

Applying for HPC resources at NHR@FAU – How to use JARDS

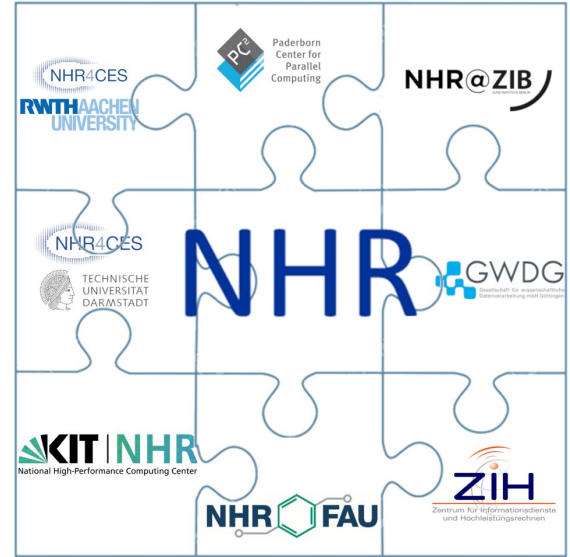
HPC-Café 12.03.2024

PD Dr. Harald Lanig

Zentrum für Nationales Hochleistungsrechnen Erlangen (NHR@FAU)



Nine NHR centers form the NHR alliance



NHR provides

- HPC resources
- Scientific/technical project support
- Performance optimization support

Application for NHR resources

- NHR resources are **open to researchers at German universities**
 - No charge!
 - For detailed information see <https://www.nhr-verein.de/en/computing-time>
- **Application** for resources through **central JARDS portal** (now available)
 - **Joint Application, Review, and Dispatch Service**, developed since 2014 at JSC
 - Researchers have to choose a **NHR center** AND **project category** which meets their requirements best
 - <https://jards.nhr-verein.de/>
- **Peer review process**
 - Scientific quality / need for Tier-2 resources must be proven
 - **Simplified review process** for projects reviewed by DFG (and others)

NHR@FAU project types and limits

Project type	GPU limits ¹ (GPU hrs)		CPU limits ¹ (mio. core-hrs)	Review	deadline
	A40	A100			
Test/Porting	< 3.000	< 3.000	< 0,5	technical	rolling call
Starter	< 10.000	< 10.000	< 1	technical	rolling call, only one time per group
Normal	6.000	4.000	1	technical rev. + 2 scientific rev.	rolling call
Pre-reviewed normal	— 60.000	— 40.000	— 10	technical rev. + resources/method	rolling call
Large Scale	60.000	40.000	10	technical rev. + 2 scientific rev.	cut-off quarterly
	— 180.000+	— 120.000+	— 30+		

¹Annual allocations

Admission to NHR and NHR@FAU systems

- At NHR@FAU, the **central application platform JARDS**
 - Is now mandatory for **Large Scale** and **Starter** projects
 - May be used for other available project categories
 - Entry point via <https://jards.nhr-verein.de/>
- You can still apply for **Test/Porting** and **Normal** projects **locally**
 - **Our NHR@FAU application form** is available at <https://doc.nhr.fau.de/nhr-application/>
 - Submit the filled template by email to: hpc-support@fau.de
- Any questions? Feel free to ask us: hpc-support@fau.de

Admission to NHR and NHR@FAU systems

- Application evaluation process
 - **Technical reviewing** by NHR@FAU staff
 - **You already get access to HPC resources!**
 - **Local Steering committee assigns reviewers** (local and external)
 - **Scientific reviewing** by local/external reviewers
 - Allocation decision by **local steering committee**
 - Exception for Large Scale projects: approval by **central NHR board** necessary
(*“Zentraler NHR-Nutzungsausschuss”*) meets 4 times/year
 - Accepted projects get a project advisor / support expert assigned
-
- From **application to decision: usually less than 3 months!**

NHR@FAU application form

- Word document (is used in shortened form also by JARDS)
 - Available via <https://doc.nhr.fau.de/nhr-application/>
- Structure
 - Part A: **Administrative Data**
 - Part B: **Scientific Project Information**
- The application form addresses:
 - scientific quality
 - justification of requested resources
 - performance / scalability of the code
 - administrative data

Project Application Form: Part A

- **Part A – Administrative Data**

- **1 General Information**

- Principal Investigator, Project Manager, institution
 - Scientific field, HPC experience

- **2 Project Information**

- Title, acronym, project type (test/normal/large) and duration
 - Pre-existing reviews, sensitive data

- **3 Technical Description**

- Requested resources (CPU, GPU, storage)
 - Application software and tools
 - Proof of efficient HPC usage

Project Application Form: Part B

- **Part B – Scientific Project Information**

- **Test/porting projects**

- Please provide a **short summary** of your test or porting project which **justifies the use of the HPC resources**. The total text should not exceed one page.
 - A half page “project description” is sufficient. Focus on HPC aspects.

- **Normal projects with granted/reviewed DFG/BMBF/EU application**

- As the scientific part of your project has already been reviewed, it is **sufficient to provide a project summary. Anyway you should make clear the amount of HPC resources you apply for**. The total text of this chapter should not exceed two pages.

- **Large projects and normal projects without existing review**

- Please provide **a scientific description of your project**. The total should not exceed 3 to 6 pages for a normal project, and 5 to 10 pages for a large project, respectively.

Project Application Form: Part B

- **Part B – Scientific Project Information**

- **4 Scientific Project Description**

- Abstract, description (all types)
 - State of the art and preliminary work, scientific goals, detailed scientific project description, detailed project plan (only large projects and normal projects without existing review)
 - Summary/statement of existing scientific reviews and justification for applied HPC resources (normal project with grant/review by DFG, BMBF, EU, etc)

Please note: **Attaching an existing review (or essential parts of it) may considerably speed-up the scientific reviewing process!**

- References

Project Application Form: Part B

- **Part B – Scientific Project Information**

- **5 Follow-up Projects**

- Resources used and results obtained so far
 - Short intermediate report and outreach

- **6 Optional Information**

- **Reviewer suggestion**
 - Awareness in the community

- **7 Final Notes**

- Acknowledgement of granted resources in publications/applications
 - Providing of publications to NHR@FAU
 - Possibility to future serve as a reviewer

How to submit an application in JARDS



Which NHR center to choose?

<https://www.nhr-verein.de/en/information-center-selection>

Information for Center Selection

All NHR centers have up-to-date HPC hardware and offer best conditions for well-scaling applications. The following is a brief description of the centers' resources as well as the consulting services offered.

Center	Description	Details	Application Guidelines
NHR@FAU	<p>NHR@FAU currently runs more than 70 000 CPU cores and offers extensive GPU resources for throughput calculations as well as moderately parallel applications (up to 8 GPUs). Available are 304 NVIDIA A100 (40/80 GB) as well as 352 NVIDIA A40 cards; the latter are particularly suitable for molecular dynamics simulations with standard packages such as GROMACS and AMBER.</p> <p>User support is known for its expertise in performance engineering for CPU and GPU nodes as well as iterative solvers. In application support, NHR@FAU has a special focus on atomistic simulations.</p>	Link	Link

<https://doc.nhr.fau.de/nhr-application/>

Calling JARDS

<https://jards.nhr-verein.de/>

Start Page

Welcome to JARDS, please choose if you want to create an application or review submitted applications.

Applications

Please select an application kind to create an application. If you do not yet know which project category and/or NHR-center are appropriate for you, please first refer to the information on the [NHR website](#).

Select Appkind *

Please select a category ▾

Open Applications

Please select a category

NHR Starter

NHR Test/Preparation

NHR Normal

NHR Large

category is intended for applicants without experience with the application procedure with performance computing, and without deeper background knowledge of high performance computing. Your application will be assigned to one of the NHR centers, from where you will receive limited HPC resources for use for one year. The goal is easy access, and to enable you to submit a successful proposal in the Normal or Large project categories.

2. NHR Test/Preparation Projects: This project category is mainly used to prepare an application; it can

Calling JARDS

Select the NHR Center

Please select an [NHR Center](#) for your computing time project. Feel free to contact info@nhr-verein.de, if you do not yet know which center fits best to you.

NHR Center Selection *

Please select the NHR Center ▾

Please select the NHR Center

NHR4CES@RWTH

NHR4CES@TUDa

NHR@ZIB

NHR@TUD

NHR@FAU

NHR@Göttingen

NHR@KIT

PC2

NHR@Süd-West

NHR Center Selection *

NHR@FAU ▾

Select Center

Calling JARDS



Electronic project application form for NHR@FAU Compute Cl
Category: NHR Large

✓ Mail sent to harald.lanig@fau.de

Login

E-mail Callback

Before you can apply for computing time we will check your identity with an automatic e-

We will send an e-mail with a link to the specified address. By using the link in this e-mail application for computing time.

Make sure to enter the same e-mail address used for previous applications, if applicable.

Login mail address

harald.lanig@fau.de

Data Privacy

☒ By using the platform, you agree to the [privacy policy](#) and consent to the collection, processing and use of your data in accordance with the applicable data protection laws and the stated provisions (according to the German Basic Law, the German Data Protection Act and the EU General Data Protection Regulation).

callback

Von jards@nhr-verein.de
jards@nhr-verein.de
An harald.lanig@fau.de
Antwort an hpc-support@fau.de
Betreff **Project application identification**

Antworten Weiterleiten Archivieren Junk L

back

This is an automatically created email. (Please do not reply to this message.)

An identification request for the application of NHR@FAU compute resources has been submitted for this email address. By clicking on the URL below, you can continue with the electronical application and confirm that you are the registered owner of this email address.

<https://jards.nhr-verein.de/jards/WEB/application/apply.php?PHPSESSID=n44drKEY=Hp17UcpEfP49PlvWxjpfOKMhjT67b5VgzWkTSfPIIdGpHBLkp8MMXAuvIil1v>

The URL is valid until 07.03.2024 17:28.

It is possible that another person specified your E-Mail address by mistake. In this case, please ignore this message.

Erlangen National High Performance Computing Center (NHR@FAU)

Email: hpc-support@fau.de

New Project Application

Electronic project application form for NHR@FAU Compute Cluster
Category: NHR Large

≡ CONTENT ▾

Application lists

Here you can create new applications by clicking the 'New Project Application' Button.
Find also your active and past projects, and your current and previous applications in the lists below.

► More information

You are logged in as: **harald.lanig@fau.de**

Please define your role (PI, PC or both) during the application process.

If this application is a request for extending an existing
computing project, please enter the project ID here



Your projects:

Search

+ New NHR Large Project Application

Access to another application kind

b101sd

Title: md simulations

Applications: 20971 FAU GPUs 12.10.2023-11.10.2024

Electronic project application form for NHR@FAU Compute Cluster

Category: NHR Large

✓ Created new application.

⚠ For the extension of existing projects, please use the "extend" button in the [Application list](#).

Choose PI and PC

Principal Investigator (PI) and Person of Contact (PC) must be chosen here for this application. To change between PI and PC, click the button.

- Your email address needs to be used either as PI or PC email address
- PI and PC email addresses need to differ
- PI is required while PC is optional
- PI is required to have at least a PhD degree or an equivalent qualification
- The PC is also the manager and technical contact of the project, who will be responsible for creating the accounts

E-mail address of principal investigator (PI) *

harald.lanig@fau.de

↓ switch PI and PC ↑

E-mail address of person of contact (PC)

☐ Apply as both, PI and PC

Application ID: 21692

1	Application list
2	Choose PI and PC
3	Show data PI
4	Project data
5	Resource Selection
6	Upload files
7	Remarks
8	Finalize

Personal Data: Principal Investigator (PI)

You can modify your own personal data [here](#). After making your changes you can use the "save profile & return to application" button to proceed with your application.

Note: The Principal Investigator (PI) must be a member of a publically funded university in Germany and must have a doctor's degree or equivalent, e.g., a Ph.D.

The PI is kindly requested to take part in reviewing other scientists' compute project proposals or otherwise to nominate a delegate who is able to thoroughly take part in the reviewing process.

Gender	Title	First name *
<input type="text" value="m"/>	<input type="text" value="Select title"/>	<input type="text" value="Harald"/>
E-mail address of principal investigator (PI) *		Phone *
<input type="text" value="harald.lanig@fau.de"/>		<input type="text" value="+4991318571112"/>
Nationalities *		
COUNTRY:		Germany
ISO CODE:		DE

Affiliation PI

Federal State *	Institution *
<input type="text" value="Bayern"/>	<input type="text" value="Universität Erlangen-Nürnberg"/>
Institute *	
<input type="text" value="Erlangen National High Performance Con"/>	

Institute name:

Erlangen National High Performance Computing Center (NHR@FAU)

Institute address

Martensstr. 1
91058 Erlangen Germany

Assigning the Person of Contact (Project Manager)

Electronic project application form for NHR@FAU Compute Cluster
Category: NHR Large

Application ID: 21692

1	Application list
2	Choose PI and PC
3	Show data PI
4	Data PC
5	Project data
6	Resource Selection
7	Upload files
8	Remarks
9	Finalize

Personal Data: Person of Contact (PC)

E-mail address of person of contact (PC)

harald.lanig@gmx.de


With the following button you can send a data request email to the given **person of contact (PC)**:

Send a data request mail to the PC

back

next

Assigning the Person of Contact (Project Manager)

The person of contact (PC) has not yet confirmed that you may  retrieve his or her personal data. Please note that this is required before the application can be finalized.

Personal Data: Person of Contact (PC)

E-mail address of person of contact (PC)

harald.lanig@gmx.de


With the following button you can send a data request email to the given **person of contact (PC)**:

Send a data request mail to the PC



An e-mail to the person of contact (PC) (harald.lanig@gmx.de) has been sent. You can now continue with the application.

Application ID: 21692

1	Application list	
2	Choose PI and PC	
3	Show data PI	
4	Data PC	
5	Project data	
6	Resource Selection	
7	Upload files	
8	Remarks	
9	Finalize	

PC needs to accept the assignment in JARDS

Von jards@nhr-verein.de
jards@nhr-verein.de

An Harald Lanig

Antwort an hpc-support@fau.de

Betreff **[JARDS] Personal data processing acknowledgement request for application no. 21692**

Antworten Weiterleiten Archivieren Junk Löschen Umleiten Mehr

16:17

S/MIME

The user harald.lanig@fau.de specified you as the person of contact (PC) for the computing time request no. 21692.

IMPORTANT: In order to proceed your approval is required.

Please login to JARDS with the following link:

<https://jards.nhr-verein.de/jards/WEB/application/config.php?appkind=nhr-1-fau#personal-data-access>

Please confirm that harald.lanig@fau.de is allowed to process your personal data under "Personal Data Access".

You can find the application in your list of "Active applications".

It is possible that another person specified your e-mail address by mistake. In this case, please ignore this message.

Best regards,
Your NHR Team

PC identity check by email callback

Login 

E-mail Callback

Before you can apply for computing time we will check your identity with an automatic e-mail call-back.

We will send an e-mail with a link to the specified address. By using the link in this e-mail you can continue with the electronic application for computing time.

Make sure to enter the same e-mail address used for previous applications, if applicable.

Login mail address

harald.lanig@gmx.de

Data Privacy

☒ By using the platform, you agree to the [privacy policy](#) and consent to the collection and processing of your data in accordance with the applicable data protection laws and the stated provisions (accounting, etc.).

callback

✓ Mail sent to harald.lanig@gmx.de

An E-mail for your identification is on the way.
This might take a few minutes. Please, also check your spam folder.
The link sent is valid for the next 30 minutes.

back

PC accepts assignment

Personal Data Access

For data privacy reasons it is required that the PI / PC grant mutual permission for the access / processing of the personal data.
Find below a list of persons who are allowed to use your personal data in a HPC compute time proposal or have requested access:

Open requests

Config

Search:

Name	E-Mail	Actions
Harald Lanig	harald.lanig@fau.de	<button>accept</button> <button>decline</button>

Showing 1 to 1 of 1 entries

Granted permissions

Config

Search:

Name	E-Mail	Actions
No data available in table		

Showing 0 to 0 of 0 entries

E-mail of the person to grant personal data access permission

add person

PC must add missing personal data

Personal Data

Gender

Title

First name *

Last name *

Phone *

Affiliation

Federal State *

Institution *

Nationalities *

select values

Institute *

Institution

Institute name:

Erlangen National High Performance Computing Center (NHR@FAU)

Institute address

Martensstr. 1
91058 Erlangen Germany

add institute

Personal Data Access

For data privacy reasons it is required that the PI / PC grant mutual permission for the access / processing of the personal data. Find below a list of persons who are allowed to use your personal data in a HPC compute time proposal or have requested access:

Open requests

Config

Search:

Name	E-Mail	Actions
No data available in table		

Showing 0 to 0 of 0 entries

Granted permissions

Config

Search:

Name	E-Mail	Actions
Harald Lanig	harald.lanig@fau.de	revoke

Showing 1 to 1 of 1 entries

E-mail of the person to grant personal data access permission

add person

save profile

PC is now registered in the JARDS database



☰ APPLICATIONS 👤 ACCOUNT ? HELP

Electronic project application form for NHR@FAU Compute Cluster
Category: NHR Large

☰ CONTENT ▾

➕ New NHR Large Project Application

[Access to another application kind](#)

Active applications:

Search:

ID: 21692

PI: harald.lanig@fau.de
PC: harald.lanig@gmx.de
Project Title:
Category: NHR Large
Center: NHR@FAU
Project ID:
Last edit: 07.03.2024 17:14



on lists

➤ 'New Project Application' Button.
rent and previous applications in the lists below.

: application process.

PI gets message about PC acceptance

Von jards@nhr-verein.de 
jards@nhr-verein.de

An harald.lanig@fau.de 

Antwort an hpc-support@fau.de 

Betreff **[JARDS] Personal data processing acknowledgement confirmed for application no. 21692**

 Antworten  Weiterleiten  Archivieren  Junk  Löschen  Umleiten

Dear Harald Lanig,

The user harald.lanig@gmx.de confirmed that you are allowed to process his/her personal data.

You can now continue editing/finalizing your application no. 21692 using the following link:

<https://jards.nhr-verein.de/jards/WEB/application/login.php?appkind=nhr-1-fau&EDITAPP=21692>

Best regards,
Your NHR Team

Also the PC can directly start editing the application

Electronic project application form for NHR@FAU Compute Cluster
Category: NHR Large



✓ Loading application 21692.

Choose PI and PC

Principal Investigator (PI) and Person of Contact (PC) must be chosen here

- Your email address needs to be used either as PI or PC email address
- PI and PC email addresses need to differ
- PI is required while PC is optional
- PI is required to have at least a PhD degree or an equivalent qualification
- The PC is also the manager and technical contact of the project, who

E-mail address of principal investigator (PI) *

harald.lanig@fau.de

↓ switch PI and PC ↑

E-mail address of person of contact (PC)

harald.lanig@gmx.de

✓ Acknowledgement to personal data processing is confirmed.

Personal Data: Principal Investigator (PI)

Note: The Principal Investigator (PI) must be a member of a publicly funded university in Germany and must have a doctor's degree or equivalent, e.g., a Ph.D.

The PI is kindly requested to take part in reviewing other scientists' compute project proposals or otherwise to nominate a delegate who is able to thoroughly take part in the reviewing process.

E-mail address of principal investigator (PI) *

harald.lanig@fau.de

PC data is now available

✓ Acknowledgement to personal data processing is confirmed.

Personal Data: Person of Contact (PC)

Warning: The Person of Contact (PC) needs an HPC Account (FAU). If you already have an account, please consider adding the account information by editing your personal data.
You can ignore this warning, if you are a new user and/or do not have an account yet.

You can modify your own personal data [here](#). After making your changes you can use button to proceed with your application.

Gender	Title	First name *	Last name *
<input type="text" value="m"/>	<input type="text" value="Dr."/>	<input type="text" value="Harald"/>	<input type="text" value="Lanig"/>
E-mail address of person of contact (PC)		Phone *	HPC Account (FAU)
<input type="text" value="harald.lanig@gmx.de"/>		<input type="text" value="+499131 8571112"/>	<input type="text"/>

Affiliation PC

Federal State *

Bayern

Institution *

Universität Erlangen-Nürnberg

Institute *

Erlangen National High Performance Con

Institute name:

Erlangen National High Performance Computing Center (NHR@FAU)

Institute address

Martensstr. 1

91058 Erlangen Germany

Entering Project Data

Project Data

If this application is a request for extending an existing computing project, please enter the project ID here

Please give the planned total duration of your research project concerning this application. This can be extended up to three years, if the project is aligned with a grant funded by DFG.

Compute period *

01.07.2024



to

30.06.2025



Project Title *

MD Simulations on Tetracycline Receptor Proteins

Please select the number of collaborators involved *

3-5



Please select the sponsorship of the project. *

none



If you have chosen 'other' specify them please:

Project Acronym: *

TetR_MD

Version of the DFG Structure

2016



Main category *

21 Biology



Sub category *

201-04 Structural Biology



Secondary main category

Choose main category



Secondary sub category

Choose sub category...



HPC Expertise *

☒ I confirm that all planned users in my compute time project have sufficient HPC experience to efficiently use Tier 2 systems.

Entering Project Data

Is this project a collaboration with further institutions of other federal states or countries? *

☐ yes ☒ no

☐ Baden-Württemberg

☐ Bayern

☐ Berlin

☐ Brandenburg

☐ Bremen

☐ Hamburg

☐ Hessen

☐ Mecklenburg-Vorpommern

☐ Niedersachsen

☐ Nordrhein-Westfalen

☐ Rheinland-Pfalz

☐ Saarland

☐ Sachsen

☐ Sachsen-Anhalt

☐ Schleswig-Holstein

☐ Thüringen

☐ Other EU country

☐ Other Non-EU country

Other applications for compute time

Please list your HPC compute proposals and projects (submitted, running, or finished) at other HPC centers in Germany that share the same or have a very similar topic. Include also proposals of other researchers involved in the current project.

Use the following table to provide the information:

							Search:
Year	Call, proposal, etc	HPC system	Project ID	Requested amount of compute time	Granted amount of compute time	Unit	Actions
<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	Please select: <input type="button" value="v"/>	<input type="button" value="x"/>

If you have several other proposals, please justify here why the current proposal should also be awarded:

0 characters (500 remaining)

Confirmation *

☒ I am aware that incomplete information may lead to a significant cutback of resources or even to the rejection of the proposal.

back

next

Resource Selection

Electronic project application form for NHR@FAU Compute Cluster
Category: NHR Large

Resource Selection

Here you can select the resources you would like to apply for.

For information about the available NHR@FAU hardware, please follow these links:

[Alex GPGPU cluster](#)

[Fritz parallel CPU cluster](#)

Afterwards, click on save or next to update the sequence of application steps and be able to enter resource details.

☒ FAU CPUs

☒ FAU GPUs

back

next

Application ID: 21692

1	Application list
2	Choose PI and PC
3	Show data PI
4	Show data PC
5	Project data
6	Resource Selection
7	CPU Resources
8	GPU Resources
9	Upload files
10	Remarks
11	Finalize

Resource Selection

Compute Resource Data FAU CPUs

For information about the **Fritz parallel CPU cluster**, please see <https://hpc.fau.de/systems-services/documentationinstructions/clusters/fritz-cluster/>.

For information about possible resources you can apply for, please see the following [overview](#).

Compute time in million core-hours for the requested period *

The maximum runtime of a production job is 24 hours!

Explanation of Requested Resources

Here is an example how such a request could look like:

I plan to run 50 MD simulations. Each simulation consists of 20 consecutive runs on 864 cores taking 24h.

Compute time demand = $50 * 20 * 864 * 24 = 20,736,000$ core-h = 21 Mio core-h on Fritz.

Five simulations can easily be run at the same time as they are independent.

For a second set of parameters, I plan to run 10 MD simulations. Each simulation consists of 25 consecutive runs on one A100 GPU taking 24h.

Compute time demand = $10 * 25 * 1 * 24 = 6,000$ A100-GPU-h.

All ten simulations are independent and can in principle run at the same time.

*

I plan to run 50 MD simulations. Each simulation consists of 20 consecutive runs on 864 cores taking 24h.

Compute time demand = $50 * 20 * 864 * 24 = 20,736,000$ core-h = 21 Mio core-h on Fritz.

Five simulations can easily be run at the same time as they are independent.

271 characters (4729 remaining)

Name and Description of the Application Software

Please describe the software you plan to use. Is it suitable for HPC and for batch processing?

*

AMBER. The package is well established at NHR@FAU.

Required System Software, Tools and Libraries

Which compilers, libraries, additional packages and tools do you need?

*

nothing

Efficient HPC Usage

Please demonstrate that your project and the software you plan to use is suited for making efficient use of an HPC.
Please indicate if you are interested in support to improve performance and/or scalability of your application!

*

AMBER is a standard software package provided by NHR@FAU.

Resource Selection

Job characteristics

Maximum Number of
simultaneously running jobs: *

Maximum main memory
demand per core (GB) *

Typical number of cores per
job *

Maximum number of cores
per job *

Artificial Intelligence (AI)/Machine Learning (ML) approach

Do you plan to employ AI/ML methods or algorithms on this resource? *

☐ yes

☒ no

back

next

Resource Selection

Compute Resource Data FAU GPUs

For information about the **Alex GPGPU cluster**, please see <https://hpc.fau.de/systems-services/documentation-instructions/clusters/alex-cluster/>.

For information about possible resources you can apply for, please see the following [overview](#).

Compute time in GPU-hours for the requested period. *

Please define how you would like to distribute the requested GPU-hours between the available GPUs:

A40

GPU hours

A100

The maximum runtime of a production job is 24 hours!

I plan to run 100 MD simulations. Each simulation consists of 25 consecutive runs on one A100 GPU taking 24h.

Compute time demand = $100 * 25 * 1 * 24 = 60,000$ A40-GPU-h.

170 characters (4830 remaining)

Name and Description of the Application Software

Please describe the software you plan to use. Is it suitable for HPC and for batch processing?

AMBER

5 characters (4995 remaining)

Application ID: 21692

- | | |
|----|--------------------|
| 1 | Application list |
| 2 | Choose PI and PC |
| 3 | Show data PI |
| 4 | Show data PC |
| 5 | Project data |
| 6 | Resource Selection |
| 7 | CPU Resources |
| 8 | GPU Resources |
| 9 | Upload files |
| 10 | Remarks |
| 11 | Finalize |

Resource Selection

Job characteristics

Maximum Number of
simultaneously running jobs: *

Typical number of GPUs per
node *

Typical number of nodes per
job *

Maximum number of nodes
per job *

Artificial Intelligence (AI)/Machine Learning (ML) approach

Do you plan to employ AI/ML methods or algorithms?

☐ yes

☒ no

Please briefly explain why you need access to the GPUs. Justify the amount of resources *

The performance of the AMBER GPU implementation is well documented and tested at NHR@FAU

88 characters (4912 remaining)

back

next

Scientific Project Description

Upload Files

For the detailed scientific project description, a template for download is provided on this [web page](#) (see the section "NHR@FAU compute time applications via JARDS" at the bottom of the page).

If you are on the way to submit a follow-up proposal, the template also includes a section for a short status report. Please discuss mainly the differences/extensions compared to the previous granting period(s) in your present project description.

Supporting material for the project proposal is optional and must be uploaded as one single file. You can also upload or include referee reports or relevant information from other funding agencies here.

Hints:

- Only PDF files are allowed for upload.
- The maximum size for a PDF file is 60 MByte.
- The number of pages for the description may be limited.

Please provide a detailed project description.

Detailed description PDF: *

Durchsuchen... Keine Datei ausgewählt.

You may upload **supporting material** for your project as a single PDF file (please include only yet unpublished material).

Supporting material PDF:

Durchsuchen... Keine Datei ausgewählt.

Application ID: 21692

1	Application list
2	Choose PI and PC
3	Show data PI
4	Show data PC
5	Project data
6	Resource Selection
7	CPU Resources
8	GPU Resources
9	Upload files
10	Remarks
11	Finalize

Scientific Project Description

How to apply for an NHR project

Via **JARDS** [↗](#)

Mandatory for Large Scale Applications! You can apply via the central online application portal **JARDS** [↗](#).

Additionally, we require some supplemental information. Please fill out this **template** [↗](#), save it as a single PDF, and upload it to **JARDS** [↗](#), when you finish your application.

Via document template (for test, porting, normal projects)

Please use this **template** [↗](#) for project applications and **send it by email from your university account** to **hpc-support@fau.de** [↗](#).

The document contains detailed information on what to fill in depending on the type of project. For further assistance contact **hpc-support@fau.de** [↗](#).

<https://doc.nhr.fau.de/nhr-application/>

Scientific Project Description

- JARDS Template **NHR@FAU-short-application-form-JARDS.docx**
 - Short form of our established application template
 - Technical Description of the project
 - Scientific Project Description
 - Follow-up Projects (if applicable)
 - Optional Information
 - Important Notes
- Upload your filled project description as PDF only to JARDS

Detailed description PDF: *

Durchsuchen... NHR@FAU-short-application-form-JARDS.pdf

Scientific Project Description



File NHR@FAU-short-application-form-JARDS.pdf successfully uploaded.

Remarks

Remarks, special requirements, consultation needed, etc.

I need help optimizing my initial setup!

40 characters (460 remaining)

Application ID: 21692

- | | |
|----|--------------------|
| 1 | Application list |
| 2 | Choose PI and PC |
| 3 | Show data PI |
| 4 | Show data PC |
| 5 | Project data |
| 6 | Resource Selection |
| 7 | CPU Resources |
| 8 | GPU Resources |
| 9 | Upload files |
| 10 | Remarks |
| 11 | Finalize |

Finalization of the application

Finalize Application

Please check all your input data on correctness by pressing the CHECK button before you press the FINALIZE button. **With finalizing your application you will no longer be able to edit this application form!**

I agree to **provide a final project report** (which might be published) which summarizes the used resources and scientific results after the project period.

☐ Accept *

I confirm the responsibility for granting access to further project members. I will ensure that citizens of countries that are subject to the export control policy of the German Federal Government have an additional authorization from the German Federal Office for **Economic Affairs and Export Control (BAFA)** before they are allowed to use the resources.

☐ Accept *

I understand that I might be contacted by German universities or research facilities in order to take part in **reviewing other scientists compute project** proposals. I am aware that I can nominate a delegate who is able to thoroughly take part in the reviewing process at all times. As a reviewer, I agree to keep personal details of the applicants and the details of the proposal confidential. I consent to the processing of the relevant application data with German universities or research facilities in order to enable the scientific peer reviewing process as specified in the data privacy agreement. In the case of delegation, I acknowledge that all responsibilities connected to the review extend to the delegate and I retain full responsibility for the processing of the review.

☐ Accept *

Finalization of the application

By applying for compute time, the principal investigator of this project confirms that in publications arising from this project the computing time granted by **NHR@FAU** will be acknowledged using this phrase:

The authors gratefully acknowledge the scientific support and HPC resources provided by the Erlangen National High Performance Computing Center (NHR@FAU) of the Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) under the NHR project <ID of your NHR@FAU project>. NHR funding is provided by federal and Bavarian state authorities. NHR@FAU hardware is partially funded by the German Research Foundation (DFG) – 440719683.

Electronic copies of these publications will be sent by e-mail to hpc-support@fau.de.

I agree to these terms.

☐ Accept *

I confirm that during the project phase **no sensitive, personal, or confidential data will be processed** on NHR@FAU systems.

☐ Accept *

The Resource Allocation Board needs a **signed version of the application form**. After pressing the FINALIZE button you will get back to the application list. There you can find this application in the list of "finalized applications". Please use the PRINT button for printing the application form, sign the form, scan the signed document and upload it using the UPLOAD SIGNED FORM button on the same page. Alternatively, you can also send it to hpc-support@fau.de, using the subject "Application for Compute Time No. 21692".

back

FINALIZE

CHECK

Coming again to finalize after saving the draft

- Visit <https://jards.nhr-verein.de/>

Start Page

Welcome to JARDS, please choose if you want to create an application or review submitte

Applications

Please select an application kind to create an application. If you do not yet know which p refer to the information on the [NHR website](#).

Select Appkind *

NHR Large



Open Applications

Select the NHR Center

Please select an [NHR Center](#) for your computing time project. Feel free to contact info@nhr-ver which center fits best to you.

NHR Center Selection *

NHR@FAU



E-mail Callback

Before you can apply for computing time we will check your identity with an automatic e-mail call-back.

We will send an e-mail with a link to the specified address. By using the link in this e-mail you can continue with the electronic application for computing time.

Make sure to enter the same e-mail address used for previous applications, if applicable.

Login mail address

harald.lanig@fau.de

Data Privacy

☒ By using the platform, you agree to the [privacy policy](#) and consent to the collection, processing and use of your personal data in compliance with the applicable data protection laws and the stated provisions (according to Article 6(1)(a) EU-GDPR I).

callback

Coming again to finalize after saving the draft

≡ CONTENT ▼

Application lists

Here you can create new applications by clicking the 'New Project Application' Button.
Find also your active and past projects, and your current and previous applications in the lists below.

► More information

You are logged in as: **harald.lanig@fau.de**

Please define your role (PI, PC or both) during the application process.

Active applications:

Search:

ID: 21692

PI: harald.lanig@fau.de

PC: harald.lanig@gmx.de

Project Title: MD Simulations on Tetracycline Receptor Proteins

Category: NHR Large

Center: NHR@FAU

Project ID:

Last edit: 08.03.2024 11:05





Coming again to finalize after saving the draft

- You can edit your application as long it is not finalized
- Directly address the section to edit via the menu:

Please provide a detailed project description.

Detailed description PDF: *

Keine Datei ausgewählt.

Latest upload: 08.03.2024 10:56  

You may upload **supporting material** for your projec

Supporting material PDF:

Keine Datei ausgewählt.

Latest upload: none

Application ID: 21692	
1	Application list
2	Choose PI and PC
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Coming again to finalize after saving the draft

✓ Thank you for your application. Your application data has been submitted.

≡ CONTENT ▾

Application lists

Here you can create new applications by clicking the 'New Project Application' Button.
Find also your active and past projects, and your current and previous applications in the lists below.
► More information

You are logged in as: **harald.lanig@fau.de**
Please define your role (PI, PC or both) during the application process.

Finalized applications:

Search:

ID: 21692

PI: harald.lanig@fau.de
PC: harald.lanig@gmx.de
Project Title: MD Simulations on Tetracycline Receptor Proteins
Category: NHR Large
Center: NHR@FAU
Project ID:
Call: 2024/3
Last edit: 08.03.2024 11:33



Application ID: 21692

1	Application list
2	Choose PI and PC
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11	Finalize

Email notification after finalization for PI and PC

Von jards@nhr-verein.de
jards@nhr-verein.de

Antworten

Allen antworten

Weiterleiten

Archivieren

Junk

Löschen

Umleiten

Mehr

An harald.lanig@fau.de

Kopie (CC) Harald Lanig

Antwort an hpc-support@fau.de

Betreff **Finalization of your compute time application with ID 21692**

11:33

S/MIME

This is an automatically generated e-mail. (Please do not reply to this message.)

The project application with ID 21692 was successfully finalized on 08.03.2024 at 11:33.

The Resource Allocation Board needs a signed version of the attached application form.

You can also print this application summary if you are logged in to the electronic project application pages using the print button from the section: "Finalized Applications".

Please sign the form, scan it and upload it using the UPLOAD SIGNED FORM button in your list of "finalized applications" in JARDS

(<https://jards.nhr-verein.de/jards/WEB/application/login.php?appkind=nhr-1-fau>).

Alternatively, you can also send it to hpc-support@fau.de. In this case, please use the e-mail subject "Application for Compute Time No. 21692".

--

Erlangen National High Performance Computing Center (NHR@FAU)

Email: hpc-support@fau.de

> 1 Anhang: application_form_21692.pdf 26,9 KB

Speichern

Need Help?

We will **help you answering your questions** about the compute time application, the submission and the reviewing process

We will also **support you porting your applications** to run effectively on our systems

In any case, contact us via hpc-support@fau.de

After submitting the application and passing the technical review, you can immediately start doing calculations (via a test/porting project account)

Standard project runtime: 12 months