



Snowlake Powers Molecular Dynamics for Medical Research Using Xilinx Alveo Accelerator Card

Snowlake’s “Yaddle MD” Molecular Dynamics Computing Engine Enables Comprehensive Molecular Dynamics Computation on a Single Alveo U200 Card

AT A GLANCE:

Shanghai Snowlake Technology Co. Ltd. was founded in 2017 and is an innovative company focusing on R&D and solutions for high-performance computing products. The company mainly provides innovative dedicated high-performance computing solutions and products for life sciences, oil and gas exploration, autonomous driving, distributed storage and other related fields.

- Industry: HPC
- Location: Shanghai, China
- Established: 2017
- Website: www.snowlake-tech.com

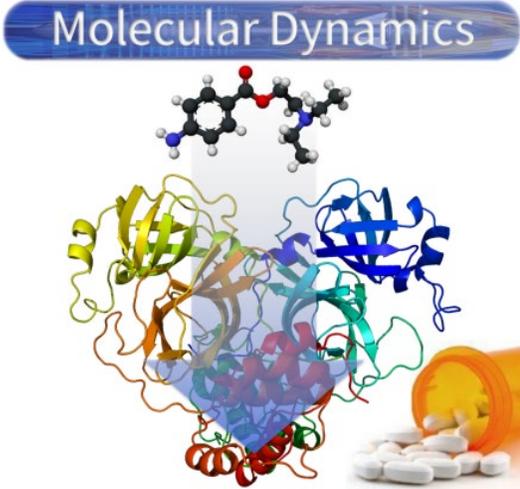


Figure 1 – Molecular dynamics modeling is used in drug research and discovery

OVERVIEW:

Snowlake Technology has developed “Yaddle MD,” a dedicated solution for molecular dynamics computing on Xilinx Alveo™ accelerator cards. With Xilinx’s Runtime Library (XRT), Yaddle provides compatibility support for commonly used molecular dynamics software and another analysis plugin via molecular dynamics APIs.

Running on Alveo, Yaddle MD performs significantly better than with CPUs and GPUs, and at a fraction of the total cost-of-ownership.

CHALLENGE:

Capital spending on drug research and discovery has grown exponentially in recent years as traditional structure-based design methods have begun to reach their limits. One of the most-exciting and innovative areas of advancement has been in motion-based drug design, or molecular dynamics simulation, which requires a heavy amount of computing power.

Previously, only large supercomputers could produce enough computing power for molecular dynamics calculations. But Snowlake wanted to build a solution that was cost- and power-efficient and achieved a significant performance boost vs. traditional supercomputers.

SOLUTION:

Drug discovery has moved to the molecular level for advancing medicine. With this level of research, scientists can better understand the role of molecules and biological processes and unlock the secrets of their interaction.

Yaddle MD is a high-performance, dedicated solution for molecular dynamics that uses a Xilinx FPGA-based Alveo U200 accelerator card to implement molecular dynamics algorithms and perform complex calculations. With this adaptive computing technology on board, Yaddle MD delivers higher performance than CPUs and GPUs to dramatically accelerate the dynamic simulation of biomolecules. Now, a single Alveo card can achieve performance once only previously achievable by supercomputers.

With Yaddle MD, users can:

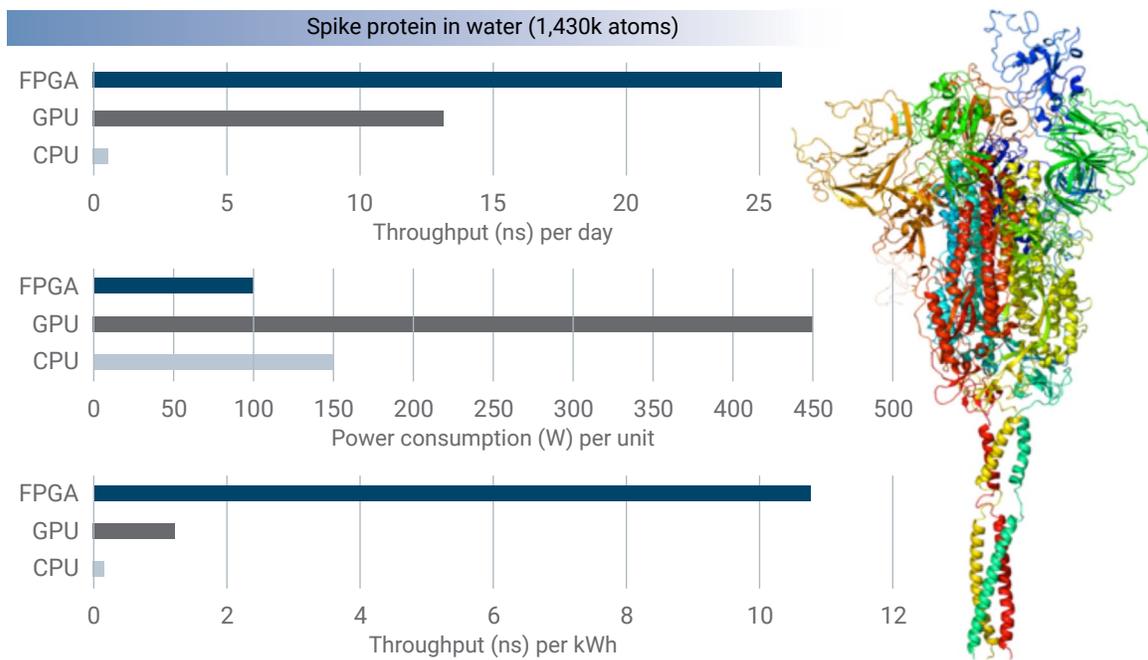
- Release CPU resources by implementing the complete computing workload of molecular dynamics on a single FPGA
- Achieve distributed pipeline calculations among atoms for non-bonded force that significantly improves computing performance
- Encode bonded information between atoms and decode them in real-time calculations
- Leverage a toolkit that provides compatibility support for common molecular dynamics software and other analysis tools, including format conversion

Xilinx Alveo U200 accelerator cards are designed to meet the constantly changing needs of the modern data center, providing up to 90X performance increase over CPUs for common workloads, including machine learning inference, video transcoding, and database search and analytics.

With complex algorithms evolving faster than silicon design cycles, it's impossible for fixed-function GPU and ASIC devices to keep pace. Built on Xilinx 16nm UltraScale™ architecture, Alveo U200 accelerator cards provide reconfigurable acceleration that can adapt to continual algorithm optimizations, supporting any workload type while reducing overall cost-of-ownership.

RESULT:

Running on Alveo accelerators, Yaddle MD achieves nearly 50X the performance of CPUs and 2X the performance of the industry's highest-performing GPUs as shown in Figure 2. At the same time, the power consumption of FPGAs is only 2/9 of GPUs and 2/3 of CPUs. Therefore, Yaddle, based on FPGAs, can offer nearly 100X the throughput of CPUs per kWh and nearly 10X the throughput of GPUs per kWh.



“Just as it’s easier to capture the details of a crime by watching a security video vs. examining live photos, molecular dynamics simulation allows drug designers to see the entire effective process of drug molecules more directly, allowing them to greatly improve the success rate of new drug development,” said Dr. Nan Sheng, chief scientist of Life Science Computing at Snowlake. “Computing performance is critical for efficiency and accuracy of molecular dynamics computing. Snowlake’s Alveo-based high-performance molecular dynamics dedicated engine, Yaddle MD, not only saves customers a lot of time, but also transforms the design of drugs based on molecular dynamics from impossible to possible.”

Snowlake is now providing Yaddle MD acceleration service through Alicloud, and its Alveo-based solutions are also available for small-scale testing development. The company also plans to pursue further speed and throughput improvements for such MD acceleration applications by scaling out simulation capabilities across multiple Alveo devices.

ADDITIONAL RESOURCES:

- [Learn More About Snowlake Technology](#)
- [Learn More About Xilinx Alveo Accelerator Cards](#)

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