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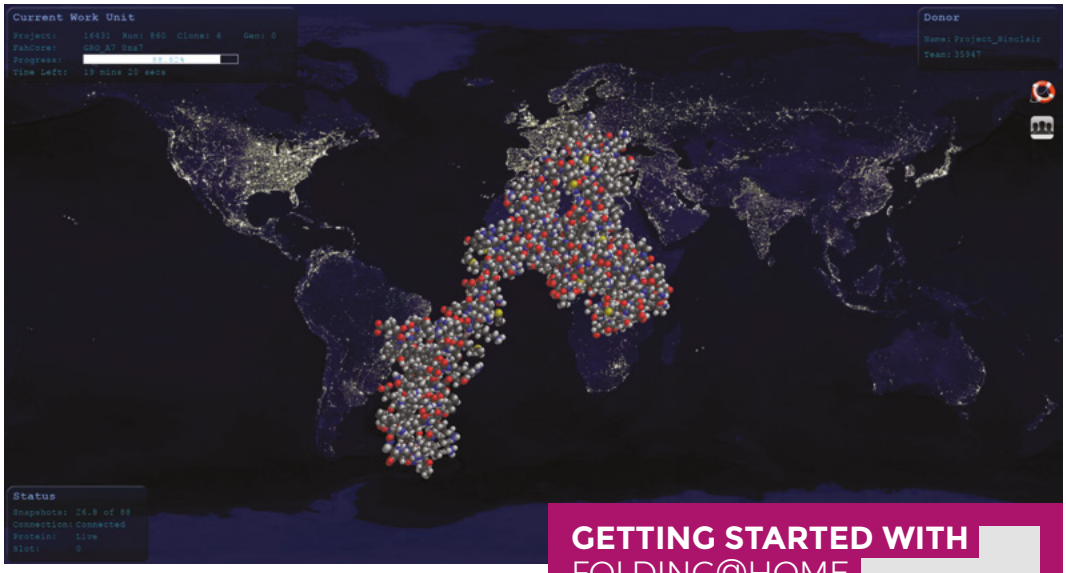
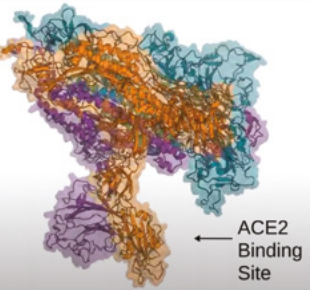
Folding@Home and the fight against COVID-19

Volunteers contribute computing power to help advance medicine



Right
The Folding@Home client viewer lets you see a visualisation of the molecule you're processing

Below
The opening motion of the 'Demogorgon' COVID-19 spike reveals the ACE2 binding site for interaction with human cells



Folding@Home is a project that allows a global volunteer network to contribute their processing power to help understand how proteins fold. This might sound obscure, but through the power of crowdsourced computing, researchers can understand how biological processes happen on a tiny scale, and from this, we can start to understand how different chemicals and agents might affect them. Traditionally, researchers studying protein folding have had to rely on expensive supercomputers to do their work. With Folding@Home, that has changed. Instead of utilising supercomputers, researchers can now submit workloads to the Folding@Home volunteer army of computers around the world and have their processing done for free. The more people that download the Folding@Home software and run it on their machines, the faster researchers can crack the secrets to challenging problems by submitting their processing jobs to the network (see box opposite).

GETTING STARTED WITH FOLDING@HOME

It's incredibly easy to get started with Folding@Home. Just head to **foldingathome.org** and download the appropriate client (available for Windows, macOS, and 64-bit Linux). Once this is installed, run the program to start folding. You can also set up a profile and join a team – various teams compete to see who can do the most work. There's a leader board at **stats.foldingathome.org/teams-monthly** and teams engage in a little friendly rivalry to see who can perform the most work units.

The easiest way of getting started with distributed computing to help fight COVID on an Arm device is to use the Fold for COVID system available from **foldforcovid.io**. It runs on a wide variety of Arm-based boards, including Raspberry Pi models 3 and 4. This is a Balena-based system that lets you download an image with everything set up and ready to go. Once you've burned the SD card, just power up your system and you're ready to go.

You can also download Folding@Home and Rosetta@Home client applications from Neocortix to volunteer your mobile phone in the efforts: **neocortix.com**.

Ben Hardwidge spoke with Dr Greg Bowman, Director of Folding@Home and Associate Professor at Washington University School of Medicine, to find out how this project – which has been backed by an all-star cast of tech industry heavyweights such as Microsoft, NVIDIA, AMD, and Arm – has been using its computing power to help the global fight against COVID-19.

"The simulation of the COVID-19 spike," says Bowman. "We've been calling it 'the Demogorgon' because of this opening motion it has – the opening of the three receptor-binding domains reminded us of the mouth of the Demogorgon from *Stranger Things*."

Analysing this opening motion was a key project for Folding@Home, as there was no way to observe it using standard experimental techniques. The aim was to understand how the COVID-19 spike protein opens up to bind to a protein called ACE2 on human cells. "Specifically, the spike has three receptor-binding domains that directly bind to ACE2," Bowman explained on his blog. "For the spike-ACE2 interaction to form, the spike's three receptor-binding domains must open up to reveal the binding interface."

In the image of the 'Demogorgon' spike on this page, each of the three proteins that form the spike has been given a different colour. These three proteins all need to spread apart to open up access to the ACE2 binding site, so that it can interact with the surface of human cells and initiate infection.

After the opening motion was visualised, the Folding@Home Twitter account explained that Folding@Home's next step was to "help figure out where the protein spends the majority of its time using thousands of simulations run by our donors. This kind of information will help to prioritise drug development efforts."

The Demogorgon isn't the only target for Folding@Home's work on COVID-19. At the moment, Bowman says Folding@Home is collaborating with Diamond (**diamond.ac.uk**) in the UK, an X-ray beamline company that's currently using macromolecular crystallography (MX) to study COVID-19.

Exploring beamline technology in depth is beyond the scope of this feature, but in basic terms, Diamond's techniques can enable researchers to observe the shape of biological molecules at atomic resolution experimentally, rather than virtually. If you head to **diamond.ac.uk/Covid-19.html**, you can see a video of how the COVID-19 crystallography setup works.

This is just the tip of the iceberg of the work Folding@Home has done to advance medicine. As well as working on COVID-19, the team has worked on Alzheimer's disease, Huntingdon's disease, cancer, and many others. You can find out more at **foldingathome.org**.

UNLOCKING THE POWER OF ARM FOR DISTRIBUTED COMPUTING WORKLOADS

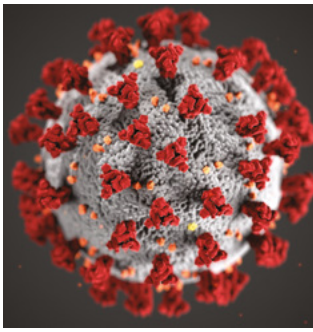
During the first half of 2020, as the COVID-19 virus began to spread, there was a concerted effort by tech industry leaders to support the efforts of Folding@Home and Rosetta@Home (a similar project to Folding@Home), the two leading distributed computing research projects. Initially, support for Arm-based devices for these projects was lacking. Recognising the opportunity to make a difference, a volunteer working group was formed by a team at Arm, working with its broader developer community and partners including Neocortix, Packet, Hivecell, and others, to perform the work necessary to bring these projects to Arm-based devices.

Traditionally, Folding@Home and Rosetta@Home have worked on desktop computers and leveraged GPUs to provide large amounts of processing power. However, the proliferation of mobile and IoT technology has caused an explosion in the availability of total compute power globally, much of it taking the form of smartphone handsets or other small devices. While more powerful desktop machines offer robust capabilities, they are outnumbered by lower-powered Arm-based machines, such as Raspberry Pi computers and mobile devices. This opportunity has led to the foundation of startups like Neocortix, who seek to offer distributed computing capabilities and platforms worldwide.

Work on Arm clients for both systems started at the beginning of 2020 with a team of experts from Neocortix, Balena, Linaro, and Arm working together to get both of these projects running on Arm machines. The Rosetta@Home version arrived first on 31 March. Since then, two Arm-based volunteer teams (crunching on Arm and Fold for COVID) have reached places 11 and 15 on the leader board (**boinc.bakerlab.org/rosetta/top_teams.php**). Not bad for teams that have only been around a few months!

Following Rosetta@Home, thanks to efforts by Neocortix, the more challenging technical implementation work to offer an Arm client for Folding@Home was completed in July 2020. At the time of writing this article, the Folding@Home client is now available for Arm devices in beta form from **foldingathome.org/beta**.

If you've got an Arm machine, why not join the effort, and together, let's get through this. ◻



Above
COVID-19 has caused suffering and chaos throughout the world in 2020

FIND OUT MORE

You can hear more about Folding@Home and how home computers are powering the future of medicine at the Arm DevSummit. Dr Greg Bowman will be speaking at 9am PDT on Tuesday 6 October. Find out more, and join for free at **hsmag.cc/fZDhrW**.

To learn more about how the COVID-19 work has been adapted to run on Arm processors such as that in Raspberry Pi, tune in to hear from Neocortix CEO Lloyd Watts at 10:50am PDT on Wednesday 7 October. Find out more and join for free at **hsmag.cc/2XoVcL**.