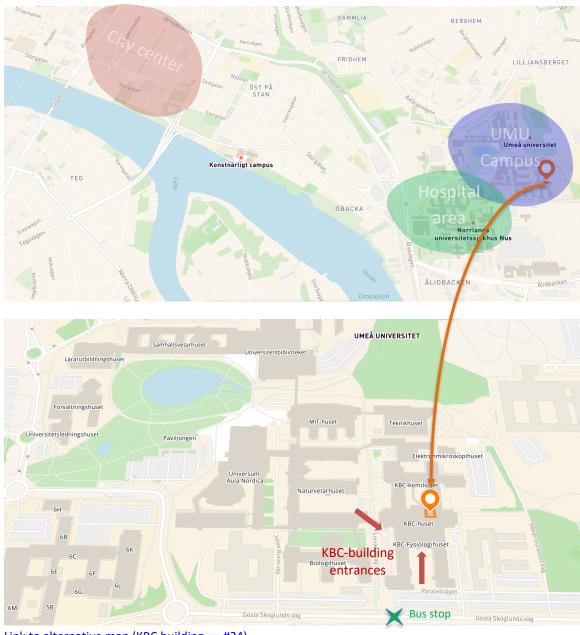
Local NAISS-USAC meeting at Umeå University

When: August 26–27 2025, Lunch-to-lunch **Zoom link:** <u>umu.zoom.us/j/62542716750</u>

Where: Stora Fokusrummet, KBC-Building, floor 3, Linnaeus väg 6

How to get there: walking 30 min from city center or by taxi to UMU campus, KBC-

building Linnaeus väg 6, or by taking the **bus** using the <u>Ultra bus app</u>



Link to alternative map (KBC building == #24)

Program

Day 1 — **Tue, Aug 26**

12:00–13:00 Lunch at Restaurant Hjortron, Universum (sign up here)

13:00–13:20 USAC – what do we do? — Michael Holmboe

13:20–13:40 NAISS – current and future capabilities — *Erik Lindahl*

13:40–14:00 1. SLU Bioinformatics Infrastructure and UPSC bioinformatics platform as NAISS power users — *Nicolas Delhomme*

14:00–14:20 2. Oxymoron? When HPC Drives Evolutionary Biology into the Real World — *Thanat Chookajorn*

14:20–14:30 Transition / setup buffer

14:30-15:00 Coffee break

15:00–15:20 3. HPC for 3D protein structure determination in Cryo-Electron Microscopy — *Suresh Banjara*

15:20–15:40 4. Unveiling a Crystal-Invisible Active Enzyme State with HPC-Powered Molecular Dynamics Simulations — *Mitul Srivastava*

15:40–16:00 5. Capturing Adenylate Kinase Dynamics with TRXSS and Ensemble Modelling — *Konstantinos Magkakis*

16:00–16:20 6. Molecular dynamics simulations of Calcium-Transporting P-type ATPases in membranes with different phospholipid compositions — *Fatemeh Sabzian*

Dinner around 18:30 for pre-registered participants, more info to come..

Day 2 — **Wed, Aug 27**

08:45-09:00 Coffee on arrival

09:00–09:20 7. Swedish Biodiversity in Time and Space (SweBITS) — Johan Stenberg

09:20–09:40 8. Scalable single-cell metagenomic analysis with Bascet and Zorn — *Johan Henriksson*

9:40–10:00 9. The energy transfer from the solar wind to the Martian ionosphere – *Xiao-Dong Wang*

10:00-10:30 Coffee break

10:30–10:50 10. Disease Aware Parameter-Efficient Fine Tuning of Vision Language Models – *Filippo Ruffini*

10:50–11:10 11. Solving Partial Differential Equations on an HPCBalaje Kalyanaraman

11:10–11:30 12. Mixed and lower precision algorithmic design for CFD and other applications – *Roman lakymchuk (Zoom presentation)*

11:30-12:00 Discussion & Wrap-up

12:00–13:00 Lunch at Restaurant Hjortron, Universum (sign up here)

13:00–16:00 Hands-on Workshop organized by HPC2N — Brigitte Brydsö

Use this link for <u>registration</u>. Contact <u>bbrydsoe@hpc2n.umu.se</u> for more info. Part 1: Advanced SLURM Usage: Tips and tricks for efficient job scheduling

Part 2: Module management: Best practices for different software environments

Will include a coffee break around 14:30