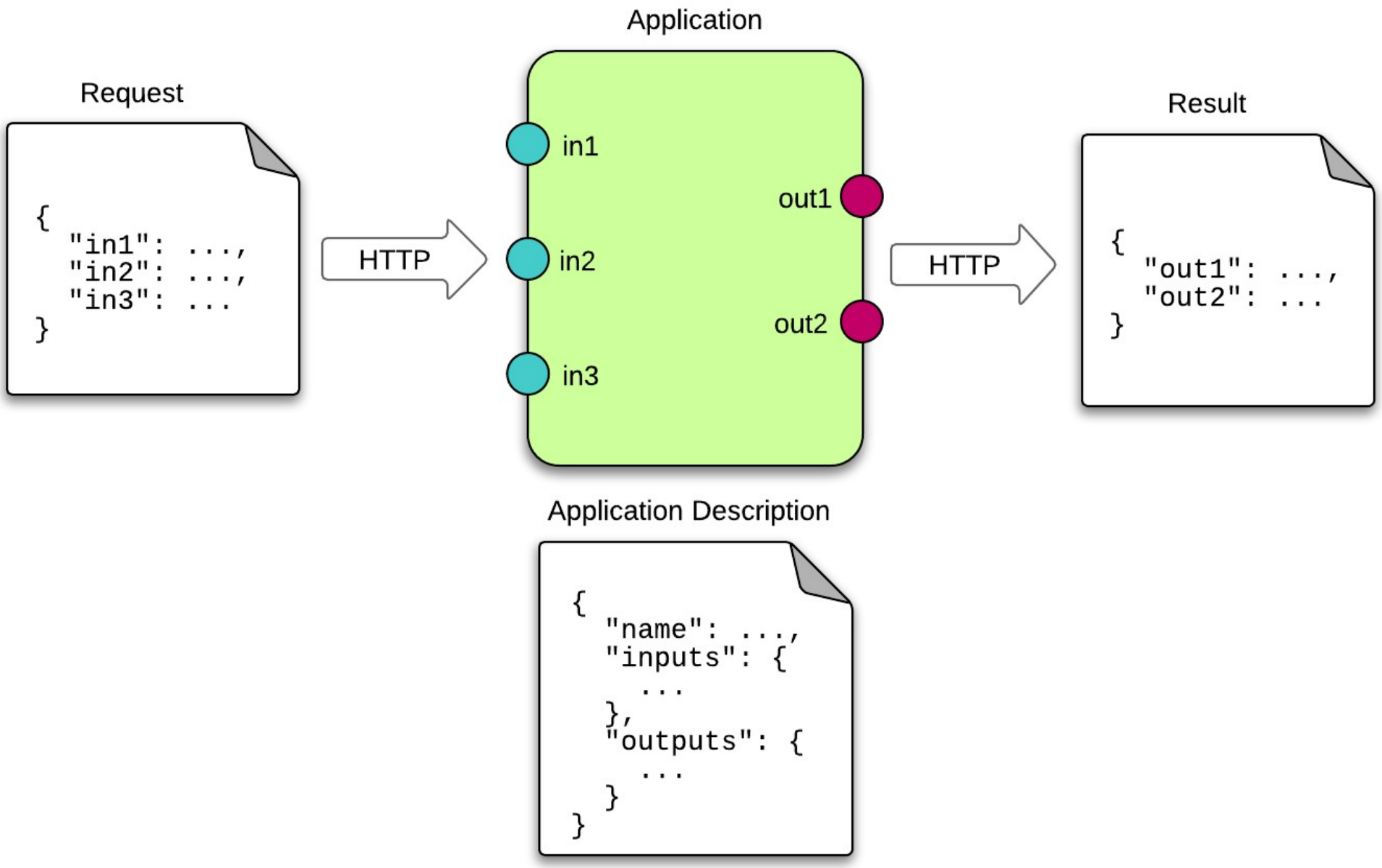
Everest (2014-...)

- Leverage cloud computing models to implement a web-based platform supporting
  - Describing and hosting computational applications as services
  - Binding applications to external computing resources
  - Running applications on arbitrary sets of resources
  - Sharing applications and resources with other users
- Platform as a Service (PaaS)
  - Accessible via web browser and REST API
  - No installation is required
- Combination of existing approaches + PaaS
  - Uniform REST interface for accessing applications
  - Web UI for application description
  - Automatic generation of web UI for application invocation

Everest Architecture



Application: Interface



POV-Ray: Parameters

POV-Ray

Edit

About | Parameters | Submit Job

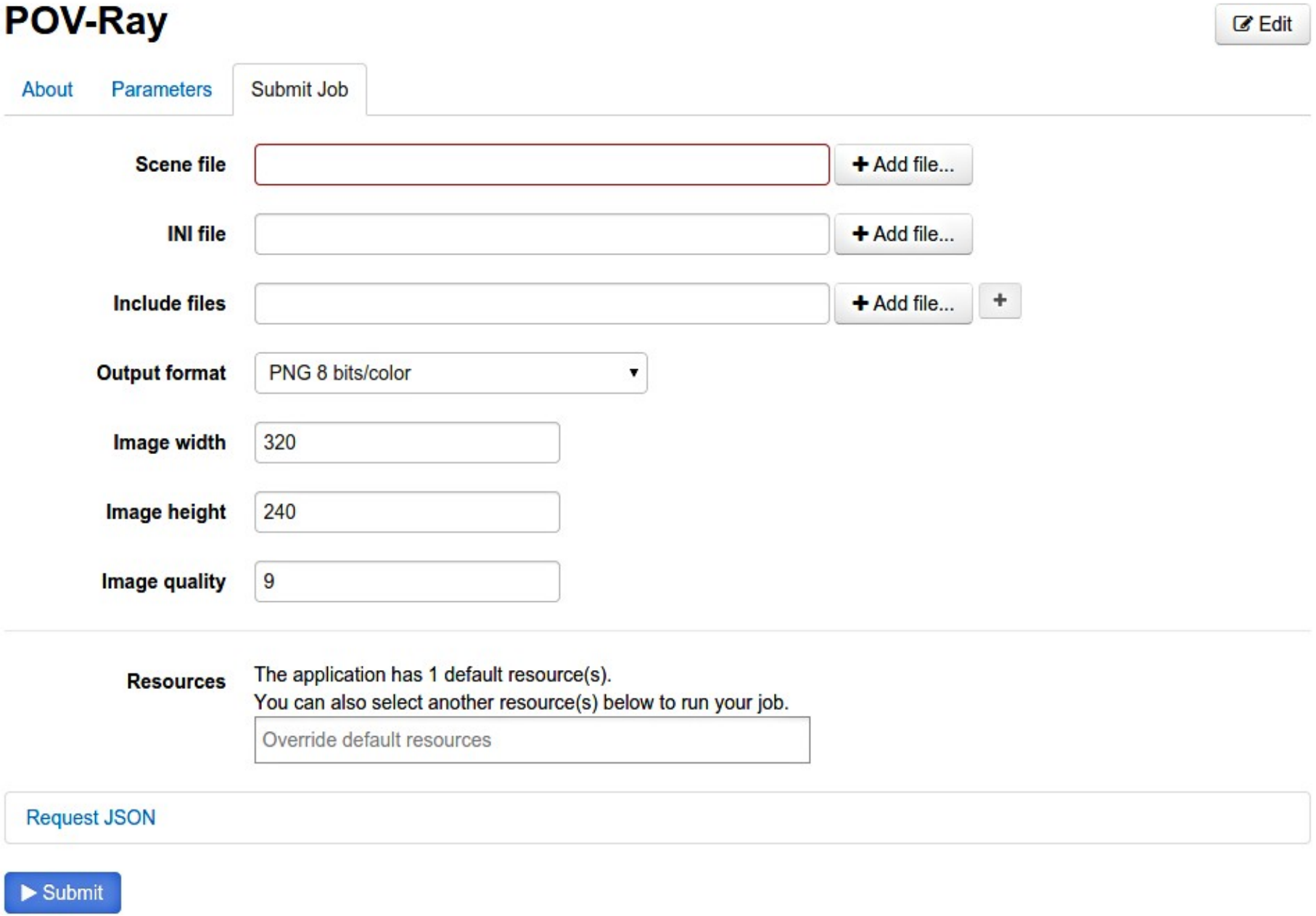
Inputs

	Title	Name	Type	Values	Default	Description
✔	Scene file	scene	URI			
	INI file	ini	URI			
	Include files	includes	array [URI]			
	Output format	format	string	C N8 N16 P T	N8	
	Image width	width	integer	[1, 2048]	320	
	Image height	height	integer	[1, 2048]	240	
	Image quality	quality	integer	[0, 11]	9	

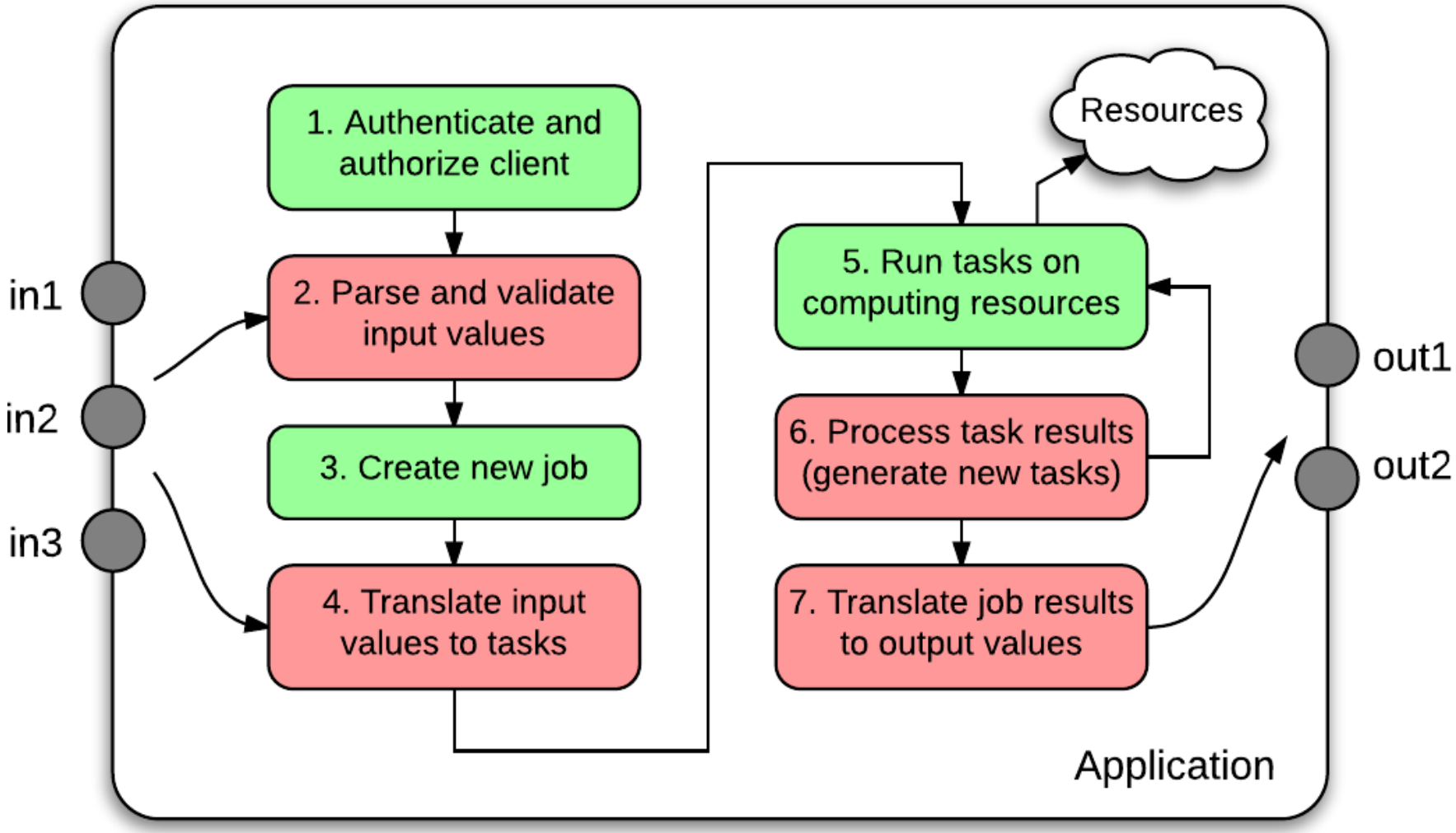
Outputs

	Title	Name	Type	Description
✔	Output image	image	URI	
✔	POV-Ray log	log	URI	

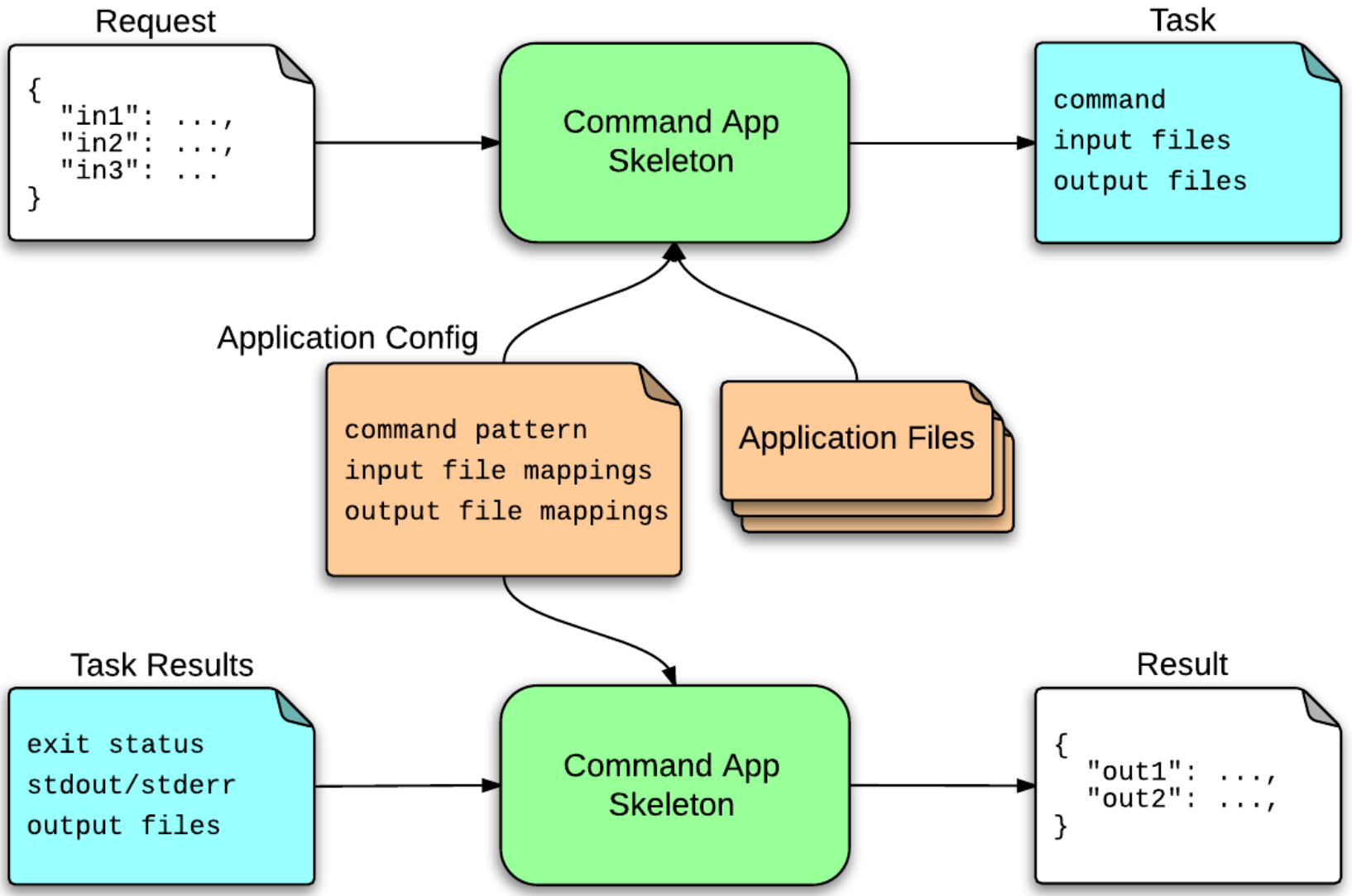
POV-Ray: Submit Form



Application: Implementation



Command Application Skeleton



POV-Ray: Configuration

POV-Ray

Metadata | Inputs | Outputs | **Configuration** | Files | Resources | Access

Command

```
./povray_run.sh +Iscene.pov +F${format} +W${width} +H${height} +Q${quality} -D +A -Oimage
```

Refer to input values as ${param}

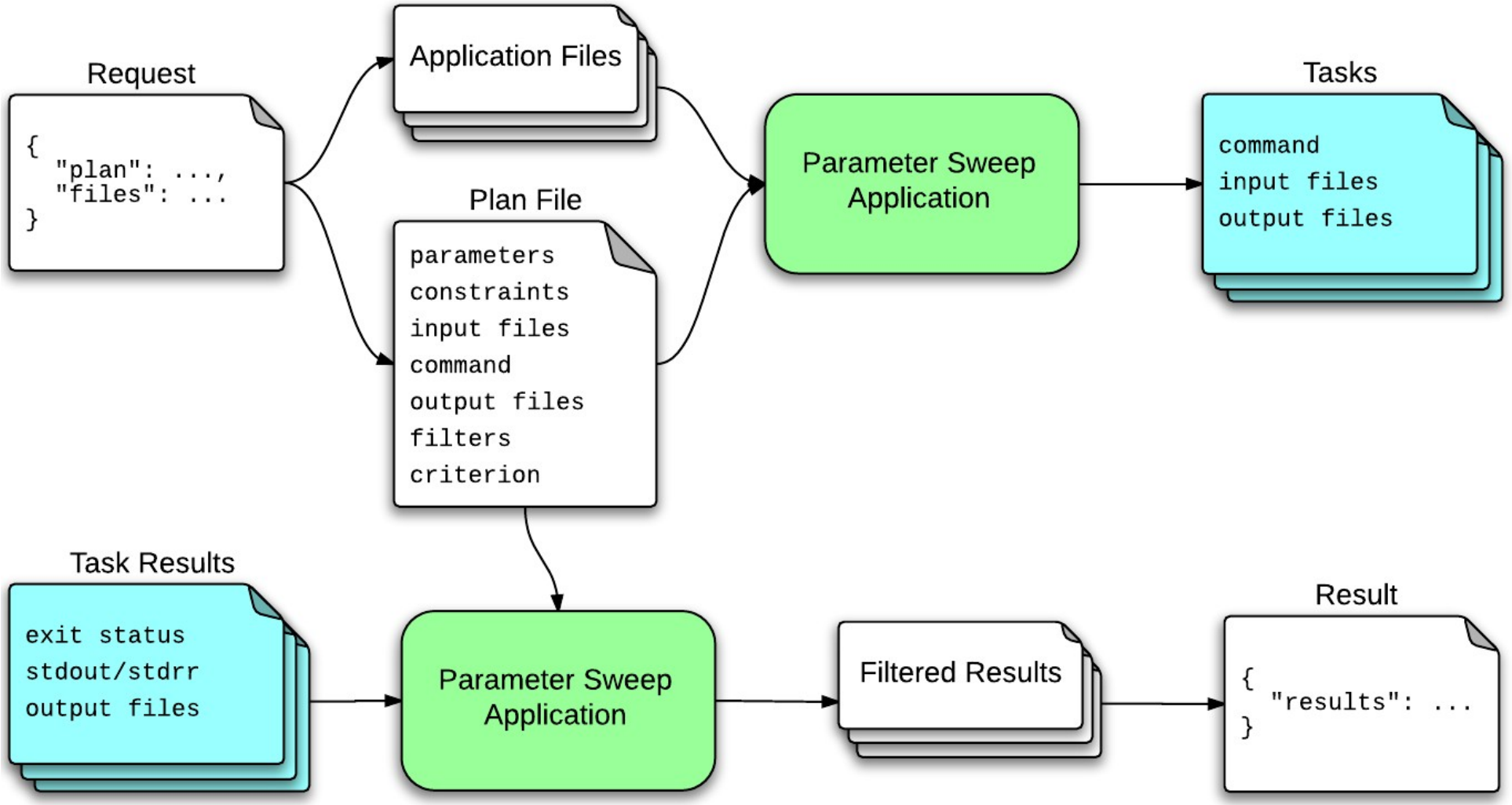
Input Mappings

Input	File	Pattern	
scene	scene.pov		🗑
ini	povray.ini		🗑
			+

Output Mappings

Output	File	Pattern	
image	image.*		🗑
log	stderr		🗑
			+

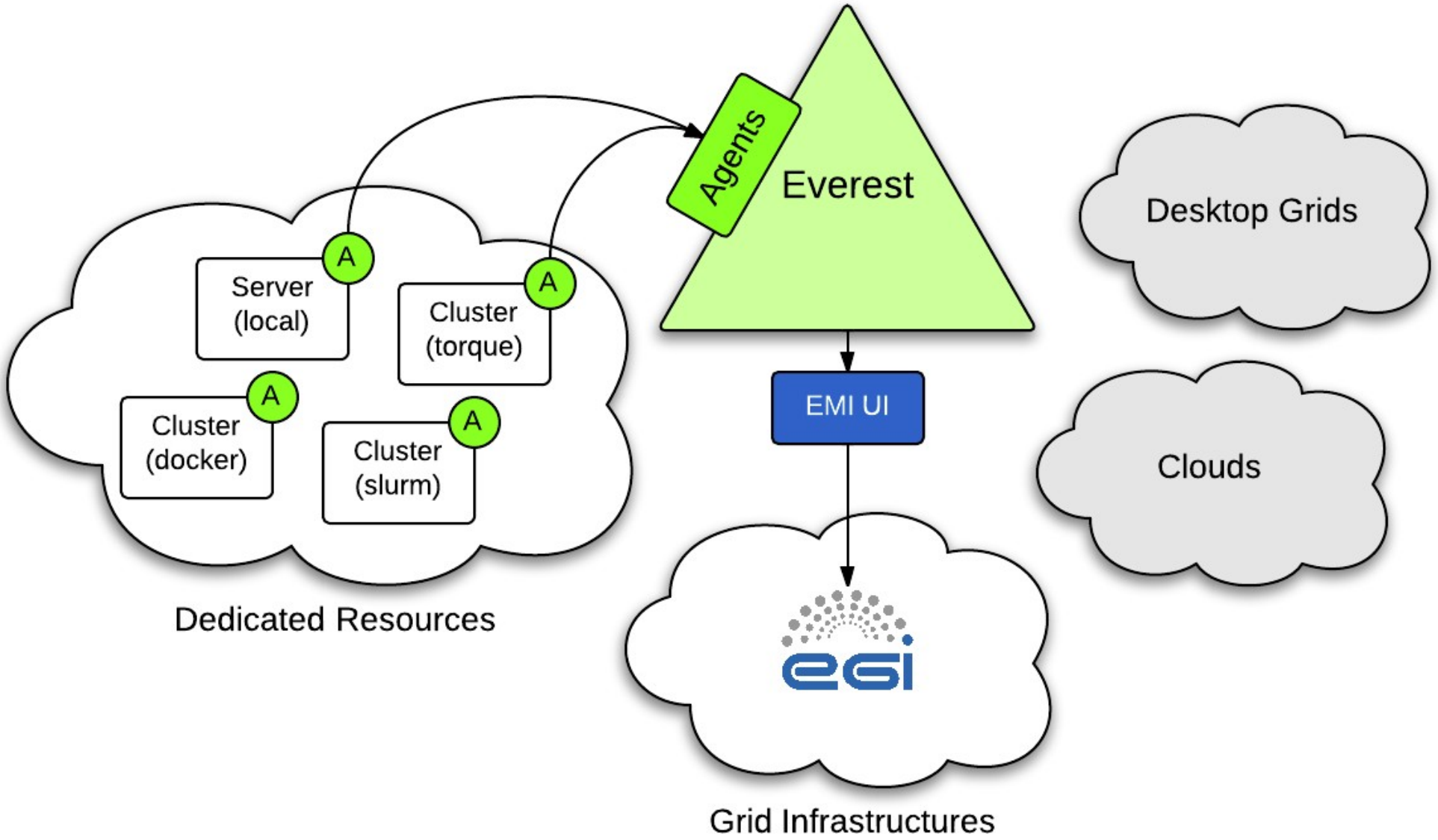
Parameter Sweep Application



Example: Virtual Screening

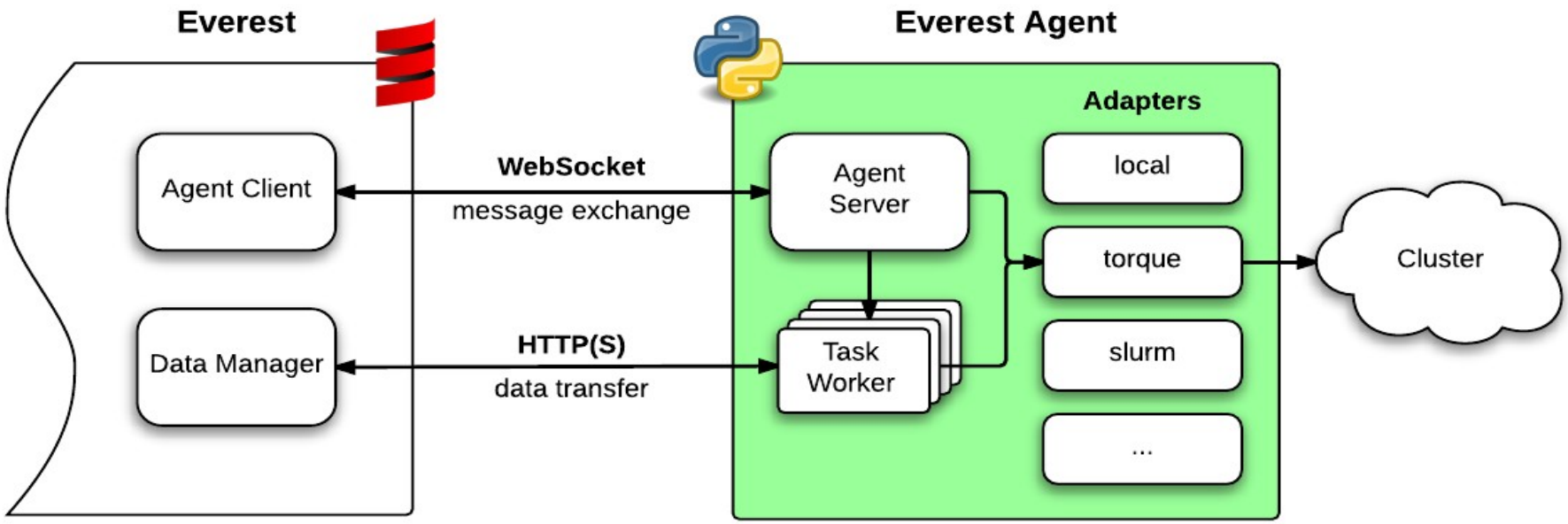
```
parameter n from 1 to 100 step 1

input_files @run.sh vina write_score.py protein.pdbqt
input_files ligand${n}.pdbqt config.txt

command ./run.sh

output_files ligand${n}_out.pdbqt log.txt @score

criterion min $affinity
```

Integration with Computing Resources

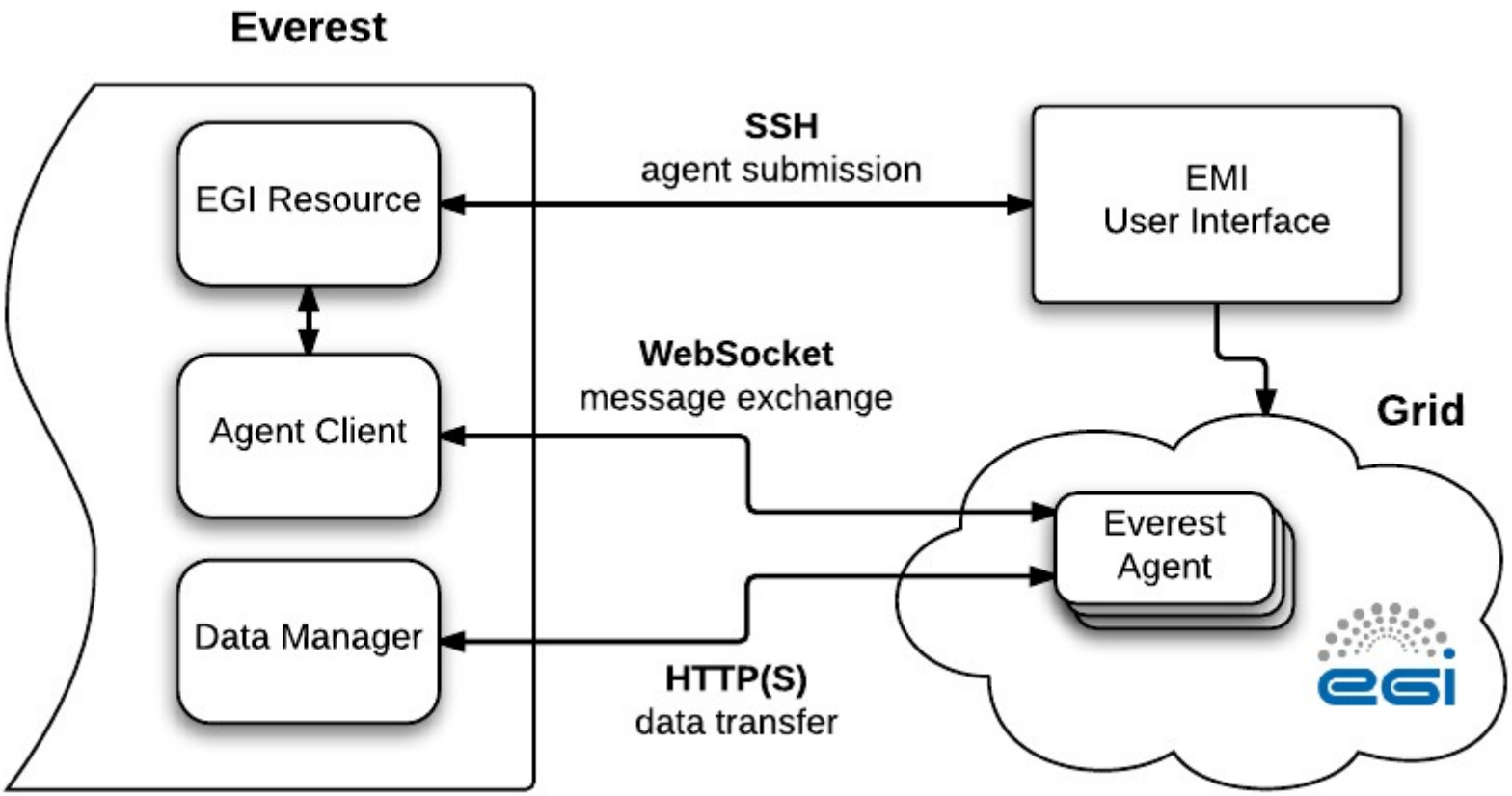


Everest Agent

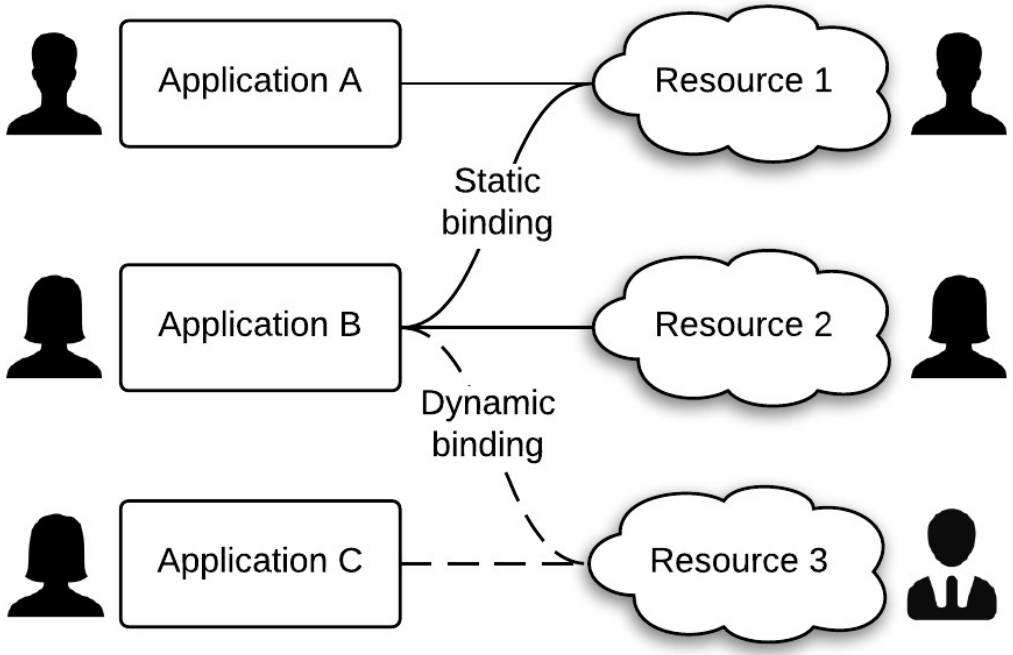
- A mediator between the resource and the platform
- Supporting servers, clusters and resources behind a firewall
- Security mechanisms: white list, execution of tasks in Docker containers
- Open Source: https://gitlab.com/everest/agent/

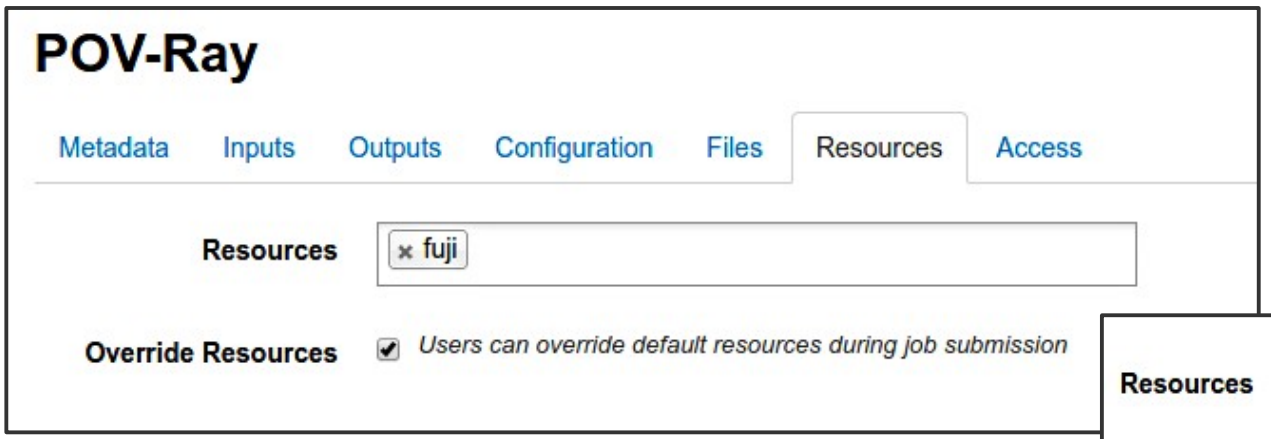


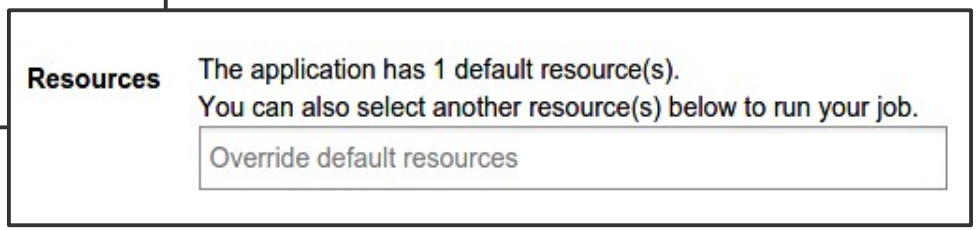
Integration with EGI



Binding Applications to Resources







Resource Binding: Challenges

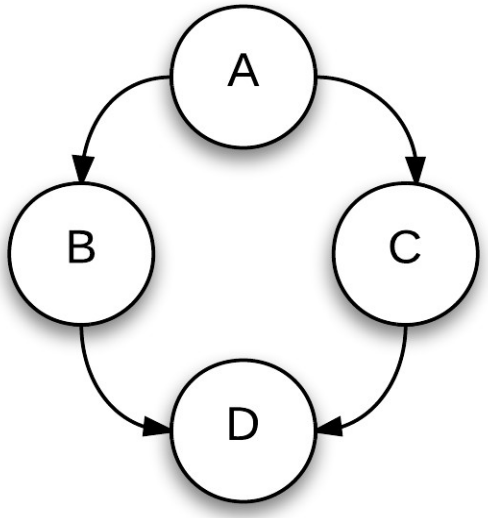
- Dynamic binding
  - Protecting users/resources from malicious/broken code
    - Common practices (trust, code signing, verification, publication)
    - Using virtualization and sandboxing solutions (Docker, Firejail)
  - Making applications portable across resources
    - Run an application in a preconfigured Docker container
    - Build a portable application package (CDE, CARE)
- Binding with multiple resources
  - Sheduling of application tasks across heterogeneous distributed computing resources

Programming Access to Applications

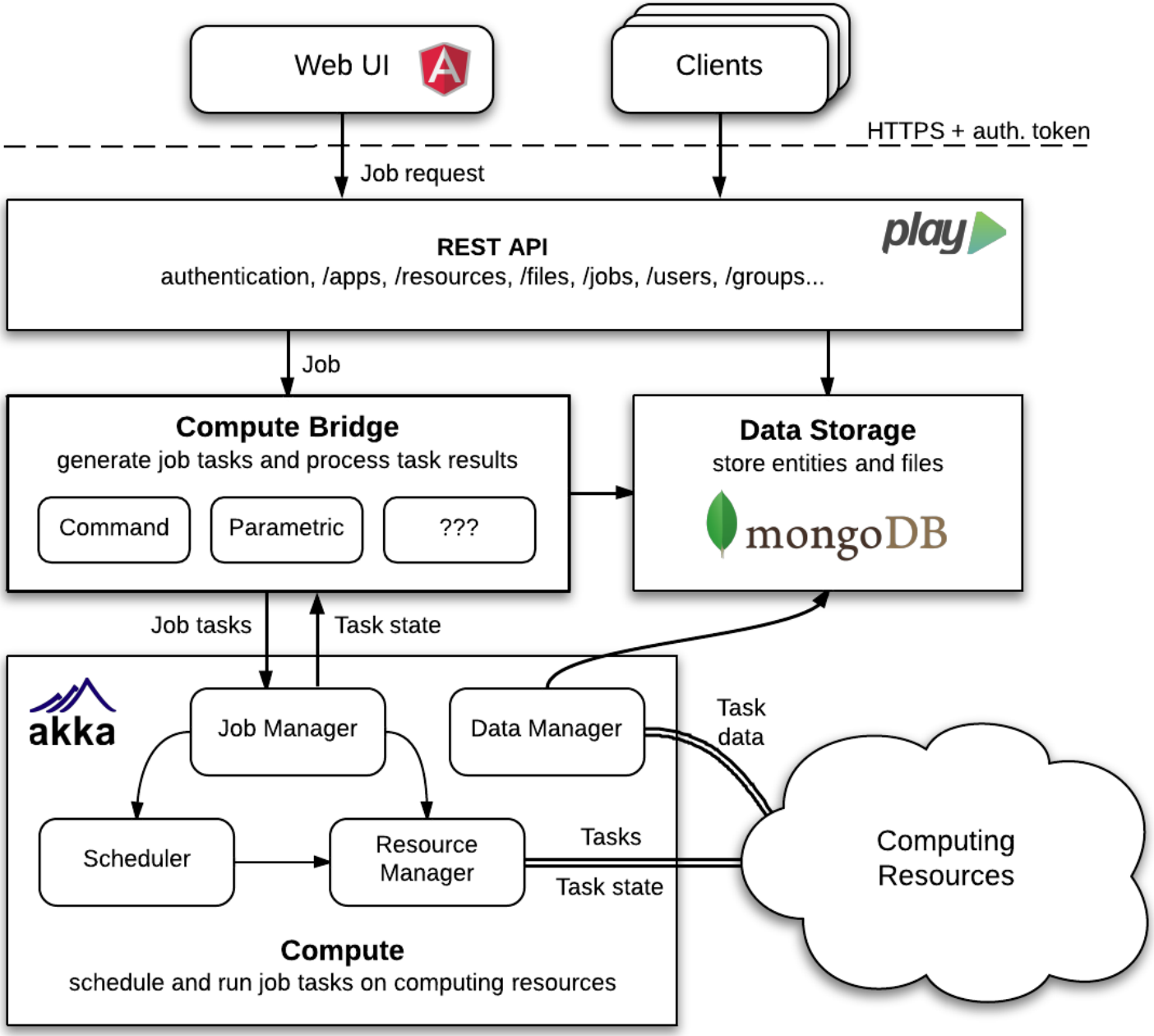
- Why?
  - Automation
    - Repetitve application runs
    - Use of multiple applications (pipelines, workflows)
  - Integration with external systems and third-party tools
- How?
  - Accessing application via web service interface (REST API)
    - HTTP + JSON, any modern programming language
  - Using client library (Python API)
    - Implemented on top of REST API

Python API

```
import everest

session = everest.Session(
  'https://everest.distcomp.org', token = '...'
)

appA = everest.App('52b1d2d13b...', session)
appB = everest.App('...', session)
appC = everest.App('...', session)
appD = everest.App('...', session)

jobA = appA.run({'a': '...'})
jobB = appB.run({'b': jobA.output('out1')})
jobC = appC.run({'c': jobA.output('out2')})
jobD = appD.run({'d1': jobB.output('out'), 'd2': jobC.output('out')})

print(jobD.result())

session.close()
```



Everest Architecture



Experimental Evaluation

- Setup
  - Single server: 2 quad-core Xeon E5620 (2.4 GHz), 24GB RAM, Ubuntu 12.04
  - Applications: Sleep, Autodock Vina, Parameter Sweep
- Raw job submission tests
  - Capable of serving 1000 concurrent clients with acceptable latencies
  - Input file uploads negatively impact throughput and latency
- End-to-end tests (complete job life cycle)
  - Job processing overhead introduced by Everest+agent is 10s of seconds
  - Could be improved to better accommodate short jobs
- Scalability tests
  - 100 agents with 10 slots running in different locations
  - Maximum observed overhead for 1000 jobs is 23 seconds
- Real application runs
  - Ad-hoc grid: 3 servers + 3 clusters (316 cores)
  - Autodock Vina, Parameter Sweep application from geophysics domain

Future Work

- Supporting more complex many-task applications
- Implementing interaction with a running application
- Integration with other types of computing resources
- Optimization of data transfer
- Efficient scheduling of applications across multiple resources
- Improving performance and scalability

Conclusion

- A web-based platform supporting scientific computing
  - Enables users with minimal skills to publish and share scientific applications as services
  - Executes applications on external resources attached by users
  - Implements decoupling of published applications from resources
  - Supports programmatic access to the platform's functionality

- More information: http://everest.distcomp.org/