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From: Training-announce <training-announce-bounces@lists.naiss.se> on behalf of training-announce@lists.naiss.se
Sent: den 4 mars 2024 09:08
To: training-announce@lists.naiss.se
Subject: [Training-announce] NAISS training "Python in an HPC environment". Training for new users of NAISS. VASP, R, Julia and programming formalism. CodeRefinery and ENCCS training.
Attachments: ATT00001.txt

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NAISS training newsletter No 19

4th March 2024

Welcome to the next edition of the NAISS training newsletter. This week we newly advertise the "Python in an HPC environment" course. Registration for the "Introduction to PDC systems course" is now available. We remind on a number of events which we previously advertised. This includes events from ENCCS.

NAISS events

- **Online training seminar: Introduction to Alvis, 11 March from 13:15 to 15:00**
- **Online introduction to running R, Python, and Julia in HPC, 12-14 March 2024**
- **Registration open for Online Training: Introduction to PDC Systems Course, 21-22 March 2024**
- **Online Workshop: VASP/EMTO Best Practices Workshop, 16 - 18 April**
- **Online training: Programming Formalisms course, 22 - 26 April 2024**
- **Online training course: Using Python in an HPC environment, UPPMAX & HPC2N, 15 May 2024**

CodeRefinery training

- **Online workshop: CodeRefinery workshop, 12-14 and 19-21 March 2024**

ENCCS training

- **The Multi-GPU Programming Bootcamp, 6-7 May**
- **The AI for Science Bootcamp, 25-26 June**
- **Publicly available training material**
- **Training events from around Europe**

NAISS training

Online training seminar: Introduction to Alvis, 11 March 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: 11 March 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 introduction to running R, Python, and Julia in HPC, 12-14 March 2024

Cooperation between HPC2N and UPPMAX

HPC2N, in cooperation with UPPMAX, is offering a three-day ONLINE training course "Introduction to running R, Python, and Julia in HPC".

Learn how to run R, Python, and Julia at Swedish HPC centres, mainly using Rackham on UPPMAX as an example. We will show you how to find and load the needed modules, how to write a batch script, as well as how to install and use your own packages, and more. The course will consist of lectures interspersed with hands-on sessions where you get to try out what you have just learned.

This course will consist of three days. Each day starts at 9:00 and closes 15:00. One day for each language.

Participation is free and open to all current and prospective users of NAISS.

Time and date: 09:00 - 15:00, 12-14 March 2024

Location: online via Zoom

- For more information and registration, see the course websites:
- HPC2N: <https://www.hpc2n.umu.se/events/courses/2024/intro-py-jl-r-fall>
- UPPMAX: <https://www.uppmx.uu.se/support/courses-and-workshops/r-python-julia>.

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Online Training: Introduction to PDC Systems Course, 21-22 March 2024

This course spans two half-days and focuses on utilising the Dardel high-performance computing (HPC) system provided by PDC. Throughout the course, we will cover fundamental information about Dardel and its usage, including an overview of the infrastructure, account management, logging in procedures, job execution, data storage, and code compilation. Specifically, we will progress from basic usage of Dardel to more advanced topics, such as exploring scientific areas where application experts can provide assistance and showcasing flagship software developed at KTH.

Time: Thu 2024-03-21 09.00 - Fri 2024-03-22 12.00

Location: Online via Zoom

For more information and access to registration please visit the event page:

<https://www.pdc.kth.se/about/events/introduction-to-pdc-systems-course-1.1320420>

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Online Workshop: VASP/EMTO Best Practices Workshop, 16 - 18 April

Cooperation between ENCCS and NAISS

NAISS and ENCCS organise the VASP/EMTO Best Practices Workshop. During the workshop we will showcase how to run the VASP (Vienna Ab-initio Simulation Package) and the EMTO (Exact Muffin-Tin Orbitals) packages efficiently on supercomputers. This workshop includes: 1) basic theory, DFT and PAW-method; 2) general introduction to VASP and EMTO, essential files and parameters, workflow; 3) running VASP at HPC centers, CPUs and GPUs (examples from NAISS); 4) performance analysis; 5) common issues; 6) post-processing tools; and 7) running VASP/EMTO calculations step-by-step on the Tetralith and Leonardo Booster clusters.

Time: 16-18 April, 10:00-15:00 (2024).

Detailed information and access to registration are handled on the ENCCS webpage: <https://enccs.se/events/vasp-emo-best-practices-workshop/>

Online training: Programming Formalisms course, 22 - 26 April 2024

Collaboration between UPPMAX and NBIS

This course aims to give life scientists, bioinformaticians, and other scientists with some experience in programming and scripting an understanding of the underlying principles of software development, design, and programming. The course aims to strengthen the understanding of more advanced programming concepts, ability to produce more reusable scripts through modular programming and to enable a better understanding of how to evaluate a script or programs performance.

We will cover an introduction to Algorithms and Data structures, Programming Paradigms especially structured and object oriented programming and to give a overview of other paradigms like functional programming. Modular development and (code) reusability, testing and optimisation.

We will cover theory with bridging practical examples and applications to enhance the theoretical understanding of the principles.

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

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>

CodeRefinery training

Online workshop: CodeRefinery workshop, 12-14 and 19-21 March 2024

Organised by CodeRefinery and partners, among which are NAISS, UPPMAX, PDC, and ENCCS

Are you writing code and managing data for your research? Do you feel like wasting too much time on manual work? Do you struggle to understand and reuse older code?

Join the CodeRefinery workshop 12-14 and 19-21 March 2024, for free and online.

The workshop covers good coding practices, reproducible research principles, and using Git for collaboration. It offers breakout room exercises with team leaders, and you can register as a team or volunteer as a team leader. But you can also follow on your own if you prefer. In-person exercise sessions are available in some locations.

For registration and more information, please visit <https://coderefinery.github.io/2024-03-12-workshop>.

ENCCS training:

The Multi-GPU Programming Bootcamp, 6-7 May

Scaling applications to multiple GPUs across multiple nodes requires one to be adept at programming models and optimisation techniques, and proficient at performing root-cause analysis using in-depth profiling to identify and minimise bottlenecks.

Topics on GPU programming covers single node multi-GPU (P2P) and multi-Node multi-GPU (GPU Direct) programming, the NVIDIA Collectives Communications Library (NCCL), and the NVSHMEM, which is a parallel programming interface based on OpenSHMEM that provides efficient and scalable communication for NVIDIA GPU clusters).

The Multi-GPU Programming Bootcamp covers step-by-step ways to improve application performance using cues from profilers and provides an understanding of the underlying technologies and communication topology needed to leverage powerful NVIDIA® libraries to extract more performance from the system.

Detailed information at ENCCS (<https://enccs.se/events/2024-05-multi-gpu-programming/>) and OpenHackathons (<https://www.openhackathons.org/s/siteevent/a0C5e000008AbEfEAK/se000316>) webpages.

Time: May 6-7, 9:00-15:00 (2024).

Link to the registration: <https://www.openhackathons.org/s/siteevent/a0C5e000008AbEfEAK/se000316>

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>.