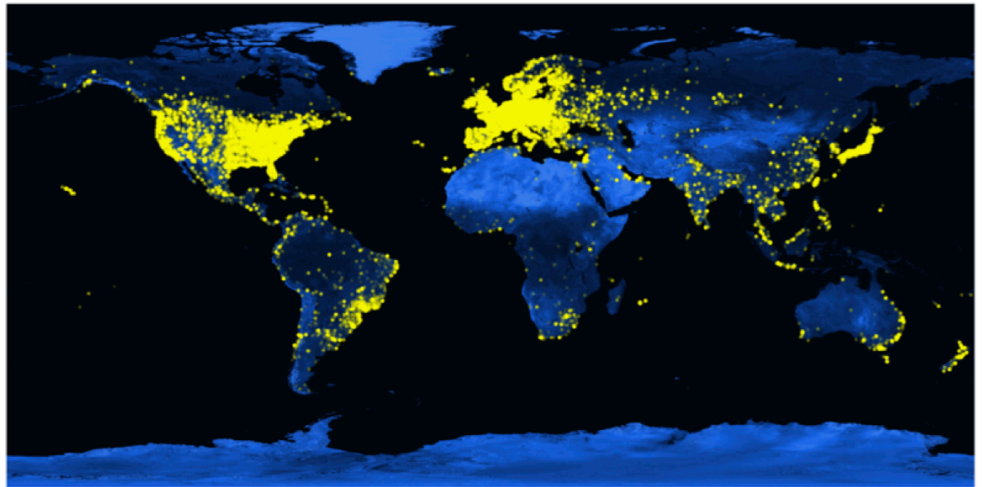**FOLDING @HOME**

Objective

To make use of HPC resources to tackle the massive data analysis for the more than 100 simulation projects now being undertaken by Folding@home.

Approach

Using Advanced Clustering's ACTblade e230, which provides up to four independent AMD EPYC compute nodes with 8 drives in one chassis. This blade combines storage, networking and computing in a single system to increase scalability and reduce datacenter complexity.

Cutting Edge Science

In its current study of the Covid-19 protein, Folding@home produces 6TB of data every hour. The project's new machines will use AMD EPYC 7742 processors providing 1,500 cpu cores. That is a notable increase over the previous system, which offered 240 cpu cores. Said Bowman: "Advanced Clustering and AMD have teamed up to create a powerful system that is optimized to run our algorithms for churning through all the data to understand how SARS-CoV-2 works and identify new therapeutic opportunities."

Covid-19 Research That Matters: Folding@home Leverages Advanced Clustering and AMD EPYC™ CPUs

Location of Folding@home users. Each yellow dot represents a unique IP address contributing to Folding@home.

Dr. Greg Bowman, an associate professor of biochemistry and molecular biophysics at Washington University School of Medicine in St. Louis, recently asked that his team of volunteer researchers turn their attention to the global effort to study Covid-19. That is no small thing.

Dr. Bowman oversees the largest crowd-sourced computational biology project the world has ever seen – called Folding@home. The project relies on the power of tens of thousands of home computers to perform the complex calculations required to simulate the dynamics of the proteins Bowman and his colleagues are studying. The Folding@home team is using 5 million devices powered by 4.5 million CPUs (31 million CPU cores) along with half a million GPUs to study Covid-19. More than 100 simulation

Dr. Greg Bowman

> "Most of the data analysis we're currently doing relies on six-year-old high performance computing machines that offer 240 cpu cores. The new machines will use AMD EPYC 7742 processors providing 1,500 cpu cores. That's a nice boost of our throughput."
>
> *- Dr. Greg Bowman, Director of Folding@Home*

projects are currently underway via Folding@-home to study the Covid-19 proteins. With all of these simulations underway, the big challenge facing Dr. Bowman and his project is data analysis. To solve that problem, he has turned to Advanced Clustering Technologies to provide high performance computing hardware equal to the task of analyzing the huge datasets.

Data-Driven Decisions
"We are bringing in 6TB of data per hour," Bowman said. "It's a huge amount of data to analyze, so we need significant hardware on our end to run the analysis. As we bring in this equipment, the question will be, 'How fast can we humans decide on the next step.' The technology is there to support us. We just need to be able to make those decisions. That's exactly where we want to be as scientists."

The HPC equipment Bowman is acquiring for his project will be quite an upgrade. The new system is built upon Advanced Clustering Technologies' ACTblade e230, which provides up to four independent AMD EPYC compute nodes with 8 drives in one chassis. This blade combines storage, networking and computing in a single system to increase scalability and reduce datacenter complexity.
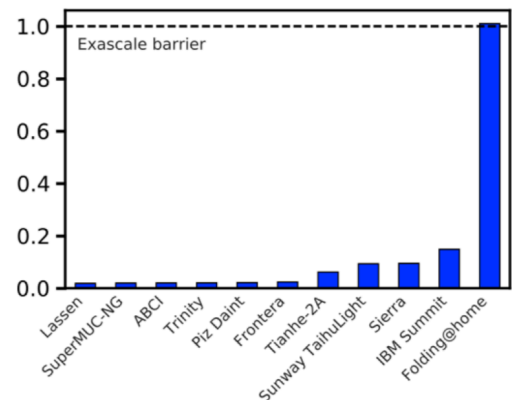
The processing speed of Folding@home and the next 10 fastest supercomputers, in exaFLOPS.

"Most of the data analysis we're currently doing relies on six-year-old high performance computing machines that offer 240 cpu cores. The new machines will use AMD EPYC 7742 processors providing 1,500 cpu cores. That's a nice boost of our throughput."

Bowman said he is excited by how high performance computing resources are able to meet the challenges of large-scale computational efforts like the one he and his volunteers currently face. "This just goes to

Case Study
Folding@Home

Dr. Bowman inspects the six-year-old high performance computing machines from Advanced Clustering that he replaced this year. The old system offered 240 cpu cores while the new one will provide 1,500 cpu cores.

show how complicated biology is," Bowman said. "This virus has 28 proteins. Humans have tens of thousands of different proteins."

The ongoing research is showing significant promise. "I am super excited about the progress we have made in studying the protein spike complex," said Dr. Bowman. "We are seeing big structural shifts. It leaves me jumping up and down with glee. The spike complex uses a conformational masking strategy, wherein it closes up on itself to protect key components of the protein from being recognized by our immune systems. To infect our cells, it has to open up and reveal these key pieces. Little is known about how this opening occurs, or what the open state looks like. Now we are seeing the whole process in our simulations."

So far, Folding@home has generated about 1 PB of data. That's about 1,000-fold more than would fit on most people's computers.

"Analyzing all that data to extract useful information, like the locations of sites that could be targeted with drugs, takes a lot of computing," Dr. Bowman said. "Advanced Clustering and AMD have teamed up to create a powerful system that is optimized to run our algorithms for churning through all the data to understand how SARS-CoV-2 works and identify new therapeutic opportunities."

Research in the future
The Folding@home project researches such modern day health challenges as cancer and Alzheimer's Disease.

"I hope that with the visibility the University is receiving with our Covid-19 work, our volunteers will stay on and drive us for results on the other public health challenges we will be addressing."

About the Folding@home Project
Folding@home is a distributed computing project designed to help scientists develop new therapeutics for a variety of diseases by simulating protein dynamics. This includes the process of protein folding and protein movements, and is reliant on the simulations run on the volunteers' personal computers. The Folding@home project is based at Washington University in St. Louis led by Dr. Greg Bowman. For more information, visit https://foldingathome.org.

About Washington University in St. Louis
Washington University in St. Louis is considered to be one of the top 10 private research universities in the nation. Virtually all faculty members engage in academic research, and more than 60% of undergraduates are involved in faculty research. The private research university is ranked 7th in the world for most cited researchers. The University received the 4th highest amount of NIH medical research grants among medical schools in 2019. The university was tied for 1st in the United States for genetics and genomics alongside Stanford and MIT in 2018. For more information, visit https://wustl.edu.

About Advanced Clustering Technologies
Advanced Clustering Technologies has been building customized, turn-key high performance computing clusters, servers and workstations since the company's founding in 2001. The company specializes in developing campus-wide supercomputers, which when fully utilized can help maintain and grow a university's competitive edge by attracting researchers and students from around the globe. Advanced Clustering's knowledgeable team of HPC experts provide phone and email support for the lifetime of your system. For more information, visit advancedclustering.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 data center. 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.