



UNIVERSITY
OF WARSAW



VIRTUAL & GLOBAL



March 23-25, 2020

CONFERENCE

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ABOUT THE ORGANISER

Interdisciplinary Centre for Mathematical and Computational Modelling (ICM), University of Warsaw was established by a resolution of the Senate of the University of Warsaw dated 29 June 1993, the Interdisciplinary Centre for Mathematical and Computer Modeling (ICM), University of Warsaw, is one of the top HPC centres 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. It has always been an active research centre with high quality research contributions in computer and computational science, numerical weather prediction, visualisation, materials engineering, digital repositories, social network analysis and other areas.

ICM's Laboratory of Visual Analysis has been successfully developing and using in-house visualisation software (VisNow) for over 20 years. Their expertise covers scientific visualisation, visual analysis, computer assisted medical diagnosis and other competence areas.

Since 1997, numerical weather prediction is the one of main activities of ICM. The numerical weather forecast for Central Europe has over 200 million visitors every year, making it one of the most popular weather services in Poland.

All of these (and other competence areas) are supported by ICM's state-of-the-art IT infrastructure. At the beginning of July 2016, ICM made available to researchers the Okeanos supercomputer — a large-scale Cray XC40 processing system. Okeanos and other HPC machines at ICM serve approximately 850 active users from about 111 different research centres. Their work makes up three hundred registered active computational grants, resulting in about 200 publications per year.



ABOUT SCFE20

This year due to exceptional circumstances related to pandemic of coronavirus and special protection measures, the conference was conducted as a **virtual event**. The participants will be able to follow the full program of the conference remotely from any place worldwide with internet access. The registration fee has been lifted to allow the widest participation.

Supercomputer Frontiers 2020 was be the sixth edition of the annual conference which run in Singapore in 2015-2017 and subsequently in 2018-2019 in Warsaw, Poland. Tentatively the main topics at this edition will be: quantum computing, connectome, optical computing, computation studies of brain, neuromorphic computing and microbiome.

Previous editions of the conference showcased a successful scientific programme with eminent plenary keynote speakers such as:

- Leon Chua (Memristor),
- Rupak Biswas (NASA),
- Paul Messina (Exascale),
- Whitfield Diffie (Cryptography),
- Dimitri Kusnezov (Personalised medicine and exascale computing),
- Karlhienz Meier (Neuromorphic computing),
- Gordon Bell (History of G. Bell Prizes),
- Alessandro Curioni (Cognitive Computing),
- Thom H. Dunning (Supercomputing).

Selected papers from earlier editions of the conference were published in special issues of Supercomputing Frontiers and Innovations, Vol 2, No 3 (2015), Vol 3, No 2 (2016), Vol 4, No 2 (2017) and Vol 5, No 2 and 3 (2018) and Vol.6 No 2 (2019).

SCIENTIFIC COMMITTEE

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Cezary REDZIK

Damian WICIK

CONFERENCE DAY 1

■ Keynote Speaker

■ Invited Speaker

■ Sponsors

9:00 — 9:10	Opening Remarks from the Chairman of the Organising Committee Marek Michalewicz, ICM UW, Poland	Google Calendar	Opening
9:10 — 10:15	A Data-Centric Approach to Extreme-Scale Ab initio Dissipative Quantum Transport Simulations Ziogas Alexandros Nikolaos, ETH Zürich	Google Calendar	PHYSICS, ASTRONOMY, COSMOLOGY
10:10 — 10:45	Accelerated Artificial Intelligence for Big-data Physics Experiments Eliu Huerta, University of Illinois at Urbana-Champaign	Google Calendar	
10:45 — 11:10	New features of superfluidity far from equilibrium: nuclear reactions, dynamics of ferrons and quantum vortices in ultracold gases Piotr Magierski, M.C.Barton, A.Bulgac, S.Jin, K.Kobuszewski, P. Kulinski, K.J.Roche, K.Sekizawa, B.Tuzemen, GWlazowski	Google Calendar	
11:10 — 11:20	Numerical tests of HARM simulations Bestin James and Agnieszka Janiuk	Google Calendar	
11:20 — 11:55	The role of Cyber-Infrastructure in Development of Africa Happy Sithole, The Council for Scientific and Industrial Research	Google Calendar	HPC IN AFRICA
11:55 — 12:30	Automated Wildlife Monitoring and Poacher Detection in Namibian Communal Conservancies Wilhelmina Nekoto, Data Engineer, Research Scientist (Computer Vision)	Google Calendar	
12:30 — 12:50	Ethiopia: The formation of a digital powerhouse of Africa. Uros Ignjacevic, General Manager of Sun Data World	Google Calendar	
12:50 — 13:10	LUNCH		
13:10 — 13:45	Optimising AI training deployments using Graph compilers and containers Karthee Sivalingam, Alfio Lazzaro, Nina Mujkanovic, HPE HPC/AI EMEA Research Lab	Google Calendar	
13:45 — 14:20	Fast and Accurate Multiscale Modeling of Platelets Guided by Machine Learning Yuefan Deng, Stony Brook University, NY	Google Calendar	MULT- AND LARGE SCALE MODELLING
14:20 — 14:45	PICongPU Performance and Scaling Results on Summit Rene Widera, Sergei Bastrakov, Alexander Debus, Marco Garten, Richard Pausch, Klaus Steiniger, Michael Bussmann and Axel Huebl	Google Calendar	
14:45 — 15:10	Templated CUDA Lattice Boltzmann Method: generic CFD solver for single and multi-phase problems Michał Dzikowski and Grzegorz Gruszczyński	Google Calendar	
15:10 — 15:20	The influence of granular layer on the stick-slip dynamics of sheared fault gouges modelled with the Discrete Element Method Piotr Klejment	Google Calendar	
15:20 — 15:30	Computational research on metal-ligand bonds stability limiting factors: the case of Rh(IX)O4+ and Rh(IX)NO3 Mateusz Domański, Łukasz Wolański, Paweł Szarek and Wojciech Grochala	Google Calendar	
15:30 — 16:05	Towards Exascale Hyperbolic PDE Engines – Are We Skating to Where the Puck Will Be? Michael Bader, Technical University of Munich	Google Calendar	
16:05 — 16:30	LUMI: the EuroHPC pre-exascale system of the North Tomasz Malkiewicz, CSC – IT Center for Science and Nordic e-Infrastructure Collaboration (NeIC)	Google Calendar	

CONFERENCE DAY 2

■ Keynote Speaker

■ Invited Speaker

■ Sponsors

9:00 — 10:00	The Human Microbiome: Big Challenges, Big Data, Big Compute Rob Knight, University of California San Diego	Google Calendar	OMICS
10:00 — 10:35	Single cell transcriptomics – new challenges for Big Data analytics Vladimir Brusic, School of Computer Science, University of Nottingham Ningbo China	Google Calendar	
10:35 — 11:10	Graphic Encoding of Macromolecules for Quantitative Classification of Protein Structure and Representation of Conformational Changes Trilce Estrada, University of New Mexico	Google Calendar	
11:10 — 11:45	Utility of Real time portable genome sequencing and HPC for global food security Laura Boykin, Cassava Virus Action Project	Google Calendar	
11:45 — 12:20	Functional dynamics of biomolecules with supercomputers Joanna Trylska, Centre of New Technologies University of Warsaw	Google Calendar	
12:20 — 12:30	Design of selective TrmD inhibitors Adam Stasiulewicz, Bartosz Trzaskowski and Joanna Sułkowska	Google Calendar	
12:30 — 12:50	LUNCH		
12:50 — 13:05	HPC Adventures: WarsawTeam around the world	Google Calendar	
13:05 — 13:40	HPC Transformation with AI Florin Manila, Senior Architect and Inventor IBM	Google Calendar	HPC SERVICES, PROVISIONING AND DELIVERY
13:40 — 14:00	Tomorrow's Supercomputers, Yesterday's Practices: Applications of cloud-backed large system emulation for supercomputer software development Łukasz Orłowski, Co-Founder and CTO of Archanan	Google Calendar	
14:00 — 14:20	Constellation® – Supercomputing at your fingertips – Delivering HPC power and expertise to all Nicolas Tonello, Constelcom Ltd	Google Calendar	
14:20 — 14:30	A hybrid HPC and Cloud platform for multidisciplinary scientific application Marian Bubak, Jan Meizner, Piotr Nowakowski, Martin Bobak, Ondrej Habala, Ladislav Hluchy, Viet Tran, Adam Belloum, Reginald Cushing, Maximilian Höb, Dieter Kranzlmüller and Jan Schmidt	Google Calendar	
14:30 — 14:40	Cyberinfrastructure Resource Integration: Advancing Local Cyberinfrastructure Through Community Best Practices Richard Knepper	Google Calendar	
14:40 — 15:05	To be announced Rick Koopman, Lenovo	Google Calendar	
15:05 — 15:25	High Performance Services for genetic research Piotr Bala, ICM UW	Google Calendar	BIOINFORMATICS
15:25 — 15:35	Ligand-dependent activity of an aminoglycoside riboswitch Marta Kulik, Takaharu Mori, Yuji Sugita and Joanna Trylska	Google Calendar	
15:35 — 15:45	Mechanism of transport of vitamin B12-peptide nucleic acids through the outer membrane of E. coli Tomasz Pierko and Joanna Trylska	Google Calendar	
15:45 — 15:55	Mutations affect the dynamics of an aminoglycoside riboswitch Piotr Chyży, Marta Kulik, Suyong Re, Yuji Sugita and Joanna Trylska	Google Calendar	
13.30 – 16.30	Tutorial OpenPOWER and Power 9	Google Calendar	
Brief agenda: 1. Power 9/OpenPOWER Features 2. WML features 3. Xilinx U50 and Edge Compute 4. Advanced accelerator features example OpenCAPI and Use cases 5. Q and A, Way forward Presenters: Florin Manila Bruno Mesnet, CAPI SNAP Proof of Concepts Team leader Jens Stapelfeldt Read more			

CONFERENCE DAY 3

■ Keynote Speaker

■ Invited Speaker

■ Sponsors

9:00 — 10:00	Emergent Atomic Switch Networks for Neuroarchitectonics James K. Gimzewski, University of California Los Angeles	Google Calendar	DATA COMMUNICATION, DISTRIBUTED COMPUTING
10:00 — 10:35	Towards the Quantum Internet: Building an entanglement-sharing quantum network Eden Figueroa, Stony Brook University	Google Calendar	
10:35 — 10:55	The historical 1st Poland-Singapore data transfer production trial over CAE-1, a behind the scene look Chin Fang, CEO of Zettar Inc.	Google Calendar	
10:55 — 11:20	Long distance geographically distributed computing cluster and High Performance Parallelex Karol Niedzielewski, Marcin Semeniuk, Jarosław Skomiał, Jerzy Proficz, Piotr Sumionka, Bartosz Pliszka and Marek Michalewicz	Google Calendar	
11:20 — 11:55	The Reality and Tremendous Opportunity of Custom, Open Source Processing Calista Redmond, Chief Executive Officer, RISC-V Foundation	Google Calendar	
11:55 — 12:30	GRAPE Supercomputer and Biosystems computational research Makoto Taiji, RIKEN Center for Biosystems Dynamics Research Osaka	Google Calendar	ARCHITECTURE
12:30 — 13:05	Technology of Real-World Analyzers (TAUR) and its practical application Jarosław Jung i Krzysztof Halagan, Lodz University of Technology	Google Calendar	
13:05 — 13:15	ARUZ – fully parallel FPGA-based data processing system Rafał Kiełbik, Krzysztof Halagan, Jarosław Jung and Zbigniew Mudza	Google Calendar	
13:15 — 13:25	Evaluation of ARM based system for HPC workloads, a case study Maciej Pawlik, Klemens Noga, Maciej Czuchry, Jacek Budzowski, Łukasz Flis, Patryk Lasoń, Marek Magryś and Michał Sterzel	Google Calendar	
13:25 — 13:45	LUNCH		
13:45 — 14:40	Vector Evolution -The path to the SX-Aurora Tsubasa Erich Focht, NEC Germany	Google Calendar	DATA-CENTRIC COMPUTING, STORAGE
14:40 — 15:05	Coarse-Grained Approach for Reconfigurable Logic in High Performance Computing Systems Zbigniew Mudza	Google Calendar	
15:05 — 15:30	The Data Vortex: From Interbellum Polish Mathematics to a Novel Topology for Connecting Cores Reed Devany, Coke Reed, Santiago Betelu and Michael Ives	Google Calendar	
15:30 — 15:55	Checkpoint/Restart Implementation for OpenSHMEM Delafrouz Mirfendereski, Barbara Chapman, Tony Curtis and Md Abdullah Shahneous Bari	Google Calendar	
15:55 — 16:30	The Data-Model Convergence: a case for Software Defined Architectures Antonino Tumeo, Pacific Northwest National Laboratory	Google Calendar	
16:30 — 17:05	Memory vs. Storage Software and Hardware: The Shifting Landscape Jay Lofstead, Scalable System Software Sandia National Laboratories	Google Calendar	SPECIAL THEMATIC SESSION: OPPORTUNITIES FOR DATA-CENTRIC COMPUTING
17:05 — 17:25	Potential of I/O-Aware Workflows in Climate and Weather Julian Kunkel	Google Calendar	
17:25 — 17:37	I/O Challenges in Data-Centric Compute Framework Ziogas Alexandros Nikolaos	Google Calendar	
17:37 — 17:54	Containers and Data-Centric Computing Jay Lofstead	Google Calendar	CLOSING
17:54 — 18:00	Closing words Marek Michalewicz, Interdisciplinary Centre for Mathematical and Computer Modeling (ICM), University of Warsaw, Poland		

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