Press release

The UK's Hartree Centre deploys Atos supercomputer for Coronavirus treatment research

London, 14 April 2020 - Atos, a global leader in digital transformation, today reveals that one of the most advanced supercomputers in the world, the powerful BullSequana X1000 installed at The Science and Technology Facilities Council (STFC) Hartree Centre, is providing supercomputing power to assist in global computational drug discovery efforts to help combat COVID-19.

The Hartree Centre team is working closely with Washington University School of Medicine who lead the Folding@home project, which allows a global community of contributors to lend unused background capacity on their personal computers to power simulations of target drug interactions. While there is plenty of compute power[1] available to run these simulations, creating the drug structures to be simulated uses complex and memory-intensive methods that requires supercomputers. Creating these drug structures has therefore become the bottleneck in using the vast amount of compute power available across Folding@home.

By using some of the capability[2] of the Hartree Centre's Atos BullSequana X1000, the team are accelerating this process and creating new drug structures to be simulated fully across Folding@home's distributed compute power.

The Atos BullSequana X1000 systems at Hartree are also being used to support the work of CompBioMed, the European Centre of Excellence in Computational Biomedicine, as part of a global effort which includes hundreds of researchers from across the US and Europe to tackle different aspects of Covid-19. As an interim measure before a vaccine can be produced, pharmaceuticals are needed that can reduce the severity of the disease or that can be used as a preventive measure. This requires thousands of compounds to be screened in the form of advanced simulations, demanding high levels of compute power. The Hartree Centre systems are being used as part of an exceptional array of

[1] Over an exaflop in aggregate
[2] 800+ nodes of Intel Knights Landing processors

supercomputers across the world that are being harnessed to undertake these simulations.

> **Alison Kennedy, Director of the STFC Hartree Centre**, said: *"We have a hugely powerful supercomputing capability at our disposal here at the Hartree Centre, so our staff were naturally looking for opportunities to contribute to global computational efforts to tackle the COVID-19 pandemic. The way the folding@home project works is to take a possible compound and use computer simulations to see how it interacts with the virus. 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."*

The team hopes to identify antiviral therapeutics that disrupt one or more of the proteins necessary for the lifecycle of COVID-19, which would help to prevent the further spread of the virus.

> **Andy Grant, Global VP, Large Strategic HPC Deals, Atos**, added: *"Whether testing new compounds or performing target drug simulations at speed, analytics supported by super computers are uniquely placed to aid in the search for potential treatments of COVID-19. The UK has consistently been at the forefront of science and medicine and it is pleasing to see this country playing a key role in what has become an enormous coordinated international endeavour."*

Atos works with the Hartree Centre, located at Daresbury Laboratory, in support of closer collaboration between academia and industry through the power of supercomputing and deep learning.

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About Atos

Atos is a global leader in digital transformation with over 110,000 employees in 73 countries and annual revenue of over € 11 billion. European number one in Cloud, Cybersecurity and High-Performance Computing, the Group provides end-to-end Orchestrated Hybrid Cloud, Big Data, Business Applications and Digital Workplace solutions. The group is the Worldwide Information Technology Partner for the Olympic & Paralympic Games and operates under the brands Atos, Atos Syntel, and Unify. In the UK & Ireland around 10,000 employees deliver business technology solutions for some of the country's largest public and private sector organisations. Atos is a SE (Societas Europaea), listed on the CAC40 Paris stock index.

The purpose of Atos is to help design the future of the information technology space. Its expertise and services support the development of knowledge, education as well as multicultural and pluralistic approaches to research that contribute to scientific and technological excellence. Across the world, the group enables its customers, employees and collaborators, and members of societies at large to live, work and develop sustainably and confidently in the information technology space.

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About Folding@home

Folding@home (F@h) is a distributed computing project for simulating protein dynamics such as protein folding and movement, essential in understanding mechanisms of disease. It brings together a community of citizen scientists who volunteer to run simulations of protein dynamics on their personal computers with insights from this work helping scientists to better understand protein interactions, providing new opportunities to develop therapeutics.

F@h released the first wave of projects for simulating protein targets for COVID-19 on 10 March 2020 and will continue to release new simulation projects as more data becomes available.

Anyone with a personal computer can contribute directly to the project

The Folding@home project is playing an essential role in understanding the mechanisms of disease, and most importantly COVID-19. It is bringing together a community of 'citizen scientists' who are volunteering to run simulations of protein dynamics on their personal computers with insights from this work helping scientists to better understand protein interactions, providing new opportunities to develop therapeutics.

Find out more about Folding@home, including what you can do to help at the website.

Information on how to get started and download the software at https://foldingathome.org/start-folding/.

The Folding@home team recently held a Reddit #AskMeAnything for the public to ask questions about the project. Read more here.