

WIGNER SCIENTIFIC COMPUTING LABORATORY GPU DAY 2022

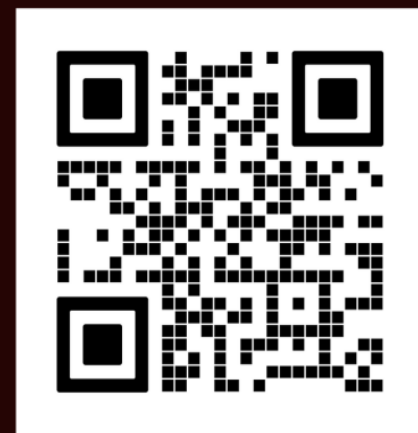
20-21. JUNE



MORE INFORMATION AND REGISTRATION:

[HTTPS://GPU DAY.COM/](https://gpuday.com/)

[HTTPS://INDICO.KFKI.HU/EVENT/1393/](https://indico.kfki.hu/event/1393/)



THE FUTURE OF MASSIVE PARALLEL AND QUANTUM COMPUTING

EMERGING ACCELERATOR PLATFORMS

IMAGE PROCESSING, COMPUTER VISION, AND RECONSTRUCTION

INDUSTRIAL APPLICATIONS

GRAPHICS, RENDERING, AND IMAGE SYNTHESIS

COMPUTING AND VISUALIZATION IN EDUCATION

QUANTUM COMPUTING SIMULATION

MACHINE LEARNING, NEURAL NETWORKS, FEATURE RECOGNITION

MANY-CORE COMPUTING IN PHYSICS AND OTHER FIELDS OF SCIENCE



WSCPs GPU Day 2022 – gpuday.com



ELKH | Eötvös Loránd
Research Network



STREAM
High Performance Computing



Programme for today/tomorrow

09:00	Opening: Opening Talk and Welcome by the Director <i>Hotel Mercure Budapest Castle Hill</i>	<i>Gergely Barnaföldi, Peter Levai</i> 09:00 - 09:20
	Accelerating massively parallel .NET code using FPGAs with Hastiayer <i>Hotel Mercure Budapest Castle Hill</i>	<i>Zoltán Lehóczky</i> 09:20 - 10:00
10:00	OpenCL Ecosystem Updates <i>Hotel Mercure Budapest Castle Hill</i>	<i>Máté Nagy-Egri</i> 10:00 - 10:40
	Coffee Break <i>Hotel Mercure Budapest Castle Hill</i>	10:40 - 11:00
11:00	ELKH Cloud vGPU challenges and implementation steps <i>Hotel Mercure Budapest Castle Hill</i>	<i>Ádám Pintér</i> 11:00 - 11:30
	Present and Future of GPU HPC in Hungary <i>Hotel Mercure Budapest Castle Hill</i>	<i>Zoltán Kiss</i> 11:30 - 11:50
12:00	Parallel Implementation of Multivariate Empirical Mode Decomposition on GPU <i>Hotel Mercure Budapest Castle Hill</i>	<i>Zeyu Wang</i> 11:50 - 12:10
	What makes us humans: Differences in the critical dynamics underlying the human and fruit-fly connectome <i>Hotel Mercure Budapest Castle Hill</i>	<i>Geza Odor</i> 12:10 - 12:30
13:00	Lunch break <i>Hotel Mercure Budapest Castle Hill</i>	12:30 - 14:00
14:00	Online data processing with GPUs in ALICE during LHC Run 3 <i>Hotel Mercure Budapest Castle Hill</i>	<i>Dr David Rohr</i> 14:00 - 14:40
	Machine learning based estimator for elliptic flow in heavy-ion collisions <i>Hotel Mercure Budapest Castle Hill</i>	<i>Suraj Prasad</i> 14:40 - 15:00
15:00	pCT Image Reconstruction – A Huge Linear Problem <i>Hotel Mercure Budapest Castle Hill</i>	<i>Akos Sudar</i> 15:00 - 15:20
	Representation learning in Artificial Intelligence <i>Hotel Mercure Budapest Castle Hill</i>	<i>Antal Jakovac</i> 15:20 - 15:40
	Coffee break <i>Hotel Mercure Budapest Castle Hill</i>	15:40 - 16:00
16:00	Machine learning methods for Schlieren imaging of a plasma channel in tenuous atomic vapor <i>Hotel Mercure Budapest Castle Hill</i>	<i>Mr Mihály András Pocsai</i> 16:00 - 16:20
	Strategies for multi-GPU PIC/MCC plasma simulation implementation on pre-exascale supercomputers <i>Hotel Mercure Budapest Castle Hill</i>	<i>Zoltán Juhasz</i> 16:20 - 16:40
	Preliminary results of the tuned HIJING++ heavy-ion event generator <i>Hotel Mercure Budapest Castle Hill</i>	<i>Balazs Majoros</i> 16:40 - 17:00
17:00	The highly increased number of protein structures calls for high performance algorithms <i>Hotel Mercure Budapest Castle Hill</i>	<i>Tamas Hegedus</i> 17:00 - 17:20

09:00	Piquasso, a comprehensive framework for optical quantum computer programming and simulation <i>Hotel Mercure Budapest Castle Hill</i>	<i>Zoltan Zimboras</i> 09:00 - 09:30
	Improving efficiency of non-Gaussian photonic circuit simulations <i>Hotel Mercure Budapest Castle Hill</i>	<i>Zoltán Kolarovszki</i> 09:30 - 09:50
10:00	Custom Tailored FPGA Boson Sampling <i>Hotel Mercure Budapest Castle Hill</i>	<i>Gregory Morse</i> 09:50 - 10:10
	Efficient quantum gate decomposition via adaptive circuit compression <i>Hotel Mercure Budapest Castle Hill</i>	<i>Peter Rakytá</i> 10:10 - 10:40
	Coffee Break <i>Hotel Mercure Budapest Castle Hill</i>	10:40 - 11:00
11:00	Studying hadronization with Machine Learning techniques <i>Hotel Mercure Budapest Castle Hill</i>	<i>Gabor Biro</i> 11:00 - 11:20
	Polynomial speedup in exact Torontonian calculation by a scalable recursive algorithm <i>Hotel Mercure Budapest Castle Hill</i>	<i>Ágoston Kaposi</i> 11:20 - 11:40
	Machine learning Hadron Spectral Functions in Lattice QCD <i>Hotel Mercure Budapest Castle Hill</i>	<i>Feiyi Liu</i> 11:40 - 12:00
12:00	Exploring SARS-CoV-2 receptor binding domain variants <i>Hotel Mercure Budapest Castle Hill</i>	<i>Ákos Gellért</i> 12:00 - 12:30
13:00	Lunch <i>Hotel Mercure Budapest Castle Hill</i>	12:30 - 14:00
14:00	Simulating gold resonant nano-antennas for nano-fusion <i>Hotel Mercure Budapest Castle Hill</i>	<i>Istvan Papp</i> 14:00 - 14:30
	Numerical Simulation of Mirages Above Water Bodies <i>Hotel Mercure Budapest Castle Hill</i>	<i>Balázs Bámer et al.</i> 14:30 - 14:50
15:00	Parallel computing for determining stable parameter domain in mechatronic applications <i>Hotel Mercure Budapest Castle Hill</i>	<i>Mr Tamás Haba</i> 14:50 - 15:10
	Full Core Pin-Level VVER-440 Simulation of a Rod Drop Experiment with the GPU-Based Monte Carlo Code-GUARDYAN <i>David Legrády</i>	15:10 - 16:00
	Coffee break <i>Hotel Mercure Budapest Castle Hill</i>	15:40 - 16:00
16:00	The resonant structure of the trans-Neptunian space <i>Hotel Mercure Budapest Castle Hill</i>	<i>Emese Kövári</i> 16:00 - 16:20
	Massively Parallel Tensor Network Algorithms <i>Hotel Mercure Budapest Castle Hill</i>	<i>Andor Menczer</i> 16:20 - 16:40
	Critical synchronization dynamics on power grids <i>Hotel Mercure Budapest Castle Hill</i>	<i>Mr Shengfeng Deng</i> 16:40 - 17:00
17:00	Application of high-performance computing for bubble simulations in sonochemistry <i>Hotel Mercure Budapest Castle Hill</i>	<i>Dániel Nagy</i> 17:00 - 17:20
	Closing <i>Hotel Mercure Budapest Castle Hill</i>	<i>Gergely Barnaföldi</i> 17:20 - 17:40



WSCLAB>_

WIGNER SCIENTIFIC COMPUTING LABORATORY

WSCLAB @ NKFIH TOP50 Research Infrastructure

17TH DECEMBER 2021.



WSCLAB @ NKFIH TOP50 Research Infrastructure

VISIT: 10TH FEBRUARY 2022.



WSCLAB's origin

12 YEARS IN PARALLEL COMPUTING (WIGNER GPU LABORATORY) & HPC @ WDC



The aim of the Wigner GPU Laboratory is to provide support for any fields in science in sense of parallel computing techniques, especially for faster numerical calculations in gravitational and high-energy physics, astronomy, astrophysics, material sciences, and detector simulations. We have started with GPU technologies in 2009, but later our aim was improved to any kind of parallel computing technology. Today, many- and multi-core, GPU, FPGA, Xeon Phi technologies are all available in the laboratory. Beside the academic environment and other institutes, we have connections to industrial partners as well.

The History of WSCLAB's Wigner GPU Laboratory

- 2005-2008 Idea of using GPU in HEP calculations
Starting of the WLCG Grid (ALICE & CMS) Tier-2 at the Wigner
- 2009 Discussion with GGB & P. Lévai & G. Debreczeni
2 main direction: HEP & Gravity
- **2010- 1st GPU Day & formation of the Wigner GPU Laboratory**
Students: M. F. Nagy-Egri & D. Berényi
- 2010- GPU Day series
- 2016- Lectures on Modern Computing in Science series
- 2016- Wigner GPU Lab Fellowship
- **2021- Wigner Scientific Computing Laboratory (NKFIH TOP50 RI)**





WSCLAB's origin

12 YEARS IN PARALLEL COMPUTING (WIGNER GPU LABORATORY) & HPC @ WDC

Since 2010, the GPU Day is a yearly international conference on massively parallel technologies and their applications and quantum computing.

Its dedicated goal is to bring together researchers from academia, developers from industry and interested students to exchange experiences and learn about novel and future technologies.

It is a unique event with focus on exchange of knowledge and expertise such topics as GPU, FPGA and quantum computing simulations.

Presentation of talks and demo desks help to draw attention to your cutting-edge solutions.

This conference is an established meeting of experts, where you can discuss methods, exchange ideas, find new collaborators and business partners.

Best place to see the Wigner GPU Lab's activity.

Our sponsors gain additional visibility at the event, on the webpage and related digital appearances including special interviews.



Barnaföldi, Gergely Gábor

LEADER OF THE LOCAL ALICE GROUP AND

Kacsokovics, Balázs

PHD STUDENT, ADMINISTRATOR

Szigeti, Balázs

MSC STUDENT, ADMINISTRATOR

Bíró, Gábor

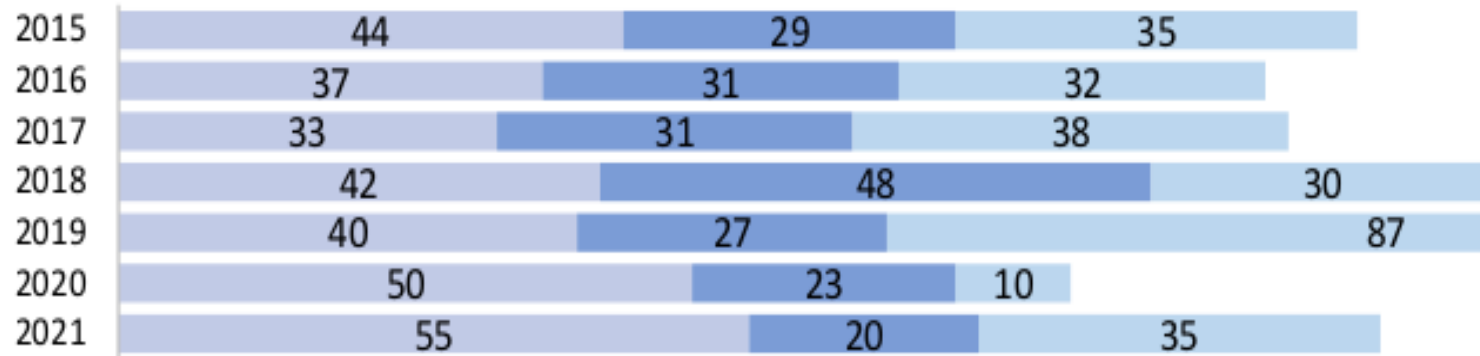
PHD STUDENT, ADMINISTRATOR



WSCLAB in numbers

KNOWLEDGE HUB: GPU_{DAY}.COM

- ✓ 6 Lectures on Modern Computing in Science
- ✓ 12 GPU Days



- ✓ 40 WSCLAB (Wigner GPU Lab) Fellowship (30 finished + 10 running)
- ✓ 33+ industrial & academic partners (Lombiq LTD, Ericsson, Khronos, CERN...)
- ✓ 35+ scientific publications and program codes

WSCLAB Projects

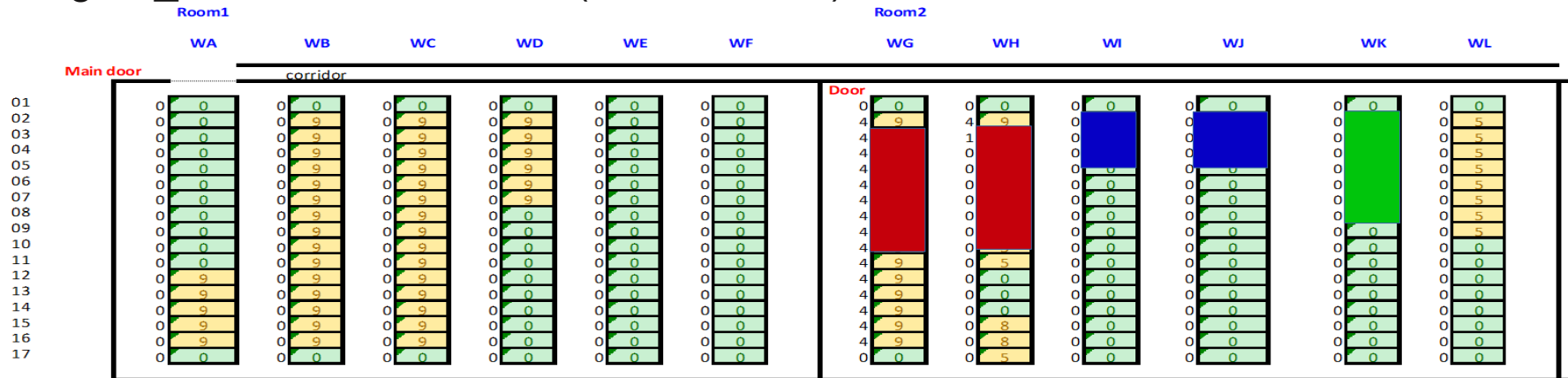
2021.12.01-2022.11.30

- ✓ Massively Parallel Classical- and Quantum Computing Simulations in HEP MassivPara@HEP (2020-2.1.1-ED-2021-00179 25M)
 - Massive parallel computing: Wigner_AF + GPULab + HIJING++
 - Quantum Computer simulations (Maxeler FPGA)
- ✓ Wigner RCP & INFRA investments @2021 (100M)
- ✓ Young Researcher's Fellowship (3M)
- ✓ Wigner GPU Labor (10M+2M non-academic)
- ✓ ALICE + CMS WLCG T2 (20M)

WSCLAB @ WDC

THE PLACE

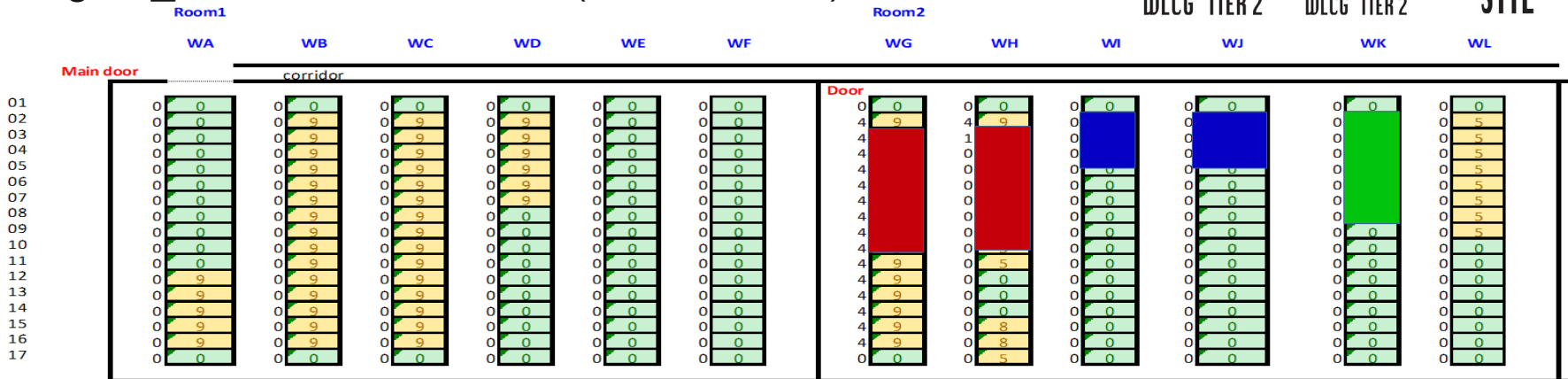
- ✓ Wigner Analysis Facility (Wigner AF)
- ✓ Wigner GPU Laboratory
- ✓ Wigner_KFKI WLCG T2 Grid (ALICE+CMS)



WSCLAB @ WDC

THE PLACE

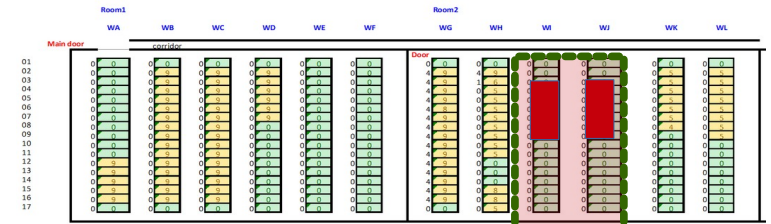
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Wigner GPU Laboratory (@WDC)

NEW HARDWARES (IN PROGRESS), HAPPY USERS

- ✓ 1) Wigner RCP investment @2021 (100M)
 - WSCLAB's GPU Lab in 2022
 - Nvidia 6xTesla T4 + Nvidia 8xA2
 - 20 TB Storage
 - 10G switch to GEANT
 - Mathematica server
 - Supermicro 8xA100 (Christmas Day)
 - Maxeller 2xFPGA for Quantum Simulations
 - **Coming (very) soon**
 - **EPYC gate server**
 - **Infiniband switch & cards**



Wigner GPU
Laboratory



Wigner GPU Laboratory (@WDC)

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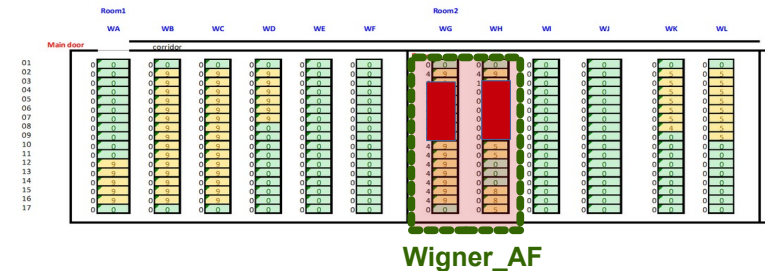


WIGNER_AF 2022Q2

NEW SPECIALIZED HEP ANALYSIS FACILITY (1ST FOR ALICE)

✓ 2) HW 9 rack of hardware

- SE: EOS config & monitoring
 - 2 redundant MGM nodes
 - 32 FST node, with 24*3 TB for each node
 - Raw capacity: ~2.6 PB
 - Usable capacity: ~1.3 PB
- WNs: configured with HTCondor, 1 single-core queue and 1 multi-core queue (for 8-core jobs)
 - 124 worker nodes, with 32 vCPU for each node
 - this pool is shared among the two queues, but the single-core queue has a limited number of maximum jobs





ALICE ANALYSIS FACILITY

WIGNER_AF 2019Q4 NEW SPECIALIZED HEP ANALYSIS FACILITY (1ST FOR ALICE)



WIGNER_AF 2020Q1

NEW SPECIALIZED HEP ANALYSIS FACILITY (1ST FOR ALICE)



Expectation:



Reality:



WIGNER_AF 2020Q1


NEW SPECIALIZED HEP ANALYSIS FACILITY (1ST FOR ALICE)

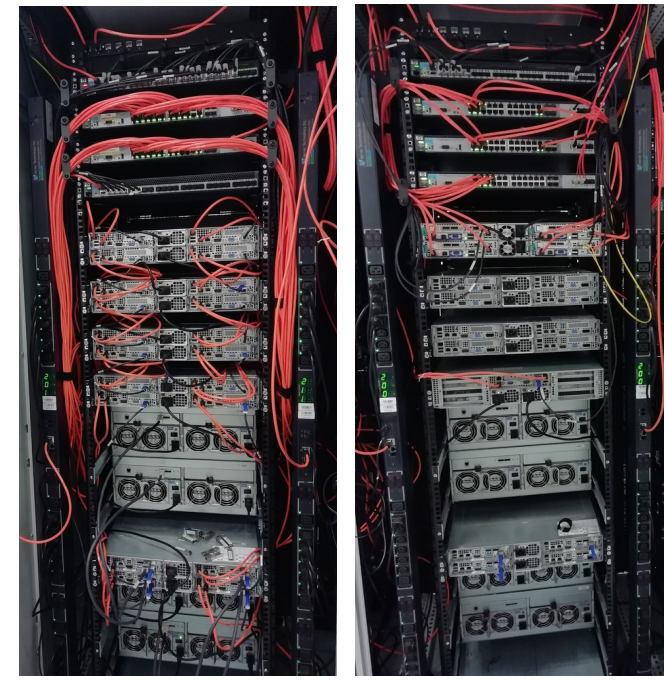


Expectation:

○ —————→ ●

Reality:

○  → ●



WIGNER_AF 2021Q2

NEW SPECIALIZED HEP ANALYSIS FACILITY (1ST FOR ALICE)

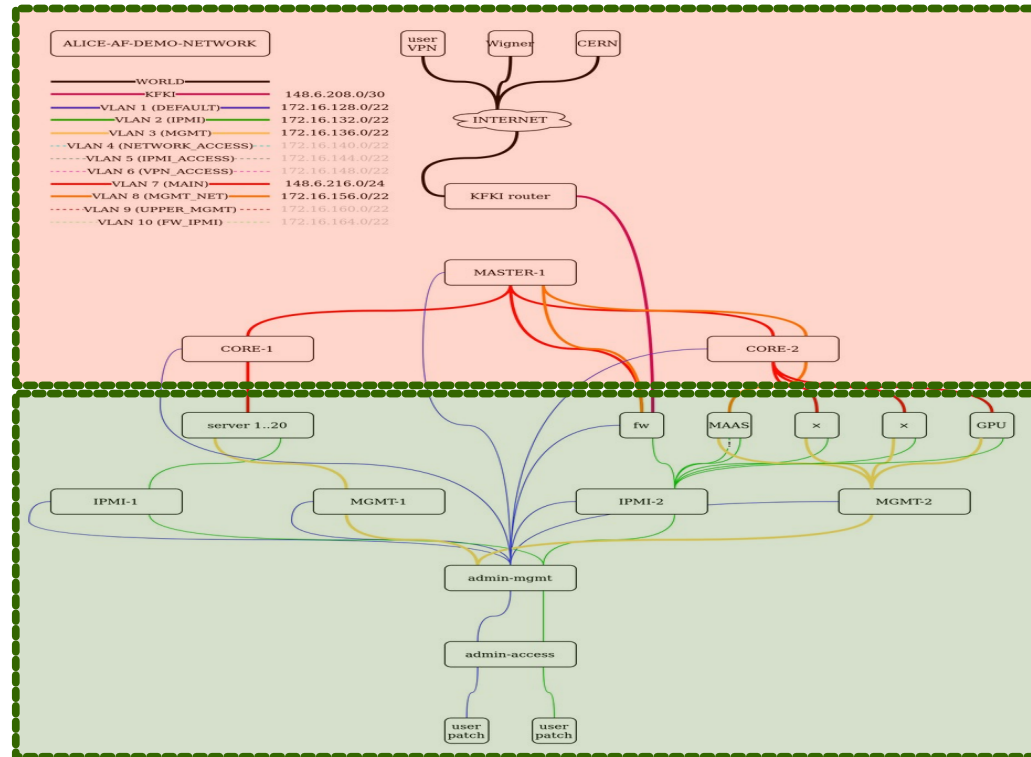


WIGNER_AF

NEW: JOINT WORK WITH HPC EXPERTS AT WDC

- ✓ WDC's services
 - Network structure
 - Fibers & routing
 - HW support
 - IPMI, MaaS
 - Security & support

- ✓ Wigner ALICE Group
 - Management
 - Use: IPMI, MaaS
 - HW monitoring
 - OS & SW



WIGNER_AF & ALICE T2 2022Q2 PERFORMANCE

✓ Wigner_AF_8_core:

✓ Wigner_AF:

✓ WIGNER_KFKI:

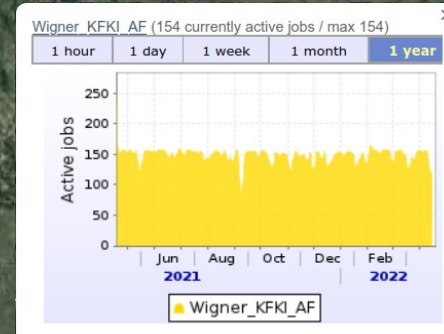


WIGNER_AF & ALICE T2 2022Q2 PERFORMANCE

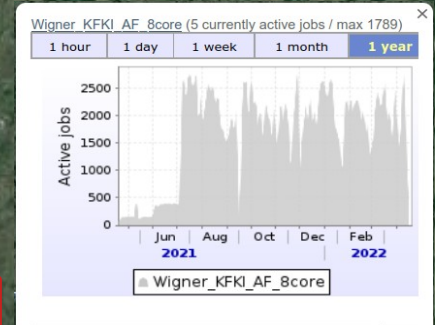
✓ Wigner_AF_8_core:



✓ Wigner_AF:



✓ WIGNER_KFKI:



WIGNER_KFKI

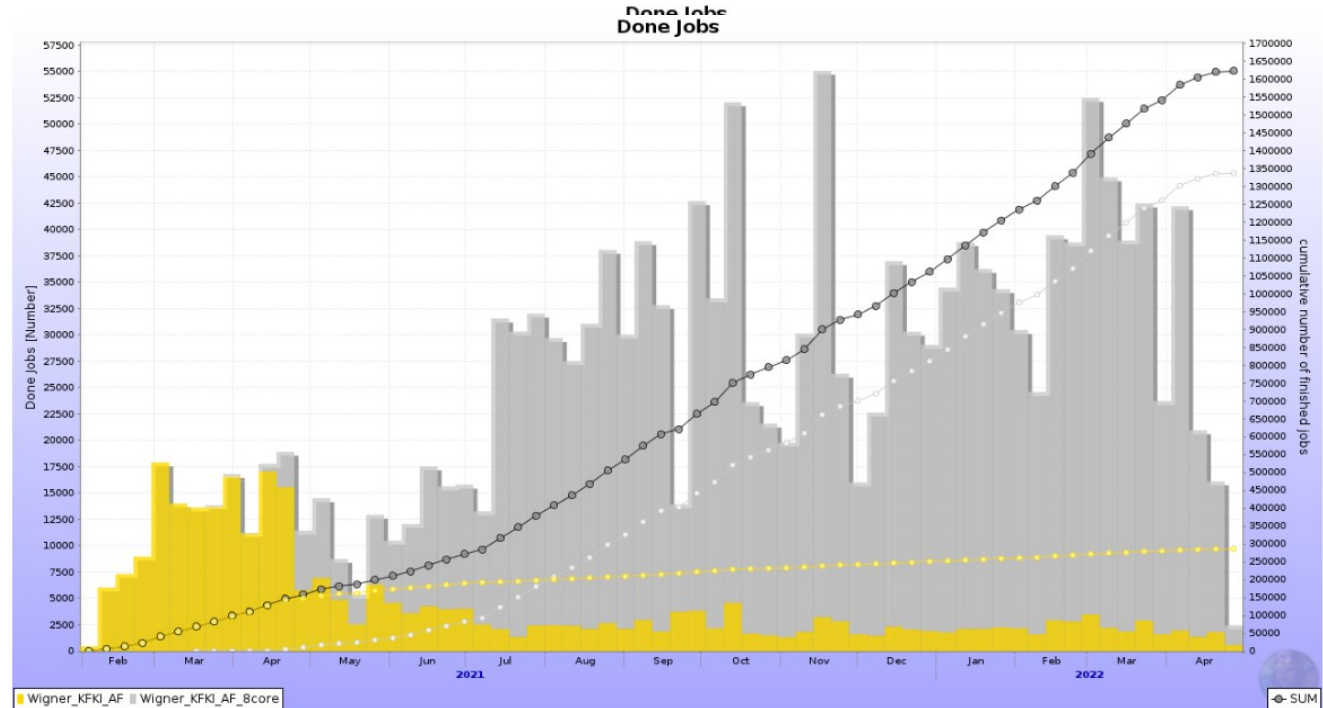
● Wigner_KFKI_AF_8core
● Wigner_KFKI_AF

WIGNER_AF & ALICE T2 2022Q2 PERFORMANCE

✓ Wigner_AF_8_core:

✓ Wigner_AF:

✓ WIGNER_KFKI:



WIGNER_AF AS IS 2022Q1 PERFORMANCE

✓ Performance & Benchmark

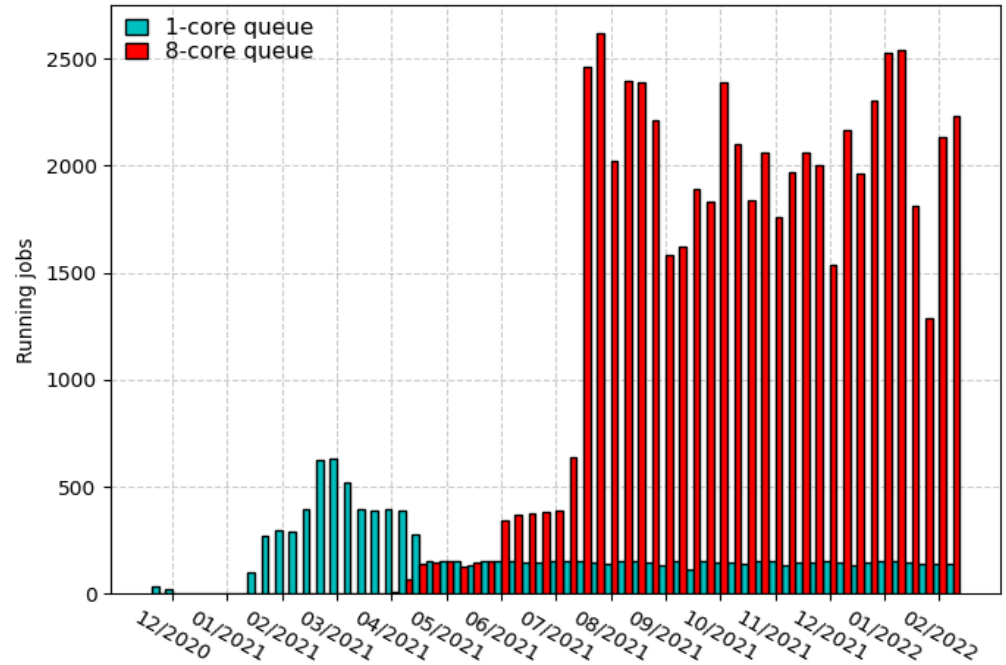
- Test of
 - 1-core pool
 - 8-core pool
 - 1-core/8-core combined pool

✓ Contribution for ALICE Coll: Public N

- Presentation an CHEP/ACAT

The Wigner ALICE Analysis Facility

Gábor Bíró^{1,2} , Gergely Gábor Barnaföldi¹ , Péter Lévai¹, Latchezar Betev³ and Jan Fiete Grosse-Oetringhaus³



WIGNER_AF AS IS 2022Q1 PERFORMANCE

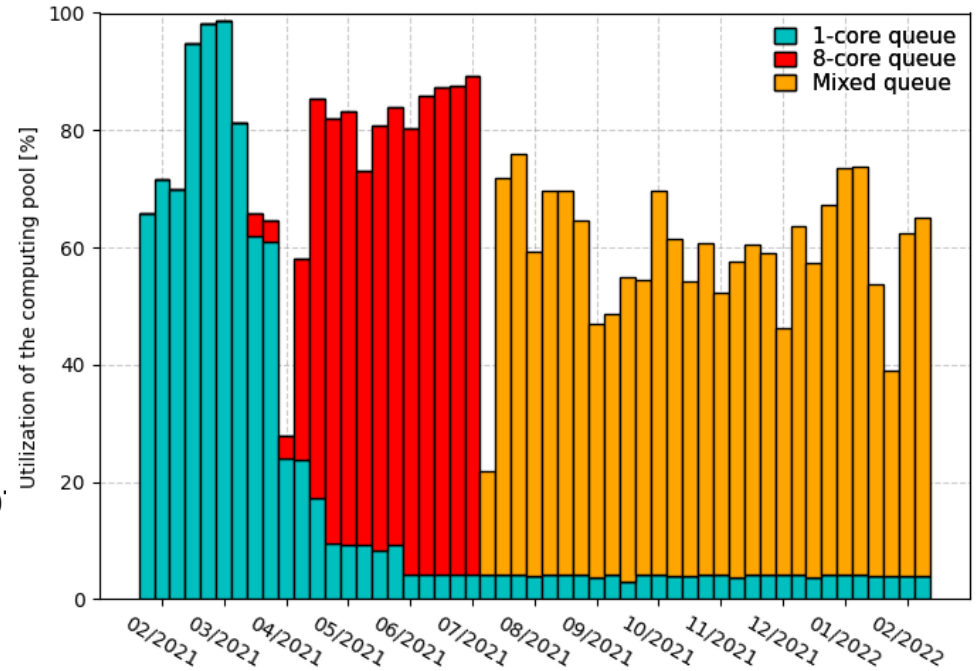
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WIGNER_AF AS IS 2022Q1 PERFORMANCE

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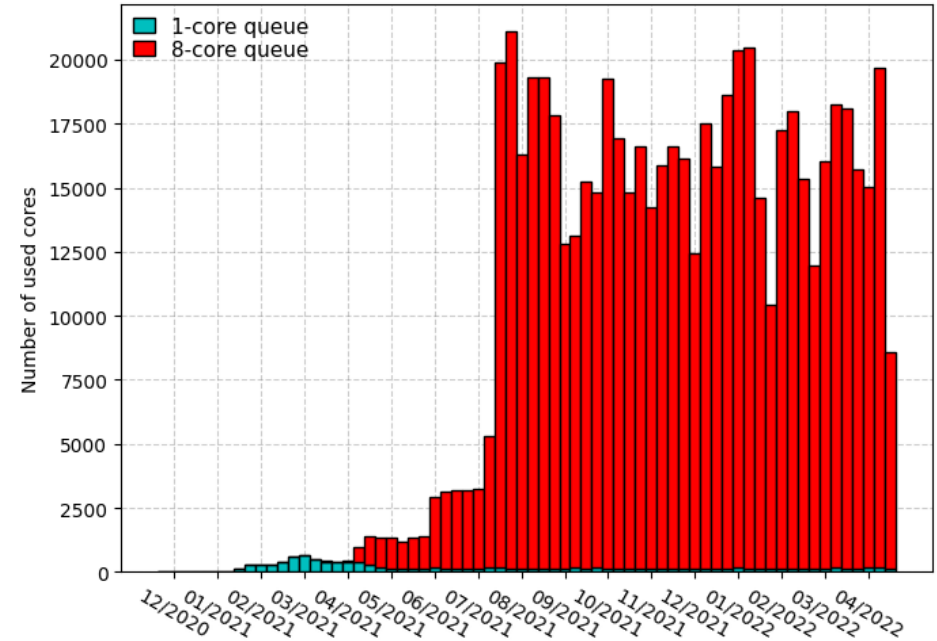
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WIGNER_AF AS IS 2022Q1 PERFORMANCE

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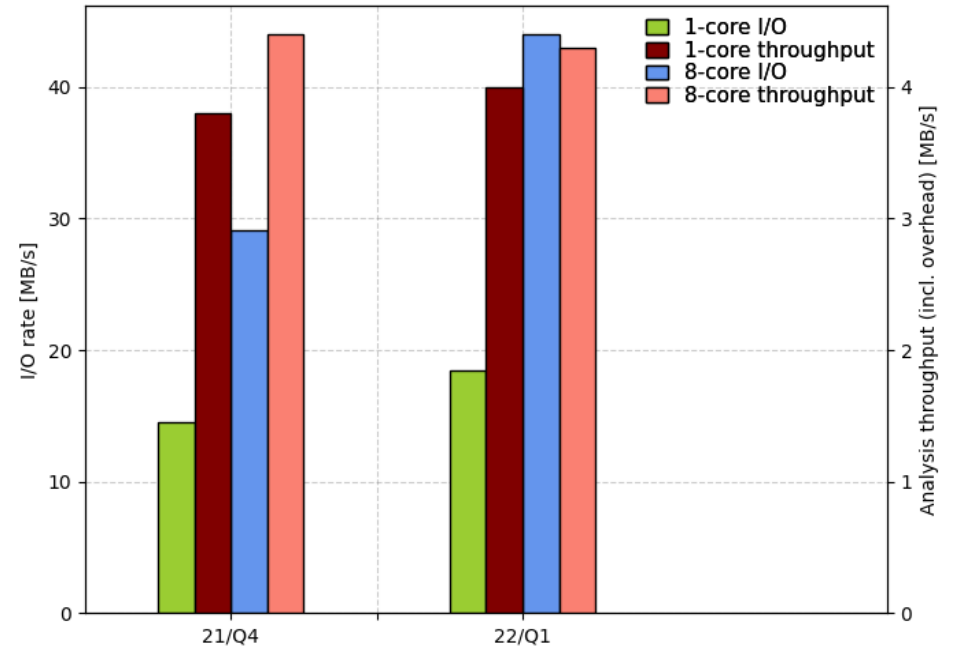
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FUTURE>_

WSCLAB's FUTURE

PLANS FOR THE FUTURE

- ✓ Short timescale
 - Finishing the running projects & make publish
 - New WSCLAB Grants for young scientists at 2022Q3
 - Restarting Lectures on Modern Computing in Science series (FPGA)
- ✓ Intermediate timescale
 - 100Gbps connection to GEANT network
- ✓ Long range plan
 - LEVENTE...