WEST AI
KI-Servicezentrum

HPC.NRW

NHR4CES
NHR for Computational Engineering Science

TECHNISCHE UNIVERSITÄT DARMSTADT | RWTH AACHEN UNIVERSITY

Application for computing time NHR4CES / HPC.NRW / RWTH / WestAI

How can I get access to supercomputers?

Tim Cramer

GREAT COMPUTING COMES WITH GREAT SUPPORT.

Introduction

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- HPC resources are expensive
  - Up to 15 Mio € per Tier-2 system (expected life time: ~5 years)
  - Local staff for administration, maintenance, support, review processes, procurements, etc.
  - ~ 1 Mio € power consumption per year / system (depending on system size)

- Funding agencies (DFG, NRW, Bund, etc.)
  - Usage only for scientific purpose (e.g. crypto mining strictly forbidden)
  - HPC operators have to ensure scientific usage
    - Computing time application & review
    - Project monitoring
    - Project reports

Roles and Tasks

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- Principal Investigator (PI)
  - Responsible for the project application
  - Needs to be a senior researcher (e.g., a leading scientist with a Dr./PhD degree)
  - Can also act as reviewer for other NHR projects
  - Has to sign the proposal
  - Responsible for status report
  - Can grant access to further Project Members (PM)

- Person of Contact (PC) *[formally known as Technical Contact (TC)]*
  - Prepares the application and the project description
  - Fills out the (online) forms
  - Manages the computing project technically
  - Can grant access to further Project Members (PM)
  - Responsible for adding members to the project

- Project Member (PM)
  - Can use the granted computing time
  - Can be ANY person selected by the PI/PC, independent of the affiliation

How to apply for computing resources

Most effort for you here, we will take care about the other steps

Not for RWTH-S / PREP / WestAI projects

Really? So complicated? I just want to do research!

→ Don’t be afraid! It is not that bad ;-)

Project Preparation 1/6

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- Effort for proposal depends on amount of required resources
- Resource estimation (allocation in Mio-Core-h)
  - Core-h := Usage / reservation of one core for one hour
  - Example Core-h: Using one compute node with 96 cores for one year (24/7):
    96 cores * 24 h * 365 days = 0.84 Mio Core-h
  - Example Memory: Many HPC systems are equipped with 2-4 GB per core.
- Trial accounts / test projects possible (“PREP”)

Project Preparation 2/6

I want to use GPUs! Why are you talking about Core-h?

- Since October 1st, 2024 you have to apply GPU resources in "GPU hours (GPU-h)“
- Note: We account all resource (internal) in Core-h for historical reasons / simplification
- Mapping Core-h ←→ GPU-h exists:

One GPU-h corresponds to 24 Core-h:

$$1\ \mathrm{GPU{-}h} \coloneqq 24\ \mathrm{Core{-}h} \Leftrightarrow 1\ \mathrm{k\,GPU{-}h} \coloneqq \frac{24}{1000}\ \mathrm{Mio\ Core{-}h}$$

- Example: Using one GPU for one year (24/7):
  1 GPU * 24 h * 365 days = 8.76 k GPU-h = 8.76 * 24/1000 Mio Core-h = 0.21 Mio Core-h

- JARDS supports you with the math ;-)

Project Preparation 3/6

– Identify a fitting project category

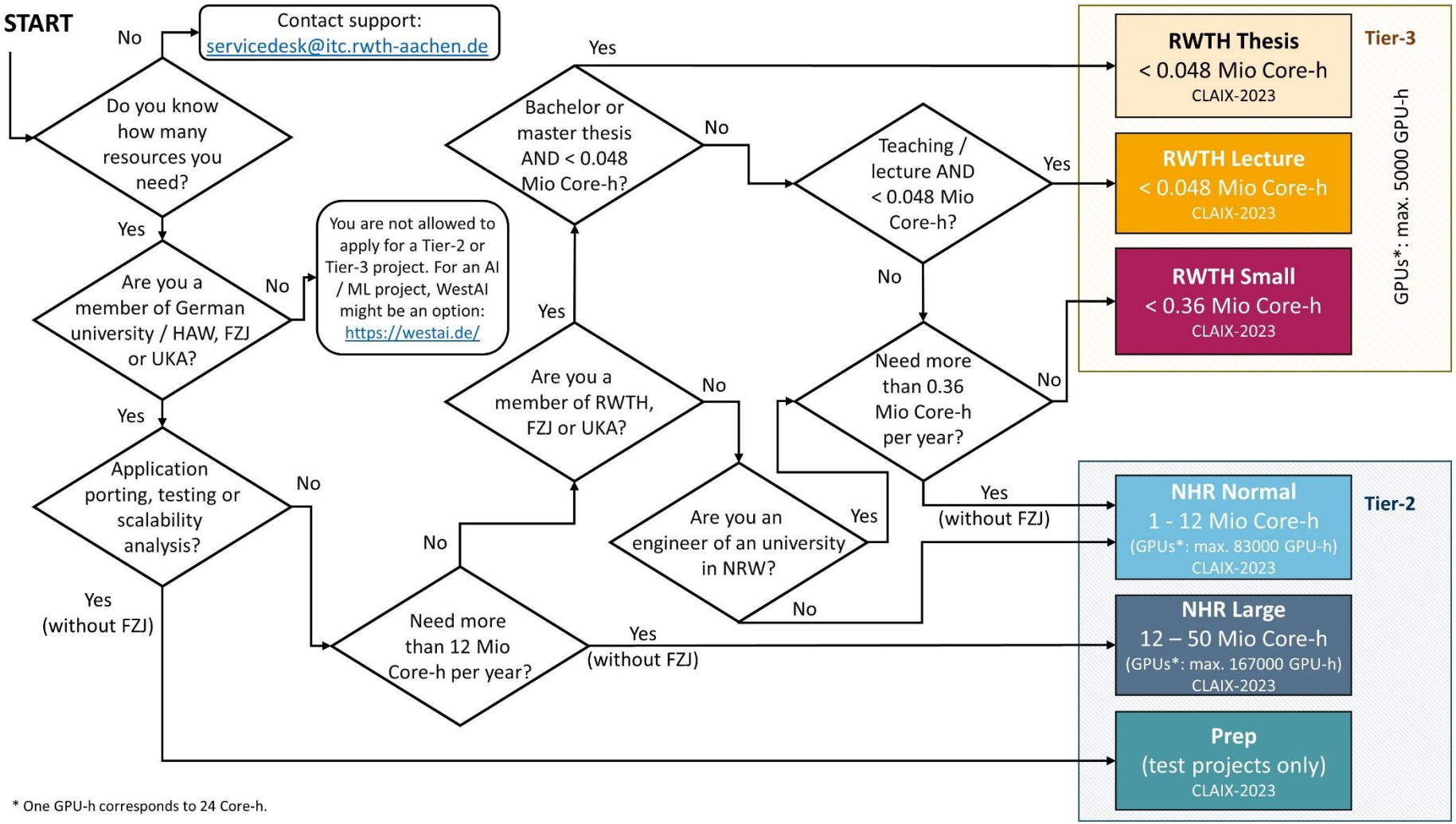
New limits

New category	Mio. Core-h *CPU* per year / project	k GPU-h *GPU* per year / project	Calls	Scientific Review	Tier
RWTH Thesis	< 0.048	< 2	Rolling	No	Tier-3
RWTH Lecture	< 0.048	< 2	Rolling	No	Tier-3
RWTH small	< 0.24	< 5	Rolling	No	Tier-3
WestAI	n.a.	< 10	Rolling	No	WestAI
NHR Prep	**Test projects only (really!)**	**Test projects only (really!)**	**Rolling**	**No**	**Tier-2**
NHR Normal	**1 – 12**	**< 83**	**4x p.a. / rolling** conditional approval as soon as scientific reviews are available	**Yes**	**Tier-2**
NHR Large	**12 - 50**	**< 167**	**4x p.a.**	**Yes**	**Tier-2**

Project Preparation 4/6

Identify a fitting project category

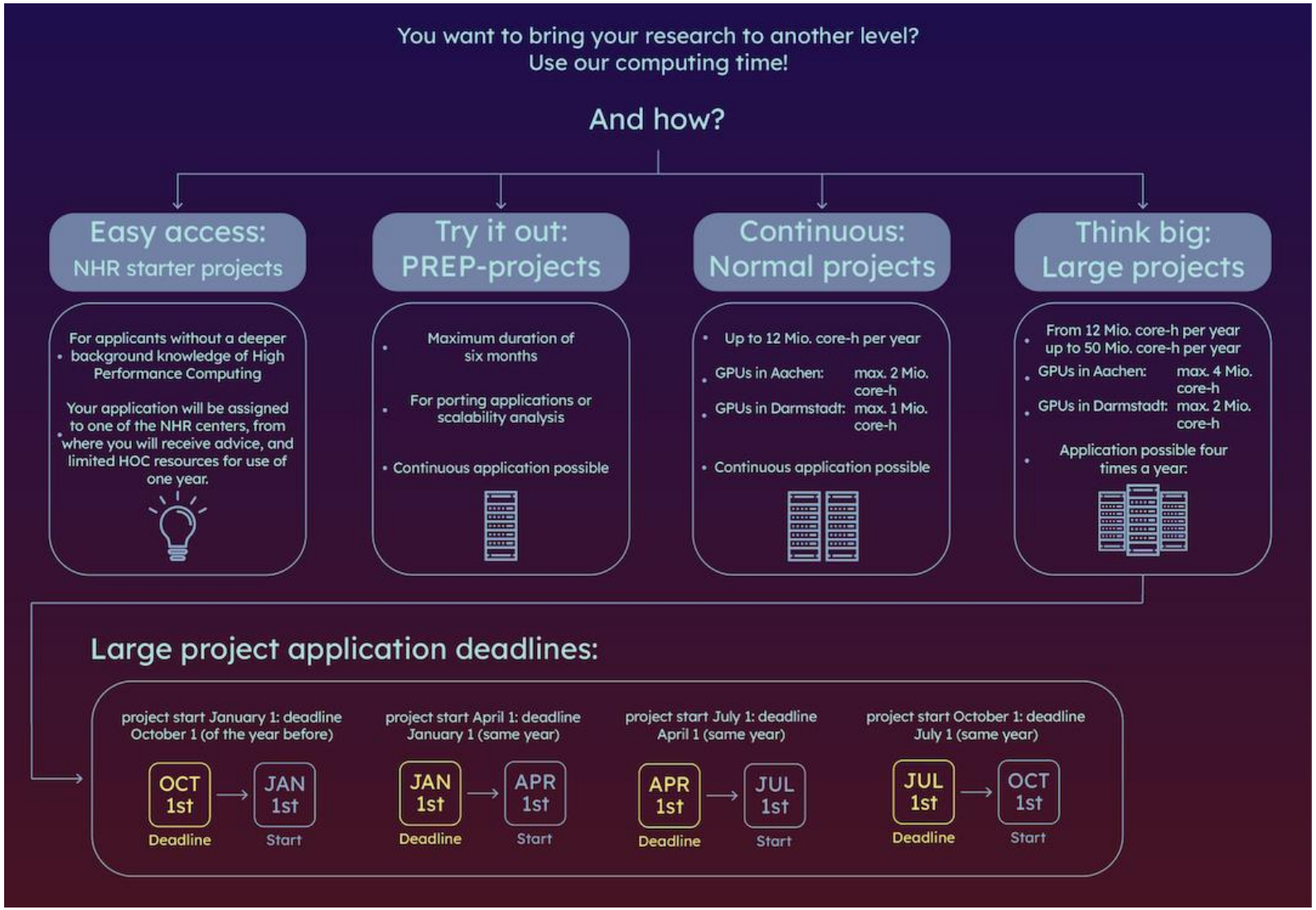
Additional option: WestAI projects



Project Preparation 6/6

NHR4CES Projects

- New step by step guide
- https://www.nhr4ces.de/hpc-access/



Proposal Submission

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1. Use the local submission system (JARDS)
   - RWTH / WestAI categories https://www.itc.rwth-aachen.de/hpc-project
   - NHR4CES: https://www.nhr4ces.de/hpc-access/

2. Principal Investigator (PI) has to sign the application in some cases

3. Send signed and scanned proposal

Formal Evaluation & Technical Review

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Formal Evaluation

- Formal aspects of a project are verified by the HPC center (e.g., Is the PI a professor or owns an Ph.D?)
- PI (or contact person) will be contacted if questions/problems show up
- Duration: usually some work days

Technical Review

- HPC experts will check your proposal for technical feasibility (e.g., availability of requested resources, software, etc.)
- Duration: up to two week

Scientific Review

- Not done for test (or smaller) projects
- We select 1-3 reviewer (=experts in the corresponding scientific domain)
- Depending on project size: Internal (=RWTH) or external experts
- Single-blind review
- Reviewers check the scientific soundness
- Duration:
  - Rolling calls: usually 4-6 weeks
  - Fixed date calls: up to 10 weeks (depending on deadlines)
- Note: If your project proposal is successful, you might be requested as review for other projects in future (also from other NHR centers!)

Resource Allocation and Monitoring 1/3

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- The Resource Allocation Board (RAB, “Vergabegremium”) decides about the resources for the project
- In case of success:
  - generate an account (if not done already)
  - add members to the approved compute project
  - prepare and submit job scripts for the project
  - obtain the project account information (quota, usage, etc.)
- Typical time for a project: One year
  - Uniform resource consumption on monthly-base expected
  - You might borrow Core-h from next month or use from last month

Resource Allocation and Monitoring 3/3

- Technically every project on the cluster has a certain budget
- Example Aachen (command line tool):
  - Sliding Window (3 months)
    - 1000 (remainder from previous month)
    + 50000 (for the current month)
    + 50000 (for next month)
    - 59000 (consumed this month)
    = 40000 Core-h left over to be consumed this month at most!

    OR:

    Core-h left over for this month*:
    50000 * -20% = -10000

```
$ r_wlm_usage -p bund1234 -q
Account:                                  bund1234
Type:                                        bund
Start of Accounting Period:             01.11.2020
End of Accounting Period:               31.10.2021
State of project:                           active
-------------------------------------------------
Quota monthly (core-h):                      50000
Remaining  core-h of prev. month:            -1000
Consumed   core-h current month:             59000
Consumed   core-h last 4 weeks:              65000
Consumable core-h (%):                         -20
Consumable core-h:                           40000
-------------------------------------------------
Total quota (core-h):                   0.600 Mio
Total consumed core-h so far:           0.500 Mio
-------------------------------------------------
Default partition:                           c18m
Allowed partitions:                     c18m,c18g
Max. allowed wallclocktime:             24.0 hours
Max. allowed cores per job:                  384
```

* 200%: No core-hours were used during the previous and the current month
-101%: The usage for the current and the previous month is > three months' quota

Project Reports

- After the project you have to provide a report about the scientific results
- Acknowledgments in related publications required

→ Both helps the HPC centers to argue for new future HPC resources

https://www.itc.rwth-aachen.de/cms/it-center/IT-Center/Publikationen/~ljja/Jahresberichte/?lidx=1

Conclusion

Questions?