AMD | STORIES

SYMMETRIC COMPUTING DISCOVERS NEW DRUGS FASTER WITH AMD EPYC™ AND RADEON INSTINCT™ TECHNOLOGY

Using AMD EPYC™ CPUs and Radeon Instinct™ GPUs, Symmetric Computing is enabling researchers to run many more protein-binding simulations a day in the quest for better medical treatments

CUSTOMER

SYMMETRIC COMPUTING

INDUSTRY

Virtual screening for drug discovery

CHALLENGES

Enhance rate of screening for binding of small molecules to target proteins.

SOLUTION

Deploy AMD EPYC™ 7601 processors and Radeon Instinct™ MI25 accelerators.

RESULTS

Faster discovery of potential drug candidates by reducing need for extremely time consuming and expensive laboratory assays.

AMD TECHNOLOGY AT A GLANCE

AMD EPYC 7601 CPU with 32 cores
Radeon Instinct MI25 GPU

Finding cures for the most common and life-threatening diseases takes a huge amount of time and effort. Theories need to be devised, potential drug regimens designed, and then there will be years of testing before a new drug can be proven to be effective, safe, and ready to be delivered to patients. But what if you could accelerate that process, using simulations on supercomputers to find the drug formulations with the best potential for success before time-consuming clinical trials begin?

This is the approach taken by Symmetric Computing in its work with medical researchers. Employing AMD EPYC processors and Radeon Instinct accelerators, Symmetric has been able to vastly speed up the process of finding potential drugs for the treatment of Alzheimer's, Parkinson's, Diabetes and other diseases.

THE NEED FOR SPEED WHEN SCREENING 500 MILLION COMPOUNDS

Symmetric Computing has been putting its ideas into practice in the Venture Development Center at the University of Massachusetts (UMass) in Boston, and one of the company's biggest focuses has been Alzheimer's disease. Symmetric has developed a Virtual Drug Discovery Platform using AutoDock Vina, NAMD, and TensorFlow. "We are using AutoDock Vina to simulate protein-ligand docking, finding where compounds bind and how tightly, to look for likely drug candidates," explains Kimberly Stieglitz, Professor Biotechnology and Chemistry at Roxbury Community Colleges.

"Then we screen the best results with Nanoscale Molecular Dynamics (NAMD) software in physiological simulated space," adds Richard Anderson, President and CTO of Symmetric Computing, Inc. "This tells us which compounds offer the best possibilities. We may take ten or even one per cent [of tested compounds] from NAMD and validate those in the lab. The idea is that this gives someone developing a new drug a better starting point."

"One of the challenges was the storage of data and lack of speed," continues Stieglitz. "I need to be able to do runs in AutoDock and then NAMD relatively quickly so I can analyze the output to know what I need to do next. And that's not possible to do on a standard system. I needed something with more speed." The simulations performed utilize a database of over 500 million small molecules with 3D structure, 23 thousand human proteins with 3D structure, alongside data on all known drugs both deployed and experimental—a huge undertaking.

These must all be tested together to see which compounds block or enhance the function of which proteins. Each compound must be tested across all human proteins because knowing, for example, that a given molecule inhibits the proteins associated with Alzheimer's isn't enough on its own; the compound may also have undesirable side effects on other human proteins that will eliminate it from being used in a drug treatment program for the disease. It's a complex, time-consuming process of trial and error that would take years if performed using laboratory-based tests alone.

"We can also put four head nodes together and get 8TB of addressable memory... With 256 cores across four servers, the EPYC platform is really a mainframe at a tenth of the cost."

Richard Anderson,
President and CTO of Symmetric Computing, Inc

This is where the AMD EPYC architecture and its fast connectivity to banks of Radeon Instinct GPU accelerators have proven so effective. Symmetric Computing's design requires highly integrated CPUs with lots of fast cores, fast access to large amounts of memory, and rapid connections to external peripheral devices providing excellent single-precision floating-point performance. The combination of AMD EPYC and Radeon Instinct technology ticks all these boxes perfectly.

MAINFRAME PERFORMANCE AT A TENTH OF THE COST

The Symmetric supercomputer design is composed of a dual-processor head node using two AMD EPYC 7601 32-core 2.7GHz CPUs with up to 4TB of memory, which is connected via a trio of InfiniBand® adapters to three GPU compute nodes. Each of these contains four Radeon Instinct MI25 accelerators managed by another AMD EPYC processor with 64GB of memory. This configuration is enabled by AMD's EPYC architecture, in particular its significantly higher PCI Express® lane count compared to competitive solutions. In dual-socket configurations, the EPYC processor has 128 PCI Express lanes for use with peripherals, 33% more two Intel® Xeon® Scalable processors in the same class.[1]

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Kimberly Stieglitz, Professor of Biotechnology and Chemistry, Roxbury Community College

The large number of EPYC processor PCI Express lanes allows Symmetric's head node to use up to four 100Gbits/sec InfiniBand adapters at full speed. Each compute node can run its four GPU accelerators at full 16x PCI Express speed alongside an InfiniBand adapter. As a result, the standard GPU cluster configuration of three compute nodes using four Radeon Instinct MI25 GPUs per node can deliver up to 300TFLOPS of half-precision and up to 150TFLOPS of single-precision performance, with the latter particularly relevant to the workloads Symmetric runs. Thanks to InfiniBand's fast throughput, the compute nodes can all access the head node's memory with up to 4TB as a shared resource.

The three InfiniBand adapters on a head node can be used for further configurations that are even more capable for memory-intensive applications, which Symmetric is calling Departmental Mainframes. "Some of the models we use are massive in terms of memory–terabytes," explains Anderson. Symmetric's Distributed Symmetric Multi-Processing platform allows the global sharing of memory across nodes to create one large pool of addressable memory. "Each EPYC processor-based head node supports up to 4TB of memory, and the fact that this is eight-channel and 2,666MHz DDR4 makes a huge difference. We can also put four head nodes together and get up to 16TB of addressable memory. This can dramatically improve performance. With 256 cores across four servers, the EPYC platform is really a mainframe at a tenth of the cost."

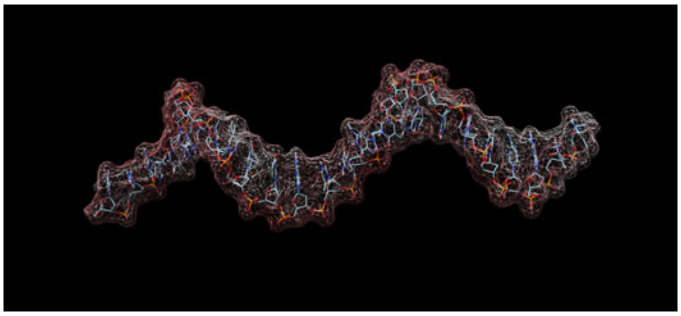
A REVOLUTION IN THE QUEST FOR NEW TREATMENTS

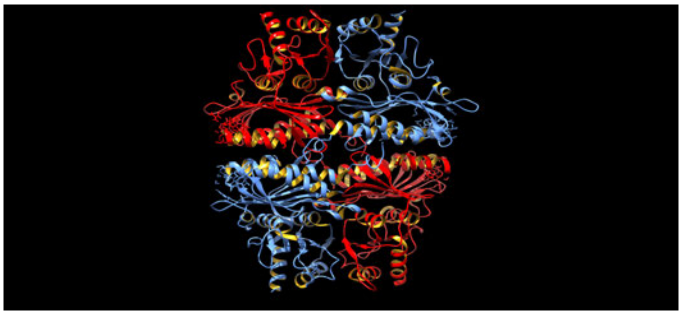
The benefits of combining EPYC CPU-powered servers and Radeon Instinct GPUs with Symmetric's supercomputing simulation approach to drug discovery are already huge, and there will be much more to come. "Thanks to this technology, we're able to identify the allosteric or control sites on a protein where small molecules bind," explains Stieglitz. "This used to be a very laborious process in the lab, but I'm now able to do it with NAMD, with speed and accuracy using the computational studies." Anderson adds as an example, that a colleague was unable to identify any allosteric sites after years of traditional research; now the Symmetric/AMD EPYC solution is discovering potential new allosteric sites using a well-defined protocol.

This has major implications for finding new, more effective therapies. The traditional approach of drug discovery by testing small molecules in the active site of a protein target can lead to drugs that have increased side effects since drugs can affect lots of different proteins, not just the one intended. Allosteric regulation can be much more specific, targeting proteins uniquely. The potential applications of this research are wide ranging, including improved treatment for HIV, reduction in the hyperparathyroidism at the end-stage of renal disease, alleviation of hypertension and heart failure, or combating opiate addiction.

The performance available from AMD EPYC processors combined with AMD Radeon Instinct GPUs is essential for this revolution in treatment discovery and other enhancements that Symmetric is launching soon. "The work we are doing on developing our whole AI platform is completely dependent on the performance of the GPU and how fast it can talk to the CPUs because that's where all the machine learning training happens," explains Anderson. "We hope to develop the AI techniques to limit the compound search space from 500 million to 50 million."

"You're not going to physically test 100 million chemicals, it's not going to happen," continues Anderson. "But with our platform, we can do the main work via the simulation. Thanks to AMD's technology, we can get the same or better performance than Intel-based servers for a quarter the price. When the 7nm EPYC processor arrives, we expect AutoDock Vina to double in performance, so we're pretty excited about that. Right now, we're screening up to 400,000 compounds a day, but we have 500 million to get through so doing twice as many will make even more of a difference."





ABOUT SYMMETRIC COMPUTING

Symmetric Computing combines high-performance computing with domain expertise in order to drive innovation. The company creates large shared-memory, many-core, symmetric multiprocessing (SMP) computers for a fraction of the cost of multi-million-dollar mainframe computers. Its GPU-intensive departmental supercomputers are ideal for scientists, engineers, economists, physicians, and designers. Symmetric's large-memory departmental mainframes provide an affordable platform for in-memory databases, big data installations, and enterprise applications. For more information, visit symmetriccomputing.com.

ABOUT AMD

For 50 years AMD has driven innovation in high-performance computing, graphics and visualization technologies—the building blocks for gaming, immersive platforms and the datacenter. Hundreds of millions of consumers, leading Fortune 500 businesses and cutting-edge scientific research facilities around the world rely on AMD technology daily to improve how they live, work and play. AMD employees around the world are focused on building great products that push the boundaries of what is possible. For more information about how AMD is enabling today and inspiring tomorrow, visit amd.com/epycserver and amd.com/instinct.

1. AMD EPYC processors have 128 I/O lanes. Two Intel Xeon Scalable processors have 96 lanes. 128 – 96 = 32 ÷ 96 = 0.33 AMD EPYC has 33% more I/O lanes. Class based on industry-standard pin-based (LGA) X86 processors. EPYC-03

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