



New “Journalists in Residence”

German science journalist **Kerstin Hoppenhaus** will be the seventh “Journalist in Residence” at HITS. For the third time, the program was announced internationally; candidates from six continents had applied, among them free journalists and editors as well. A jury consisting of science journalists and scientists from universities, Max Planck Institutes and HITS, selected Kerstin Hoppenhaus for 2018. She will join the institute in July 2018. Hoppenhaus studied biology and directing. For more than ten years, she has been working as a freelance director for documentary, research movies and online projects.

The jury also chose New York City-based **Dr. Andreas von Bubnoff** who will come to HITS in 2019. The German-born free science journalist is a molecular biologist by training and has been living in the United States for 20 years.



HITS researchers decode the Axolotl genome

After five years, the HITS junior group “Computational Biology” is bringing its work to a close with spectacular results: Together with colleagues from Dresden and Vienna, they succeeded in decoding the genomes of the Mexican salamander Axolotl and the flat worm *Schmidtea mediterranea*. Both animals are important organisms in regeneration research, their genomes were considered as extremely hard to decipher. Therefore, the HITS researchers developed an entirely new code (see Portrait).



“Thanks to our donor Klaus Tschira we had plenty of time and no publication pressure.”

Dr. Siegfried Schloissnig, HITS junior group Computational Biology (2013-2018).

HITS



Habilitation for HITSter

The astrophysicist **Dr. Rüdiger Pakmor** successfully completed the habilitation process at Heidelberg University. At the end of January, the faculty committee of physics and astronomy presented him the certificate of *venia legendi*. Rüdiger Pakmor has been at HITS since October 2010, working in the Theoretical Astrophysics group (TAP, head: Prof. Volker Springel). He develops novel numerical methods and applies them, among others, to galaxy formation and supernova explosions. Pakmor co-authors several publications and big cosmological simulations, like “Auriga” and “IllustrisTNG”. Since February 1, 2018, he has been holding a “staff scientist” position at HITS. After alumnus Prof. Christoph Pfrommer, this is the second habilitation attained by a HITSter.

“Golden Spike Award” for Volker Springel

Again, the steering committee of the High Performance Computing Center Stuttgart, HLRS chose **Prof. Volker Springel** (TAP) for the “HLRS Golden Spike Award”. The decision criteria for the awarded projects are scientific relevance and optimal usage of HPC equipment in terms of optimization, parallelization and overall performance. Volker Springel was awarded for his work in the “The Illustris++ Project: The Next Generation of Cosmological Hydrodynamical Simulations of Galaxy Formation” (see “Portrait”).



New staff members and visiting scientists

Administration: Irina Zaichenko, accounting

MBM: Isabel Martin, PhD student

MCM: Dr. Ariane Nunes-Alves, visiting scientist (Heidelberg University)

Prof. Huan-Xiang Zhou, visiting scientist (Florida State University, USA)

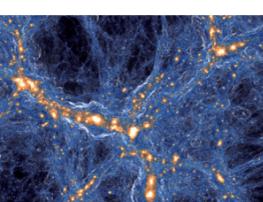
NLP: Kevin Alex Mathews, PhD student (HITS scholarship)

SDBV: Dr. Sucheta Ghosh, research associate

HITS groups

Astroinformatics (AIN), Computational Biology (CBI), 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 Computing (SCO), Scientific Databases and Visualization (SDBV), Theoretical Astrophysics (TAP).

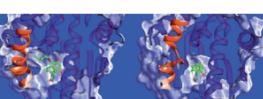
HITSTERS



How black holes shape the cosmos

An international team of astrophysicists led by HITS researcher **Prof. Volker Springel** (Theoretical Astrophysics) gained new insights into the cosmic evolution. They calculated how black holes influence the distribution of dark matter, how heavy elements are produced and distributed throughout the cosmos, and where magnetic fields originate. The “Illustris – The Next Generation” (IllustrisTNG) simulation includes some of the physical processes, which play a crucial role, for the very first time in such an extensive simulation. At its intersection points, the cosmic web of gas and dark matter hosts galaxies quite similar to the shape and size of real galaxies. For the first time, hydrodynamical simulations could directly compute the detailed clustering pattern of galaxies in space. Comparisons with observational data demonstrate the high degree of realism of IllustrisTNG. In addition, the simulations predict how the cosmic web changes over time, in particular in relation to the underlying “back bone” of the dark matter cosmos.

V. Springel et al.: “First results from the IllustrisTNG simulations: matter and galaxy clustering”, published in: MNRAS, Feb 1st, 2018.

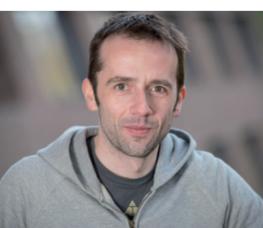


A matter of mobility: a new strategy for drug discovery?

A joint study of a cancer target protein reveals an unusual relation between binding site flexibility and drug-target lifetime. “We were really surprised”, says HITS researcher **Prof. Rebecca Wade** (Molecular and Cellular Modeling), “when we found out that an important contributor to the long residence times was the greater mobility of the helical region of the binding pocket when the inhibitor bound.” Now, scientists can consider less rigid protein targets and identify molecules that stabilize more mobile forms of the protein upon binding – somewhat like a ski boot with an adaptable inner liner that continually adjusts to the foot. The findings of this study suggest a new way to find more effective drug candidates with optimal kinetic and thermodynamic properties.

Protein conformational flexibility modulates kinetics and thermodynamics of drug binding. Amaral M, Kokh D, Wegener A, Bomke J, Buchstaller HP, Eggenweiler HM, Matias P, Wade RC, Frech M. Nature Communications 8, Article number: 2276 (2017).

RESEARCH



Siegfried Schloissnig: “I had sufficient time to do diligent quality work”

The blue box on the sidebar is filling up with books and documents: After five years at HITS, Siegfried Schloissnig is preparing to leave his office within the HITS building. “We have successfully accomplished our mission and my work style is to explore unknown terrain”, the 38-year-old bioinformatician states while gazing out the window and over the park with its huge sequoia. It has actually been a mammoth task he had to master together with his team members Philipp Bongartz, Philipp Kämpfer, Martin Pippel and Sean Powell in the last five years. The scientists have decoded the genome both of the Mexican salamander Axolotl and the flat worm *Schmidtea mediterranea* in collaboration with colleagues from Vienna and Dresden. Both animals are important organisms in regeneration research. The research results have been published in the scientific journal “Nature” and have eventuated in significant response from the media.

Schloissnig and his team have been developing an entirely new software program to reconstruct a genome from extremely large amounts of highly repetitive genetic information. With 32 billion base pairs the Axolotl genome is ten times larger than the human genome. “When it comes to the flat worm, everything seemed to be identically at first due to the numerous repetitions”, Schloissnig explains. But in the end the scientists succeeded. “Now colleagues in the laboratory can really work with the Axolotl genome,” Schloissnig rejoices. “Before, everything was a guessing game, but now the puzzle has been put together.”

Siegfried Schloissnig, born in Klagenfurt, studied computer science at the KIT and obtained his doctorate in human biology at the University of Heidelberg. He then worked at the EMBL Heidelberg as a PostDoc and joined HITS in 2013 as head of the new junior group “Computational Biology”. The group’s task ends with two “Nature”-publications. Schloissnig’s next career move will take him back to Austria, where he will supervise the IT department of regeneration research at the Institute for Molecular Pathology (IMP) in Vienna. “Working at HITS has truly been a privilege because it allowed us to pursue our work undisturbed and in pleasant surroundings”, Schloissnig concludes. “And thanks to our donor, Klaus Tschira, we had plenty of time and no publication pressure.” The blue box has been packed meanwhile – it’s time to head off.

Imprint | Dr. Peter Saueressig (V.i.S.d.P.), Saueressig@h-its.org, Tel. +49 6221 533 245
Photos: HITS, Gülay Keskin, IllustrisTNG, IMP | www.h-its.org

PORTRAIT

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Heidelberger Institut für
Theoretische Studien



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