7th International Conference
"Distributed Computing and Grid-technologies in Science and Education" (GRID'2016)

Automation of Distributed Scientific Computations with Everest

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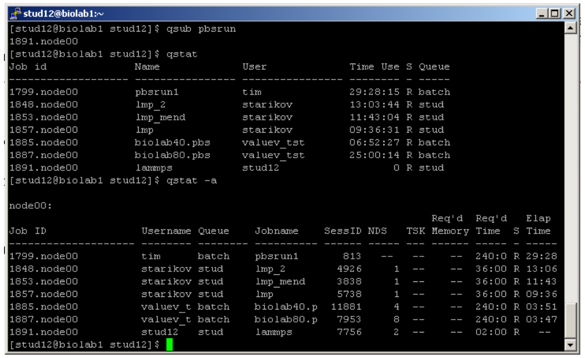
Motivation

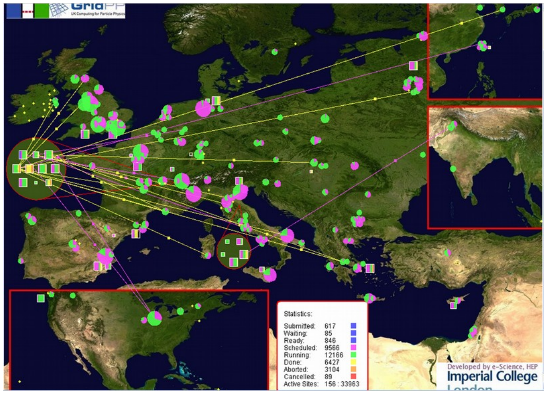
- Modern science and engineering require the use of advanced computational tools and high-performance resources for simulation, data analysis, etc.
- The specialized information technologies are crucial for supporting research and automation of routine activities in such complex environments
- However, small and medium laboratories lack the human and financial resources needed to acquire and operate such technologies

Common Problems and Solutions

- Running computations on HPC resources
- Integration of multiple computing resources
- Sharing of computing applications
- Combined use of multiple applications
- Running large parameter sweep experiments

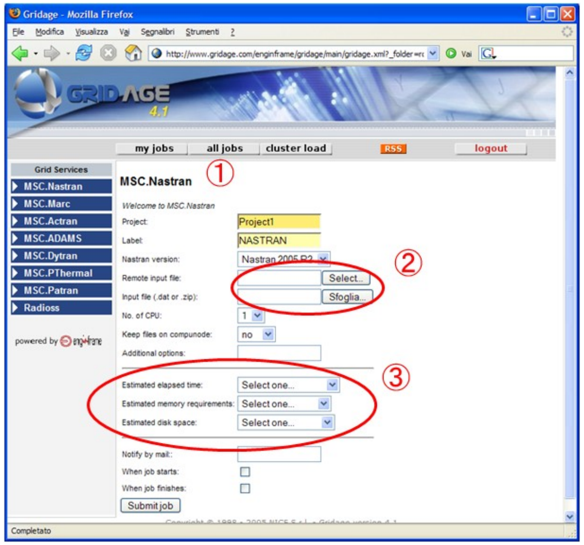


```
[stud12@biolab1 stud12]$ qsub pbsrun
1891.node00
[stud12@biolab1 stud12]$ qstat
Job id               Name             User             Time Use S Queue
-------------------- ---------------- ---------------- -------- - -----
1799.node00          pbsrun1          tim              29:28:15 R batch
1848.node00          lmp_2            starikov         13:03:44 R stud
1853.node00          lmp_mend         starikov         11:43:04 R stud
1857.node00          lmp              starikov         09:36:31 R stud
1885.node00          biolab40.pbs     valuev_tst       06:52:27 R batch
1887.node00          biolab80.pbs     valuev_tst       25:00:14 R batch
1891.node00          lammps           stud12                  0 R stud
[stud12@biolab1 stud12]$ qstat -a

node00:
                                                            Req'd  Req'd   Elap
Job ID               Username Queue    Jobname    SessID NDS   TSK Memory Time  S Time
-------------------- -------- -------- ---------- ------ ----- --- ------ ----- - -----
1799.node00          tim      batch    pbsrun1       813    --  --     -- 240:0 R 29:28
1848.node00          starikov stud     lmp_2        4926     1  --     -- 36:00 R 13:06
1853.node00          starikov stud     lmp_mend     3838     1  --     -- 36:00 R 11:43
1857.node00          starikov stud     lmp          5738     1  --     -- 36:00 R 09:36
1885.node00          valuev_t batch    biolab40.p  11881     4  --     -- 240:0 R 03:51
1887.node00          valuev_t batch    biolab80.p   7953     8  --     -- 240:0 R 03:47
1891.node00          stud12   stud     lammps       7756     2  --     -- 02:00 R   --
[stud12@biolab1 stud12]$
```


GridPP
UK Computing for Particle Physics
Developed by e-Science, HEP
Imperial College London

Statistics:

Submitted:	617	🟦
Waiting:	85	🟦
Ready:	846	🟦
Scheduled:	9566	🟪
Running:	12166	🟩
Done:	6427	🟨
Aborted:	3104	🟧
Cancelled:	89	🟥
Active Sites:	156 : 33963	



MSC.Nastran

Welcome to MSC.Nastran

Project: Project1

Label: NASTRAN

Nastran version: Nastran 2005 R2

Remote input file:

Input file (.dat or .zip):

No. of CPU: 1

Keep files on compunode: no

Additional options:

Estimated elapsed time: Select one...

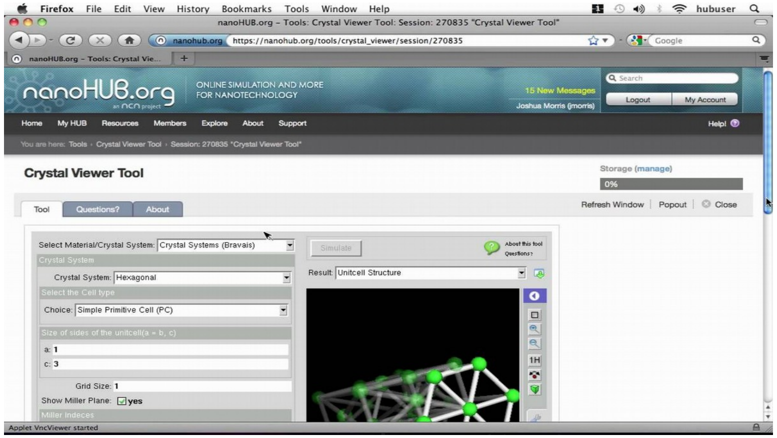
Estimated memory requirements: Select one...

Estimated disk space: Select one...

Notify by mail:

When job starts: □

When job finishes: □



Crystal Viewer Tool

Select Material/Crystal System: Crystal Systems (Bravais)

Crystal System

Crystal System: Hexagonal

Select the Cell type

Choice: Simple Primitive Cell (PC)

Size of sides of the unitcell(a = b, c)

a: 1

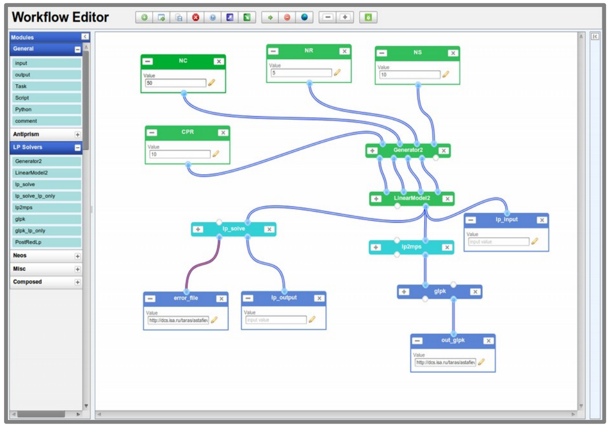
c: 3

Grid Size: 1

Show Miller Plane: ☑ yes

Miller Indeces

Result: Unitcell Structure



Proposed Approach

- Use cloud computing models (SaaS, PaaS) to provide researchers with access to required solutions via remotely accessible services
  - Minimal requirements for technical expertise or local infrastructure
  - Support discovery within small and medium labs
  - Accelerate work by automating routine activities

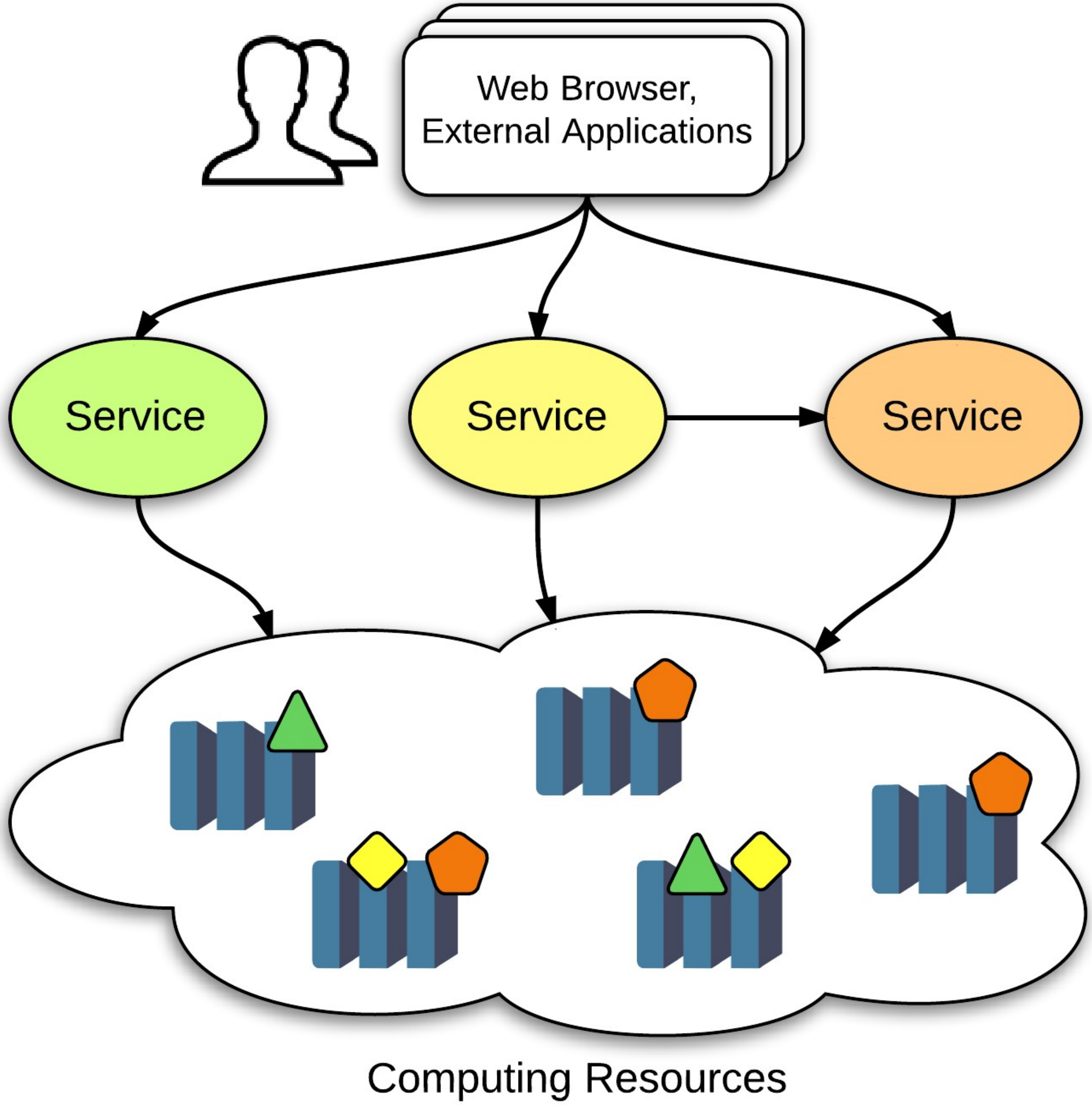
A Similar Vision from Globus Team

We are convinced that the Discovery Cloud represents the future of scientific computing. Once realized, it will allow any researcher, in any laboratory, to access, via intuitive interfaces, a rich set of services that collectively automate and accelerate common research activities.

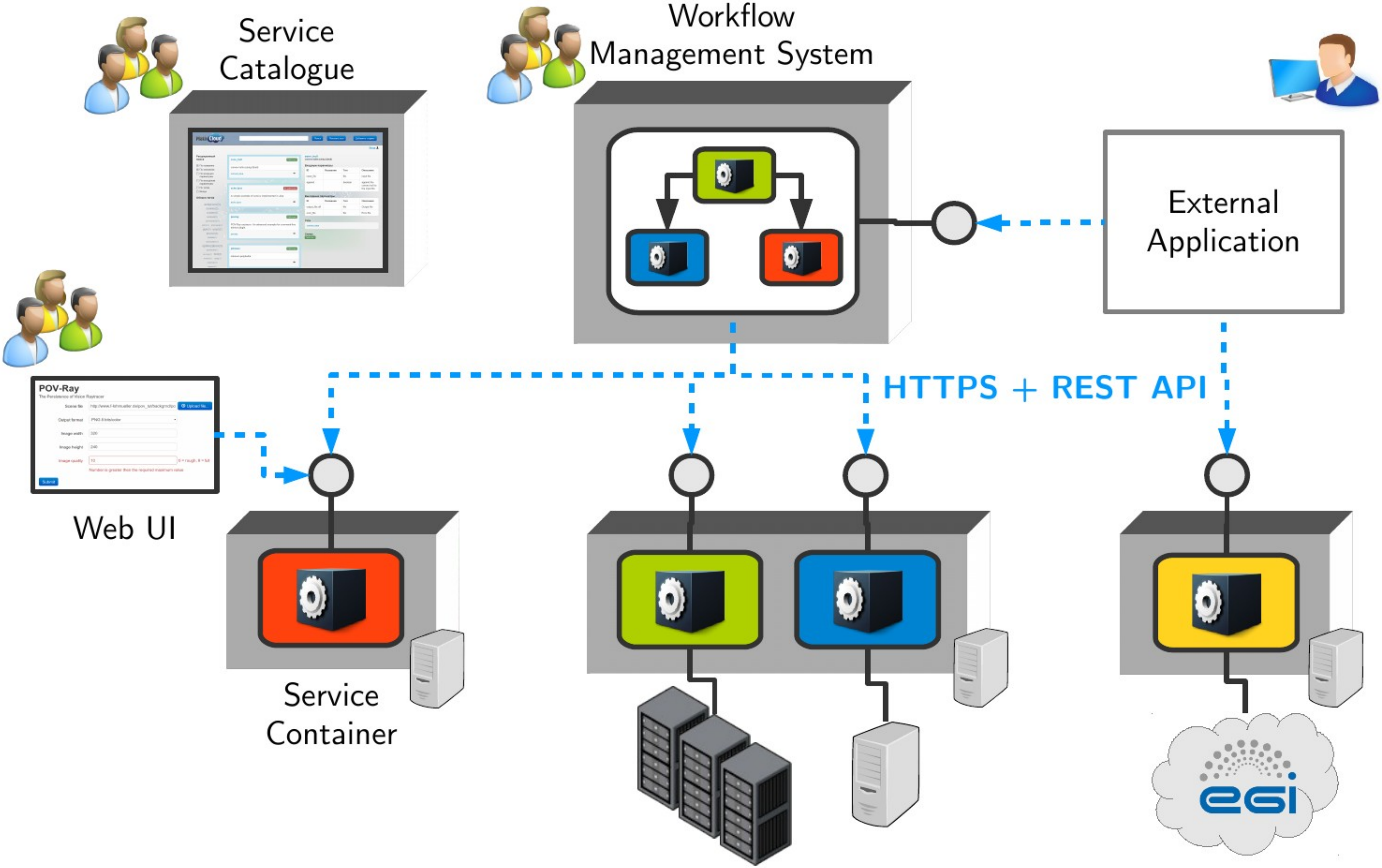
Researchers working within SMLs will be able to discover any computational, software, or data resource relevant to their research; track and organize data consumed and produced by their research; access and run powerful modeling and simulation software; and collaborate with colleagues regardless of location - all without installing software, acquiring storage systems or computational infrastructure, or employing IT staff to operate and maintain hardware and software.

Foster, I., Chard, K., & Tuecke, S. (2016, April). The Discovery Cloud: Accelerating and Democratizing Research on a Global Scale. In 2016 IEEE International Conference on Cloud Engineering (IC2E) (pp. 68-77). IEEE.

Computational Services



MathCloud (2009-2012)



POV-Ray

The Persistence of Vision Raytracer

Scene file: http://www.f-lohmueller.de/pov_tut/backgrnd/po

Output format: PNG 8 bits/color

Image width: 320

Image height: 240

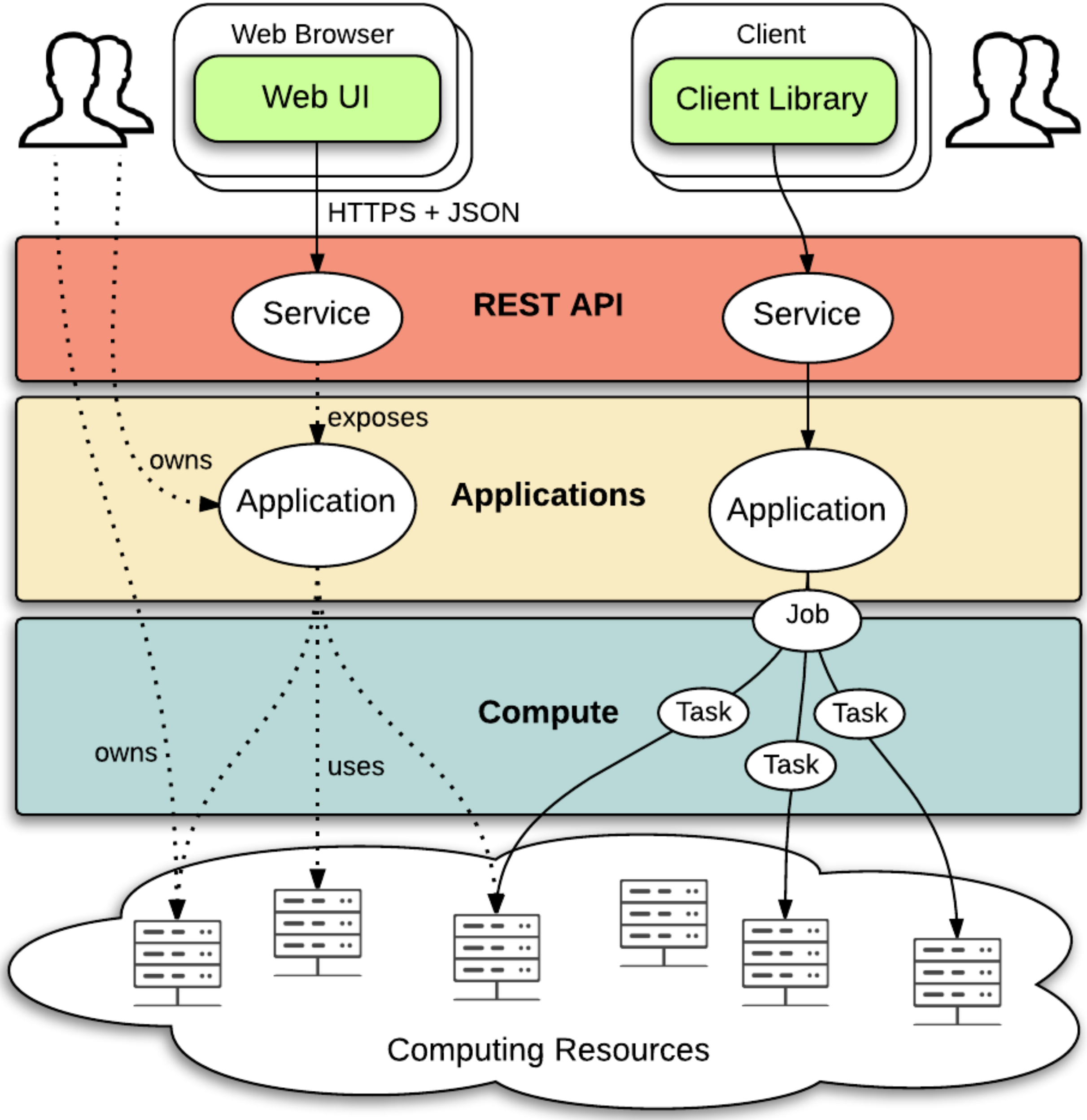
Image quality: 10 — 0 = rough, 9 = full

Number is greater than the required maximum value

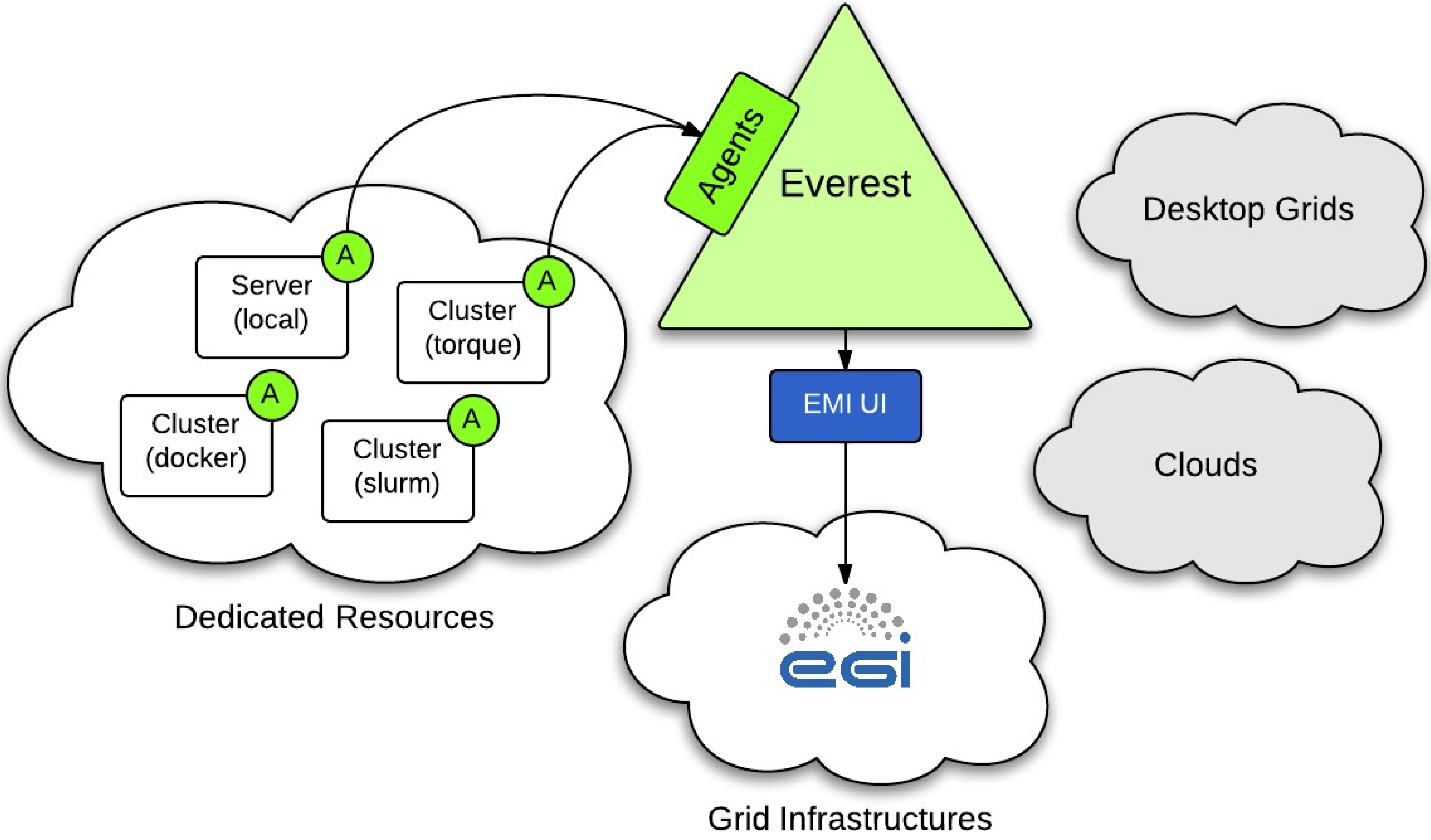
Everest (2013-...)

- Web-based platform supporting
  - Publication of 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
  - Remote access via web browser and REST API
  - Single platform instance can be accessed by many users
  - No installation is required
- Public instance with open registration
  - http://everest.distcomp.org/

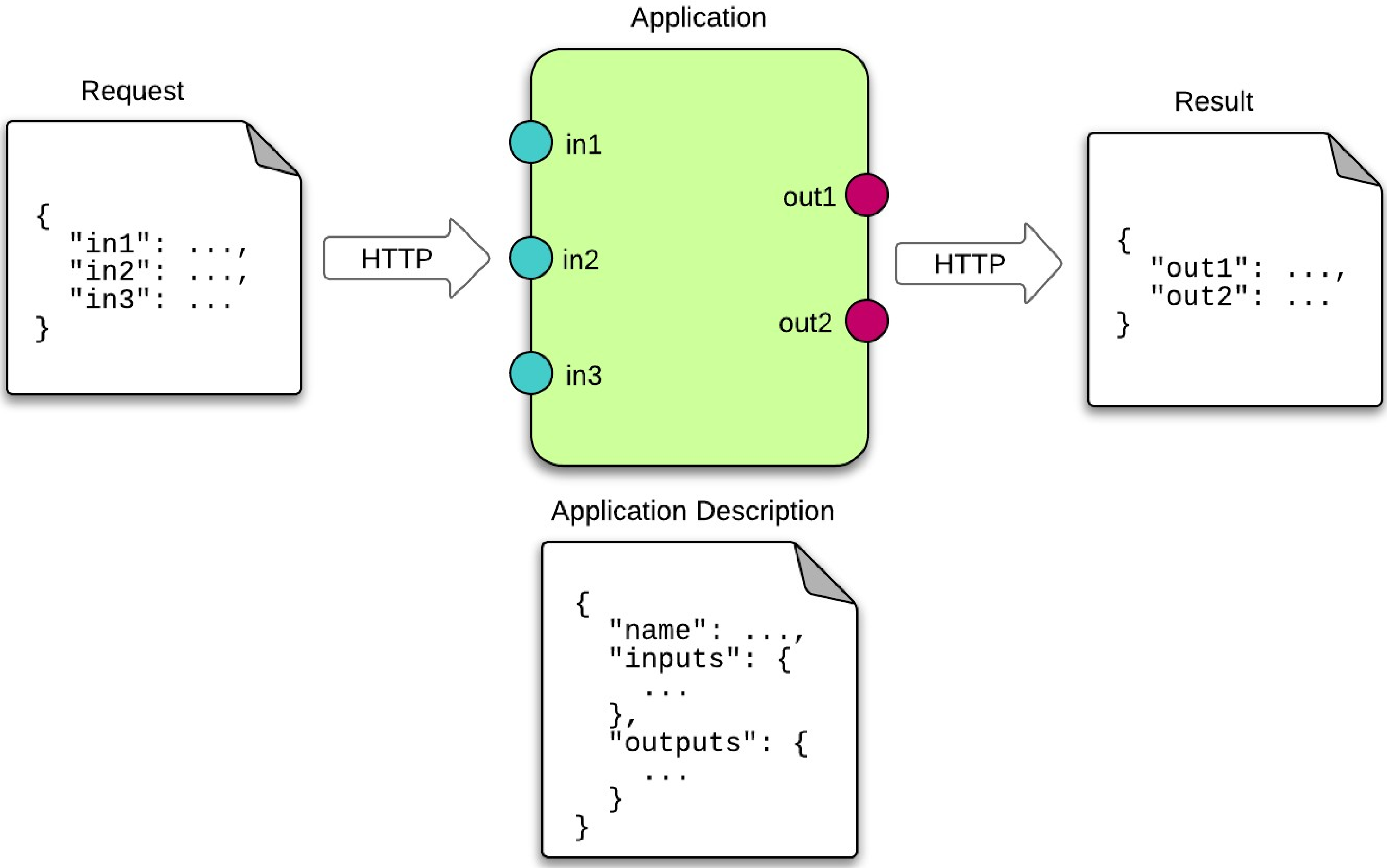
Everest Architecture



Integration with Computing Resources



Application



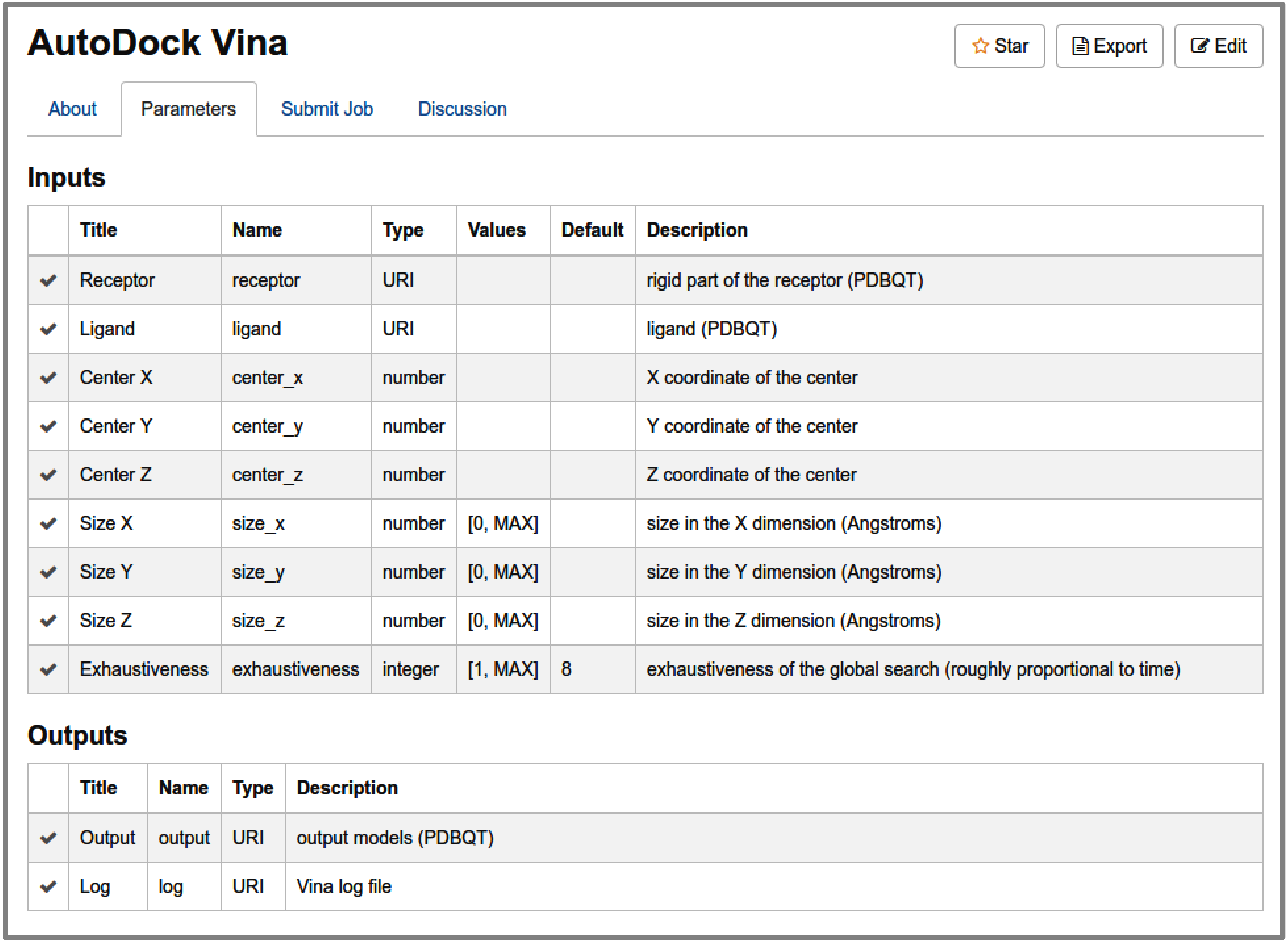
```
{
  "in1": ...,
  "in2": ...,
  "in3": ...
}
```

```
{
  "out1": ...,
  "out2": ...
}
```

```
{
  "name": ...,
  "inputs": {
    ...
  },
  "outputs": {
    ...
  }
}
```

Supported Application Types

- Command
  - Generic template for applications with command-line interface
  - Single compute task
- Parameter Sweep
  - Generic service for running parameter sweep experiments
  - Large number of independent compute tasks
  - Experimental support for coordination between tasks
- Workflow
  - Composition of multiple applications
  - Multiple jobs with dependencies (described using Python API)
  - Can be published as a new application



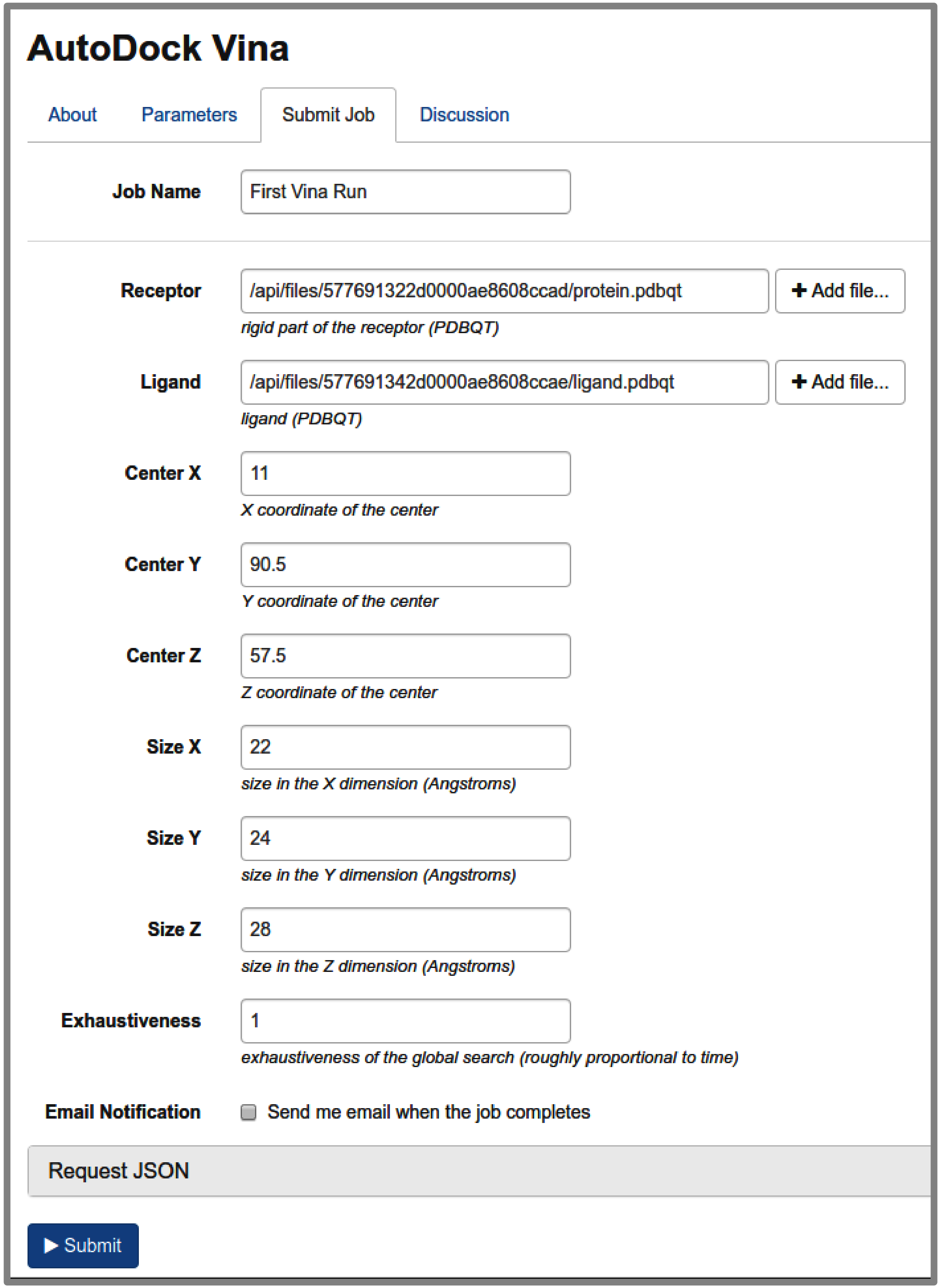
AutoDock Vina

Inputs

	Title	Name	Type	Values	Default	Description
✓	Receptor	receptor	URI			rigid part of the receptor (PDBQT)
✓	Ligand	ligand	URI			ligand (PDBQT)
✓	Center X	center_x	number			X coordinate of the center
✓	Center Y	center_y	number			Y coordinate of the center
✓	Center Z	center_z	number			Z coordinate of the center
✓	Size X	size_x	number	[0, MAX]		size in the X dimension (Angstroms)
✓	Size Y	size_y	number	[0, MAX]		size in the Y dimension (Angstroms)
✓	Size Z	size_z	number	[0, MAX]		size in the Z dimension (Angstroms)
✓	Exhaustiveness	exhaustiveness	integer	[1, MAX]	8	exhaustiveness of the global search (roughly proportional to time)

Outputs

	Title	Name	Type	Description
✓	Output	output	URI	output models (PDBQT)
✓	Log	log	URI	Vina log file



AutoDock Vina

Job Name First Vina Run

Receptor /api/files/577691322d0000ae8608ccad/protein.pdbqt
rigid part of the receptor (PDBQT)

Ligand /api/files/577691342d0000ae8608ccae/ligand.pdbqt
ligand (PDBQT)

Center X 11
X coordinate of the center

Center Y 90.5
Y coordinate of the center

Center Z 57.5
Z coordinate of the center

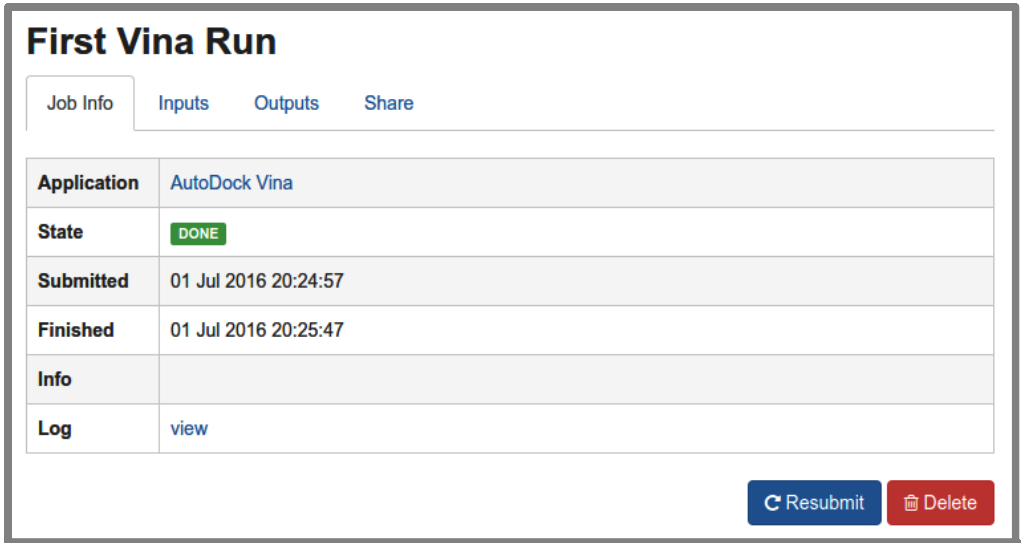
Size X 22
size in the X dimension (Angstroms)

Size Y 24
size in the Y dimension (Angstroms)

Size Z 28
size in the Z dimension (Angstroms)

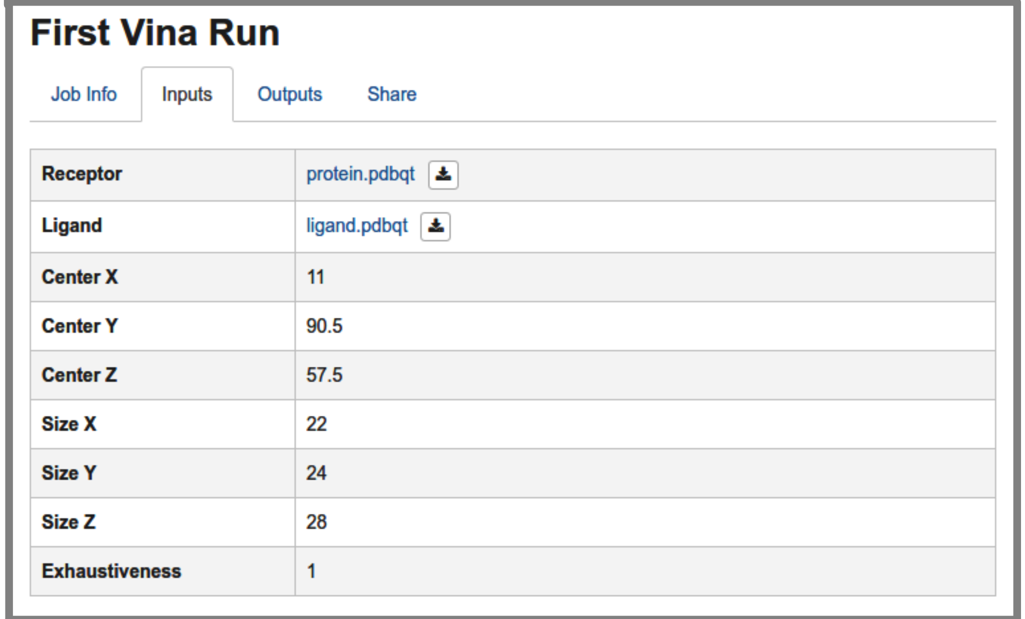
Exhaustiveness 1
exhaustiveness of the global search (roughly proportional to time)

Email Notification □ Send me email when the job completes



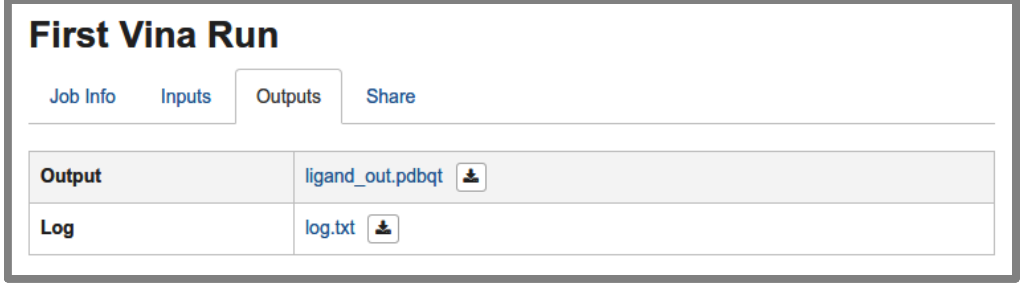
First Vina Run

Application	AutoDock Vina
State	DONE
Submitted	01 Jul 2016 20:24:57
Finished	01 Jul 2016 20:25:47
Info	
Log	view



First Vina Run

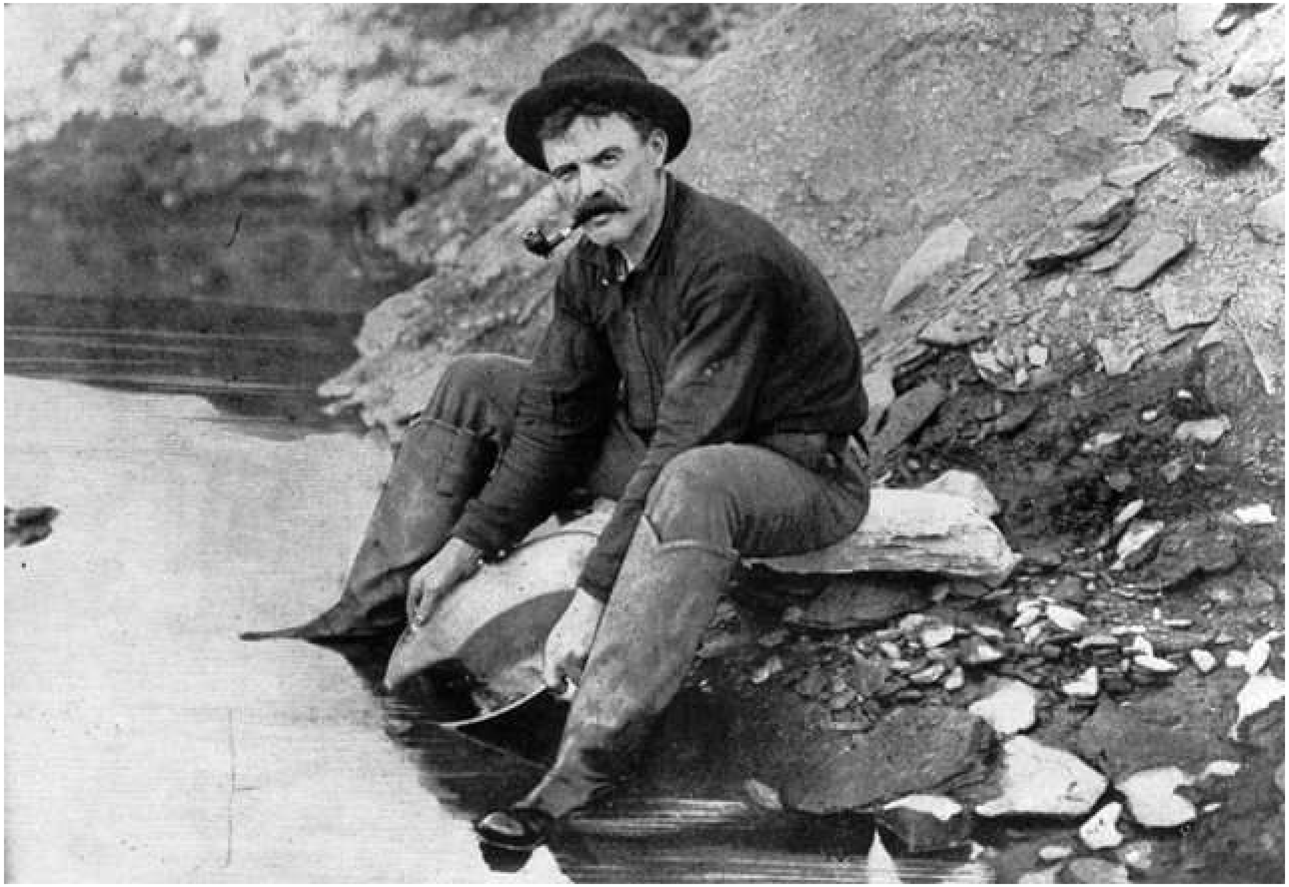
Receptor	protein.pdbqt
Ligand	ligand.pdbqt
Center X	11
Center Y	90.5
Center Z	57.5
Size X	22
Size Y	24
Size Z	28
Exhaustiveness	1



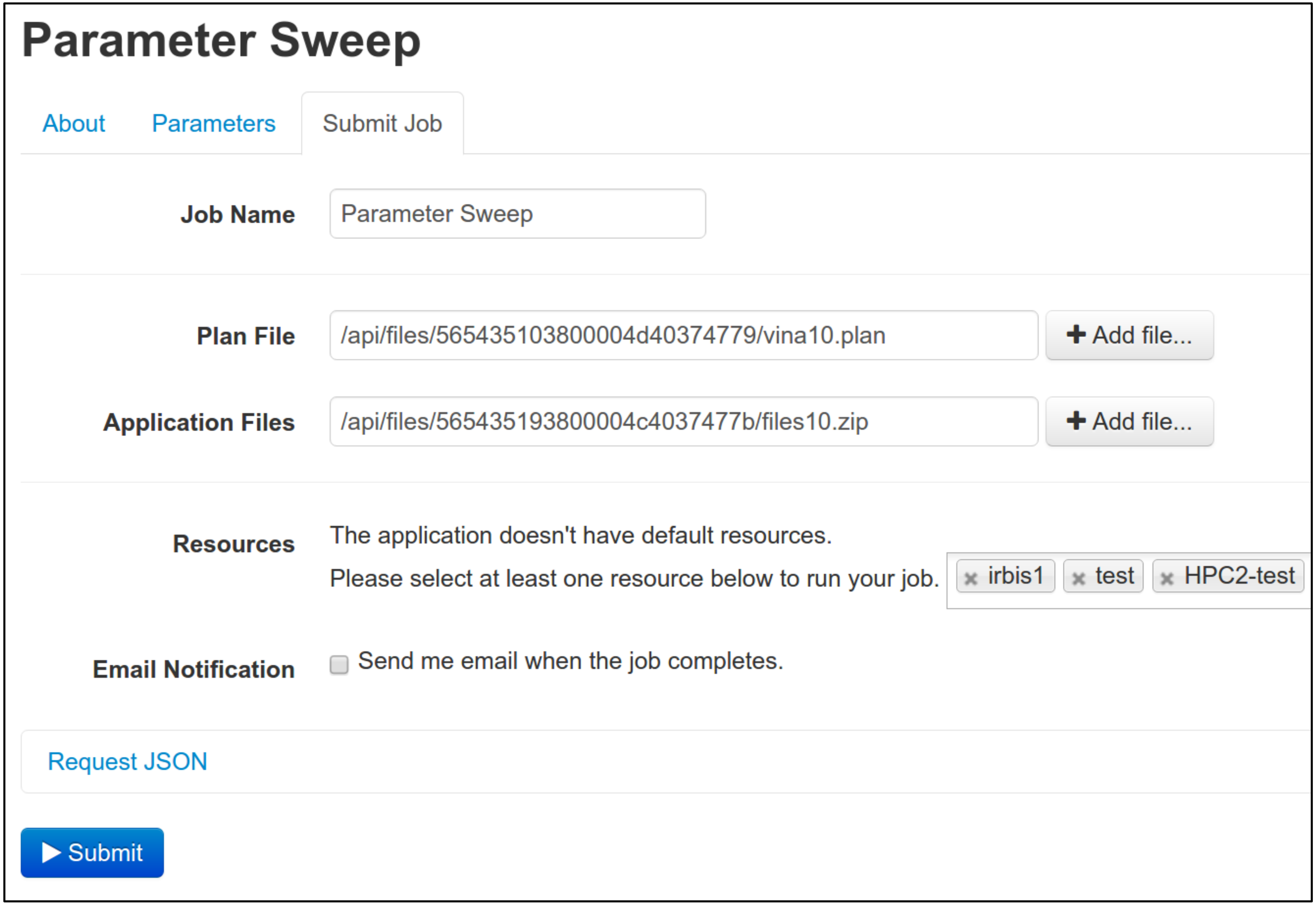
First Vina Run

Output	ligand_out.pdbqt
Log	log.txt

Parameter Sweep Experiments



Parameter Sweep Service



Parameter Sweep

Job Name: Parameter Sweep

Plan File: /api/files/565435103800004d40374779/vina10.plan

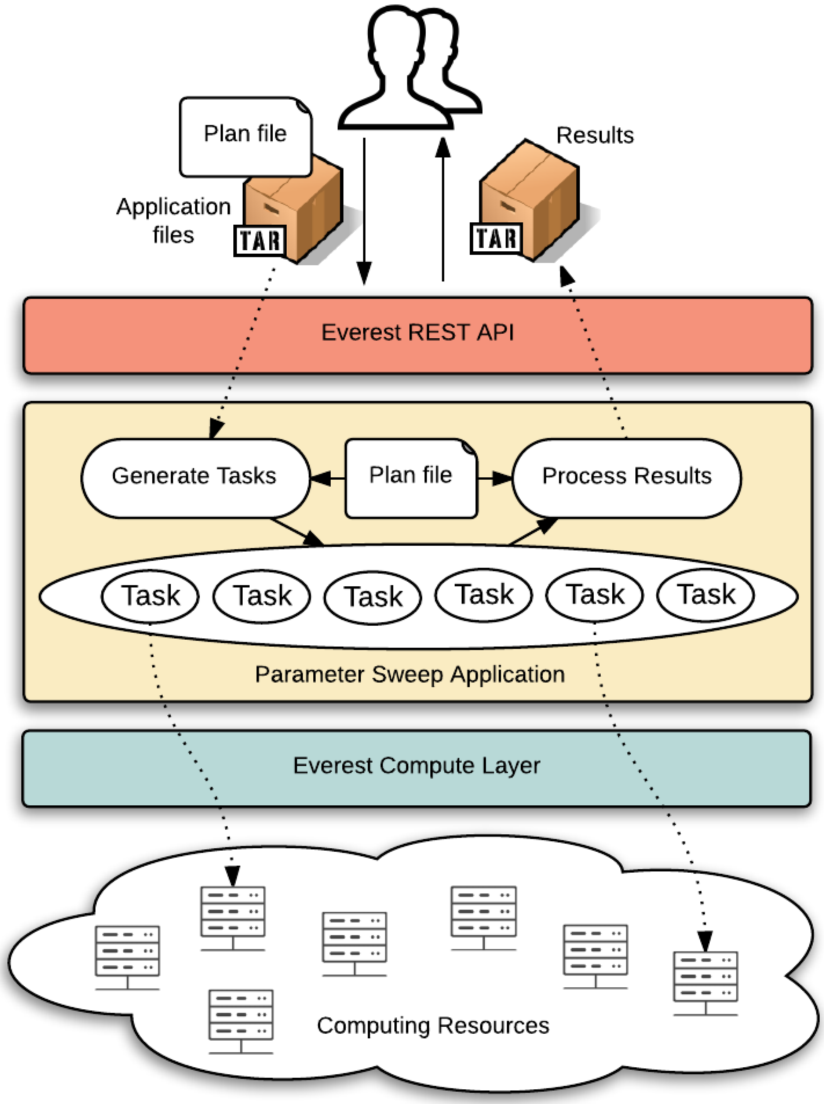
Application Files: /api/files/565435193800004c4037477b/files10.zip

Resources: The application doesn't have default resources.
Please select at least one resource below to run your job. × irbis1 × test × HPC2-test

Email Notification: □ Send me email when the job completes.

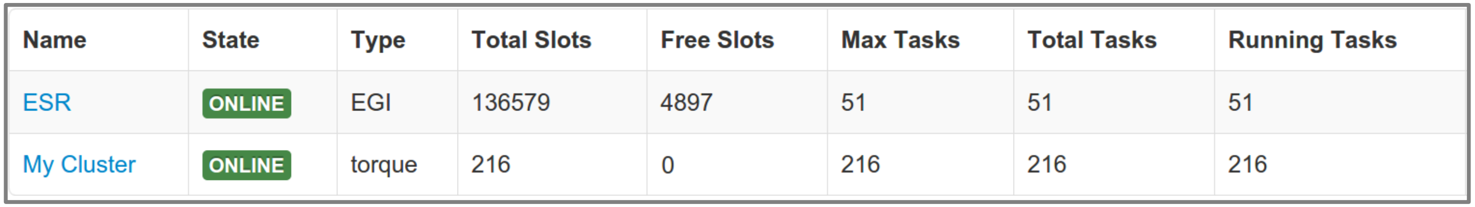
Parameter Sweep Service

```
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
```

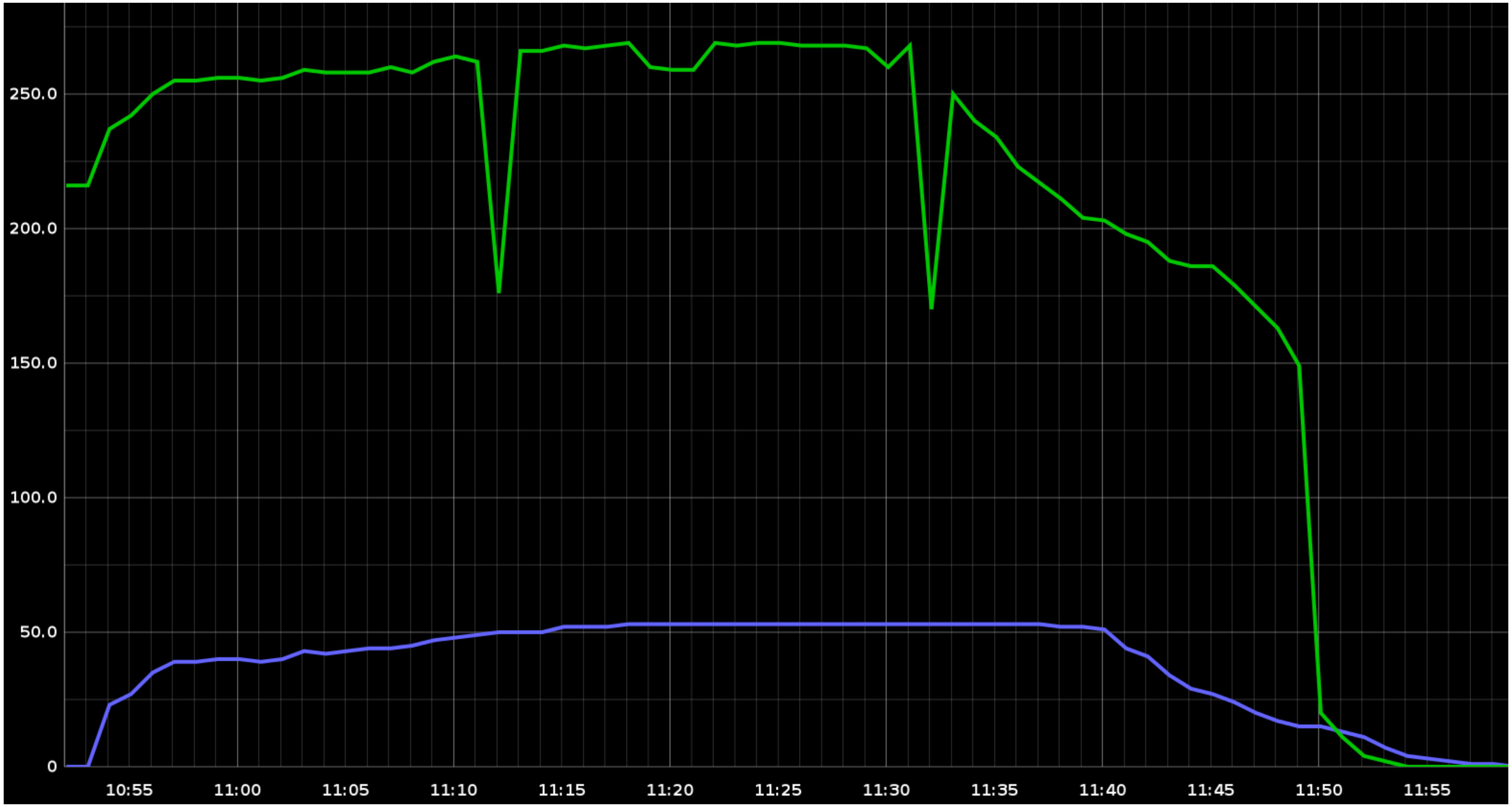


Using Multiple Computing Resources

- Geophysical parameter sweep experiment running on HPC cluster and EGI VO

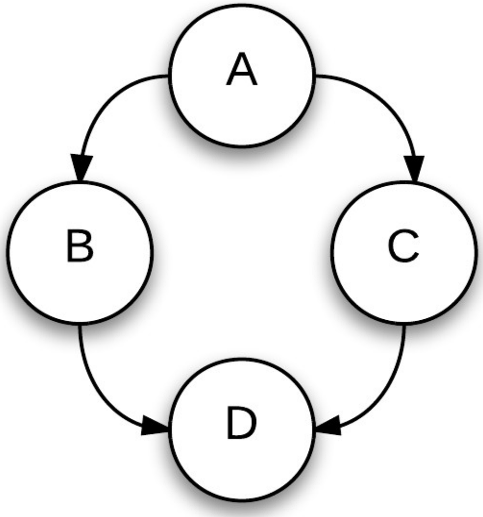


Name	State	Type	Total Slots	Free Slots	Max Tasks	Total Tasks	Running Tasks
ESR	ONLINE	EGI	136579	4897	51	51	51
My Cluster	ONLINE	torque	216	0	216	216	216

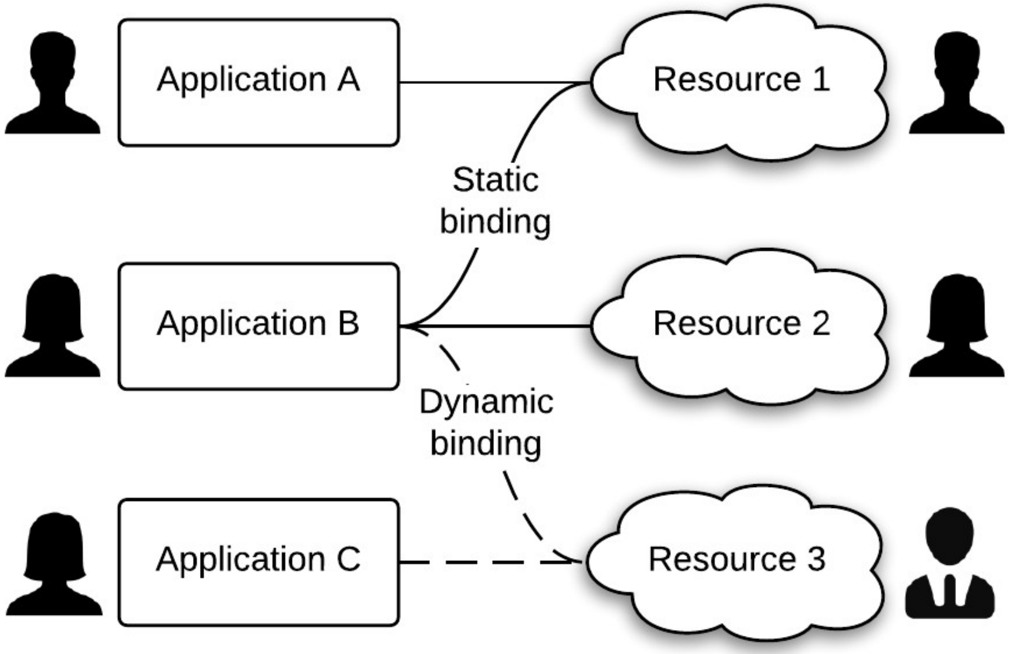


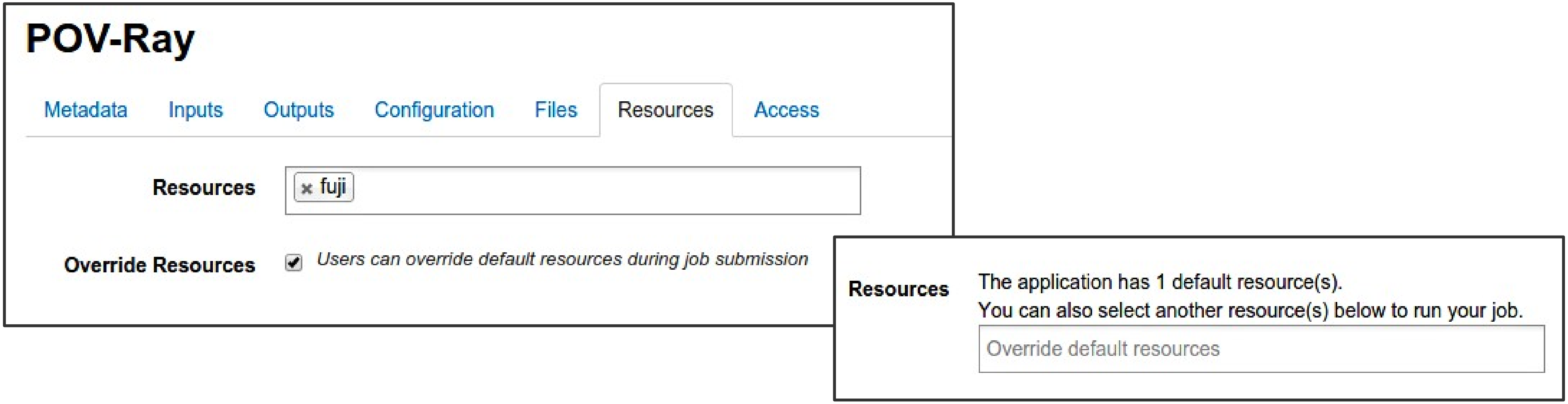
Application Composition (Workflows)

```
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()
```



Binding Applications to Resources





POV-Ray

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

Resources × fuji

Override Resources ☑ *Users can override default resources during job submission*

Resources The application has 1 default resource(s).
You can also select another resource(s) below to run your job.

Override default resources

Current Status

- Project results are presented on several conferences
  - PaCT'2013, CLOSER'2014, GRID'2014, ISPDC'2015, RussianSCDays'2015
- Project website and public platform instance
  - http://everest.distcomp.org/
  - 274 users, 79 applications, 46 resources
- Used in several research projects and educational activities
  - Distributed optimization, computer simulation, parameter study, plasma physics, geophysics, bioinformatics
  - Teaching parallel and distributed computing

Future Directions

- Suport for Big Data applications
- Integration with clouds
- Advanced scheduling across distributed resources
- Enabling portable applications
- Sustainability models

Conclusion

- Automation of computational activities increases research productivity but requires a sophisticated infrastructure
- Cloud-based services and platforms providing researchers with access to required infrastructure will accelerate innovation in small and medium labs
- Everest is an example of such platform supporting publication, execution and composition of computing applications in a distributed environment

http://everest.distcomp.org/