



Parallel Programming in Computational Engineering and Science (PPCES)

HPC Training Event 2025

March 10th-14th, 2025 | Aachen

Dr. Marc-André Hermanns, Dr. Christian Terboven,
Dr. Jannis Klinkenberg, Dr. Sandra Wienke



Who We Are? – Organizations

- **NHR4CES**: NHR for Computational Engineering Science
 - NHR = National High Performance Computing: alliance of 9 German universities to provide resources and competencies to scientists at all German universities
 - RWTH + TU Darmstadt = NHR4CES: focus on computational engineering sciences
- **IT Center** of RWTH Aachen University, HPC team
 - Provides consulting and training services for HPC users
 - Conducts own HPC research and lecturing (Chair for High Performance Computing)
- **HPC.NRW**: The North Rhine-Westphalian Competence Network for HPC
 - Connection of expertise of the large HPC centers (Tier 2) with the consulting services of smaller centers (Tier 3)
- **EDIH Rheinland**: European Digital Innovation Hub
 - Advice on Digitalization, Artificial Intelligence and High Performance Computing
 - Focus on small and medium-sized enterprises, Start-ups, Spin-offs and public facilities
- **WestAI**: AI services from NRW for Germany
 - Consulting services and access to hardware resources on Nvidia H100 for academia as well as small and medium-sized enterprises*



* constraint to research and exploration activities

PPCES Overview

- Annual one-week workshop since 2011
- Content
 - Lectures: contents generally applicable
 - Lab exercises: executed on RWTH's HPC cluster "CLAIX"
 - Applying learned concepts in practice (with help from supervisors)
 - Individual discussions possible
- Materials on website: <https://blog.rwth-aachen.de/itc-events/en/event/ppces-2025/>
 - Additionally: [Introduction to HPC](#) (architecture, storage, compute time, slurm,...)
- Catering is sponsored by NEC

 **Orchestrating a brighter world**

NEC

PPCES Overview

MPI		OpenMP		Machine Learning	Legend
Mon, March 10th	Tue, March 11th	Wed, March 12th	Thu, March 13th	Fri, March 14th	
		Start: 9:00h			
					lecture/ lab
10:30 – 11:00	10:30 – 11:00	10:30 – 11:00	10:30 – 11:00	10:30 – 11:00	break
12:40 – 14:00	12:30 – 14:00	12:30 – 14:00	12:30 – 14:00	12:30 – 14:00	
15:30 – 16:00	15:30 – 16:00	15:30 – 16:00	15:30 – 16:00	15:30 – 16:00	
		End: 17:00h			

HPC Cluster CLAIX-2023 (Tier-2 + Tier-3)

Theoretical Peak Performance CPUs	2.6 + 1.4 PFlops
Theoretical Peak Performance GPUs	4.4 + 0.7 PFlops
Available resources CPUs	346 + 185 Mio Coreh
Available resources GPUs	27 + 4 Mio Coreh (1 GPU-h == 24 Core-h)
HPC Segment	412 + 220 HPC nodes 2-socket Intel Sapphire Rapids (Xeon 8468, 2x48 cores, 2.1 GHz) <ul style="list-style-type: none"> • 470 nodes with 256 GB • 160 nodes with 512 GB • 2 nodes with 1024 GB
ML Segment	32 + 5 ML nodes 2-socket Intel Sapphire Rapids (Xeon 8468, 2x48 cores, 2.1 GHz, 256 GB) 4x NVIDIA H100 96 GB HBM2e per node
Interactive Segment	One ML node with MIG configuration (e.g., for JupyterHub usage)
Fabric	Infiniband NDR network 2:1 blocking
Storage	29 PB Lustre Storage (HPCWORK) 1.1 PB GPFS (HOME/WORK) BEEOND on SSDs (1.4 TB per node)



Additional WestAI resources:
15 ML nodes

Accessing CLAIX – Hardware

Dedicated hardware (and accounting) for the workshop

- 4 CLAIX-2023-HPC nodes
- 10 CLAIX-2023-ML nodes

	MPI & OpenMP	ML/DL
Advanced reservation	PPCES-m	PPCES-g
Compute time project	lect0138	

Example in batch script file:

```
#SBATCH -reservation=PPCES-m
#SBATCH -account=lect0138
```

Login nodes (full list [here](#))

- login23-x-1.hpc.itc.rwth-aachen.de (X-Server, remote desktop sessions, [web access possible](#))
- login23-x-2.hpc.itc.rwth-aachen.de (X-Server, remote desktop sessions, [web access possible](#))
- login23-2.hpc.itc.rwth-Aachen.de
- login23-3.hpc.itc.rwth-Aachen.de

Accessing CLAIX – Accounts

Members of RWTH (or affiliated persons)

- HPC account required: <https://regapp.itc.rwth-aachen.de/>
 - Two-factor-authentication (2FA) required
- If provided during survey, all permissions for dedicated hardware have already been granted
- **If not, please contact the IT center staff during the lab session!**

External participants

- Temporary account and SSH key was sent to you by e-mail
 - Account: `hpclab[01-20]`
 - Key: Linux format (pem) or PuTTY/pageant format (ppk)
 - **If you didn't get an e-mail, please contact the IT Center staff during the lab session!**
- Password: will be provided during the lab sessions
- Hpclab accounts have all permissions for dedicated hardware

See Handout: **HPC Cluster Access** for further details

The screenshot shows a handout page titled "HPC Cluster Access for External Users". At the top, there are logos for NHR4 CES, HPC.NRW, EDIH Rheinland, WEST AI KI-Servicezentrum, IT Center, and RWTH AACHEN UNIVERSITY. The page is divided into several sections:

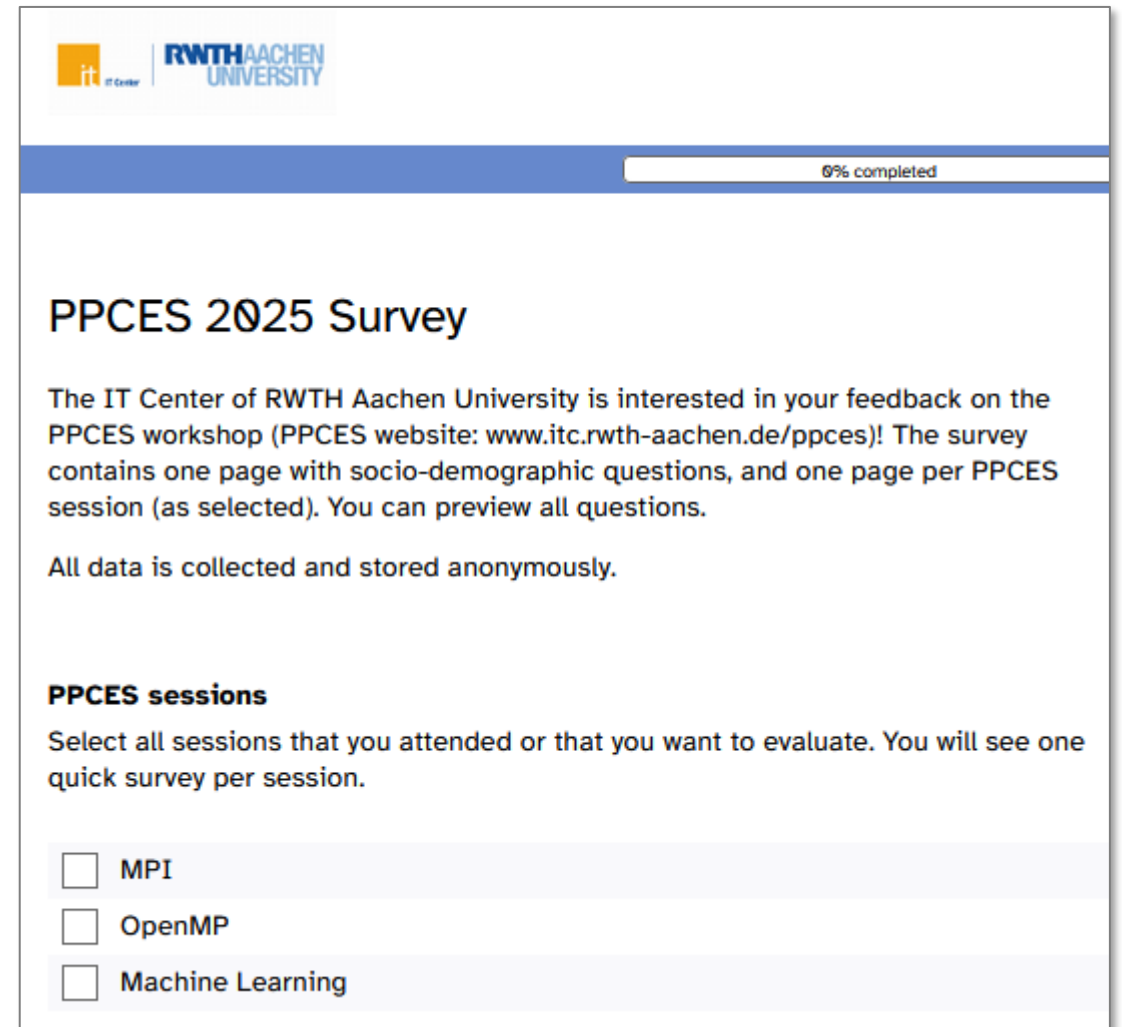
- Links:** A box containing four links: [1] FastX, [2] pageant, [3] PuTTY, and [4] WinSCP.
- Basic Information:** A list of items including SSH (private) keys and HPC account names.
- Linux Users:** Instructions for access via SSH, including a terminal command and a note about login nodes.
- Windows Users:** A section titled "Option 1: Remote Desktop Access with the FastX Desktop Client [1]" which includes a list of steps for setting up the client and connecting. To the right of this text is a screenshot of a Windows system tray icon for the FastX Desktop Client, with a context menu open showing options like "View Keys", "Add Key", "Remove All Keys", etc.

At the bottom right, there is a small screenshot of the "Edit Connection" dialog box in PuTTY, showing the "Host" field set to "ssh" and the "User" field set to "hpclab-<no>".

Evaluation – Feedback Wanted!



PPCES Evaluation Form
(open until March 30th, 2025)
<https://s2survey.net/ppces2025>



The screenshot shows the survey interface with the RWTH Aachen University logo and IT Center branding at the top. A progress bar indicates 0% completion. The main heading is "PPCES 2025 Survey". The introductory text explains the survey's purpose and provides the website URL. Below this, it states that data is collected anonymously. The "PPCES sessions" section lists three options: MPI, OpenMP, and Machine Learning, each with an unchecked checkbox.

PPCES 2025 Survey

The IT Center of RWTH Aachen University is interested in your feedback on the PPCES workshop (PPCES website: www.itc.rwth-aachen.de/ppces)! The survey contains one page with socio-demographic questions, and one page per PPCES session (as selected). You can preview all questions.

All data is collected and stored anonymously.

PPCES sessions

Select all sessions that you attended or that you want to evaluate. You will see one quick survey per session.

- MPI
- OpenMP
- Machine Learning