

**SUPERCOMPUTING FRONTIERS
EUROPE 2021**

JULY 19-23, 2021

POST-CONFERENCE REPORT

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ABOUT THE ORGANISER

Established by a resolution of the Senate of the University of Warsaw dated 29 June 1993 the **Interdisciplinary Centre for Mathematical and Computational Modelling (ICM) University of Warsaw**, is one of the top HPC centers in Poland.

ICM is engaged in serving the needs of a large community of computational researchers in Poland through provision of HPC and grid resources, storage, networking and expertise. ICM is involved in an interdisciplinary scientific research based on mathematical modeling, computer simulations, multi-scale and large-scale calculations, and teaching in the above areas.

The popular **meteo.pl weather portal** for the last 27 years has been providing the most accurate weather predictions for Poland and is being visited about 200 million times a year. ICM researchers created **decision support tool for global civil aviation** (in collaboration with ICAO). Since May 2020, ICM has been supporting the Polish Government and crisis management authorities in Poland by providing short and long term predictions of the epidemic in Poland using ICM **Epidemiological Model for the COVID-19**. ICM plays a crucial role in securing access for Polish scientists from over 500 institutions to the entire body of scientific literature by maintaining the **Virtual Library of Science**. ICM networking team has participated in a number of **cutting edge networking solutions**, both for high throughput and low latency requirements. In 2019, ICM engineers have established a production 100Gbps connection over 20.000 km CAE-1 (Collaboration Asia Europe-1) line between Warsaw and Singapore.

A WORD FROM THE CHAIRMAN

We are witnessing a very interesting period of intense, concerted and carefully planned European engagement in the global supercomputing development. At this seventh edition of Supercomputing Frontiers Europe 2021 we've heard reports on the progress and activities of EuroHPC Joint Undertaking as well as reports from several major European HPC Centres. Irene Qualters from Los Alamos National Laboratory provided the current US Department of Energy perspective on supercomputing technology and science. This year we focused on some of the major game changers in our field: Cloud HPC and interplay of AI, ML and HPC.

Several reports in "Focus on India" and "Focus on Africa" themes informed us on notable computing activities in these important regions of the world. SCFE 2021 was again run as a virtual conference but this has helped us reach a much wider audience of over 800 registrants from 77 countries. We are on the right track to establish SCFE as a permanent forum for exchange of new ideas and discussion of emerging technologies in supercomputing.



MAREK MICHALEWICZ
CHAIRMAN



SCIENTIFIC COMMITTEE

PROGRAMME CHAIR

Marek Michalewicz, ICM University of Warsaw

MEMBERS

Jean-Thomas Acquaviva, Data Direct Networks Storage

Michael Bader, Technical University of Munich

Piotr Bala, ICM University of Warsaw

Natalie Bates, Energy Efficient HPC Working Group

Maciej Brodowicz, CREST, Indiana University

Vladimir Brusic, University of Nottingham

Michael Bussman, Helmholtz-Zentrum Dresden-Rossendorf

Choong-Seock Chang, Princeton University

Maciej Cytowski, Pawsey Supercomputing Centre

Bronis de Supinski, Lawrence Livermore National Laboratory

Ewa Deelman, University of Southern California

Vassil Dimitrov, University of Calgary

Jack Dongarra, University of Tennessee

Nicola Ferrier, Argonne National Laboratory

Grzegorz Gruszczynski, ICM University of Warsaw

Nicola Ferrier, Argonne National Laboratory

John L. Gustafson, National University of Singapore

Michal Hermanowicz, ICM University of Warsaw

Wojciech Hellwing, Center for Theoretical Physics PAS

Torsten Hoefler, ETH Zurich

Eliu Huerta Escudero, University of Chicago and Argonne National Laboratory

Daniel S. Katz, University of Illinois at Urbana-Champaign

Scott Klasky, Oak Ridge National Laboratory

Kimmo Koski, CSC – IT Center for Science Ltd

Tomasz Kosciolk, University of California

Julian Kunkel, University of Reading

James Lin, Shanghai Jiao Tong University

Gerald Lofstead, Sandia National Laboratories

Ronald Luijten, Data Motion Architecture & Services GmbH

Allen D. Malony, University of Oregon

Madhav Marathe, Virginia Bioinformatics Institute, Virginia Tech

Bruno Michel, IBM Zurich Research Laboratory

Richard Murphy, Gem State Informatics, Inc.

Jaroslav Nabrzyski, University of Notre Dame

Manish Parashar, University of Utah

Ivo F. Sbalzarini, TU Dresden & Max Planck Institute of Molecular Cell Biology and Genetics

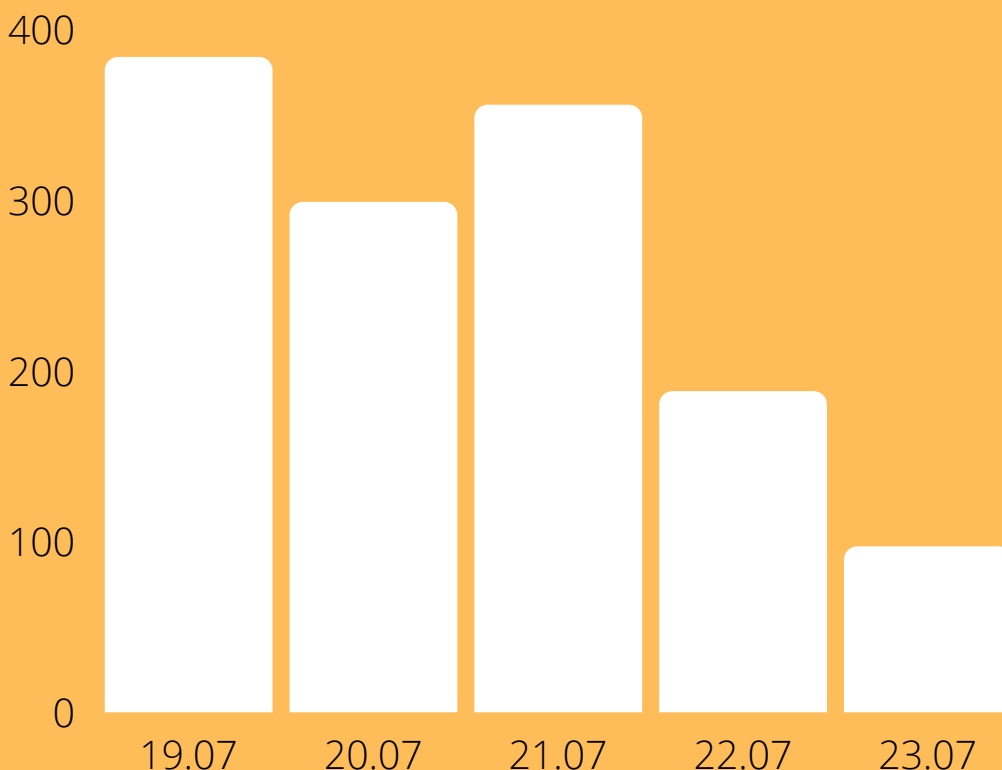
Sven-Bodo Scholz, Heriot-Watt University

Rick Stevens, Argonne National Laboratory & The University of Chicago

Vladimir Voevodin, Lomonosov Moscow State University

Roman Wyrzykowski, Czestochowa University of Technology

Alexandros Nikolaos Ziogas, ETH Zurich



VISITORS

The chart shows the number of unique logins during each day of SCFE21 conference. First three days attracted, on average, 346 visitors, while the workshops had engaged 188 and 97 people respectively.

SCFE 2021 STATS

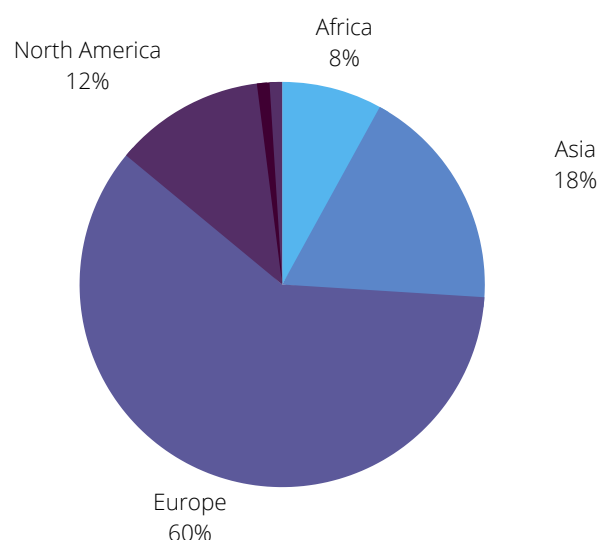
The number of registrations amounted to 834 people from 77 countries (67 countries in 2020) and the number of unique visits during the event summed up to 775.

The conference gathered 43 distinguish speakers including 4 keynote speakers: Irene Qualters from Los Alamos National Laboratory, Anders Jensen, the Executive Director of the EuroHPC JU, Hiroaki Kitano from The Systems Biology Institute and Roberto Car, the recipient of the 2020 ACM Gordon Bell Prize, from Princeton University.

SCFE21 had the pleasure to be joined by 8 excellent chairmen/chairwoman: Marek Michalewicz [ICM UW], Norbert Meyer [PSNC], Karolina Szafranek [ICM UW], Dirk Pleiter [KTH Royal Institute of Technology], Ronald Luijten [Data Motion Architecture & Services], Taisuke Boku [University of Tsukuba], Wlodzislaw Duch [Nicolaus Copernicus University] and Sharan Kalwani [Senior Member IEEE].

The event featured two special segments: 'Focus on Africa' and 'Focus on India' where scientists from Uganda, Botswana, South Africa and India were breaking the geographical barriers in HPC development and integration prompting heightened interest in the conference in Africa and Asia.

Attendees per continent showed below.



834

The number of registrations for
the Supercomputing Frontiers
Europe 2021

755

The number of unique visits
during the entire event
(conference + workshops)

41%

The percentage of registrations
from universities from around
the world

59%

The percentage of registrations
from industry companies, media
and not specified

CONFERENCE DAY 1

First day of Supercomputing Frontiers Europe 2021 focused on current and future initiatives within Europe, the States and Africa. The conference hosted two **keynote speakers: Anders Jensen**, the executive director of EuroHPC JU and **Irene Qualters**, the associate laboratory director of Los Alamos National Laboratory. One of the last segments was a roundtable talk moderated by Addison Snell from InterSect360 Research.

"At European Processor Initiative we have one overall objective which is to develop a complete EU designed high-end microprocessor, addressing supercomputing and edge-HPC segments."



Jean- Marc Denis

Chair of the Board, European Processor Initiative

THE THEMATIC BLOCKS

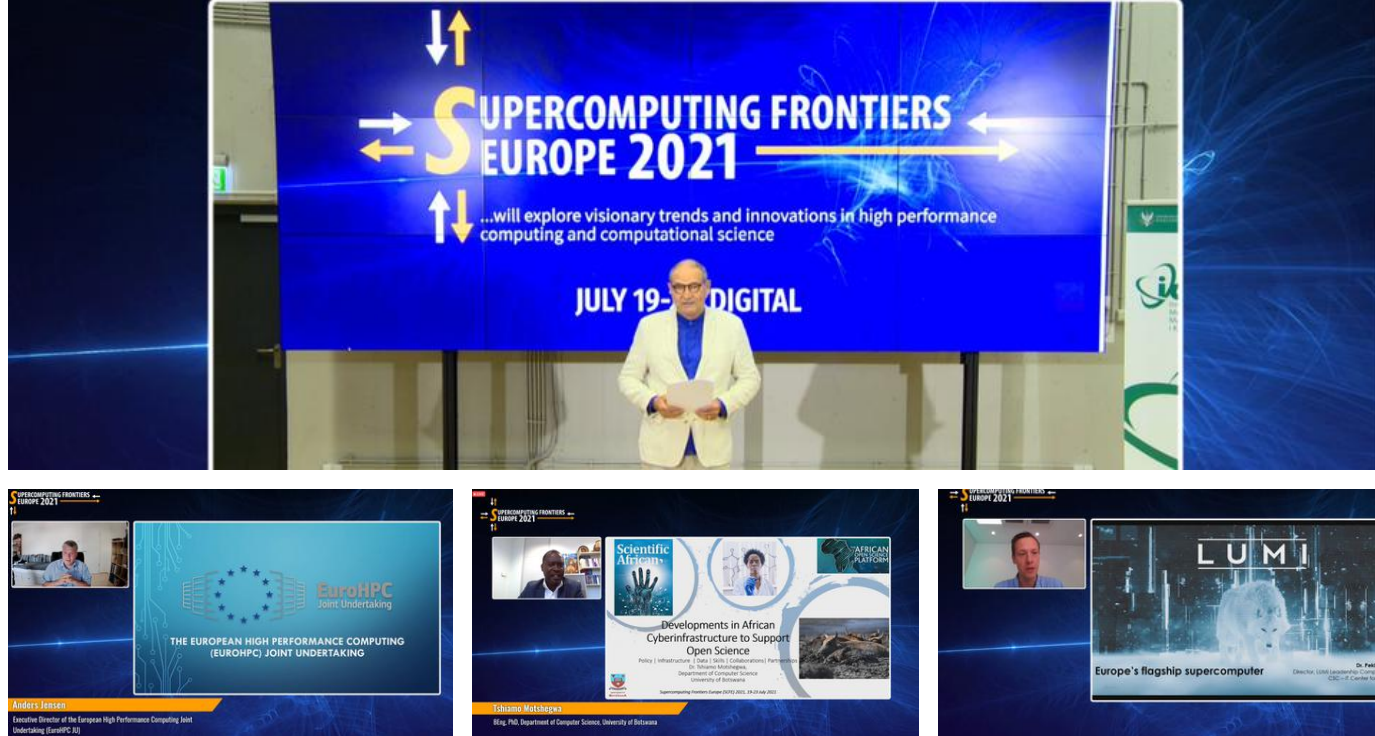
- **European Initiatives** [featuring CASUS, EuroHPC JU, LUMI, FF4EuroHPC, LRZ, European Processor Initiative]
- **African Initiatives** [feat. University of Botswana]
- **US perspective** [feat. Los Alamos National Laboratory]
- **Industry perspective** [Roundtable panel on Industry trends for HPC and AI with Addison Snell]
- **Students and education** [feat. Warsaw Team]

"As we go towards exascale computing , lot of the large -scale HPC will start looking like hyper-scale deployments."



Gaurav Kaul

Solutions Architect AI & HPC
Hewlett Packard Enterprise



SPEAKERS IN ORDER OF PRESENTATION - DAY 1

MAREK MICHALEWICZ

Opening words

KEYNOTE: ANDERS JENSEN

"EuroHPC JU at full throttle"

VALENTIN PLUGARU

MeluXina – a new generation supercomputer

KEYNOTE: IRENE QUALTERS

"The Enduring Role of HPC: Advancing Science and Engineering"

PEKKA MANNINEN

LUMI: Europe's flagship supercomputer

JEAN-MARC DENIS

"Future Supercomputers are game changers for processor architecture. Why?"

TOMI ILIJAS

FF4EuroHPC: Enabling SMEs to benefit from HPC – Open Call 2

GAURAV KAUL

"Memory and Interconnect Interplay in System Architecture"

HERBERT HUBER

Energy efficient supercomputing at LRZ

MACIEJ BRZEŹNIAK

"National Data Storage"

ATTILA CANGI

Data-driven Surrogate Modeling of Matter under Extreme Conditions

ROUNDTABLE WITH ADDISON SNELL

"Industry trends for HPC and AI"

TSHIAMO MOTSHEGWA

Developments in African Cyber-infrastructure to Support Open Science & Open Data

PATRYCJA KRZYNA, MAREK MASIAK, MAREK SKIBA

"Warsaw Team: Student participation in HPC competitions amidst a global pandemic"

ROUNDTABLE

Addison Snell invited three distinguished speakers to the roundtable discussion where the panelists were asked about the industry trends for HPC, AI and cyber-infrastructure. The idea of openness was one of the main points of the debate. The viewers were exposed to three different, yet very similar and insightful perspectives: Anders Jenses representing Europe, Irene Qualters- USA and Tshiamo Motshegwa- Africa.

"As analysts, we seek out any opportunity to talk to visionary leaders about the state and direction of the HPC market. SCFE21 provided that opportunity, on a global level."



Addison Snell
Chief Executive Officer
InterSect360 Research





"There is a strong drive within Europe to wanting to get back into the microprocessor development (...), we just want to also be able to produce our own processors and reacquire the know-how."



Anders Dam Jensen
Executive Director
EuroHPC JU



"Some of the areas which are using AI are not represented by massive data, we actually have sparse data and the use cases around AI may be diverse enough to support the range of options - Cloud, sensor, Edge."



Irene Qualters
Assoc. Laboratory Director
LANL



Tshiamo Motshegwa
Dept. of Computer Science
University of Botswana

CONFERENCE DAY 2

Second day provided an interesting perspective on Meteo topic, thanks to speakers from South Africa, India and Poland. Featured talks from 'Focus on Africa' and 'Focus on India' attracted many new viewers and expanded the reach of SCFE21. Another frontier which was crossed during the conference was the merger of Cloud and HPC with talks from Kate Keahey, Wolfgang Gentzsch, Edward Hsu, Tara Madhyastha and Neil Thompson.

"Africa Union 2063 mentioned climate change as risk factor (..), so the way to try and deal with is to reduce the impact associated with extreme weather to have early warning system."



Mary-Jane Bopape

Senior manager
South African Weather Service

THE THEMATIC BLOCKS

- **Meteo** [featuring C-DAC, South African Weather Service, Centre of Numerical Weather Prediction at Institute of Meteorology and Water Management]
- **Material** [feat. The Institute of Mathematical Sciences, University of Limpopo, South Africa]
- **Sponsor talks** [feat. HPE, NEC]
- **HPC & Cloud** [feat. Argonne National Lab; UberCloud; Rescale; RONIN]

"How a researcher can create a self-service HPC cluster that's auto scaling just for themselves, that is one of the fundamental features that enables scalability for researchers and is a motivation for using the Cloud."



Tara Madhyastha

Principal Research Scientist
RONIN

LIVE  **↑ ↓**





**High Performance Computing
Built for Cloud**

Using an Intelligent Control Plane Approach

Edward Hsu
Chief Product Officer, Rescale

Edward Hsu
Chief Product Officer at Rescale

SPEAKERS IN ORDER OF PRESENTATION - DAY 2

AKSHARA JAYANAND KAGINALKAR

"Connecting the dots: urban environment models, HPC-Cloud, climate resilient Indian smart cities"

MARY-JANE BOPAPE

"Implementation of the SADC Cyber-Infrastructure Framework: focus on weather modelling"

BOGDAN ROSA

"Computational challenges in modelling cloud microphysical processes"

PINAKI CHAUDHURI

"Studying amorphous materials via large-scale computing"

PHUTI NGOEPE

"Simulated synthesis, characterisation and performance of nanostructured metal oxide electrodes for energy storage"

NICOLAS DUBÉ

"A Vision for the Post-Exascale Era"

ERICH FOCHT

"Programming Heterogeneity"

KATE KEAHEY

"Chameleon: Taking Science from Cloud to Edge"

WOLFGANG GENTZSCH

"Using distributed HPC technology for building an automated, self-service, truly multi-cloud simulation platform"

EDWARD HSU

"High Performance Computing Built For Cloud Using an Intelligent Control Plane Approach"

TARA MADHYASTHA

"RONIN: Secure Self-service High Performance Research Computing in the Cloud"

NEIL THOMPSON

"The approximate future of computing"

CONFERENCE DAY 3

The last day of the conference included two **keynote lectures** from **Hiroaki Kitano** [SBI] and **Roberto Car** [Princeton University]. It started out with invited talks from Onur Mutlu and Sunita Chandrasekaran, who concluded the conference by saying- "It covered a broad range of topics including HPC. Quantum computing, AI/DL/ML and interdisciplinary science! (...) it was fun to present on the best practices of software development!".

"What we are trying to do, by 2050, is to build AI systems which can make major scientific discovery, highly autonomously, that's worth Nobel Price in Physiology and Medicine."



Hiroaki Kitano
President
The Systems Biology Institute

THE THEMATIC BLOCKS

- Software [University of Delaware; NAG]
- CFD [Jawaharlal Nehru Centre for Advanced Scientific Research]
- AI & Materials [Citrine Informatics]
- Hardware [AMD, Xilinx]
- Quantum Computing [D-Wave]
- Genomics [BRECA, Lenovo]
- I/O, storage, interconnects [DDN, Cornelis Networks]

"We worked very hard to improve the efficiency of ab-initio molecular dynamic simulation and finally we found that this can be done by using machine learning."



Roberto Car
Recipient of the 2020 ACM
Gordon Bell Prize
Princeton University

SPEAKERS IN ORDER OF PRESENTATION - DAY 3

ONUR MUTLU

"Intelligent Architectures for Intelligent Systems"

SUNITA CHANDRASEKARAN

"Best practices for a productive (yet performance) software development"

FOUZHAN HOSSEINI

"Meet the POP CoE: Getting insight into HPC code behavior"

SANTOSH ANSUMALI

"Towards CFD at Exa-scale"

KEYNOTE: HIROAKI KITANO

"Nobel Turing Challenge – Creating the Engine of Scientific Discovery"

BRYCE MEREDIG

"Designing next-generation materials with machine learning"

ANDREW KING

"What a Computational Performance Advantage Means for the Future of Practical Quantum Computing"

DAUDI JJINGO

"A review of computational data science applications in Uganda"

MIGUEL TEROL PALENCIA

"Lenovo Scalable Architectures for Genomics Analytics"

THOMAS BLUM

"Taking a closer look at AI I/O"

PHIL MURPHY

"Cornelis Networks Omni-Path: Purpose Built High-Performance Fabrics for HPC/HPDA/AI"

KARL PODESTA

"Supercomputing on Azure Powered By AMD EPYC"

TOMASZ WAZNY, RAFAL TYMKOW

"The biggest HPC implementation on the Central and Eastern Europe, PCSS business case"

KEN O'BRIEN

"Innovative Computing-Architectures with FPGAs"

KEYNOTE: ROBERTO CAR

"Innovative Computing-Architectures with FPGAs"

MAREK MICHALEWICZ

Closing words



MACHINE LEARNING BASED AB-INITIO MOLECULAR DYNAMICS

Roberto Car
Princeton University



Virtual Conference, July 19-23 (2021), Warsaw (Poland)

Roberto Car

Professor at Department of Chemistry, Princeton University

WORKSHOPS

DAY 4

The 4th day of SCFE21 started off with a workshop delivered by the Systems Biology Institute. During the 3-hour tutorial the presenters together with the viewers explored the text mining approaches for biological sciences powered by machine learning models. SBI has developed the Taxila tool to mine textual data to generate hypotheses and empower the engine of scientific discovery.

Next was the QCG- PilotJob, where presenters from Poznan Supercomputing and Networking Center were explaining in an easy, efficient and unified way how to execute a large number of tasks on various types of computing resources.

The last workshop of the day was held by Huawei, which consisted of two presentations. The first one showed how to use technologies based on Huawei AI technology and Dorado mass storage in a modern way and the second one was an introduction to Huawei's OceanStor Pacific next-gen HPDA storage, which offers a variety of professional solutions for customers across different industries.



The Systems Biology Institute

Speakers: Sucheendra Kumar Palaniappan and Samik Ghosh

Title: *Creating an engine of scientific discovery- Taxila: Analyzing text in biological context*



Poznan Supercomputing and Networking Center

Speakers: Bartosz Bosak, Piotr Kopta, Tomasz Piontek, Wojciech Szeliga

Title: *Overcome limitations of Scheduling Systems with QCG-PilotJob*



Huawei Poland

Speaker: Arkadiusz Giedrojć

Title: *Huawei AI technology and Dorado Mass Storage in a modern way*

Speaker: Zhihao Tang

Title: *Oceanstor pacific next generation HPDA storage*

WORKSHOPS

DAY 5

The last day of Supercomputing Frontiers Europe 2021 comprised of three insightful workshops delivered by Lenovo, Interdisciplinary Centre for Mathematical and Computational Modelling (ICM) University of Warsaw and Huawei Poland.

The goal of Lenovo's workshop was to bring clarity into the current state of accelerators and to equip attendees with tools helping them evaluate the available GPUs choices. Specifically, the tutorial reviewed accelerators from Nvidia and other vendors and compared their performance, performance/Watt and price/performance across AI workloads and beyond.

Scientists from ICM University of Warsaw prepared a tutorial on VisNow- a tool for data processing, visualization and visual analysis – an open source generic platform based on data flow paradigm. The goal of this tutorial was to introduce the audience to the concept of visual analysis, and show basic ideas of scientific visualization.

Closing the event was a workshop from Huawei on resolving a pandemic created problem: hybrid learning/working. With artificial intelligence inside, Huawei IdeaHub turns every room into a smart room.



Lenovo

Speaker: Miro Hodak

Title: *How to select the right GPU for the specific AI workloads*



ICM University of Warsaw

Speakers: Bartosz Borucki, Jędrzej Nowosielski, Krzysztof Nowiński

Title: *Advanced scientific visualization with VisNOW platform*



Huawei Poland

Speaker: Piotr Pawlikowski

Title: *Hybrid learning with AI powered Huawei Ideahub solution – the new style of smart education*

TESTIMONIALS

"SFE21 was an excellent conference covering a broad range of topics including HPC initiatives, Cloud, Edge, AI and Quantum Computing. Bringing the international community together during the pandemic and creating a good experience using a virtual platform is hard and the organizing team did a fantastic job to this end. I am glad I had the opportunity to attend this conference and enjoyed giving a talk on how to get insight into HPC code behavior. Thank you SFE21 team!"

Fouzhan Hosseini
Performance Optimisation and Productivity Manager
NAG



The conference was exceptionally organised, covering diverse, current and relevant topics in relation to cutting edge data and compute intensive theory, technologies, ecosystems and applications. The conference was attended by a globally diverse audience and provided invaluable networking opportunities to foster collaborations. It provided industry engagement, panel discussions and hands-on training workshops

Tshiamo Motshegwa
Lecturer, Department of Computer Science
University of Botswana



Supercomputing Frontiers Europe 2021 was a well organised conference providing an excellent balance of high performance computing "trade-craft" talks and interesting scientific talks. The talks were all informative and I learnt something from each one of them. Some topic areas were new for me and challenged my thinking – which is exactly the purpose of this Conference I believe. Many of the speakers were very engaging and have prompted me to continue to learn about the topics after the conference. This is the essence of attending a conference – virtual or otherwise!

Clem Lau
Senior consultant, Founder
Xlink Media



Now that SCFE21 is over, I want to thank the conference organizers for a perfect conference, with many great talks about different HPC Initiatives, HPC architectures and components, including Cloud, Edge, AI, and Quantum Computing, amazing and novel HPC applications, and outstanding speakers. And last but not least a perfectly smooth organization with an excellent digital conference platform.

Wolfgang Gentzsch
President
The UberCloud



ACKNOWLEDGEMENT

Supercomputing Frontiers Europe 2021 had the privilege to receive the honorary patronage of:

- Ministry of Economic Development, Labour and Technology;
- Digital Affairs - Chancellery of the Prime Minister;
- Rector of the University of Warsaw;
- The National Centre for Research and Development;
- National Information Processing Institute (OPI);
- Center for Advanced Systems Understanding (CASUS).

The conference was supported by Polish Media Partners:

- ITwiz;
- Forum Akademickie.

Worldwide Media Partners:

- HPC Wire, Datanami, Enterprise AI, HPC Wire Japan;
- Inside HPC;
- Intersect 360 Research, This Week in HPC.

SCFE21 partnered with **ISC High Performance** (the biggest HPC event in Europe), **Quantum AI Foundation** (Warsaw Quantum Computing Group meetings organiser) and **RISC-V** (a free and open ISA enabling a new era of processor innovation through open standard collaboration).



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DDN is the premier provider of high-performance storage solutions, and was voted #1 in high-performance storage for AI and HPC computing in 2020. With DDN, data-centric organisations can analyze much larger datasets, and bring innovative products and services to market more quickly, while maximizing the value of complex, distributed datasets. DDN's unique parallel architecture is designed for the most demanding data-intensive environments, accelerating peta-scale data sets for deep learning models. Over the last two decades, DDN has become the data management provider of choice for over 10,000 customers across HPC, AI and analytics, government, life sciences, energy and financial services. www.ddn.com



Huawei in Poland has been operating for 17 years providing information and communication technologies in areas:

- Telecommunications networks – Huawei Carrier Business Group
- Network solutions, IT, AI, cloud services, Data Center Facility, Photovoltaics and Solar Inverters – Huawei Enterprise Business Group
- Consumer Devices – Huawei Consumer Business Group

Huawei operates around the world, employing over 194 000 employees, serving more than three trillion people. Every year, Huawei spends about 30% of its revenue on development and research. In the last 10 years, it has been a budget of around 300 trillion pln, and in 80 R&D centres Huawei currently has 96 000 people working. Huawei Enterprise is based on cooperation with Distributors and Partners by ensuring that they participate in attractive partner, training and marketing programs. www.e.huawei.com



Lenovo is a Fortune Global 500 company with a turnover of \$ 47 billion and a global technology leader in intelligent digital transformation. Lenovo Infrastructure Solutions Group offers ThinkSystem and ThinkAgile solutions that provide the most robust technology foundation for an efficient, reliable and secure data center on the market. It is a comprehensive portfolio of servers, storage, networking solutions and software that seamlessly integrate and collaborate in any environment, enabling rapid deployment and shorter waiting times for additional business benefits. The industry recognition that Lenovo has earned, as the #1 Top 500 supercomputer provider in the world, illustrates its strong commitment to HPC. www.lenovo.com

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Cornelis Networks™ is a leading independent provider of purpose-built high-performance fabrics enabling HPC, AI, and HPDA customers solve the world's toughest challenges. The new Cornelis™ Omni-Path Express™ suite delivers accelerated performance at scale with the best performance price in the industry, powering the fastest supercomputers on the planet that enable breakthroughs in science and engineering. Our design embraces open source including native OFI that offer enhanced performance and a definitive choice to the high-performance compute community.

www.cornelisnetworks.com



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