

Computing Time and Data Processing Using Supercomputers

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IT4Innovations National Supercomputing Center

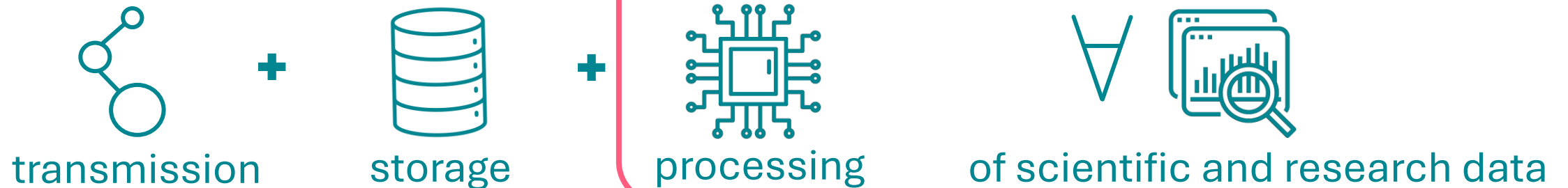
03. 12. 2025



Co-funded by
the European Union

e-INFRA CZ

- unique research and development e-infrastructure in the Czech Republic
- provides capacities and resources for:

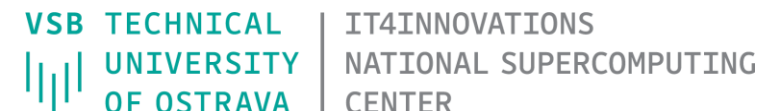


- cooperation of **three national e-infrastructures**:

- CESNET (Prague)
 - CERIT-SC (ICS MUNI)
- + institutes of the CAS
+ universities



- IT4Innovations National Supercomputing Center





Computational resources e-INFRA CZ – MetaCentrum

- National distributed computing environment (coordinated by CESNET)
- Resources provided by CESNET + CERIT-SC + institutes of the CAS + universities
 - Shared access
 - Benefits for owners of participating resources
- **Free to use, registration available at any time, immediate access**
- **Training available upon request, even for small groups**
vorel@cesnet.cz ; meta@cesnet.cz





Examples of user projects – MetaCentrum

- Computational chemistry
- Material and structural simulation
- Simulation of flow of gases and liquids
- Recognition and speech generation
- Physical Geodesy
- Ecological modeling
- Video processing
- Data Mining
- Analysis of medical images



How to Get Access – Metacentrum

- **Get Account:**

- **e-INFRA CZ Account** intended for all persons affiliated with an academic institution from the Czech Republic (eduID.cz).
 - Go to <https://metavo.metacentrum.cz/en/application/form>.
 - Select a member academic institution you are affiliated with.
 - Fill out the e-INFRA CZ Account information (username, password and ssh key(s)).
 - New applications are manually approved within a few working days.
- Persons not eligible for an e-INFRA CZ account have to contact the [user support](#) team.
- All accounts are valid till 02. 02. YYYY => request for account renewal each year.



Accessing the MetaCentrum

- [Read the documentation.](#)
- **Software:** free / general licenses / private licenses
- **Access:**
 - **Grid computing** – access via command-line interface in a terminal (OpenPBS scheduler)
 - **GUI** – access via graphical user interface
 - Open OnDemand:
 - Galaxy
 - Jupyter notebook
 - **Cloud computing** (OpenStack)
 - **Container** platform Kubernetes
- [AI via API](#) on **local hardware**
 - Llama 3.3
 - Deepseek R1
 - Llama 4, ...





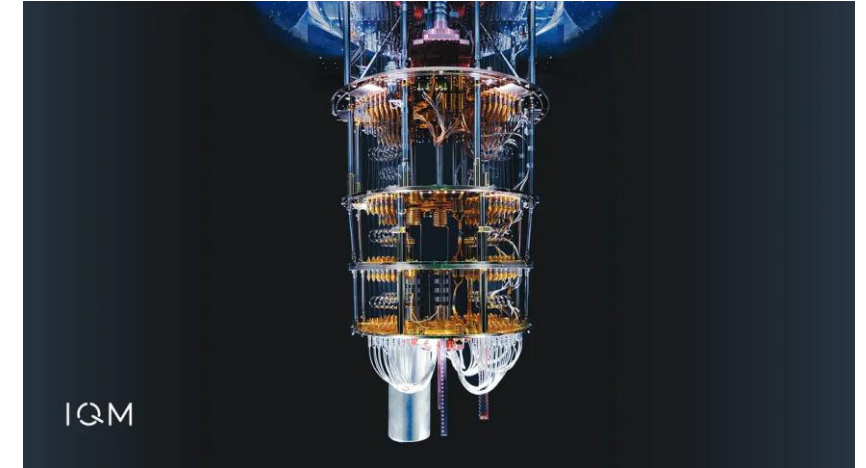
Computational resources e-INFRA CZ – IT4I

IT4Innovations National Supercomputing Center:

- High-Performance Computing (HPC)
- High-Performance Data Analysis (HPDA)
- Artificial Intelligence (AI)
- Quantum Computing (QC)

Resources:

Karolina	Barbora	NVIDIA DGX-2	VLQ
15.7 PFlop/s	849 TFlop/s	2 PFlop/s pro AI	24 qubitů
HPC + HDPA	HPC + HDPA	AI + HPC	QC
2021	2019	2019	2025



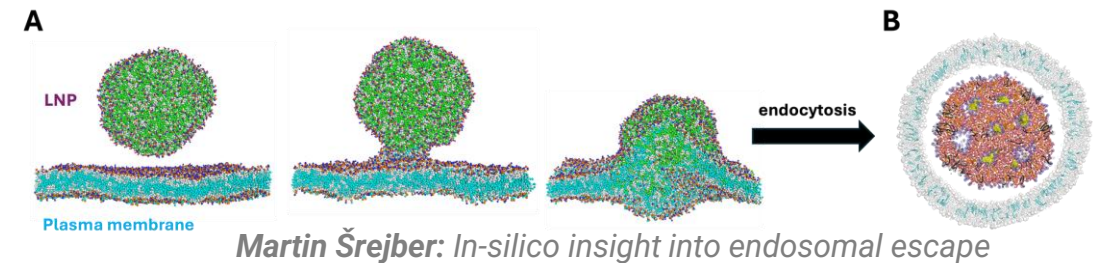
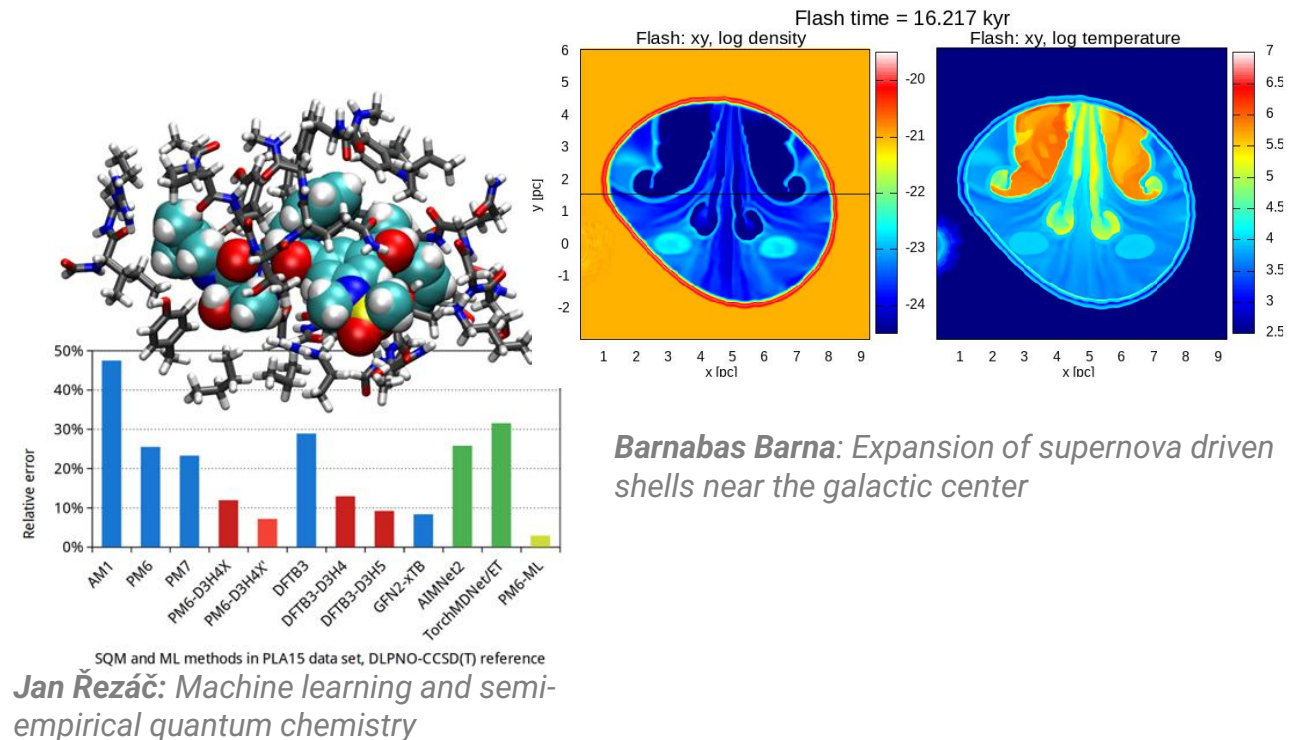
+ **LUMI Supercomputer** – IT4I is a member of the LUMI consortium, giving the Czech research community access to the most powerful supercomputer in Europe (531.5 PFlop/s).

IT4Innovations computing resources - **free** for academic institutions and other research organizations in CZ



Examples of user projects – IT4I

- Bioinformatics, drug design, DNA sequence analysis, protein modelling
- Big data processing, use for machine learning, artificial intelligence (e.g. large language models LLM)
- Virtual reality, video rendering, image processing
- Medium and long-term weather forecasting, climate change modelling
- Mathematical and physical calculations, new materials design
- Simulations in various industries (CFD)
- Digital twins, e.g. human brain model, earth model
- Quantum computing, etc.





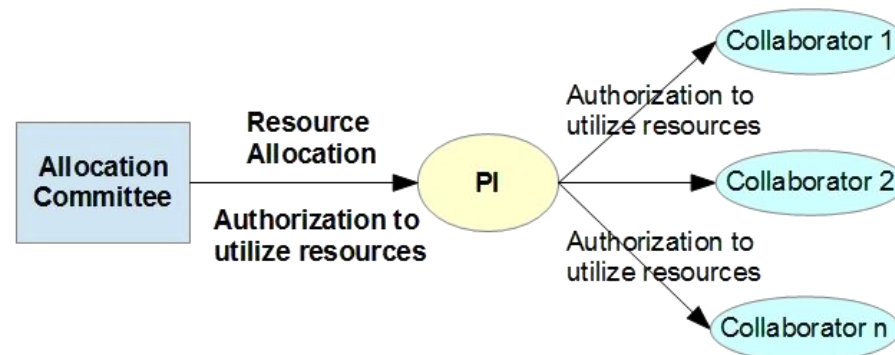
How to Get Access – IT4I

- **Get Account:**

- **e-INFRA CZ Account** intended for all persons affiliated with an academic institution from the Czech Republic (eduID.cz).
 - Go to <https://signup.e-infra.cz/fed/registrar/?vo=IT4Innovations>
 - Select a member academic institution you are affiliated with.
 - Fill out the e-INFRA CZ Account information (username, password and ssh key(s)).
- **IT4I Account** (persons not eligible for an e-INFRA CZ account).

- **Get Project** (or Project Membership):

- Academic researchers may apply via Open Access Competitions.
- Commercial and non-commercial institutions may also apply via the Directors Discretion.





How to Get Project – IT4I

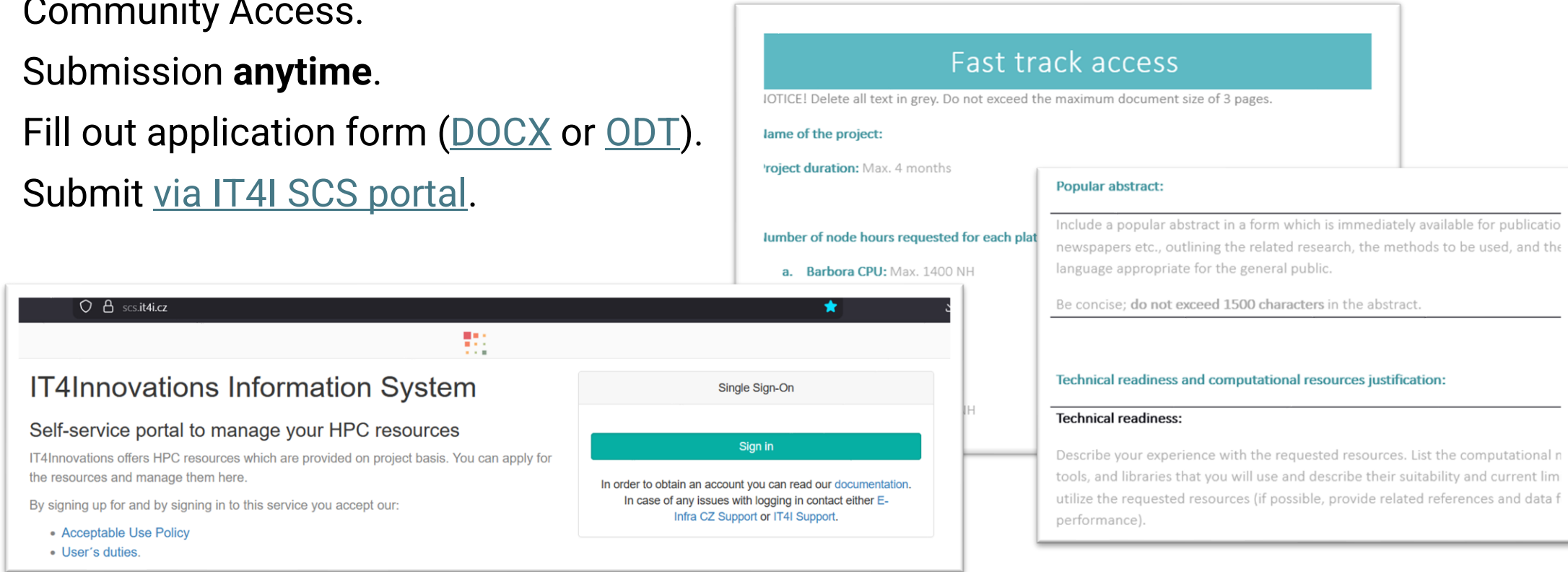
- Fill out a **request for allocation** at [IT4I SCS portal](#).
- Several access types (new users have to ask for Fast Track Access for the first time).

Access category	Access type	Duration of allocation and main deadlines
Open access	Open Access Grant Competition	12, 24 or 36 months; 3 x a year (February, June, and October); decision within 55 days
	Institutional and Community Access	12, 24 or 36 months; decision within 55 days
	Fast Track Access	max. 4 months; submission at any time; decision within 7 days
Access for thematic use of capacities	Important Societal Challenges	max. 12 months; submission at any time; decision within 30 days
	Teaching and Educational Activities	max. 12 months; submission at any time; decision within 30 days
	In-house Infrastructure Research	max. 12 months; submission at any time; decision within 30 days
	Rental of Computational Resources	duration as per contract; submission at any time
	Contract research	duration as per contract; submission at any time
LUMI	IT4Innovations Open Access Grant Competition and EuroHPC JU Grant Competitions	



Fast Track Access – IT4I

- Solving simpler, short-term computational tasks, testing concepts, debugging and developing applications, and for research, development, and innovation activities.
- Primary objective – **preparation** for the Open Access Grant Competition or Institutional and Community Access.
- Submission **anytime**.
- Fill out application form ([DOCX](#) or [ODT](#)).
- Submit [via IT4I SCS portal](#).



The image displays the IT4Innovations Information System portal and an application form. The portal, accessed via scs.it4i.cz, features a 'Single Sign-On' section with a 'Sign in' button and links to documentation and support. The application form, titled 'Fast track access', includes fields for project name, duration, and node hours, along with sections for a popular abstract, technical readiness justification, and technical readiness details.

Fast track access

NOTICE! Delete all text in grey. Do not exceed the maximum document size of 3 pages.

Name of the project:

Project duration: Max. 4 months

Number of node hours requested for each platform:

a. **Barbora CPU:** Max. 1400 NH

Popular abstract:

Include a popular abstract in a form which is immediately available for publication in newspapers etc., outlining the related research, the methods to be used, and the language appropriate for the general public.

Be concise; do not exceed 1500 characters in the abstract.

Technical readiness and computational resources justification:

Technical readiness:

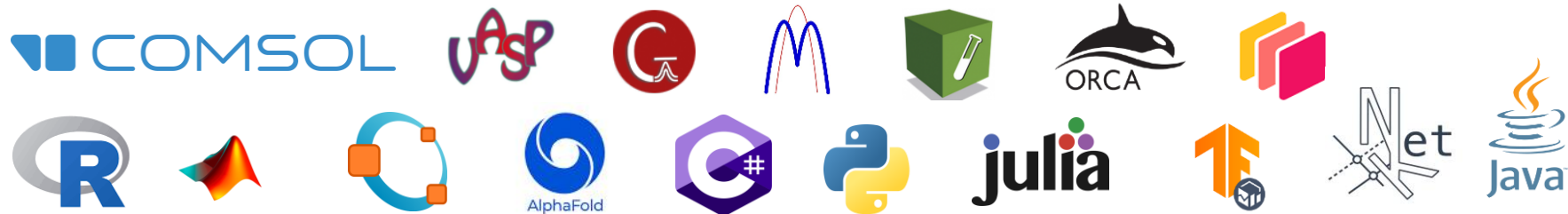
Describe your experience with the requested resources. List the computational tools, and libraries that you will use and describe their suitability and current limitations. If possible, provide related references and data from previous performance.



Accessing the IT4I clusters

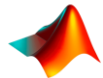
- [Read the documentation.](#)

- **Software:**



- **Access:**

- **SSH Access** – access via command-line interface in a terminal (SLURM scheduler)
- **GUI** – access via graphical user interface

- Open OnDemand:         
- Virtual Network Computing (VNC)

- **Cloud computing** (OpenStack)

- **Lexis** – launching computations with automatic data upload via a web interface, no terminal needed. 



SSH Access

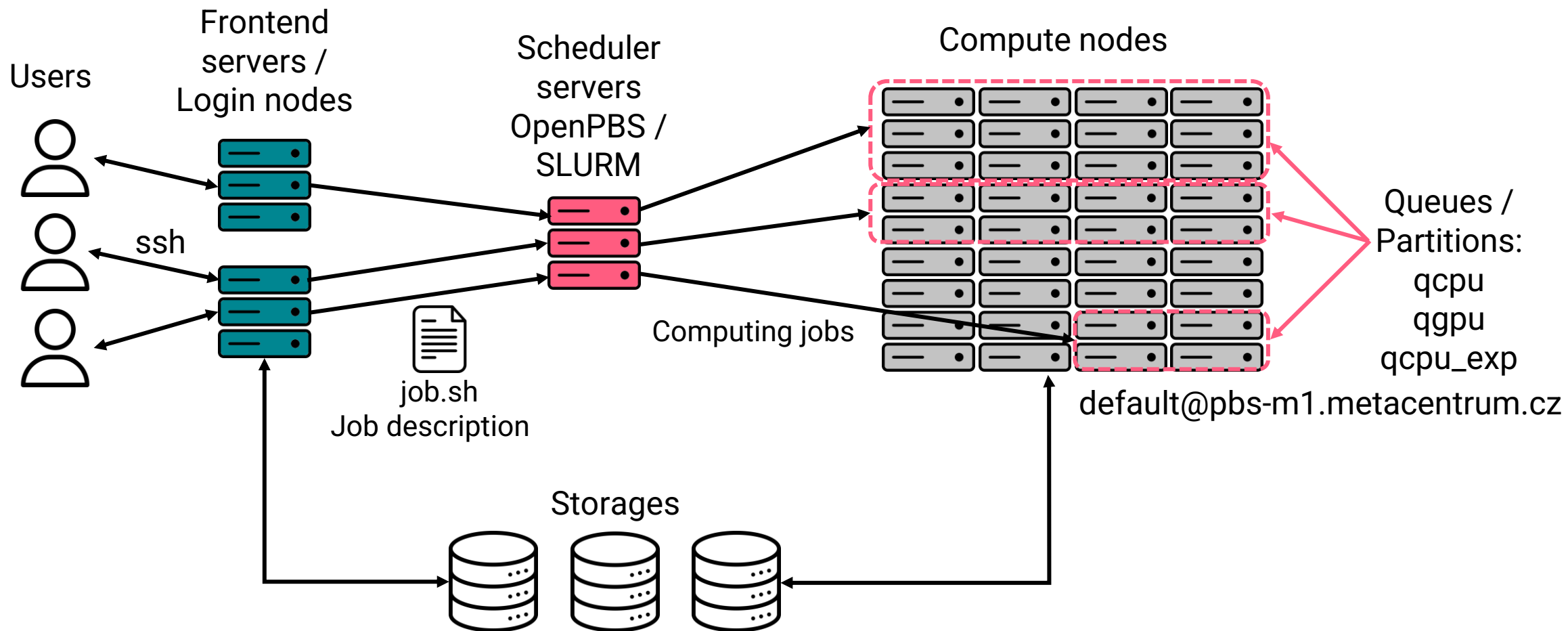
- Authentication by private key only.

Windows	Linux
Generate private and public keys via PuTTY Key Generator	Generate private and public keys
Assign private key to your e-infra profile	Assign private key to your e-infra profile
Set up PuTTY client	Create config SSH file
Connect to clusters	Connect to clusters

- Access the resources via command-line interface in a terminal (CLI).



How it works



ALL work MUST to be performed on compute nodes!



How it works – MetaCentrum

Pick the one that is closest to your physical location
(city) to minimise network lag



Users



ssh

Frontend server alias	Physical location	Native home
charon.metacentrum.cz	Liberec	/storage/liberec3-tul
elmo.metacentrum.cz	Praha	/storage/praha5-elixir
nympha.metacentrum.cz	Plzeň	/storage/plzen1
oven.metacentrum.cz	Brno	/storage/brno2
perian.metacentrum.cz	Brno	/storage/brno2
skirit.metacentrum.cz	Brno	/storage/brno2
tarkil.metacentrum.cz	Praha	/storage/praha1
tilia.metacentrum.cz	Průhonice	/storage/pruhonice1-ibot
zenith.metacentrum.cz	Brno	/storage/brno12-cerit

Queues

Unless you have a reason to send job to a specific queue, do not specify any.

default@pbs-m1.metacentrum.cz



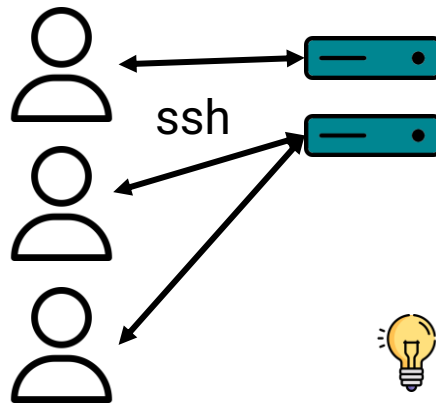
In case your favourite frontend is down or going just too slow, do not hesitate to use another one.



How it works – IT4I



Users



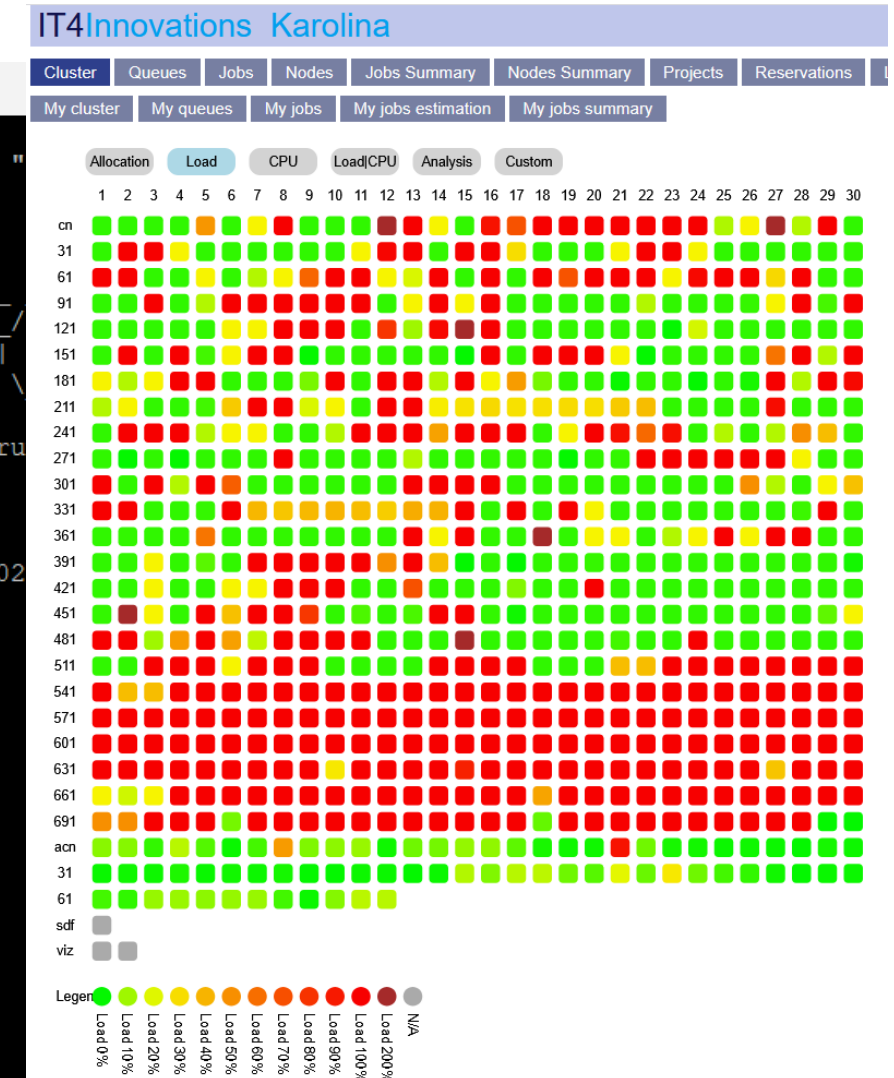
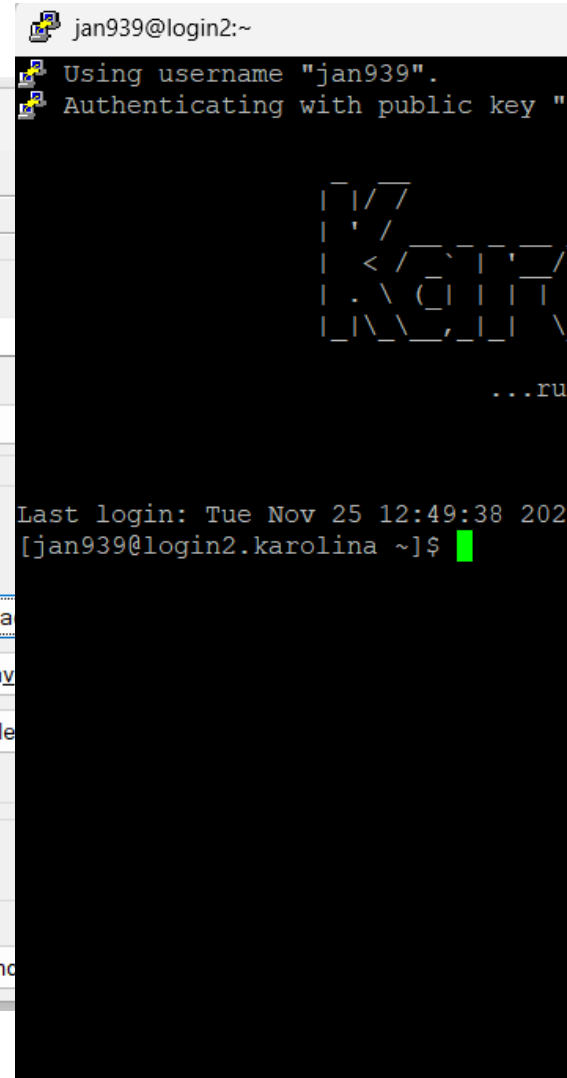
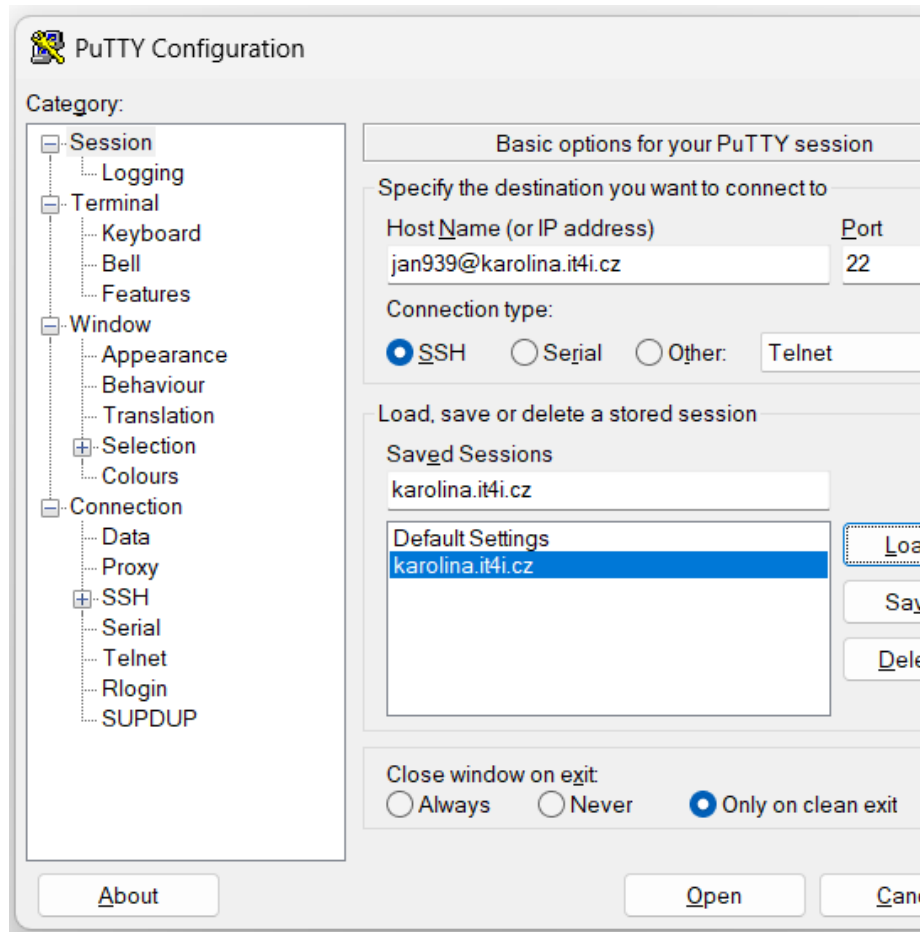
Frontend server alias	Physical location	Storage
karolina.it4i.cz	Ostrava	/home; /scratch; /mnt/projX
barbora.it4i.cz	Ostrava	/home; /scratch; /mnt/projX



The DGX-2 machine is integrated into Barbora cluster, it can be accessed from Barbora login nodes `barbora.it4i.cz` through the Barbora scheduler queue `qdgx` as a compute node `cn202`.



How it works – IT4I





Graphical User Interface: Open OnDemand

- Interactive interface to remote computing resources via web browser.
- MetaCentrum:
 - Login with academic identity.
 - [Metacentrum Open OnDemand instance](#)
- IT4Innovations:
 - Connect to [IT4I VPN](#).
 - Login with e-INFRA credentials.
 - Karolina: <https://ood-karolina.it4i.cz/>
 - Barbora: <https://ood-barbora.it4i.cz/>



OnDemand provides an integrated, single access point for all of your HPC resources.

Pinned Apps A featured subset of [all available apps](#)

 ANSYS System Installed App	 Blender System Installed App	 Code Aster System Installed App	 Code Server System Installed App
 Gnome Desktop System Installed App	 Jupyter (+IJulia) System Installed App	 MATLAB System Installed App	 ParaView System Installed App

Home / My Interactive Sessions / Jupyter (+IJulia)

- Interactive Apps
 - AI Tools
 - ComfyUI
 - Ollama + Open WebUI
 - vLLM + Open WebUI
 - Desktops
 - Karolina Login Mate
 - Karolina Login XFCE
 - Gnome Desktop
 - GUIs
 - ANSYS
 - Blender
 - ParaView
 - TorchStudio
 - Servers
 - Code Server
 - Jupyter (+IJulia)**
 - MATLAB

Jupyter (+IJulia)

This app will launch a [Jupyter](#) server using [Python](#) on the [Karolina](#) cluster.

Project

fta-25-65

Your project id

Partition

qcpu

Number of hours

1

Nodes

1

Tasks

1

GPUs

1

The setting is only valid for the GPU node

Mode

Session was successfully created.

✕

Home / My Interactive Sessions

- Interactive Apps
- AI Tools
- ComfyUI
- Ollama + Open WebUI
- vLLM + Open WebUI
- Desktops
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- Karolina Login XFCE
- Gnome Desktop
- GUIs
- ANSYS
- Blender
- ParaView
- TorchStudio
- Servers
- Code Server

Jupyter (+Julia) (3422490)1 node | 128 cores | Starting

Created at: 2025-11-28 12:48:10 CET

Time Remaining: 59 minutes

Session ID: 30fcbb63-ed64-4cbc-b49e-3374417e3bc3

Delete

Your session is currently starting... Please be patient as this process can take a few minutes.

ood-karolina.it4i.cz/node/cn070.karolina.it4i.cz/9051/lab/tree/Untitled.ipynb

File Edit View Run Kernel Tabs Settings Help

Filter files by name

Name	Modified
assets	57s ago
after.sh	57s ago
before.sh	57s ago
config.py	52s ago
Y: connection.yml	43s ago
job_script_conten...	57s ago
job_script_option...	57s ago
output.log	now
script.sh	57s ago
• Untitled.ipynb	now
user_defined_con...	57s ago

Untitled.ipynb

Notebook Python 3 (ipykernel)

[]:



LEXIS - Easy access to data management and HPC

<https://docs.lexis.tech/index.html>

How to supercompute:

- Set up an account
- Pick a supercomputer
- Fill out a request for allocation
- Get it approved
- Set up a SSH key
- Know how to use Linux terminal
- Login in to the Supercomputer
- Learn how to launch jobs in SLURM
- Learn about modules
- Learn about storages and data transfer
- ... finally compute something



```
Using username "jan939".
Authenticating with public key "katerina.martinov"

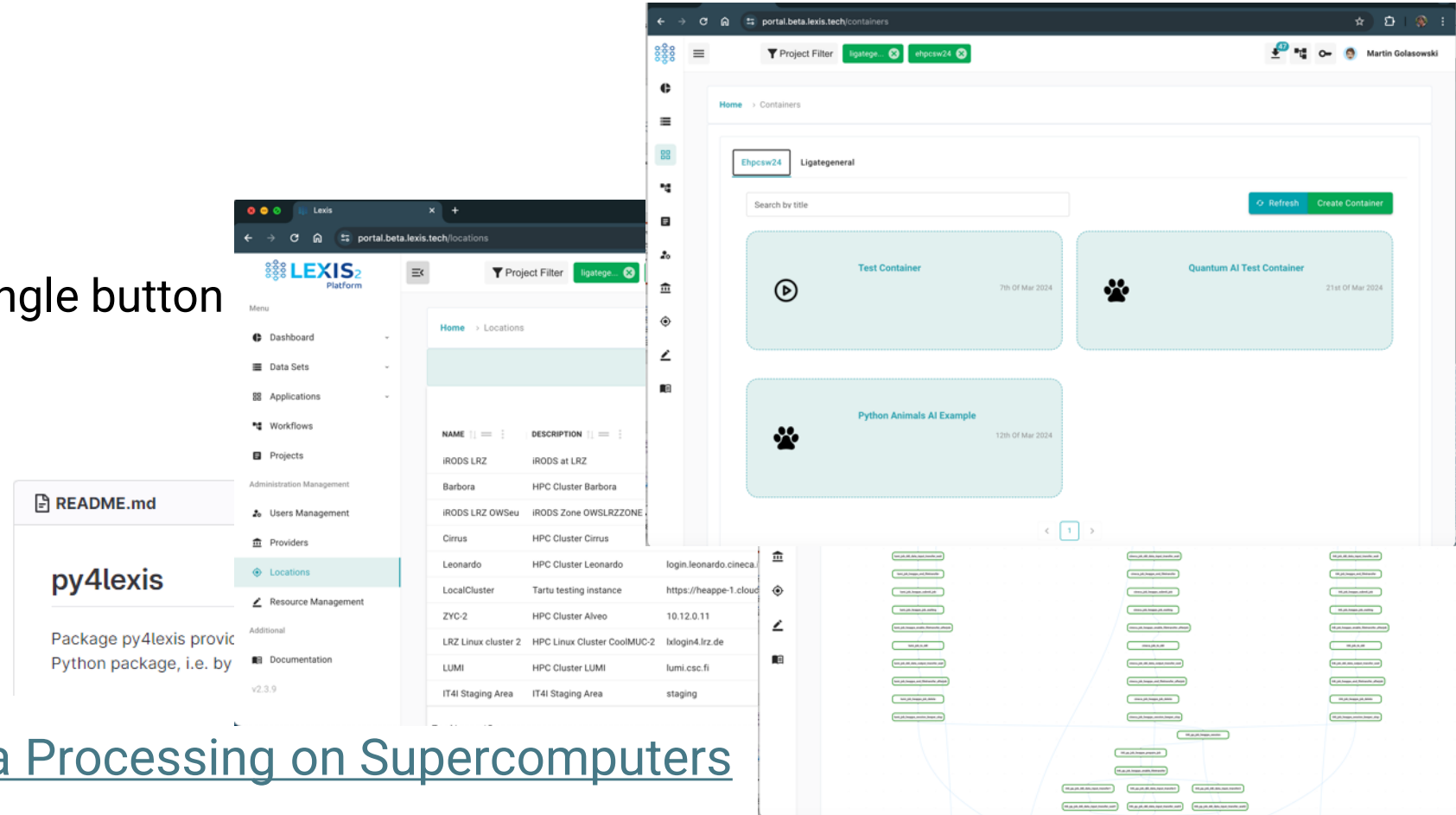
Karolina
...running on Rocky 8.X

Last login: Tue Nov 25 12:49:38 2025 from 158.196.113.114
[jan939@login2.karolina ~]$
```



LEXIS - Easy access to data management and HPC

- Web interface
- Allocations at one place
- Across multiple clusters
- Launch applications with a single button
- Get logs
- Manage data in iRODS
- Use common web login
- ... and many more
- Training available: [Big Data Processing on Supercomputers](#)



The image displays three overlapping screenshots related to the LEXIS platform. The top-right screenshot shows the 'Containers' page of the LEXIS portal, featuring a search bar, a 'Refresh' button, and a 'Create Container' button. Below these are three container cards: 'Test Container' (7th Of Mar 2024), 'Quantum AI Test Container' (21st Of Mar 2024), and 'Python Animals AI Example' (12th Of Mar 2024). The bottom-left screenshot shows the 'Locations' page, which lists various HPC clusters and their details in a table. The bottom-right screenshot shows the 'py4lexis' package documentation, including a 'README.md' file and the package description: 'Package py4lexis provic Python package, i.e. by v2.3.9'.

NAME	DESCRIPTION
iRODS LRZ	iRODS at LRZ
Barbora	HPC Cluster Barbora
iRODS LRZ OWSeu	iRODS Zone OWSLRZZONE
Cirrus	HPC Cluster Cirrus
Leonardo	HPC Cluster Leonardo
LocalCluster	Tartu testing instance
ZYC-2	HPC Cluster Alveo
LRZ Linux cluster 2	HPC Linux Cluster CoolMUC-2
LUMI	HPC Cluster LUMI
IT4I Staging Area	IT4I Staging Area

What to remember

1. Computing resources provided by e-INFRA are for free.

(academic institutions and other research organizations in CR)

2. There is always someone who can help you.

[MetaCentrum support](#), [IT4Innovation support](#), [EOSC-CZ Training Centre](#), [IT4Innovations Training Centre](#)

3. Acknowledge your computing resources in research publications.

Computational resources were provided by the e-INFRA CZ project (ID:90254), supported by the Ministry of Education, Youth and Sports of the Czech Republic.

Thank you for your attention



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