

Running Parameter Sweep Applications on Everest Cloud Platform

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Parameter Sweep Applications

Distinct features of Parameter Sweep applications

- They involve some input set of computational parameters
- They run multiple computations (tasks) for various combinations of the input parameters' values (usually the cartesian product)
- The result of the Parameter Sweep computation is the set of all of the tasks' computations

Parameter Sweep Web Service

Everest^β

Applications

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Parameter Sweep

About

Parameters

Submit Job

Plan File

+ Add file...

Application Files

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Resources

The application doesn't have default resources.

Please select at least one resource below to run your job.


fuji

Request JSON

▶ Submit

Parameter Sweep Web Service

Everest^β

 Applications

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 About

Job 53ab9a9132000075004b11d3

[Job Info](#)

[Inputs](#)

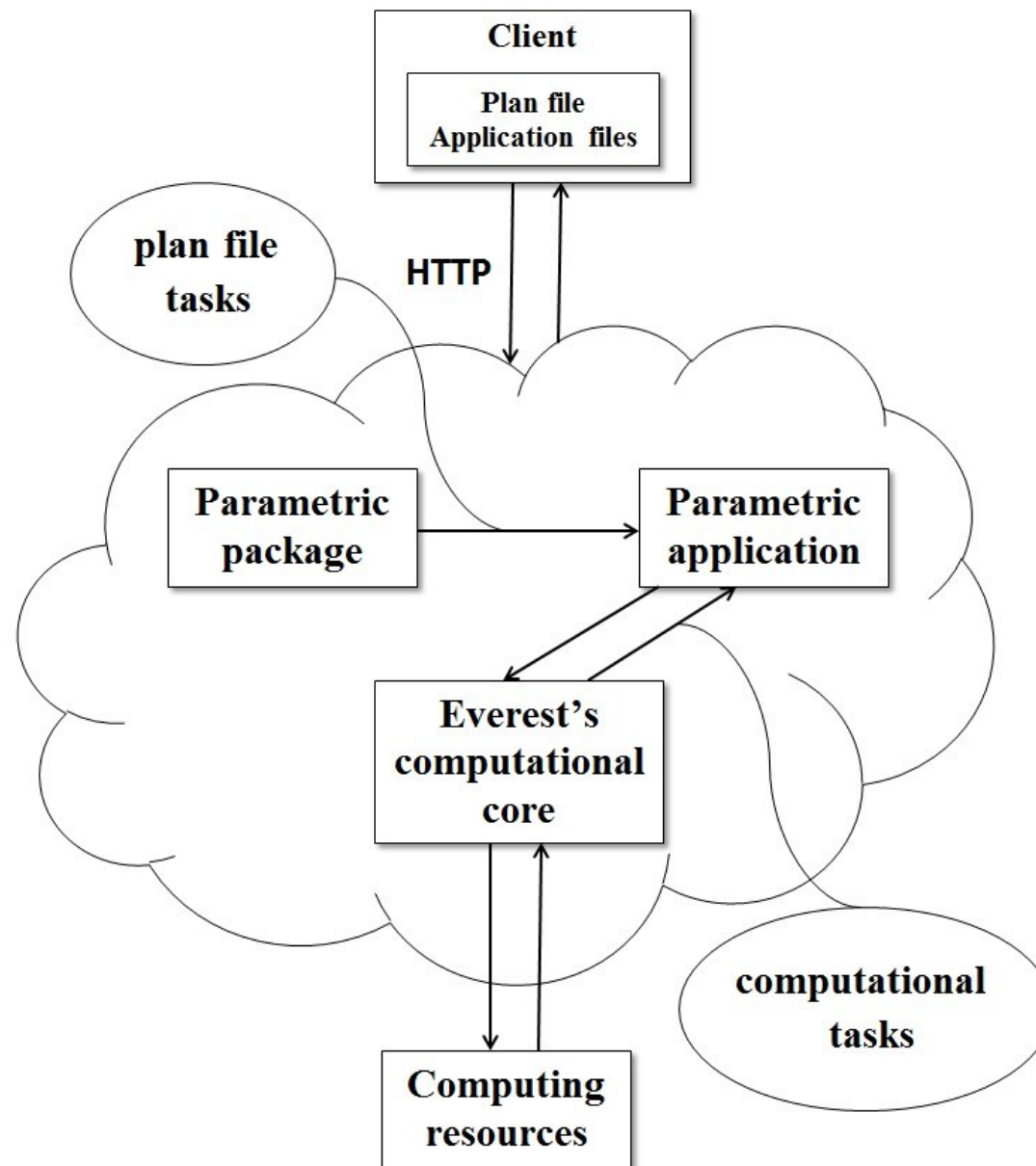
[Outputs](#)

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Results

[results.zip](#)

Parameter Sweep Web Service



Plan File

Plan file is a text description of the parameter sweep computation.

Plan file includes the following directives

- Parameter
- Constraint
- Input files
- Substitute files
- Command
- Output files
- Filter
- Criterion

Plan File (1)

parameter p1 from 1 to 11 step 2

parameter p2 0.1 4.56 3.0 5.667

parameter p3 file1 "my file 2" anotherFile

parameter p4 "some text" text anotherText

constraint value $\$p1^2 - \sin(\$p2) \leq$
 $\text{sqrt}(\$p1)$, $\$p1 + 5*\$p2 > 10$, $\$p1\%3 = 1$

constraint index $\$p3 = \$p4$

Plan File (2)

```
input_files $p3 file2 MyScript
```

```
substitute_files MyScript
```

```
command /bin/sh MyScript
```

```
output_files output1 output2
```


Plan File (3)

```
filter  $\{\text{output1:x1}\}^2 \leq$   
     $\text{sqrt}(\{\text{output2:x2}\}), \{\text{output1:x2}\} +$   
     $5 * \{\text{output2:x2}\} > 10$ 
```

```
criterion max  $\{\text{output1:x1}\}^2 +$   
     $\text{cos}(\{\text{output1:x2}\}) +$   
     $5 * \{\text{output2:x2}\}$ 
```

Example

parameter n from 1 to 10 step 1

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

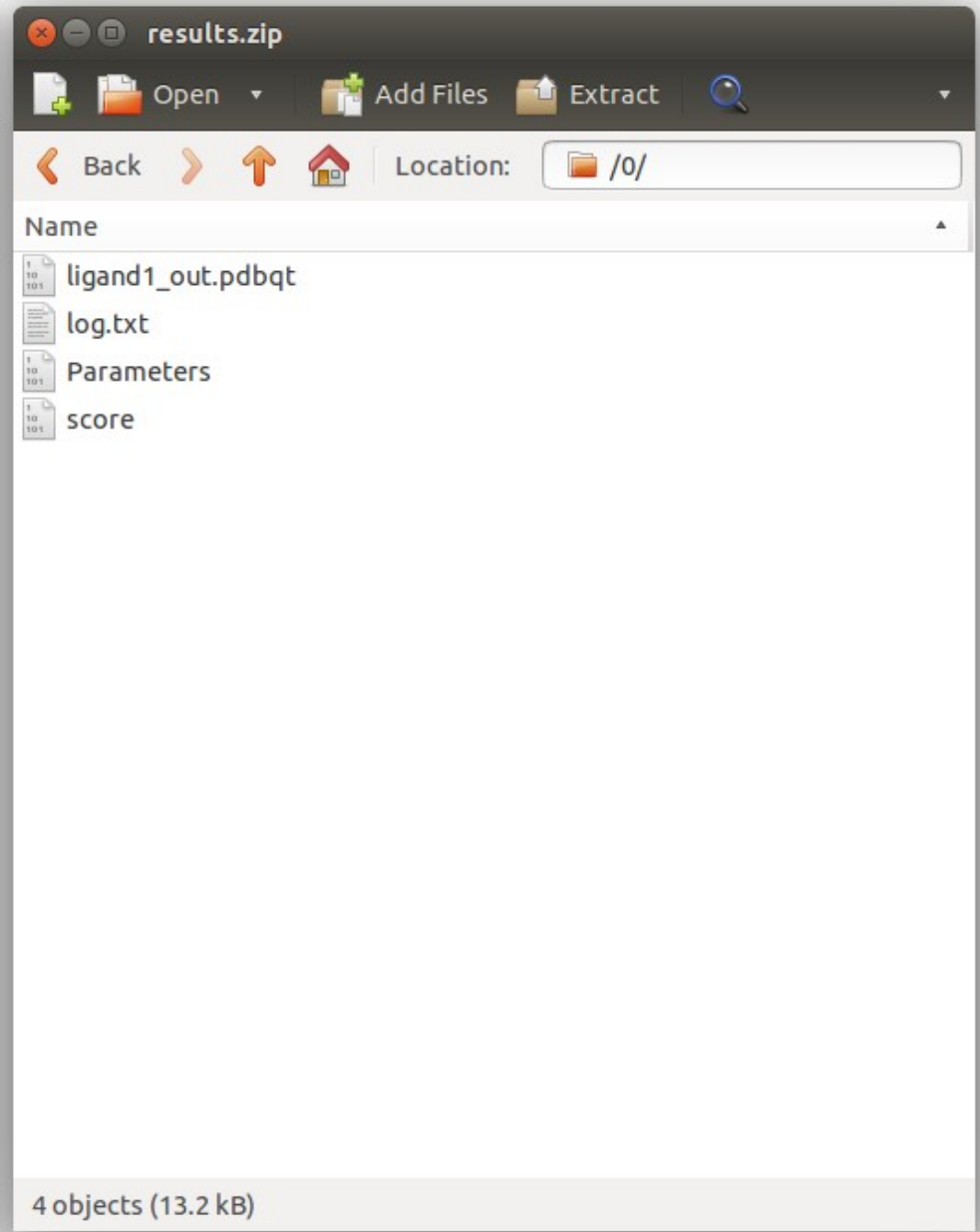
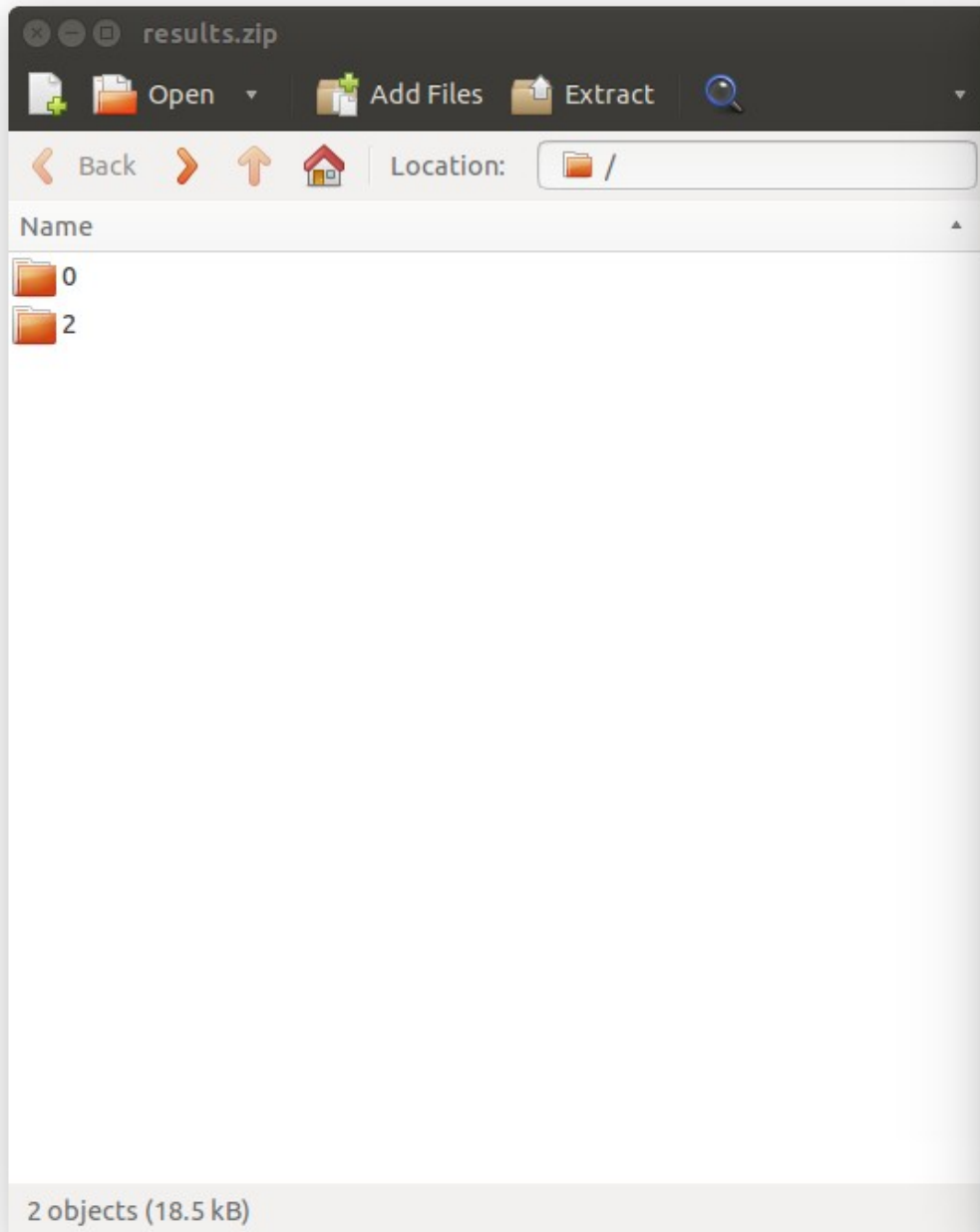
substitute_files run.sh

command ./run.sh

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

criterion min \${score:affinity}

Example



Future Work

- Convenient web interface for the plan file creation
- Advanced scheduling of multi-task jobs in Everest
- Evaluation and application case studies

Thank you for your attention!