

## Mikael Carp

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## NAISS training newsletter No 22 19th April 2024

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Welcome to the next edition of the NAISS training newsletter.

NAISS provides an overview on all training events on the events webpage: <https://www.naiss.se/events/>

### NAISS training

- **Online training and support event: “NSC introduction to Tetralith/Sigma”, 23 April 2024 at 10:00**
- **Online training seminar: Introduction to Alvis, 23 April from 13:15 to 15:00**
- **Online webinar: Introduction to Code-Saturne, 26 April 2024**
- **Online training course: Introduction to Pandas for data science, LUNARC, 13 - 14 May 2024**
- **Online training course: Using Python in an HPC environment, UPPMAX & HPC2N, 15 May 2024**
- **Online training: Snakemake Hackathon, 22nd May**
- **Online hackathon: Bianca In-Depth: Improve Your Handling of Sensitive Research Data, 24 May 2024**
- **Online training: UPPMAX Introductory Course, 27-30 August 2024**

### Tuesday Tools & Techniques for High Performance Computing

- **Episode 2: Day-to-day working on clusters, 23 April 2024**
- **Episode 3: Containers on clusters, 7 May 2024**
- **Episode 4: Parallelization and workflows, 14 May 2024**

### Online interactive support and discussion forum:

- **NAISS Zoom-in - a virtual open-house, 25 April from 14:00 until 15:00**

### ENCCS training

- **The AI for Science Bootcamp, 25-26 June**
  - **Publicly available training material**
  - **Training events from around Europe**
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## NAISS training

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**Online training and support event: “NSC introduction to Tetralith/Sigma”, 23 April 2024 at 10:00**

An online event with two parts:

- A short introduction suitable for new users to the NSC Tetralith (NAISS) and Sigma (LiU) clusters. Topics include the module system, submitting jobs, working with Python, allocating GPU:s for simulations or graphics and other useful information.
- An open session for questions with several NSC application experts attending.

Feel free to join (and leave) whenever depending on your interest. The online event is open for all present and prospective NSC users.

Time: 23 Apr 2024, 10:00 - ca. 11:15 Introduction, ca 11:15 - Open session

Zoom link: <https://liu-se.zoom.us/j/6988980503?pwd=MExuQS9iRGpKazhzQi81Y2wwV0xrdz09>

The presentation will be available on the event webpage:  
[https://www.nsc.liu.se/support/Events/NSC\\_intro\\_Apr2024/](https://www.nsc.liu.se/support/Events/NSC_intro_Apr2024/)

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**Online training seminar: Introduction to Alvis, 23 April from 13:15 to 15:00**

This seminar is for new and prospective users of the NAISS cluster for AI/ML, Alvis. You will learn all that you need to know to get started on the system.

Time: 23 April 13:15  
Location: <https://chalmers.zoom.us/j/64201336538>

For more information visit <https://www.c3se.chalmers.se/#current-and-upcoming-events>

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**Online webinar: Introduction to Code-Saturne 26 April 2024**

A free open-source code for CFD applications. This webinar is suitable for researchers who already have experience using Computational Fluid Dynamics (CFD) codes. While this webinar is primarily geared for R&D personnel from the industrial/business arena, academic researchers and research software engineers with expertise in the CFD area are also welcome to attend.

When: Fri 2024-04-26, 15.00 - 16.00

Where: online via Zoom

For more information please visit: <https://www.pdc.kth.se/about/events/webinar-introduction-to-code-saturne-1.1323572>

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**Online training course: Introduction to Pandas for data science, LUNARC, 13 - 14 May 2024**

Pandas is a powerful, popular Python package for cleaning, manipulating, and statistically analyzing large tabular data sets. It is particularly useful in preparation for AI/ML applications and publication-ready visualization. Originally developed for financial panel data, it is now used by data scientists in a huge variety of fields, from marketing to medicine to astronomy. Pandas is capable of handling data sets of several Gigabytes.

This course will introduce the core Pandas data types, basic input/output routines, data selection and filtering, data inspection and cleaning methods, built-in and user-defined functions for data manipulation, hierarchical data structures, and some built-in visualization methods. There will be a mix of static examples and live demonstrations via Jupyter notebook, and exercises will be provided to complement the lecture materials.

For more information and access to registration, please visit <https://www.lunarc.lu.se/learning-more/training-courses/introduction-to-pandas-for-data-science-13-14-may-2024/>

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**Online training course: Using Python in an HPC environment, UPPMAX & HPC2N, 15 May 2024**

This course aims to give a brief, but comprehensive introduction to using Python in an HPC environment. You will learn how to use modules to load Python, how to find site installed Python packages, as well as how to install packages yourself. In addition, you will learn how to use virtual environments, write a batch script for running Python, use Python in parallel, and how to use Python for ML and on GPUs.

The course is a cooperation between UPPMAX and HPC2N. The instructors will use UPPMAX's systems for demos and there will be hands-on exercises for the participants.

This course will consist of lectures interspersed with hands-on sessions where you get to try out what you have just learned.

Remote/online participation: The course will be completely online and we will use Zoom. More information about connecting and such will be sent to the participants close to the course.

The goal for the course is that you will be able to

- Load Python modules and site-installed Python packages
- Create a virtual environment and install your own Python packages to it
- Write a batch script for running Python
- Use Python in parallel
- Use Python for ML
- Use GPUs with Python

Prerequisites: familiarity with the LINUX command line, basic Python

For more info and registration, please visit:

<https://www.hpc2n.umu.se/events/courses/2024/spring/python-in-hpc>  
<https://www.uppmx.uu.se/support/courses-and-workshops/HPC-python>

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**Online training: Snakemake Hackathon, 22nd May**

*Collaboration between CSC, Aalto University, PDC, ENCCS, and UPPMAX*

Abstract: Snakemake is a common entry tool in the world of computational workflows, especially in Bioinformatics. The tool is designed to support you in setting up a workflow system, which opposed to a "your favorite language here" script, helps you keep track of your processes. For Snakemake, the user has to define inputs and outputs and the tool will figure out the order of steps and which steps can be run in parallel.

This Hackathon is open for all, free of charge and independent of field of Science and it is all about getting your own workflows to the supercomputer (Puhti, Mahti, Lumi or other).

Time: 22nd May, 09:00-14:00 (2024).

Detailed information at webpage: [https://ssl.eventilla.com/snakemake\\_hack](https://ssl.eventilla.com/snakemake_hack)

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**Online hackathon: Bianca In-Depth: Improve Your Handling of Sensitive Research Data, 24 May 2024**

Are you already working with sensitive data in your research and feel that your workflows can be improved? If yes, welcome to 1 day hackathon where you'll learn smarter ways of working on the Bianca cluster. We will tell you how to do file transfer from a terminal, advanced SLURM, using IDEs (i.e. RStudio and/or VSCode), and installing custom software and packages.

The workshop will consist of short lectures and the content will be driven by questions from the participants.

To attend this course, we expect you to be able to login to Bianca, submit a Slurm bash script, and know how to transfer files.

You do not need to be a member of a NAISS-SENS project in order to join the workshop. A SUPR course project will be available to all participants.

When: Friday, May 24, 2024

Where: online via Zoom

For more information and registration please visit: <https://www.uppmx.uu.se/support/courses-and-workshops/bianca-hackathon-2024>.

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### **Online course: UPPMAX Introductory Course, 27-30 August 2024**

This 4-day course provides an introduction to the high-performance computing (HPC) environment offered at UPPMAX.

It offers an overview on how the systems work and covers skills from basic Linux usage to more advanced tips and tricks, including Python scripting.

Participation is open to all existing and prospective NAISS users.

When: August 27-30, 2024

Where: online via Zoom

For more information and registration, please visit: <https://www.uppmx.uu.se/support/courses-and-workshops/uppmx-introductory-course>.

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## **Tuesday Tools & Techniques for High Performance Computing**

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### **Online Training: Tuesday Tools & Techniques for High Performance Computing, April-May, 2024**

Cooperation between NAISS, Aalto University, CSC, NRIS, and CodeRefinery.

Do you use supercomputers in your research work? Are you curious about making your computing faster and more efficient? Join us for TTT4HPC: four self-contained episodes on best practices in High Performance Computing. This is a great chance to enhance your computational skills. What you will learn is also used a lot outside academia whenever large scale computations are needed.

Episodes are self-contained, you can join only for the episodes that are useful for your research.

#### **Episode 2 - 23/04/2024 - Day-to-day working on clusters**

Content: focus on software development on HPC, syncing data, interactive work with HPC, vscode

#### **Episode 3 - 07/05/2024 - Containers on clusters**

Content: focus on containers with Apptainer/Singularity, how to build containers for HPC, how to work with the filesystem, other practical examples with containers

**Episode 4 - 14/05/2024 - Parallelization and workflows**

Content: focus on parallelization with HPC, efficient parameter sweeps, workflow automation, hyperscaling pitfalls

For more information and registration, please visit <https://scicomp.aalto.fi/training/scip/ttt4hpc-2024/index.html>.

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**Online interactive support and discussion forum:**  
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**NAISS Zoom-in - a virtual open-house, 25 April from 14:00 until 15:00**

You are invited to a virtual meeting room. Inside the meeting room we like to discuss services offered by NAISS and how they can be used for your computational needs, help you process your data and visualise your results. Participants are highly encouraged to pose their own questions.

We also expect to have experts available from [C3SE](#), [HPC2N](#) and [LUNARC](#), to discuss the University operated HPC services at Chalmers, Umeå and Lund University.

The zoom-link for the session on 25th April is: <https://lu-se.zoom.us/j/63229059195?pwd=MzBOK2ZKeVhkOHRab3B5d1pRZExLZz09>

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**ENCCS training:**  
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**The AI for Science Bootcamp, 25-26 June**

Abstract: The AI for Science Bootcamp provides a step-by-step overview of the fundamentals of deep neural networks and walks attendees through the hands-on experience of building and improving deep learning models for applications related to scientific computing and physical systems defined by differential equations.

The material will cover more advanced topics, such as physics-informed neural networks (PINNs) and operator learning and make use of tools like NVIDIA Modulus to develop and train the models. Furthermore, this online bootcamp is a hands-on learning experience where we will guide you through step-by-step instructions with teaching assistants on hand to help throughout.

Detailed information at ENCCS (<https://enccs.se/events/ai-for-science-bootcamp/>) and OpenHackathons (<https://www.openhackathons.org/s/siteevent/a0C5e000008AbEaEAK/se000315>) webpages.

Time: June 25-26, 9:00-13:30 (2024).

Link to the registration: <https://www.openhackathons.org/s/siteevent/a0C5e000008AbEaEAK/se000315>

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*ENCCS also asked us to publicise their online training material overview*

**Publicly available training material:**

ENCCS develops and maintains a library of training material on topics in HPC, AI and Quantum Computing which is suitable for self-paced learning. Find the library at <https://enccs.se/lessons/>.

**Training events from around Europe**

Many HPC centres and National Competence Centres around Europe offer diverse HPC training workshops open to anyone in Europe, many of which are online. Upcoming workshops can be found at <https://hpc-portal.eu/upcoming-events-courses>.