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Keynote: Research Software and Its Developers: Insights Gained and Future Directions

Tuesday 25 February 2025 13:15 (1 hour)

Simulation software packages are fundamental for advancing modern scientific research. These tools vary widely in scale, from a few thousand lines of code to millions, demanding significant human expertise and computational resources for their development and long-term maintenance. Yet, despite this critical role, both the developers and the process of scientific software development are often underappreciated in academic settings.

In this talk, I will explore aspects and challenges specific to scientific code development within academia, aiming to stimulate a broader discussion around several core questions: Is the current academic model the most effective way to develop research software? How much should society invest in building and maintaining research software? What strategies can we adopt to ensure that scientific code is robust and reliable? What unique questions and obstacles do scientific software development projects encounter? Furthermore, how can we ensure the long-term accessibility, maintenance, and reproducibility of simulation software and simulation results?

Drawing on two decades of experience as a co-developer and co-manager of the DFTB+ quantum mechanical atomistic simulation software, and as an active member of the Fortran developer community, I will share some lessons learned so far and offer some views on the future of research software engineering.

I want to participate in the youngRSE prize

Presenter: Dr ARADI, Bálint (University of Bremen)