

HITSters are part of new faculty at Heidelberg University

With the aim of pooling its expertise in the field of technology and engineering as well as expanding its range of research and subjects in

The focus here is not on traditional technologies, however, but on innovative engineering approaches. The Faculty went into operation on 1 October 2021. The founding dean is Guido Kanschat, who is a member of the management board of the Interdisciplinary

lar Biomechanics), and **Vincent Heuveline** (Data Mining and Uncertainty Quantification) are part of the new Faculty. These researchers bring with them their vast expertise in computational research on biomolecular systems and materials as well as in engineering mathematics and high-performance computing and are also members of the IWR. Additionally, Rebecca Wade is a member of the Center of Molecular Biology Heidelberg (ZMBH) and is also one of the IWR directors.

The Faculty of Engineering Sciences comprises the areas of computer engineering, engineering molecular systems, and carbon-based materials sciences in addition to molecular biotechnology. These high-profile areas are enhanced by the presence of more scientists from cross-disciplinary research centers at the University: the IWR, the Center for Molecular Biology, the Biochemistry Center, and the BioQuant Center.



a dynamically developing field of competence, Heidelberg University has founded a new faculty: the Faculty of Engineering Sciences.

Center for Scientific Computing (IWR). HITS group leaders **Rebecca Wade** (Molecular and Cellular Modeling), **Frauke Gräter** (Molecu-



Via Data

The HITS blog can be found on the "Scilogs" portal at <https://scilogs.spektrum.de/via-data/>.

HITS

And again: "Highly Cited Researcher" at HITS

For six years running, HITS group leader **Alexandros Stamatakis** (CME) has been named one of the most cited researchers worldwide, according to this year's "Highly Cited Researchers" list by the U.S. company Clarivate Analytics. The ranking is an important indicator for the impact of a researcher's scientific publications. Stamatakis is listed in the ranking with a primary affiliation at



HITS, his secondary affiliation is the Karlsruhe Institute of Technology (KIT). He appears in the category "Cross-Field." It comprises researchers with substantial influence across several fields during the last decade. With this category, the ranking takes into account that bleeding edge research areas are often interdisciplinary.

Searching for a way out of the brain fog caused by COVID-19

HITS is a partner in the new EU-funded research program BRAVE, which has proposed that the problem of COVID-19 brain inflammation be tackled by computer-de-



signed molecules. The project was selected for European Commission (EC) funding after a call by the Human Brain Project (HBP) that encouraged the use of the HBP and EBRAINS infrastructure for COVID-19-related research. The University of Turin (Italy) serves as the project coordinator, with the other partners being the University of Pavia (Italy), the Forschungszentrum Jülich (Germany), and the MCM Group (Leader: **Rebecca Wade**) at HITS.

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New employees and visiting scientists

Master's students:

Vincent Bronner (SET); Marco Vetter, Freyja Walberg (both PSO); Xinyi Zhang (CME)

Pre-docs:

Lynn Buchele, Quentin Coppée (both TOS); Alexander Holas (PSO); Wei Liu (NLP); Stiv Llenga (CCC); Micaela Menegaldo (AIN); Anastasis Togkousidis (CME)

Post-docs:

Eva Laplace (SET); Ghulam Qadir (CST)

Administrative Services:

Yashasvini Balachandra (Controlling)

Visiting scientists:

Marcel Meyer, Heidelberg University, Germany (MBM); Melanie Schienle, KIT Karlsruhe, Germany (CST); Dandan Wei, CSC Scholarship, China (SET)

HITS groups 12/2021: *Astroinformatics (AIN), Computational Carbon Chemistry (CCC), Computational Molecular Evolution (CME), Computational Statistics (CST), Data Mining and Uncertainty Quantification (DMQ), Groups and Geometry (GRG), Molecular Biomechanics (MBM), Molecular and Cellular Modeling (MCM), Natural Language Processing (NLP), Physics of Stellar Objects (PSO), Scientific Databases and Visualization (SDBV), Stellar Evolution Theory (SET), Theory and Observations of Stars (TOS).*

HITSters

More than the sum of its parts: Combining models to improve COVID-19 forecasts

Sometimes, it is possible to obtain a clearer picture by combining different approaches in a collaborative way. Scientists from the German-Polish COVID-19 Forecast Hub took this approach when evaluating the strengths and weaknesses of forecasting models and assessed whether combined ensemble forecasts can improve upon single-model predictions. The study has been published in Nature Communications and featured in the journal's Editors' Highlights.

"We created a comparison platform for different models and fostered the exchange between modeling teams with the goal of improving individual models and their overall combined prediction," stated **Melanie Schienle**, professor of Statistics and Econometrics at KIT and a current guest scientist at HITS who leads the project team together with CST group leader **Tilmann Gneiting**. The Forecast Hub follows an open science approach. It evaluates forecasts and preserves the entire history of the model outputs. "Models often look a bit better than they are when applied in retrospect, and we wanted to avoid that pitfall," added **Johannes Bracher** (HITS and KIT), the first

author of the study. "We publicly specified the rules of the comparison in advance, similar to in pharmaceutical or medical trials."

The study period covers the onset of the second wave in Germany and Poland, from 12 October to 19 December 2020. This



period is characterized by tightening non-pharmaceutical interventions, which subsequently led to a decrease in cases in Poland as well as to a plateau and a renewed increase in cases in Germany. Thirteen independent teams provided probabilistic real-time forecasts of COVID-19 cases and deaths for lead times of one to four weeks. Overall, ensemble forecasts showed good relative performance – especially in terms of uncertainty quantification

– and were typically on par with the best single-model predictions. Moreover, their performance was less variable across different weeks. "Thus, we can clearly see the benefit of this collaborative approach, which provides more stable performance," said Johannes Bracher. "It's like the famous quote by Aristotle: 'The whole is more than the sum of its parts.'"

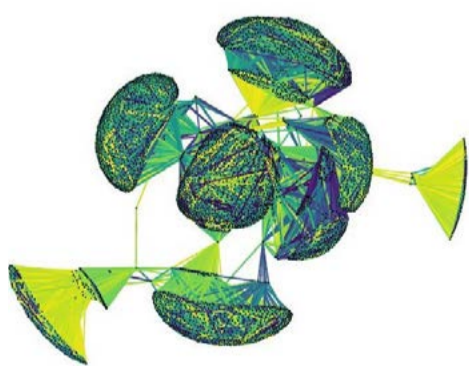
The evaluations also highlight the fact that COVID-19 remains highly challenging to predict, and ensemble prediction is also sometimes off target. "Overall, the predictions were very heterogeneous across models, so different models did not agree at all about what was going to happen next," Melanie Schienle added. "By considering the different forecasts together, we can gain a more realistic assessment of the degree of uncertainty."

Publication: Bracher, J., Wolfram, D., Deuschel, J. et al. A pre-registered short-term forecasting study of COVID-19 in Germany and Poland during the second wave. Nat Commun 12, 5173 (2021). <https://doi.org/10.1038/s41467-021-25207-0>

Research

Beyond the limits: The HITS Lab

An essential characteristic of HITS is its interdisciplinarity. Collaboration across disciplinary boundaries, however, is challenging. While interdisciplinary work at HITS is already ongoing, the Institute aims to address this challenge more intensively. One tool to foster collaboration is called the HITS Lab – an internal funding program for projects in which at least two groups from different disciplines at HITS come together to work on a shared topic. The participating groups can hire researchers as part of the HITS Lab, and these researchers are – in turn – jointly supervised by the respective group leaders. Four HITS Lab projects have been launched by the autumn of 2021.



"HITS is home to many a scientific beacon," stated HITS Scientific Director **Frauke Gräter**. "With the HITS Lab, we aim to seek new approaches in the voids between these beacons and to build bridges between scientific cultures."

The first project began at the end of 2019, when Frauke Gräter (MBM) and **Michael Strube** (NLP)

together with Vera (from the English Department at Heidelberg University) – working within the framework of a project at the Marsilius Kolleg at Heidelberg University – asked, "Does the quality of writing influence scientific impact?" Also at the end of 2019, Michael Strube, **Wolfgang Müller** (SDBV), and colleagues obtained funding from the BMBF for the DeepCurate project. The scientific idea came from the HITS Lab initiative, as well.

Two other HITS Lab projects began in 2020: Emulation in Simulation is a collaboration between Frauke Gräter, **Friedrich Röpke** (PSO), and **Tilmann Gneiting** (CST) with the aim of estimating partial results via the clever use of machine-learning techniques – so-called emulators – and thereby of reducing computational effort.

Another project, Geometry and Representation Learning, is a collaborative effort between **Anna Wienhard** (GRG), Michael Strube (NLP), and their groups that investigates the use of non-Euclidean geometries within natural language processing. This project has gained visibility in the machine-learning community. Two papers have already been published and successfully presented at international conferences on machine learning (NeurIPS 2020, IICML 2021). A third publication was recently accepted as a spotlight presentation at the NeurIPS Machine Learning Conference from 10–13 December.

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Beyond the limits



The Charts