

Distribution of protein simulations on machines

Sridhar, Dept of Biochemistry

Example commandline of one simulation job

```
nohup /work/sridhar/rosetta/rosetta_source/bin/match.linuxiccrelease @/gpfs/DS3524-1/WORK/sridhar/scripts/  
myscripts/test_jobdistribution/general_match.flags -match:geometric_constraint_file /gpfs/DS3524-1/WORK/  
sridhar/scripts/myscripts/test_jobdistribution/Orgpho_S_H_DE_oxya_FP1_match.cst -s /lab/shared/scaffolds/pb/  
1pbp/1pbp_nohet_1_relax.pdb -match:scaffold_active_site_residues /lab/shared/scaffolds/pb/1pbp/  
1pbp_nohet_1.pdb_0.pos > log &
```

pb/1pbp/1pbp_nohet_1.pdb_0.pos

Input file:

1pbp

2gbp

1abe

2uvh

....

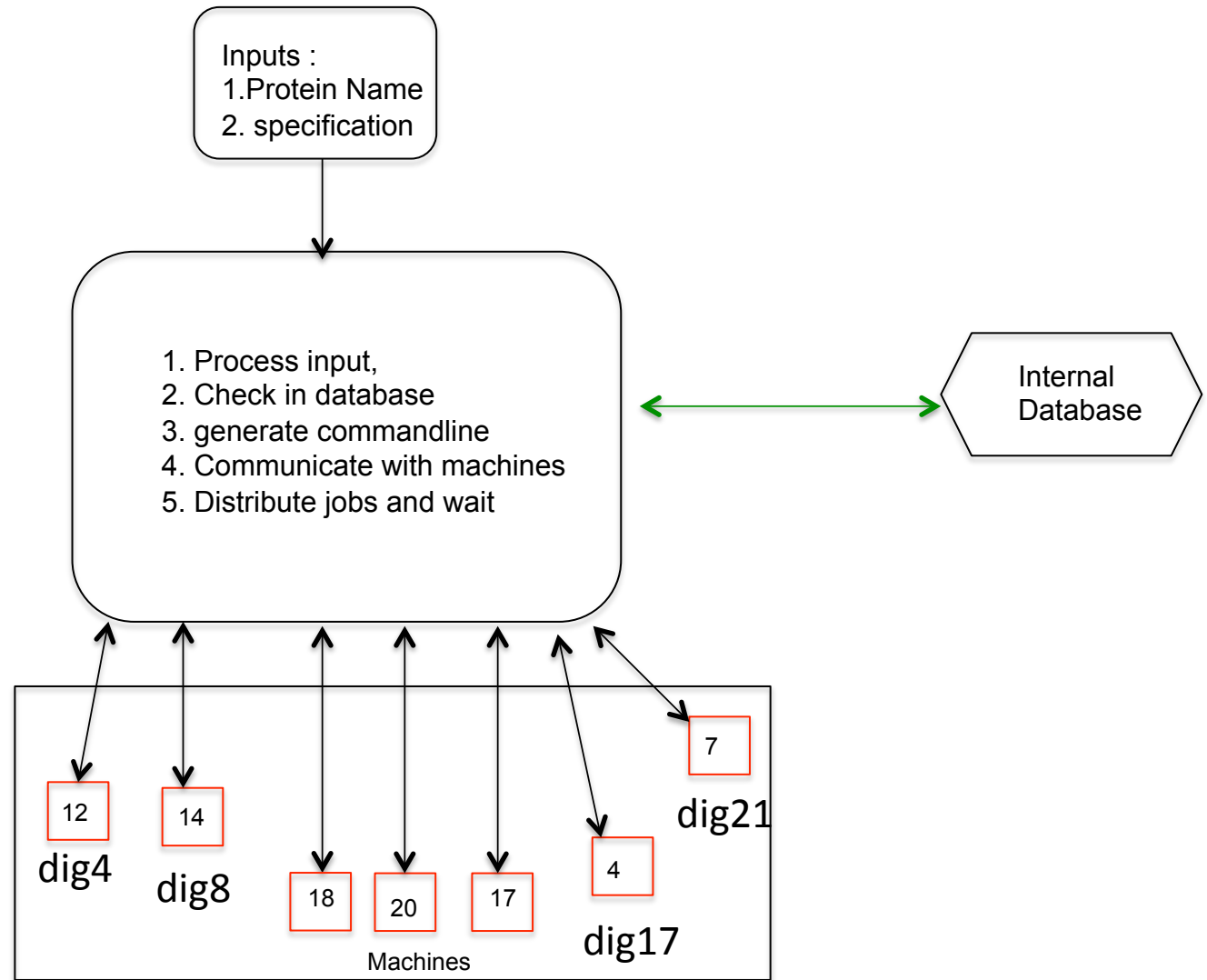
....

....

Submitting 10 jobs manually would be easier

But submitting 1000 jobs is painful to do manually.

A python script to automate distribution of jobs and have check on them would be ideal



```
[sridhar@dig3 test_jobdistribution]$ ./Job_Distribution.py -file pdblast -cstfile Orgpho_S_H_DE_oxya_FP1_match.cst --nodes 20
Total jobs is more than available nodes, jobs will submitted as nodes become free
Submitting jobs -- Iteration 0
submitting 16vp to dig4
submitting 1a8s to dig4
1a8v does not exists in /lab/shared/scaffolds/
submitting 1aa6 to dig4
1af7 does not exists in /lab/shared/scaffolds/
submitting 1aj6 to dig4
submitting 1ajk to dig4
1ajo does not exists in /lab/shared/scaffolds/
submitting 1ake to dig4
submitting 1aky to dig4
submitting 1al3 to dig4
submitting 1alq to dig4
submitting 1am7 to dig4
submitting 1amu to dig4
submitting 1anx to dig4
submitting 1aop to dig4
submitting 1aqm to dig4
1auq does not exists in /lab/shared/scaffolds/
1avs does not exists in /lab/shared/scaffolds/
1axn does not exists in /lab/shared/scaffolds/
submitting 1ayx to dig4
submitting 1azo to dig4
submitting 1b0y to dig4
submitting 1b54 to dig4
submitting 1b56 to dig4
submitting 1b6g to dig5
Submitting jobs -- Iteration 1
submitting 1b80 to dig4
submitting 1b8l to dig4
submitting 1ba3 to dig4
submitting 1bf6 to dig4
submitting 1bff to dig4
submitting 1bi0 to dig4
submitting 1bin to dig4
submitting 1bob to dig4
submitting 1bs0 to dig4
submitting 1bs1 to dig4
submitting 1bwk to dig4
submitting 1bx4 to dig4
1bx6 does not exists in /lab/shared/scaffolds/
1bxv does not exists in /lab/shared/scaffolds/
submitting 1byq to dig4
1c1k does not exists in /lab/shared/scaffolds/
submitting 1c8x to dig4
submitting 1cc4 to dig4
submitting 1cjh to dig4
submitting 1cke to dig4
1clc does not exists in /lab/shared/scaffolds/
submitting 1cr5 to dig4
submitting 1cs3 to dig5
submitting 1cwv to dig5
Submitting jobs -- Iteration 2
submitting 1cxy to dig4
submitting 1cy5 to dig4
1cyx does not exists in /lab/shared/scaffolds/
submitting 1cza to dig4
submitting 1d2m to dig4
submitting 1d3g to dig4
submitting 1d4o to dig4
submitting 1d5t to dig4
1dbu does not exists in /lab/shared/scaffolds/
submitting 1dbw to dig4
1dcq does not exists in /lab/shared/scaffolds/
```

Before execution

```
[sridhar@dig3 test_jobdistribution]$ ls
general_match.flags  general_match_VX.flags  Job_Distribution.py*  Job_Distribution.pyc  match.cst  Orgpho_S_H_DE_oxya_FP1_match.cst
pdblist  pdb.list  pdblist2  pdblist3  subs.flags  test2  testkill.py*  trash/  VX.conf.pdb  VXS.params
[sridhar@dig3 test_jobdistribution]$
```

Execution

```
[sridhar@dig3 test_jobdistribution]$ ./Job_Distribution.py -file pdblist -cstfile Orgpho_S_H_DE_oxya_FP1_match.cst -nodes 20
total jobs is more than available nodes, jobs will submitted as nodes become free
```

After execution

```
[sridhar@dig3 test_jobdistribution]$ ls
16vp/ 1aky/ 1avs/ 1b8l/ 1bwk/ 1cke/ 1d2m/ 1dhy/ 1dvj/ 1e2w/ 1eaz/ 1elj/          pdblist2
1a8s/ 1al3/ 1axn/ 1ba3/ 1bx4/ 1clc/ 1d3g/ 1dk0/ 1dyo/ 1e42/ 1efd/  general_match.flags      pdblist3
1a8v/ 1alq/ 1ayx/ 1bf6/ 1bx6/ 1cr5/ 1d4o/ 1dki/ 1dyp/ 1e5k/ 1eh6/  general_match_VX.flags  subs.flags
1aa6/ 1am7/ 1azo/ 1bff/ 1bxv/ 1cs3/ 1d5t/ 1dlw/ 1dyq/ 1e6c/ 1ej1/  Job_Distribution.py*    test2
1af7/ 1amu/ 1b0y/ 1bi0/ 1byq/ 1cwv/ 1dbu/ 1dly/ 1dyr/ 1e6z/ 1ej2/  Job_Distribution.pyc    testkill.py*
1aj6/ 1anx/ 1b54/ 1bin/ 1cl1/ 1cxy/ 1dbw/ 1dm1/ 1e0c/ 1e7z/ 1ej8/  match.cst                trash/
1ajk/ 1aop/ 1b56/ 1bob/ 1c8x/ 1cy5/ 1dcq/ 1dmg/ 1e0s/ 1e8c/ 1ejd/  Orgpho_S_H_DE_oxya_FP1_match.cst  VX.conf.pdb
1ajo/ 1aqm/ 1b6g/ 1bs0/ 1cc4/ 1cyx/ 1dd9/ 1ds1/ 1e1m/ 1e9m/ 1ek8/  pdblist                  VXS.params
1ake/ 1auq/ 1b80/ 1bs1/ 1cjw/ 1cza/ 1ddg/ 1dv8/ 1e25/ 1eaq/ 1el1/  pdb.list
[sridhar@dig3 test_jobdistribution]$
```

```
from Job_Distribution import *

hostlist = get_hostlist(4,27)
onlinedigs = online_digs(hostlist)
killalldigs(onlinedigs)
```

```
[sridhar@dig3 test_jobdistribution]$ ./testkill.py
killing jobs in dig4
Connection to dig4 closed by remote host.
killing jobs in dig5
Connection to dig5 closed by remote host.
killing jobs in dig6
Connection to dig6 closed by remote host.
killing jobs in dig7
Connection to dig7 closed by remote host.
killing jobs in dig8
Connection to dig8 closed by remote host.
killing jobs in dig9
Connection to dig9 closed by remote host.
killing jobs in dig10
Connection to dig10 closed by remote host.
killing jobs in dig11
Connection to dig11 closed by remote host.
killing jobs in dig12
Connection to dig12 closed by remote host.
killing jobs in dig13
Connection to dig13 closed by remote host.
killing jobs in dig14
Connection to dig14 closed by remote host.
killing jobs in dig15
Connection to dig15 closed by remote host.
killing jobs in dig16
Connection to dig16 closed by remote host.
killing jobs in dig17
Connection to dig17 closed by remote host.
killing jobs in dig18
Connection to dig18 closed by remote host.
killing jobs in dig19
Connection to dig19 closed by remote host.
killing jobs in dig20
Connection to dig20 closed by remote host.
killing jobs in dig21
Connection to dig21 closed by remote host.
killing jobs in dig22
Connection to dig22 closed by remote host.
killing jobs in dig23
Connection to dig23 closed by remote host.
killing jobs in dig24
Connection to dig24 closed by remote host.
killing jobs in dig25
Connection to dig25 closed by remote host.
killing jobs in dig26
Connection to dig26 closed by remote host.
```