

1.) start
bigjobs

Replica-Exchange
Master
(async-re.py)

2.) start repex agents as
subjobs

BigJob
(bigjob.py)

Resource

BigJob Agent
(bigjob_agent.py)

Repex Agent
(async-
re_agent.py)

3.) Spawn NAMD/
6.) Restart NAMD

NAMD

5.) post result/
search for exchange partner

4.) collect results

5.) post result/
search for exchange partner

Advert
Service

Resource

BigJob Agent
(bigjob_agent.py)

Repex Agent
(async-
re_agent.py)

3.) Spawn NAMD/
6.) Restart NAMD

NAMD

4.) collect results

5.) post result/
search for exchange partner