EXXACT

CASE STUDY

Exxact GPU Cluster Accelerates Cancer Research at Notre Dame

BACKGROUND

With more people becoming afflicted with cancer every year, Notre Dame scientists are working to create personalized cancer vaccine therapies with the assistance of computational modeling. The acquisition of a GPU-based compute cluster from Exxact Corporation has dramatically accelerated simulations for Notre Dame cancer researchers. The cluster is maintained by the Notre Dame Center for Research Computing which is an innovative and multidisciplinary research environment.

CRC
CENTER FOR RESEARCH COMPUTING

The research effort is led by Professor Brian Baker, Associate Dean for Research and Graduate Studies in the College of Science and Professor of Chemistry and Biochemistry. Baker and a vastly talented team of biophysicists, biochemists, and immunologists are relying on GPU computing power to develop new immunotherapeutics.

Cory Ayres, a biochemistry graduate student, leads the computational production while being co-advised by Professor Baker and Professor Steven Corcelli from the Department of Chemistry and Biochemistry. Ayres focuses his research on molecular dynamics (MD) studies of T-Cell receptors (TCRs) and major histocompatibility complex proteins bound to peptide antigens (pMHCs).

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SITUATION

To develop new immunotherapeutics, Ayres must examine the interactions of the TCR and pMHC proteins using AMBER Molecular Dynamics software, which will allow him to determine the role that these motions play in molecular recognition. He will also need to perform molecular dynamics simulations to identify neoepitopes, the part of an antigen recognized by the immune system, that is the most immunogenic.

CHALLENGE

AMBER is one of the most widely used applications for biochemists and other scientists who focus on molecular dynamics research. However, AMBER also requires a tremendous amount of computing power to drive its simulations. Baker and Ayers were previously using only CPUs to power their MD simulations, which allowed them to simulate only about a nanosecond a day.

SOLUTION

To accelerate the results for cancer research, the Notre Dame scientists closely collaborated with the Center for Research Computing, Exxact and AMBER GPU Development Lead, Dr. Ross Walker, to develop a solution fully optimized for AMBER. A key feature of AMBER is the ability to leverage NVIDIA GPUs to massively accelerate complex molecular simulations. As the sole provider of AMBER Certified MD Systems, Exxact's team of engineers configured an AMBER Optimized Cluster Solution featuring 40 NVIDIA Maxwell–based GPU accelerators in 10 Intel-based servers.

With a GPU cluster in place, the Notre Dame Research team can now simulate up to 1.2 microseconds a day, allowing research to advance at a factor of 1,000 times faster than when they initially started. The increased computational throughput helps Bakers's team run even more simulations to help determine whether a given neoantigen will stimulate an anti-tumor immune response. These accelerated simulations, made possible by Exxact's GPU cluster, will aid in ultimately identifying which neoepitopes may be useful as cancer vaccine components. If successful, this research will lead to significant advances in the fight against cancer and possibly even patient-specific, personalized vaccines in the future.

> "The Exxact team's expert knowledge of GPU computational systems coupled with their close coordination with scientific software developers (such as the AMBER team) made designing, deploying, tuning, and operating this high performance research cluster an outstanding experience."
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> *Paul R. Brenner, PhD, P.E., Center for Research Computing, The University of Notre Dame*