

LECTURES ON MODERN SCIENTIFIC PROGRAMMING



MACHINE LEARNING, NEURAL NETWORKS, FEATURE RECOGNITION

FIELD PROGRAMMABLE GATE ARRAYS

HANDS-ON SESSIONS

QUANTUM COMPUTING SIMULATION

QUANTUM MACHINE LEARNING AND SIMULATIONS

MANY-CORE COMPUTING IN PHYSICS AND OTHER FIELDS OF SCIENCE

WIGNER SCIENTIFIC COMPUTING LABORATORY

LECTURES ON MODERN SCIENTIFIC PROGRAMMING

14-15. NOVEMBER 2022.

MORE INFORMATION AND REGISTRATION:

[HTTPS://INDICO.KFKI.HU/EVENT/1409](https://indico.kfki.hu/event/1409)



Programme for today/tomorrow

09:00	Opening Wigner RCP	Gergely Barnaföldi et al. 09:00 - 09:05	
	Introduction to Machine Learning	Gabor Biro	
	Wigner RCP	09:05 - 10:00	
10:00	Coffee Break Wigner RCP	10:00 - 10:20	
	Machine Learning Hands-On Session	Gabor Biro	
11:00			
12:00	Wigner RCP	10:20 - 12:30	
	Lunch Break		
13:00			
	Wigner RCP	12:30 - 14:00	
14:00	Introduction to FPGA	Erno David	
	Wigner RCP	14:00 - 15:00	
15:00	Simulation of quantum computers via FPGA based data-flow engines	Peter Rakyta	
	Wigner RCP	15:00 - 16:00	
16:00	Coffee Break Wigner RCP	16:00 - 16:20	
	Hands-On Session		
17:00	Wigner RCP	16:20 - 17:30	
09:00	Introduction to Quantum Computing	Zoltan Zimboras	
	Wigner RCP	09:00 - 10:00	
10:00	Coffee Break Wigner RCP	10:00 - 10:20	
	Quantum Computing Hands-On Session	Márton Karácsony et al.	
11:00			
12:00	Wigner RCP	10:20 - 12:30	
	Lunch Break		
13:00			
	Wigner RCP	12:30 - 14:00	
14:00	Introduction to Quantum Machine Learning	Michael Spannowsky	
	Wigner RCP	14:00 - 16:00	
15:00			
	Wigner RCP	16:00 - 16:20	
16:00	Coffee Break Wigner RCP	16:00 - 16:20	
	Quantum Machine Learning Hands-On Session	Márton Karácsony et al.	
17:00	Wigner RCP	16:20 - 17:30	



WSCLAB> —

WIGNER SCIENTIFIC COMPUTING LABORATORY





WSCLAB's origin

13 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 Early years: 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 @ NKFIH TOP50 Research Infrastructure

START: 17TH DECEMBER 2021.



WSCLAB @ NKFIH TOP50 Research Infrastructure

VISIT: 10TH FEBRUARY 2022.





WSCLAB's origin

13 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.



WIGNER SCIENTIFIC COMPUTING LABORATORY

GPU DAY 2022

20-21. JUNE



MORE INFORMATION AND REGISTRATION:

[HTTPS://GPUDAY.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

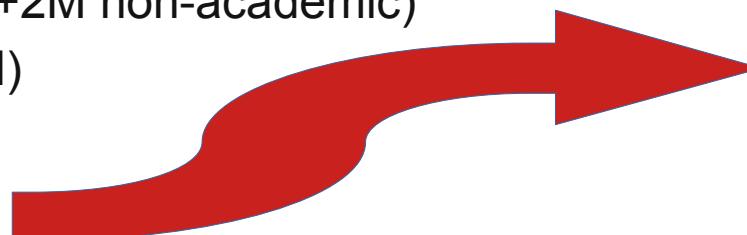
MANY-CORE COMPUTING IN PHYSICS AND OTHER FIELDS OF SCIENCE



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 Laboratory (10M+2M non-academic)
- ✓ ALICE + CMS WLCG T2 (20M)
- ✓ Ongoing & finished projects



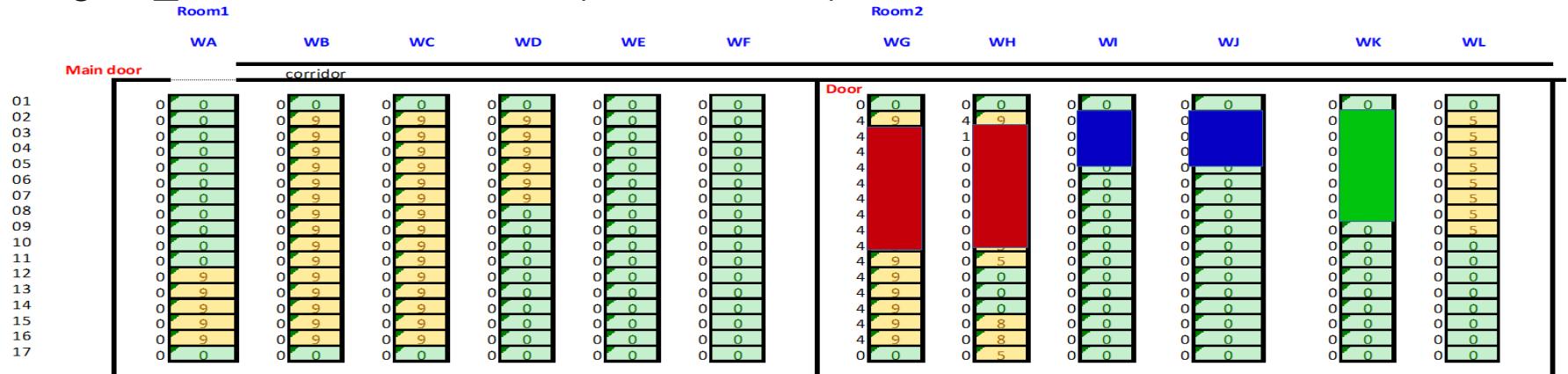


HARDWARES>_

WSCLAB @ WDC

THE PLACE

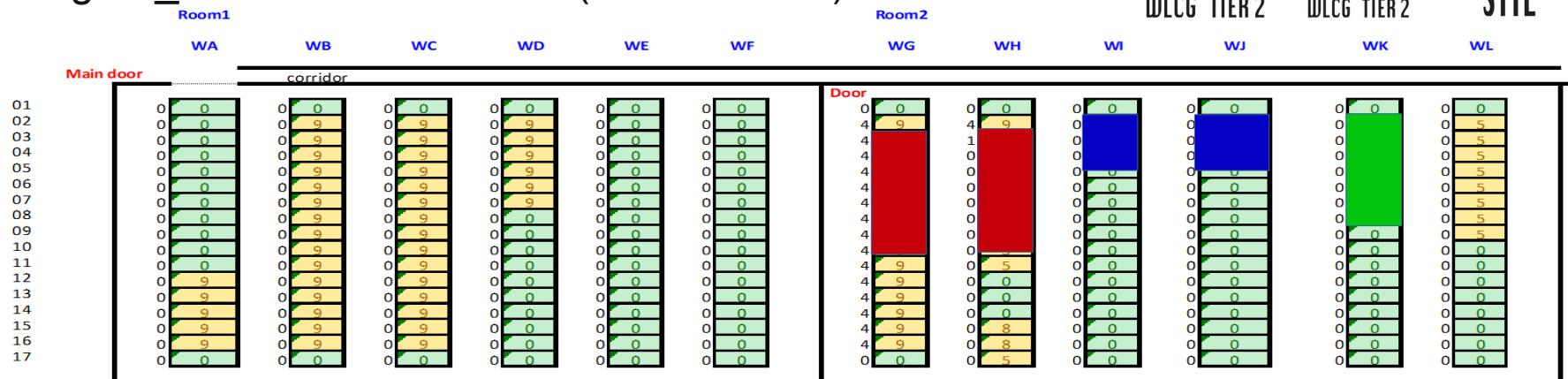
- ✓ Wigner Analysis Facility (Wigner AF)
- ✓ Wigner GPU Laboratory
- ✓ Wigner_KFKI WLCG T2 Grid (ALICE+CMS)



WSCLAB @ WDC

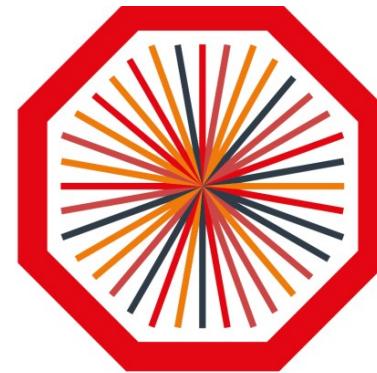
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wigner



ALICE

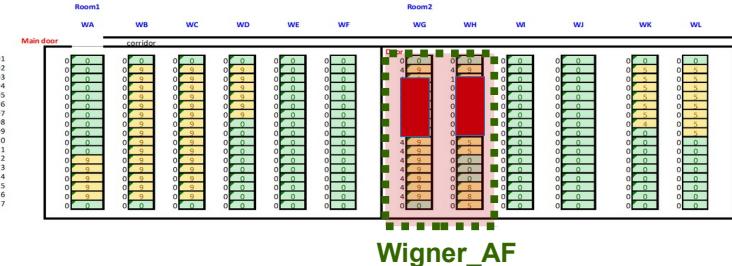
ANALYSIS FACILITY

WIGNER_AF 2022Q2

NEW SPECIALIZED HEP ANALYSIS FACILITY (1ST FOR ALICE)

✓ 1) 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



WIGNER_AF & ALICE T2 2022Q2

PERFORMANCE

- ✓ Wigner_AF_8_core:

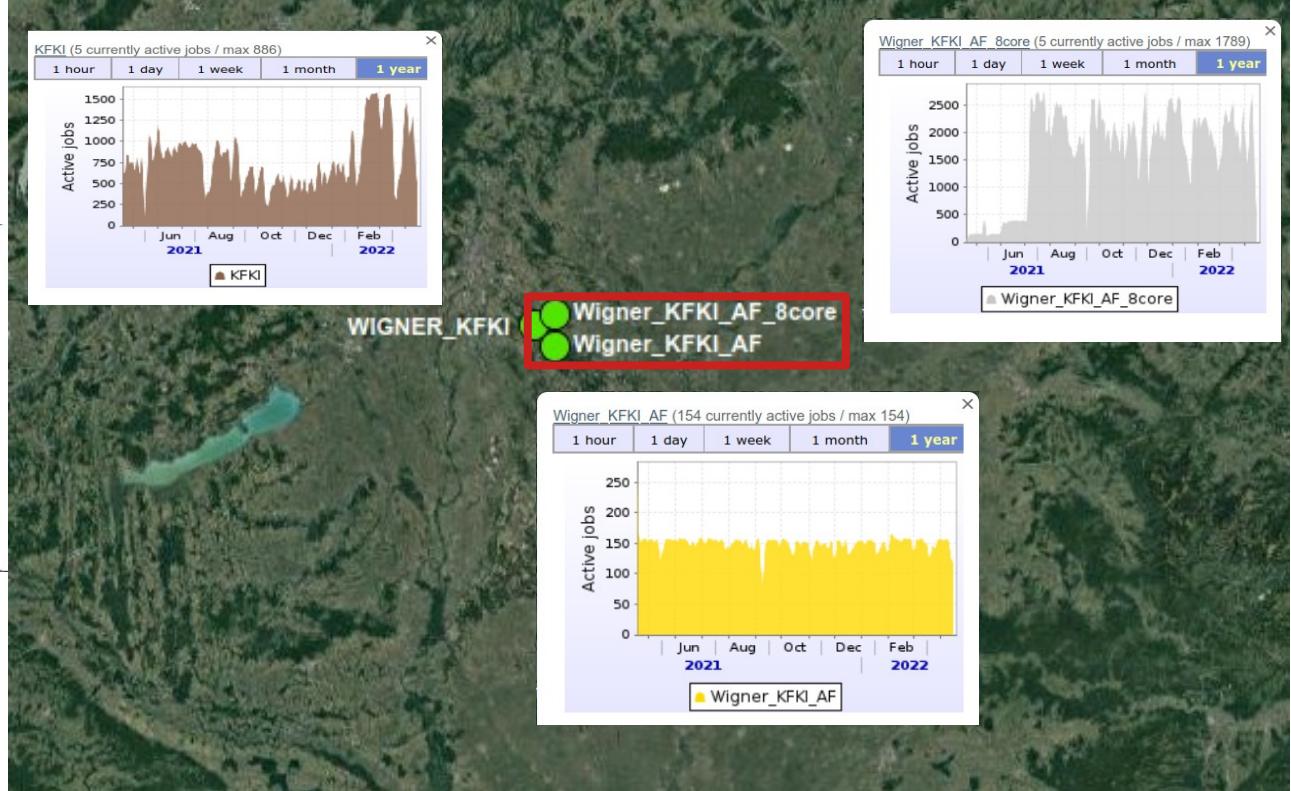
- ✓ Wigner_AF:

- ✓ WIGNER_KFKI:



WIGNER_AF & ALICE T2 2022Q2 PERFORMANCE

✓ Wigner_AF_8_core:

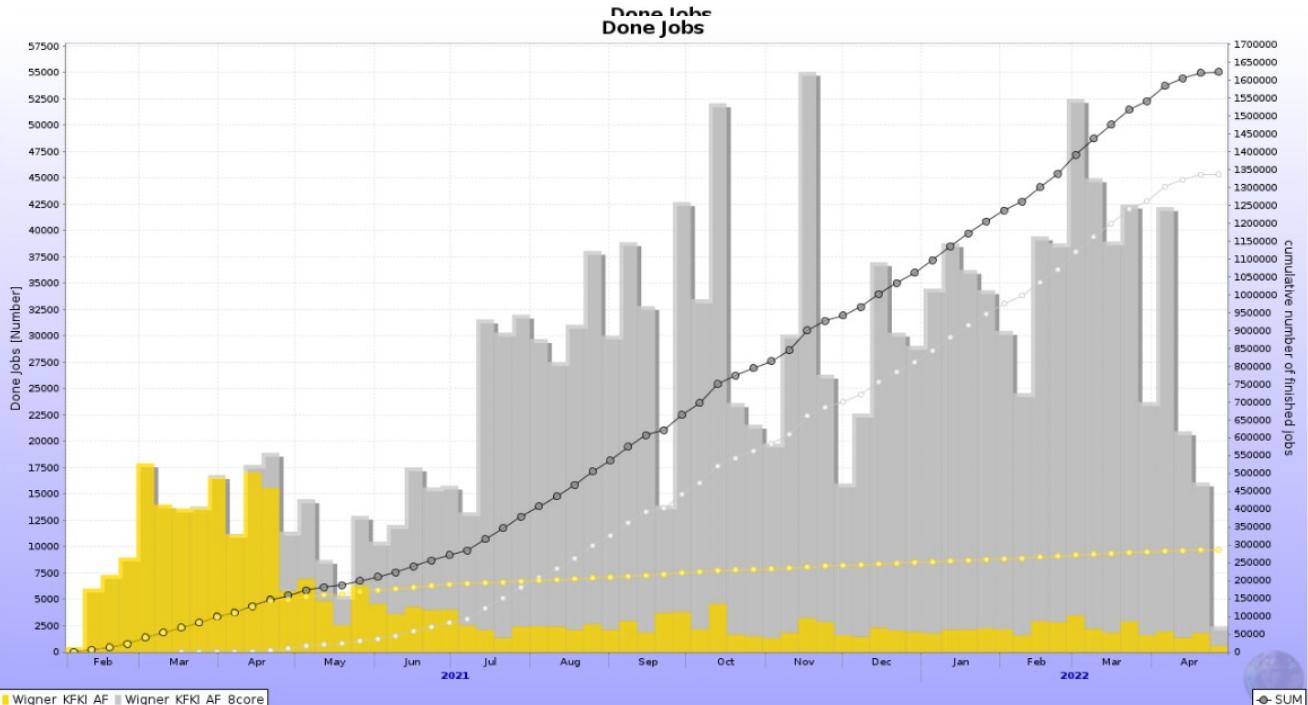


✓ Wigner_AF:

✓ WIGNER_KFKI:

WIGNER_AF & ALICE T2 2022Q2 PERFORMANCE

✓ Wigner_AF_8_core:



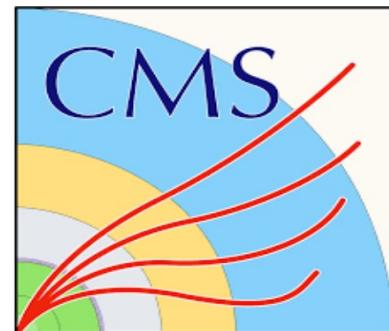
✓ Wigner_AF:

✓ WIGNER_KFKI:



ALICE

WLCG TIER 2



wigner
((O)) VIRGO
WLCG TIER 2



SITE

WIGNER WLCG T2s, 2022Q1

2006: WLCG T2 ALICE & CMS, 2022: VIRGO & EUPRAXIA

✓ 2) International Projects

- CERN ALICE & CMS T2:
 - 3000 vCPU + 2 GB/vcore RAM
 - Usable SE capacity: ~2.0 PB
 - 1-1 single core queue
- VIRGO T2 SITE
 - 1600 vCPU + 5120 TB RAM
 - Usable SE capacity: ~1.0 PB





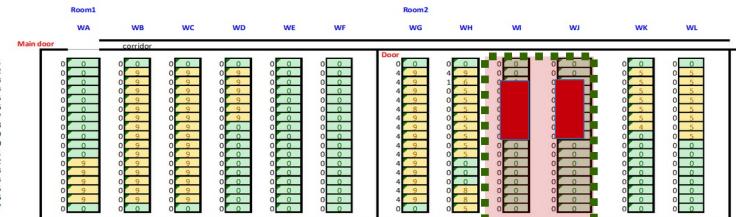
GPU Laboratory

Wigner GPU Laboratory (@WDC)

NEW HARDWARES (IN PROGRESS), HAPPY USERS

✓ 3) 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 (Xilinx Alveo)
- Coming (very) soon
 - EPYC gate server
 - Infiniband switch & cards

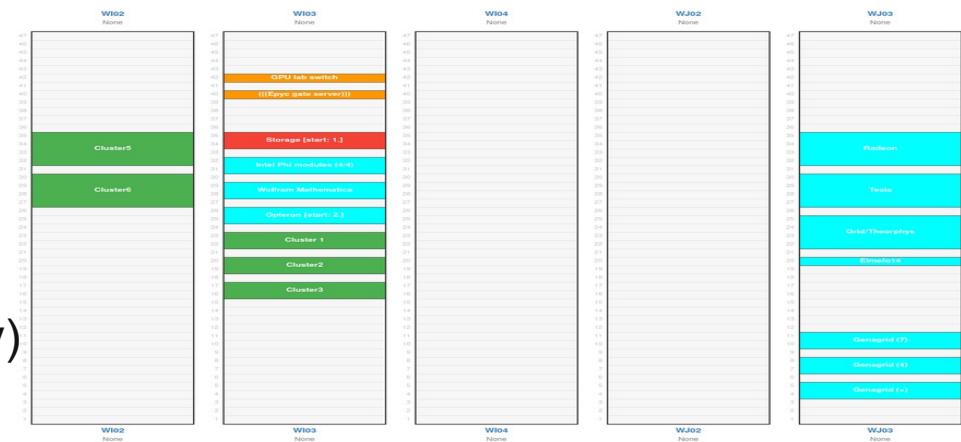


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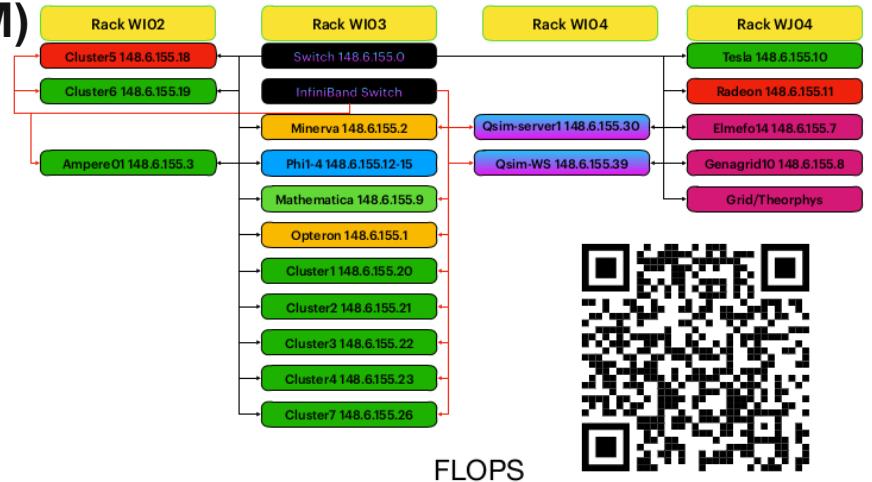


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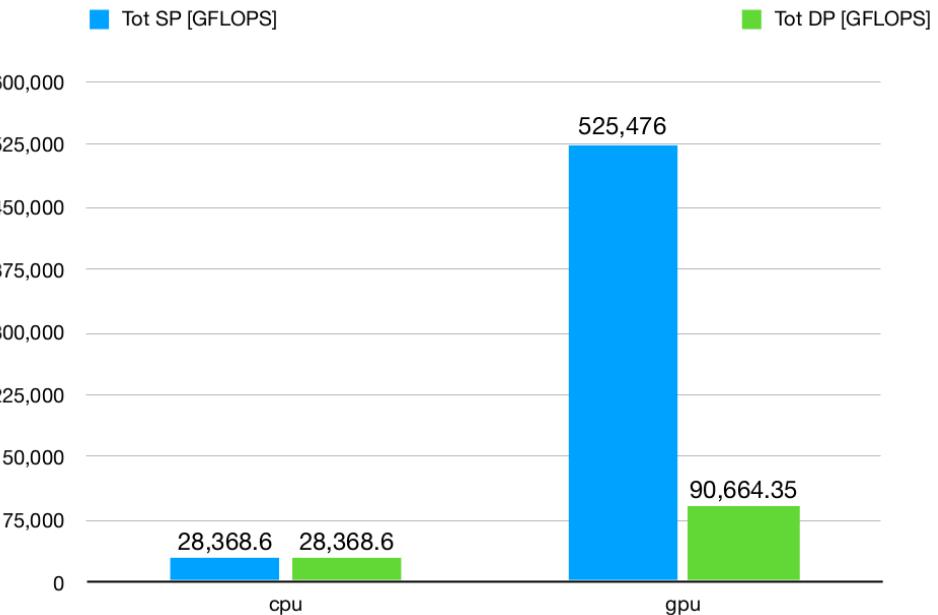
	cpu	gpu	Total Mem
Tot SP [GFLOPS]	28,368.6	525,476	3,056 GB
Tot DP [GFLOPS]	28,368.6	90,664	

Wigner GPU Laboratory (@WDC)

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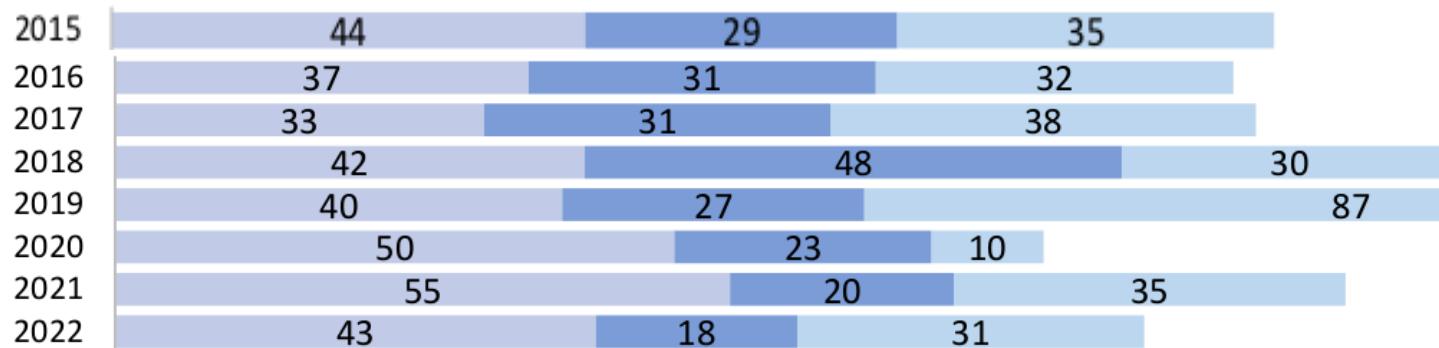
RESULTS>_



WSCLAB in numbers

KNOWLEDGE HUB: GPUDAY.COM

- ✓ 7 Lectures on Modern Computing in Science (will come fall 2022)
- ✓ 12 GPU Days



- ✓ 40 WSCLAB (Wigner GPU Lab) Fellowship (31 finished + 9 running) → new round
- ✓ 33+ industrial & academic partners (Lombiq LTD, Ericsson, Khronos, CERN...)
- ✓ 35+ scientific publications and program codes

WSCLAB's SCIENTIFIC RESULTS

BASED ON THE PROJECTS

✓ Finished Projects

- Projects from various scientific fields:
- Astronomy & Astrophysics, Physics, Biochemistry, Life & Medical Sciences, Etology/Ornitology, Computational Sciences & Quantum Computing



✓ List of Publications

- More than 35 publications & public codes





FUTURE>_

WSCLAB's FUTURE IS IN YOUR HAND

- ✓ **What are the WSCLAB services**
 - Knowledge hub for scientific computing solutions
 - Dedicated GPU & FPGA server hosting & services
 - Tutorial series & teaching
 - Advising highly-parallel computing
 - PhD/PostDoc projects

- ✓ **How to apply**
 - Visit wsclab.wigner.hu

Grant Opportunity

The GPU-Lab wishes to provide an opportunity for researchers to produce academic output with the Lab's monetary, infrastructural and technical support. Applications must always aim on publishing the achieved results.

[APPLICATION](#) [WE OFFER](#)

The application must contain a CV with emphasis on the scientific field knowledge and the programming experiences and a detailed plan of the proposed research project in not more than 2 pages detailing the following points:

- Project title and abstract in English
- Short introduction to the scientific problem
- Weekly plan breakdown
- CPU/GPU and FPGA time and development/user support needs
- Knowledge and experience in programming languages and parallel computing technologies
- Publication and other scientific outcome of the project



WSCLAB's FUTURE

PLANS FOR THE FUTURE

✓ **Short timescale**

- Finishing the running projects & make them publish
- New WSCLAB Grants for young scientists at 2022Q3
- Lectures on Modern Computing in Science series (FPGA) → fall 2022

✓ **Intermediate timescale**

- 100Gbps connection to GEANT network

✓ **Long range plan**

- Closely related to the KIFÜ's LEVENTE project & Quantum Computing



STREAM
High Performance Computing



Cerntech



IN2P3
INSTITUT NATIONAL DE PHYSIQUE NUCLÉAIRE
ET DE PHYSIQUE DES PARTICULES



epam



ELKH | Eötvös Loránd
Research Network



K H R O N O S
GROUP
CONNECTING SOFTWARE TO SILICON

SZÉCHENYI 2020

ERICSSON



UNIVERSITY OF
OXFORD





THX>_





BACKUP> _

Wigner GPU Laboratory (@WDC)

HARDWARE DETAILS

		db	Single Precision [GFLOPS]	Double Precision [GFLOPS]	Tot SP [GFLOPS]	Tot DP [GFLOPS]
CPU	AMD EPYC 7742	2	2,513		2,513	5,026.0
GPU	NVIDIA A100-SXM4 HBM2e 80GB	8	19,490.00		9,746.00	155,920.00
Memory	64GB Samsung 3200MHz DDR4 ECC Registered DIMM	32	64 GB			sum: 2,048 GB
Modell	Supermicro A+ Server 4124GO-NART+					
Alaptop	H12DGO-6					

Qsim-server1

		db	Single Precision [GFLOPS]	Double Precision [GFLOPS]	Tot SP [GFLOPS]	Tot DP [GFLOPS]
Alaptop	GIGABYTE MZ92-FS0-00					
CPU	AMD EPYC 7543	2	1433.6		1433.6	2,867.2
FPGA	Maxeler FPGA (Xilinx Alveo U250)	2	2,035		2,035	4,071
Memory	16GB Micron 3200MHz DDR4 ECC RDIMM	16	16 GB			sum: 256 GB

Qsim-workstation

		db	Single Precision [GFLOPS]	Double Precision [GFLOPS]	Tot SP [GFLOPS]	Tot DP [GFLOPS]
Alaptop	Supermicro M12SWA-TF					
CPU	AMD Ryzen Threadripper PRO 3955WX	1	998.4		998.4	998.4
FPGA	Maxeler FPGA (Xilinx Alveo U250)	1	2,035		2,035	2,035
Memory	16GB SK Hynix 3200MHz DDR4 ECC RDIMM	4	16 GB			sum: 64 GB

Wigner GPU Laboratory (@WDC)

HARDWARE DETAILS

		db	Single Precision [GFLOPS]	Double Precision [GFLOPS]	Tot SP [GFLOPS]	Tot DP [GFLOPS]
Alaplap	ESC8000 G4					
CPU	Intel® Xeon Gold 5122	2	460.8	460.8	921.6	921.6
GPU	AMD Radeon RX Vega 64	6	8,286	518	49,716	3,108
Memory	16GB Micron DDR4 2666MHz ECC	12	16 GB		sum:	192 GB

Cluster 6

		db	Single Precision [GFLOPS]	Double Precision [GFLOPS]	Tot SP [GFLOPS]	Tot DP [GFLOPS]
Alaplap	ESC8000 G4					
CPU	Intel® Xeon Gold 5122s	2	460.8	460.8	921.6	921.6
GPU	NVIDIA Tesla T4	8	8,141	254	65,128	2,035
Memory	16GB Micron DDR4 2666MHz ECC	12	16 GB		sum:	192 GB

Cluster 7

		db	Single Precision [GFLOPS]	Double Precision [GFLOPS]	Tot SP [GFLOPS]	Tot DP [GFLOPS]
Alaplap	4124GS-TNR					
CPU	AMD EPYC™ 7302	2	768.0	768.0	1,536.0	1,536.0
GPU	NVIDIA® A2	8	4,531.0	70.8	36,248.0	566.4
Memory	16GB Micron 3200MHz DDR4 ECC RDIMM	16	16 GB		sum:	256 GB

Wigner GPU Laboratory (@WDC)

HARDWARE DETAILS

Phi 1 – 4

		db	Single Precision [GFLOPS]	Double Precision [GFLOPS]	Tot SP [GFLOPS]	Tot DP [GFLOPS]
Alaplap	Intel® Xeon Server Compute Module					
CPU	Intel® Xeon 7250		3046	3046	12,184.0	12,184.0
Memory	16GB Micron DDR4 2666MHz ECC	6	8GB		sum:	48 GB

Mathematica

		db	Single Precision [GFLOPS]	Double Precision [GFLOPS]	Tot SP [GFLOPS]	Tot DP [GFLOPS]
Alaplap	ESC4000 G4S					
CPU	AMD EPYC 7502P	1	1,585.0	1,585.0	1,585.0	1,585.0
GPU	NVIDIA GeForce GTX 980 Graphics	2	4,612	144	9,224	288
	Nvidia GeForce GTX 1080 Ti	2	11,340	354	22,680	709
Memory	32GB Kingston 3200MHz DDR4 ECC Reg CL22 DIMM	8	32 GB		sum:	256 GB

		db	Single Precision [GFLOPS]	Double Precision [GFLOPS]	Tot SP [GFLOPS]	Tot DP [GFLOPS]
Alaplap	ASUS RS924A-E6/RS8					
CPU	AMD Opteron™ 6376	4	294.3	294.3	1,177.2	1,177.2
GPU	AMD Radeon R9 270X Graphics	2	2,560	160	5,120	320
Memory	32GB 1333MHz DDR3L ECC Reg CL9 DIMM	4	32 GB		sum:	128

EPYC Kapugép

		db	Single Precision [GFLOPS]	Double Precision [GFLOPS]	Tot SP [GFLOPS]	Tot DP [GFLOPS]
Alaplap	Supermicro 1014S-WTRT					
CPU	AMD EPYC™ 7262	1	409.6	409.6	409.6	409.6
Memory	16GB Micron 3200MHz DDR4 ECC RDIMM	8	8 GB		sum:	64