Together against COVID-19

The current SARS-CoV-2 pandemic presents immense challenges both to society and to each individual. JSC, together with its partners in the Gauss Centre for Supercomputing and in PRACE, is doing its part to tackle these challenges: through a fast, unbureaucratic process, they are offering computing time and support on their HPC facilities to experts involved in studies dealing with the spread of the virus or with research on a medical or molecular level. Interested scientists can address their requests to Thomas Lippert (th.lippert@fz-juelich.de). JSC has already started supporting and cooperating closely with researchers investigating this new virus.

Together with Heidelberg University and the Frankfurt Institute for Advanced Studies, models and algorithms are being developed to predict the course of both the current but also of future possible pandemics. These models will enable researchers to answer the question of how targeted interventions, such as the reduction and readmission of human-to-human contact or the quarantining of infected persons, influence the spread of the virus.

On the medical and molecular level, computer-aided drug design (CADD) is a highly effective method to identify active ingredients against the virus. JSC, together with the Barcelona Supercomputing Centre and CINECA in Bologna, is supporting the European EXSCALATE4-CORONAVIRUS (E4C) project by providing computing resources on its HPC systems. A team of researchers with the participation of Paolo Carloni (Forschungszentrum Jülich, Computational Medicine – IAS-5/INM-9) and Giulia Rossetti (IAS-5/INM-9 and RWTH Aachen University) has already started corresponding screenings on the JURECA supercomputer. The aim of E4C is to identify molecules capable of targeting the SARS-CoV-2 virus, as well as to develop an effective tool for combatting future pandemics.

The group led by Birgit Strodel (Forschungszentrum Jülich, Structural Biochemistry – IBI-7) is also using CADD with the aim of identifying possible inhibitors of the COVID-19 main protease enzyme. The group plans to partner with experimental groups to assess both the *in vitro* and *in vivo* inhibitory capabilities of the most promising compounds with a view to speedy development for the treatment of COVID-19 infections. JSC is supporting the project by providing computing time on JURECA.

Finally, JSC is currently in contact with further research groups, for instance at Osnabrück University, the Max Delbrück Center for Molecular Medicine in Berlin, and Forschungszentrum Jülich, in order to explore possibilities for supporting their research on COVID-19.

Contact: Prof. Thomas Lippert, th.lippert@fz-juelich.de

Basic Operations at JSC from 19 March

In accordance with the preventive measures against the spread of the coronavirus published by the Board of Directors of Forschungszentrum Jülich on 17 March, JSC is adapting its range of services and switching to basic operations. Please check https://fz-juelich.de/ias/jsc/basic-op regularly for updates.

HPC systems and support:
The HPC systems are fully in operation. However, only half of the administrator team is on site to maintain them. The entire user support team is currently working from home. To report problems with the HPC systems and for support in using the supercomputers, please use the email address sc@fz-juelich.de (ticket system).

The support phone number, +49 2461-61-2828, is currently diverted to an answering machine; recorded messages are immediately forwarded as voice messages to sc@fz-juelich.de and then processed further.

Dispatch services can still be reached during the usual opening hours – whether on site in building 16.4., room 201, by phone on +49 2461 61-5642, or by email at dispatch.jsc@fz-juelich.de.

JuNet network services and IT security:
The number of on-site employees in the areas of network and IT security has been halved. Your usual contact persons can still be reached by email. If you experience any network issues, you can reach the network helpdesk as usual at +49 2461 61-6440 or by email at junet@fz-juelich.de.