Eugen Hruska, Ph.D.

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Research

2020 - · · · Postdoctoral Research Associate, Emory University

Investigating the behavior of the molecule-solvent interface.

Determined optimal adaptive sampling strategies for folding proteins and the upper limit for speed up with adaptive sampling. Developed open-source package ExTASY, a scalable and open-source adaptive sampling platform enabling deep learning: github.com/ClementiGroup/ExTASY. Showed adaptive sampling reaches accurate protein folding and protein dynamics.

2012 **Bachelor student, University of Regensburg**

Localized interaction interface between proteins central to polycystic kidney disease with NMR.

Education

2014 – 2020 Ph.D., Physics, Rice University

Thesis title: Adaptive sampling of Conformational Dynamics

Advisor: Cecilia Clementi

2012 – 2014 **Bachelor**, Biochemistry, University of Regensburg

Bachelor, Physics, University of Ilmenau

Thesis title: NMR-spectroscopic Analysis of Interaction between Polycystin-2 and mDia1 Advisor: Hans R. Kalbitzer

Research Publications

- 1 **Hruska**, **E.** (2020). *Adaptive sampling of conformational dynamics* (Doctoral dissertation). Rice University. **6** https://scholarship.rice.edu/handle/1911/108744
- **Hruska**, E., Balasubramanian, V., Ossyra, J. R., Jha, S., & Clementi, C. (2019). Extensible and scalable adaptive sampling on supercomputers. *arXiv preprint arXiv:1907.06954*.

 https://arxiv.org/abs/1907.06954v1
- Hruska, E., Abella, J. R., Nüske, F., Kavraki, L. E., & Clementi, C. (2018). Quantitative comparison of adaptive sampling methods for protein dynamics. *The Journal of Chemical Physics*, 149(24), 244119. https://doi.org/10.1063/1.5053582
- Balasubramanian, V., Bethune, I., Shkurti, A., Breitmoser, E., **Hruska**, **E.**, Clementi, C., Laughton, C., & Jha, S. Extasy: Scalable and flexible coupling of md simulations and advanced sampling techniques. In: *2016 ieee 12th international conference on e-science (e-science)*. IEEE. 2016, 361–370. https://ieeexplore.ieee.org/document/7870921

Awards

2012 Student award, German Physical Society

Scholarship, German Academic Scholarship Foundation, most prestigious scholarship in Germany

High School

Gold medal, International Physics Olympiad, top high school physics competition, rank top 50 in world

2011 Gold medal and Best Experiment, World Physics Olympiad

2007-2008 Gold medal, International Junior Science Olympiad, top science competition aged 15 and under

2010 Ronze medal, International Biology Olympiad, top high school biology competition

2009 Ronze medal, International Young Physicists' Tournament

Teaching Experience

Teaching Assistant, Rice University
PHYS 700 lab, Supervised experimental lab and evaluated students' progress.

Service

Coach for U.S. Physics Team preparing top 20 US high school students representing USA in high school level international physics competition

■ Taste of Science organizing scientific outreach events for the general public

Tutor for international science competitions, preparing promising students

Other

Languages 📕 English - fluent, German - native, Slovak - native

Coding Python (5+ years): tensorflow, pytorch (deep learning, GPUs), sklearn (machine learning), pyemma (markov state models), openmm (molecular dynamics), radical cybertools (HPC), bash, ŁTĘX, ...

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