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Join the Fight Against COVID-19 with Your PC

The battle against the COVID-19 contagion highlights the heroic efforts of healthcare professionals and other frontline workers. As these heroes bravely perform their duties, those of us sheltered at home can do our share in helping find a cure to this infectious disease.

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Anyone with computing power to spare can take part in the Folding@Home (F@H) project, which is hunting down drug targets in the novel coronavirus. F@H needs massive processing power to be able to run simulations of how proteins fold and interact with potential drugs to treat COVID-19.

Proteins are complex molecules – made up of atoms – that perform most of the work in cells. Scientists are leveraging F@H to better understand the structure of proteins and how they behave. In particular, scientists want to know how atoms in a protein move relative to one another, as this can reveal binding sites or other potential drug sites.

As conventional lab-based experiments may not be enough to work out protein structures, the F@H project is there to support scientists with this task. Luckily, a growing army of “citizen scientists” is turning out to join the project. Starting with around 30,000 computers a few months ago, the project saw its total network expand to more than 400,000 since the coronavirus pandemic began.

This has raised F@H processing power to nearly2.5 "exaflops", or more than the combined capacity of the world’s top 500 supercomputers. F@H is spearheaded by the Washington University School of Medicine. Proponents noted that drug-target simulations require careful planning and design before they are carried out. The preparatory work also takes a huge amount of computing power, which is provided by the UK Science and Technology Facilities Council (STFC), through its Atos supercomputer located at Hartree Centre.

STFC says its involvement and support will help generate potential drugs more quickly as these will be widely distributed across a large network of F@H users.

“The way this project works is to take a possible compound and use computer simulations to see how it interacts with the virus,” STFC director Alison Kennedy explained. “It’s not a way to provide a vaccine, but if suitable antiviral compounds are identified, it could help to treat patients who have contracted the virus, which could help them to get better more quickly and reduce the burden on critical healthcare services.”

Meanwhile, scientists at the Hong Kong University of Science and Technology are also using the distributed computing power of F@H to search for other compounds that could hit those targets.

Source: pharmaphorum

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Published on : Tue, 21 Apr 2020

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