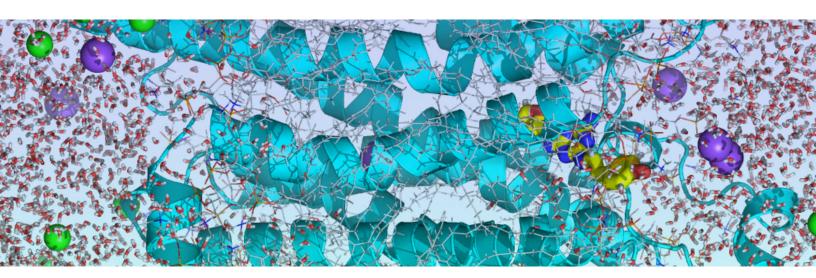




Democratizing Access to Next Generation Computer-Aided Drug Discovery Technologies with an HPC GPU Cluster



Background

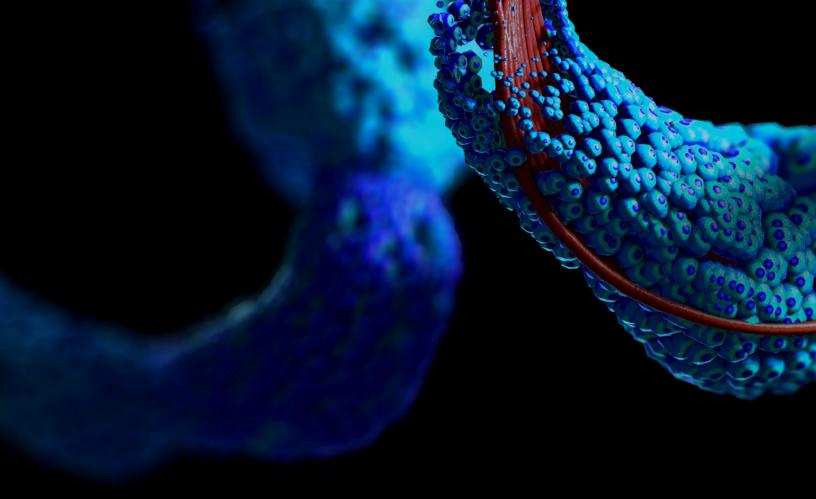
The use of AI, computational modeling, and simulation in drug discovery dates back to at least the 1960s. Despite this long history, their impact has only been felt in recent years with the dramatic increase in computational power and data availability. Nowadays, modern *in silico* approaches are required in virtually all drug discovery campaigns and have the potential to significantly improve on slow traditional approaches that involve multi-year iterative design, synthesis, and testing, of drug candidates.

Modern computer simulation software, like molecular dynamics, was developed on the x86 CPU platform. CPUs, however, were designed to execute a broad range of instructions and execute instruction sets sequentially. Performing the same numerical calculations repeatedly proved extremely difficult and slow. This meant that heavy scientific workloads required clusters of hundreds of CPU cores for even small-scale molecular dynamics simulations.

NVIDIA developed the first mainstream GPU able to advance computer graphics. Since pixels on a screen have little relation to one another, the calculations could be grouped and processed independently, known as parallelization.

GPU parallel computing was revolutionary and could be applied to numerous areas in addition to graphics and image processing. In 2007, NVIDIA developed CUDA, a parallel computing platform and programming model that enabled software to harness parallelization in GPUs for general-purpose processing, increasing the efficiency of several types of numerical computation exponentially.

General-purpose computing on GPUs was very well suited for molecular dynamics due to the extensive independent calculations within these simulations. Like pixels on a screen, many of the numerical calculations needed to model the motion of molecules in a simulation could be evaluated independently of each other. By using CUDA, scientists could now leverage the power of GPUs for molecular dynamics simulation. Porting molecular dynamics to GPUs could effectively multiply the performance of CPU-only configurations by one hundredfold.



Situation

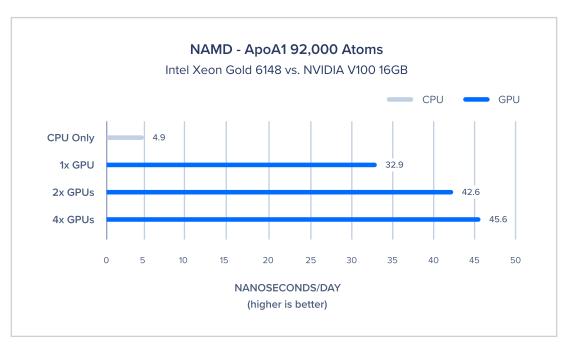
With GPUs presenting significant performance gains for scientific computing, there needed to be a way to bring these innovative benefits to the masses. As a world-class leader in computer-aided drug design (CADD), artificial intelligence drug design (AIDD), and molecular dynamics simulation, TandemAI CTO Albert Pan recognized the rise of computation in drug discovery and the need for simpler and more efficient ways to model drug interactions so that

"With the significant increase in computational power and data in recent years, computer-aided drug design and Al have become an indispensable part of any drug discovery effort," said Pan.

There is a high barrier to entry, however, to CADD and AIDD. In particular, building an entire high-performance computing infrastructure from scratch, especially for early stage companies with lower budgets, less commercial space, and limited in-house knowledge in managing a large-scale HPC GPU cluster, is very difficult.

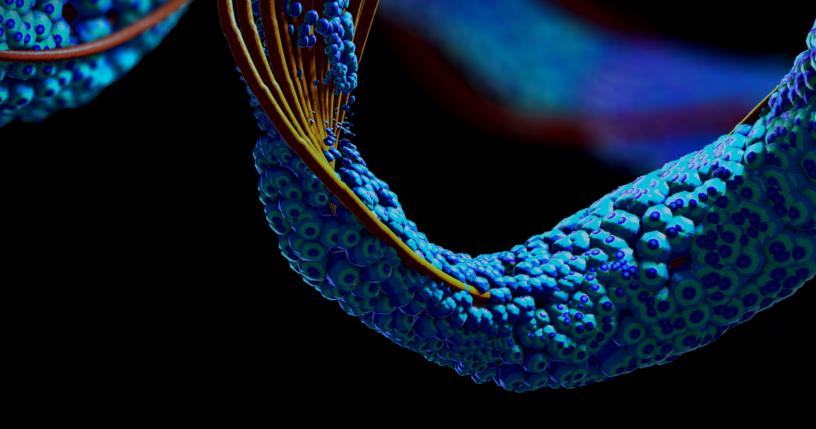
TandemAl's goal for CADD and AIDD as well as molecular dynamics simulation was not to gatekeep the immense benefits modern-day computing could have for drug discovery, but instead, to democratize access to these cutting edge

Benchmarks



CPU vs GPUs presenting a huge performance gain





Challenge

Running molecular dynamics simulations is a unique challenge when it comes to science and computing. Computer science has quickly interwoven itself within the pharmaceutical industry in the past decade with CADD and AIDD tools being used extensively in the drug discovery process. These tools can be difficult to master and have multiple barriers to entry.

CTO Albert Pan and Head of HPC Xinyu Que sought to lower the barrier of entry to computer-aided drug discovery by democratizing access to the most advanced tools. To do this they needed to leverage a powerful enough computing system that enabled concurrent molecular dynamics simulations and delivered cutting edge drug discovery methods to their users.

They wanted to deliver their expertise as a service to companies and research institutions to help them avoid the large start-up costs needed to leverage these approaches effectively.

This meant that TandemAl's computing solution had to incorporate custom-tailored high-performant hardware to revolutionize and accelerate the discovery of drugs for the world's top research institutions and biotech companies.



Solution

The TandemAl team turned to Exxact Corporation to build their custom HPC cluster. Exxact proved to be responsive and knowledgeable in the life science and molecular dynamics fields of research, working with TandemAl to supply a custom-configured cluster with high-performance GPU computing power and high bandwidth network connectivity.

TandemAl worked with Exxact to configure a 48U Turnkey GPU Cluster powered by NVIDIA RTX GPUs dedicated to accelerating scientific computing. Powered by 64 NVIDIA RTX A4500s and extensive high throughput 100GB networking, TandemAl is now able to run multi-tenant usage of multiple large-scale simulations with ease.

TandemAl's collaborative team of scientists work with biotech companies and the global scientific community. They provide easy access to cutting edge CADD software as well as a massive wet lab for researchers and scientists to discover and develop successful pre-clinical drug candidates in a faster and more efficient way. A core technology offered by TandemAI is free-energy perturbation (FEP), a precise and accurate digital assay built on top of molecular dynamics simulations for predicting proteinsmall molecule binding affinities.

TandemAl's large-scale and highly efficient wet lab operations integrate seamlessly with their computational tools. This integration of "dry/wet" cycles combines computational and experimental data to optimize the accuracy of their predictions with the use of AI and machine learning.

With the computing infrastructure supplied by Exxact, TandemAI can run hundreds of computationally intensive digital assays every day. Providing these extremely fast calculations as a service can enable the discovery of groundbreaking drug innovations for scientists from around the world.

" The Exxact Team's turnkey GPU cluster and customer service enabled us to scale up and hit the ground running during the early days of TandemAI when we were still building out the TandemAI team."

TandemAl CTO Albert Pan