



One Lab – Many Project WSCLAB

LECTURES ON MODERN SCIENTIFIC PROGRAMMING 2023
TOWARDS EXASCALE HIGH-PERFORMANCE COMPUTING



LECTURES ON MODERN SCIENTIFIC PROGRAMMING



HUN-REN
Hungarian Research Network



nkfih



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 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.



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'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.



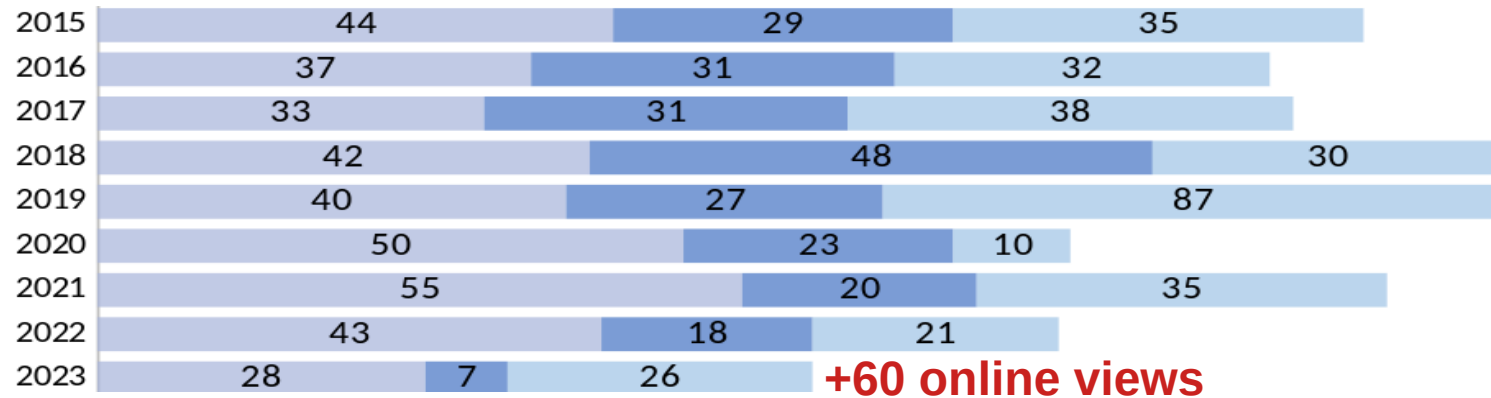


PROJECTS>_

WSCLAB GPULAB 2023 in numbers

KNOWLEDGE HUB: GPUDAY.COM

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



- ✓ 55 WSCLAB (Wigner GPU Lab) Fellowship (46 finished + 9 running)
- ✓ 35+ industrial & academic partners (Lombiq LTD, Ericsson, Khronos, CERN...)
- ✓ 65+ 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

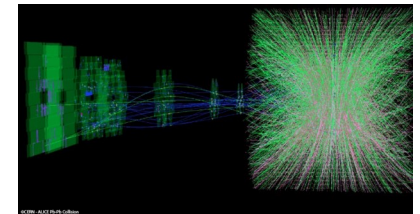
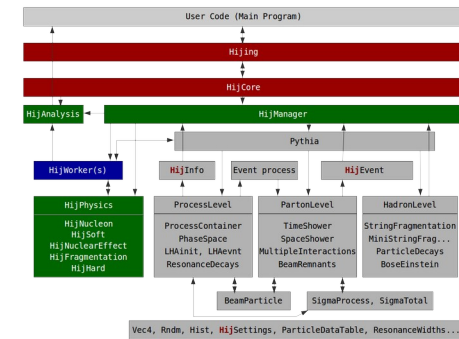
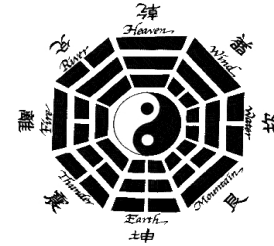
- More than 60 publications & public codes



WSCLAB's SCIENTIFIC PROJECTS

PHYSICS (15)

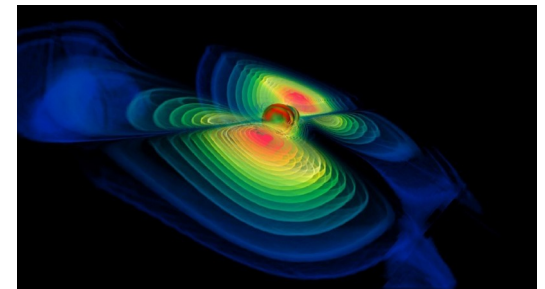
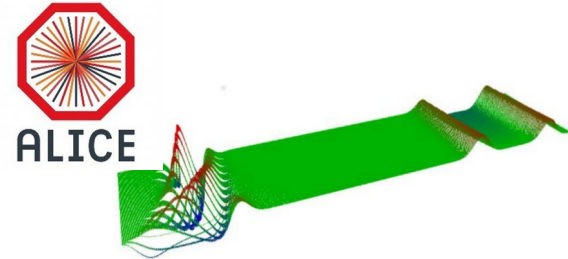
- ✓ Simulating the photo-ionisation of Rubidium atoms
- ✓ High Performance Computing for Nanofusion
- ✓ High performance Monte Carlo simulations of high-energy heavy-ion collisions
- ✓ Modelling non-linear optics by machine learning techniques
- ✓ Nanoplasmonic Laser Fusion
- ✓ Generation of Gravitational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

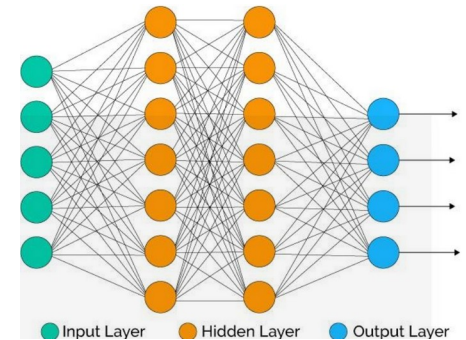
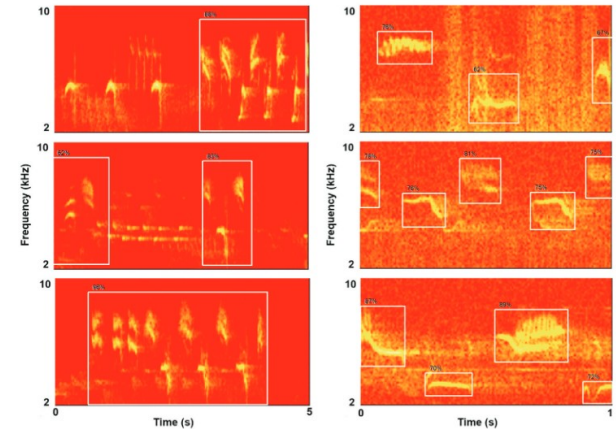
- ✓ Optimization and Development of High-performance Computing pipeline to search for gravitational radiation from rotating NS by means of GPU-based Hardware Accelerators
- ✓ ALICE TCP GEM QA – GPU-accelerated image analysis
- ✓ Viscous corrections from linearized Boltzmann transport
- ✓ Parallelized 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 (5)

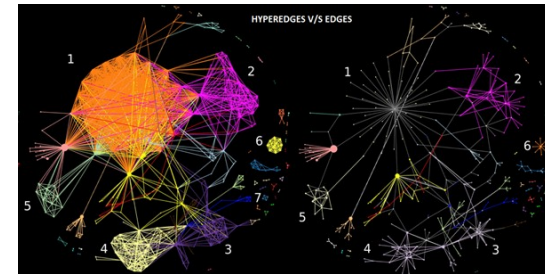
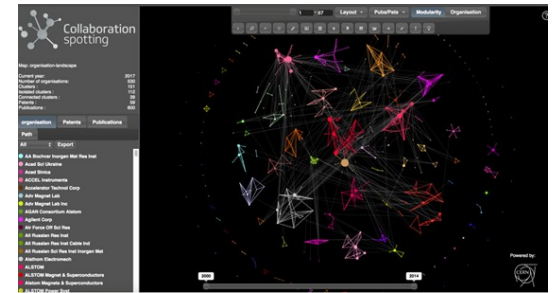
- ✓ Analysis of the spatial structure of SARS-CoV-2 protein using machine learning methods
- ✓ Quantum chemical study of the hydrolysis of oxidized endogenous psychedelic N,N-dimethyltryptamine
- ✓ N,N-dimethyltryptamine metabolism by the monoamine oxidase enzyme-A
- ✓ In silico studies to uncover the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

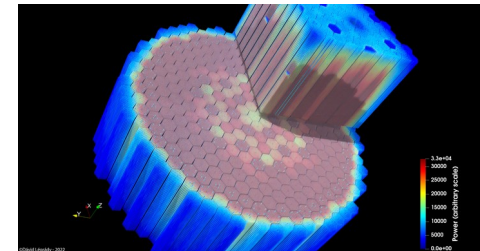
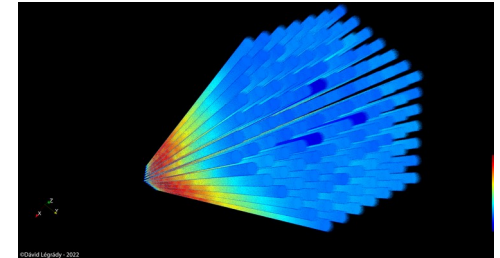
- ✓ 3D iterative image reconstruction software developed for proton computed tomography imaging
- ✓ Biasing the GUARDYAN GPU-based Monte Carlo code using space-, energy- and angle-dependent adjoint function
- ✓ Implementing Hastlayer support for Xilinx SoC Zynq FPGA family II.
- ✓ Evaluation of proton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



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 Hungaria 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

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 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



WSCLAB>_



WIGNER SCIENTIFIC COMPUTING LABORATORY







NEXT LEVEL: SciComp

INSTITUTE FOR SCIENTIFIC COMPUTING ASSOCIATION

Institute of Scientific Computing

INSTITUTE FOR SCIENTIFIC COMPUTING

The Institute was founded in March 2023 in the Ceremonial Hall of the Hungarian Academy of Sciences with the participation of over 100 prominent scientists, who are members of leading research institutions and universities in Hungary, representing various fields of scientific computations. Following the preparations, our Association was officially registered in August 2023.



HUN-REN
Hungarian Research Network





NEXT LEVEL: SciComp

INSTITUTE FOR SCIENTIFIC COMPUTING ASSOCIATION

The Institute was founded in March 2023 in the Ceremonial Hall of the Hungarian Academy of Sciences with the participation of over 100 prominent scientists, who are members of leading research institutions and universities in Hungary, representing various fields of scientific computations. Following the preparations, our Association was officially registered in August 2023.

Our aim is to support and promote the development of scientific computations in Hungary and to establish it as a scientific discipline.

Through the establishment of the organization, we intend to provide a professional forum, network, and community platform for researchers and developers actively engaged in the field of scientific computations.

We interpret scientific computations in the broadest sense, including scientific data mining, simulation, machine learning, artificial intelligence, and various numerical methods carried out with scientific rigor and precision, as well as their application in the fields of humanities, natural sciences, and social sciences.

We consider scientific computations as an independent scientific field that requires expertise in algorithms, mathematics, hardware, software, and the relevant applied sciences.

The Institute is a horizontal organization that seeks to achieve its goals through the voluntary and collaborative efforts of its members working at universities, research institutions, and corporate research centers.





NEXT LEVEL: SciComp



OUR ACTIVITIES

The Institute of Scientific Computing conducts various activities to support researchers, e)

Our goal is to promote dialogue among researchers and establish professional and perso scientific computing methods in their work or contribute to innovation in this field.

BUILDING CONNECTIONS AND RESEARCH

The Institute provides a platform where its members can build connections and share their research results.

We encourage our members to participate in professional discourse and publish their research results. Additionally, we publish research topics for theses, dissertations, scientific student research, and PhD topics.

CONFERENCE ORGANIZATION AND KNOWLEDGE DISSEMINATION

The Institute regularly organizes conferences, workshops, and seminar series on scientific computing.

Participation in professional events offers a great opportunity for professionals in the field to exchange knowledge and experience. In addition to organizing such events, the Institute collaborates with educational and professional organizations to provide courses and lectures for high school teachers to support the teaching of scientific computing.

Our association will hold its first conference on November 7-8, 2023. Learn more and find the registration link under the [Conference](#) section.

JOB OPPORTUNITIES

The Institute also supports career development in the field of scientific computing.

We regularly post job opportunities, professional/summer internship applications, internship job postings, and other job openings.

PROJECTS

The Institute initiates projects for high school students and teachers to support those interested in scientific computing and introduce them to practical applications.

The Institute of Scientific Computing is committed to advancing the field of scientific computing and spreading knowledge. We take pride in bringing together the scientific computing community and supporting the development of the field.





THX>_

