New HITS Journalist in Residence: Jackson Ryan

Jackson Ryan, an award-winning Australian science journalist, has joined HITS as its 13th Journalist in Residence. He began his residency in April 2025.

Ryan holds a PhD in pharmaceutical and medical science and has over eight years of experience as both a staff and freelance science writer. He was a global science editor at CNET (2019-2023) and a science and tech reporter at ABC until early 2024. He has reported on a wide range of scientific topics, including astronomy, climate and Earth sciences, biology, health, physics, and the influence of big tech. His in-depth coverage of climate change in Antarctica earned him Australia's prestigious Eureka Prize for Sci-



ence Journalism in 2022. At present, he serves as president of the Science Journalists Association of Australia and works independently, with bylines in The New York Times, The Guardian, The Saturday Paper, The Monthly, and Nature.

During his time at HITS, Ryan plans to focus on a central theme: scientific integrity and public trust in science. His goal is to research, develop, and write a series of longform stories for general readers, academics, and fellow science journalists, exploring the increasingly complex relationship society has with science. He is especially interested in the reliability of large datasets and hopes to learn from German researchers how they approach issues of scientific misconduct.

Beyond his own project, Ryan is similarly looking forward to connecting with German and other European science journalists to strengthen international ties. He has already given a talk on "Science, Fiction: Uncovering Research Misconduct Without Eroding Trust" at Heidelberg University in May and will give another public talk later this year.



Via Data

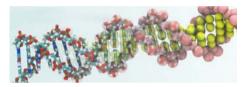
The HITS blog can be found on the "Scilogs" portal at https://scilogs.spektrum.de/via-data/.



HITS

Shaken and stirred: 1st Martini User Meeting

The Main-Neckar Martini User Meeting 2025 took place on 13-14 February at Studio Villa Bosch in Heidelberg and convened over 40 researchers from the Main-Neckar region to discuss the Martini Coarse-Grained force field, a widely used simulation method in biomolecular and soft matter physics.



The event featured expert talks, a poster session, and a panel discussion on recent developments and applications of the field, which is developed and maintained by the Martini Force-Field Initiative, an international collaboration of researchers.

Fabian Grünewald, HITS Independent Postdoc, co-organized the event together with Sebastian Thallmair (Frankfurt Institute for Advanced Studies - FIAS). Grünewald studied chemistry at the University of Groningen, the Netherlands, where he also received his PhD with honors in physical/



computational chemistry. He joined HITS in October 2023 and collaborates closely with the MBM and the MLI groups. He develops molecular simulation methods

to design and optimize RNA-delivery nanoparticles, focusing on their structure and targeting the ability and stability for applications in nanomedicine.

New employees and visiting scientists

Master students: Visiting scientists:

Communications: HITS Journalist in Residence: Pranavandhan Upendranath (SET), Arkaprahbha Roy (PSO), Gregory Jung (TOS) Raphael Hirschi (Klaus Tschira Guest Professor, Keele University, UK), Maximilian Ludwig (DMQ), Constanza Vasquez Venegas (AIN) Helena Camilleri (Team Assistance) Jackson Ryan (Australia)

HITS groups (06/2025): 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).

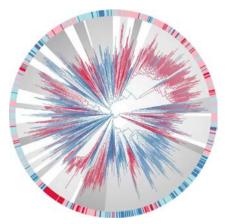
HITSters

Unfolding the origins: A history of bacterial evolution

A particular challenge for the team was the lack of "maximum age calibrations" - estimates for the earliest possible appearance of bacterial lineages. However, the team leveraged Earth's geochemical record, which preserves signatures of microbial metabolism, as a complementary source of historical data.

estimating the timing of those transfers - key to unraveling how and when certain microbial traits evolved. The analyses performed using his tools were instrumental in anchoring the evolutionary timeline proposed in the study.

Understanding the early evolution of microbial life has long posed a challenge due to the patchy fossil record and the absence of reliable age markers for key bacterial groups. An international team of researchers has traced the evolution of Earth's bacterial biosphere, spanning the past 4 billion years in a new study published in "Science". Benoit Morel, an alumnus of the Computational Molecular Evolution (CME) group at HITS, played a pivotal role in identifying the timeline of key microbial milestones.



Integrative approaches to dating early bacterial evolution

One of the most important moments in Earth's biological history was the Great Oxidation Event (GOE), which happened around 2.4 billion years ago. During this time, oxygen levels in the atmosphere rose sharply, mainly due to cyanobacteria developing the ability to produce oxygen through photosynthesis. This major change had a big impact on life, as many organisms had to adapt to living with oxygen.

Led by scientists at Eötvös Loránd University, Budapest, the research team used the timing of this atmospheric transformation to help calibrate the bacterial phylogenetic tree, focusing on when aerobic metabolism first emerged. At HITS, Benoit Morel developed a software capable of inferring horizontal gene transfers between ancestral species and

Aerobic bacteria existed long before the Great **Oxidation Event**

One of the team's most striking findings is that the earliest aerobic bacteria appeared nearly 900 million years before the GOE, during the Archaean eon. This discovery reshapes our understanding of microbial evolution and Earth's oxygenation history.

The framework developed in this study not only sheds light on the ancient past of aerobic bacteria but also offers a powerful new way to trace the evolution of microbial traits in relation to Earth's geochemical record - a valuable tool for future investigations into the deep history of life.

Davín, A., Wooddcroft, B., Soo, R., Morel, Murali, R., Schrempf, D., Clark, J., Álvarez-Carretero, S., Boussau, B., Moody, E., Szántho, L., Richy, E., Pisani, D., Hemp, J., Fischer, W., Donoghue, P., Spang, A., Hugenholtz, P., Williams, T., Szöllősi, G.: A geological timescale for bacterial evolution and oxygen adaptation. In: Science, 4 Apr 2025, Vol 388, Issue 6742.

Research

Beyond the limits – Lu Yang, HITS Visiting Scientist

Lu Yang, Professor at the School of Statistics, University of Minnesota, USA, joined the Computational Statistics (CST) group in February 2025. During her three-month stay as a Visiting Scientist, she delved into interdisciplinary research at HITS. In this interview, she discusses how statistical methodology shapes real-world decision-making, reflects on the key insights she has gained during her time at the institute, and offers a glimpse into the exciting challenges she plans to pursue next.

Statistical methodology can often feel abstract to those outside the field. Can you share an example of how your work might influence real-world decisions or innovations?

My research in statistics is largely motivated by insurance applications. For example, in one of my recent papers we developed a method to help insurance companies determine a loss reserve using micro level data, as more and more detailed data became available in recent years.



What's one recent development in statistics or data science that you find particularly exciting - or even a little concerning - and why?

The explosion of AI of course. Statistics and data science are the backbone of AI. It provides parallel opportunities in statistics and data science. But it also poses many challenges and issues when it comes to its effective and responsible use.

Looking back on your time as a visiting scientist at HITS, what has been the most surprising or inspiring aspect of your experience - scientifically or personally? I've been amazed by how collegial the environment at HITS is. I didn't expect to

have so many opportunities to interact with fellow scientists and colleagues as a visiting scientist.

As you prepare to leave HITS, what challenges or big questions in statistical methodology are you most eager to tackle next?

I learned a lot about forecast calibration from the CST group, which I believe is an important and interesting area in statistics. I'm eager to apply those methods to evaluate and refine models for different types of data and also contribute to this area by developing tools.

How did you spend your free time during your stay in Heidelberg?

I took some German classes offered by HITS and I went to some concerts. I also made use of the convenient location of Heidelberg and traveled around Europe quite a bit, e.g. Amsterdam, Leuven, Austria and southern Spain, which was a lot of fun.

Imprint | Dr. Peter Saueressig (Vi.S.d.P.), saueressig@h-its.org, Tel. +49 6221 533 245 | Pictures: HITS, Davin et al. (aus: "Science", 4 Apr 2025, Vol 388, Issue 6742) | www.h-its.org





