

Program

SeRC 17:th Annual Meeting, May 6-7 2026, Skogshem & Wijk,
Lidingö, Stockholm

Theme: Software

Wednesday May 6

- 11:50 (Sharp) **Chartered buses** leave from KTH, in front of Lindstedtsv 3 (registration needed)
- 12:30 **Lunch**
- 13:30-13:45 **Welcome**
Dan Henningson, KTH
- 13:45-14:15 **HPC and AI landscape in Sweden**
Erik Lindahl, KTH, LiU & SU
Salla Franzén, AI4S
- 14:15-14:20 **Structure of the meeting**
Shahab Mirjalili, KTH
- Session 1**
- 14:20-14:35 **From SMILES to transition states with VeloxChem**
Bastian van Hoorn, KTH
- 14:35-14:50 **Reeb Spaces: A Topological Tool for Exploring Electron Density and Chemical Bonding**
Petar Hristov & Mohit Sharma, LiU
- Keynote 1**
- 14:50-15:35 **Arbor -- At the crossroads between scales**
Thorsten Hater, Forschungszentrum Jülich
- Session 2 (Poster & Video Session + Coffee)**
- 15:35-15:50 **Masters students introductions**
- 15:50-17:00 **Posters & Videos + Coffee**
- Session 3**
- 17:00-17:15 **Software for Exploring Complex Energy Landscapes in Spin Systems**
Anna Delin, KTH
- Keynote 2**
- 17:15-18:00 **Using physics to extract maximum information from noisy sparse flow data**
Matthew Juniper, Cambridge University
- 19:00 **Dinner**

Thursday May 7

Session 4

09:00-09:25 **KTH Center for Scientific Computing (KCSC)**
Patrick Norman, KTH

09:25-09:40 **TDEP: Toward GPU-Accelerated Finite-Temperature Lattice Dynamics**
Utkarsh Singh, LiU

Keynote 3

09:40-10:25 **Gracemaker: a tool for building graph atomic cluster expansion for atomistic simulations**
Anton Bochkarev, Ruhr Universität Bochum

10:25 **Coffee**

Session 5

11:00-11:15 **Fast Multipole Method for Scalable Electrostatics in GROMACS**
Umair Sadiq, KTH

Keynote 4

11:15-11:45 **Herding Cats at Exascale: The Development and Maintenance of Neko**
Niclas Jansson, KTH

11:45-12:00 **Navigating the hardware shift: atmospheric modelling in heterogeneous architectures**
Lorenzo Luca Donati, SU

12:00-12:15 **Closure (The Future of SeRC)**
Dan Henningson, KTH

12:30 **Lunch**

13:30 (Sharp) **Chartered buses** leave from Skogshem & Wijk for KTH (registration needed)

Connected meeting:

Wednesday May 6 10:00-12:30 SeRC Steering group and Advisory group meeting