Molecular Dynamics Applications with BigPanDA

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Molecular Dynamics

- Professor Kwangho Nam at University of Texas at Arlington
- CHARMM + custom-compiled software: CPU + GPU application for simulating enzyme catalysis, conformational change, and ligand binding/release
- Jobs use full node (all cores on CPU and also the GPU) and can be customized to fit 40-60 minutes wall time
- Depending on the type of projects, it can expand beyond 500 nodes on Titan; currently, it uses 60 ~ 124 nodes for each project, which can be combined to run using more nodes.

Payload tests

- 2 tests with single job pilot were conducted in summer 2017
- CHARMM to generate and analyze a molecular simulations. (CPU+GPU)
  - 124 nodes with walltime=30min out:2.4Gb
  - 124 nodes with walltime=90min out:5.8Gb
- First tests were considered as successful by Dr. Kwangho Nam

Plans

- Target is multi-node backfill
  - Choose 40 minute maximum walltime - no interference with ATLAS
- Need a “top layer” that automates submission of the jobs that will target 30-45 minute duration backfill
  - First priority for Sean, along with learning to use multi-job backfill pilot
- May need some task management (ProdSys-like) capabilities
  - Some jobs depend on the completion of previous jobs
  - Would like to automate this with scripts (done manually now)
  - For now scripts are ok (maybe even the same submission scripts mentioned above) - but may need ProdSys capabilities later
- Schedule - we want to start submitting tasks in ~2 weeks

Thank you!