Faster Discoveries with High Performance Computing for Life Sciences

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Introduction

HPC is the aggregation of computer power that solves problems whether too large or time-consuming to process by standard computers.

Various terms come along as we speak of HPC, including **supercomputers**, **clustering**, **high-throughput computing**, and **grid computing**. Despite many names, HPC is a set of computations, storage, network resources, and workload schedulers that allow processing immense volumes of data superfast in a parallel mode. HPC can also utilize machine learning, deep learning, and other tools to drive the outcomes further.

HPC and Life Sciences

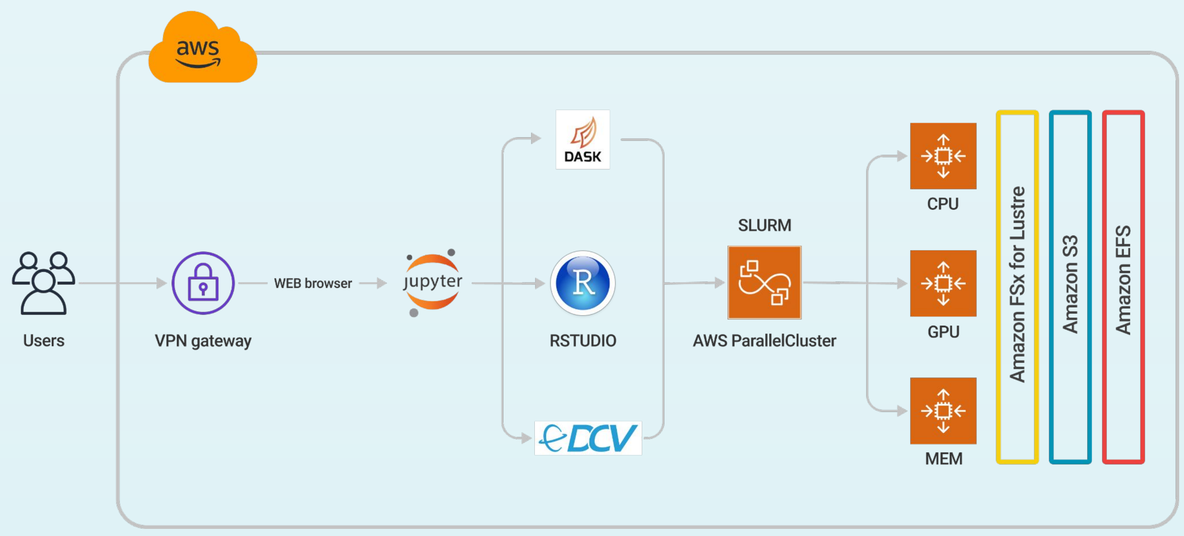
HPC is a breakthrough element for biotech and biopharma companies to unfold R&D faster and more productively. Researches can set high expectations and compute vast data rapidly to unlock insights and value.

Quantori HPC Accelerators

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.

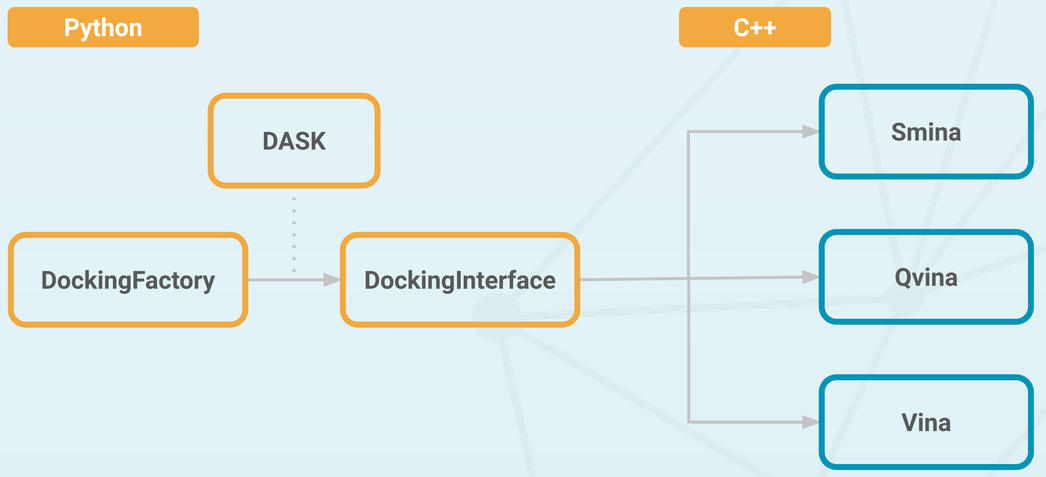


Docking Factory Accelerator

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.

HPC Platform for Cell Image Analysis

Challenge: A U.S. genomics company working with cellular structure analysis asked Quantori to help them seamlessly shift all of their computations to the cloud due to a lack of sufficient onsite resources.

Solution: Quantori introduced the HPC platform, optimized the client’s applications for AWS hardware, migrated the on-premise pipelines to AWS, provided support for any type of instances with HPC approach and made the image analysis efficient and scalable, allowed scaling up to thousands of CPUs with no need for scientists to know AWS or CLI/Web interfaces, integrated easy access to DSFWorld with HPC.

Outcome: The HPC approach provided support for any type of instances and made the image analysis scalable and more efficient. The scientists are able to operate without knowledge of AWS or CLI/Web interfaces and enabling them to cost-effectively process hundreds of public datasets in real-time, instead of weeks.

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