Challenges of Forecasting COVID-19 During the 2nd Wave in 2020

Short-term forecasts of COVID-19 case numbers for the next 1–4 weeks can be a valuable tool for deciding which measures are necessary to prevent an oversubscription of hospital beds and ICUs, but how reliable are these predictions?

In "A pre-registered short-term forecasting study of COVID-19 in Germany and Poland during the second wave" published in *Nature Communication* (DOI: 10.1038/s41467-021-25207-0), scientists from JSC together with colleagues from Europe and the USA analyse their predictions collected for Germany and Poland as part of the German–Polish forecasting hub (https://kitmetricslab.github.io/forecasthub/forecast) during the second wave of COVID-19 (12 October – 19 December 2020). In the study, individual forecast performance is compared to the quality of ensemble forecasts, in which the individual forecasts are combined. The confidence interval of the ensemble forecasts provides good coverage, i.e. the 50 % confidence interval covers about 50 % of the data. The predictions of the ensemble compare well against the best single-model prediction and seem less prone to outliers.

The team's contributions to the German–Polish forecasting hub are now also included in the European Covid-19 Forecast Hub at https://covid19forecasthub.eu/.

Contact: Dr. Jan Meinke, j.meinke@fz-juelich.de

Disentangling the Switching Behaviour of Membrane Receptors

Molecular receptors in membranes control many processes in living cells and are also used as targets for drugs. Membrane receptors are activated by the binding of messenger substances known as ligands. Many membrane receptors are made up of different subunits, each of which can bind a ligand. This makes the activation mechanism complex.

In a recent publication in *Proceedings of the National Academy of Sciences*, entitled "Thermodynamic profile of mutual subunit control in a heteromeric receptor" (DOI: 10.1073/pnas.2100469118), a team of scientists including Prof. Gohlke from JSC at Forschungszentrum Jülich and Heinrich Heine University Düsseldorf, Prof. Benndorf from Jena University Hospital, and Prof. Schulz from Schmalkalden University of Applied Sciences carried out a very original functional analysis of the switching behaviour of the tetrameric CNG channel, which is involved in olfaction. The channel consists of four subunits that the authors concatenated, resulting in 12 configurations with permutated subunit order. Gohlke's group helped to develop an understanding of the most likely spatial subunit arrangement with molecular simulations. The energetic interaction of the various subunits at these receptors was precisely described using site-directed mutagenesis, functional electrical measurement, and mathematical analysis with complex Markov models.

The strategy described in the publication is also suitable for analysing other membrane receptors, which allows information to be gleaned on how ligands, including drugs, can switch such receptors on or off. The work was funded within DFG Research Group 2518, "Functional dynamics of ion channels and transporters – DynIon".

Contact: Prof. Holger Gohlke, h.gohlke@fz-juelich.de

Interpretation of Biomolecular Data Driven by Swarm Intelligence

The detailed structure of biomolecules is of key interest in understanding their crucial roles and interactions in the human body. In order to develop new drugs, for example, researchers must first determine these structures in complex experiments. However, the data obtained from such experiments is sometimes ambiguous and cannot be uniquely assigned to a specific structure. Scientists from JSC, KIT, DKFZ, and the University of Duisburg-Essen have jointly developed an AI-based method to evaluate such ambiguous data with the help of data-driven molecular simulations. This method is based on the concept of swarm learning in AI research. A supercomputer simulates many swarm members at the same time on over 1000 processors. Each member tests different parameter combinations and weights of the experimental data with a complementary physics-based computer

model. According to Marie Weiel, a doctoral researcher and leading author of the study, a crucial ingredient is the communication that takes place between the swarm members to cooperatively find an optimal solution, which is essential for the best possible interpretation of the data as molecular structures. The method thus delivers very accurate structures and at the same time uses the available computing resources – in this case JUWELS and the HPC cluster at KIT – very efficiently. The results were published in the journal *Nature Machine Intelligence* (DOI: 10.1038/s42256-021-00366-3).

Contact: Prof. Alexander Schug, al.schug@fz-juelich.de

New DFG Project FMhub Started

The performance of today's simulation software originates from increased parallelism instead of increased clock frequency. As a result, a sustainable software design is required to harvest the available parallelism. The rapid increase in diverse and hierarchically parallel hardware as well as the advent of accelerators (e.g. GPUs) make it harder for the maintainers of such simulation codes to retain flexibility and high performance for all parts of the code. In recent years, many communities therefore parted from the monolithic application approach and moved towards a collection of highly specialized components.

The new DFG-funded FMhub project aims to provide an open-source fast multipole method (FMM) for the scientific community as a flexible C++ library called FMSolvr to compute long-range interactions. The code will be made available together with community-building tools such as version control, a bug tracker, continuous integration, and deployment tools as well as comprehensive documentation. In contrast to high-level modifications, the parallelization layer of FMSolvr will also be addressed. By decoupling three integral parts (intracore, intranode, and internode parallelism), the goal is to increase maintainability and portability. The separation of these parallelization layers will allow the exchange of parallelization strategies arising in the future, e.g. different vectorization libraries or tasking frameworks. This modularization also aims to increase the decoupling of algorithmic components within the library to increase flexibility.

Together with Prof. Matthias Werner and his team from Chemnitz University of Technology, researchers at JSC will employ software engineering techniques to work towards these goals. The project started in September 2021 and will run for three years.

Contact: Dr. Ivo Kabadshow, i.kabadshow@fz-juelich.de

New EuroHPC JU Project ADMIRE

Exascale is heralded as a major breakthrough in computing that will pave the way for excellence in science and engineering, machine learning, and artificial intelligence. Its realization comes with a cohort of challenges, especially in processing and managing extremely large data sets. The legacy flat storage systems on classic HPC architectures are no longer capable of dealing with the emerging data-intensive computing requirements of applications. To address these concerns, hierarchical storage systems have been developed to balance computation and storage performance. However, there is still a need for adequate software interfaces which can leverage these HPC I/O architectures. It is in this area that the ADMIRE project (Adaptive Multi-tier Intelligent Data Manager for Exascale) will play a key role by creating an active I/O stack that exploits all layers of HPC I/O. This will be achieved by implementing an intelligent global coordination mechanism, malleability of computation and I/O, and the integrated scheduling of storage resources. An operational software-defined framework will be developed based on scalable monitoring and control, with aligned control and data paths as well as embedded control points which orchestrate the system components and applications. The envisioned framework will be co-designed by the project partners with several use cases from diverse scientific areas, including climate/weather, life sciences, remote sensing, software heritage, and deep learning.

ADMIRE is coordinated by Universidad Carlos III de Madrid (Spain). JSC will contribute to the work packages “Application Co-Design” (WP7), “Intelligent Controller” (WP6), and “Dissemination and Exploitation” (WP8). JSC is the lead partner for WP7, which will produce an enhanced version of the existing applications based on the co-design methodology developed during the project lifetime. ADMIRE is funded through the EuroHPC Joint Undertaking and is co-funded by the German Ministry for Education and Research (BMBF). The project formally started on 1 April 2021 and will last for three years.

Contact: Dr. Shahbaz Memon, m.memon@fz-juelich.de

Second Virtual PRACE Summer of HPC

The Summer of HPC (SoHPC) programme, now in its ninth year, allowed over 60 university students from all scientific disciplines to spend two months working remotely with PRACE partner organizations. In addition to allowing students to work on research projects in a multidisciplinary and international environment, the aim of the SoHPC programme is to promote and disseminate scientific culture among the upcoming generation of researchers, encouraging the students participating in the programme to become the computational scientists of tomorrow. Furthermore, through the participants’ sharing of their experiences in blog posts and video presentations, the programme aims to ensure that the students themselves become ambassadors for supercomputing at their respective institutions.

This year, three students – namely Arthur Guillec (France), Tristan Michel (France), and Marc Túnica (Spain) – joined JSC remotely for the summer to gain first-hand experience in day-to-day research. After an online training week for all students hosted by the Irish Centre for High-End Computing in Dublin, the three students teamed up and started working on their assigned projects at JSC. Arthur and Tristan were supervised by Ivo Kabadshow and worked on parallelizing the Fast Multipole Method with HPX, while Marc was supervised by Marcel Rodekamp and dealt with High Performance Quantum Fields. They produced two video presentations that can be found at https://bit.ly/3C1PoqS and at https://bit.ly/3lEk7Uv.

Contact: Dr. Ivo Kabadshow, i.kabadshow@fz-juelich.de