

# WIGNER SCIENTIFIC COMPUTING LABORATORY

## GPU DAY 2024

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30-31. MAY

MORE INFORMATION AND REGISTRATION:

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

[HTTPS://INDICO.KFKI.HU/EVENT/1567/](https://indico.kfki.hu/event/1567/)





# 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

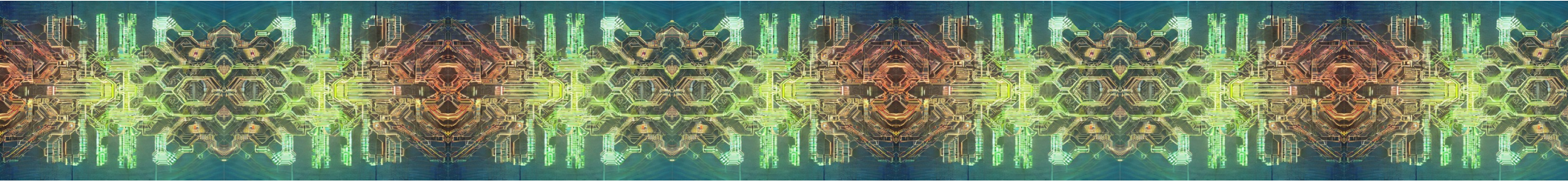
MACHINE LEARNING, NEURAL NETWORKS, FEATURE RECOGNITION

MANY-CORE COMPUTING IN PHYSICS AND OTHER FIELDS OF SCIENCE

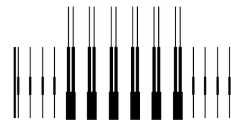
# Gener8



# One Lab – Many Project Review of The WSCLAB



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



**MTA**  
Centre  
of Excellence



**ROLE>\_**

# WSCLAB's origin

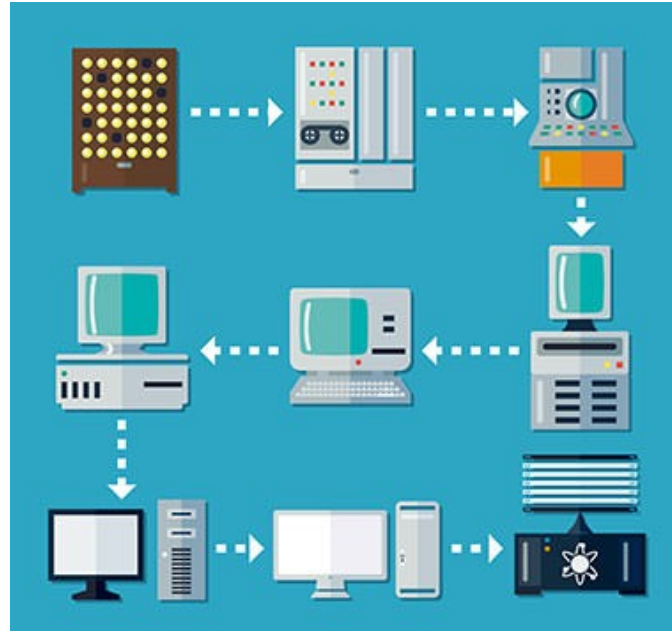
14 YEARS IN PARALLEL COMPUTING (WIGNER GPU LABORATORY) & HPC @ WDC

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

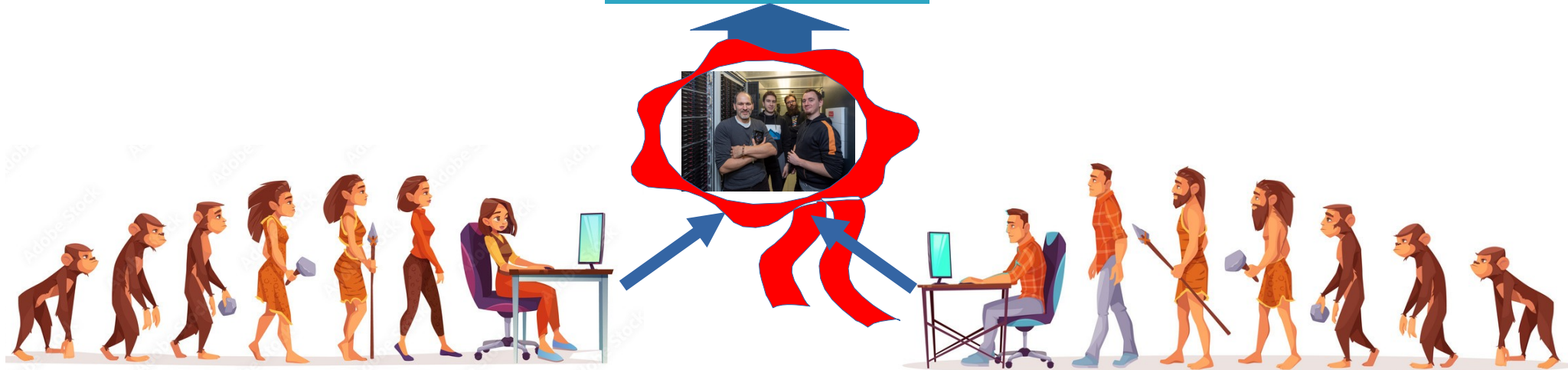
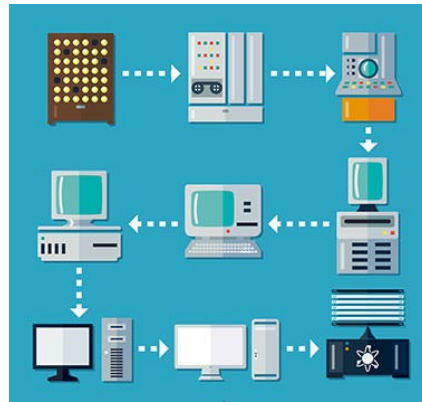
14 YEARS IN PARALLEL COMPUTING (WIGNER GPU LABORATORY) & HPC @ WDC





# 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- 1<sup>st</sup> 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: 17<sup>TH</sup> DECEMBER 2021.





# WSCLAB's origin

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

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*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.*





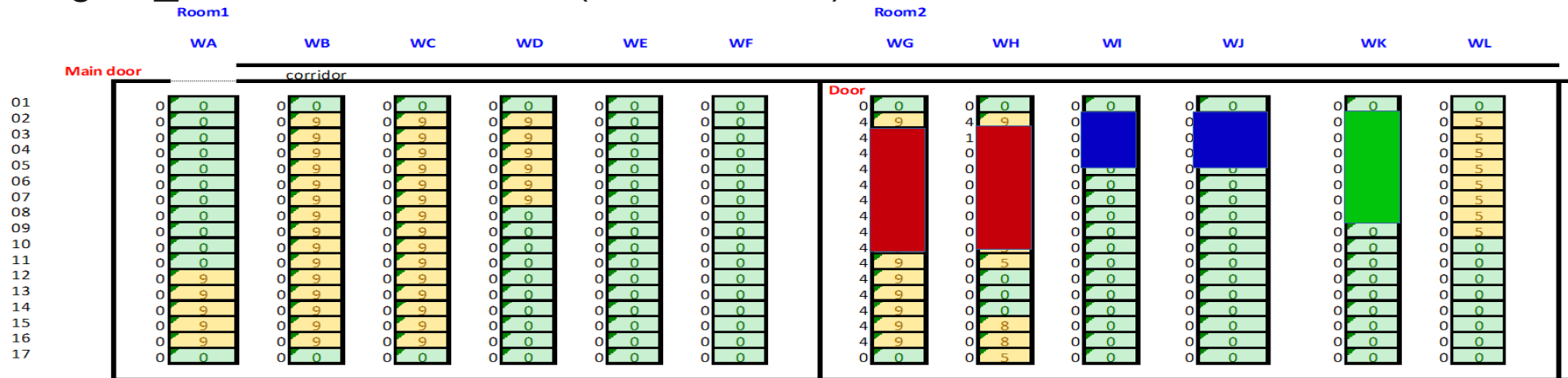


**HARDWARES>\_**

# WSCLAB @ WDC

## THE PLACE

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









**EVENTS>\_**

# GPU Days so far...

## GPU nap 2010

MTA KFKI Részecske- és Magfizikai Kutatóintézet

XII. Budapest, Konkoly-Thege Mikós út 29-33

2010 június 4.

(Előjelentkezés szükséges: <http://gpu.kfki.hu>)



### Program kivonat:

- Ismerkedés a GPU programozással, gyakorlat
- Grafikus kártyák, mint asztali szuperszámítógépek
- Molekuladinamika számítások GPU-val
- Rács QCD és részecskefizikai alkalmazások
- GPU a kísérleti és elméleti gravitációkutatásban

**gpu 2011**  
GPU programozás a tudományos kutatásokban

MTA KFKI Részecske- és Magfizikai Kutatóintézet  
XII. Budapest, Konkoly-Thege Mikós út 29-33  
2011 június 15-16.

PROGRAM:

- 09:00 Regisztráció
- 09:30 Bemutató
- 10:00 GPU az IKT-tudományban
- 10:30 Munkahelyi feladatmegoldás
- 11:00 Szakmai előadások
- 11:30 Munkahelyi feladatmegoldás
- 12:00 Ebéda
- 13:00 Szakmai előadások
- 13:30 Munkahelyi feladatmegoldás
- 14:00 Ebéda
- 15:00 GPU a fizikában
- 15:30 Munkahelyi feladatmegoldás
- 16:00 Záró beszéd
- 16:30 Regisztráció

MTA KFKI Részecske- és Magfizikai Kutatóintézet  
XII. Budapest, Konkoly-Thege Mikós út 29-33  
2011 június 15-16.

**gpu@2012**  
GPU programozás a tudományos kutatásokban

MTA KFKI Részecske- és Magfizikai Kutatóintézet  
XII. Budapest, Konkoly-Thege Mikós út 29-33  
2012 június 14-15.

PROGRAM:

- 09:00 Regisztráció
- 09:30 Bemutató
- 10:00 GPU az IKT-tudományban
- 10:30 Munkahelyi feladatmegoldás
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- 14:00 Ebéda
- 15:00 GPU a fizikában
- 15:30 Munkahelyi feladatmegoldás
- 16:00 Záró beszéd
- 16:30 Regisztráció

**gpu@2013**  
GPU programozás a tudományos kutatásokban

MTA KFKI Részecske- és Magfizikai Kutatóintézet  
XII. Budapest, Konkoly-Thege Mikós út 29-33  
2013 június 13-14.

PROGRAM:

- 09:00 Regisztráció
- 09:30 Bemutató
- 10:00 GPU az IKT-tudományban
- 10:30 Munkahelyi feladatmegoldás
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- 16:00 Záró beszéd
- 16:30 Regisztráció

**FUTURE OF MANY-CORE COMPUTING IN SCIENCE**

**GPU DAY 2014**  
GPU programozás a tudományos kutatásokban

MTA KFKI Részecske- és Magfizikai Kutatóintézet  
XII. Budapest, Konkoly-Thege Mikós út 29-33  
2014 június 11-12.

PROGRAM:

- 09:00 Regisztráció
- 09:30 Bemutató
- 10:00 GPU az IKT-tudományban
- 10:30 Munkahelyi feladatmegoldás
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- 16:00 Záró beszéd
- 16:30 Regisztráció

**GPU DAY 2015**  
The Future of Many-Core Computing in Science

MTA KFKI Részecske- és Magfizikai Kutatóintézet  
XII. Budapest, Konkoly-Thege Mikós út 29-33  
2015 május 20-21.

PROGRAM:

- 09:00 Regisztráció
- 09:30 Bemutató
- 10:00 GPU az IKT-tudományban
- 10:30 Munkahelyi feladatmegoldás
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- 16:00 Záró beszéd
- 16:30 Regisztráció

**6TH GPU DAY**  
The Future of Many-Core Computing in Science

2ND JUN  
3RD JUN

MTA KFKI Részecske- és Magfizikai Kutatóintézet  
XII. Budapest, Konkoly-Thege Mikós út 29-33  
2016 június 2-3.

PROGRAM:

- 09:00 Regisztráció
- 09:30 Bemutató
- 10:00 GPU az IKT-tudományban
- 10:30 Munkahelyi feladatmegoldás
- 11:00 Szakmai előadások
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- 15:30 Munkahelyi feladatmegoldás
- 16:00 Záró beszéd
- 16:30 Regisztráció

**GPU DAY 2019**  
The Future of Computing, Graphics and Data Analysis

11-12 07 2019

MTA KFKI Részecske- és Magfizikai Kutatóintézet  
XII. Budapest, Konkoly-Thege Mikós út 29-33  
2019 július 11-12.

PROGRAM:

- 09:00 Regisztráció
- 09:30 Bemutató
- 10:00 GPU az IKT-tudományban
- 10:30 Munkahelyi feladatmegoldás
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- 16:30 Regisztráció

**WIGNER GPU LABORATORY PRESENTS GPU DAY 2021**  
10-11. NOVEMBER

MORE INFORMATION AND REGISTRATION:  
[HTTPS://GPUDAY.COM/](https://gpuday.com/)  
[HTTPS://INDICO.KFKI.HU/EVENT/1330/](https://indico.kfki.hu/event/1330/)

KEYNOTE SPEAKERS: ALBERTO DI MEGLIO, OSKAR MENCER  
THE FUTURE OF MASSIVE PARALLEL AND QUANTUM COMPUTING

EMERGING ACCELERATOR PLATFORMS  
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QUANTUM COMPUTING SIMULATION  
MACHINE LEARNING, NEURAL NETWORKS, FEATURE RECOGNITION  
MANY-CORE COMPUTING IN PHYSICS AND OTHER FIELDS OF SCIENCE

**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

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**WIGNER SCIENTIFIC COMPUTING LABORATORY GPU DAY 2023**  
15-16. MAY

MORE INFORMATION AND REGISTRATION:  
[HTTPS://GPUDAY.COM/](https://gpuday.com/)  
[HTTPS://INDICO.KFKI.HU/EVENT/1482/](https://indico.kfki.hu/event/1482/)





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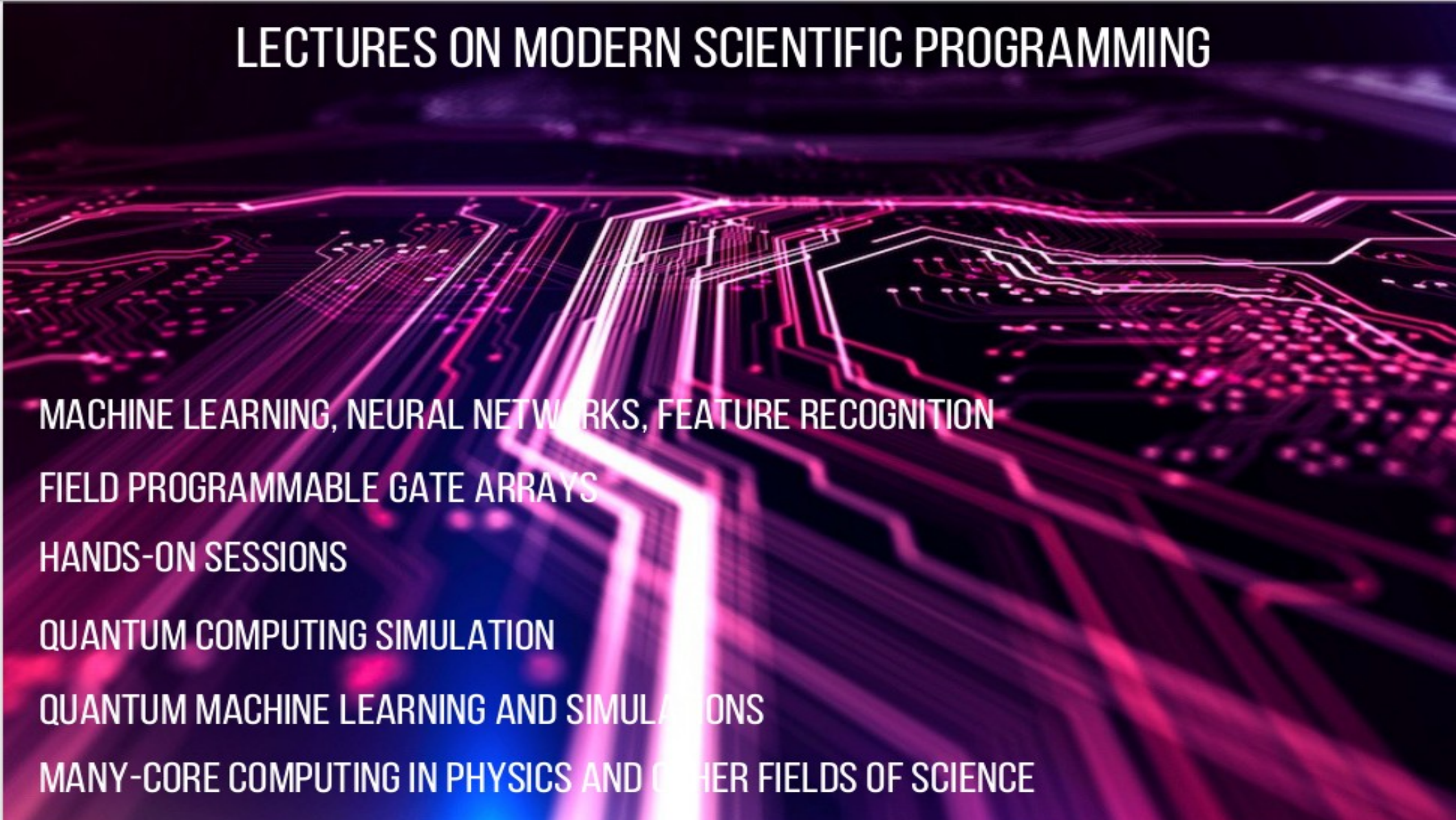
MACHINE LEARNING, NEURAL NETWORKS, FEATURE RECOGNITION

MANY-CORE COMPUTING IN PHYSICS AND OTHER FIELDS OF SCIENCE





# 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

Why GitHub? Team Enterprise Explore Marketplace Pricing Search Sign In Sign up

**wigner GPU Lab**  
Research group centered around massively parallel scientific calculations.  
Budapest, Hungary <http://gpu.wigner.mta.hu/>

Repositories 6 Packages People Projects

## OpenCL-Primer

Documentation on how to get started with OpenCL programming

BSD-3-Clause 0 0 0 0 Updated on Sep 26, 2019

## SYCL-PRNG

A pseudo random number generator library written against the SYCL API.

C++ 1 4 1 0 Updated on Jun 11, 2019

## Teaching

Material used for teaching.

C++ 8 43 6 (1 issue needs help) 0 Updated on Jun 7, 2019

## HaladoAlkProg

Code samples for the "Haladó Alkalmazott Programozás" course

C++ MIT 0 0 0 Updated on May 15, 2019

## LOMSP

Sample codes from the Lectures On Modern Scientific Programming series

C++ 1 1 0 0 Updated on Feb 14, 2018

## SchwarzschildRaytracer

Raytracer in the Schwarzschild metric for visualization

C++ 1 0 0 0 Updated on Jun 2, 2017

**wigner GPU Lab** 54 subscribers SUBSCRIBE

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GitHub



# PROJECTS>\_



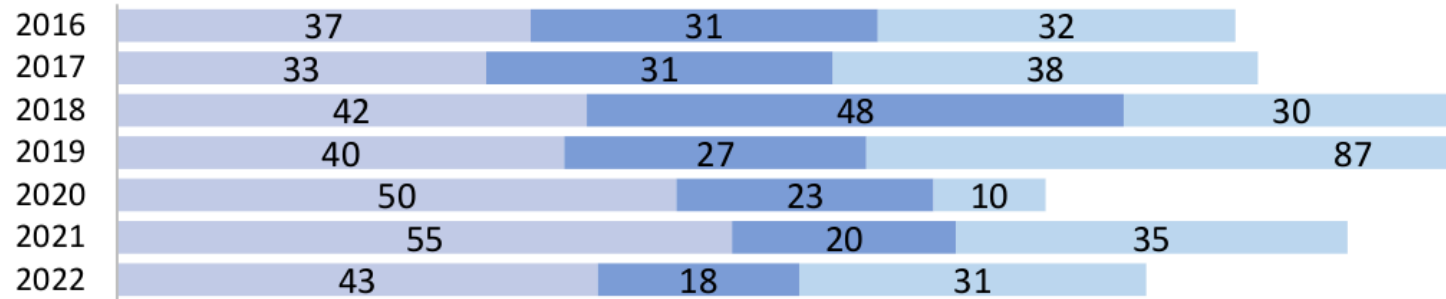




# WSCLAB in numbers

KNOWLEDGE HUB: GPU DAY.COM

## ✓ 14 GPU Days

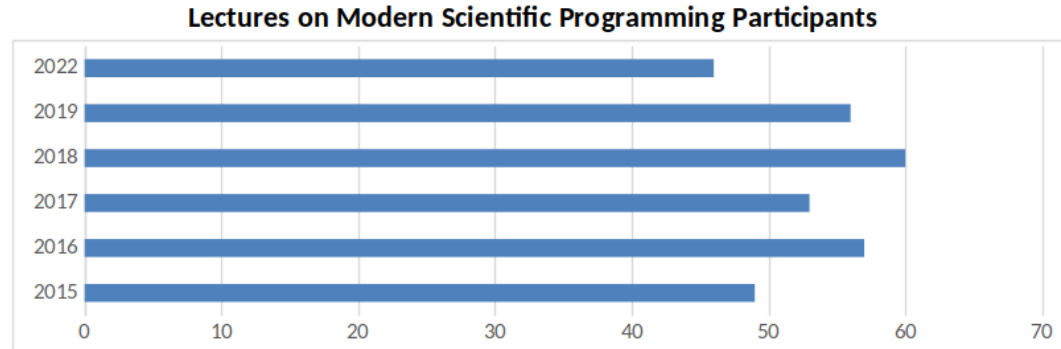


- ✓ 9 Lectures in Modern Computing in Science
- ✓ 55+ WSCLAB (Wigner GPU Lab) Fellowship
- ✓ 35+ industrial & academic partners (Lombiq LTD, Ericsson, Khronos, CERN...)
- ✓ 70+ scientific publications and program codes

# WSCLAB in numbers

KNOWLEDGE HUB: GPU DAY.COM

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- ✓ 55+ WSCLAB (Wigner GPU Lab) Fellowship
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- ✓ 70+ scientific publications and program codes

# 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)

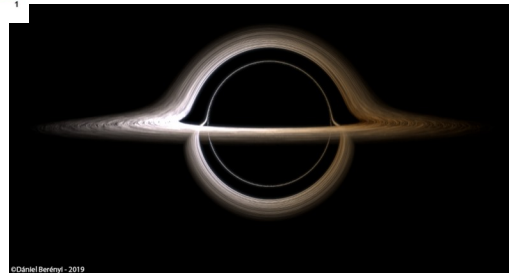
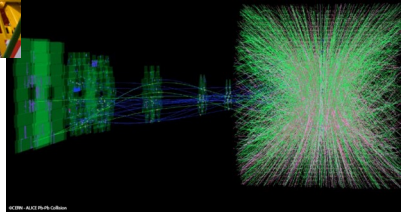
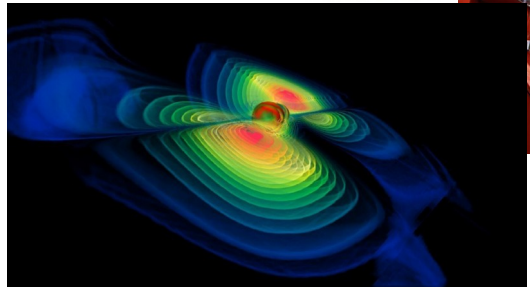
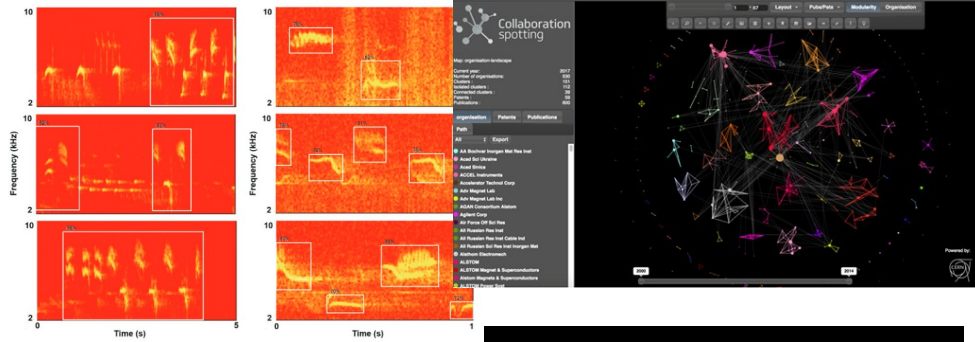
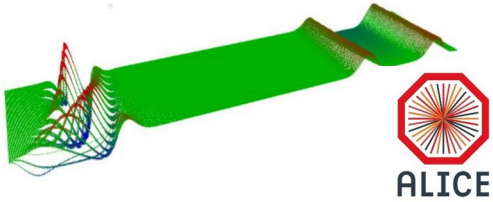
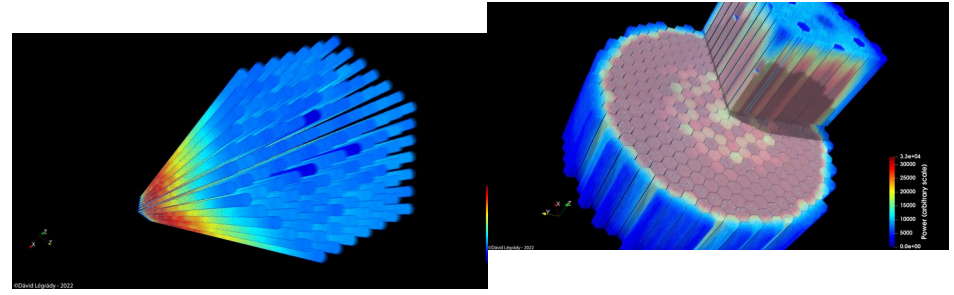
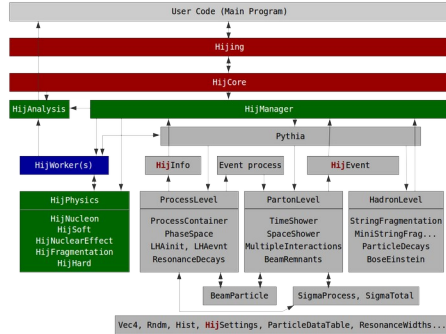


### ✓ List of Publications

- More than 70 publications & public codes

# WSCLAB's SCIENTIFIC PROJECTS

## FEW SELECTED ONES







**FUTURE>\_**

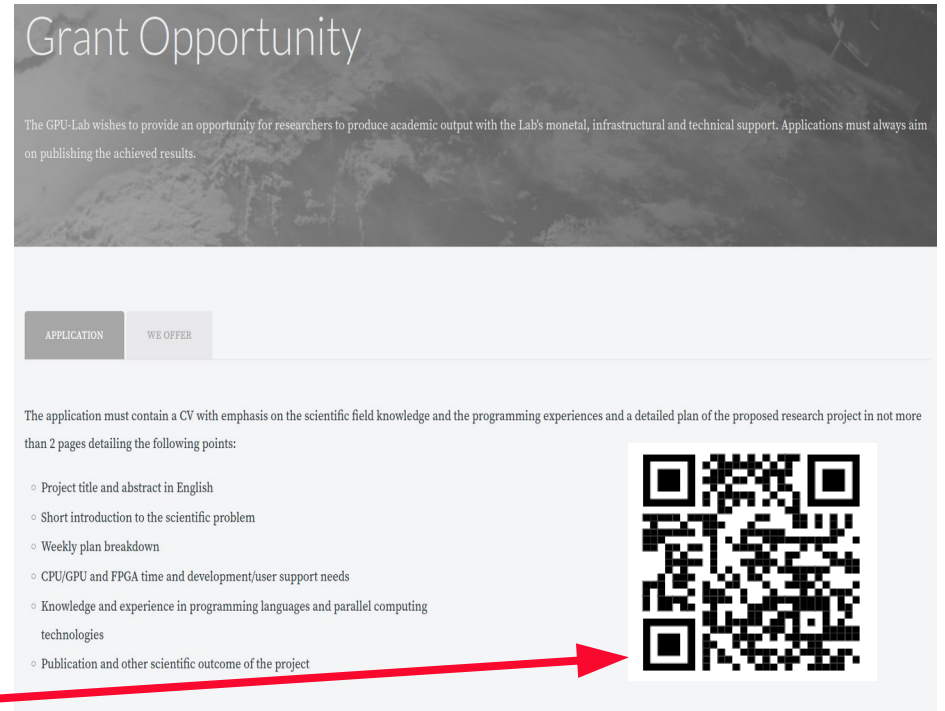
# WSCLAB's FUTURE IS IN YOUR HAND

## ✓ 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](http://wsclab.wigner.hu)



Grant Opportunity

The GPU-Lab wishes to provide an opportunity for researchers to produce academic output with the Lab's monetal, 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

A red arrow points from the text 'Visit wsclab.wigner.hu' to a QR code located in the bottom right corner of the webpage screenshot.

# WSCLAB's FUTURE

## PLANS FOR THE FUTURE

### ✓ Short timescale

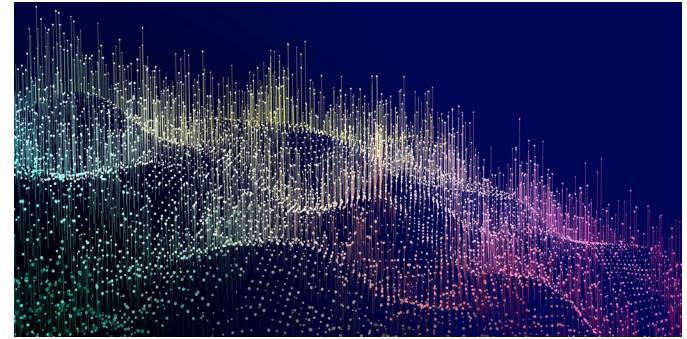
- New WSCLAB Grants for young scientists for 2024
- GPU Day 2024 series (30-31 May 2024)
- Lectures on Modern Computing in Science series (in fall 2024) on LLM in Science

### ✓ Intermediate timescale

- Further local HW developments & cloud solutions

### ✓ Long range plan

- Closely related to the EuroHPC LEVENTE project including Quantum Computing & Quantum simulations





HUN  
REN



HUN-REN  
Hungarian Research Network



HPC @hu  
Kompetencia Központ



STREAM  
High Performance Computing



Cerntech



IN2P3  
INSTITUT NATIONAL DE PHYSIQUE NUCLÉAIRE  
ET DE PHYSIQUE DES PARTICULES



ELKH | Eötvös Loránd  
Research Network

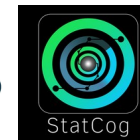


KRONOS  
GROUP  
CONNECTING SOFTWARE TO SILICON

SZÉCHENYI 2020



UNIVERSITY OF  
OXFORD





# WSCLAB>\_



WIGNER SCIENTIFIC COMPUTING LABORATORY





THX>\_





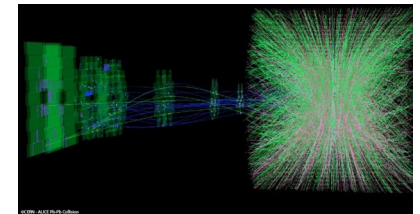
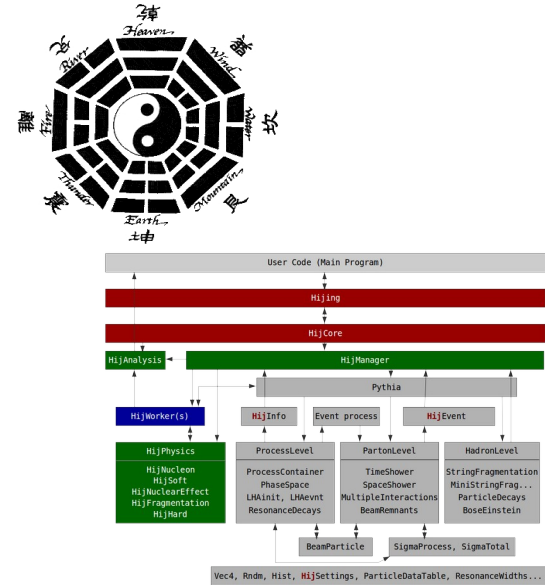
**BACKUP>\_**



# WSCLAB's SCIENTIFIC PROJECTS

## FEW SELECTED ONES

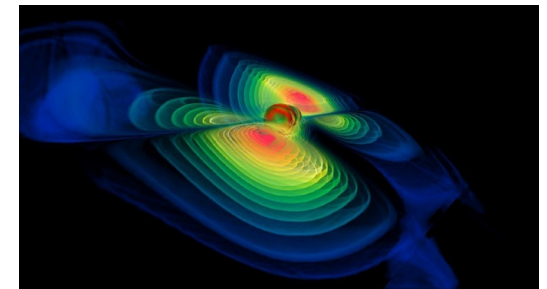
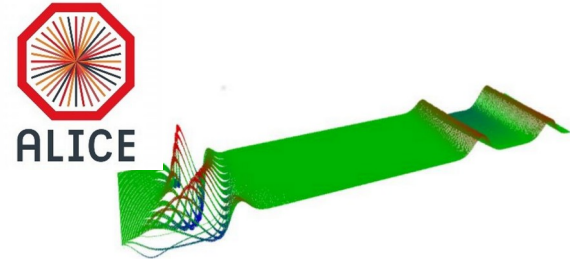
- ✓ Simulating the photo-ionisation of Rubidium atoms
- ✓ **High Performance Computing for Nanofusion**
- ✓ High performance Monte Carlo simulations of high-energy heavy-ion collisions
- ✓ **Modelling non-linear optics by machine learning techniques**
- ✓ Generation of Gravitational Wave Signals with 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

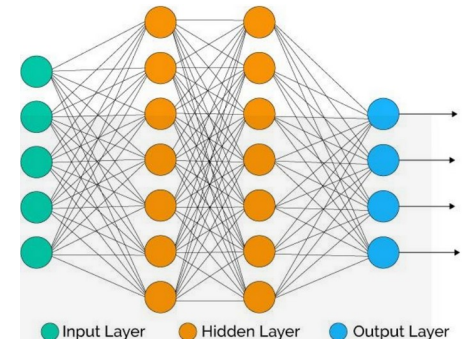
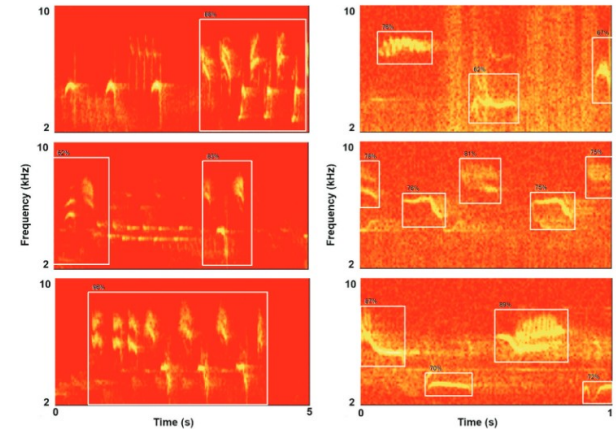
- ✓ Optimization and Development of High-performance Computing pipeline to search for gravitational radiation from rotating NS by means of GPU-based Hardware Accelerators
- ✓ ALICE TCP GEM QA – GPU-accelerated image analysis
- ✓ Viscous corrections from linearized Boltzmann transport
- ✓ Parallelized 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

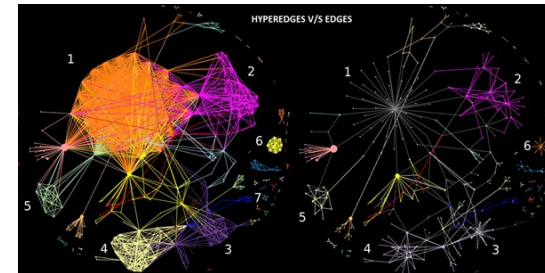
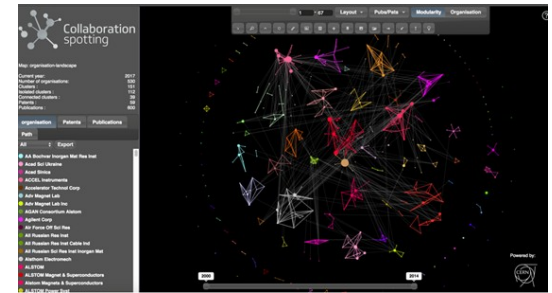
- ✓ **Analysis of the spatial structure of SARS-CoV-2 protein using machine learning methods**
- ✓ Quantum chemical study of the hydrolysis of oxidized endogenous psychedelic N,N-dimethyltryptamine
- ✓ N,N-dimethyltryptamine metabolism by the monoamine oxidase enzyme-A
- ✓ In silico studies to uncover 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.

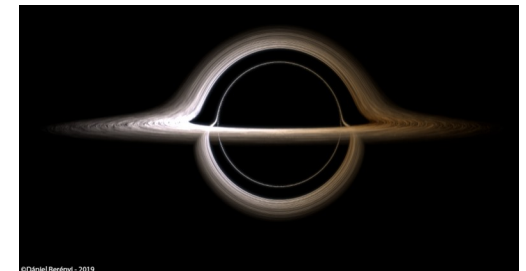
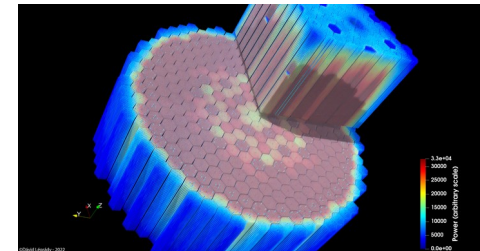
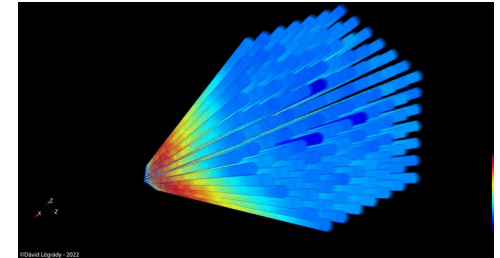




# WSCLAB's SCIENTIFIC PROJECTS

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**