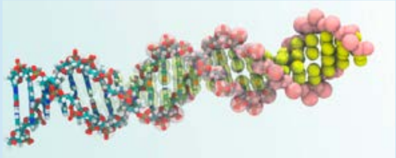
Meeting the Next Generation of Researchers: HITS at HLF25

From 15–18 September 2025, the 12th Heidelberg Laureate Forum (HLF) took place at Heidelberg University. Around 200 carefully selected early-career researchers in mathematics and computer science attended. The conference offered a unique opportunity to meet and exchange ideas with laureates of the Abel Prize, Turing Award, Fields Medal, and other prestigious international awards. As part of the program, the Science Hub Showcase offered companies and research institutions the opportunity to present their work in short elevator-pitch style presentations. **Kai Polsterer**, Scientific Director at HITS, introduced the institute in just three slides and three minutes. He highlighted HITS' research focus and explained opportunities for collaboration.

During the event, the HITS booth at the heart of the conference venue attracted numerous inquisitive and highly motivated researchers. These interactions provided an excellent opportunity to discuss career aspirations and the diverse programs and initiatives offered by HITS.

The forum not only strengthened connections with emerging talents in mathematics and computer science, but also highlighted the ongoing commitment of the Heidelberg Laureate Forum Foundation (HLFF) and its associated partners to advancing research and supporting the next generation of scientific leaders.



Main-Neckar Martini User Meeting 2026
19–20 March 2026
Registration for this event will open on 1 January.
https://martini-workshop2026.h-its.org/

HITS

Fair and Faithful Language Processing: New Independent Postdoc

Computer scientist **Vagrant Gautam** joined HITS as an Independent Postdoc in September 2025. Born in Canada, Vagrant was raised in India and Singapore and returned to Canada to study computational linguistics at Simon Fraser University. Vagrant earned a PhD at the Faculty of Mathematics and Computer Science at Saarland University, Germany, with a dissertation on "Fair and Faithful Processing of Referring Expressions in English."
At HITS, Vagrant will collaborate closely with the Natural Language Processing (NLP) group. Vagrant's research focuses on both technical and social aspects of language technology: from developing linguistically informed methods for reference resolution and pronoun use, to critically examining concepts such as fairness, bias, and democratization in NLP and machine learning.

A Decade of Impact: HITSter Among World's Most Cited Researchers

Phylogeny, biodiversity, and research policy – areas that drive computer scientist and HITS group leader **Alexandros Stamatakis**. According to Clarivate's "Highly Cited Researchers" list, he has now ranked among the most cited researchers in his field for the tenth consecutive year.
In the ranking, he is listed with his primary affiliation at the Foundation for Research and Technology – Hellas (FORTH), where he has advanced computational biodiversity research in Crete in recent years. His secondary affiliation is with HITS. Stamatakis develops scalable software for analyzing large biological datasets, has reconstructed phylogenies of birds and insects, and is active in research policy – promoting, among other initiatives, the "Brain Gain" to Greece and a national program to support female professors.

New employees and visiting scientists

Master students:	Elias Huber (MLI), David Sichma (MLI), Dominik Sucker (MLI), Korinna Riccarda Bayer (PSO), Utkarsh Jain (SET), Rui Zhan (SET)
PhD students:	Levi Miederer (MCM), María Inmaculada Moyano Rejano (TOS), Tobias van Lier (TOS)
Postdoc:	Julius Steuer (NLP)
Visiting scientist:	Constanza Vásquez Venegas (AIN)

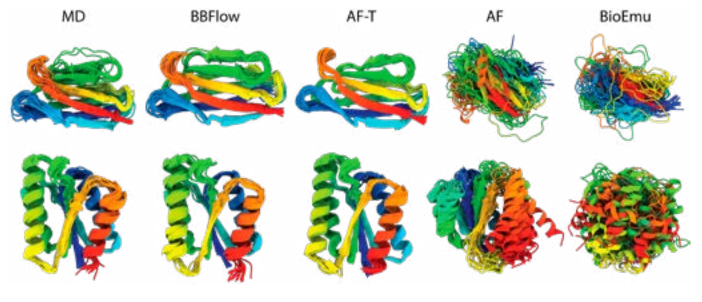
HITS groups (12/2025): *Astroinformatics (AIN), Computational Molecular Evolution (CME), Computational Statistics (CST), Data Mining and Uncertainty Quantification (DMQ), Machine Learning and Artificial Intelligence (MLI), Molecular and Cellular Modeling (MCM), Natural Language Processing (NLP), Physics of Stellar Objects (PSO), Scientific Databases and Visualization (SDBV), Stellar Evolution Theory (SET), Theory and Observations of Stars (TOS).*

HITSters

Designing Flexible Proteins: The Journey from GAFL to FliPS and BBFlow

Proteins, often called the molecular machines of life, perform essential tasks in living organisms. Their functions depend on both their three-dimensional shapes and their flexibility. Designing proteins has long been a challenge in computational biology. Thanks to recent advances in machine learning, structural biology, and generative modeling, scientists are able to not only predict protein folding but also design entirely new proteins.

Tailoring Protein Flexibility with FliPS
In July 2025, researchers from HITS and the Max Planck Institute for Polymer Research (MPIP) introduced a new machine-learning framework called FliPS (Flexibility-Conditioned Protein Structure Design with Flow Matching). FliPS enables the design of proteins with customizable flexibility patterns – including ones rarely seen in nature.
"Many natural proteins perform their functions so effectively because they can carry out specific movements and are rigid or flexible in just the right places," says **Leif Seute**, PhD student in the Machine Learning and Artificial Intelligence (MLI) group. "We can now generate new proteins that mimic this key property." MLI group leader **Jan Stühmer** adds: "FliPS extends last year's GAFL (Geometric Algebra Flow Matching) model." GAFL is three times faster than comparable methods and closely resembles natural proteins. FliPS shows how flexibility can serve as a design criterion for proteins. Researchers can now create proteins tailored to specific needs – they can move, bend, or adapt as required. This opens up new possibilities for de novo protein engineering.



The team also recently introduced its latest model, BBFlow (Backbone Flow), a deep generative model that predicts protein dynamics.

FliPS and BBFlow – Two Complementary Models
BBFlow is a flow-matching model that captures a protein's three-dimensional structure based on its backbone geometry – the spatial arrangement of a protein's main chain of atoms. It is 40 times faster than the current state-of-the-art model AlphaFlow, while offering comparable accuracy. Unlike conventional methods that rely on evolutionary sequence information, BBFlow does not require such data. It predicts protein dynamics directly from their structure, making it particularly well-suited for new or synthetic proteins that lack natural counterparts.
"While BBFlow forecasts protein dynamics, FliPS designs new proteins with specific dynamic properties. BBFlow can then filter the best candidates generated by FliPS," says **Nicolas Wolf**, first author of the paper. Understanding protein dynamics is crucial for developing new drugs, therapies, and materials. Protein design combines biochemistry, physics, and computer science, allowing the molecular language of life to be deciphered and applied in medicine and technology.

N. Wolf, L. Seute, V. Viliuga, S. Wagner, J. Stühmer, F. Gräter. Learning conformational ensembles of proteins based on backbone geometry. NeurIPS, 2025.

Research

Beyond the limits – Jackson Ryan, HITS Journalist in Residence 2025

Australian science journalist Jackson Ryan joined HITS in April 2025 as the 13th Journalist in Residence. During his six-month stay, he gave an internal seminar for HITS researchers and a public talk at the Deutsch-Amerikanisches Institut (dai) on "Insights from Antarctica." Prior to his departure, he recorded a video interview for the institute's social media channels, sharing his most memorable encounters and emphasizing the need to "think beyond yourself."

What inspired you to join the Journalist in Residence program at HITS?
You don't really get an opportunity to do something like this in Australia. It's great to be able to come to a beautiful place like Heidelberg and do it. As the President of the Science Journalists Association of Australia, I'm eager to use this opportunity to learn more about Germany's science journalism landscape and to bring those insights and experiences back to Australia.

If you had to sum up your residency in just three words, which would you choose?
I'm not really the kind of guy who sums things up in three words, but I would say: really – bloody – awesome. Three actual words though: Motivating, energizing and world-class.

What was your most memorable encounter at HITS?
There are many memorable encounters. I could speak about getting beers with Kai Polsterer, the HITS scientific director. But I think the most rewarding encounters are the ones you don't expect to have, particularly with young researchers. There are lots of young researchers who are interested in science journalism and science communication and just running into them in the corridor – those are the most memorable encounters for me.

How did this residency shape your views on connecting scientists and journalists globally, and what did you take away from it?
For me this experience was about expanding my horizons. I came here with a project I was really interested in. The connections that I've made with scientists and other journalists have strengthened that project. I've learned to slow down and listen. I'm a fast-paced guy, I'm always working on a lot of projects. But slowing down and listening to people will really support the journalism that comes out of this project.

What advice would you give aspiring journalists who want to follow a similar path or apply for this program?
I have two pieces of advice: First, think big in every project you take on. Even if you doubt you can do it – you can. Just go for it. Second, think beyond yourself. Don't focus only on your own professional development; consider how you can truly support science journalism and strengthen the ecosystem worldwide.

What's next?
Once I finish here, the plan is to build a dashboard for journalists in Australia and across the world, that can help them filter out cases of research misconduct and retractions. If I can build that resource, I think it will be much easier for journalists across the world to report on research misconduct even if they haven't had the background in doing so.

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Beyond the limits

HITS

The Charts

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