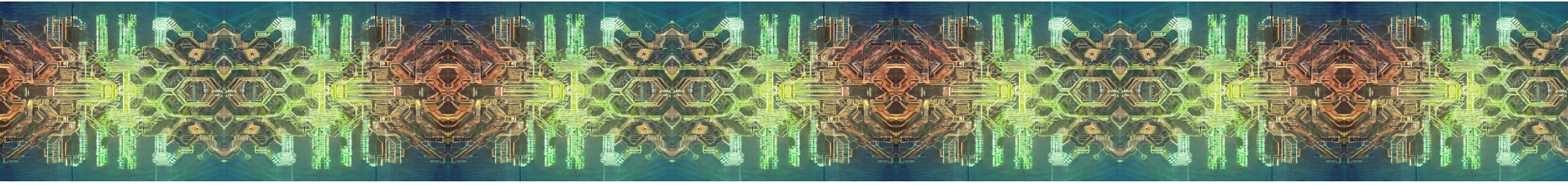
One Lab – Many Project
Review of the WSCLAB's Projects



Gergely Gábor Barnaföldi
WSCLAB, Wigner Reseach Centre for Physics

MTA
Centre
of Excellence

ROLE>_

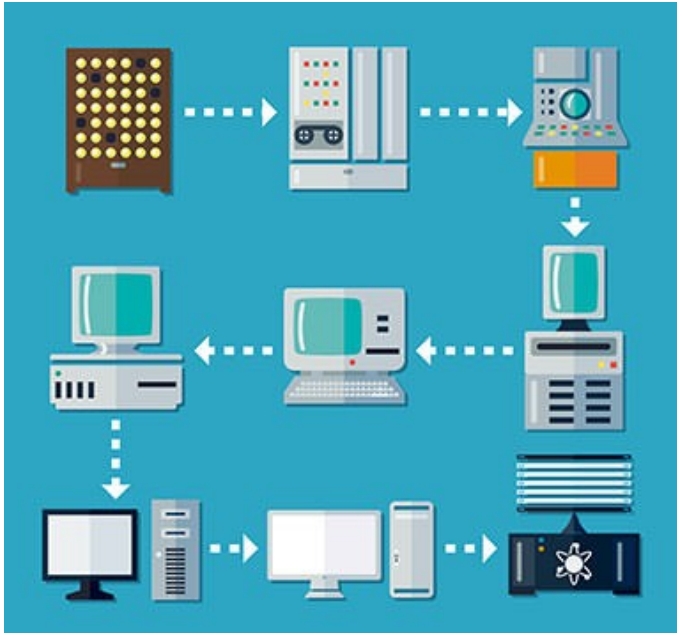
WSCLAB's origin

14 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.

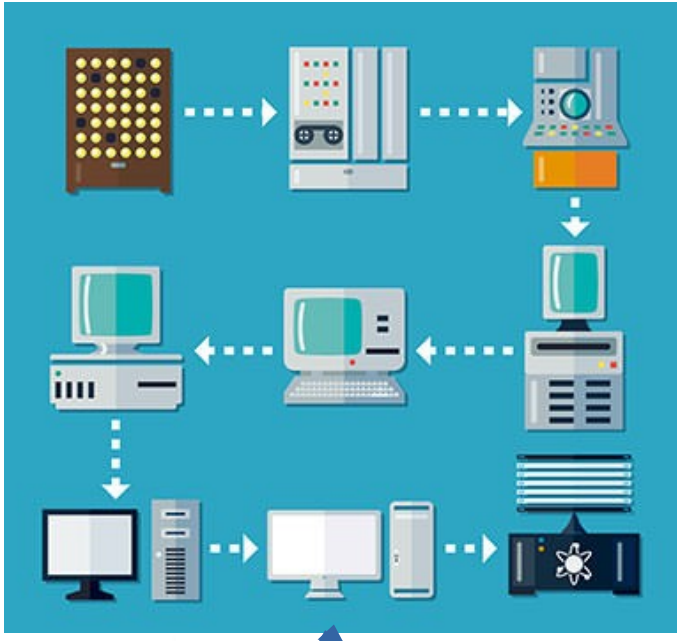
WSCLAB’s role

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



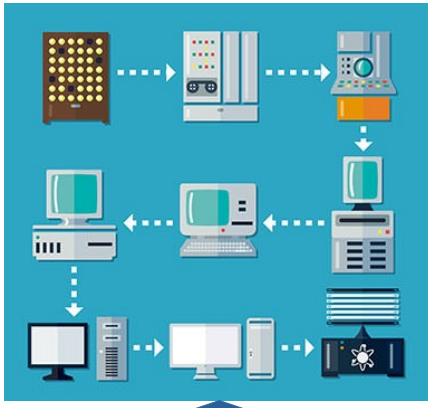
WSCLAB's role

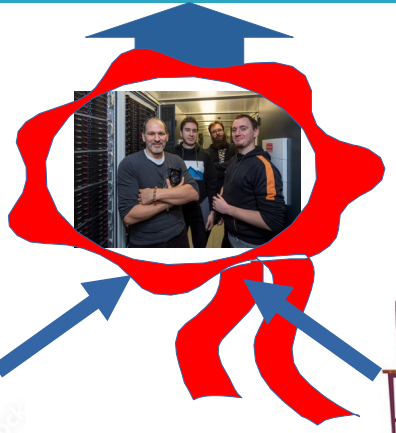
14 YEARS IN PARALLEL COMPUTING (WIGNER GPU LABORATORY) & HPC @ WDC



WSCLAB's role

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





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.

CERTIFICATE of RECOGNITION

This is to certify that

WIGNER Scientific Computing Laboratory (WSCLAB)

is recognized as an

EXCELLENT RESEARCH INFRASTRUCTURE in HUNGARY

in terms of its scientific performance and international collaboration.

Awarded by

the National Research, Development and Innovation Office Budapest, Hungary

on the 16th of December, 2021

Dr. István Szabó
Vice President for Science and International Affairs

NATIONAL RESEARCH, DEVELOPMENT AND INNOVATION OFFICE HUNGARY

WSCLAB's origin

14 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.

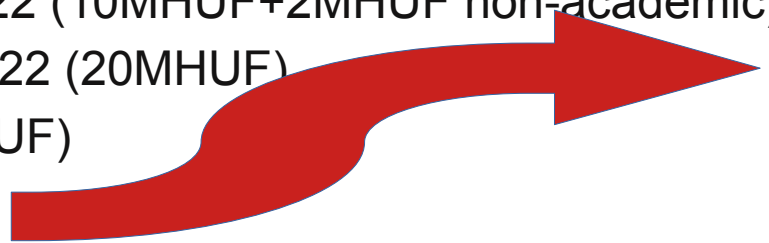
Best place to see the Wigner GPU Lab's activity.

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

WSCLAB Upgrade Projects

2021.12.01-2024.12.06

- ✓ Massively Parallel Classical- and Quantum Computing Simulations in HEP MassivPara@HEP (2020-2.1.1-ED-2021-00179 25MHUF)
  - Massive parallel computing: Wigner_AF + GPULab + HIJING++
  - Quantum Computer simulations (Maxeler FPGA)
- ✓ Wigner RCP & INFRA investments @2021 (100MHUF)
- ✓ Young Researcher's Fellowship @2022 (3MHUF)
- ✓ Wigner GPU Laboratory @2022 (10MHUF+2MHUF non-academic)
- ✓ ALICE + CMS WLCG T2 @2022 (20MHUF)
- ✓ 100GBps links @2023 (20MHUF)



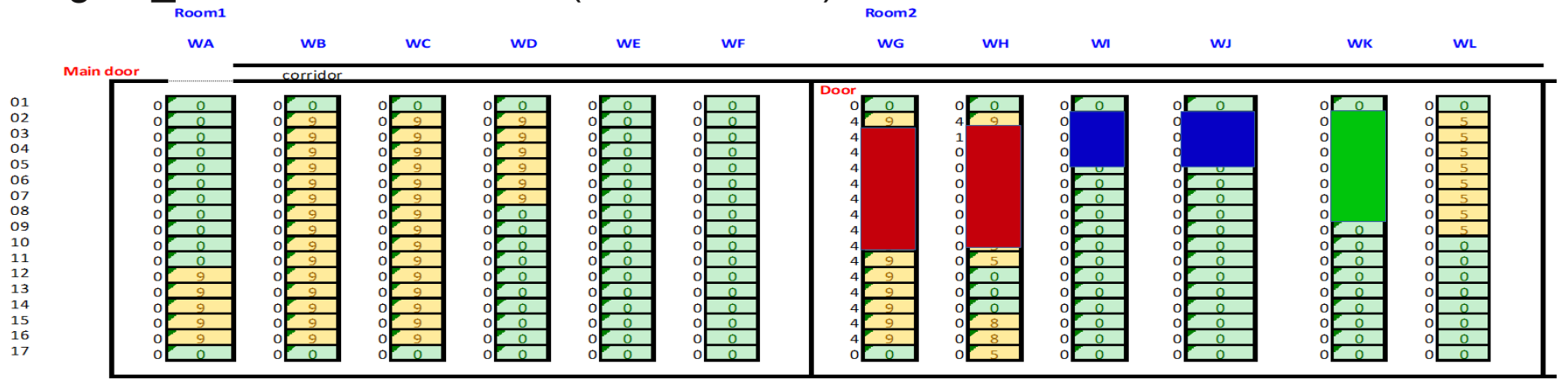
- ✓ Ongoing & finished projects

HARDWARES>_

WSCLAB @ WDC

THE PLACE

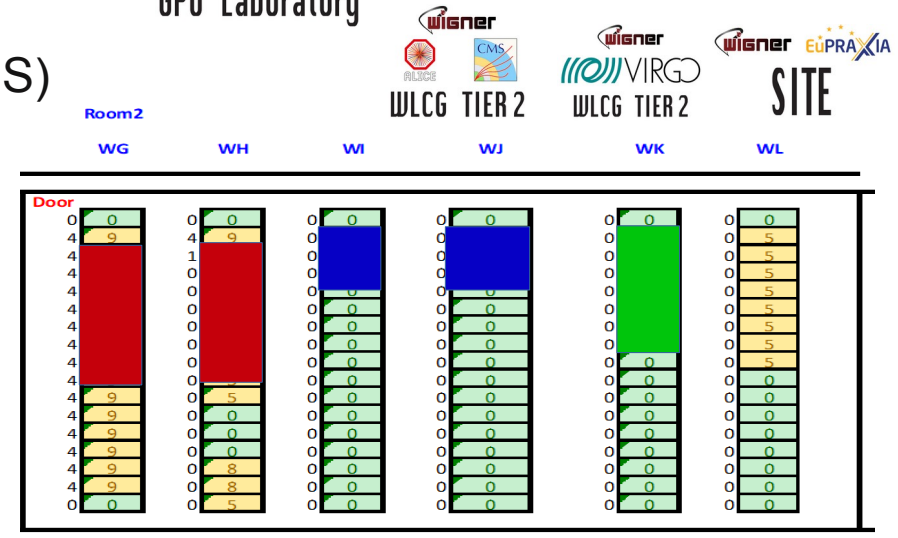
- ✓ Wigner Analysis Facility (Wigner AF)
- ✓ Wigner GPU Laboratory
- ✓ Wigner_KFKI WLCG T2 Grid (ALICE+CMS)

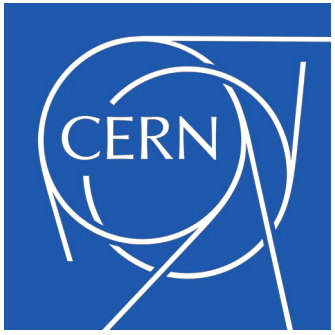


WSCLAB @ WDC

THE PLACE

- ✓ Wigner Analysis Facility (Wigner AF)
- ✓ Wigner GPU Laboratory
- ✓ Wigner_KFKI WLCG T2 Grid (ALICE+CMS)
- ✓ New: LIGO/VIRGO
- ✓ New: EuPRAXIA





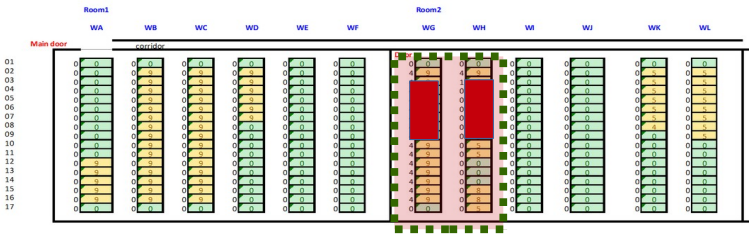
ANALYSIS FACILITY

WIGNER_AF

NEW SPECIALIZED HEP ANALYSIS FACILITY (1ST FOR ALICE)

ALICE ANALYSIS FACILITY

- ✓ **1) HW 9 rack of hardware**
  - SE: EOS config & monitoring
    - 100Gbps link to GEANT
    - 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
    - Pool is shared among two queues, but the single-core queue is limited



Wigner_AF

WIGNER_AF & ALICE T2 2022Q2

PERFORMANCE

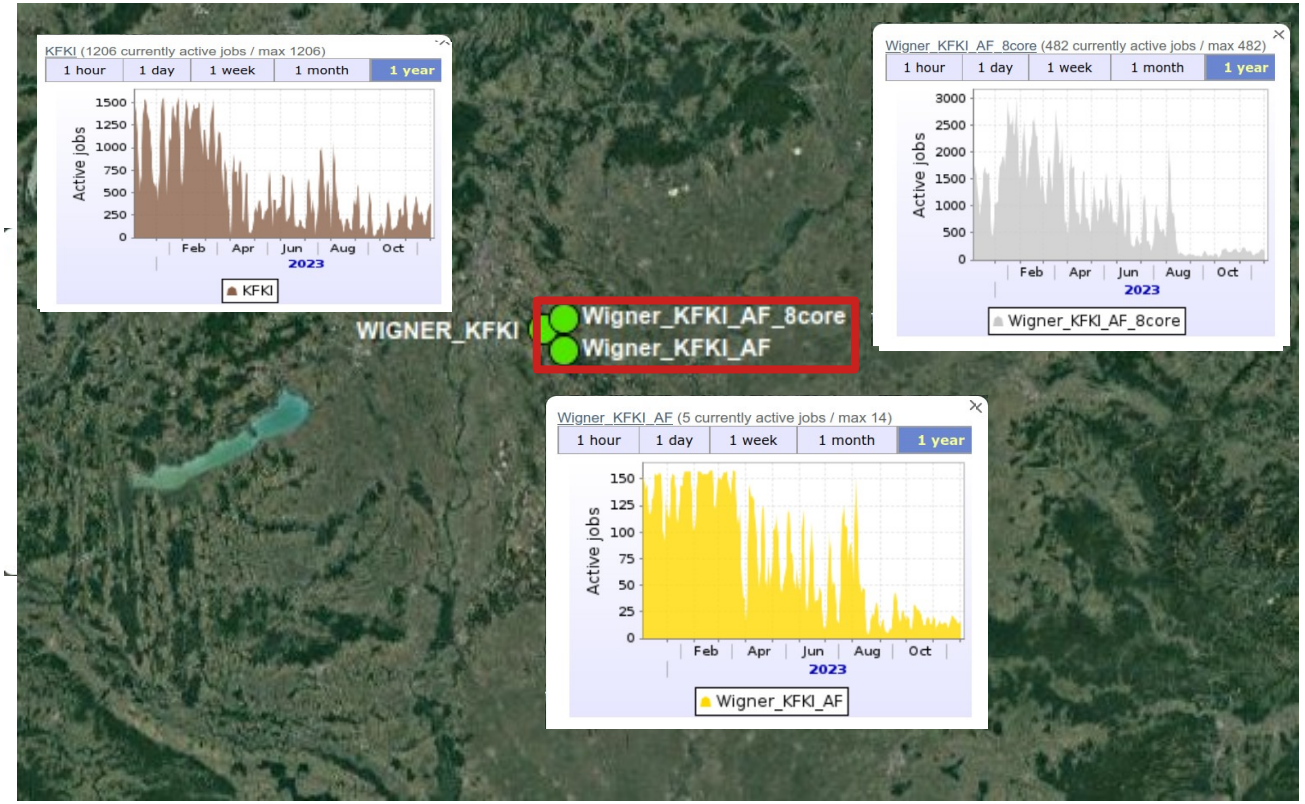
- ✓ Wigner_ AF_8_core:
- ✓ Wigner_AF:
- ✓ WIGNER_KFKI:

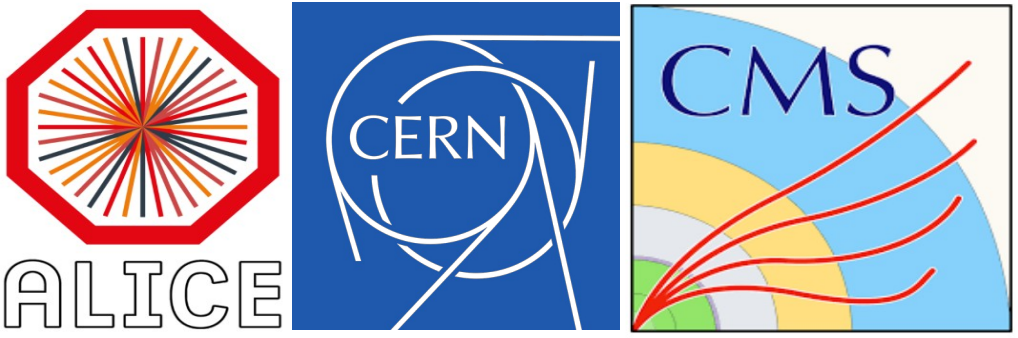
The Wigner ALICE Analysis Facility

Gábor Bíró[1,2], Gergely Gábor Barnaföldi[1], Péter Lévai[1], Latchezar Betev[3] and Jan Fiete Grosse-Oetringhaus[3]

WIGNER_AF & ALICE T2
PERFORMANCE

- ✓ Wigner_ AF_8_core:
- ✓ Wigner_AF:
- ✓ WIGNER_KFKI:





WLCG TIER 2

WLCG TIER 2

SITE

WIGNER WLCG T2s, 2022Q1

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

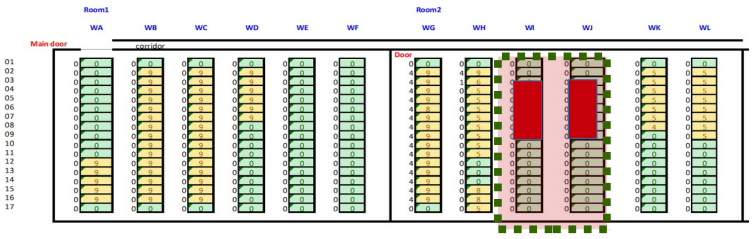
- ✓ **2) International Projects**
  - CERN ALICE & CMS T2:
    - 100 Gbps link to GEANT
    - 3000 vCPU + 2 GB/vcore RAM
    - Usable SE capacity: ~2.0 PB
    - 1-1 single core queue
  - VIRGO T2 SITE
    - 1600 vCPU + 5120 TB RAM
    - Usable SE capacity: ~1.0 PB

GPU Laboratory

Wigner GPU Laboratory (@WDC)
HARDWARES

GPU Laboratory

- ✓ **3) Wigner WSCLAB's GPU Lab picks**
  - 20 TB Storage Element
  - 100 Gbps switch to GEANT
  - Mathematica WN server
  - Supermicro EPYC +8x A100
  - EPYC + 6x Nvidia Tesla T4
  - EPYC + 8xNvidia A2
  - Maxeller 2xFPGA (Xilinx Alveo)
  - EPYC gate server
  - Infiniband switch & cards



Wigner GPU Laboratory

Wigner GPU Laboratory (@WDC)

HARDWARES

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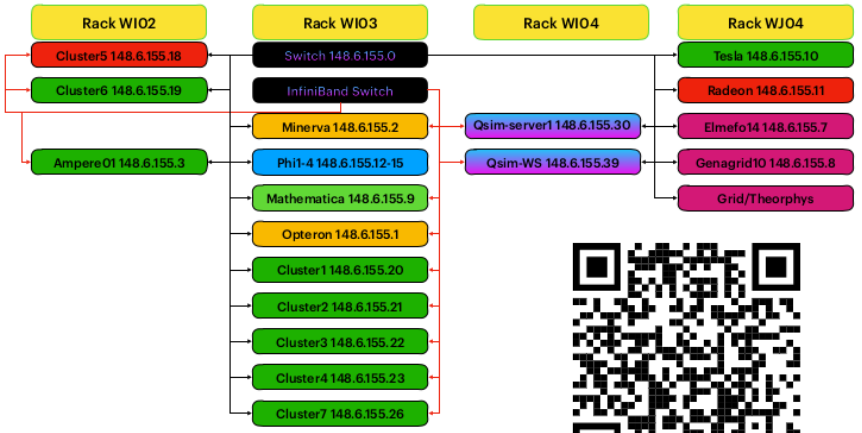

	cpu	gpu	Total Mem
Tot SP [GFLOPS]	28,368.6	525,476	3,056 GB
Tot DP [GFLOPS]	28,368.6	90,664	

Wigner GPU Laboratory (@WDC)
HARDWARES

GPU Laboratory

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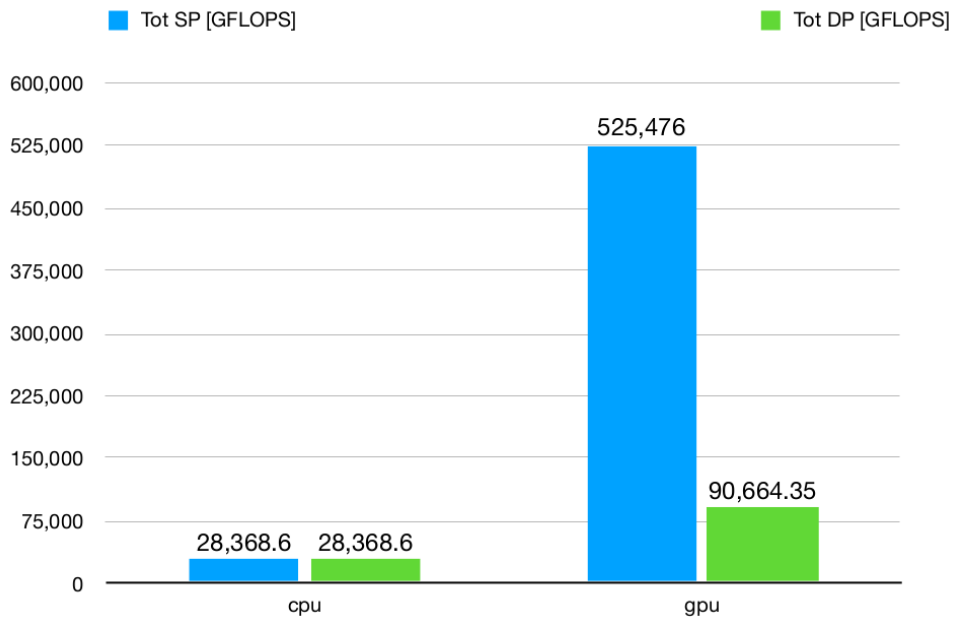


EVENTS>_

WIGNER SCIENTIFIC COMPUTING LABORATORY

GPU DAY 2022

THE FUTURE OF MASSIVE PARALLEL AND QUANTUM COMPUTING

EMERGING ACCELERATOR PLATFORMS

IMAGE PROCESSING, COMPUTER VISION, AND RECONSTRUCTION

INDUSTRIAL APPLICATIONS

GRAPHICS, RENDERING, AND IMAGE SYNTHESIS

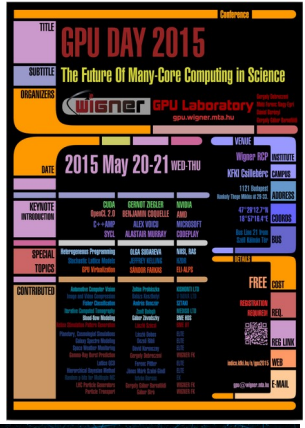
COMPUTING AND VISUALIZATION IN EDUCATION

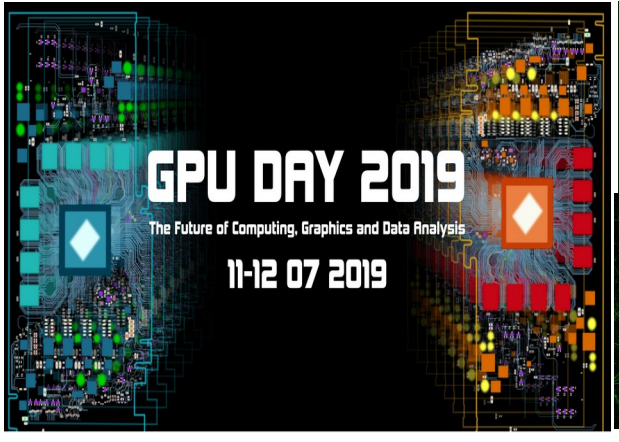
QUANTUM COMPUTING SIMULATION

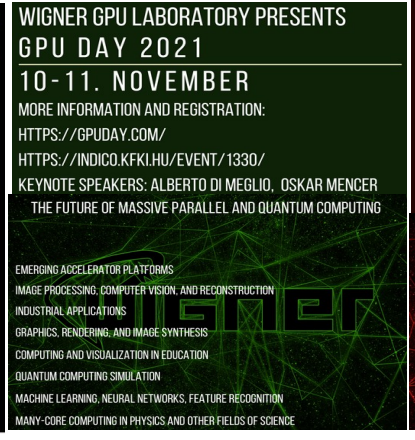
MACHINE LEARNING, NEURAL NETWORKS, FEATURE RECOGNITION

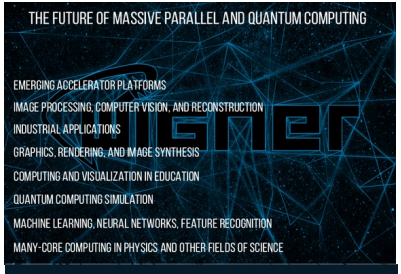
MANY-CORE COMPUTING IN PHYSICS AND OTHER FIELDS OF SCIENCE

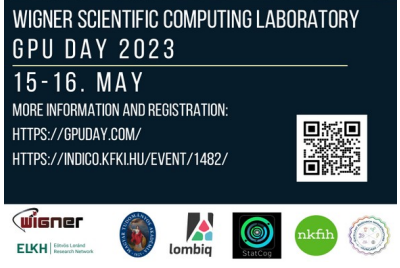
GPU Days so far...



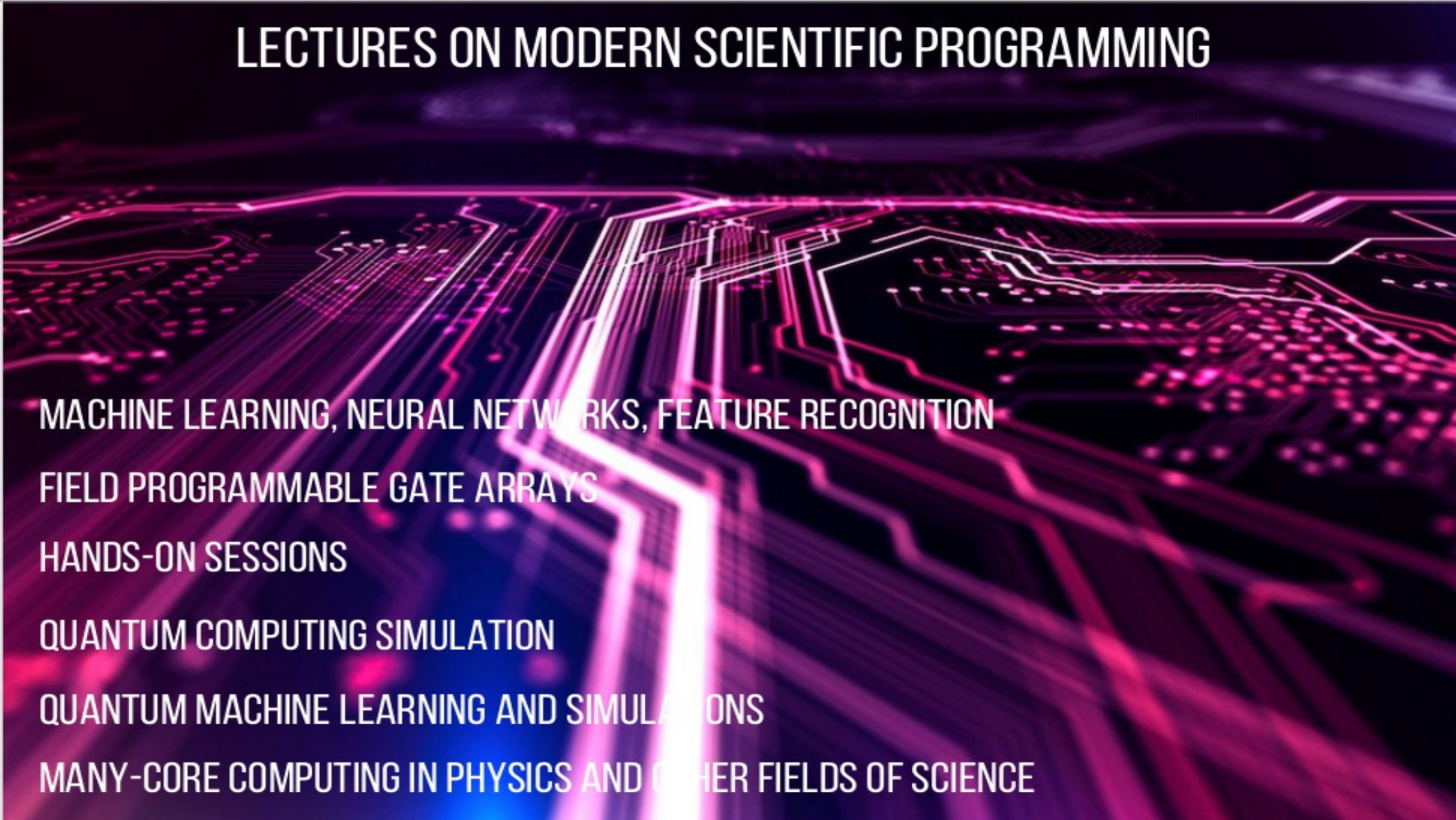








LECTURES ON MODERN SCIENTIFIC PROGRAMMING



MACHINE LEARNING, NEURAL NETWORKS, FEATURE RECOGNITION

FIELD PROGRAMMABLE GATE ARRAYS

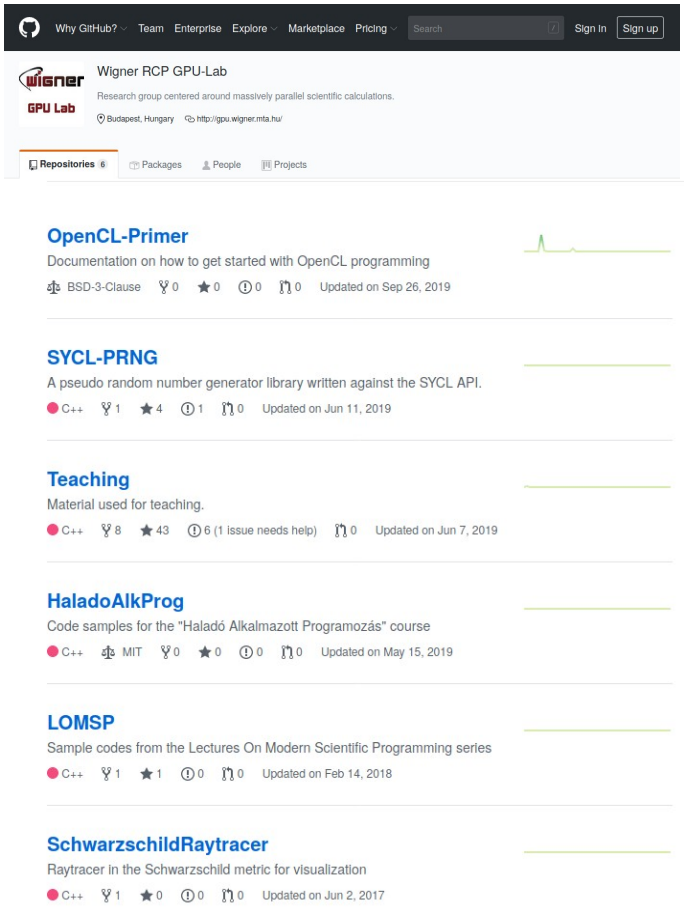
HANDS-ON SESSIONS

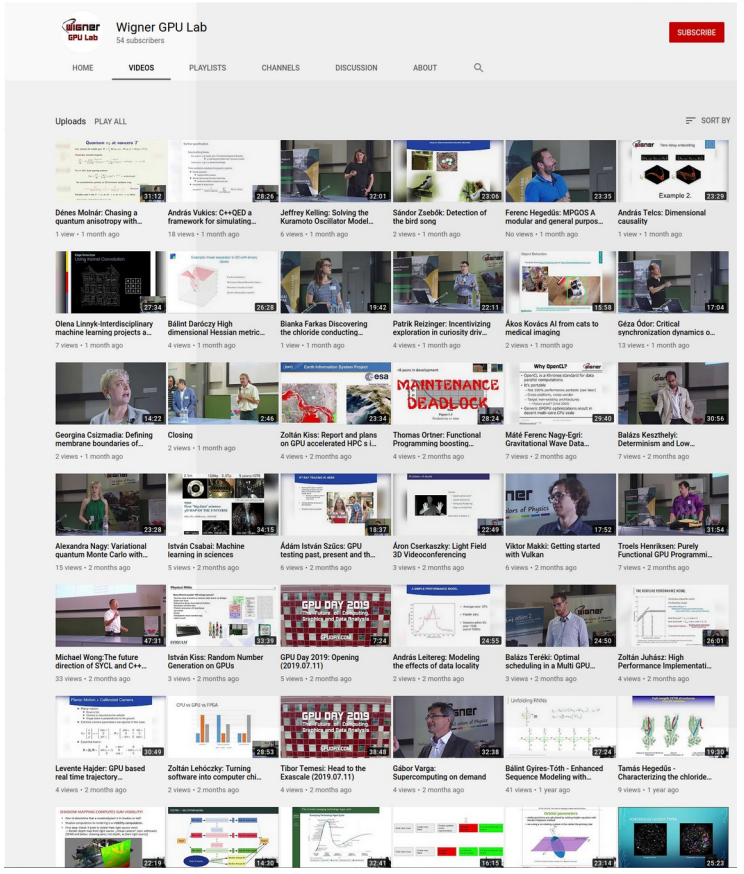
QUANTUM COMPUTING SIMULATION

QUANTUM MACHINE LEARNING AND SIMULATIONS

MANY-CORE COMPUTING IN PHYSICS AND OTHER FIELDS OF SCIENCE

WSCLAB's EDUCATIONAL MATTERS





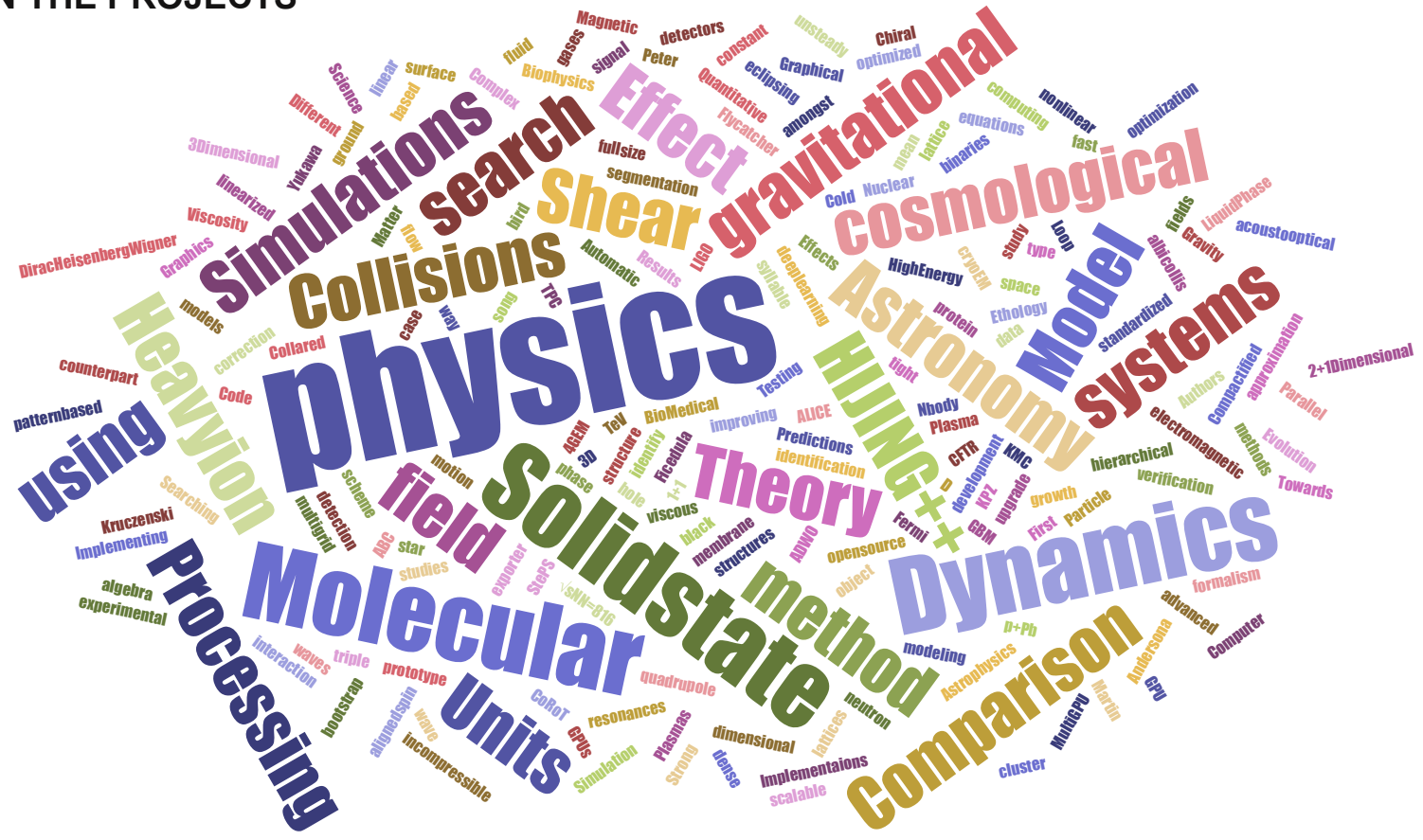
YouTube HU

GitHub

PROJECTS>_

WSCLAB's SCIENTIFIC RESULTS

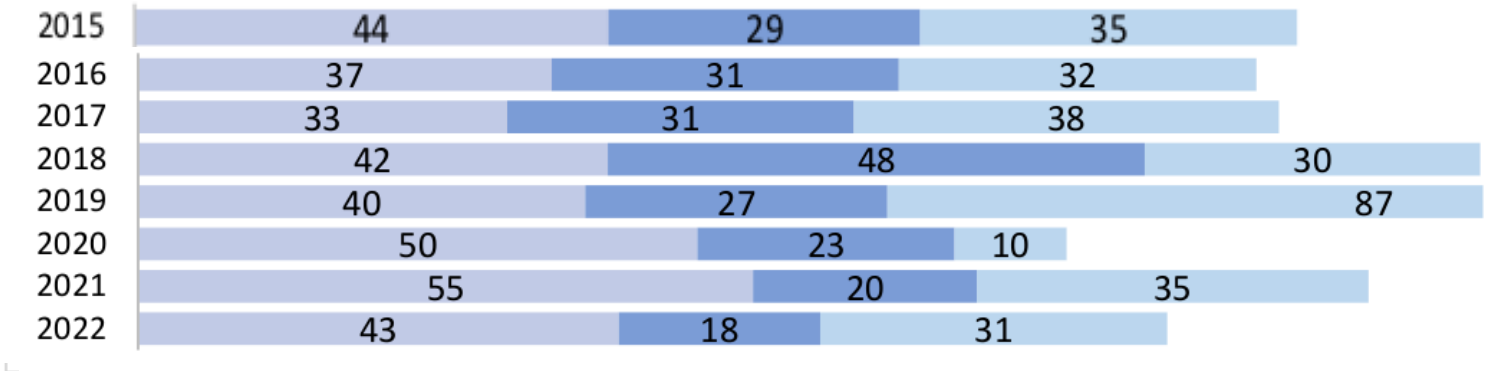
BASED ON THE PROJECTS



WSCLAB in numbers

KNOWLEDGE HUB: GPUDAY.COM

- ✓ 9 Lectures on Modern Computing in Science
- ✓ 13 GPU Days



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

WSCLAB's SCIENTIFIC RESULTS

BASED ON THE PROJECTS

✓ **Finished Projects from various fields**

- Astronomy & Astrophysics (12)
- Physics (15)
- Biochemistry (5)
- Life & Medical Sciences, Etology/Ornitology (5)
- Computational Sciences, Imaging, Simulations (11)
- Quantum Computing (6)

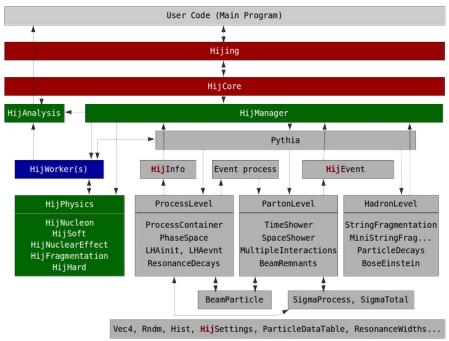
✓ **List of Publications**

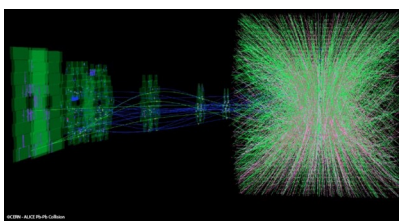
- More than 60 publications & public codes

WSCLAB's SCIENTIFIC PROJECTS

FEW SELECTED ONES

- ✓ Simulating the photo-ionisation of Rubidium atoms
- ✓ **High Performance Computing for Nanofusion**
- ✓ High performance Monte Carlo simulations of high-energy heavy-ion collisions
- ✓ **Modelling non-linear optics by machine learning techniques**
- ✓ Generation of Gravitational Wave Signals with Parallel methods
- ✓ Studying Hadronization by Machine Learning Techniques
- ✓ Modelling of polygons on rotating fluid surface with the parameters of real-life experiments

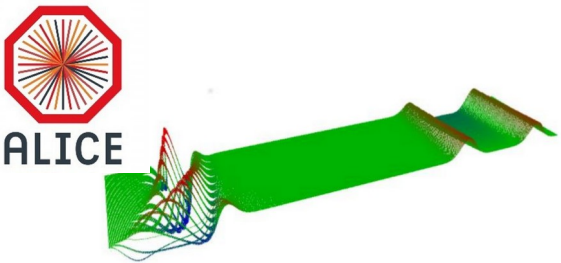


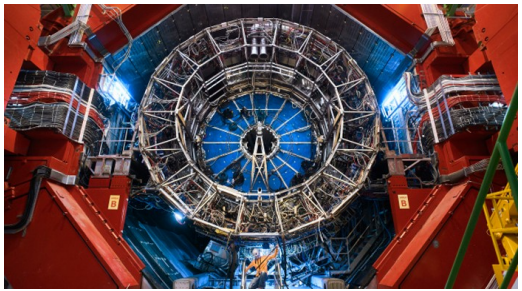


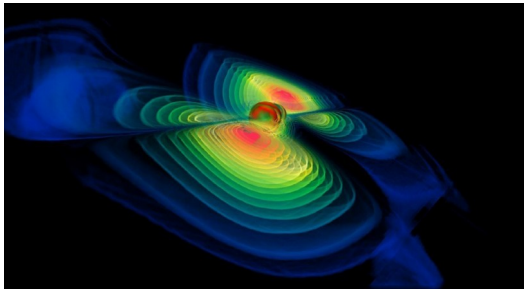
WSCLAB's SCIENTIFIC PROJECTS

PHYSICS (15)

- ✓ Optimalization and Development of High-performance Computing pipeline to search for gravitational radiation from rotating NS by reans of GPU-based Hardware Accelerators
- ✓ ALICE TCP GEM QA – GPU-accelerated image analysis
- ✓ Viscous corrections from linearized Boltzmann transport
- ✓ Parallelized Transport and Corrections to Equilibrium Phase Space Distributions
- ✓ Numerical Studies of Lattice Loop Equations in Pure Gauge Theory
- ✓ Construction of known waveforms – like OJ287 – with PYCBC
- ✓ Detection estimates for gravitational binary sources



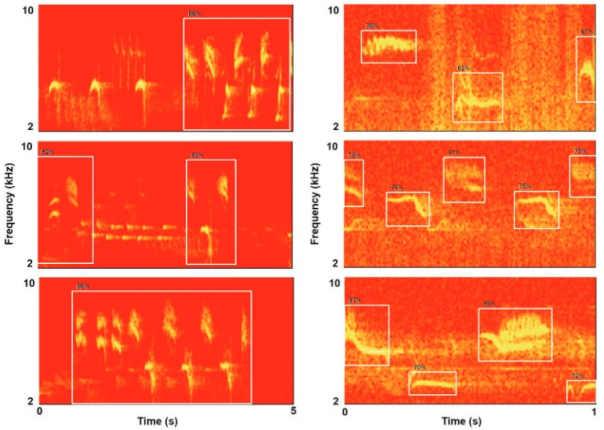


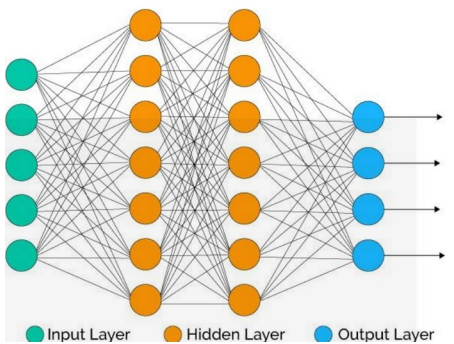


WSCLAB's SCIENTIFIC PROJECTS

LIFE SCIENCES, CHEMISTRY, ORNITOLOGY (5)

- ✓ **Analysis of the spatial structure of SARS-CoV-2 protein using machine learning methods**
- ✓ Quantum chemical study of the hydrolysis of oxidized endogenous psychedelic N,N-dimethyltryptamine
- ✓ N,N-dimethyltryptamine metabolism by the monoamine oxidase enzyme-A
- ✓ In silico studies to uncover the effect of CFTR mutants causing cystic fibrosis
- ✓ **Detection of the songs of collared flycatcher (Ficedula albicollis) with the help of deep neural networks**

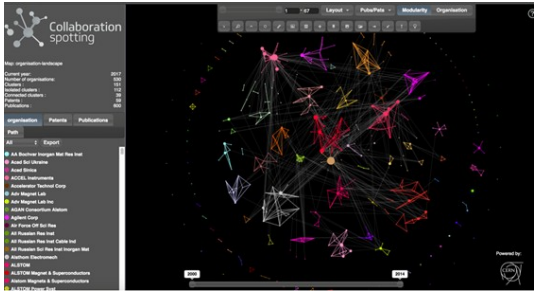


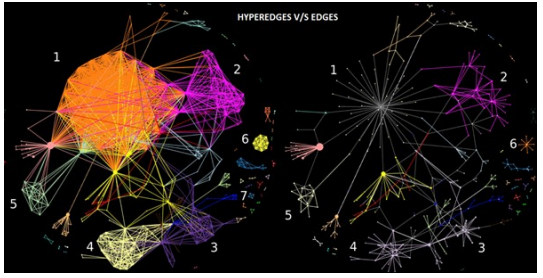


WSCLAB's SCIENTIFIC PROJECTS

IMAGING, SIMULATIONS, COMPUTING (11)

- ✓ 3D iterative image reconstruction software developed for proton computed tomography imaging
- ✓ Biasing the GUARDYAN GPU-based Monte Carlo code using space-, energy- and angle-dependent adjoint function
- ✓ **Evaluation of proton tomography measurements with neural networks for hadron therapy**
- ✓ Stochastic causality
- ✓ Implementing Hastlayer support for Xilinx SoC Zynq FPGA family I. And II.

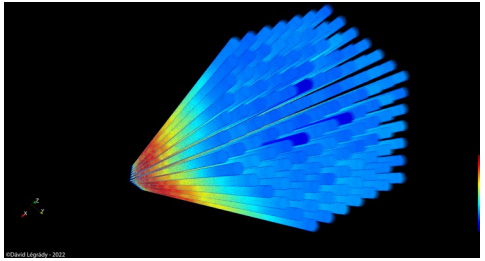


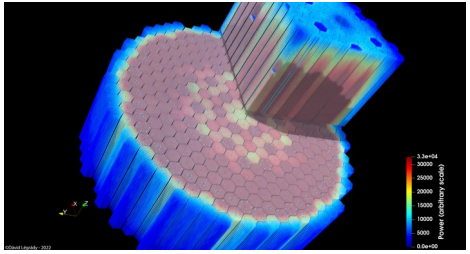


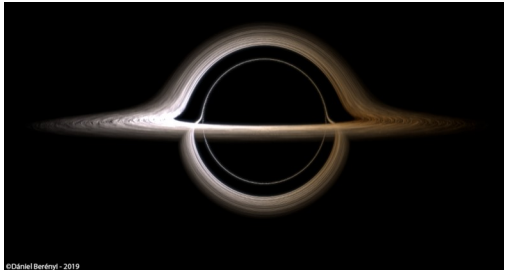
WSCLAB's SCIENTIFIC PROJECTS

IMAGING, SIMULATIONS, COMPUTING (11)

- ✓ **Full Core Pin-Level VVER-440 Simulation of a Rod Drop Experiment with the GPU-Based Monte Carlo Code GUARDYAN**
- ✓ Eötvös balance camera photo evaluation
- ✓ Implementing support for high-performance Microsoft Catapult FPGAs in the Hastlayer .NET high-level synthesis toolbox
- ✓ **Graph visualization of the human brain's structural and functional organization**
- ✓ Data processing algorithm development for parallel architectures







WSCLAB's SCIENTIFIC PROJECTS

ASTRONOMY, ASTROPHYSICS, COSMOLOGY (12)

- ✓ **Examination of seasonal polar ice cap edge in the southern hemisphere of Mars**
- ✓ A dynamical survey of trans-Neptunian space I. mean motion resonances with Neptune
- ✓ A dynamical survey of the trans-Neptunian space II.: Diffusion and stability
- ✓ Entropy based stability analysis of planetary systems retrieved from scalar time series
- ✓ **Shock waves in partially ionised prominence plasmas**
- ✓ Statistical study of mean motion resonances and physical properties of Hungarian asteroids using FAIR
- ✓ The evolution of sunspots I. Lifetime and asymmetric evolution

WSCLAB's SCIENTIFIC PROJECTS

ASTRONOMY, ASTROPHYSICS, COSMOLOGY (12)

- ✓ **Study of Cosmological Large Scale Structure with GPU-accelerated N-body Simulations**
- ✓ Light curve modeling of close binary and multiple systems
- ✓ Investigation of the K2 Mission's Star System's Eclipse Mean Times
- ✓ Large Scale Lightcurve Analysis
- ✓ The study of the effect of the cosmological constant with the GW150914

WSCLAB's SCIENTIFIC PROJECTS

QUANTUM COMPUTING & TECHNOLOGY (6)

- ✓ Polynomial speedup in Torontonian calculation by a scalable recursive algorithm
- ✓ **Highly optimized quantum circuits synthesized via data-flow engines**
- ✓ Efficient quantum gate decomposition via adaptive circuit compression
- ✓ Approaching the theoretical limit in quantum gate decomposition
- ✓ GPU based simulation of strongly correlated quantum systems
- ✓ **Accelerating Quantum Computer Simulators with GPUs**

FUTURE>_

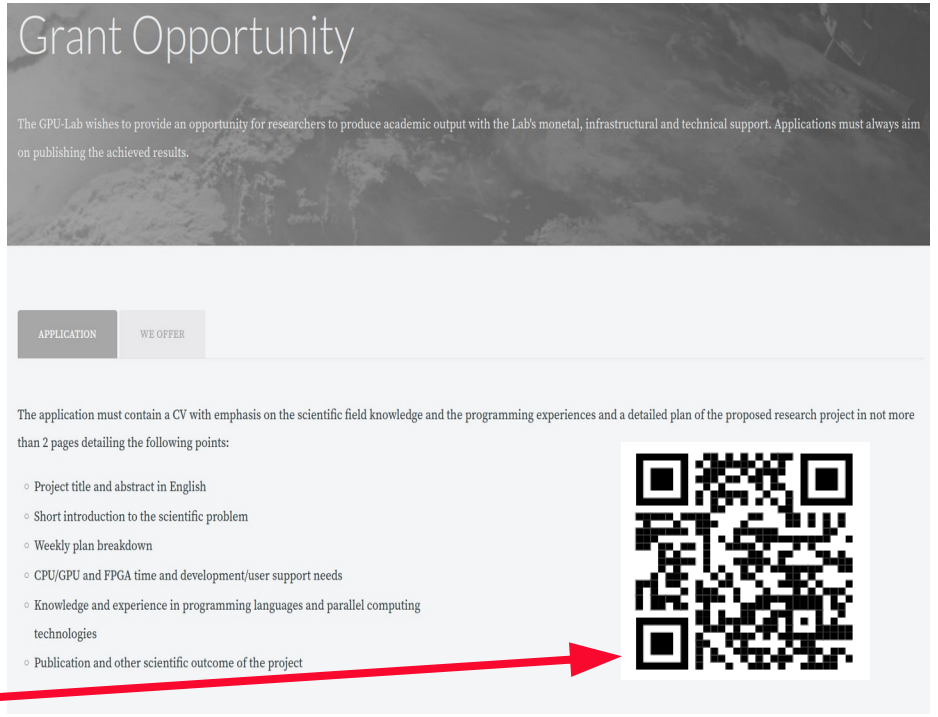
WSCLAB's FUTURE
IS IN YOUR HAND

✓ **What are the WSCLAB services**

- Knowledge hub for scientific computing solutions
- Dedicated GPU & FPGA server hosting & services
- Quantum Computing simulations
- Tutorial series & teaching
- Advising highly-parallel computing
- PhD/PostDoc projects

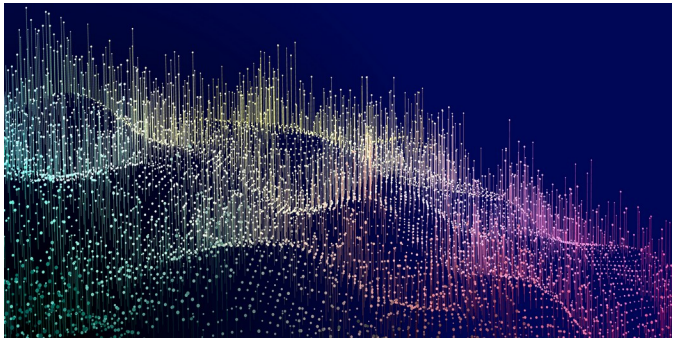
✓ **How to apply**

- Visit wsclab.wigner.hu



WSCLAB's FUTURE

PLANS FOR THE FUTURE



- ✓ **Short timescale**
  - New WSCLAB Grants for young scientists for 2024
  - GPU Day 2024 series (in May/June 2024)
  - Lectures on Modern Computing in Science series (in fall 2024)

- ✓ **Intermediate timescale**
  - Further local HW developments & cloud solutions

- ✓ **Long range plan**
  - Closely related to the EuroHPC LEVENTE project including Quantum Computing & Quantum simulations

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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	5,026.0
GPU	NVIDIA A100-SXM4 HBM2e 80GB	8	19,490.00	9,746.00	155,920.00	77,968.00
Memory	64GB Samsung 3200MHz DDR4 ECC Registered DIMM	32	64 GB		sum:	2,048 GB
Modell	Supermicro A+ Server 4124GO-NART+					
Alaplap	H12DGO-6					

Qsim-server1

		db	Single Precision [GFLOPS]	Double Precision [GFLOPS]	Tot SP [GFLOPS]	Tot DP [GFLOPS]
Alaplap	GIGABYTE MZ92-FS0-00					
CPU	AMD EPYC 7543	2	1433.6	1433.6	2,867.2	2,867.2
FPGA	Maxeler FPGA (Xilinx Alveo U250)	2	2,035	2,035	4,071	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]
Alaplap	Supermicro M12SWA-TF					
CPU	AMD Ryzen Threadripper PRO 3955WX	1	998.4	998.4	998.4	998.4
FPGA	Maxeler FPGA (Xilinx Alveo U250)	1	2,035	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	8 GB		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