WIGNER SCIENTIFIC COMPUTING LABORATORY

GPU DAY 2024

30-31. MAY

MORE INFORMATION AND REGISTRATION:

HTTPS://GPUDAY.COM/

HTTPS://INDICO.KFKI.HU/EVENT/1567/

HUN REN WIGNER

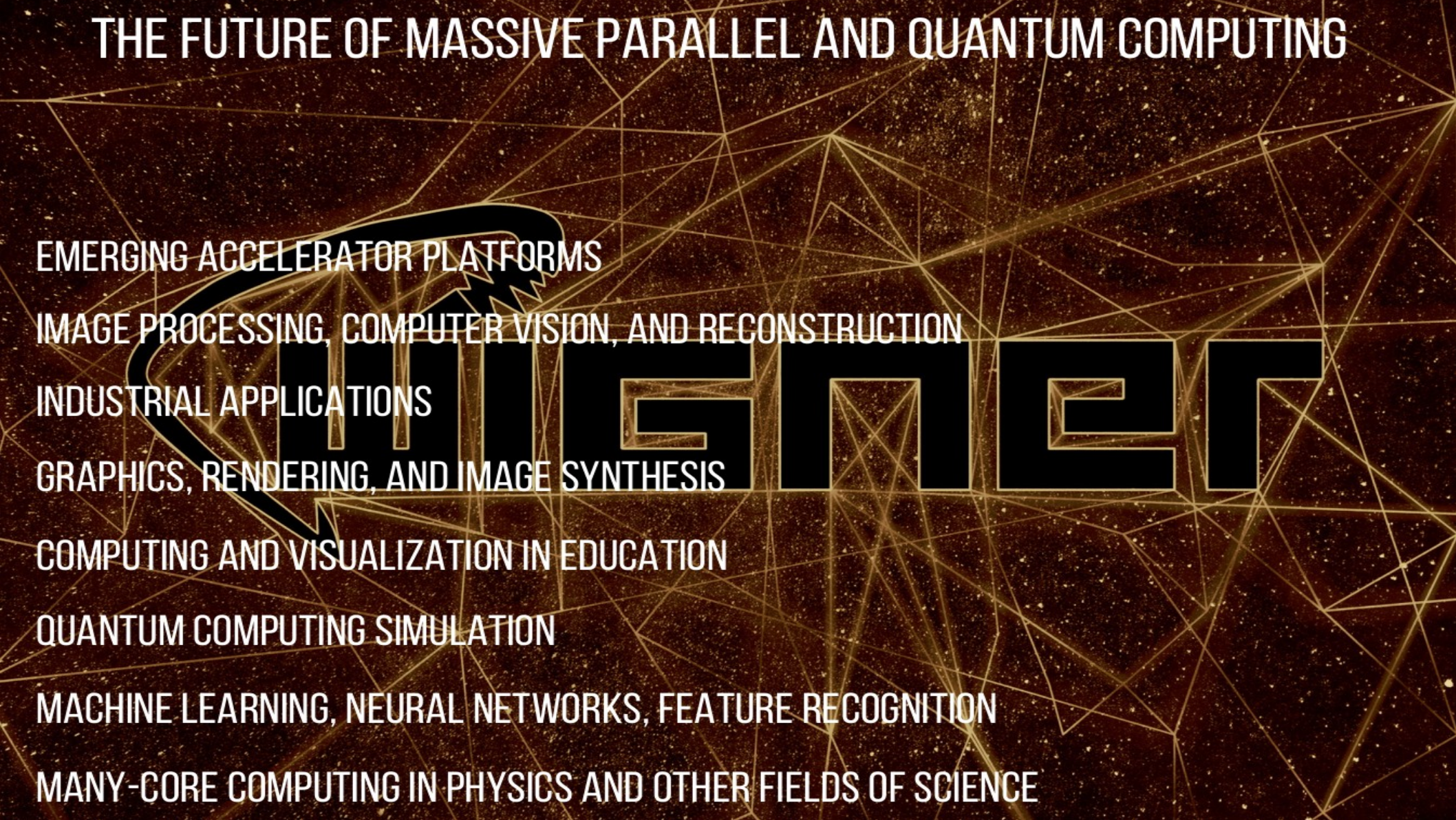
HUN-REN Hungarian Research Network

HPC @hu Kompetencia Központ

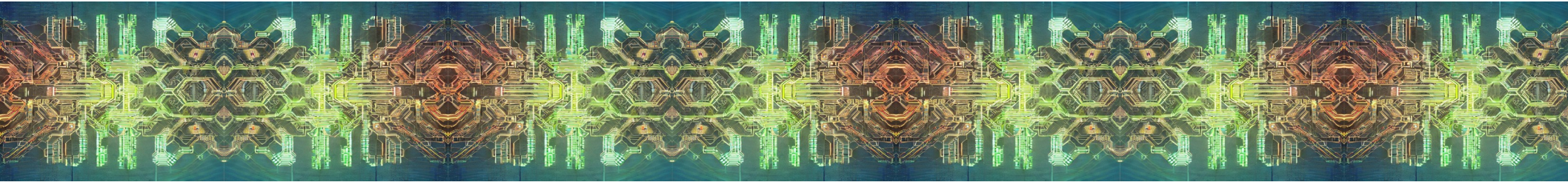
KIFÜ

lombiq

THE FUTURE OF MASSIVE PARALLEL AND QUANTUM COMPUTING



One Lab – Many Project
Review of The WSCLAB



Gergely Gábor Barnaföldi
WSCLAB, HUN-REN Wigner Reseach Centre for Physics

MTA
Centre
of Excellence

ROLE>_

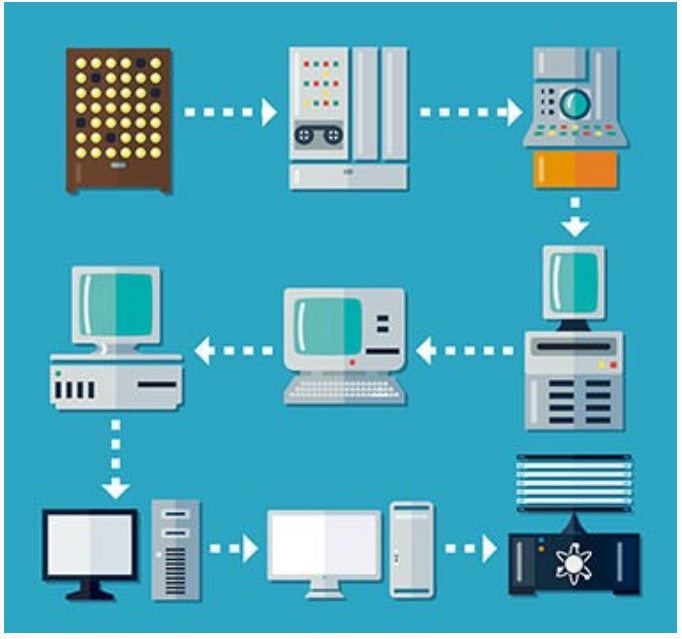
WSCLAB's origin

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.

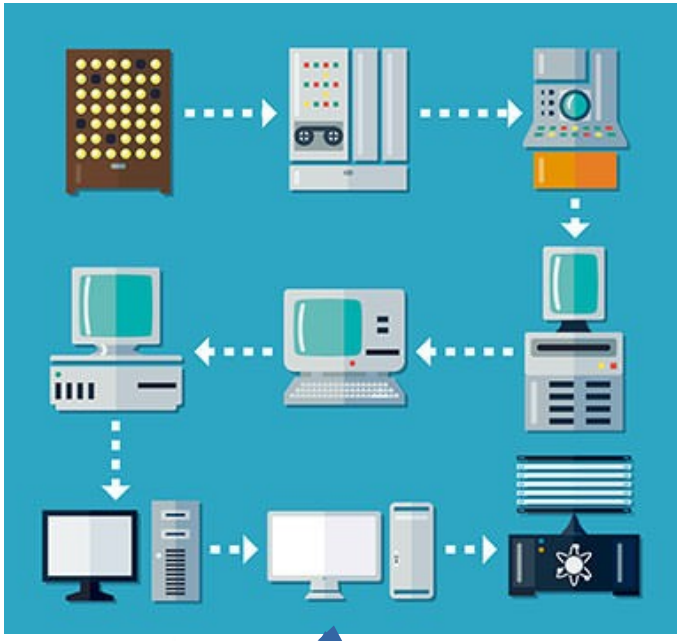
WSCLAB’s role

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



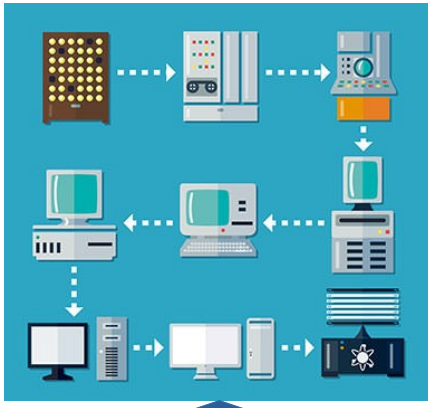
WSCLAB's role

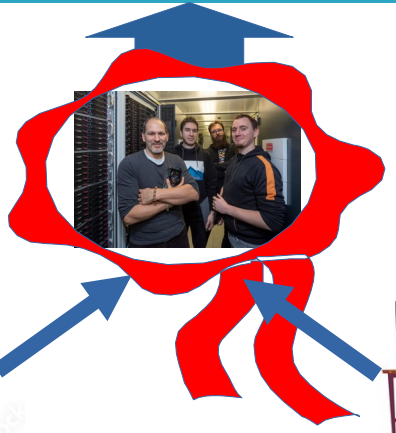
14 YEARS IN PARALLEL COMPUTING (WIGNER GPU LABORATORY) & HPC @ WDC



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.

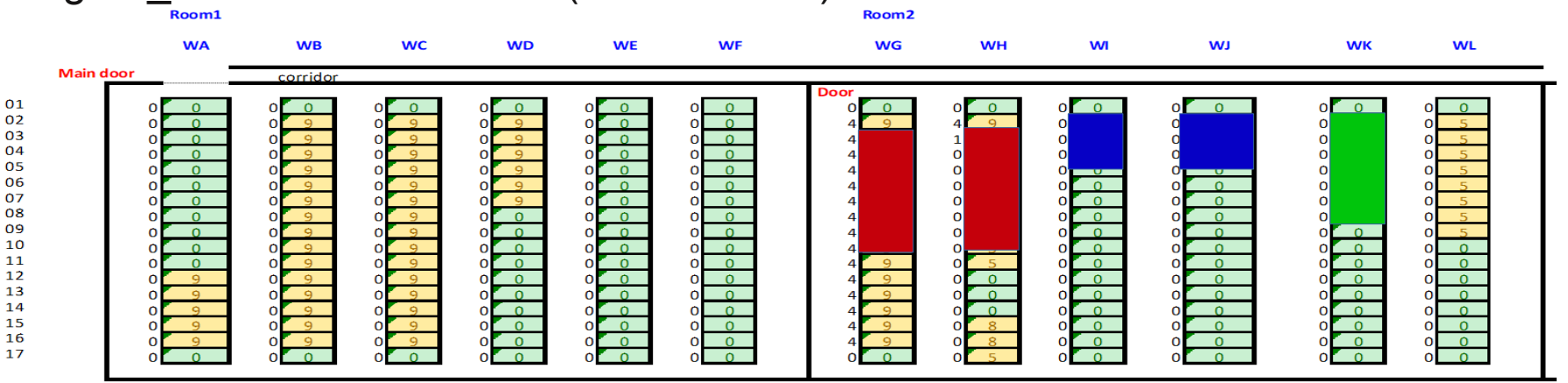
Our sponsors gain additional visibility at the event, on the webpage and related digital appearances including special interviews.

HARDWARES>_

WSCLAB @ WDC

THE PLACE

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

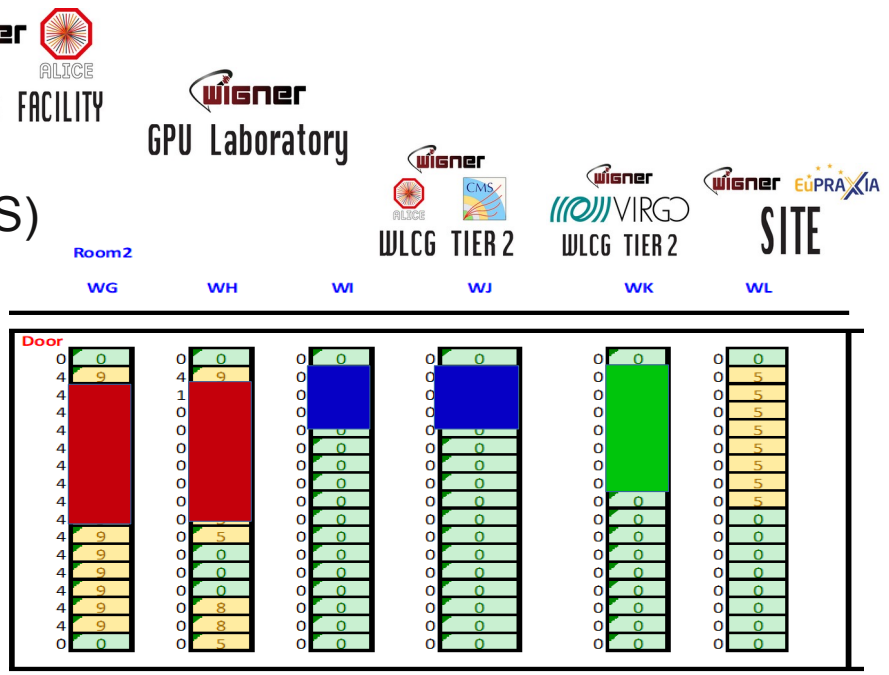


WSCLAB @ WDC

THE PLACE

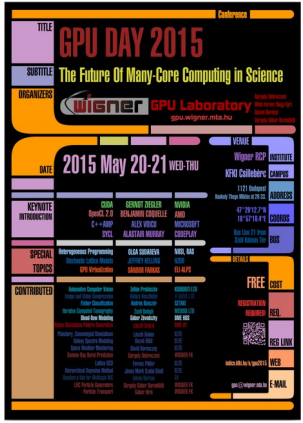
- ✓ Wigner Analysis Facility (Wigner AF)
- ✓ Wigner GPU Laboratory
- ✓ Wigner_KFKI WLCG T2 Grid (ALICE+CMS)
- ✓ New: LIGO/VIRGO
- ✓ New: EuPRAXIA

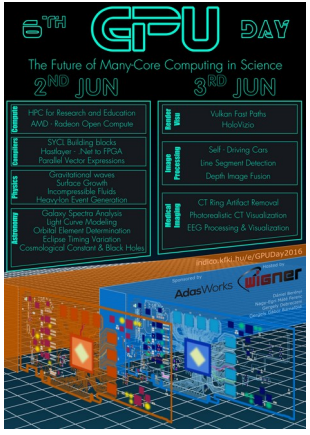
SERVING LARGE-SCALE EU & WORLDWIDE SCIENTIFIC COMMUNITIES

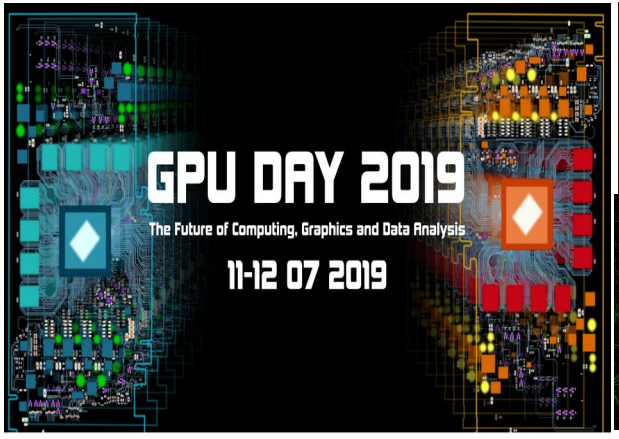


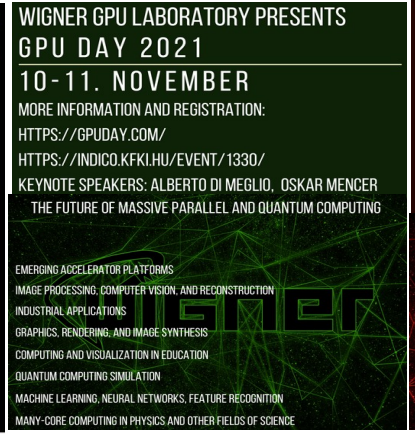
EVENTS>_

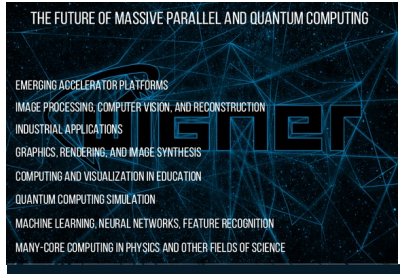
GPU Days so far...

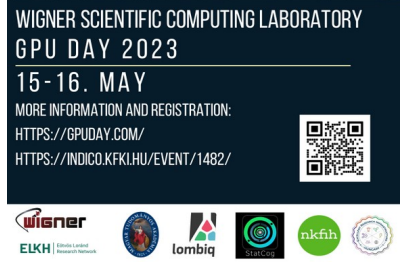












WIGNER SCIENTIFIC COMPUTING LABORATORY

GPU DAY 2024

EMERGING ACCELERATOR PLATFORMS

IMAGE PROCESSING, COMPUTER VISION, AND RECONSTRUCTION

INDUSTRIAL APPLICATIONS

GRAPHICS, RENDERING, AND IMAGE SYNTHESIS

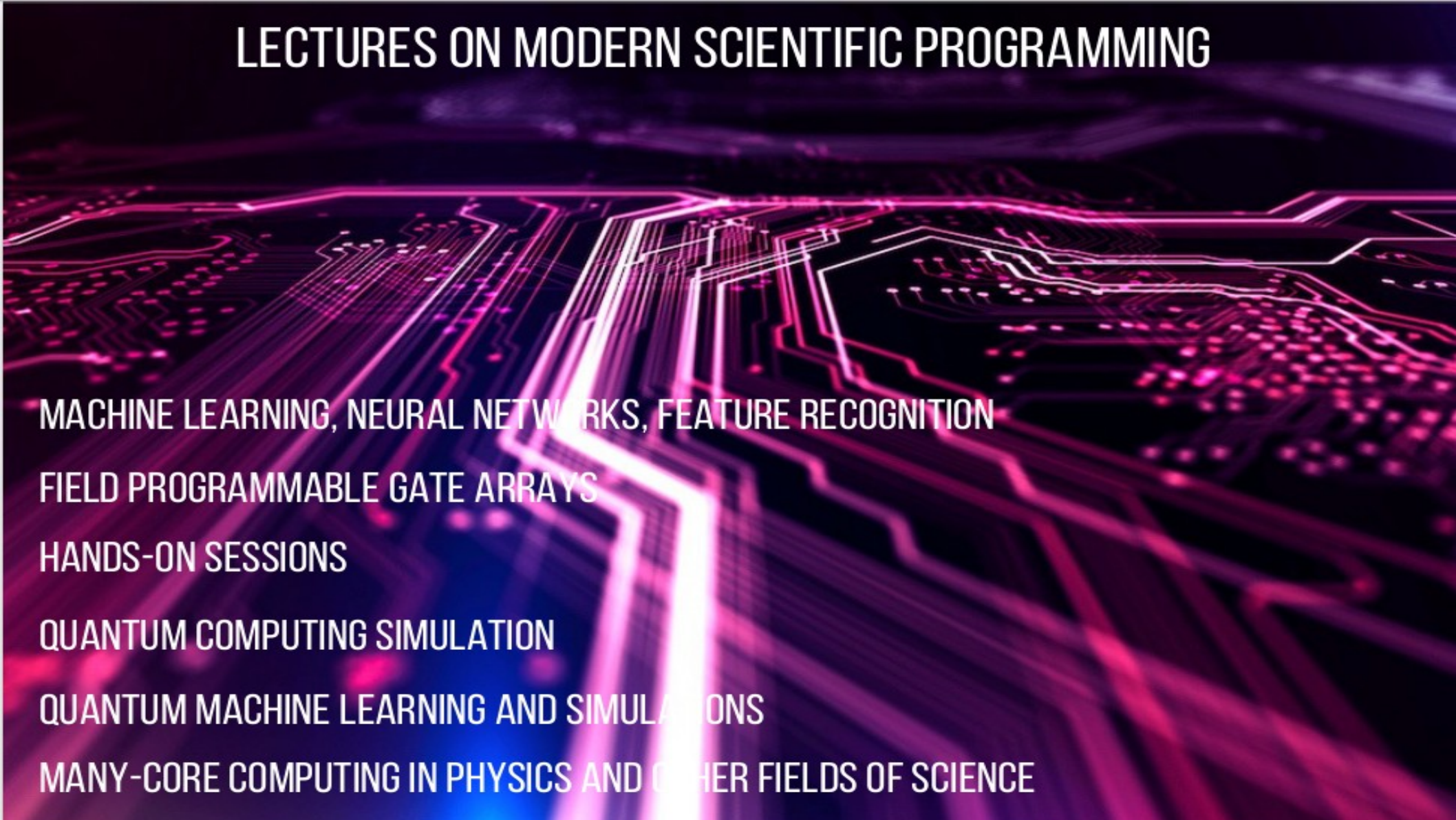
COMPUTING AND VISUALIZATION IN EDUCATION

QUANTUM COMPUTING SIMULATION

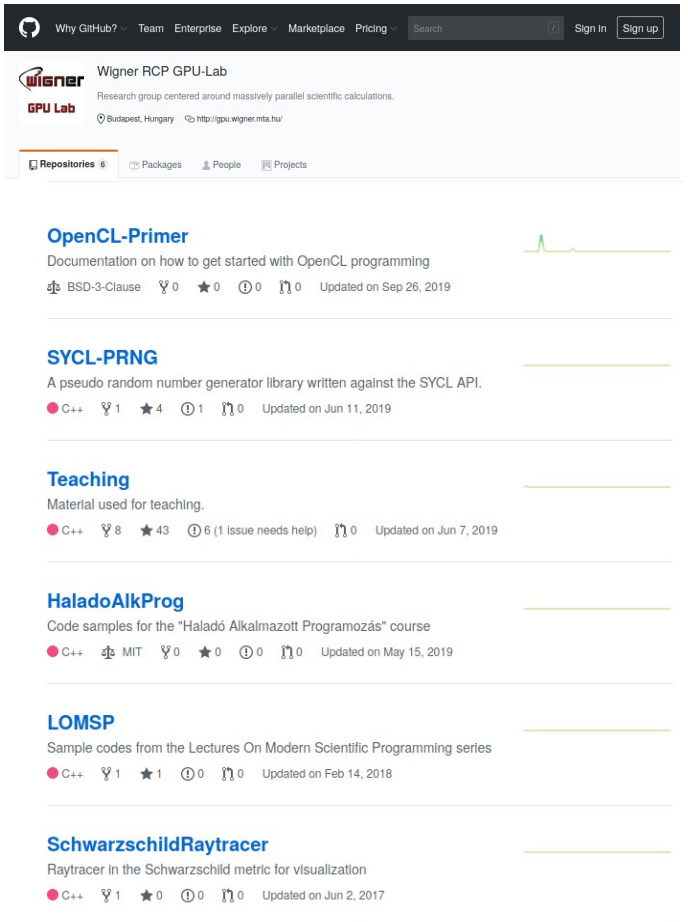
MACHINE LEARNING, NEURAL NETWORKS, FEATURE RECOGNITION

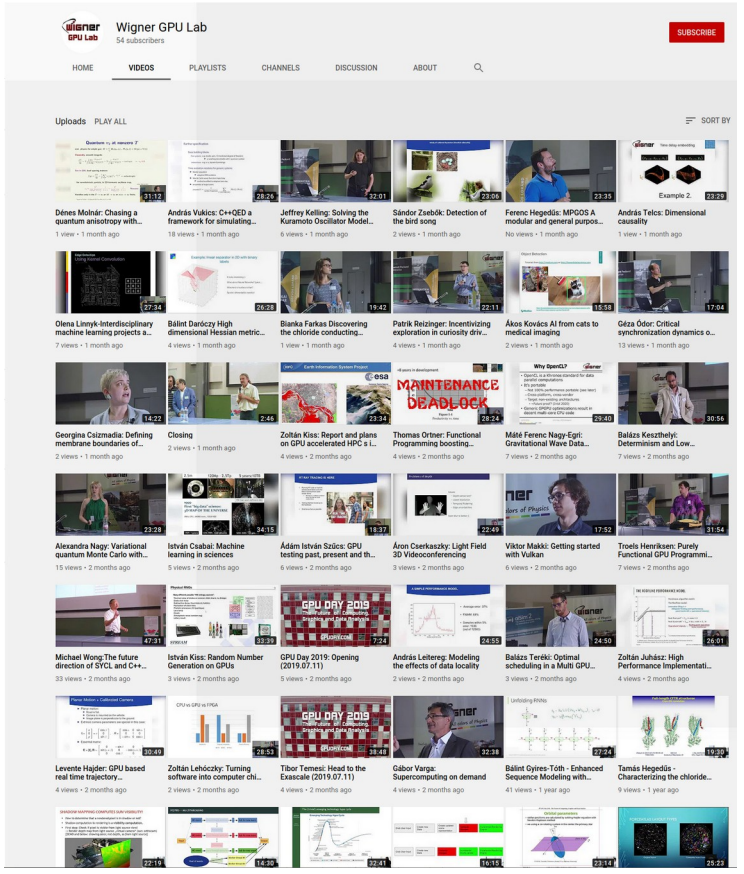
MANY-CORE COMPUTING IN PHYSICS AND OTHER FIELDS OF SCIENCE

LECTURES ON MODERN SCIENTIFIC PROGRAMMING



WSCLAB's EDUCATIONAL MATTERS





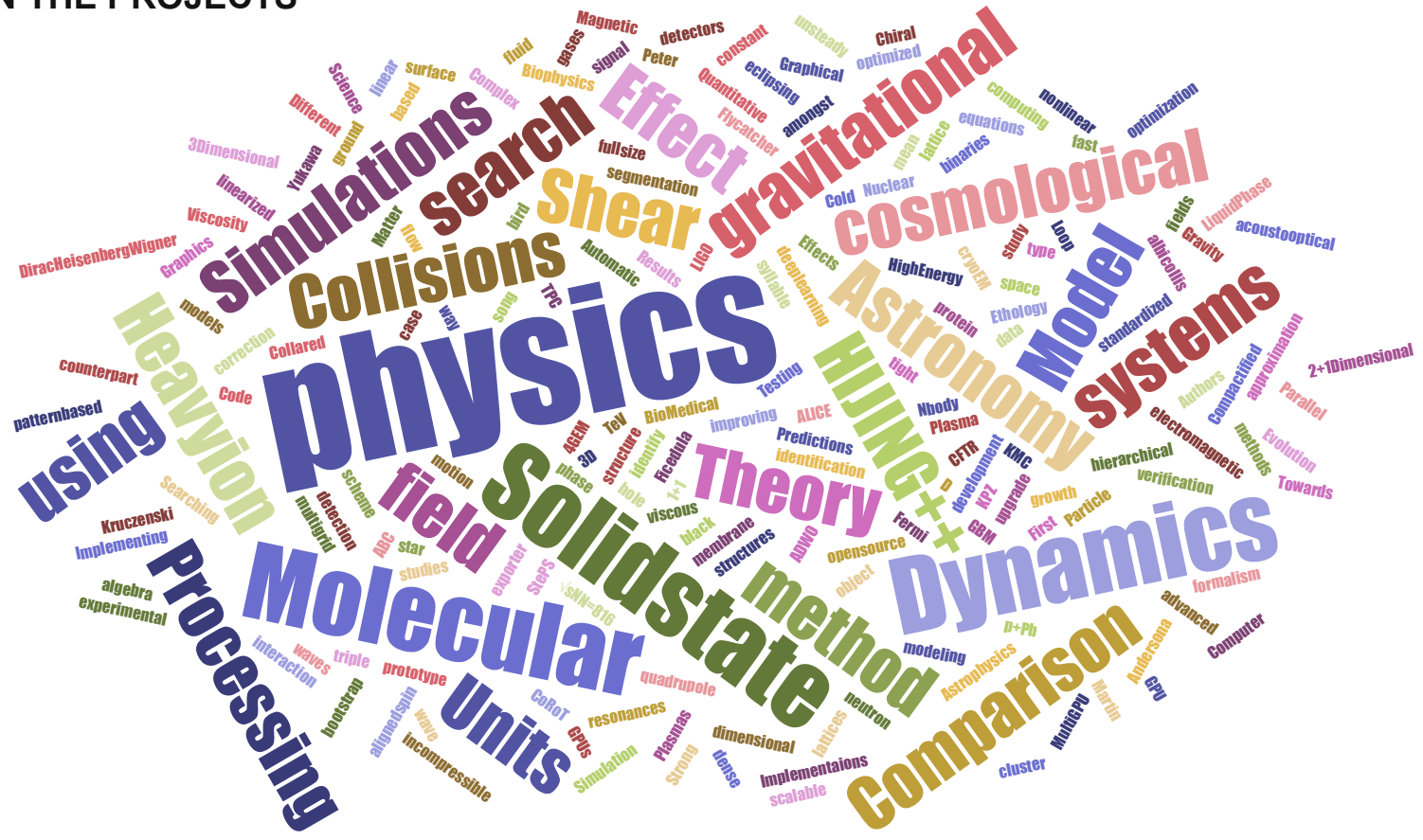
YouTube HU

GitHub

PROJECTS>_

WSCLAB's SCIENTIFIC RESULTS

BASED ON THE PROJECTS



WSCLAB in numbers

KNOWLEDGE HUB: GPUDAY.COM

- ✓ 14 GPU Days

- ✓ 9 Lectures in Modern Computing in Science
- ✓ 55+ WSCLAB (Wigner GPU Lab) Fellowship
- ✓ 35+ industrial & academic partners (Lombiq LTD, Ericsson, Khronos, CERN...)
- ✓ 70+ scientific publications and program codes

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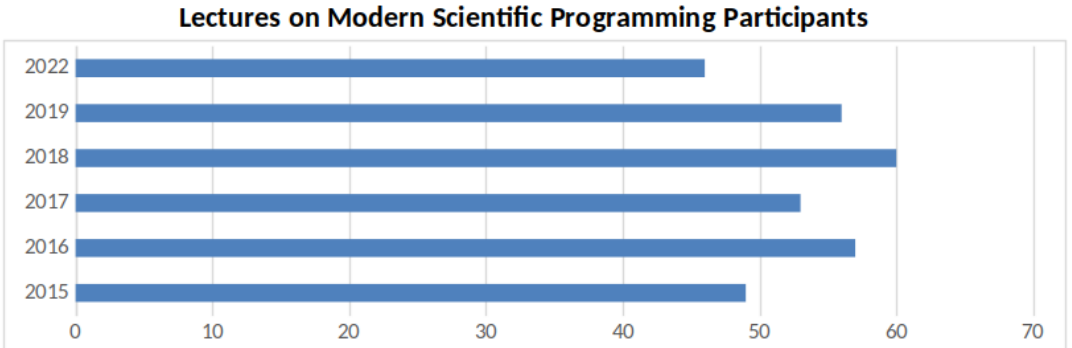

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WSCLAB's SCIENTIFIC RESULTS

BASED ON THE PROJECTS

✓ **Finished Projects from various fields**

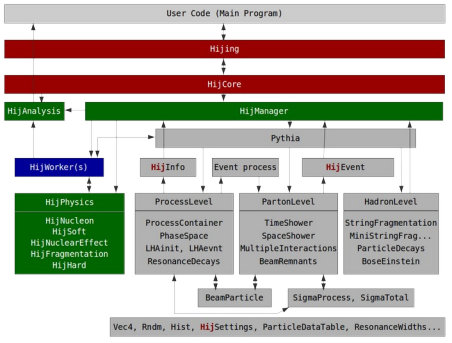
- Astronomy & Astrophysics (16)
- Physics (30)
- Biochemistry (6)
- Life & Medical Sciences, Etology/Ornitology (7)
- Computational Sciences, Imaging, Simulations (13)
- Quantum Computing (9)

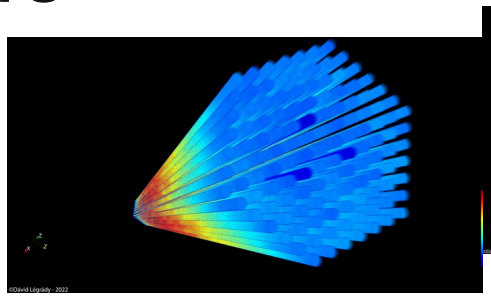
✓ **List of Publications**

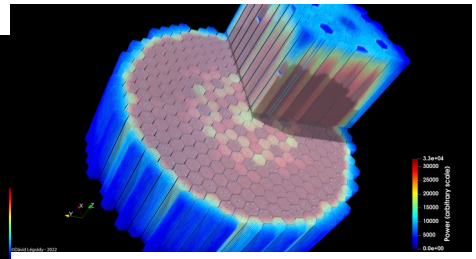
- More than 70 publications & public codes

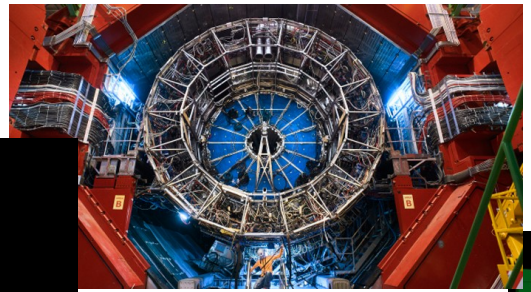
WSCLAB's SCIENTIFIC PROJECTS

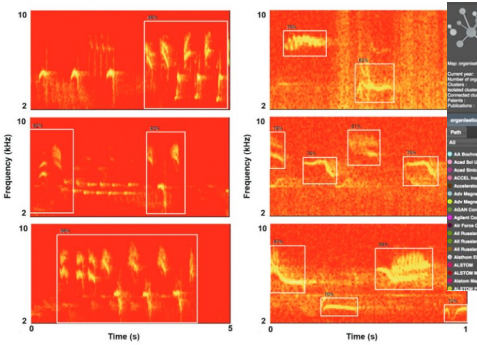
FEW SELECTED ONES

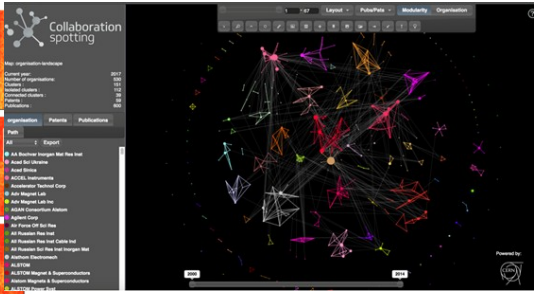


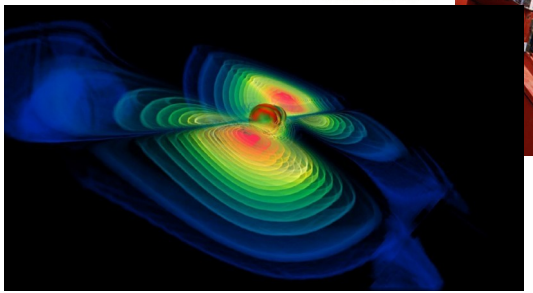


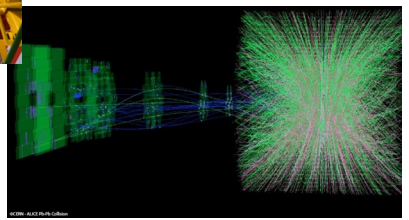


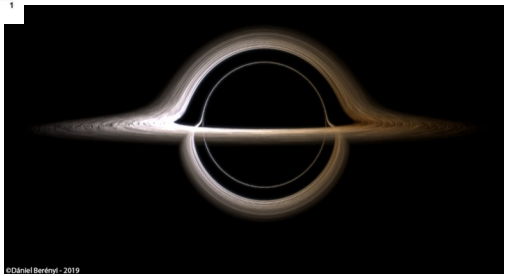












FUTURE>_

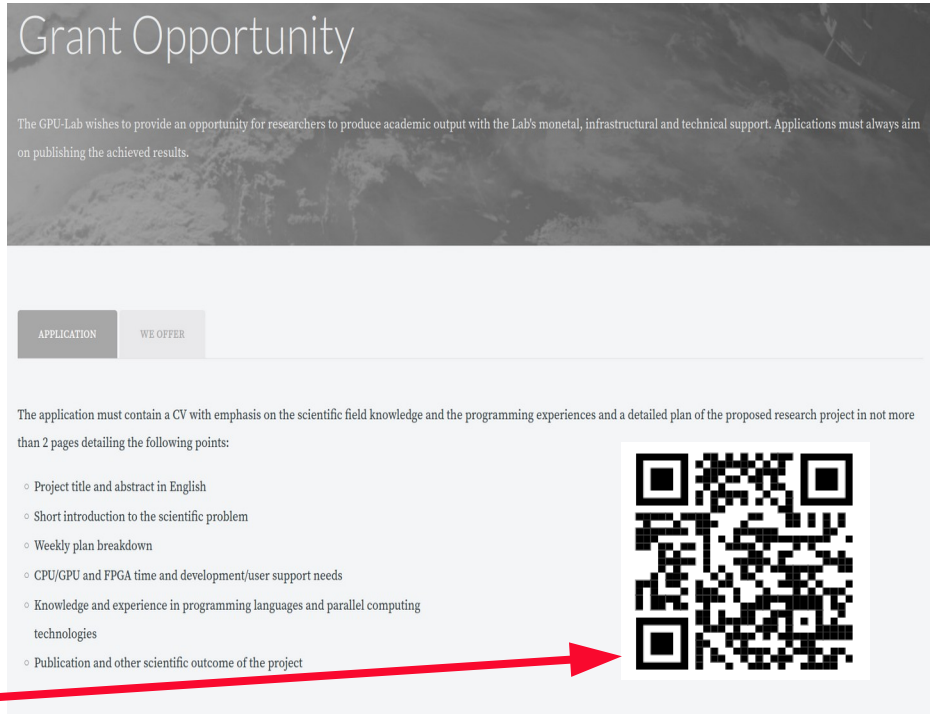
WSCLAB's FUTURE
IS IN YOUR HAND

✓ **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

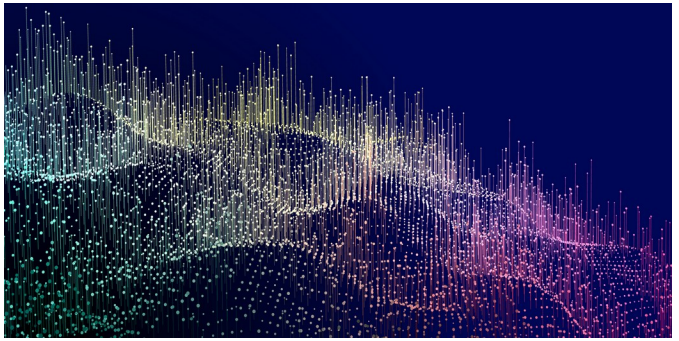
✓ **How to apply**

- 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 (30-31 May 2024)
- Lectures on Modern Computing in Science series (in fall 2024) on LLM in Science

✓ **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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Kompetencia Központ
EXCELLENT RESEARCH INFRASTRUCTURE HUNGARY
Lombiq
UNIVERSITAS BUDAPESTINENSIS DE ROLANDO EÖTVÖS NOMINATA
ik
silicon computers
STREAM
High Performance Computing
UNIVERSITAS BUDAPESTINENSIS DE SEMMELWEIS NOMINATA 1769
AIMOTIVE
nkfih
codeplay
IFIN-HH
CERN
Cerntech
Collaboration spotting
CERN openlab
IN2P3
INSTITUT NATIONAL DE PHYSIQUE NUCLÉAIRE ET DE PHYSIQUE DES PARTICULES
QNL
Quantum Information National Laboratory
HUNGARY
UNIVERSITY OF HELSINKI
KONKOLY
CAMK PAN
ALICE
epam
PURDUE
UNIVERSITY
MAGYAR TUDOMÁNYOS AKADÉMIA 1825
ELKH
Eötvös Loránd Research Network
l'Observatoire de Paris
KHRONOS GROUP
CONNECTING SOFTWARE TO SILICON
SZÉCHENYI 2020
ERICSSON
UNIVERSITY OF OXFORD
StatCog

WSCLAB>_

WIGNER SCIENTIFIC COMPUTING LABORATORY


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EXCELLENT RESEARCH INFRASTRUCTURE
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THX>_


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KIFÜ


lombiq


GitHub

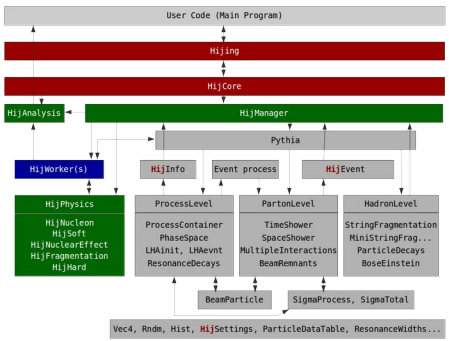

YouTube

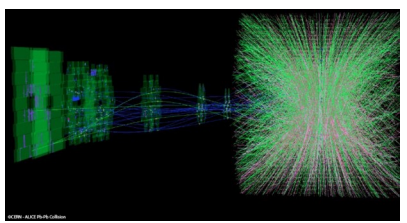
BACKUP>_

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

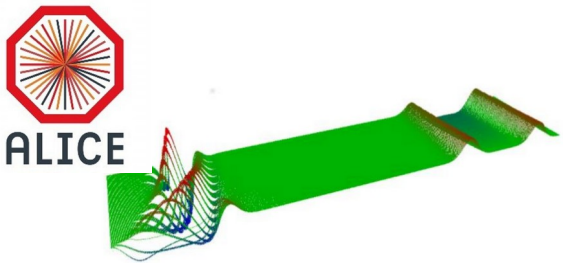


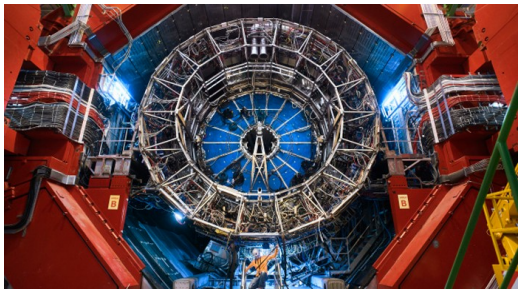


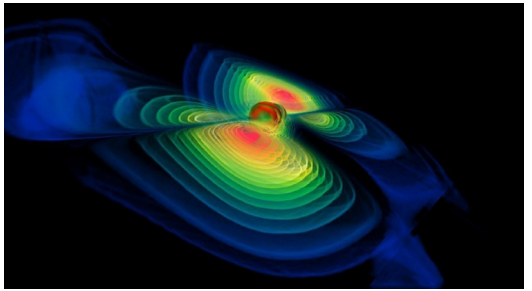
WSCLAB's SCIENTIFIC PROJECTS

PHYSICS

- ✓ 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



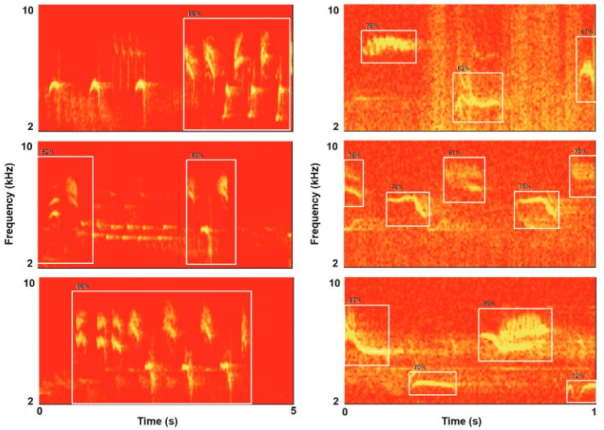


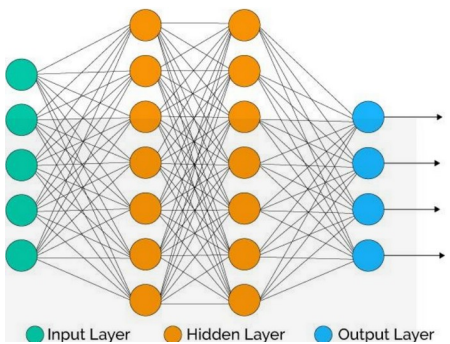


WSCLAB's SCIENTIFIC PROJECTS

LIFE SCIENCES, CHEMISTRY, ORNITOLOGY

- ✓ **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**

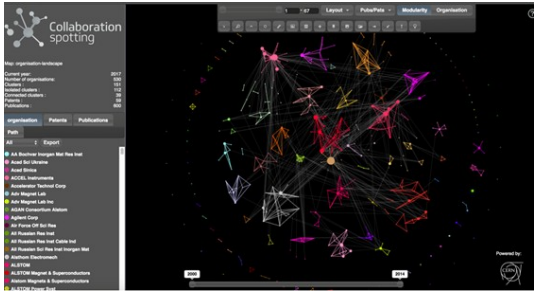


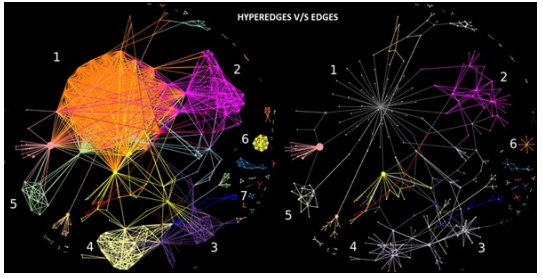


WSCLAB's SCIENTIFIC PROJECTS

IMAGING, SIMULATIONS, COMPUTING

- ✓ 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.

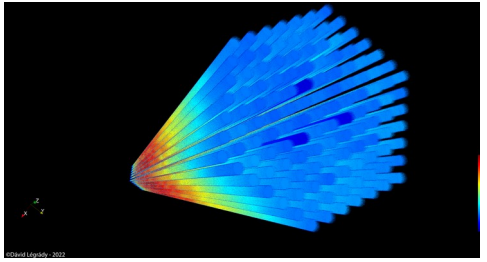


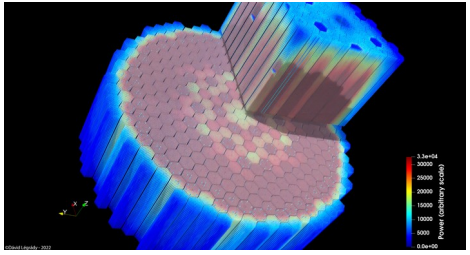


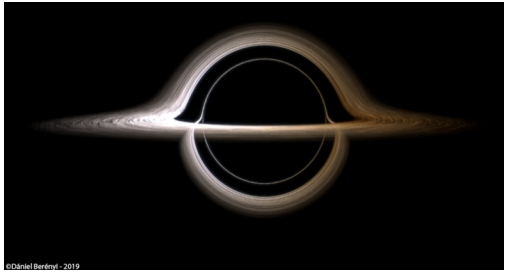
WSCLAB's SCIENTIFIC PROJECTS

IMAGING, SIMULATIONS, COMPUTING

- ✓ **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

- ✓ **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

- ✓ **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

- ✓ 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**