



One Lab Many Project

Review of the WSCLAB's Projects

Gergely Gábor Barnaföldi
WSCLAB, Wigner Research Centre for Physics

Support: NKFIH 2020-2.1.1-ED-2021-00179



ELKH | Eötvös Loránd
Research Network



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. Debrecezeni

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.



G.G. Barnafoldi: AIME 2022

WSCLAB @ NKFIH TOP50 Research Infrastructure

VISIT: 10TH FEBRUARY 2022.



G.G. Barnafoldi: AIME 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.

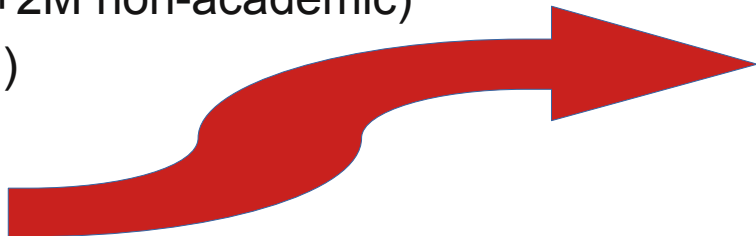
Our sponsors gain additional visibility at the event, on the webpage and related digital appearances including special interviews.



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



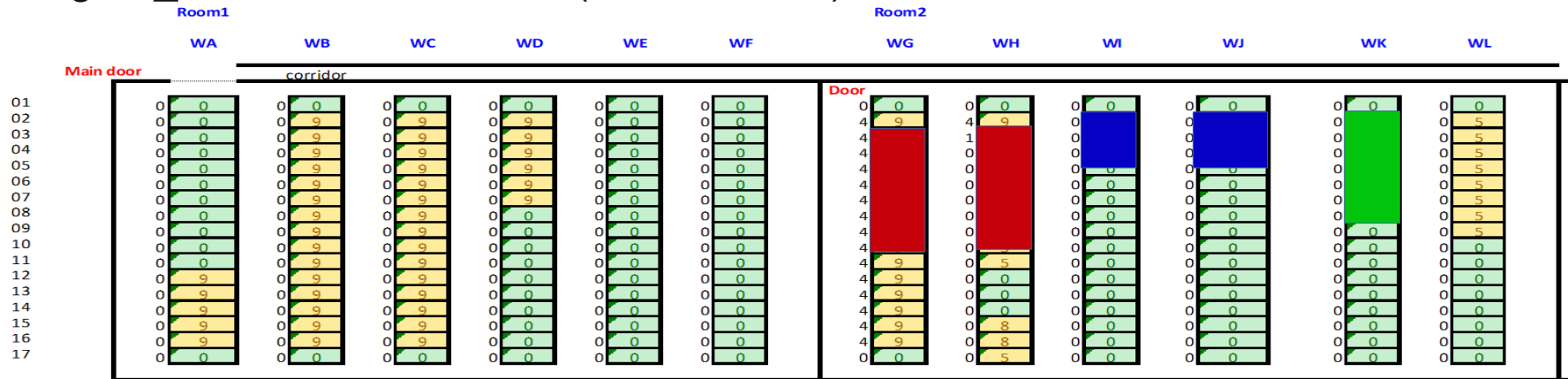


HARDWARES>_

WSCLAB @ WDC

THE PLACE

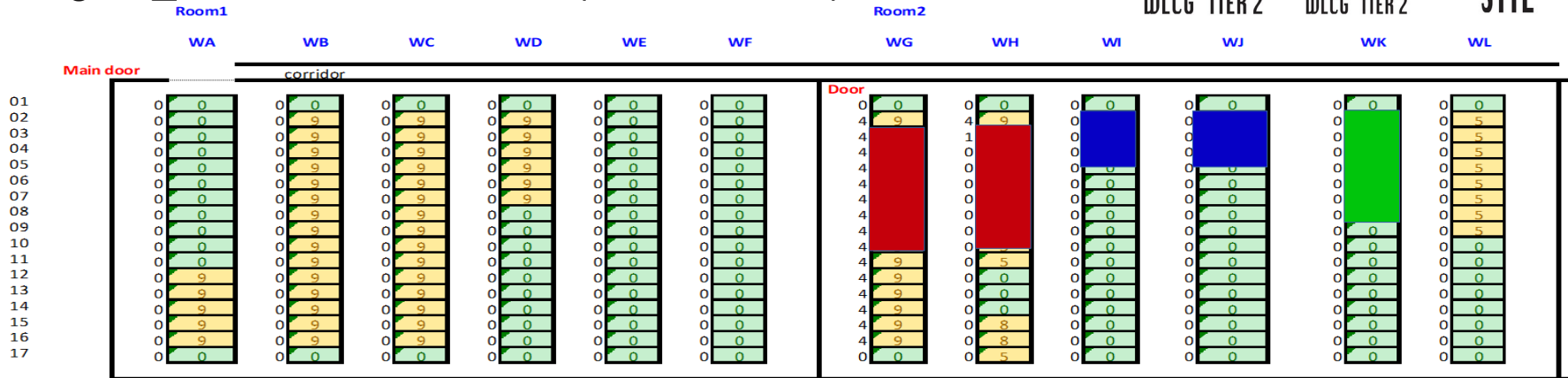
- ✓ Wigner Analysis Facility (Wigner AF)
- ✓ Wigner GPU Laboratory
- ✓ Wigner_KFKI WLCG T2 Grid (ALICE+CMS)



WSCLAB @ WDC

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ALICE

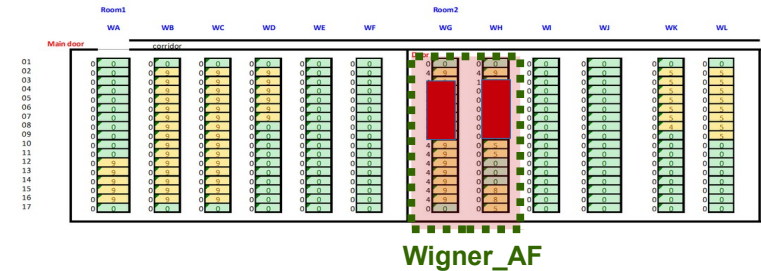
ANALYSIS FACILITY

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:

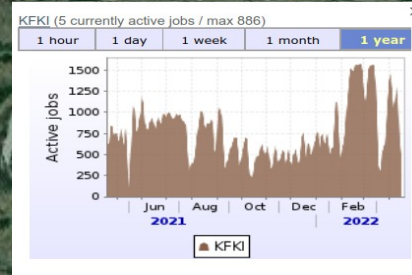
✓ Wigner_AF:

✓ WIGNER_KFKI:

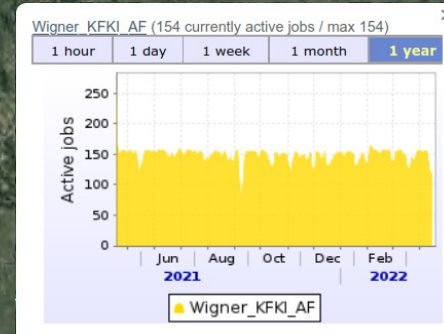


WIGNER_AF & ALICE T2 2022Q2 PERFORMANCE

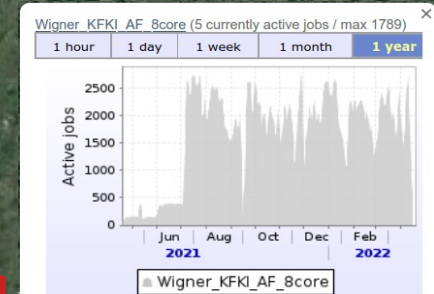
✓ Wigner_AF_8_core:



✓ Wigner_AF:



✓ WIGNER_KFKI:



WIGNER_KFKI

Wigner_KFKI_AF_8core

Wigner_KFKI_AF

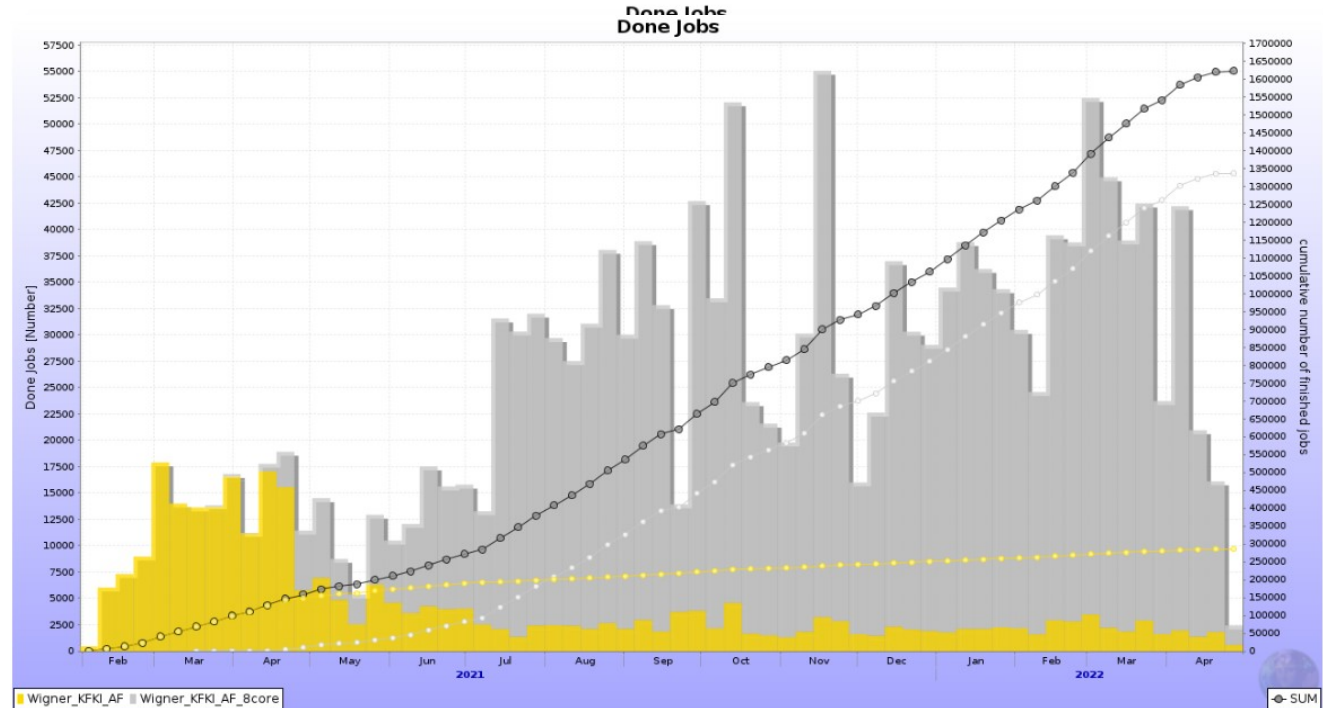
WIGNER_AF & ALICE T2 2022Q2

PERFORMANCE

✓ Wigner_AF_8_core:

✓ Wigner_AF:

✓ WIGNER_KFKI:



WIGNER_AF AS IS 2022Q1 PERFORMANCE

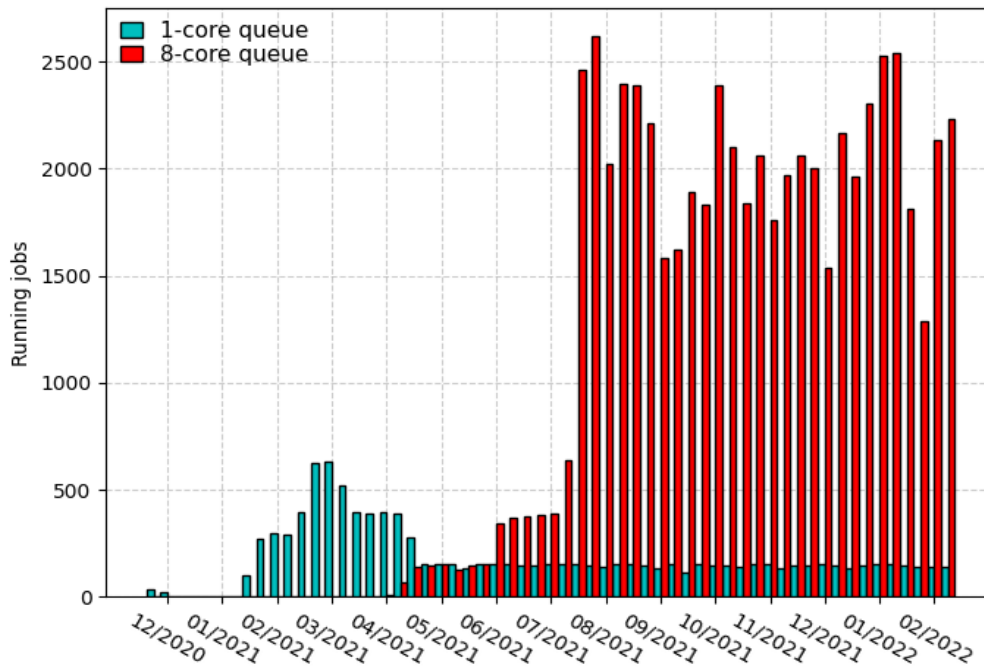
✓ Performance & Benchmark

- Test of
 - 1-core pool
 - 8-core pool
 - 1-core/8-core combined pool

✓ Contribution for ALICE Coll: Public N

- Presentation an CHEP/ACAT

The Wigner ALICE Analysis Facility



Gábor Bíró^{1,2}, Gergely Gábor Barnaföldi¹, Péter Lévai¹, Latchezar Betev³ and Jan Fiete Grosse-Oetringhaus³

WIGNER_AF AS IS 2022Q1

PERFORMANCE

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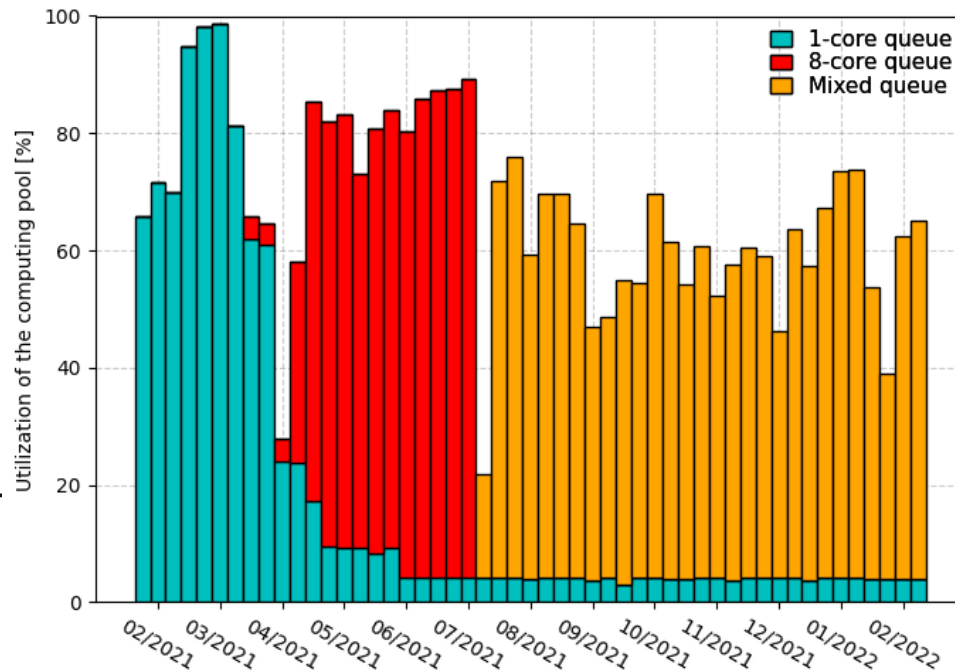
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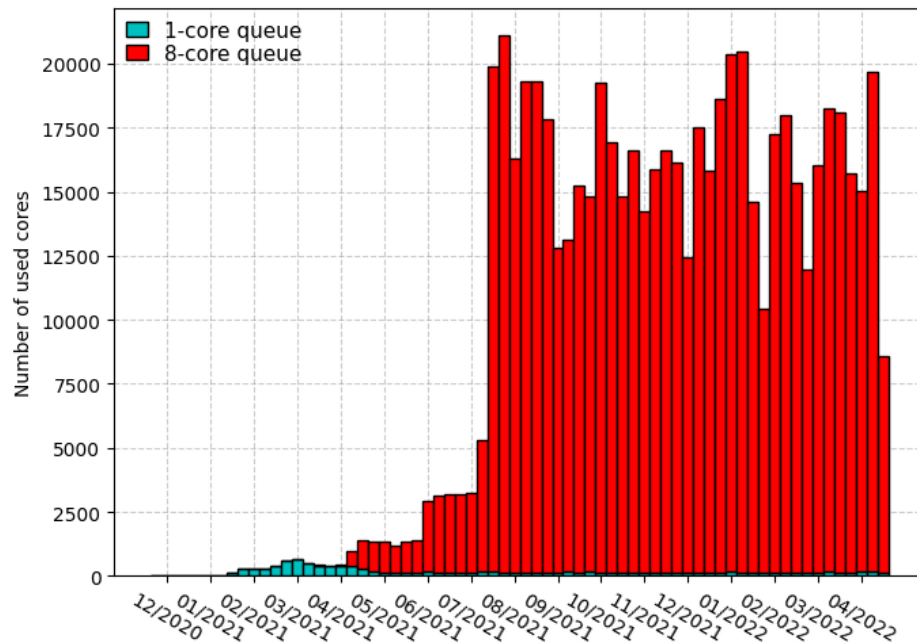
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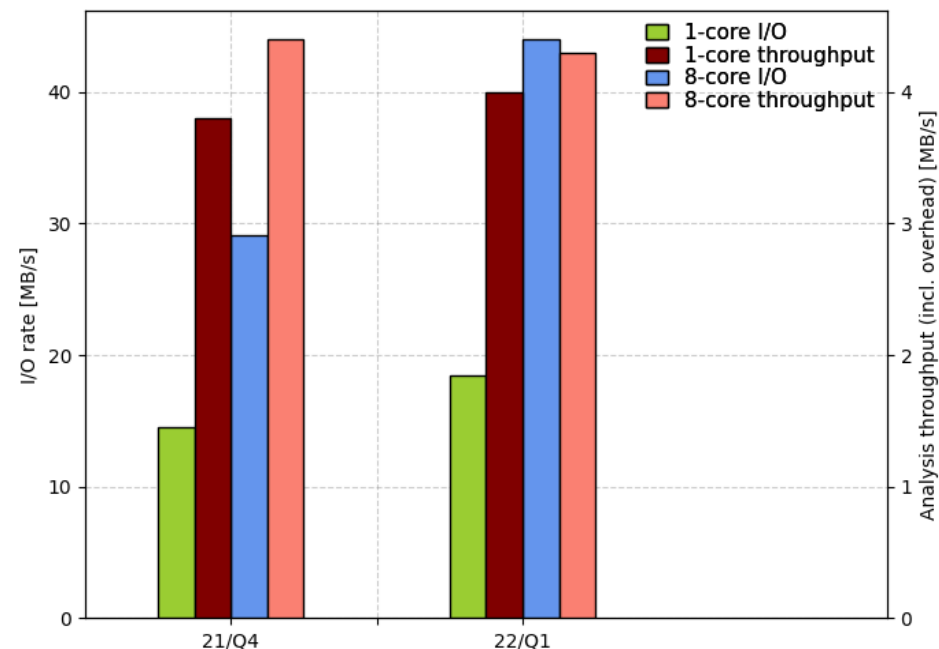
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ALICE



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:
 - 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



WL01	WL02	WL03	WL04	WL05	WL06	WK01	WK02	WK03	WK04	WK05	WK06	WK07	WK08	WK09	WK10	WK11	WK12	WK13	WK14	WK15	WK16	WK17	WK18	WK19	WK20	WK21	WK22	WK23	WK24	WK25	WK26	WK27	WK28	WK29	WK30	WK31	WK32	WK33	WK34	WK35	WK36	WK37	WK38	WK39	WK40	WK41	WK42	WK43	WK44	WK45	WK46	WK47	WK48	WK49	WK50	WK51	WK52	WK53	WK54	WK55	WK56	WK57	WK58	WK59	WK60	WK61	WK62	WK63	WK64	WK65	WK66	WK67	WK68	WK69	WK70	WK71	WK72	WK73	WK74	WK75	WK76	WK77	WK78	WK79	WK80	WK81	WK82	WK83	WK84	WK85	WK86	WK87	WK88	WK89	WK90	WK91	WK92	WK93	WK94	WK95	WK96	WK97	WK98	WK99	WK100	WK101	WK102	WK103	WK104	WK105	WK106	WK107	WK108	WK109	WK110	WK111	WK112	WK113	WK114	WK115	WK116	WK117	WK118	WK119	WK120	WK121	WK122	WK123	WK124	WK125	WK126	WK127	WK128	WK129	WK130	WK131	WK132	WK133	WK134	WK135	WK136	WK137	WK138	WK139	WK140	WK141	WK142	WK143	WK144	WK145	WK146	WK147	WK148	WK149	WK150	WK151	WK152	WK153	WK154	WK155	WK156	WK157	WK158	WK159	WK160	WK161	WK162	WK163	WK164	WK165	WK166	WK167	WK168	WK169	WK170	WK171	WK172	WK173	WK174	WK175	WK176	WK177	WK178	WK179	WK180	WK181	WK182	WK183	WK184	WK185	WK186	WK187	WK188	WK189	WK190	WK191	WK192	WK193	WK194	WK195	WK196	WK197	WK198	WK199	WK200	WK201	WK202	WK203	WK204	WK205	WK206	WK207	WK208	WK209	WK210	WK211	WK212	WK213	WK214	WK215	WK216	WK217	WK218	WK219	WK220	WK221	WK222	WK223	WK224	WK225	WK226	WK227	WK228	WK229	WK230	WK231	WK232	WK233	WK234	WK235	WK236	WK237	WK238	WK239	WK240	WK241	WK242	WK243	WK244	WK245	WK246	WK247	WK248	WK249	WK250	WK251	WK252	WK253	WK254	WK255	WK256	WK257	WK258	WK259	WK260	WK261	WK262	WK263	WK264	WK265	WK266	WK267	WK268	WK269	WK270	WK271	WK272	WK273	WK274	WK275	WK276	WK277	WK278	WK279	WK280	WK281	WK282	WK283	WK284	WK285	WK286	WK287	WK288	WK289	WK290	WK291	WK292	WK293	WK294	WK295	WK296	WK297	WK298	WK299	WK300	WK301	WK302	WK303	WK304	WK305	WK306	WK307	WK308	WK309	WK310	WK311	WK312	WK313	WK314	WK315	WK316	WK317	WK318	WK319	WK320	WK321	WK322	WK323	WK324	WK325	WK326	WK327	WK328	WK329	WK330	WK331	WK332	WK333	WK334	WK335	WK336	WK337	WK338	WK339	WK340	WK341	WK342	WK343	WK344	WK345	WK346	WK347	WK348	WK349	WK350	WK351	WK352	WK353	WK354	WK355	WK356	WK357	WK358	WK359	WK360	WK361	WK362	WK363	WK364	WK365	WK366	WK367	WK368	WK369	WK370	WK371	WK372	WK373	WK374	WK375	WK376	WK377	WK378	WK379	WK380	WK381	WK382	WK383	WK384	WK385	WK386	WK387	WK388	WK389	WK390	WK391	WK392	WK393	WK394	WK395	WK396	WK397	WK398	WK399	WK400	WK401	WK402	WK403	WK404	WK405	WK406	WK407	WK408	WK409	WK410	WK411	WK412	WK413	WK414	WK415	WK416	WK417	WK418	WK419	WK420	WK421	WK422	WK423	WK424	WK425	WK426	WK427	WK428	WK429	WK430	WK431	WK432	WK433	WK434	WK435	WK436	WK437	WK438	WK439	WK440	WK441	WK442	WK443	WK444	WK445	WK446	WK447	WK448	WK449	WK450	WK451	WK452	WK453	WK454	WK455	WK456	WK457	WK458	WK459	WK460	WK461	WK462	WK463	WK464	WK465	WK466	WK467	WK468	WK469	WK470	WK471	WK472	WK473	WK474	WK475	WK476	WK477	WK478	WK479	WK480	WK481	WK482	WK483	WK484	WK485	WK486	WK487	WK488	WK489	WK490	WK491	WK492	WK493	WK494	WK495	WK496	WK497	WK498	WK499	WK500	WK501	WK502	WK503	WK504	WK505	WK506	WK507	WK508	WK509	WK510	WK511	WK512	WK513	WK514	WK515	WK516	WK517	WK518	WK519	WK520	WK521	WK522	WK523	WK524	WK525	WK526	WK527	WK528	WK529	WK530	WK531	WK532	WK533	WK534	WK535	WK536	WK537	WK538	WK539	WK540	WK541	WK542	WK543	WK544	WK545	WK546	WK547	WK548	WK549	WK550	WK551	WK552	WK553	WK554	WK555	WK556	WK557	WK558	WK559	WK560	WK561	WK562	WK563	WK564	WK565	WK566	WK567	WK568	WK569	WK570	WK571	WK572	WK573	WK574	WK575	WK576	WK577	WK578	WK579	WK580	WK581	WK582	WK583	WK584	WK585	WK586	WK587	WK588	WK589	WK590	WK591	WK592	WK593	WK594	WK595	WK596	WK597	WK598	WK599	WK600	WK601	WK602	WK603	WK604	WK605	WK606	WK607	WK608	WK609	WK610	WK611	WK612	WK613	WK614	WK615	WK616	WK617	WK618	WK619	WK620	WK621	WK622	WK623	WK624	WK625	WK626	WK627	WK628	WK629	WK630	WK631	WK632	WK633	WK634	WK635	WK636	WK637	WK638	WK639	WK640	WK641	WK642	WK643	WK644	WK645	WK646	WK647	WK648	WK649	WK650	WK651	WK652	WK653	WK654	WK655	WK656	WK657	WK658	WK659	WK660	WK661	WK662	WK663	WK664	WK665	WK666	WK667	WK668	WK669	WK670	WK671	WK672	WK673	WK674	WK675	WK676	WK677	WK678	WK679	WK680	WK681	WK682	WK683	WK684	WK685	WK686	WK687	WK688	WK689	WK690	WK691	WK692	WK693	WK694	WK695	WK696	WK697	WK698	WK699	WK700	WK701	WK702	WK703	WK704	WK705	WK706	WK707	WK708	WK709	WK710	WK711	WK712	WK713	WK714	WK715	WK716	WK717	WK718	WK719	WK720	WK721	WK722	WK723	WK724	WK725	WK726	WK727	WK728	WK729	WK730	WK731	WK732	WK733	WK734	WK735	WK736	WK737	WK738	WK739	WK740	WK741	WK742	WK743	WK744	WK745	WK746	WK747	WK748	WK749	WK750	WK751	WK752	WK753	WK754	WK755	WK756	WK757	WK758	WK759	WK760	WK761	WK762	WK763	WK764	WK765	WK766	WK767	WK768	WK769	WK770	WK771	WK772	WK773	WK774	WK775	WK776	WK777	WK778	WK779	WK780	WK781	WK782	WK783	WK784	WK785	WK786	WK787	WK788	WK789	WK790	WK791	WK792	WK793	WK794	WK795	WK796	WK797	WK798	WK799	WK800	WK801	WK802	WK803	WK804	WK805	WK806	WK807	WK808	WK809	WK810	WK811	WK812	WK813	WK814	WK815	WK816	WK817	WK818	WK819	WK820	WK821	WK822	WK823	WK824	WK825	WK826	WK827	WK828	WK829	WK830	WK831	WK832	WK833	WK834	WK835	WK836	WK837	WK838	WK839	WK840	WK841	WK842	WK843	WK844	WK845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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



Wigner GPU
Laboratory



Wigner GPU Laboratory (@WDC)

NEW HARDWARES (IN PROGRESS), HAPPY USERS

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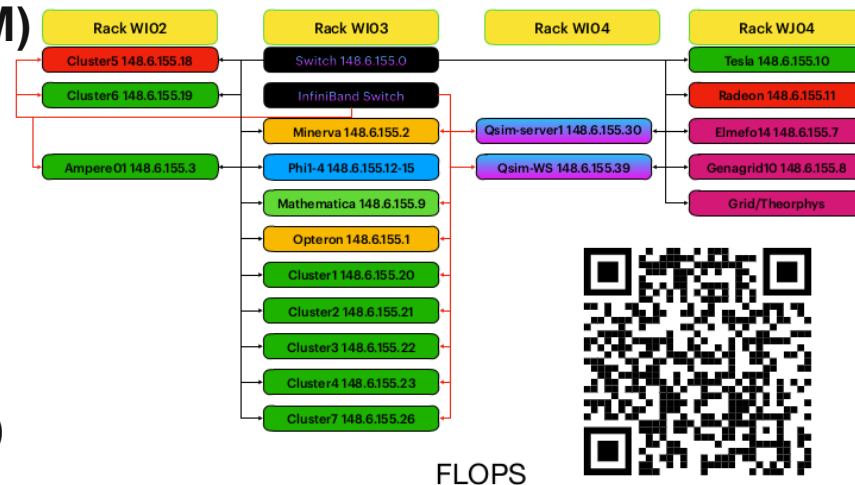


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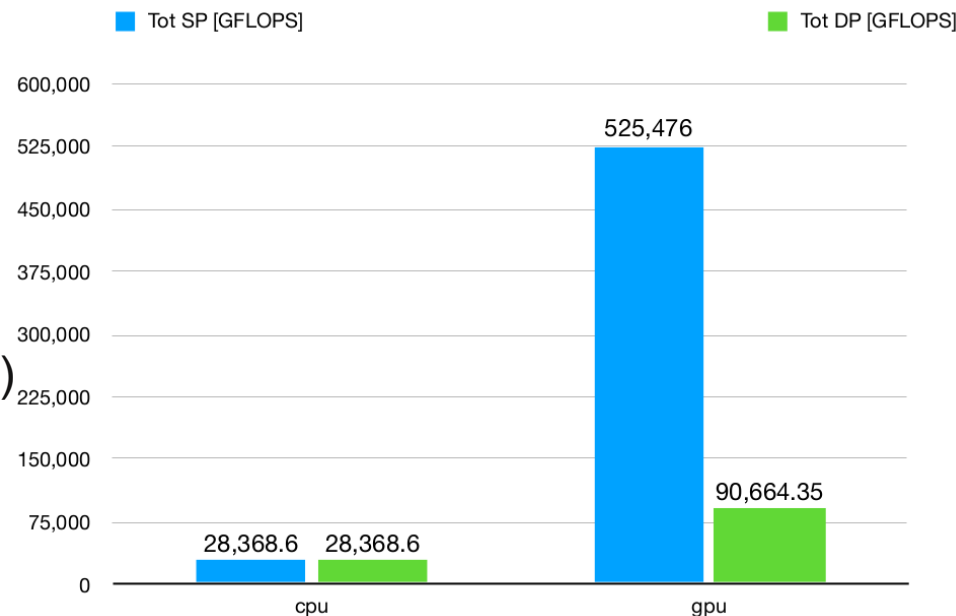
	cpu	gpu	Total Mem
Tot SP [GFLOPS]	28,368.6	525,476	3,056 GB
Tot DP [GFLOPS]	28,368.6	90,664	

Wigner GPU Laboratory (@WDC)

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





EVENTS>_

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

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

[illegible][illegible]

- 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

THE FUTURE OF MANY-MANY CORES IN SCIENCE

The event is supported by:

- wigner
- silicon computers
- AMD
R1000
- SOLIDANGLE

WINE:
WINEBOT RESEARCH CENTER
FOR PHYSICS OF THE H.A.S.T.

H-1121 BUDAPEST, HUNGARY
KISMETI UTCA 10/105. ST. 30. 33.
MANY DATA CENTER

WEB & REGISTRATION:
GPU.WIGNER.MTA.HU
E-MAIL:
GPU@WIGNER.MTA.HU

PROGRAM:

- 8:00 AM REGISTRATION - ENTRY TO THE CONGRESS
- 9:00 AM - GETTING FROM THE CONGRESS REGISTRATION PLAZA TO THE HALL
- 9:30 AM - THE FUTURE OF THE PHYSICAL SIMULATION AT CERN
- 10:00 AM - CERN/MS/2014/001
- 10:30 AM - THE FUTURE COMPUTING WITH SCALIN CORES
- 11:00 AM - SCALIN CORES
- 11:30 AM - SCALIN CORES
- 12:00 PM - LUNCH
- 1:30 PM - AMD IN TRANSFORMING SYSTEM ARCHITECTURES: SOFTWARE AND BUILDING BLOCKS
- 2:00 PM - SCALIN CORES
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[illegible]

6TH GPU DAY



The Future of Many-Core Computing in Science

2ND JUN 3RD JUN

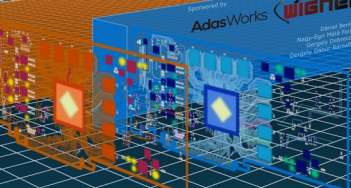
Symposium	HPC for Research and Education AMD - Radeon Open Compute
Lectures	SYCL Building blocks Haskell - Next to FGPA Parallel Vector Expressions
Topics	Gravitational waves Surface Growth Incompressible Fluids Heavy-Ion Event Generation
Astronomy	Galaxy Spectra Analysis Light Curve Modeling Orbital Element Determination Eclipse Timing Variation Cosmological Constant & Black Holes

Speaker Bio	Volkan Fost Paths HoloViz.io
Topic Processing	Self - Driving Cars Line Segment Detection Depth Image Fusion
Medical Imaging	CT Ring Artifact Removal Photorealistic CT Visualization EEG Processing & Visualization

indico.kit.edu/gpuDay2016 powered by

AdasWorks is a joint project of the Wigner Research Center for Physics and the Institute for Information Technology at the Hungarian Academy of Sciences.



GPU DAY 2019

The Future of Computing, Graphics and Data Analysis

11-12 07 2019

WIGNER SCIENTIFIC COMPUTING LABORATORY GPU DAY 2022

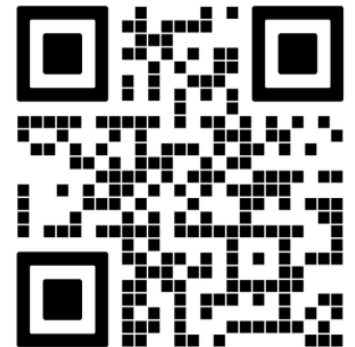
20-21. JUNE



MORE INFORMATION AND REGISTRATION:

[HTTPS://GPU DAY.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



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)



LECTURES ON MODERN SCIENTIFIC PROGRAMMING



ELKH | Eötvös Loránd
Research Network



MACHINE LEARNING, NEURAL NETWORKS, FEATURE RECOGNITION

FIELD PROGRAMMABLE GATE ARRAYS

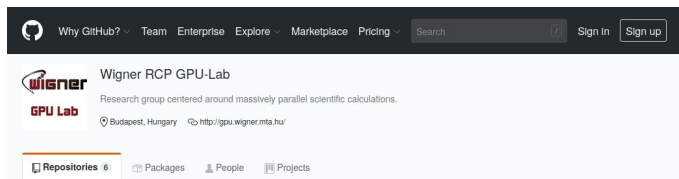
HANDS-ON SESSIONS

QUANTUM COMPUTING SIMULATION

QUANTUM MACHINE LEARNING AND SIMULATIONS

MANY-CORE COMPUTING IN PHYSICS AND OTHER FIELDS OF SCIENCE

WSCLAB's EDUCATIONAL MATTERS



OpenCL-Primer

Documentation on how to get started with OpenCL programming

BSD-3-Clause 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 1 (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

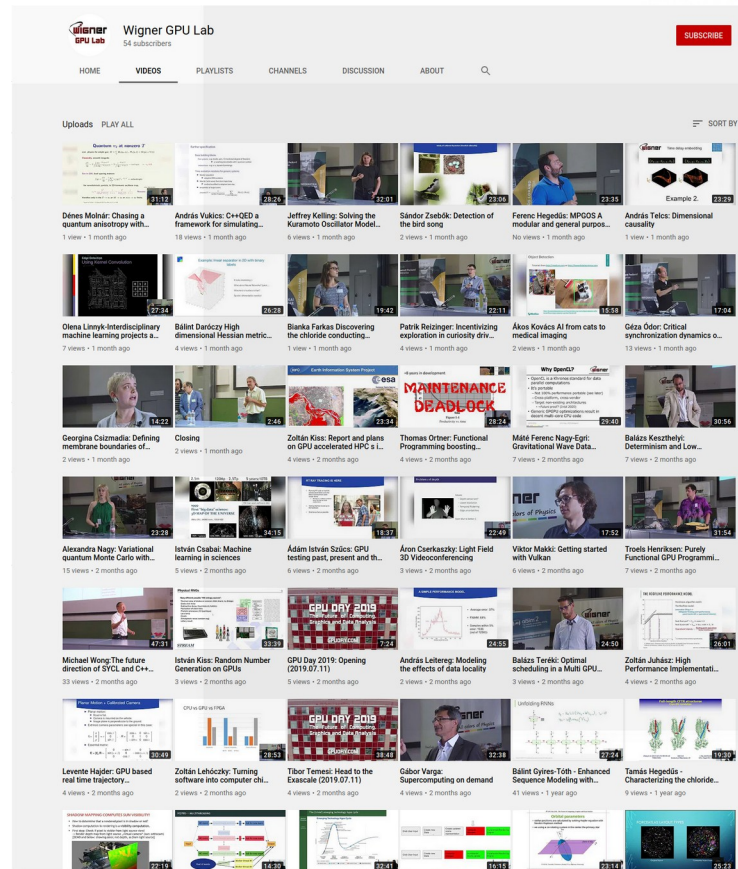
Sample codes from the Lectures On Modern Scientific Programming series

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

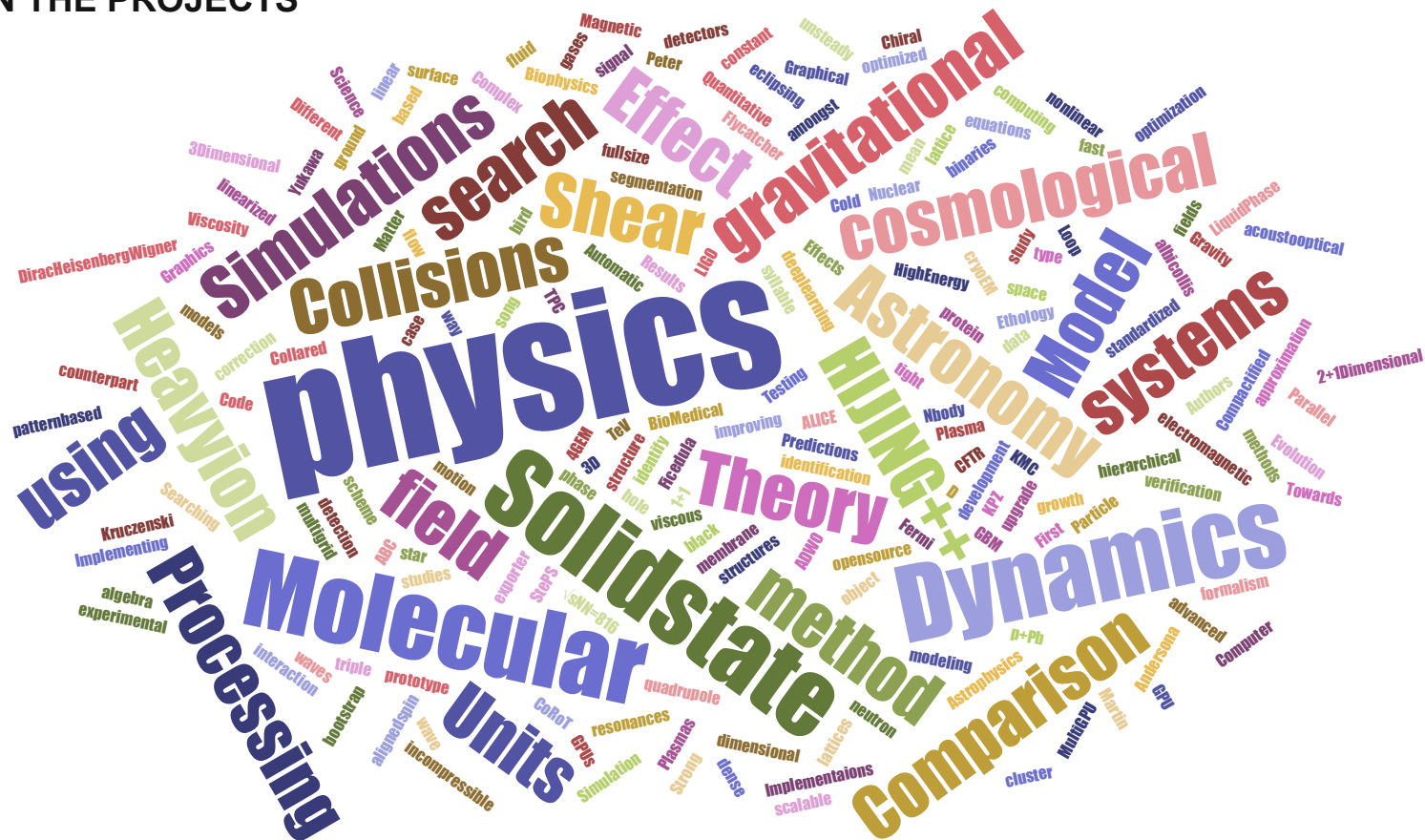


GitHub



PROJECTS>_

WSCLAB's SCIENTIFIC RESULTS

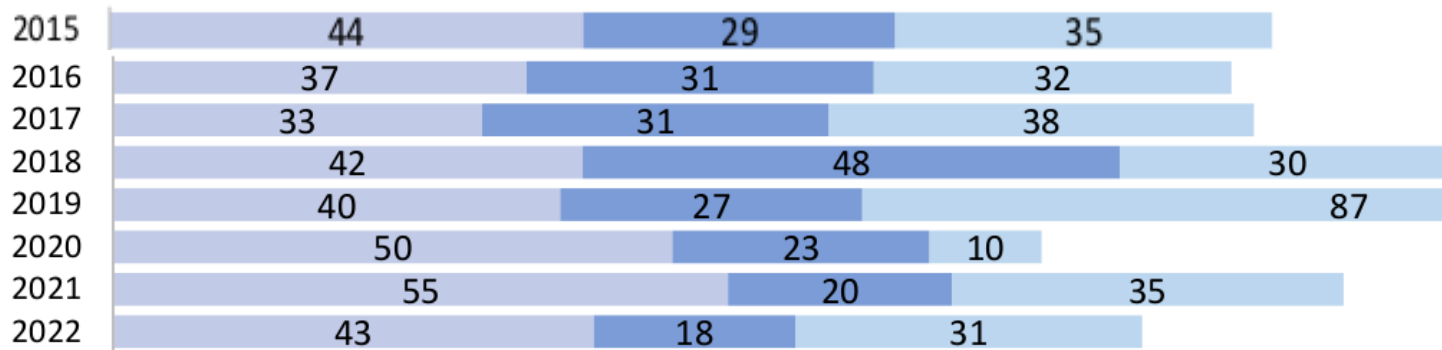




WSCLAB in numbers

KNOWLEDGE HUB: GPU DAY.COM

- ✓ 7 Lectures on Modern Computing in Science
- ✓ 12 GPU Days



- ✓ 40 WSCLAB (Wigner GPU Lab) Fellowship (40 finished + 9 running)
- ✓ 33+ industrial & academic partners (Lombiq LTD, Ericsson, Khronos, CERN...)
- ✓ 50+ 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

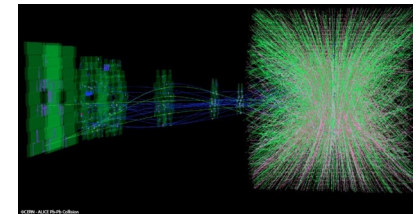
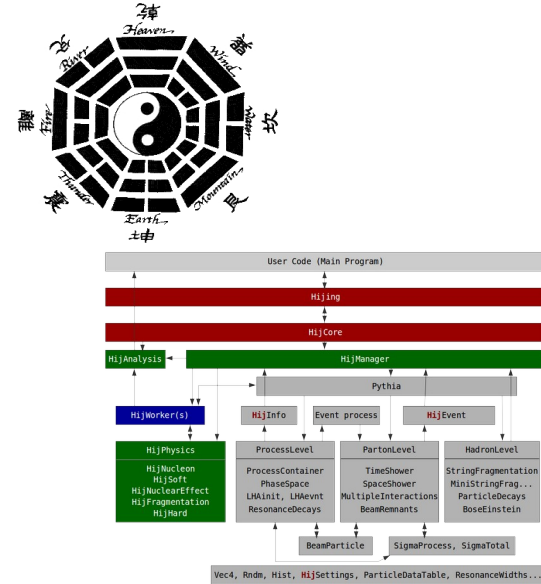
- More than 40 publications & public codes



WSCLAB's SCIENTIFIC PROJECTS

PHYSICS (15)

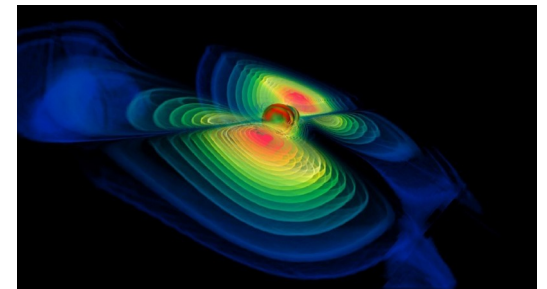
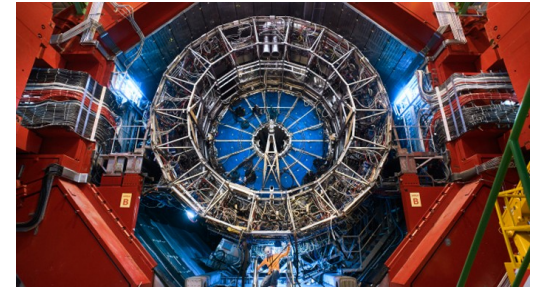
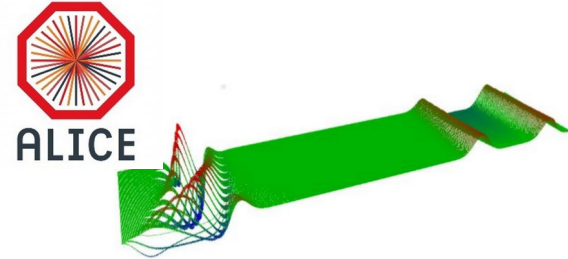
- ✓ Simulating the photo-ionisation of Rubidium atoms
- ✓ High Performance Computing for Nanofusion
- ✓ High performance Monte Carlo simulations of high-energy heavy-ion collisions
- ✓ Modelling non-linear optics by machine learning techniques
- ✓ Nanoplasmonic Laser Fusion
- ✓ Generation of Gravitational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

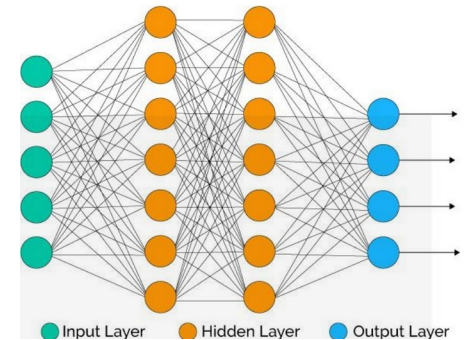
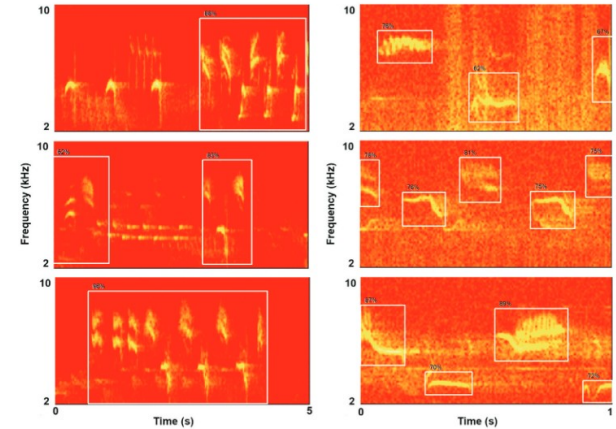
- ✓ Optimization and Development of High-performance Computing pipeline to search for gravitational radiation from rotating NS by means of GPU-based Hardware Accelerators
- ✓ ALICE TCP GEM QA – GPU-accelerated image analysis
- ✓ Viscous corrections from linearized Boltzmann transport
- ✓ Parallelized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

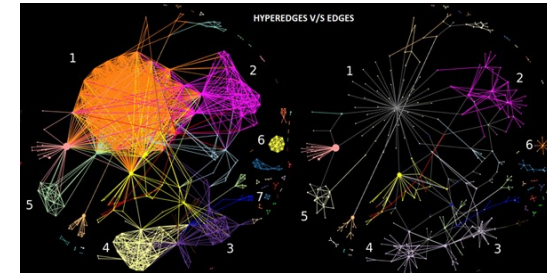
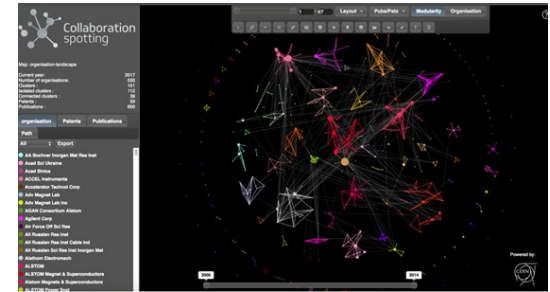
- ✓ Analysis of the spatial structure of SARS-CoV-2 protein using machine learning methods
- ✓ Quantum chemical study of the hydrolysis of oxidized endogenous psychedelic N,N-dimethyltryptamine
- ✓ N,N-dimethyltryptamine metabolism by the monoamine oxidase enzyme-A
- ✓ In silico studies to uncover the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

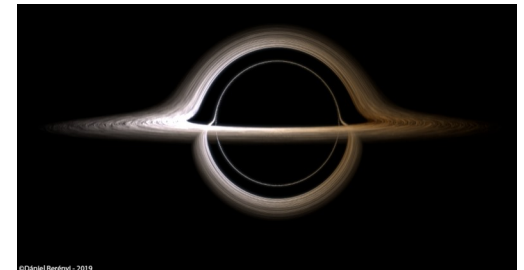
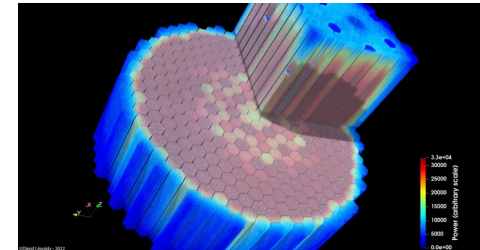
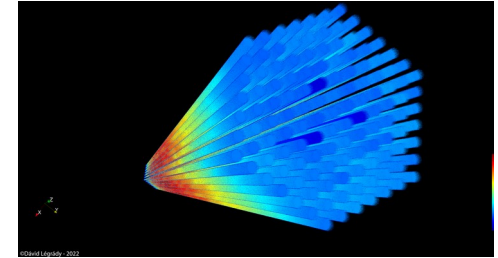
- ✓ 3D iterative image reconstruction software developed for proton computed tomography imaging
- ✓ Biasing the GUARDYAN GPU-based Monte Carlo code using space-, energy- and angle-dependent adjoint function
- ✓ Implementing Hastlayer support for Xilinx SoC Zynq FPGA family II.
- ✓ Evaluation of proton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

→ See Talks tomorrow Z. Zimborás et al



FUTURE>_

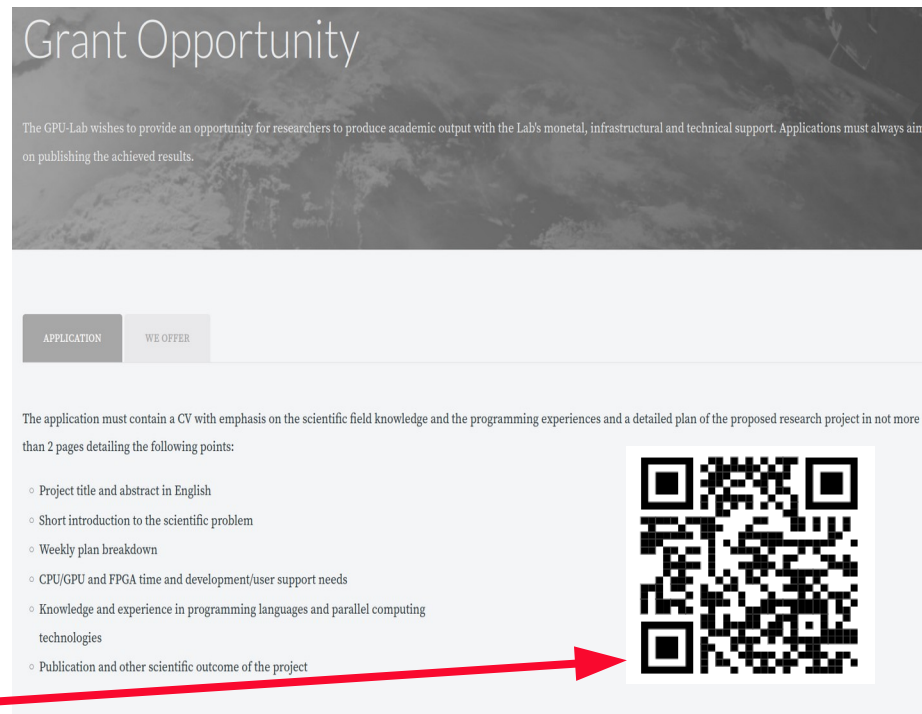
WSCLAB's FUTURE IS IN YOUR HAND

✓ 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



The screenshot shows a webpage titled "Grant Opportunity". The header text states: "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." Below this, there are two tabs: "APPLICATION" (selected) and "WE OFFER". The main content area under the "APPLICATION" tab specifies: "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:" followed by a bulleted list of requirements. A red arrow points from the URL in the list below to a QR code on the right side of the page.


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's FUTURE

PLANS FOR THE FUTURE

✓ **Short timescale**

- Finishing the running projects & make them publish
- New WSCLAB Grants for young scientists at 2023Q1
- GPU Day & Lectures on Modern Computing in Science series in 2023
- 100Gbps connection to GEANT network

✓ **Intermediate timescale**

- Further hardware developments

✓ **Long range plan**

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

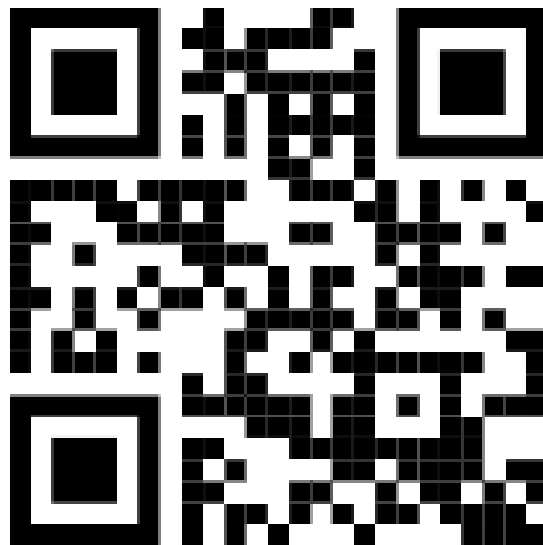




WSCLAB>_



WIGNER SCIENTIFIC COMPUTING LABORATORY



ELKH | Eötvös Loránd
Research Network





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	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

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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



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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

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		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