Faster Discoveries with the “Docking Factory” Accelerator for Molecular Docking

Mikhail Serkov
Senior Director, HPC Services

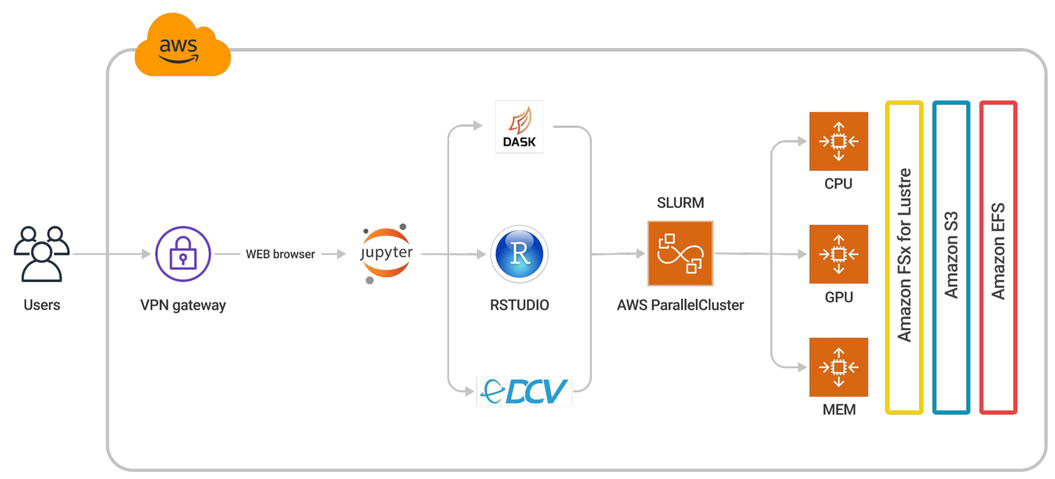
One of the biggest challenges in drug discovery is high throughput docking. Compound libraries have grown and it is often a task to screen millions or even billions of compounds in a reasonable time. It is important not only to have the computation resource but also to make sure that the resource is efficiently utilized by the docking software.

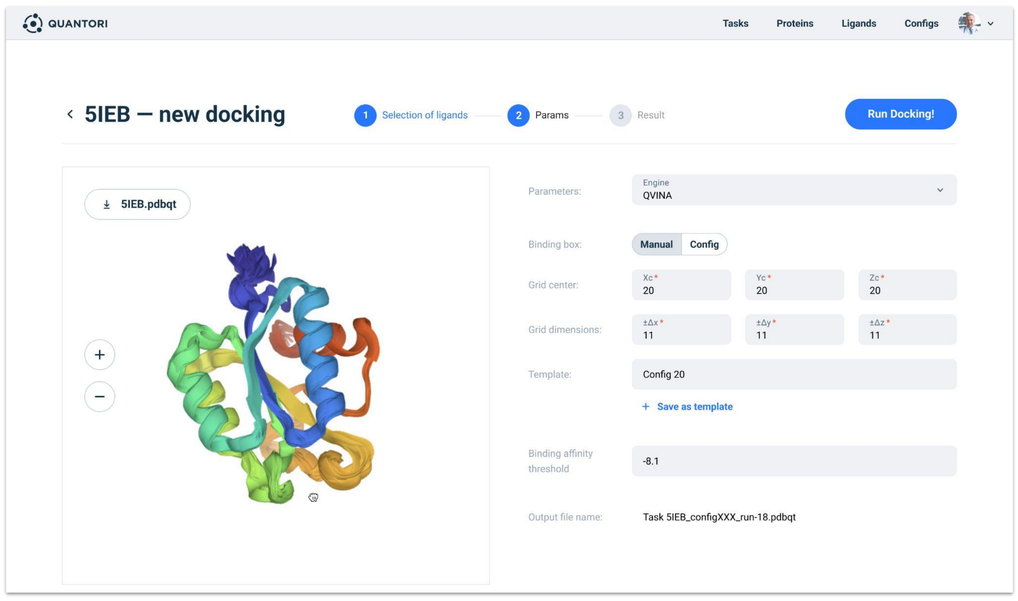
Quantori introduces the “Docking Factory" accelerator for molecular docking. The accelerator enables cost-effective high throughput docking on existing on-prem HPC clusters and/or cloud resources, allowing scientists to focus on the research and advance rapidly.

Computation Platform Accelerator

This “high performance computation platform” accelerator helps accelerate scientific research with HPC technologies without focusing on infrastructure.

With flexible design, it could be integrated with the majority of tools used for computation in Genomics, CryoEM, computational chemistry, and other areas – depending on the research focus.





Docking Factory Accelerator

The Docking Factory accelerator provides researchers with a convenient framework and tool for molecular docking.

Molecular docking is one of the most frequently used methods in structure-based drug design. There are many different algorithms to perform docking and no unified way of running it. Each tool comes with its own set of parameters, features, and scoring functions.

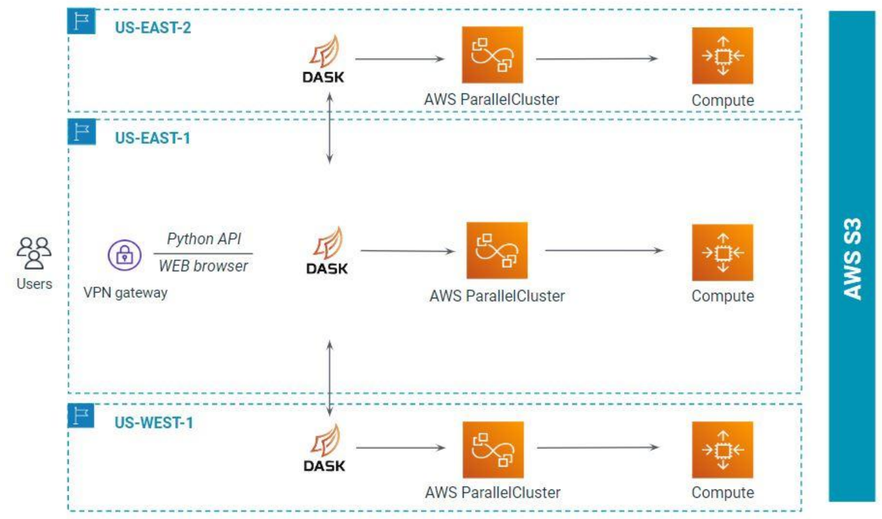
With this Docking Factory accelerator – a user can easily analyze results from the run using RStudio/Jupyter without switching context, which saves a lot of time.

HPC Platform for Molecular Docking

Challenge: A life sciences company was operating a platform built on ARM architecture with EC2 Spot Instances to reduce the compute costs and improve the application output. Quantori’s challenge was to rapidly develop HPC compute environments using AWS ParallelCluster, an open-source cluster management tool.

Solution: Qauntori implemented an HPC infrastructure accelerator for macromolecular docking of tertiary and quaternary proteins, which enabled scientists to work exclusively within their research environments with AWS ParrallelCluster, Jupyter Notebooks, complators and docking tools including AutoDock, Smina, and QVina. This powerful platform can scale from small runs with a few thousand ligands, up to millions without reconfiguration.

Outcome: The life sciences company gained a cost-effective and highly performant system for running docking computations.



Library size: 250000 ligands
Docking pipeline: qvina + smina
Total dockings: 500000

Cost: ~$10 using on-demand c6g.16xlarge instances
Time: 30 minutes on 1024 CPU cores

contact@quantori.com
+1(617) 225-4353

quantori.com