

Erik Lindahl

Session 2

Title: Hardware limits & opportunities for the future of biomolecular simulation

Abstract:

Classical molecular dynamics simulations of large molecules such as proteins, lipids or DNA have long been among the largest users of HPC resources worldwide. The field has benefitted tremendously from performance advances in computing in general, and accelerators in particular; what was once a niche endeavor in theoretical physics is now broadly used e.g. in the pharmaceutical industry. I will talk about the heterogeneous acceleration algorithms we have developed in the GROMACS code in particular to improve strong scaling by utilizing advanced GPU interconnects. However, as we are reaching iteration times for complete steps well below 100 microseconds, we also need to face the grim realities of physics that latencies will not keep going down. I will discuss some potential ways around this, including both ensemble models and machine-learning methods to sample conformations in parallel rather than serial.

Bio:

Erik Lindahl obtained a Master of Science from Lund University in 1995, followed by a PhD degree in Theoretical Biophysics from the KTH Royal Institute of Technology in Stockholm 2001, and postdoctoral work at Groningen University, Stanford University and Institut Pasteur.

He holds professorships of biophysics both at Stockholm University and KTH, and leads a mixed computational and experimental research environment located at Science for Life Laboratory site. The research in the Lindahl lab is focused on advancing the state of the art of both methodology of biomolecular simulations and applications to membrane proteins, in particular understanding and altering properties of the voltage and ligand gated ion channels responsible for nerve impulse transmission. Lindahl's team has written the GROMACS molecular dynamics simulation toolkit, and they are also involved in developing the RELION code to perform molecular reconstruction in cryo-electron microscopy. Since 2025 he is the director of the National Academic Infrastructure for Supercomputing in Sweden.