

Parallel Programming in Computational Engineering & Science (PPCES) 2024



TECHNISCHE
UNIVERSITÄT
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NHR for
Computational
Engineering
Science

Welcome & Organization

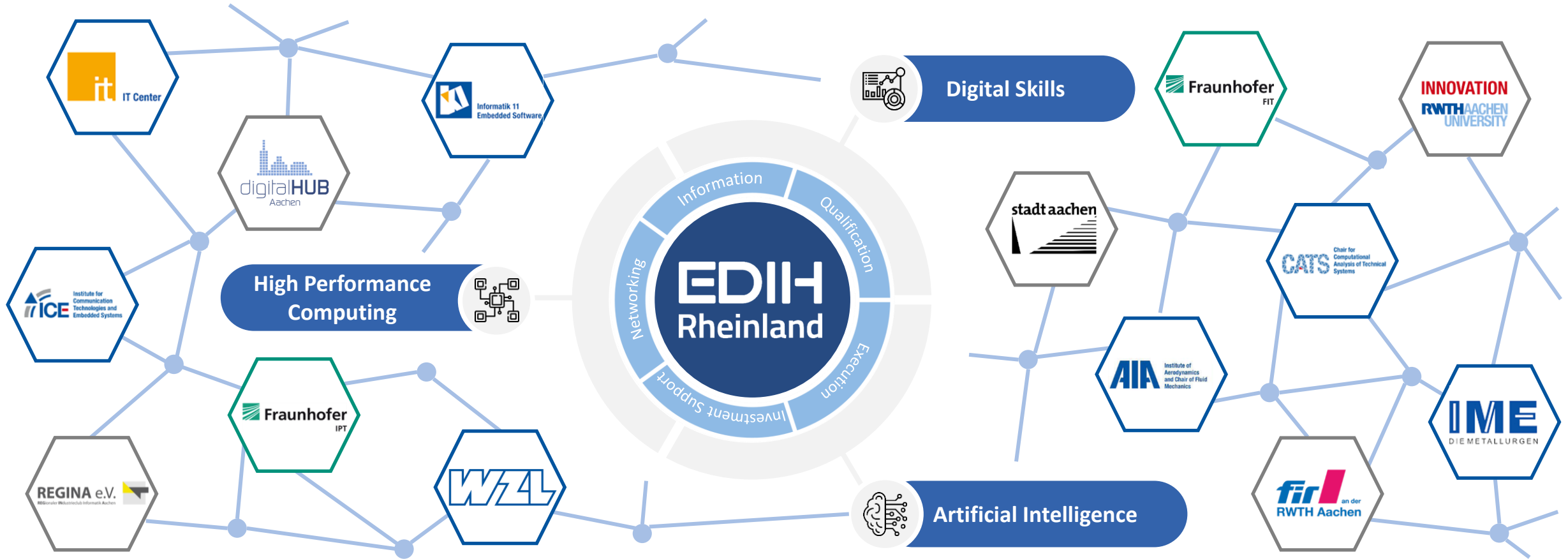
About PPCES

- Annual one-week workshop since 2011
- Lectures: contents generally applicable
 - Presenting contents of a certain topic
 - Short general discussion at the end
- Lab exercises: executed on RWTH's CLAIX HPC cluster
 - 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-2024/>
 - Additionally: [Introduction to HPC](#) (architecture, storage, compute time, slurm,...)
- Catering is sponsored by NEC



 Orchestrating a brighter world

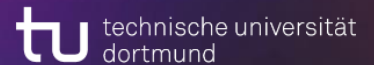
NEC



Das EDIH Rheinland bietet einen einfachen Zugang zu innovativen und zukunftsorientierten Technologien.

WestAI

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Agenda

OpenMP		MPI		Machine Learning
Mon, March 11th	Tue, March 12th	Wed, March 13th	Thu, March 14th	Fri, March 15th
		Start: 9:00h		
10:10 – 10:40	10:30 – 11:00	10:30 – 11:00	10:30 – 11:00	10:30 – 11:00
12:00 – 13:30	12:00 – 13:30	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		

Legend

lecture/ lab
break

CLAIX-2023 (Tier3 + Tier2)

HPC Segment	<p>412 + 220 HPC nodes 2-socket Intel Sapphire Rapids (Xeon 8468, 2x48 cores, 2.1 GHz)</p> <ul style="list-style-type: none"> • 470 nodes with 256 GB • 160 nodes with 512 GB • 2 nodes with 1024 GB <p>→ 2.6 + 1.4 PFlop/s (theoretical peak performance)</p>
ML Segment	<p>32 + 5 ML nodes 2-socket Intel Sapphire Rapids (Xeon 8468, 2x48 cores, 2.1 GHz, 256 GB)</p> <p>4x NVIDIA H100 96 GB HBM2e per node</p> <p>→ 4.4 + 0.7 PFlop/s (theoretical peak performance)</p>
Interactive Segment	Additional nodes with smaller GPUs (e.g., for JupyterHub usage)
Fabric	Infiniband NDR network (OPA) 2:1 blocking
Storage	26 PiB Lustre Storage BEEOND on SSDs (1.4 TB per node)



[Hardware overview on IT Center Help](#)

Accessing the CLAIR HPC Cluster

Accounts

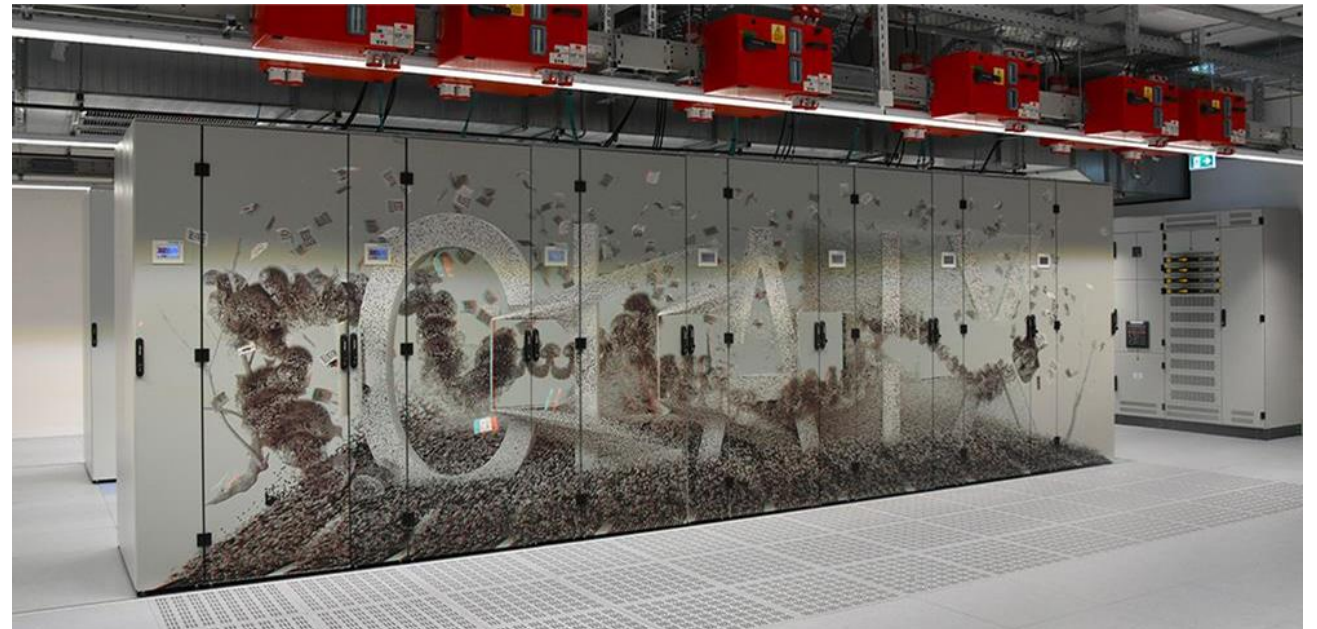
Members of RWTH (or affiliated persons)

- [HPC account required:](https://regapp.itc.rwth-aachen.de/)
https://regapp.itc.rwth-aachen.de/
- [Two-factor-authentication](#) (2FA) required

External participants

- Temporary account will be provided

Dedicated hardware for the workshop



	OpenMP days	MPI days	ML day
Advanced reservation	PPCES24	PPCES24MPI	PPCES24GPU
Compute time project	lect0113	supp0006	lect0114

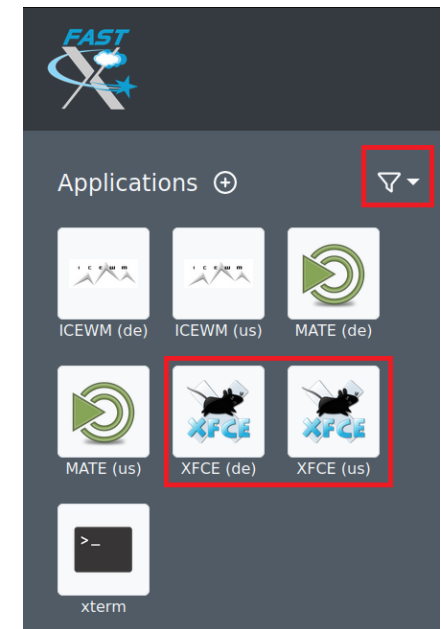
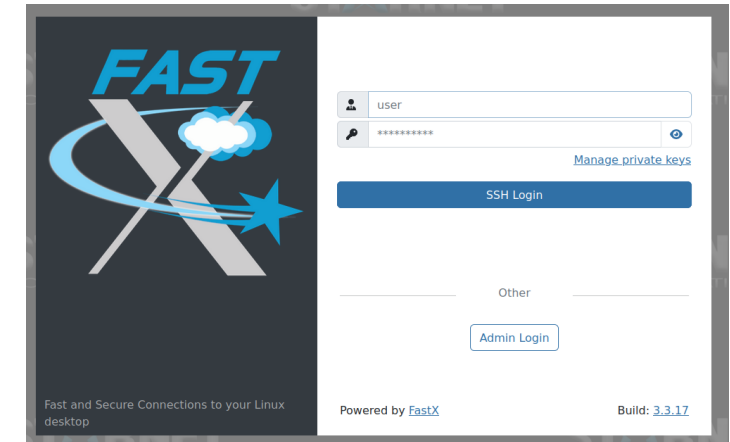
Example in batch script file:

```
#SBATCH -reservation=PPCES24
#SBATCH -account=lect0113
```

Remote Desktop Access

FastX3 (desktop client or browser)

- Browser client: <https://login23-x-2.hpc.itc.rwth-aachen.de:3300>
- Desktop client: login nodes (see next slide)
- Select the correct application
 - Recommended: XFCE
 - May need to select “all applications” in Filter at the top right corner of the Application box
- Start the session
 - Click on the session (may have to click twice)
- Open up a terminal
 - Bottom of the screen
 - Click the “terminal” icon



Cluster Access

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

- login23-x-2.hpc.itc.rwth-aachen.de (CLAIX-2023, X-Server)
- login23-2.hpc.itc.rwth-Aachen.de (CLALIX-2023)
- login23-3.hpc.itc.rwth-Aachen.de (CLAIX-2023)
- login18-2.hpc.itc.rwth-aachen.de (CLAIX-2018)
- login18-3.hpc.itc.rwth-aachen.de (CLAIX-2018)

Access via SSH

Access from within the RWTH network / eduroam via ssh:

- `ssh -Y ab123456@login23-x-2.hpc.itc.rwth-aachen.de`
- GitBash for Windows: <https://git-scm.com/download/win>

Cluster Access: External Participants Only!

Account

- Username: `hpclab[01-50]`
 - Distribution of accounts by speaker/helpers
- Password: see paper sheet

Access

- Login node: `login18-beta.itc.hpc.rwth-aachen.de`
 - Use desktop client or
 - Web interface: <https://login18-beta.hpc.itc.rwth-aachen.de:3300>
- Jump from there to a CLAIX-2023 frontend node (see node list on previous slide)

```
ssh -Y hpclab[01-50]@login23-2.hpc.itc.rwth-aachen.de
```

Note: Do not store any private/ sensitive data on the cluster

Evaluation



Feedback Wanted!



PPCES Evaluation Form

(valid until March 29th, 2024)

<https://s2survey.net/ppces2024/>

The screenshot shows the survey interface. At the top left, there are logos for 'itc.rwth-aachen.de' and 'RWTH AACHEN UNIVERSITY'. A progress bar at the top right indicates '0% completed'. The main heading is 'PPCES 2024 Survey'. Below this, a paragraph explains that the IT Center of RWTH Aachen University is interested in feedback on the PPCES workshop, with a link to the website. It states the survey contains socio-demographic questions and one page per session. A note mentions that all data is collected and stored anonymously. Under the heading 'PPCES sessions', there is a list of three sessions with checkboxes: OpenMP, MPI, and Machine Learning.

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0% completed

PPCES 2024 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.

- OpenMP
- MPI
- Machine Learning