## Call for "HITS Journalist in Residence" is open

HITS has launched a new round of applications for the Journalist in Residence" program 2020/2021. It offers a stay of three to six months for each year, with a compensation of € 5,000 per month. The program is geared towards science journalists with at least five years of experience and a focus on the natural sciences and technology. One of its goals is to encourage dialogue between journalists and researchers, thus providing journalists with a better understanding of the way research works and how researchers think. Journalists are not expected to publish anything related to HITS in return. Instead, the program supports free and independent journalism. The deadline for applications is 10 September 2019.

Since 2012, HITS has hosted seven "Journalists in Residence"– from the U.S., Spain, Germany, and India – many of them utilized their stay to start long-term projects. For example, science journalist Volker Stollorz wrote the concept for a German Science Media Center during his stay at HITS. In 2016, the "Science Media Center Germany" was established.

## The Anniversary: COMBINE Meeting

The "Computational Modeling in Biology" Network (COMBINE) was founded ten years ago as an initiative to coordinate the development of the various community standards and formats in systems biology, synthetic biology and related fields. For the 10th anniversary, the network members will meet at the Studio Villa Bosch in Heidelberg from 15-19 July. COMBINE 2019 will be a workshop-style event with invited lectures, oral presentations and posters, but also reserving enough time for afternoon breakout sessions. It will include talks about the COMBINE standards and presentations of tools using these standards and similar topics. The meeting is organized by international members of the network, including **Martin Golebiewski** and **Wolfgang Müller** from the Scientific Databases and Visualization (SDBV) group at HITS. More information: www.co.mbine.org

**"We are thinking beyond the limits of our research fields."** Wolfgang Müller, HITS Scientific Director

## Two Humboldt Fellows at HITS

Since 2012, HITS has been the host for eight fellows of the Humboldt foundation. This year, the institute was glad to welcome two more "Humboldtians": After a first stay last year, **Prof. Kevin Hinkle** (University of Dayton, Ohio/USA) has returned to the MBM group for another three months as a postdoctoral fellow to pursue research on bio-polymers under tension, using multi-scale approaches. **Dr. Ariane Nunes-Alves** was awarded a Capes-Humboldt Research Fellowship for postdoctoral research for two years, beginning on 1 July 2019. She has been working as a postdoc researcher in the MCM group since 2018. Her research focus is on methods to predict the residence time for drugs that are bound to proteins.
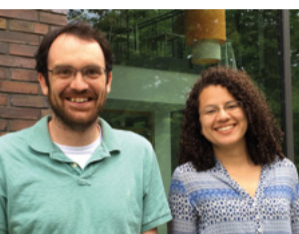
## HITSters "on board"

Recently, MCM group leader **Prof. Rebecca Wade** has been appointed to the Editorial Board of the Journal of Chemical Information and Modeling (JCIM) from the beginning of 2019. MCM postdoc researcher **Dr. Ariane Nunes-Alves** has been appointed to the Early Career Board of the same outlet, an American Chemical Society Journal.

## New employees and visiting scientists

**CME:**   Johanna Wegmann, master's student
**CST:**   Dr. Timo Dimitriadis, employee
**MBM:**   Fabian Kutzki, visiting scientist / Martin Richter, master's student / Dr. Nicholas Michelarakis, employee /
           Dr. Markus Kurth, Postdoc
**MCM:**   Anton Hanke, bachelor's student
**PSO:**   David Bubeck, master's student
**SDBV:**  Natalia Simous, employee

*HITS groups (07/2019)*
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).

## "Deep learning" and mathematical statistics: Interdisciplinarity bears fruit



Almost four years ago, members of the two HITS research groups Astroinformatics (AIN) and Computational Statistics (CST) began an exchange of scientific ideas that led to two publications: **Dr. Sebastian Lerch** (CST) developed a neural network that provides better temperature predictions than classical standard methods. Lerch had been inspired by an internal seminar on machine learning at HITS held by **Dr. Antonio D'Isanto** (AIN). At the same time, Antonio D'Isanto and **Dr. Kai Polsterer** (both from AIN) developed a new method for predicting photometric redshift using deep learning techniques. The prediction quality exceeds that of all previous reference methods because the AIN group uses the "continuous ranked probability score" (CRPS), a mathematically and statistically based quality measure with which the CST group works.

"We developed our ideas together for over a year," recalls Sebastian Lerch, who adopted the approaches of his AIN colleagues in the construction of the neural network. The basic idea of the later publication had been previously unknown in the field, which is one reason that the work published in the "Monthly Weather Review" is one of the most read current publications in this leading scientific journal.

"We had intensive discussions with our colleagues about the prediction quality of machine learning systems," reports AIN Group Leader Kai Polsterer. "It turned out that the CRPS might be a good solution – and it was." With this new method, astronomers can now predict redshift, a cosmological measure a age and distance - for all celestial objects, be they stars, galaxies, or quasars.

"The close proximity of the meeting points at HITS (such as the café bar) was very helpful," emphasizes Sebastian Lerch, who now heads his own research group at KIT. Kai Polsterer adds that "the family atmosphere and the openness towards other fields play into the idea of interdisciplinarity at HITS."

*Rasp, S. and S. Lerch: Neural networks for post-processing ensemble weather forecasts, Mon. Weather Rev., Vol. 146, Nov. 2018. DOI: 10.1175/mwr-d-18-0187.1*
*D'Isanto, A. and KL Polsterer: Photometric redshift via deep learning. Astronomy & Astrophysics, Vol. 609, Jan. 2018. DOI: 10.1051/0004-6361/201731326*
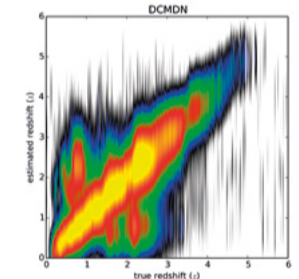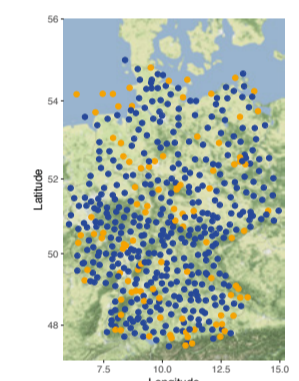
## Wolfgang Müller: "We think outside the box!"

When Wolfgang Müller assumed leadership of the group "Scientific Databases and Visualization" (SDBV) almost ten years ago, he was entering new territory. "Until then, I had had very little involvement with biological processes," recalls the physicist and doctor of computer science. However, he had gained vast experience with efficient, interactive search methods in complex data, such as images, and Müller found it exciting to work with "real" users instead of hypothetical usage scenarios.

Theory, experiments, and practice have played equal roles in Wolfgang Müller's career: He wrote his physics diploma thesis on bursting bubbles in soap foam and earned his computer science diploma with a thesis on data mining. In 2001, Müller obtained his doctorate at the Université de Genève on content-based image retrieval, later completing post-doctoral research at the University of Bamberg in 2008. He then worked as a developer at "Freiheit.com" in Hamburg, where he developed together with colleagues a website that millions of people still use today.

Müller's interdisciplinary profile fit well with the SDBV Group, where experienced biologists, biochemists, and chemists work together with software developers on the integration of data into the life sciences.

The group focuses on developing the reaction kinetics database SABIO-RK and managing data in national and international research projects and initiatives, such as de.NBI, LiSyM, FAIRDOM, and MESI-STRAT. HITS database specialists contribute their many years of experience – from which the data management platform SEEK emerged alongside SABIO-RK – as part of the transnational FAIRDOM project. "We want users to exchange their data according to the FAIR principle," says Wolfgang Müller, "which means that the data should be Findable, Accessible, Interoperable, and Reusable."

Müller's group is also committed to data standards in research. It is active in the COMBINE (COmputational Modeling in Biology NEtwork) network, which promotes the development of various standards and formats in systems biology, synthetic biology, and related disciplines. HITS will host the 10th COMBINE Meeting, which will bring together leading scientists and members of organizations such as ISO and DIN from 15–19 July 2019.

The proverbial idea of thinking outside the box also aids Wolfgang Müller in his function as HITS Scientific Director, which he will hold for a rotation of two years from the beginning of 2019. "We are thinking outside the box more and more," the 49-year-old states as he reflects upon the increasing number of interdisciplinary projects and publications from the HITS research groups. "We can certainly do even better. After all, as our motto states: 'Think beyond the limits!'"

Heidelberger Institut für
Theoretische Studien

HITS

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