DELL Technologies intel

Crowdsourced Supercomputing

The Folding@home distributed computing project has created an exascale supercomputer — and is putting it to work in the fight against COVID-19 and other diseases.

FOLDING @HOME

Scientific Research | United States

Business needs

Folding@home draws on the collective processing power of more than a million client systems to support data- and compute-intensive scientific simulations.

Solutions at a glance

- Highly heterogeneous environment
- Globally distributed computing using client PCs
- On-premises and cloud servers

Business results

- Unlocking the secrets of COVID-19 and other diseases
- Enabling the visualization of complex protein dynamics
- Making massive amounts of compute available to scientists
- Showcasing the power of a global community

At its peak in 2020, the Folding@home distributed computing network grew to

2.4 exaflops

With a surge in participation in 2020, the Folding@home community grew to more than

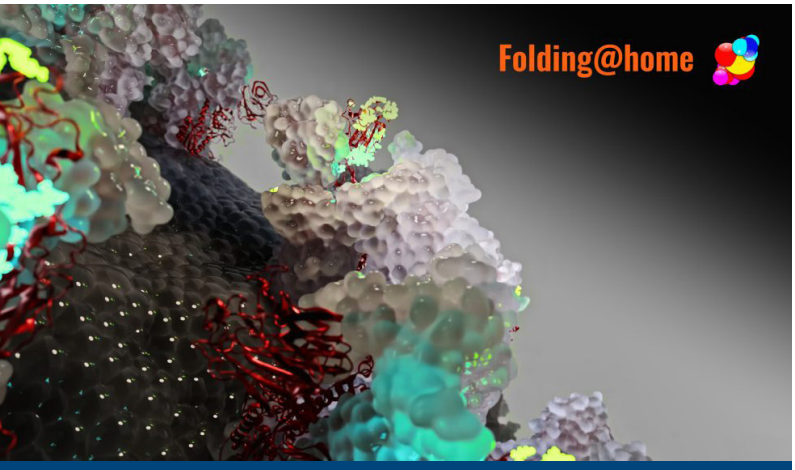
1 million contributors

Simulating protein dynamics — with lots of help

Folding@home is a distributed computing project for simulating protein dynamics, including the process of protein folding and the movements of proteins implicated in a variety of diseases. Folding refers to the way proteins are assembled in the cells that make up a human body. These proteins, which keep us healthy, assemble themselves by folding. But when they misfold, there can be serious consequences to a person's health.

Like cars and other machines in our world, proteins have myriad moving parts. However, there is no microscope for watching them in action. To visualize the movement of these molecular machines, scientists rely on computer simulations, which provide a way to see what's happening under the hood. But there's a catch: These simulations require an enormous amount of computational power — on the scale of a supercomputer.

To overcome this barrier in the road to scientific discovery, the Folding@home project harnesses the unused processing power of personal computers made available by volunteers around the world. To join the project, volunteers download a software app that runs small parts of much larger simulations for the Folding@home project. On the backend servers, the project's algorithms piece together the parts to create a composite simulation that allows scientists to better understand the biology of processes they can't observe directly.



Join the fold

The Folding@home distributed computing project invites anyone with a computer and an Internet connection to volunteer their personal computer to simulate proteins. To start folding, visit Folding@home.

> "Everyone with any brand of PC can join the fight against COVID-19 by sharing your unused computer power with @FoldingAtHome."
>
> *— Michael Dell, Founder and CEO, Dell Technologies*[1]

1 Twitter, Michael Dell tweet, March 26, 2020.

Fighting COVID-19 with exascale computing

In the years since its launch in 2000, the Folding@home project has broadened its focus to encompass a wide range of current biomedical problems, according to project director Dr. Greg Bowman, Associate Professor of Biochemistry & Molecular Biophysics at Washington University of St. Louis.

"We still work with protein folding, but now we focus more on understanding diseases, such as SARS and the SARS-CoV-2 virus, which is responsible for the COVID-19 disease," Dr. Bowman says. "We also use simulations to directly aid in the design of new antiviral drugs. We're doing similar things with the Ebola virus and proteins involved in Alzheimer's disease and cancer."

Currently, the Folding@home project is actively involved in the global effort to find a cure for COVID-19. In response to the pandemic, a huge wave of citizen scientists joined Folding@home to make their computers available to help researchers understand how the SARS-CoV-2 virus works and to identify new therapeutic opportunities.

"In under three months we had over a million new devices join the Folding@home project," Dr. Bowman notes. "With this, we were able to understand the moving parts of every possible protein from the virus and capture large structural changes."

With the surge of new participants, Folding@home's distributed computing network grew to encompass approximately 2.4 exaflops of computational power. That's more raw computing power than the world's largest 500 traditional supercomputers combined.[2] This level of theoretical performance earned the system the distinction of being the world's first exascale computer.[3]

"Within a couple of months, we had something like a hundredfold growth in participation in Folding@home," Dr. Bowman says. "And we had five times the performance of the world's fastest supercomputer, and that was with a

2 Folding@home via Twitter, @foldingathome, April 13, 2020.

3 Folding@home, "Citizen Scientists Create An Exascale Computer To Combat Covid-19," July 26, 2020.

very conservative estimate of what we had available on the Folding@home network. This scale allows us to do calculations that are inconceivable by any other means."

Support from the tech industry

When it experienced the huge surge in volunteer participation in 2020, Folding@home came face to face with some backend challenges, including network limitations. At that point, many tech companies, among others, stepped up and offered additional resources to the project, which has servers scattered around the world, including some in cloud installations.

"A lot of tech organizations, like Dell Technologies, reached out to us and asked, 'How can we help?'" Dr. Bowman says. "And that was really instrumental in our ability to make progress and harness this opportunity."

Today, teams from Dell Technologies are part of the legions of volunteers who make their unused processing cycles available to Folding@home. The project tracks the contributions of each of its volunteer teams, in terms of active CPUs, work unit counts and more. (For an example, see the Team: Dell Technologies report.)

VMware, a Dell Technologies company, is also actively involved in the Folding@home project. Its contributions include a VMware vSphere Appliance that contains the Folding@home client software. When a user configures the software and deploys the appliance, the Folding@home client is up and running and ready to go to work.

"We've got an incredible community — here in the United States and all around the world — contributing to the scientific process of understanding the COVID virus and our other research pursuits," Dr. Bowman says. "In terms of our volunteers, they are literally everywhere that is inhabited by human beings. This outpouring of support has been extraordinary."

A Readers' Choice Award

In December 2020, Folding@home was recognized with the HPCwire Readers' Choice Award for Best Use of HPC in Response to Societal Plights. In announcing the award, the HPCwire staff noted:

"The pandemic resulted in an unprecedented marshalling of HPC resources in order to tackle the Herculean computational tasks that faced medical and epidemiological researchers throughout the year. One of the earliest movers on this front was Folding@home, a crowdsourced research computing service that aggregates computational power provided by citizen scientists. Folding@home achieved historic levels of aggregate power during the pandemic thanks to millions of volunteer CPUs and GPUs — and then used that power to simulate the movements of SARS-CoV-2's critical proteins, a key task for drug design."

Sharing the learnings

One of the beauties of our scientific and high performance computing communities is an innate drive to share learnings in order to push all things forward. That's the way it is with the global Folding@home community.

"Folding@home has enabled hundreds of scientific papers that have been peer reviewed and published on all the different types of problems we have tackled," Dr. Bowman says. "It's driven big advances in protein folding, and it has contributed a great deal to the fight against COVID-19, the Ebola virus, Alzheimer's disease and cancer, among other problems."

In the spirit of sharing its learnings and resources, the project makes its open-source software programs and simulation models available on GitHub, Open Science framework, and AWS public datasets.

"We're all about teamwork, and the belief that together we can accomplish more than any of us could achieve on our own," Dr. Bowman says. "That's the way it was when we started down this path 20 years ago, and that's the way it is today."

The Folding@home distributed computing project is based at the Washington University School of Medicine in St. Louis, under the directorship of Dr. Greg Bowman. Drs. John Chodera from Memorial Sloan-Kettering Cancer Center and Vince Voelz from Temple University are also active in helping manage the project. Together, their three labs are the primary drivers of Folding@home. To learn more about the project, visit foldingathome.org.