

Two New Research Groups Established at the John von Neumann Institute for Computing in Jülich

The three founding partners of the John von Neumann Institute for Computing (NIC)—namely the Forschungszentrum Jülich (FZJ), Deutsches Elektronen-Synchrotron DESY Zeuthen and GSI Helmholtzzentrum für Schwerionenforschung Darmstadt—support supercomputer-oriented research and development through research groups dedicated to selected fields of physics and other natural sciences. Recently, two new groups have formed for the field of computational biology, but place their respective emphases on different aspects.

The NIC research group, “Computational Biophysical Chemistry” began work at FZJ at the end of April, 2017. The group is headed by Holger Gohlke from Heinrich Heine University Düsseldorf. Prof. Gohlke obtained his diploma in chemistry from the Technische Universität Darmstadt and his PhD from the Philipps-Universität Marburg. He subsequently conducted postdoctoral research at The Scripps Research Institute, La Jolla, USA. After appointments as an assistant professor in Frankfurt and a professor in Kiel, he moved to Düsseldorf in 2009. Prof. Gohlke was awarded the “Innovationspreis in Medizinischer und Pharmazeutischer Chemie” (innovation award for medicinal and pharmaceutical chemistry) by the German Chemical Society (GDCh) and the German Pharmaceutical Society (DPhG), the Hansch Award of the Cheminformatics and QSAR Society, and the Novartis Chemistry Lectureship. His current research focuses on the understanding, prediction, and modulation of interactions involving biomolecules and supramolecules from a computational perspective. Prof. Gohlke’s group

develops and applies techniques founded in structural bioinformatics, computational biology, and computational biophysics. In line with these research interests, the group is excited about the possibility of a dual affiliation with the Jülich Supercomputing Centre (JSC) and the Institute of Complex Systems/Structural Biochemistry (ICS-6). This will pave the way to bridging the supercomputing capabilities of the JSC with the structural biochemistry capabilities of the ICS-6 in order to address complex questions regarding the structure, dynamics, and function of biomolecules and supramolecules.



The other new group, “Computational Structural Biology” is led by Alexander Schug. It became operational in September, 2017 and is affiliated with the JSC. Dr. Schug studied physics at the University of Dortmund and obtained his PhD 2005 at the Forschungszentrum Karlsruhe and the University of Dortmund. Afterwards, he has worked as Postdoctoral Scholar in Kobe (Japan) and San Diego (US) before becoming an Assistant Professor in Chemistry (Umeå, Sweden). In 2011, he



returned to Germany to head a research group at the Karlsruhe Institute of Technology (KIT). Dr. Schug has received multiple awards, including a FIZ Chemie Berlin Preis from the GdCH and a Google Faculty Research Award 2016. His general research interests include theoretical biophysics, biomolecular simulations, and high-performance computing. In this role, his group leverages the incredible, constantly growing capabilities of HPC by integrating data from multiple sources in simulations to gain new insight about topics ranging from biomolecular structure and dynamics at atomic resolution to understanding neural cell tissue growth and differentiation. As understanding these properties is key to understanding biological function, this work promises to provide significant new insight with impact in fields ranging from basic molecular biology to pharmacological and medical research.

Further information about these new and all other NIC research groups can be found on our web site [1].

Reference

- [1] **John von Neumann Institut:**
http://www.john-von-neumann-institut.de/nic/EN/Research/ResearchGroups/_node.html

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