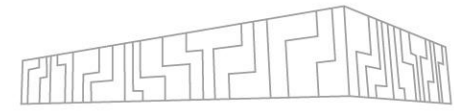




# 7<sup>TH</sup> USERS' CONFERENCE OF IT4INNOVATIONS

30–31 OCTOBER 2023  
IT4INNOVATIONS, OSTRAVA

# 2023 – UPDATES AND OPPORTUNITIES

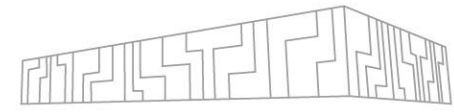


| NEW SERVICES

| NEW SYSTEMS

| LUMI-Q QUANTUM

# SLURM SCHEDULER



## Complete switchover to Slurm

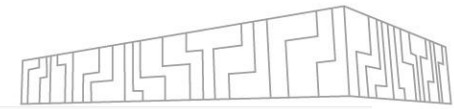
- Slurm on Barbora, Karolina and Complementary systems
- Complete integration to accounting and SCS
- Removed legacy queues, check: `$ sinfo -s`
- Still optimizing the queue policies: fairsharing and backfilling
- <https://docs.it4i.cz/general/job-submission-and-execution/>

## Scheduler status view

- `$ squeue [--time] -all ; squeue -u uname`
- <https://extranet.it4i.cz/rsweb/karolina/queues?user=uname>

(Includes electricity stats, see O. Vysocky 17:00)

# SLURM SCHEDULER



https://docs.it4i.cz/general/job-submission-and-execution/

120%

General

Search

scs/docs.it4i.cz

General Storage Clusters Software Clouds

## General

- Get Access >
- Get Project
- Manage Your Profile >
- Access Services >
- Run Jobs ▾
  - Introduction
  - Job Submission and Execution ▾
    - [General](#)
    - Karolina Specific
  - Resources Allocation >
  - Job Priority
  - Capacity Computing >
- Other Services >
- Technical Information >
- Satisfaction and Feedback
- Energy Saving
- DICE
- LUMI
- Support

## Job States

[↑ Back to top](#)

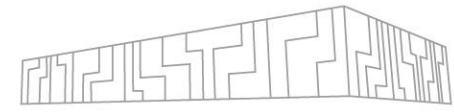
The most common job states are (in alphabetical order):

Code	Job State	Explanation
CA	CANCELLED	Job was explicitly cancelled by the user or system administrator. The job may or may not have been initiated.
CD	COMPLETED	Job has terminated all processes on all nodes with an exit code of zero.
CG	COMPLETING	Job is in the process of completing. Some processes on some nodes may still be active.
F	FAILED	Job terminated with non-zero exit code or other failure condition.
NF	NODE_FAIL	Job terminated due to failure of one or more allocated nodes.
OOM	OUT_OF_MEMORY	Job experienced out of memory error.
PD	PENDING	Job is awaiting resource allocation.
PR	PREEMPTED	Job terminated due to preemption.
R	RUNNING	Job currently has an allocation.

## Table of contents

- Introduction
- Getting Partition Information
- Running Interactive Jobs
- Running Batch Jobs
  - Job Script
  - Job Submit
  - Job Environment Variables
- Job Management
  - Getting Job Information
  - [Job States](#)
  - Modifying Jobs
  - Deleting Jobs
- Faq
  - Invalid Account

# HYPERQUEUE



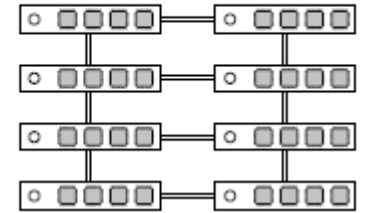
## Problem:

- Large amount of jobs?
- Very large amount of small jobs?
- Only 1 or few cores per job needed?
- Complicated job dependencies?

Many simple tasks



Slurm/PBS Cluster

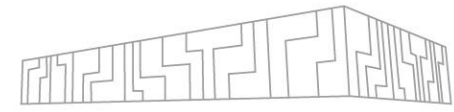


**Answer: Use hq!**

<https://it4innovations.github.io/hyperqueue/stable/>

<https://docs.it4i.cz/general/capacity-computing/#hyperqueue>

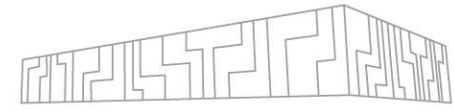
# E-INFRA CLOUD AT KAROLINA



## Announcing e-INFRA CLOUD service at Karolina

- Available to all active IT4I users (users attached to project)
- 22 Cloud nodes (configuration like cn[001-720])
- <https://horizon.ostrava.openstack.cloud.e-infra.cz/>
- Small resources available by default, including IP address
- Connectivity to Karolina login
- <https://docs.it4i.cz/cloud/einfracz-cloud/>
- IF more resources needed, **apply!**

# E-INFRA CLOUD AT KAROLINA



Project

Project / Compute / Overview

API Access

Compute

## Overview

Overview

Instances

Images

Key Pairs

Server Groups

Volumes

Network

Identity

### Limit Summary

#### Compute



Instances  
Used 1 of 10



VCPUs  
Used 1 of 20



RAM  
Used 2GB of 50GB



Volumes  
Used 1 of 10



Volume Snapshots  
Used 0 of 10



Volume Storage  
Used 20GB of 1000GB

#### Network



Floating IPs  
Allocated 0 of 1



Security Groups  
Used 2 of 10



Security Group Rules  
Used 10 of 100



Networks  
Used 0 of 1



Ports  
Used 1 of 10

### Usage Summary

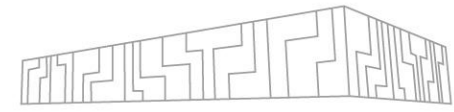
Select a period of time to query its usage:

The date should be in YYYY-MM-DD format.

2023-10-29 to 2023-10-30

Active Instances: 1

# IT4I DATA TRANSFERS AND STORAGE



## Improved connectivity to LUMI supercomputer

- Updated network parameters on Karolina and LUMI system
- New routing between IT4I and CSC proposed
- 3x speedup
- Use parallel transfers:

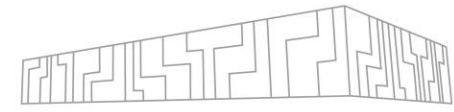
<https://docs.it4i.cz/general/shell-and-data-access/?h=xargs#data-transfer>

## S3 Services

- S3 access to PROJECT and CL3 (total capacity 33PB)  
<https://docs.it4i.cz/storage/proj4-storage/>



# KAROLINA GUI - OPENONDEMAND



 FortiClient VPN + <https://ood-karolina.it4i.cz/>

Browser address bar: [https://ood-karolina.it4i.cz/pun/sys/dashboard/batch\\_connect/sessions](https://ood-karolina.it4i.cz/pun/sys/dashboard/batch_connect/sessions)



KAROLINA Files Jobs Clusters Interactive Apps My Interactive Sessions Help Logged in as jansik Log Out

Session was successfully created. ✕

Home / My Interactive Sessions

**Interactive Apps**

Desktops

-  Karolina Login Mate
-  Karolina Login XFCE

**Karolina Login Mate (64897.host)** 1 node | 53 cores | Running

**Host:** [>\\_login1.karolina.it4i.cz](#) Delete

**Created at:** 2022-11-03 08:55:16 CET

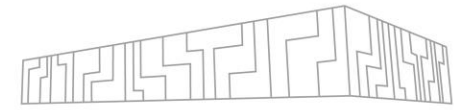
**Time Remaining:** 1 hour and 35 minutes

**Session ID:** [dfd5e0d0-d806-49b2-90e1-0e7d0a7f4786](#)

Compression 0 (low) to 9 (high) | Image Quality 0 (low) to 9 (high)

Launch Karolina Login Mate View Only (Share-able Link)

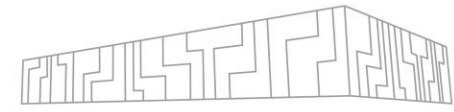
# KAROLINA GUI - OPENONDEMAND



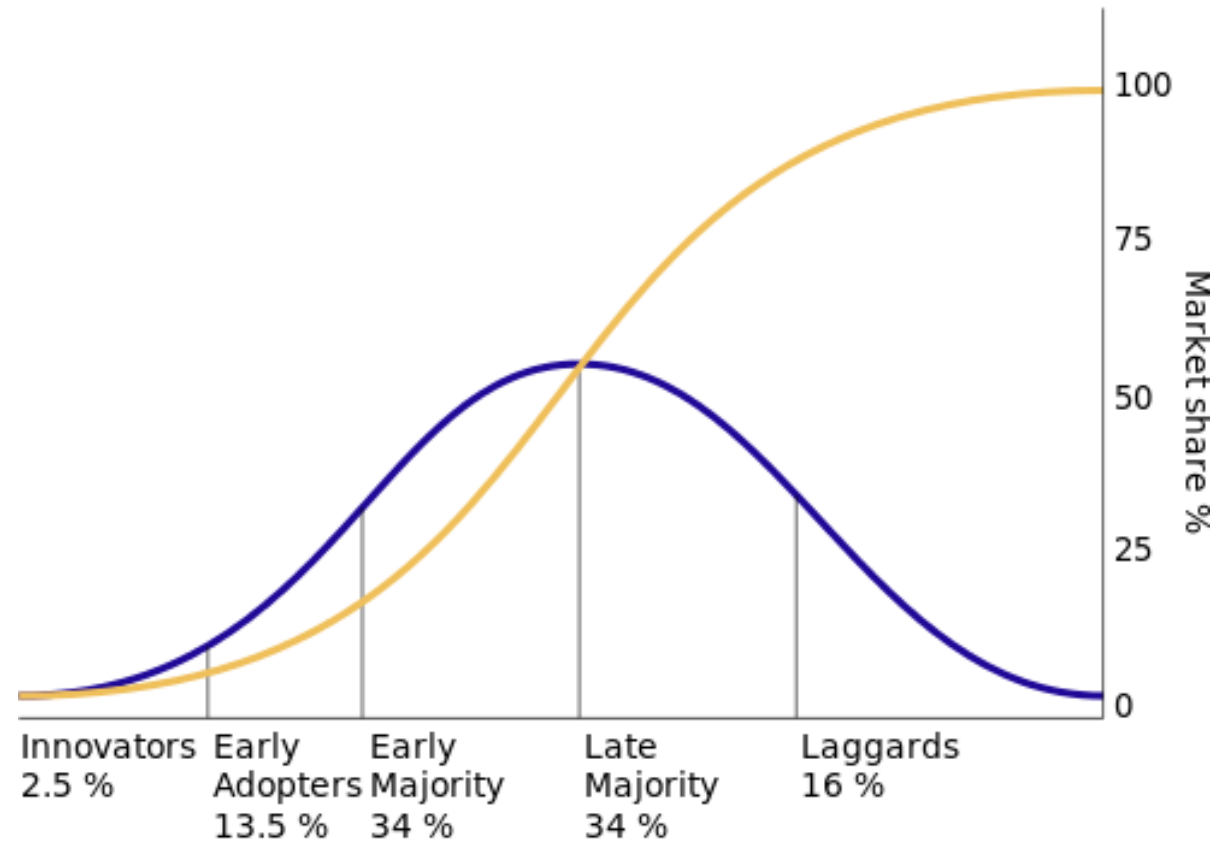
The screenshot displays the MATLAB R2021a academic use interface with several windows open:

- Code Editor (mbi-blas.c):** Shows C code for a Lorenz attractor simulation using OpenMP. The code includes memory allocation, matrix initialization, and a loop for iterations. It uses `omp_get_wtime()` for timing and `omp_get_thread_num()` for thread identification.
- Command Window:** Contains MATLAB commands: `na = linspace(-10,10,1000); xt = exp(-t./10).*sin(5*t); yt = exp(-t./10).*cos(5*t); p = plot3(xt,yt,t); na = linspace(-10,10,1000); t = linspace(-10,10,1000); xt = exp(-t./10).*sin(5*t);`
- Figure 1:** A 3D plot of the Lorenz attractor, showing a complex, chaotic trajectory in a 3D space.
- Mate Terminal:** Shows the execution of the MATLAB script: `matlab & bg; cd work; cd lorenz; gvim mbi-blas.c`
- Arm Forge 23.0.2:** A configuration window for the Arm Forge environment, showing options for OpenMP threads, CUDA, Memory Debugging, and Submit to Queue.

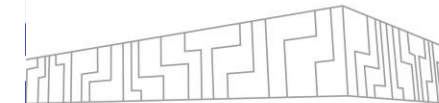
# COMPLEMENTARY SYSTEMS



Targeted at perspective technology to provide „innovator/early adopter“ advantage in the Rogers curve sense.



# COMPLEMENTARY SYSTEM 2



## Clusters

Karolina >

Barbora >

NVIDIA DGX-2 >

Complementary Systems >

Introduction

Accessing CS

Specification

Complementary System Job Scheduling

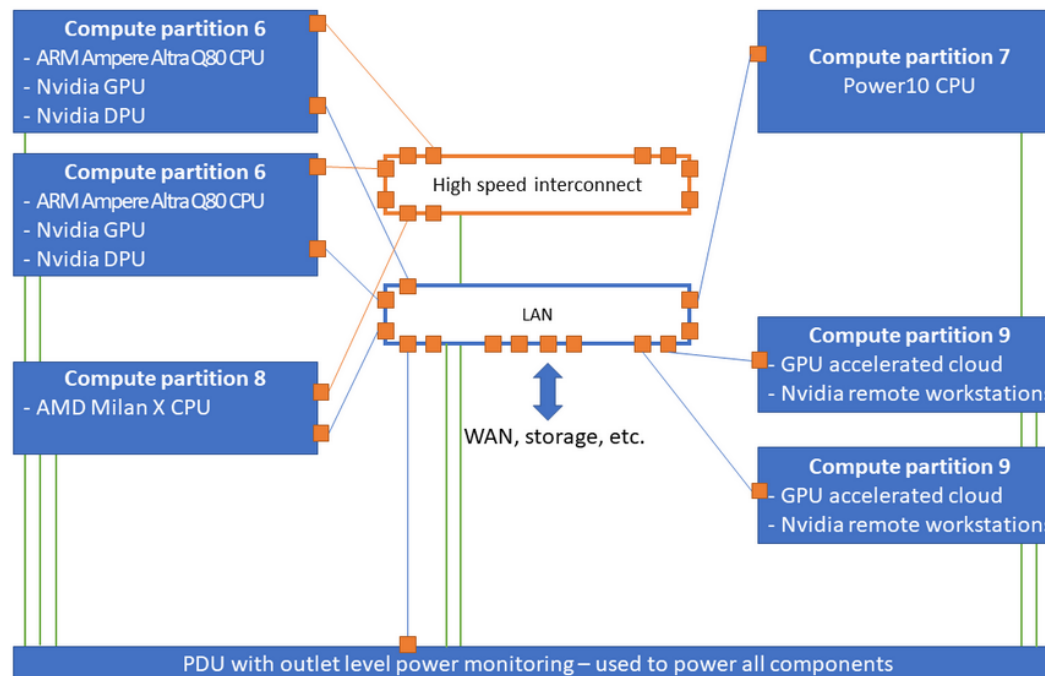
Guides >

Archive >

## Complementary Systems 2

Second stage of complementary systems implementation comprises of these partitions:

- compute partition 6 - based on ARM technology + CUDA programmable GPGPU accelerators on ampere architecture + DPU network processing units
- compute partition 7 - based on IBM Power10 architecture
- compute partition 8 - modern CPU with a very high L3 cache capacity (over 750MB)
- compute partition 9 - virtual GPU accelerated workstations



Ta

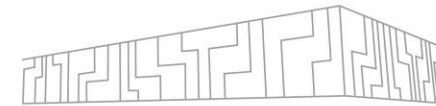
Co

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Av

# NEW SYSTEMS, MCIII

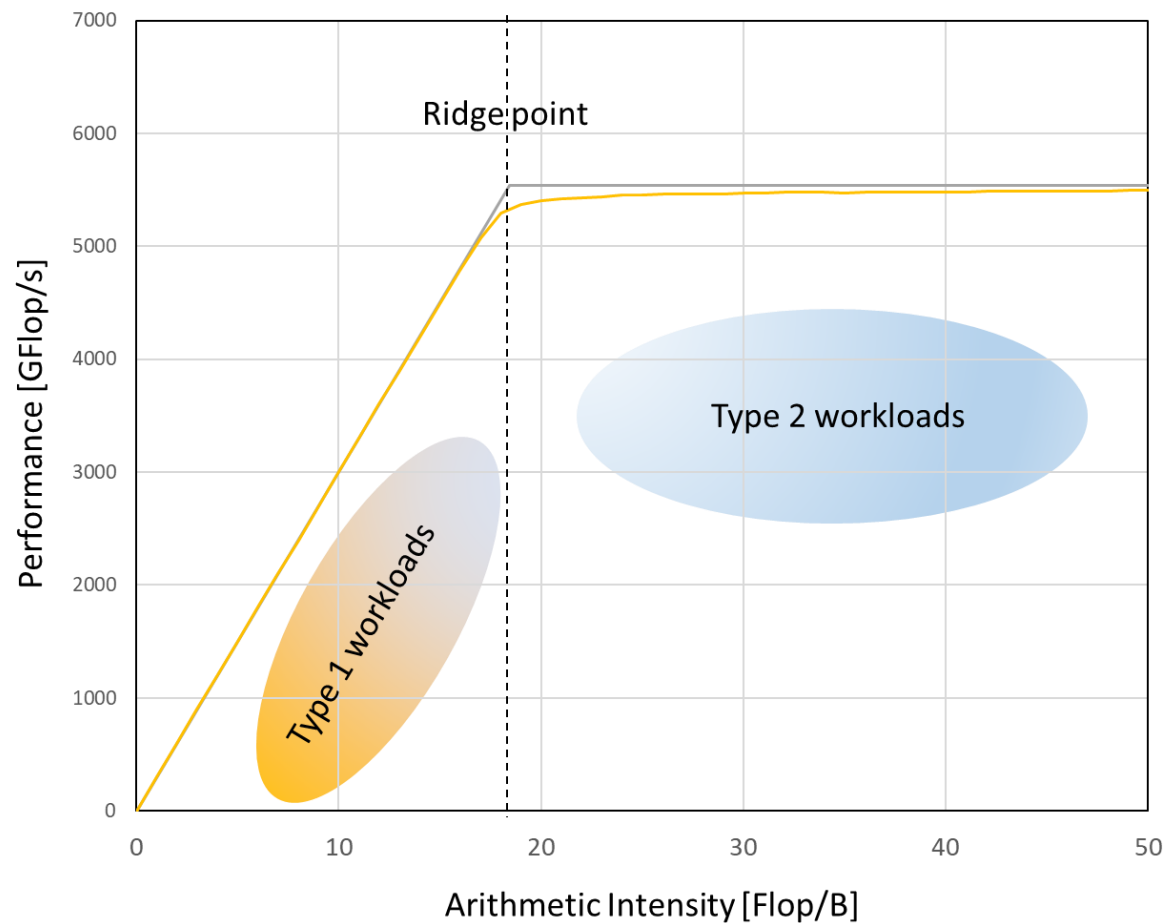


Compute		180 nodes
Home		25 TB
Scratch		300 TB
Login		2 nodes
Mgmt		2 nodes
Infiniband	200 GBps	194 ports
LAN		196 ports

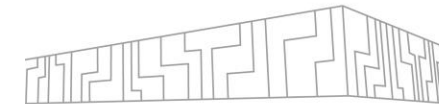
## HBM Memory

x86\_64 architecture

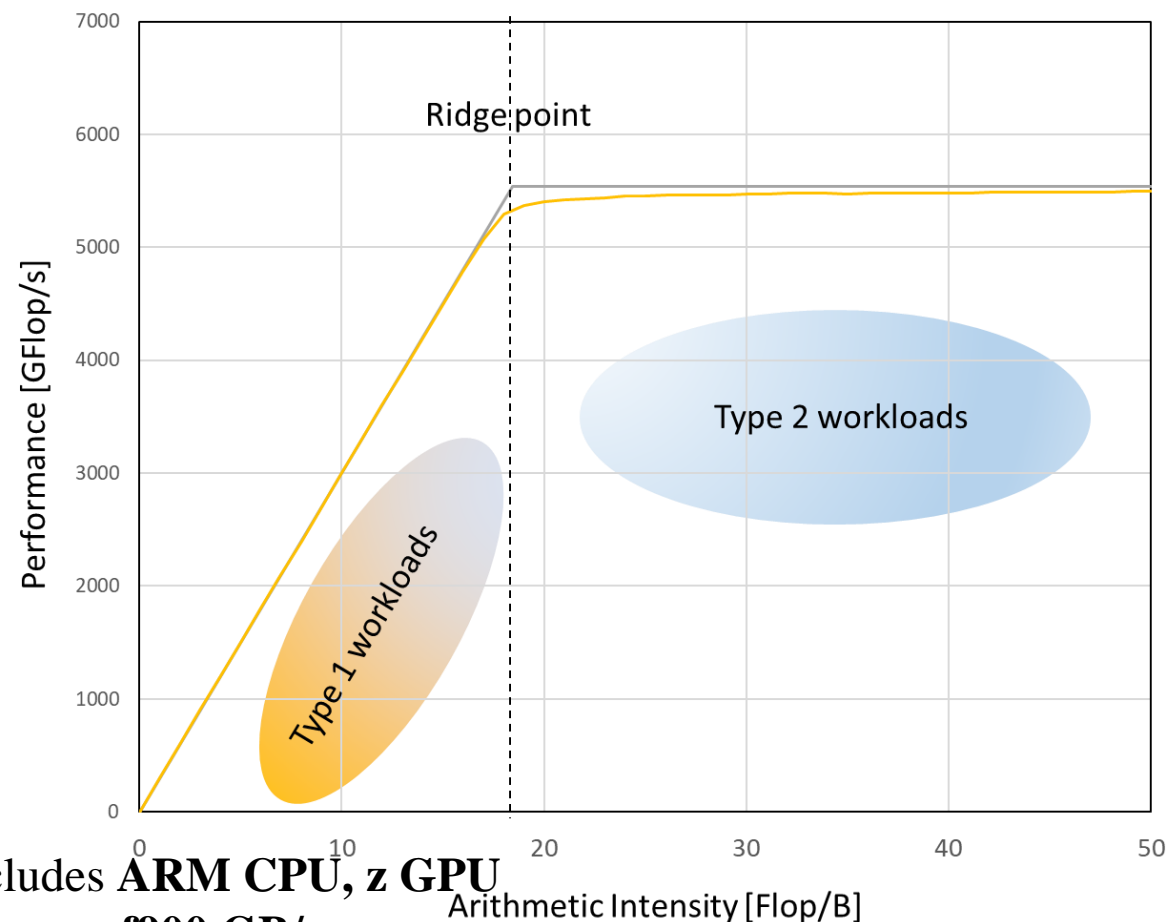
HBM2 mem 64 GB, 1,2 TB/s, 1,2 PFlop/s



# NEW SYSTEMS, VCIII



CPU		300 nodes
<b>Accel</b>		74 nodes
Home		25 TB
Scratch		2000 TB
Login		4 nodes
Mgmt		4 nodes
Infiniband		530 ports
LAN		460 ports



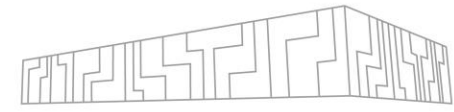
**x86\_64 architecture** 4x Grace Hopper NVIDIA, includes ARM CPU, z GPU

**ARM architecture** memory perf 4 TB/s a z memory perf 900 GB/s.

**NVIDIA Architecture** Total 18 PFlop/s.

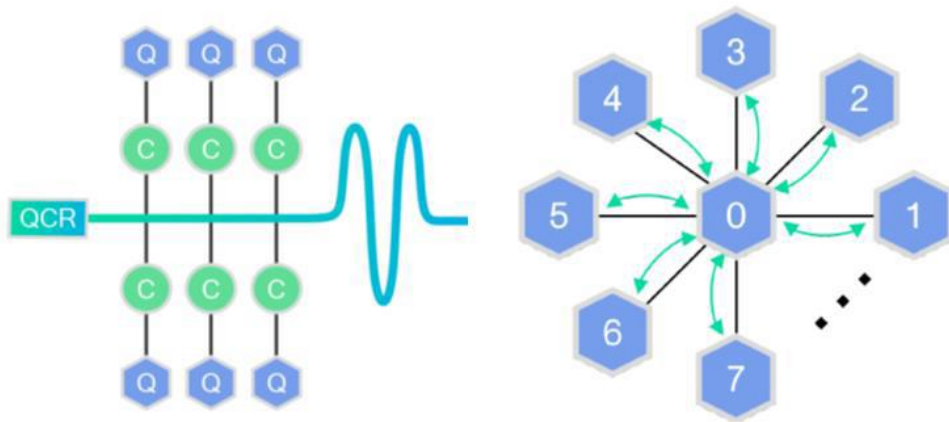
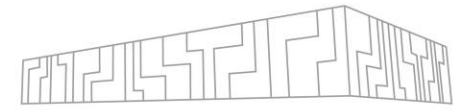
GRACE+HOPPER

# LUMI-Q PROGRESS



- LUMI-Q Hosting agreement (procurement and hosting) signed June 2023
- LUMI-Q Operational costs grant agreement in final stages before signature
- LUMI-Q Consortium agreement provided to partners, collecting feedback to v2, up to 3.11.2023
- LUMI-Q Integration costs grant application submitted 28.9.2023, project name EuroQHPC-Integration. The project includes all 6 hosting entities, led by GENCI
- LUMI-Q RFP prepared and submitted to EuroHPC JU on 16.10.2023.

# LUMI-Q TECHNOLOGY

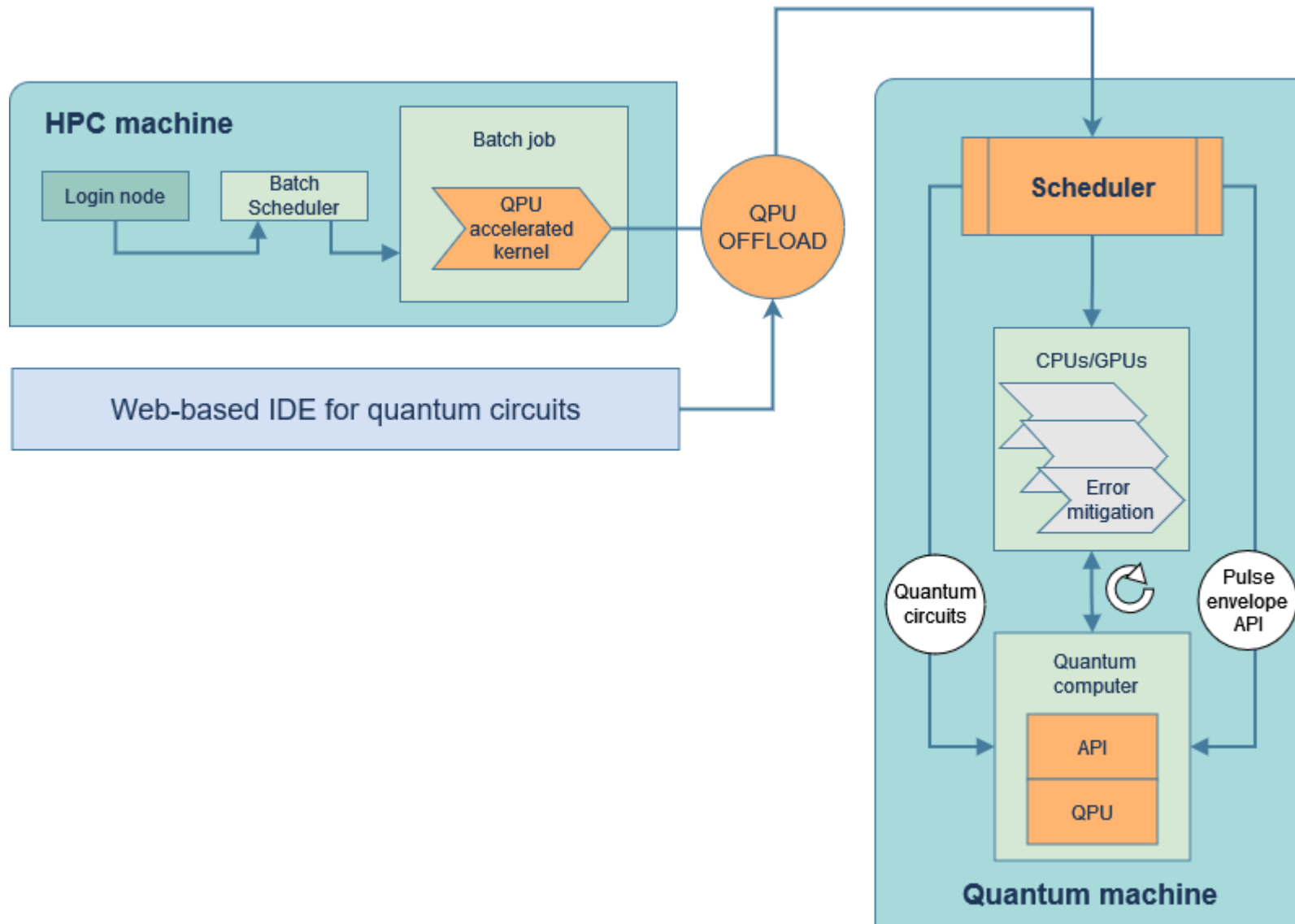
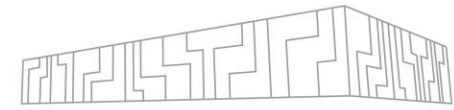


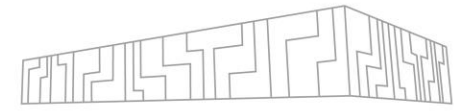
- Star-shape qubit topology, one-to-all qubit connectivity,
- Strong reduction of SWAP operations count
- High complexity quantum algorithms possible
- Massive advancement compared to anything presently available
- Increased performance

Operation	SWAP ops 12 qubits in 3x4 grid	SWAP ops 12 qubits LUMI-Q grid
Two qubit gates	11	2
Two qubit gates, all pairs	45	26
3-qubit GHZ state	11	2
One simulation step of all-to-all spin system	45	26



# LUMI-Q EUROHPCQS-INTEGRATION





<https://events.it4i.cz/>

**Nov 21**

[ONLINE] IO-SEA: Automated Workflows and Benchmarks with JUBE in IO-SEA and Beyond

**Nov 08**

[HYBRID] Parallel Computing with MATLAB and Scaling MATLAB Code to the HPC Cluster (EuroCC)



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