

CBI 学会 2020 年大会 スポンサーセッション
SS-05 CH3

日時 : 10 月 29 日 (木) 10:00 – 11:30

MD in Orion: A Parallel Universe

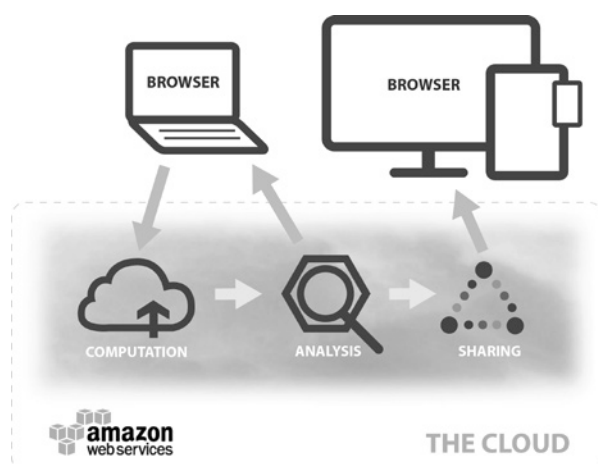
Christopher Bayly

Head of MD solutions, OpenEye Scientific Software Inc.

The new technology of OpenEye's Orion makes it easier for non-experts to leverage the capabilities of the Cloud to do highly parallel computing. This encourages us to re-think our science to come up with more highly parallelized methods and workflows. This presentation will focus on how we do this in two areas relevant for Molecular Dynamics (MD) in ligand design: Relative Binding Free Energy (RBFEE) calculations, and a faster cheaper MMPBSA-based method designed to offer a higher throughput approximate score earlier in the pipeline.

A Cloud Native Platform for Computer-Aided Drug Design

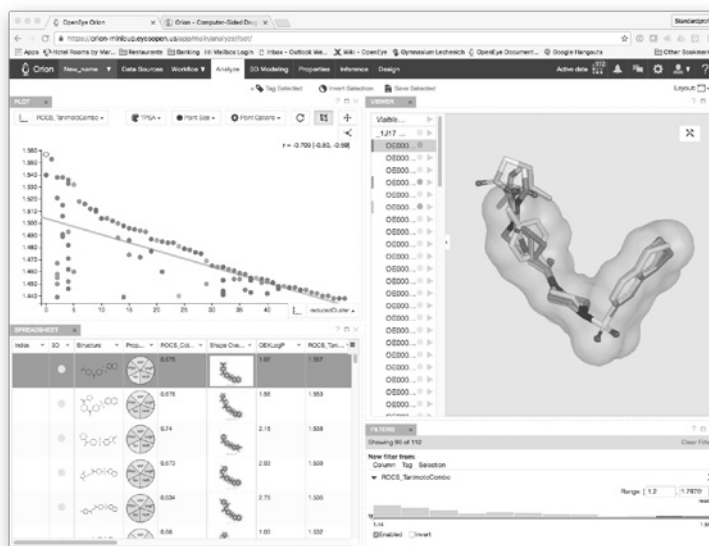
Orion is our reimagining of computational drug discovery and design powered by the cloud. It includes all of OpenEye's software, extensive tools for data visualization and communication, useful data sources and task-oriented workflows, all in a robust, scalable, cloud environment. Orion is a 'cloud native' platform in that all elements of Orion reside on, Amazon Web Services (AWS):



- Easy, scalable, maintenance-free
- Access to hundreds, thousands, or even tens of thousands of CPUs
- Unlimited storage and archiving via reliable networks
- World-class data-security. Access directly through the customer's relationship with AWS, or indirectly through OpenEye

Features

- Scalable environment via Amazon Web Services (AWS)
- Access to ALL OpenEye computational software and toolkits
- Results sharing via chat and text-like environment with access privileges
- Easily handles large-scale computation including data analysis and file handling
- Seamless access to third party code



www.eyesopen.com