Science and journalism: HITS at "Wissenswerte" in Heidelberg

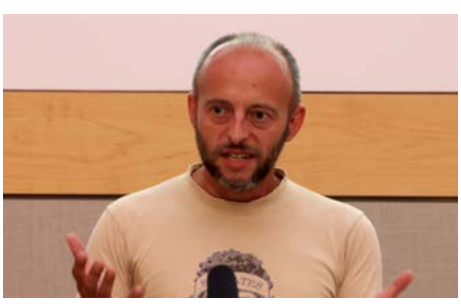
From 30 October to 1 November 2024, the largest conference for science journalism in the German-speaking world (Wissenswerte) was held in Heidelberg for the first time. More than 300 participants attended the conference on the University premises, where the program offered high-level panel discussions, lectures and workshops on current journalistic and academic topics.

Among other Heidelberg-based institutions, HITS was also present with a booth – a good occasion to network and introduce the institute to interested science journalists. Particularly noteworthy was a new format called "Science Insight", with short presentations on current scientific topics, where one HITSter had the opportunity to showcase his research. "Generating Proteins with Flow Matching and Geometric Algebra" was the title of the short talk by **Leif Seute**, a PhD student in the Machine Learning and Artificial Intelligence (MLI) group at HITS. He completed his master's degree in theoretical and computational physics at the University of Heidelberg and specialized in geometric deep learning for molecular science. In his talk, he emphasized the crucial role of proteins as a building block of life and demonstrated how computer-aided design of proteins opens up new possibilities in the development of drugs, vaccines or sensors.

Via Data
New HITS Blog Article on „Scilogs" about „Digital Baby Twins" - Elaine Zaunseder (DMQ)
https://scilogs.spektrum.de/via-data/doppel-leben-digital-baby-twins/

HITS

Time and again: Alexandros Stamatakis named Highly Cited Researcher



For nine consecutive years, HITS group leader **Alexandros Stamatakis** (CME) has been named one of the world's most cited researchers by Clarivate Analytics. The ranking recognizes researchers whose publications are among the top 1% in citations within their fields. The current list includes approximately 6,900 designations of researchers from 59 countries. Stamatakis is ranked with a primary affiliation at the Foundation for Research & Technology – Hellas (FORTH) in Crete, Greece, where he leads an ERA (European Research Area) Chair project focused on computational biodiversity research, while maintaining a secondary affiliation with HITS.

Alexandros Stamatakis develops software for analyzing huge biological datasets. His research focus lies on the development of scalable methods and software for the analysis of molecular sequence data. His work has significantly advanced evolutionary biology. Since 2010, he has led the "Computational Molecular Evolution" research group at HITS and has been a full Professor for High Performance Computing at Karlsruhe Institute of Technology (KIT) since 2012. During the ERA Chair project, he remains an associated group leader at HITS and a full professor on leave at KIT, where he continues his teaching activities.

New employees and visiting scientists

Postdocs:	Beni Egressy (MLI), Georgios Lioutas (PSO), Kushal Singh (MCM)
PhD students:	Torben Berndt (MLI), Catarina Corte-Real (AIN), Rimpa Pal (HITS Scholarship, DMQ)
Master student:	Tobias van Lier (TOS)
Research Associate:	Arno Fricke (SDBV)
Visiting scientist:	Veronica Agaeva (PSO, Heidelberg University)

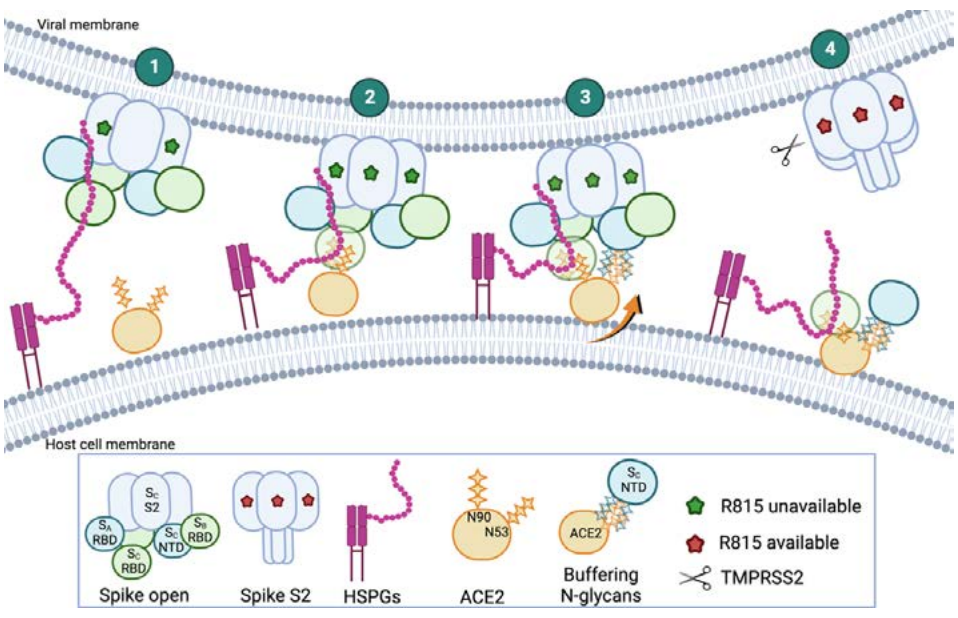
HITS groups (12/2024): *Astroinformatics (AIN), Computational Molecular Evolution (CME), Computational Statistics (CST), Data Mining and Uncertainty Quantification (DMQ), Machine Learning and Artificial Intelligence (MLI), Molecular Biomechanics (MBM), Molecular and Cellular Modeling (MCM), Natural Language Processing (NLP), Physics of Stellar Objects (PSO), Scientific Databases and Visualization (SDBV), Stellar Evolution Theory (SET), Theory and Observations of Stars (TOS).*

HITSters

Polysaccharides as Accomplices in SARS-CoV-2 infection

An international team of scientists at Heidelberg Institute for Theoretical Studies (HITS) and Heidelberg University has published new findings on how specific polysaccharides act as "accomplices" in the SARS-CoV-2 infection mechanism. The study, published in Proceedings of the National Academy of Sciences USA (PNAS), highlights the critical role played by specific polysaccharides expressed on the host cell surfaces called heparan sulfate and on the protein N-glycans. These polysaccharides were previously thought to only assist the virus by helping its spike protein bind to the host cell receptor ACE2. However, their varying expression in different cells and individuals appears to influence susceptibility to the virus.

"We were interested in gaining a deeper understanding of how heparan sulfates are involved in the SARS-CoV-2 infection mechanism and how they relate to host cell susceptibility," says HITS group leader



Rebecca Wade. Using atomic-level molecular simulations, the researchers explored how heparan sulfate and N-glycans strengthen the interaction between the spike protein and ACE2. "Only by using simulations could we analyze the molecular details and see that heparan sulfate and N-glycans synergistically stabilize the spike/ACE2 complex," says **Giulia Paiardi**, the study's first author.

This discovery opens up new therapeutic possibilities for combating SARS-CoV-2. "If we can develop suitable heparan sulfate mimetics, we might be able to prevent the virus from binding to and entering human cells," concludes Rebecca Wade.

Research

Frauke Gräter: "I will miss HITS."

How does it feel to leave HITS after having spent almost a third of one's life there, and to move on to lead a Max Planck Institute? "For me, it's the right step at the right time," says **Frauke Gräter**, "but I'm leaving with a heavy heart." The biophysicist, and longtime leader of the HITS research group Molecular Biomechanics, will assume her new role as director at the Max Planck Institute for Polymer Research in Mainz as of January 2025.
More than 15 years ago, she first met HITS founder Klaus Tschira during an interview for a group leader position at EML Research, HITS' predecessor institute. She was surprised — by his curiosity, his warmth, and his love for science. "Klaus Tschira reassured me that one can do research out of pure love for the subject, and that basic research is essential for gaining knowledge." At that time, Gräter was returning from Shanghai, where she had led a junior group at a partner institute of the Max Planck Society. She had previously worked at the Max Planck Institute for Biophysical Chemistry in Göttingen and at Columbia University in New York. That first conversation in the fireplace room of the Villa Bosch led to many others, as the new group "Molecular Biomechanics" was a key component of HITS, which Klaus Tschira founded on the new campus a few months later. "Freedom and autonomy, being able to set one's own research agenda without micromanagement — this was the prevailing atmosphere I've experienced."

From Spider Silk to Collagen: Full Force in Protein Research
Frauke Gräter's research goal has been to understand how mechanical forces influence biological processes, especially in proteins. Through studies on the structure of spider silk and blood coagulation, she actively contributed to the institute's early years, witnessing its growth from 5 to 13 groups and — after the founder's passing in 2015 — the transition and consolidation into sustainable, resilient structures that both preserve and build upon the founder's legacy. She played a significant role in this as Scientific Director of HITS in 2021 and 2022.

As a scientist, she was successful during this period as well. In 2017, she received the "PRACE Ada Lovelace Award" for outstanding contributions to high-performance computing and, in 2020, an ERC Consolidator Grant for her research on the protein collagen, which gives stability to connective tissues in bones, ligaments, and skin. Together with Rebecca Wade — "a fantastic colleague" — she developed the SIMPLAIX project, which combines simulations with AI.
The institute also holds personal memories for her: "The great food in the cafeteria and the beautiful park, where we could have professional discussions or just sit together — sometimes even in winter, with mulled wine and guitar music."
"HITS has great potential," Frauke Gräter summarizes. "As a relatively small, interdisciplinary institute, it's like a speedboat, able to quickly take on and advance new research directions, thanks in part to the funding by the Klaus Tschira Stiftung."
What will Frauke Gräter take with her to Mainz? "So much of what I've experienced at HITS: the openness to unconventional collaborations, the sense of open spaces that foster communication, and the drive to bring science to the public. I will miss HITS!"

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Pictures: HITS, Paiardi G. et al.

Beyond the limits