UNIVERSITY OF WARSAW

icm

SUPERCOMPUTING FRONTIERS EUROPE 2018

March 12-16, 2018

CONFERENCE REPORT

SUPERCOMPUTINGFRONTIERS.EU

CONTENTS

03
ABOUT
THE ORGANISER

04
ABOUT
THE CONFERENCE

05
SCIENTIFIC COMMITTEE

06
ORGANISING COMMITTEE

07- 26
CONFERENCE

27
WORKSHOPS

35
ACKNOWLEDGEMENT

36
SPONSORS

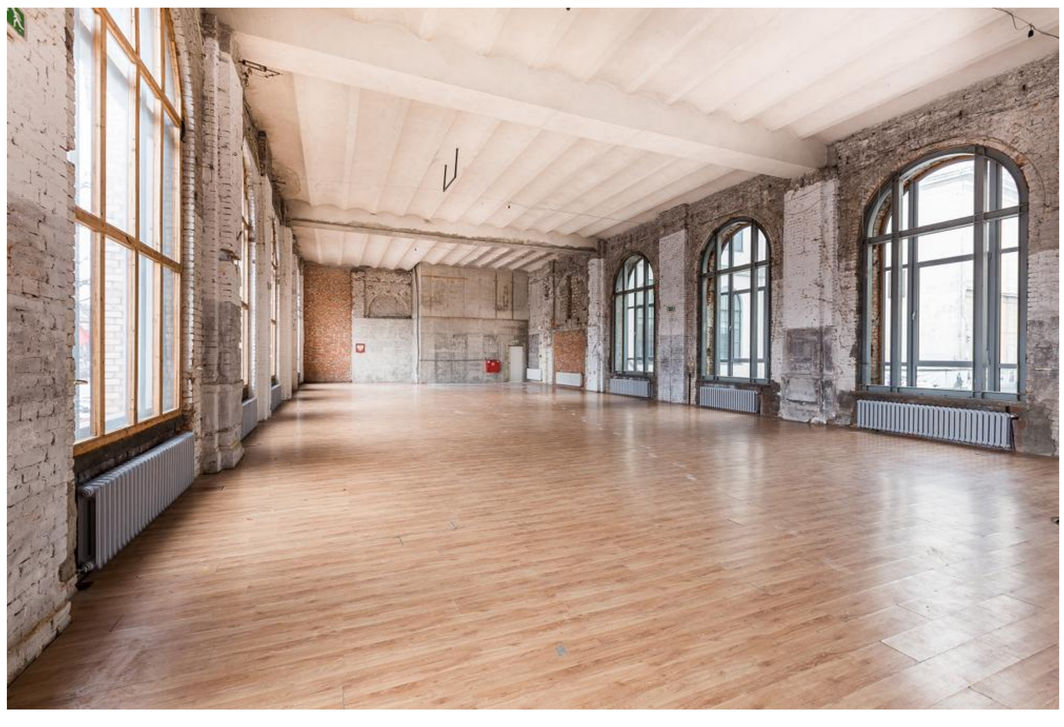
ABOUT THE ORGANISER

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.

Supercomputing Frontiers Europe will be held for the first time in Warsaw, the capital of Poland. It is the largest city in Poland and the centre of economic, political and cultural events. Warsaw is a metropolis full of life and, at the same time, a city with a unique history. A quarter of its surface is occupied by green spaces, it is also the centre of culture for every taste and every budget.

The conference venues is:
Nałęcz Institute of Biocybernetics and Biomedical Engineering, Polish Academy of Sciences.

We invite all conference participants for a **conference banquet**, which will take place on the second day of the conference on Tuesday, 13th March at 6:30PM. The venue is a historic The Reduta Bank Polski Hall. The winter mood will be warmed by a well-known DJ Eltron John who will create an exceptional musical experience.



ABOUT SCFE18

Supercomputer Frontiers 2018 is the next edition of the annual conference in Singapore. This time organized in Warsaw - for the first time in Eastern Europe. It is a platform for the thought leaders from both academia and industry to interact and discuss the visionary ideas, the most important global trends and substantial innovations in supercomputing. The inaugural conference held in March this year showcased a successful scientific program with spectacular plenary keynote speakers like Prof. Gordon Bell, Dr Alessandro Curioni, Prof. Thom H. Dunning, Jr., Dr Haohuan Fu, Prof. John Gustafson, Prof. Maciej Andrzej Brodowicz, Prof. David Daniel Donofrio, Mr Kenneth P. Jacobsen, Prof. Richard Cameron Murphy, Prof. John Marshall Shalf, Dr Isaac R. Nassi.

The themes for Supercomputing Frontiers 2018 are:

- Supercomputing applications in domains of critical impact in economic and human terms, and

especially those requiring computing resources approaching Exascale;

- Big data science merging with supercomputing with associated issues of I/O, high bandwidth networking, storage, workflows and real time processing;
- Architectural complexity of Exascale systems with special focus on supercomputing interconnects, interconnect topologies and routing, and interplay of interconnect topologies with algorithmic communication patterns for both numerically intensive computations and big data; and
- Any other topic that pushes the boundaries of supercomputing to exascale and beyond.

SCIENTIFIC COMMITTEE

PROGRAMME CHAIR

Marek Michalewicz, ICM University of Warsaw

MEMBERS

George BECKETT
EPCC, University of Edinburgh, UK
Pete BECKMAN
Argonne National Laboratory / University of Chicago, USA
Taisuke BOKU
University of Tsukuba, Japan
Lindsay BOTTEN
Australian National University, Australia
Alessandro CURIONI
Zurich Research Laboratory, Switzerland
Maciej CYTOWSKI
Pawsey Supercomputing Centre, Australia
Bronis DE SUPINSKI
Lawrence Livermore National Laboratory, USA
Yuefan DENG
Stony Brook University, USA
Jack DONGARRA
University of Tennessee, USA
Thomas Harold Jr DUNNING
University of Illinois, USA
John FEO
Pacific Northwest National Laboratory, USA
John GUSTAFSON
A*STAR and National University of Singapore, Singapore
Robert HARRISON
IACS, Stony Brook University, USA
William HARROD
Advanced Scientific Computing Research, USA
Wojciech HELLWING
Center for Theoretical Physics, Polish Academy of Sciences, Poland
David KAHANER
Asian Technology Information Program (ATIP), USA
Daniel S. KATZ
NCSA, University of Illinois, USA
Scott KLASKY
Oak Ridge National Laboratory, USA
Patricia KOVATCH
Icahn School of Medicine at Mount Sinai, USA
Michael KRAJECKI
CReSTIC, Université de Reims Champagne–Ardenne, France
Henryk KRAWCZYK
Centrum Informatyczne Trójmiejskiej Akademickiej Sieci Komputerowej, Poland
Julian KUNKEL
Universität Hamburg, Germany
Krzysztof KUROWSKI
Poznan Supercomputing and Networking Center, Poland
Jysoo LEE
KAUST Supercomputing Core Lab, Saudi Arabia
Madhav MARATHE
Network Dynamics and Simulation Science Laboratory, USA
Satoshi MATSUOKA
Tokyo Institute of Technology, Japan
Richard MURPHY
Micron, USA
Marek NIEZGÓDKA
Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw (ICM), Poland
Gabriel NOAJE
NVIDIA Corporation, Singapore
Jacek OKO
Wrocław University of Science and Technology, Poland
Witold RUDNICKI
Interdisciplinary Centre for Mathematical and Computational Modelling, University of Warsaw (ICM), Poland
Sven-Bodo SCHOLZ
Heriot–Watt University, UK
Thomas SCHULTHESS
ETH Zurich / CSCS, Switzerland
John SHALF
Lawrence Berkeley National Laboratory, USA
Horst SIMON
Lawrence Berkeley National Laboratory, USA
Happy SITHOLE
Centre for High Performance Computing, South Africa
Thomas STERLING
Indiana University, USA
Rick STEVENS
Argonne National Laboratory, USA
Maciej STROIŃSKI
Poznan Supercomputing and Networking Center, Poland
John A. TAYLOR
Commonwealth Scientific and Industrial Research Organisation, Australia
Vladimir VOEVODIN
Research Computing Centre, Lomonosov Moscow State University, Russia
Kazimierz WIATR
Akademia Górniczo-Hutnicza, Polska
Roman WYRZYKOWSKI
Częstochowa University of Technology, Poland

ORGANISING COMMITTEE

GENERAL CHAIR

Marek Michalewicz
ICM University of Warsaw

MEMBERS

Maciej CHOJNOWSKI

Joanna JĘDRASZCZYK

Mateusz NEUMANN

Jacek PIECHOTA

Jan PIOTROWSKI

Jarosław SKOMIAŁ

Luiza SKRAJNA-IWAŃCZYK

Maciej STRYBEL

Maciej SZPINDLER

CONFERENCE DAY 1

■ Keynote Speaker ■ Invited Speaker ■ Sponsors

8:00 — 9:00	Registration		
9:00 — 10:00	Simultac Fonton **Thomas Sterling, Indiana University, USA**	ARCHITECTURES	Ch.: **Marek Niezgódka**
10:00 — 10:45	In an era of big data, is it time to update scientific content, software code and hardware architecture in one fell swoop? — the advent of processor-in-memory architecture Bob Bishop, EMU Technology Inc., USA	ARCHITECTURES	Ch.: **Marek Niezgódka**
10:45 — 11:05	BREAK		
11:05 — 11:50	Computing with Data Flow Engines: The Next Step for Supercomputing Tobias Becker, Maxeler Technologies, USA	ARCHITECTURES	Chair: **Dimitri Kusnezov**
11:50 — 12:35	Objective, innovation and impact of the energy-efficient DOME MicroDataCenter Ronald P. Luijten, IBM Zurich Research Laboratory, Switzerland	ARCHITECTURES	Chair: **Dimitri Kusnezov**
12:35 — 12:50	Vortex-topology Messaging: Data Vortex for high performance middleware Ryan Quick and Arno Kolster, Providentia Worldwide, USA/Canada	ARCHITECTURES	Chair: **Dimitri Kusnezov**
12:50 — 13:05	Efficiency analysis of a hybrid supercomputer Desmos with Angara interconnect Vladimir Stegailov *et al.*, Joint Institute for High Temperatures of the Russian Academy of Sciences, Russia	ARCHITECTURES	Chair: **Dimitri Kusnezov**
13:05 — 13:20	Elbrus processors performance for fast Fourier transform and computational materials science codes Denis Dergunov, Vladimir Stegailov and Alexey Timofeev, Higher School of Economics, Russia	ARCHITECTURES	Chair: **Dimitri Kusnezov**
13:20 — 14:20	LUNCH		
14:20 — 15:05	Internet of Things Nicola Ferrier, Argonne National Laboratory, USA	IOT	Chair: **Henryk Krawczyk**
15:05 — 15:35	Applying DDN to machine learning Frederic Lemaire, DDN	IND.SPONSORS	Chair: **Henryk Krawczyk**
15:35 — 15:50	HPC Storage and Big Data – Solving the I/O challenge Torben Kling Petersen, Cray	IND.SPONSORS	Chair: **Henryk Krawczyk**
15:50 — 16:05	Data Challenge Influencing New Architecture (Gen-Z) Michal Klimeš, HPE	IND.SPONSORS	Chair: **Henryk Krawczyk**
16:05 — 16:25	BREAK		
16:25 — 16:45	Software Ecosystem for Arm-based HPC Florent Lebeau, ARM	IND.	Chair: **Krzysztof Kurowski**
16:45 — 17:00	Facilitate HPC Operation and Administration via Cloud Nejc Bat, Arctur d.o.o., Slovenia; Ji Qing, Sugon, China; presented by Miha Verlič, Arctur d.o.o., Slovenia	CLOUD&GRID	Chair: **Krzysztof Kurowski**
17:00 — 17:15	Supercomputing with the PLGrid Infrastructure: a Tool for Open Science Jacek Kitowski *et al.*, AGH University of Science and Technology, Poland	CLOUD&GRID	Chair: **Krzysztof Kurowski**
17:15 — 17:30	Towards Near-Data Processing for Clouds – Challenges and Future Direction Gaurav Kaul *et al.*, Amazon, UK	CLOUD&GRID	Chair: **Krzysztof Kurowski**
18:30 — 21:30	CONFERENCE BANQUET, AT REDUTA BANKU POLSKIEGO		

SPEAKERS IN ORDER OF PRESENTATION

DAY 1 | MONDAY, MARCH 12

Precision Medicine as an Accelerator for Next Generation Supercomputing

Dimitri Kusnezov Department of Energy, USA

Dr. Kusnezov received A.B. degrees in Physics and in Pure Mathematics with highest honors from UC Berkeley. Following a year of research at the Institut fur Kernphysik, KFA-Julich, in Germany, he attended Princeton University earning his MS in Physics and Ph.D. in theoretical physics. At Michigan State University, he conducted postdoctoral research and then became an Instructor. He joined the faculty of Yale University as an assistant professor in theoretical physics, becoming an associate professor and has served as a visiting professor at numerous universities around the world. Dr. Kusnezov has published over 100 articles and edited 2 books. After more than a decade at Yale, he left academia to pursue federal service at the National Nuclear Security Administration and is a member of the Senior Executive Service. He has served in multiple positions within the NNSA, was nominated by the President to serve in the National Nuclear Security Administration, and he currently serves as Chief Scientist.

Supercomputing for Fast Learners: How Warsaw Team got to the finals in three major Student Cluster Competitions in China, USA and Germany

Adam Sobecki University of Warsaw

Adam Sobecki is a sophomore student studying Computer Science at the University of Warsaw. He is proficient in programming languages such as C/C++, CUDA, Java, Python, Haskell, OCaml and really loves problem solving. His major areas of interest in Computer Science are Algorithms and Data Structures, High Performance Computing, Machine Learning and Deep Learning. He is also up-to-date with new technologies. His hobbies are scuba diving and swimming.

Dominik Psujek Technical University of Warsaw

Dominik Psujek is a Computer Science student at Warsaw University of Technology. He is interested in computer security, networks, low and big-scale computer infrastructures and managing them. He is a part of Warsaw Team since September 2017 as a technician and server administrator. Other interests include electronic and rock music, as well as fantasy and criminal books and stories.

Marcin Mielniczuk University of Warsaw

Marcin Mielniczuk is studying Mathematics and Computer Science at the University of Warsaw. For him, the essence of these fields is problem solving, which he is really fond of. He is a cryptography and free software enthusiast. He is a polyglot – speaks fluently in 4 languages and is currently learning one more. In his free time he likes wandering off the beaten track, reading books and playing the guitar.

SPEAKERS IN ORDER OF PRESENTATION

DAY 1 | MONDAY, MARCH 12

Supercomputing Security or Supercomputing for Security

Whitfield Diffie Turing Award 2015, USA

Bailey Whitfield 'Whit' Diffie (born June 5, 1944) is an American cryptographer and one of the pioneers of public-key cryptography. Diffie and Martin Hellman's 1976 paper New Directions in Cryptography introduced a radically new method of distributing cryptographic keys, that helped solve key distribution—a fundamental problem in cryptography. Their technique became known as Diffie–Hellman key exchange. The article stimulated the almost immediate public development of a new class of encryption algorithms, the asymmetric key algorithms.

After a long career at Sun Microsystems, where he became a Sun Fellow, Diffie served for two and a half years as Vice President for Information Security and Cryptography at the Internet Corporation for Assigned Names and Numbers (2010–2012). He has also served as a visiting scholar (2009–2010) and affiliate (2010–2012) at the Freeman Spogli Institute's Center for International Security and Cooperation at Stanford University.

Together with Martin Hellman, Diffie won the 2015 Turing Award, widely considered the most prestigious award in the field of computer science. The citation for the award was: "For fundamental contributions to modern cryptography. Diffie and Hellman's groundbreaking 1976 paper, 'New Directions in Cryptography', introduced the ideas of public-key cryptography and digital signatures, which are the foundation for most regularly-used security protocols on the internet today.

source: https://en.wikipedia.org/wiki/Whitfield_Diffie

Delivering trust, privacy and unprecedented scale in distributed systems

Luke Barton Kalypton, UK

Luke's expertise spans 25+ years in the IT infrastructure and services market with emphasis in Security, IoT and Payments. He's focused on taking fledgling companies through the usual growth challenges to acquisition stage. He's highly experienced in identifying new business opportunities, creating strategic business partnerships and delivering business outcomes.

Performance evaluation of NLFSR enumeration onheterogeneous environments

Janusz Szmidt Military University of Technology, Poland

Janusz Szmidt, Ph.D, is mostly interested in application of number theory to cryptology. His interest is in cryptanalysis of hash functions, cryptographically strong elliptic curves, investigation and construction of nonlinear feedback shift registers which serve as pseudo-random generators of binary de Bruijn sequences with application to cryptography and communication.

SPEAKERS IN ORDER OF PRESENTATION

DAY 1 | MONDAY, MARCH 12

Distributed calculations in heterogeneous untrusted network

Łukasz Gleń Golem Factory, Poland

Lukasz Glen is an analyst and researcher at Golem Factory. He took his first steps in cryptocurrency and blockchain in 2015 with probabilistic nanopayments scheme creation. A year ago, Glen left the smart grid and smartmetering industry to fully concentrate his efforts on Golem. His activities within the Golem project range from distributed networks, Ethereum contracts to computation correctness problems. Glen holds a PhD in Mathematics, and is able to successfully merge his technical and industrial expertise with a scientific approach.

When HPC meets AI meets cloud

Jeff Watters Intel, USA

Jeff Watters holds the position of Director of Product Strategy in Intel's Technical Computing Initiative Organization. He is responsible for driving technical computing requirements into Intel's various ingredient teams and influencing product roadmap decisions. Since receiving his BSEE from the University of Illinois in 1986, Jeff has had a continuous career in processor and system design roles. Early days were spent designing systems for Compaq Computer Corporation before transferring to Intel Corporation to enable ecosystem partner solutions using Intel processor products. Jeff managed Intel's Asia Pacific Technical Sales force while living in Taiwan, directed the internationally-spread server applications engineering team after returning to the US, and lastly, setting the definition for various DCG processor products including the Xeon Phi roadmap. Jeff is highly interested in the future of high performance computing in light of new algorithmic paradigms, such as machine learning and data analytics, and the advent of the cloud democratization of HPC datacenters. Jeff's current role focuses on these new HPC trends and the requirements that will drive product definition for 2020 through 2024.

Advanced theoretical techniques to overcome drug-resistant bacteria

Joanna Sułkowska University of Warsaw, Poland

Joanna I. Sulkowska, Ph. D and her group are interested in development of multi dimensional models for the analysis of energy landscape of proteins with complex structures, as proteins with non trivial topology; development of analytical methods as direct coupling analysis (DCA). Scientific interests: theoretical models of the energy landscape of proteins; analytical methods and bioinformatics tools to predict protein structures and folding mechanisms; mechanical properties of proteins, degradation and translation; protein ligand interactions, membrane proteins; applications of mathematical knot theory to proteins and nucleic acids.

SPEAKERS IN ORDER OF PRESENTATION

DAY 1 | MONDAY, MARCH 12

Accelerating scientific discoveries in protein bioinformatics with Microsoft Azure cloud platform

Dariusz Mrozek Microsoft

High performance computing with coarse-grained model of biological macromolecules

Emilia A. Lubecka University of Gdańsk, Poland

Emilia A. Lubecka is Assistant Professor in the Institute of Informatics, Faculty of Mathematics, Physic and Informatics, of the University of Gdańsk. She obtained a Sc. degree in computer science (with honors) from Gdańsk University of Technology in 2013, a Ph.D. in chemistry from University of Gdańsk in 2014. She worked as research analyst in Academic Computer Center in Gdańsk, TASK, 2014-2015. She is a member of the European Peptide Society and the Polish Biochemical Society. Her main scientific interests are proteins folding mechanisms, prediction of proteins structures, high performance computing and coarse-grained models of biomolecules. Currently, she is working on UNRES force filed (collaboration with prof. A. Liwo, Faculty of Chemistry, University of Gdańsk).

(Super)Computing for all Humankind

Petros Koumoutsakos ETH Zurich, Switzerland

Petros Koumoutsakos received his Diploma (1986) in Naval Architecture at the National Technical University of Athens and a Master's (1987) at the University of Michigan, Ann Arbor. He received his Master's (1988) in Aeronautics and his PhD (1992) in Aeronautics and Applied Mathematics from the California Institute of Technology. He conducted postodoctoral studies at the Center for Parallel Computing (Caltech, 1992-1994) and at the Center for Turbulence Research (Stanford U./NASA Ames, 1994-1997). He was appointed as Chair for Computational Science at ETH Zurich in 2000.
Petros has been elected Fellow of the American Society of Mechanical Engineers (ASME), the American Physical Society (APS) and the Society of Industrial and Applied Mathematics (SIAM). He is recipient the Advanced Investigator Award by the European Research Council (2013) and led the team that won the ACM Gordon Bell prize in Supercomputing (2013).

Multiscale urban air quality numerical modelling, simulation and advanced visualisation

Andrzej A. Wyszogrodzki Institute of Meteorology and Water Management

Andrzej A. Wyszogrodzki received M.Sc. and Ph.D. degrees from the University of Warsaw, Poland, in physics in 1996 and 2001, respectively. Afterwards, he spent 3 years as a postdoctoral fellow at the Los Alamos National Laboratory in New Mexico, USA and one year at the IBM T. J. Watson Research Center, Yorktown Heights, USA. In 2005 he went to Boulder, Colorado, to work as a project scientist at the National Center for Atmospheric Research (NCAR). In September 2013 he joined the Institute of Meteorology and Water Management - National Research Institute in Warsaw, Poland as a head of the department of the Numerical Weather Forecasting with COSMO model.

Michał Kulczewski Poznań Supercomputing and Networking Center

Michal Kulczewski works in the Applications Department at Poznan Supercomputing and Networking Center since 2005. He received his M.Sc. degree in Computer Science, Computer Network and Distributed Systems, from the Poznan University of Technology, Poland in 2005. His research interests include mainly numerical weather predictions, modelling air quality in urban environments, code optimization, programming multi- and many-core computing systems, advanced in-situ data analysis and visualisation.

High-Performance Computing in geophysics: application of the discrete element method to materials failure problem

Piotr Klejment Institute of Geophysics Polish Academy of Sciences, Poland

My adventure with supercomputing has started during PhD Studies. I am working on PhD Thesis at Institute of Geophysics Polish Academy of Sciences and my area of interest is numerical modelling of materials in geophysical applications. In this research, the Discrete Element Method is used, which requires huge computational resources. That is the reason why our team takes advantage of Okeanos Supercomputer power. We study wide variety of geophysical issues like earthquake nucleation, rocks strength and mechanics, hydraulic fracturing, ice fracturing or glaciers calving, to name a few. In all of those areas I found very useful my physical, mathematical and programming background obtained from my studies connected with solid state physics at Warsaw University of Technology, Faculty of Physics.

CONFERENCE DAY 2

■ Keynote Speaker ■ Invited Speaker ■ Sponsors

8:00 — 9:00	Registration		
9:00 — 10:00	Simultac Fonton **Thomas Sterling, Indiana University, USA**	ARCHITECTURES	Ch.: **Marek Niezgódka**
10:00 — 10:45	In an era of big data, is it time to update scientific content, software code and hardware architecture in one fell swoop? — the advent of processor-in-memory architecture Bob Bishop, EMU Technology Inc., USA		
10:45 — 11:05	BREAK		
11:05 — 11:50	Computing with Data Flow Engines: The Next Step for Supercomputing Tobias Becker, Maxeler Technologies, USA	ARCHITECTURES	Chair: **Dimitri Kusnezov**
11:50 — 12:35	Objective, innovation and impact of the energy-efficient DOME MicroDataCenter Ronald P. Luijten, IBM Zurich Research Laboratory, Switzerland		
12:35 — 12:50	Vortex-topology Messaging: Data Vortex for high performance middleware Ryan Quick and Arno Kolster, Providentia Worldwide, USA/Canada		
12:50 — 13:05	Efficiency analysis of a hybrid supercomputer Desmos with Angara interconnect Vladimir Stegailov *et al.*, Joint Institute for High Temperatures of the Russian Academy of Sciences, Russia		
13:05 — 13:20	Elbrus processors performance for fast Fourier transform and computational materials science codes Denis Dergunov, Vladimir Stegailov and Alexey Timofeev, Higher School of Economics, Russia		
13:20 — 14:20	LUNCH		
14:20 — 15:05	Internet of Things Nicola Ferrier, Argonne National Laboratory, USA	IOT	Chair: **Henryk Krawczyk**
15:05 — 15:35	Applying DDN to machine learning Frederic Lemaire, DDN	IND.-SPONSORS	
15:35 — 15:50	HPC Storage and Big Data – Solving the I/O challenge Torben Kling Petersen, Cray		
15:50 — 16:05	Data Challenge Influencing New Architecture (Gen-Z) Michal Klimeš, HPE		
16:05 — 16:25	BREAK		
16:25 — 16:45	Software Ecosystem for Arm-based HPC Florent Lebeau, ARM	IND.	Chair: **Krzysztof Kurowski**
16:45 — 17:00	Facilitate HPC Operation and Administration via Cloud Nejc Bat, Arctur d.o.o., Slovenia; Ji Qing, Sugon, China; presented by Miha Verlič, Arctur d.o.o., Slovenia	CLOUD&GRID	
17:00 — 17:15	Supercomputing with the PLGrid Infrastructure: a Tool for Open Science Jacek Kitowski *et al.*, AGH University of Science and Technology, Poland		
17:15 — 17:30	Towards Near-Data Processing for Clouds – Challenges and Future Direction Gaurav Kaul *et al.*, Amazon, UK		
18:30 — 21:30	CONFERENCE BANQUET, AT REDUTA BANKU POLSKIEGO		

SPEAKERS IN ORDER OF PRESENTATION

DAY 2 | TUESDAY, MARCH 13

Simultac Fonton

Thomas Sterling Indiana University, USA

Dr. Thomas Sterling holds the position of Professor of Intelligent Systems Engineering at the Indiana University (IU) School of Informatics and Computing as well as the Chief Scientist and Associate Director of the Center for Research in Extreme Scale Technologies (CREST). Since receiving his Ph.D from MIT in 1984 as a Hertz Fellow Dr. Sterling has engaged in applied research in fields associated with parallel computing system structures, semantics, and operation in industry, government labs, and academia. Dr. Sterling is best known as the “father of Beowulf” for his pioneering research in commodity/Linux cluster computing. He was awarded the Gordon Bell Prize in 1997 with his collaborators for this work. He was the PI of the HTMT Project sponsored by NSF, DARPA, NSA, and NASA to explore advanced technologies and their implication for high-end system architectures. Other research projects included the DARPA DIVA PIM architecture project with USC-ISI, the Cray Cascade Petaflops architecture project sponsored by the DARPA HPCS Program, and the Gilgamesh high-density computing project at NASA JPL. Thomas Sterling is currently engaged in research associated with the innovative ParalleX execution model for extreme scale computing to establish the foundation principles to guide the co-design for the development of future generation Exascale computing systems by the end of this decade. ParalleX is currently the conceptual centerpiece of the XPRESS project as part of the DOE X-stack program and has been demonstrated in proof-of-concept in the HPX runtime system sofware. Dr. Sterling is the co-author of six books and holds six patents. He was the recipient of the 2013 Vanguard Award. In 2014, he was named a fellow of the American Association for the Advancement of Science.

In an era of big data, is it time to update scientifc content, softtare code and hardtare architecture in one fell stoop? - the advent of processor-in-memory architecture

Bob Bishop EMU Technology Inc., USA

Bob Bishop spent 40 years in the technical, engineering and scientific computing business, and was responsible for building and operating the international aspects of Silicon Graphics Inc., Apollo Computer Inc., and Digital Equipment Corporation. To accomplish this task, he lived with his family in five countries: USA, Australia, Japan, Germany and Switzerland. He was Chairman and CEO of SGI from 1999 to 2005.

Bishop has been involved in a wide range of global initiatives including the advisory boards for EU's Human Brain Project, National ICT Australia (NICTA), Multimedia Super Corridor of Malaysia, University Tenaga Nasional (Uniten), and UCLA's Laboratory for Neural Imaging (LONI). He is a Fellow of the Australian Davos Connection and an elected member of the Swiss Academy of Engineering Sciences.

Bishop earned a B.S. (First Class Honors) in mathematical physics from the University of Adelaide, Australia, an M.S. from the Courant Institute of Mathematical Sciences at New York University, and received his D.S. honoris causa from the University of Queensland.

In 2006, Dr. Bishop was awarded the NASA Distinguished Public Service Medal for his role in building simulation facilities that helped NASA's space shuttle fleet return-to-flight afer the 2003 Columbia disaster.

Bishop is Chairman & Founder of BBWORLD Consulting Services Sàrl and President & Founder of The ICES Foundation (International Centre for Earth Simulation), both Geneva-based organisations. He serves on the board of EMU Technology Inc..

Bob Bishop spent 40 years in the technical, engineering and scientific computing business, and was responsible for building and operating the international aspects of Silicon Graphics Inc., Apollo Computer Inc., and Digital Equipment Corporation. To accomplish this task, he lived with his family in five countries: USA, Australia, Japan, Germany and Switzerland. He was Chairman and CEO of SGI from 1999 to 2005.

Bishop has been involved in a wide range of global initiatives including the advisory boards for EU's Human Brain Project, National ICT Australia (NICTA), Multimedia Super Corridor of Malaysia, University Tenaga Nasional (Uniten), and UCLA's Laboratory for Neural Imaging (LONI). He is a Fellow of the Australian Davos Connection and an elected member of the Swiss Academy of Engineering Sciences.

Bishop earned a B.S. (First Class Honors) in mathematical physics from the University of Adelaide, Australia, an M.S. from the Courant Institute of Mathematical Sciences at New York University, and received his D.S. honoris causa from the University of Queensland.

In 2006, Dr. Bishop was awarded the NASA Distinguished Public Service Medal for his role in building simulation facilities that helped NASA's space shuttle fleet return-to-flight afer the 2003 Columbia disaster. Bishop is Chairman & Founder of BBWORLD Consulting Services Sàrl and President & Founder of The ICES Foundation (International Centre for Earth Simulation), both Geneva-based organizations.

Computing with Data Flot Engines: The Next Step for Supercomputing

Tobias Becker Maxeler Technologies, USA

Dr. Tobias Becker is the Head of MaxAcademy at Maxeler Technologies where he coordinates various research activities and Maxeler's university program. Before joining Maxeler he been has held positions as a researcher in the Department of Computing at Imperial College London, and at Xilinx, Inc. He received a Ph.D. degree in Computing from Imperial College London and a Dipl. Ing. degree in Electrical Engineering from the Technical University of Karlsruhe (now KIT). His research work covers topics in reconfigurable computing, custom accelerators, self-adaptive systems, low-power optimisations, and financial applications.

SPEAKERS IN ORDER OF PRESENTATION

DAY 2 | TUESDAY, MARCH 13

Objective, innovation and impact of the energy-effcient DOME MicroDataCenter

Ronald P. Luijten IBM Zurich Research Laboratory, Switzerland

Ronald P. Luijten, senior IEEE member, received his Masters of Electronic Engineering with honors from the University of Technology in Eindhoven, Netherlands in 1984. In the same year he joined the systems department at IBM's Zurich Research Laboratory in Switzerland. He has contributed to the design of various communication chips, including PRIZMA high port count packet switch and ATM adapter chip sets, culminating in a 15-month assignment at IBM's networking development laboratory in La Gaude, France as lead-architect, from 1994-95. He lead the OSMOSIS optical switch demonstrator project for the DOE in close collaboration with Corning, inc. from 2004 to 2007. His team also contributed the congestion control mechanism to the converged enhanced Ethernet standard and is worked on the network validation of IBM's HPC systems. He currently manages the IBM DOME microDataCenter team. Ronald's personal research interests are in datacenter architecture, design and performance ('Data Motion in Data Centers'). He holds more than 25 issued patents, and has co-organized 7 IEEE conferences. Over the years (32), IBM has awarded Ronald with three outstanding technical achievement awards and a corporate patent award.

Vortex-topology Messaging: Data Vortex for high performance middleware

Ryan Quick Providentia Worldwide, USA

Ryan Quick received degrees in English and Philosophy from Vanderbilt University. He has been active in the Internet and Linux communities since the early 1990s. He focused on distributed systems for the last 25 years, with special attention to the interaction between applications, operating systems, and the hardware and networks underlying them. Ryan holds patents for messaging middleware systems, and pioneers bridging High Performance Computing technologies with enterprise best-practices. His HPC work for real-time analytics garnered provisional patents and awards. He is recognized for innovation in hardware and application design, messaging ontology, and event-driven systems. Currently, he brings machine learning, real-time streaming, set selection, and digital signal processing technologies to predictive analytics for self-healing in command and control systems.

SUPERCOMPUTING FRONTIERS EUROPE 2018

SPEAKERS IN ORDER OF PRESENTATION

DAY 2 | TUESDAY, MARCH 13

Effciency analysis of a hybrid supercomputer Desmos with Angara interconnect

Vladimir Stegailov Joint Institute for High Temperatures of the Russian Academy of Sciences, Russia

Vladimir Stegailov is currently the head of department in Joint Institute for High Temperatures of Russian Academy of Sciences and a professor in Moscow Institute of Physics and Technology and Higher School of Economics. Vladimir Stegailov received PhD (2004) and DrSc (2012) degrees from Moscow Institute of Physics and Technology. His principal research interests include high performance computing in materials science, development of theoretical approaches for multi-scale modelling and simulation, atomistic modelling of condensed phase (molecular dynamics and ab initio approaches). In 2016, Vladimir received the Presidential prize in science and innovation for young scientists. He is the author of more than 80 publications in peer reviewed journals.

Elbrus processors performance for fast Fourier transform and computational materials science codes

Alexey Timofeev Joint Institute for High Temperatures of the Russian Academy of Sciences, Russia

Alexey Timofeev is a head of laboratory in Joint Institute for High Temperatures of Russian Academy of Sciences and an assistant professor in Moscow Institute of Physics and Technology and Higher School of Economics. Alexey completed his Ph.D. at Joint Institute for High Temperatures of Russian Academy of Sciences in 2011 and his undergraduate studies at Moscow Institute of Physics and Technology. His research interests include high performance computing in materials science, plasma modelling and simulation. In 2010, Alexey received the gold Medal in science for students. He is the author of more than 15 publications in peer-reviewed journals.

Internet of Things

Nicola Ferrier Argonne National Laboratory, USA

Nicola Ferrier received her doctorate from Harvard University in 1992. Afer postdoctoral fellowships at Oxford University and Harvard, she joined the Department of Mechanical Engineering at the University of Wisconsin (UW)-Madison in 1996. She became an associate professor in 2003 and professor in 2009. She received the NSF CAREER award (1997) and the UW Vilas Associates Professorship (1999) and the UW Honored Instructor Award (2009). She joined the Mathematics and Computer Science Division at Argonne in 2013.

Ferrier's research interests are in the use of computer vision (digital images) to control robots, machinery, and devices, with applications as diverse as medical systems, manufacturing, and projects that facilitate "scientific discovery" (such as her recent project using machine vision and robotics for plant phenotype studies).

SPEAKERS IN ORDER OF PRESENTATION

DAY 2 | TUESDAY, MARCH 13

Applying DDN to machine learning

Frederic Lemaire DDN

HPC Storage and Big Data – Solving the I/O challenge

Torben Kling Petersen Cray

HPE techology innovations: from Gen-Z to 'The machine'

Michal Klimeš HPE

Software Ecosystem for Arm-based HPC

Florent Lebeau ARM

Florent Lebeau is a staf applications engineer at ARM providing efective customer training across a broad range of debugging, profiling and optimization tools. Having worked in HPC for many years, Florent brings valuable knowledge and experience in the practical use of parallel programming and development tools, joining the ARM HPC Tools team afer working as an engineer for Allinea Sofware and at CAPS enterprise, where he developed profiling tools for HMPP Workbench and provided training on parallel technologies. Florent graduated from the University of Dundee with an MSc in Applied Computing.

Facilitate HPC Operation and administration via Cloud

Miha Verlič Arctur d.o.o., Slovenia

Miha Verlič is a HPC & system administrator at Arctur. He has over 15 years of experiences in wide range of fields - Linux, networking, databases, services, monitoring. His knowledge in multiple areas gives him a complete overview of a complex ecosystem such as HPC cluster and in-depth understanding how every element works. His experiences help him with debugging, optimizations and keeping systems running 24/7. The vast experience and knowledge has proven to be invaluable also in the development of EasyOP, the HPC management system that he will be presenting.

SPEAKERS IN ORDER OF PRESENTATION

DAY 2 | TUESDAY, MARCH 13

Supercomputing with the PLGrid Infrastructure: a Tool for Open Science

Jacek Kitowski AGH University of Science and Technology, Poland

Jacek Kitowski, full professor of computer science, Head of the Computer Systems Group at the Department of Computer Science of the AGH University of Science and Technology, Cracow and Head for international afairs and the Director of Polish Consortium PL-Grid for development of computing infrastructure for scientific research at ACK Cyfronet AGH, Cracow.

He is the author or co-author of about 250 scientific papers. His topics of interest include large-scale computations, multiprocessor architectures, high availability systems, distributed computing, Grid/Cloud services and Grid/Cloud storage systems, knowledge engineering. Member of Ministry Expert Body for Scientific Investments (2015-2019) Polish representative to Computing RRB (WLCG) nominated by Minister of Science and Higher Education (since 2017).

Towards Near-Data Processing for Clouds – Challenges and Future

Gaurav Kaul Amazon, UK

Gaurav Kaul is a Solution Architect for HPC and AII in AWS. He works with customers in Europe who are looking to migrate and optimize their workloads on AWS. He joined AWS from Intel where he worked as a Systems architect and worked on server and systems for HPC for various ODMs. He has completed his MS in Computer Science from the University of Manchester. He lives in London, UK.

CONFERENCE DAY 3

■ Keynote Speaker ■ Invited Speaker ■ Sponsors

8:00 — 9:00	Registration		
9:00 — 10:00	Neuromorphic computing – From biology to user facilities **Karlheinz Meier, Heidelberg University, Germany**	NEURO,	Chair: **Thomas Sterling**
10:00 — 10:45	The Start of the Journey from Digital to Quantum Computing Robert Ewald, D-Wave, USA	QUANTUM C,	
10:45 — 11:00	From Spin Chemistry to Quantum Computing – Early Experience with Quantum Computing at the University of Notre Dame's Center for Research Computing Mariya Vyushkova, Jarek Nabrzyski and Alexander Vyushkov, University of Notre Dame, USA		
11:00 — 11:20	BREAK		
11:20 — 12:05	Manycore Accelerators beyond GPU Architecture Benoit Dupont de Dinechin, Kalray, France	ARCH,	Chair: **Artur Binczewski**
12:05 — 12:50	Next Generation Software Defined Services and the Global Research Platform: A Software Defined Distributed Environment For High Performance Large Scale Data Intensive Science Joe Mambretti, Northwestern University, USA	NET,	
12:50 — 13:00	Progress Report: Connecting Poland to Scientific Data Superhighway Jarosław Skomiał, Interdisciplinary Centre for Mathematical and Computer Modeling (ICM), University of Warsaw, Poland		
13:00 — 13:20	Implementing integrated photonics in supercomputing centers interconnect Krzysztof Kawecki, Infinera & FCA	INFRA,	
13:20 — 14:20	LUNCH		
14:20 — 15:05	Nonlinear partial differential equations, gravity, cosmology and supercomputing Baojiu Li, Durham University, UK	COSMOLOGY	Chair: **Wojciech Hellwing**
15:05 — 15:25	Individual time-stepping in cosmological simulations: A challenge for strong scaling and domain decomposition algorithms Matthieu Schaller, Leiden Observatory, Netherlands		
15:25 — 15:45	Numerical simulations of black hole accretion in gamma ray bursts Agnieszka Janiuk and Konstantinos Sapountzis, Center for Theoretical Physics, Polish Academy of Sciences, Poland; Ireneusz Janiuk		
15:45 — 16:05	Copernicus Complexio simulations Sownak Bose *et al.*, Harvard-Smithsonian Center for Astrophysics, USA		
16:05 — 16:20	Machine learning and astronomical big data Maciej Bilicki, Leiden Observatory, Netherlands		
16:20 — 16:35	Performance of Julia programming language in HPC simulation of the cosmic ray transport in the heliosphere Anna Wawrzynczak-Szaban, Renata Modzelewska-Łagodzin and Agnieszka Gil-Świderska, Siedlce University of Natural Sciences and Humanities, Poland		
16:35 — 16:55	BREAK		
16:55 — 17:25	Cognitive Discovery: How AI can dramatically change the way we do R&D Costas Bekas, IBM	INFRA,	Chair: **Krzysztof Kurek**
17:25 — 17:40	Towards exascale simulations of quantum turbulence in Fermi superfluids: status and challenges Gabriel Wlazłowski *et al.*, Warsaw University of Technology, Poland	APPLICATIONS	
17:40 — 17:55	The application of HPC solutions for the plasma impurities diagnostics for the thermal fusion reactors Rafał Krawczyk *et al.*, Warsaw University of Technology, Poland		
17:55 — 18:10	How a supercomputer can unravel the structure of hadrons? Piotr Korcyl, Jagiellonian University, Poland		
18:10 — 18:15	Closing words Marek Michalewicz, Interdisciplinary Centre for Mathematical and Computer Modeling (ICM), University of Warsaw, Poland	CLOSING	

SUPERCOMPUTING FRONTIERS EUROPE 2018

SPEAKERS IN ORDER OF PRESENTATION

DAY 3 | WEDNESDAY, MARCH 14

Neuromorphic computing – From biology to user facilities

Karlheinz Meier Heidelberg University, Germany

Karlheinz Meier was appointed full professor of physics at Heidelberg University in 1992, where he co-founded the Kirchhoff-Institute for hhysics. He has more than 25 years of experience in experimental particle physics, including design of a large-scale electronic data processing system that enabled the discovery of the Higgs Boson in 2012. Around 2005 he became interested in large-scale electronic implementations of brain-inspired computer architectures. His group pioneered several innovations in the field. He led 2 major European initiatives, FACETS and BrainScaleS. In 2009 he was one of the initiators of the European Human Brain hroject (HBh) that was approved in 2013. In the HBh he leads the subproject on neuromorphic computing with the goal of establishing brain-inspired computing paradigms as research tools for neuroscience and generic hardware systems for cognitive computing. In the HBh he is a member of the project directorate and vice-chair of the science and infrastructure board.

The Start of the Journey from Digital to Quantum Computing

Robert Ewald D-Wave, USA

Robert “Bo” Ewald leads D-Wave’s international business as hresident and is responsible for global customer operations for the company. Mr. Ewald has a long history with other leading technology organizations, government projects, and industry efforts. He has experience in large and startup businesses having been the CEO of visualization and HhC leader Silicon Graphics Inc., hresident of supercomputing leader Cray Research, hresident and CEO of Linux pioneer Linux Networx and Executive Chairman of herceptive hixel, Inc. He started his career at the Los Alamos National Laboratory where he led the Computing and Communications Division. He has served on the boards of directors of both public and private companies and has participated in numerous government and industry panels and committees. He was appointed to the hresident’s Information Technology Advisory Council by both the Clinton and Bush administrations.

From Spin Chemistry to Quantum Computing – Early Experience with Quantum Computing at the University of Notre Dame’s Center for Research Computing

Jarek Nabrzyski University of Notre Dame, USA

Jarek Nabrzyski is the Director of the Center for Research Computing (CRC), Concurrent hrofessor of Computer Science and Engineering at the University of Notre Dame, as well as the Director of a newly founded Quantum Computing Lab in the CRC. Before joining Notre Dame in 2009 Nabrzyski was the the Executive Director of the Louisiana Center for Computation and Technology and, before that, he managed the Scientific Application Department at the hoznan Supercomputing and Networking Center in hoznań, holand. Nabrzyski has received M.Sc. and hh.D. in Computer Science and Engineering from the hoznan University of Technology. His research interests cover scientific computing, distributed resource management and scheduling, and broad aspects of reproducibility in science.

SPEAKERS IN ORDER OF PRESENTATION

DAY 3 | WEDNESDAY, MARCH 14

Manycore Accelerators beyond GPU Architecture

Benoît Dupont de Dinechin Kalray, France

Benoît Dupont de Dinechin is Chief Technology Officer of Kalray. He is the Kalray VLIW core main architect, and the co-architect of the Multi-hurpose hrocessing Array (MhhA) processors. Benoît also defined the Kalray sofware roadmap and contributed to its implementation. Before joining Kalray, Benoît was in charge of Research and Development of the STMicroelectronics Sofware, Tools, Services division, and was promoted to STMicroelectronics Fellow in 2008. hrior to STMicroelectronics, Benoît worked at the Cray Research park (Minnesota, USA), where he designed the sofware pipeliner of the Cray T3E production compilers. Benoît earned an engineering degree in Radar and Telecommunications from the Ecole Nationale Supérieure de l'Aéronautique et de l'Espace (Toulouse, France), and a doctoral degree in computer systems from the University hierre et Marie Curie (haris) under the direction of hrof. h. Feautrier. He completed his post-doctoral studies at the McGill University (Montreal, Canada) at the ACAhS laboratory led by hrof. G. R. Gao.

Next Generation Software Defined Services and the Global Research Platform: A Software Defined Distributed Environment For High Performance Large Scale Data Intensive Science

Joe Mambretti Northwestern University, USA

Joe Mambretti is Director of International Center for Advanced Internet Research (iCAIR) at Northwestern University. He is also Director of MREN, a high-performance network interlinking organizations providing services in seven upper-midwest states. iCAIR, created in partnership with a number of major high-tech corporations, designs and implements large-scale services and infrastructure for data-intensive applications (metro, regional, national, and global). With its research partners, iCAIR has established multiple national and international network research testbeds that are used to develop new architecture and technology for dynamically provisioned communication services and networks, including those based on lightpath switching and 100G paths. He is also Director of the StarLight facility in Chicago; the hrincipal Investigator (hI) of an National Science Foundation (NSF) project to develop an international Sofware Defined Network Exchange (SDX); the hI of the NSF-funded International Global Environment for Network Innovations (iGENI); the hI of the NSF-funded StarWave, a multi 100G communications exchange facility; the hI of several research projects to create 100G services, network testbeds, and facilities; the hI of several national and international network testbeds; the hI of an NSF-funded GENI project that developed the world's first SDX prototype; and, co-hI of the Chameleon NSFCloud testbed. He is the author of many articles and the co-editor of Grid Networks: Enabling Grids With Advanced Communications Technology, published by Wiley.

SPEAKERS IN ORDER OF PRESENTATION

DAY 3 | WEDNESDAY, MARCH 14

Progress Report: Connecting Poland to Scientific Data Superhighway

Jarosław Skomiał Interdisciplinary Centre for Mathematical and Computer Modeling (ICM), University of Warsaw, Poland

Implementing integrated photonics in supercomputing centers interconnect

Krzysztof Kawecki Infnera & FCA

Nonlinear partial differential equations, gravity, cosmology and supercomputing

Baojiu Li Durham University, UK

Individual time-stepping in cosmological simulations: A challenge for strong scaling and domain decomposition algorithms

Matthieu Schaller Leiden Observatory, Netherlands

Dr. Schaller obtained his PhD at the Institute for Computational Cosmology in Durham (UK) where he worked of galaxy formation and cosmological simulations. In collaboration with experts in the school of computer science, he lead the development of the next-generation code named SWIFT. This new simulation software was designed from scratch to run on the largest HPC clusters using modern technologies to exploit the latest architecture changes. Some of these innovations will be presented in this talk. Dr. Schaller is now a VENI post-doctoral fellow at the University of Leiden (Netherlands) where he pursues the development of SWIFT and plans simulations for ESA's future Euclid satellite mission.

SPEAKERS IN ORDER OF PRESENTATION

DAY 3 | WEDNESDAY, MARCH 14

Numerical simulations of black hole accretion in gamma ray bursts

Agnieszka Janiuk Center for Theoretical Physics, Polish Academy of Sciences, Poland

Graduated from the Faculty of physics at University of Warsaw, Department of Astronomy. Received her PhD under Doctoral Studies at Nicolaus Copernicus Astronomical Center, Polish Academy of Sciences (CAMK, graduated with honors).

She obtained several scientific fellowships, including pre-doctoral positions in Scuola Internazionale Superiore di Studi Avanzati in Trieste, Harvard Smithsonian Center for Astrophysics, post-doc at Max Planck Institut fuer Astronomy and Astrophysics in Munich, several short-term scientific visits in Inter University Center for Astronomy and Astrophysics in Pune and post-doc at University of Nevada, Las Vegas.

Habilitated in Astronomy in CAMK in Warsaw in April 2011. Since October 2011 works in the Center for Theoretical physics (CFT), first as an Assistant Professor (adjunct), from Autumn 2011 as an Associate Professor.

In the years 2011-2015, she served as the Deputy Head of Center for Theoretical Physics. She is a member of the Polish Astronomical Society (in the period of 2009-2011 was in the Managing Board of the Society), member of the International Astronomical Union, and, since 2015, elected as a member of the Astronomy Committee of the Polish Academy of Sciences. She is also a member of the National Council of Astroparticle Physics in Poland.

From 2016, she is a member of the European Astronomical Society. In the years 2009-2014 she took part in the COST (European Cooperation in Science and Technology) Action Mh0905 on the “Black holes in the Violent Universe” and served as the Managing Committee member and Poland’s representative for this Action.

From 2016, she is a member of the Science Advisory Board of the Athena X-ray mission.
She specializes in astrophysics of accretion disks in compact binary systems, active galactic nuclei and the origin of Gamma Ray Bursts, as well as nucleosynthesis of heavy elements in these objects. She is an author and co-author of over 100 scientific publications devoted to relativistic computational astrophysics.

SUPERCOMPUTING FRONTIERS EUROPE 2018

SPEAKERS IN ORDER OF PRESENTATION

DAY 3 | WEDNESDAY, MARCH 14

Copernicus Complexio simulations

Sownak Bose Harvard-Smithsonian Center for Astrophysics, USA

Sownak Bose writes about himself: “I am an astrophysicist at the Harvard-Smithsonian Center for Astrophysics, where I am currently an ITC Fellow. Before this, I obtained my PhD in astrophysics from the Institute for Computational Cosmology in Durham University, preceded by an undergraduate Masters degree in Physics from the University of Oxford. My research involves the study of dark matter and dark energy, and how they influence the formation of structure in the Universe through the use of large cosmological simulations on supercomputers.”

Machine learning and astronomical big data

Maciej Bilicki Leiden Observatory, Netherlands

Dr. Maciej Bilicki is a cosmologist who works with big data from the largest astronomical surveys. His research covers many areas of the study of the large-scale structure of the Universe, including applications of various machine-learning methodologies to extract astronomical information which is difficult or even impossible to obtain with more traditional methods. Together with his collaborators, he uses these novel approaches to robustly estimate distances to millions of far-away galaxies, as well as to automatically classify extragalactic sources in datasets encompassing of the order of billion objects detected over the entire sky. Dr. Bilicki is currently a research associate at the Leiden Observatory in the Netherlands, as well as a part-time research assistant at the Astrophysics Division of the National Centre for Nuclear Research in Warsaw, Poland.

Performance of Julia programming language in HPC simulation of the cosmic ray transport in the heliosphere

Anna Wawrzyńczak–Szaban Siedlce University of Natural Sciences and Humanities, Poland

Assistant Professor at Institute of Computer Sciences of Siedlce University and in National Centre for Nuclear Research, holand. Anna Wawrzyńczak–Szaban received her M.Sc. in Mathematics and Ph.D. in Physics. Her scientific interests focus on performing large-scale simulations solving realistic problems posed by physical and engineering sciences. One of these problems is the non-stationary motion of charged particles in the 3D inhomogeneous magnetic field. She puts particular attention on the application of the stochastic approach to model heliospheric cosmic ray transport during high solar activity periods. Her area of interest also covers the application of Bayesian statistics and heuristics methods in stochastic event reconstruction. Presently she leads the Polish National Science Centre grant “Accurate and approximate algorithms for large-scale stochastic simulation.” Results of her research were published in about 20 high-rank scientific journals and presented at over 40 international conferences.

SPEAKERS IN ORDER OF PRESENTATION

DAY 3 | WEDNESDAY, MARCH 14

Cognitive Discovery: iow AI can dramatically change the way we do R&D

Costas Bekas IBM

Towards exascale simulations of quantum turbulence in Fermi superfuids: status and challenges

Gabriel Wlazłowski Warsaw University of Technology, Poland

Gabriel Wlazłowski (Ph. D.) is physicist at Warsaw University of Technology (Poland). He is interested in studies of dynamics of various superfluid Fermi system, ranging from ultra-cold atomic gases through nuclear systems to neutron stars. Since 2013, together with collaborators from University of Washington (USA) and Warsaw University of Technology, he has been developing extension of density functional theory to superfluid and superconducting systems that can fully utilize the advanced capabilities of modern leadership class supercomputers. Presently, his group is conducting studies using systems like Piz Daint (CSCS, Switzerland), Titan (ORNL, USA) and Tsubame3.0 (GSIC Center, Japan).

The application of HPC solutions for the plasma impurities diagnostics for the thermal fusion reactors

Rafał Krawczyk Warsaw University of Technology, Poland

Rafał Krawczyk is employed as an assistant and a PhD student in Institute of Electronic System, Warsaw University of Technology. He specializes in implementing server and accelerator based processing for intensive computing loads in large scale physics experiments. He participated in the LHCb detector upgrade at CERN. The topic of his current work is providing a fast, heterogeneous high-performance and high-throughput device with real-time constraints for the WEST thermal fusion reactor diagnostics for French Alternative Energies Commission in Cadarache. The work is conducted in the framework of EUFOfusion project, with long-term objective of constructing the ITER - the first fully operational thermonuclear power plant. For the SCFE 2018, joint studies of his and the research team will be presented.

How a supercomputer can unravel the structure of hadrons?

Piotr Korcyl Jagiellonian University, Poland

Piotr Korcyl about himself: “I'm theoretical physicist working at the Jagiellonian University in the field of elementary particles. I'm using Monte Carlo simulations of Quantum Chromodynamics to explore the structure of particles such a protons and neutrons. I finished my PhD at the Jagiellonian University. I was a postdoc at DESY (Deutsches Elektronen-Synchrotron) Zeuthen, I was awarded a Fulbright Fellowship and spent half a year at the Columbia University in New York and eventually I was a postdoc in the largest Lattice QCD group in Germany at the University of Regensburg. I'm a member of the CLS and RQCD collaborations and I'm using the largest supercomputer facilities in Europe, such as JUQUEEN, superMUC, Marconi, and Prometheus and OKEANOS in Poland. During my postdoc at the University of Regensburg I participated in the development of the QhACE2 supercomputer prototype, one of the most energy-efficient Intel Knights Landing machine.”

WORKSHOPS
DAY 4

TUTORIAL 1:
D-WAVE SYSTEMS: AN INTRODUCTION TO PROGRAMMING A QUANTUM COMPUTER

Time:
9.00am – 1.00pm

Breaks:
Morning Tea Break – 10.30am – 11.00am
Lunch Break – 1.00pm – 2.00pm

Presenters:
- Andy Mason, *Sales Director, D-Wave Europe*
- Sheir Yarkoni, *Technical Analysist, D-Wave Europe*

Abstract:
Quantum computing has progressed from ideas and research to implementation and product development. There are multiple physical devices capable of providing controllable evolution of a quantum wavefunction which could form the basis for a quantum computer. The 2000-qubit D-Wave System uses an annealing/adiabatic architecture which natively solves discrete optimization, and probabilistic machine learning problems.

Our goal is to expand attendees' understanding of quantum computing as implemented on the D-Wave System and where it fits in a computing environment (or maybe work flow).

Important Notes:
Participants will have access to 128 qubit simulators (using their own laptops) and the opportunity to implement a number of programming examples as well as view live demos on a 2000 qubit D-Wave System.
It is recommended attendees
have knowledge comparable to an M.Sc. or higher in computer science, mathematics or physics or equivalent, or otherwise have sufficient familiarity with algorithms and data structures and experience implementing algorithms
in C/C++, Matlab or Python.

WORKSHOPS
DAY 4

TUTORIAL 2:
INTRODUCTION TO NUMERICAL COMPUTING WITH JULIA

Time:
1:30pm – 5.00pm

Brief agenda:

1. What makes Julia fast – language design principles.
2. Explanation of the sample computational problem that will be solved during the workshop.
3. Parallel computing in Julia on a single machine.
4. Using Julia in AWS Cloud.
5. Using Julia on ICM computing cluster.

Presenters:

- Bogumił Kamiński, *SGH Warsaw School of Economics, Poland*
- Przemysław Szufel, *SGH Warsaw School of Economics, Poland*

Abstract:
Julia language was designed to deliver dramatic improvements in simplicity, speed, scalability, and productivity to solve massive computational problems. The goal of this workshop is to give the participants hands-on experience of running massively distributed numerical experiments using Julia language. The example problem is a large scale stochastic simulation-optimization task (a description of the employed algorithms is presented in this paper). The computations will be presented on two environments: ICM computing cluster and a Spot Fleet of EC2 instances in the AWS Cloud. We will show how to build and run a cluster having at least 100 nodes in Julia language.

Important Notes:
If participants want to run the computations themselves it is advised that they have a notebook with SSH client installed and an AWS account (free coupons for computations on AWS will be provided).

WORKSHOPS
DAY 4

TUTORIAL 3:
ADVANCED SCIENTIFIC VISUALIZATION WITH VISNOW PLATFORM

Time:
9:00am – 12.30pm

Brief agenda:

1. Introduction to Scientific Visualization and Visual Analysis.
2. Visualization systems and paradigms
3. Generic data structures
4. Introduction to VisNow
5. Hands-on Session #1 – 2D data visualization
6. Hands-on Session #2 – 3D data visualization
7. Hands-on Session #3 – Vector data visualization
8. Hands-on Session #4 – Unstructured data visualization.

Presenters:

- Bartosz Borucki, *Interdisciplinary Centre for Mathematical and Computational Modelling University of Warsaw, Poland*
- Krzysztof Nowiński, *Interdisciplinary Centre for Mathematical and Computational Modelling University of Warsaw, Poland*

Abstract:

Visual analysis is one of the most powerful tools for data exploration and interpretation. It takes advantage of visualization techniques and allows scientists to work with their research data in interactive and intuitive way. In today's HPC environment and Big Data era, data analysis techniques, together with visualization, gain on importance. However, the amounts of data and the sizes of single datasets impose the need for adequate software tools.

In this tutorial we will address this problem by providing participants with strong tool for data processing, visualization and visual analysis – VisNow, an open source generic platform based on data flow paradigm. The goal of this tutorial is to introduce the audience to the concept of visual analysis, show basic ideas of scientific visualization and to go step-by-step through several case studies in hands-on sessions based on our platform. Problems of visualization of common HPC data structures, including 2-D and 3-D, scalar and vector, regular and unstructured data will be covered and adequate elements of the software described to give participants the basics of VisNow usage.

WORKSHOPS
DAY 4

TUTORIAL 4:
HIGH PERFORMANCE COMPUTING AND BIG DATA ANALITICS WITH PCJ AND JAVA

Time:
1:30pm – 5.00pm

Brief agenda:
The half dayr tutorial comprises three parts parts, with time for discussion at the included coffee breaks. The tutorial is organized in the form of hands-out with the short introduction. We would like to get participants involved
in the programming of simple examples provided by the organizers as well as computational kernels brought by the participants.

1. Part 1 (1 hour) briefly covers the PGAS programming model and presents details of the PCJ library. It provides overview of the library and presents examples of the typical programming tasks. Examples of the parallelization
2. of the most popular programming kernels will be provided.
3. Part 2 (1.5 hour) is design as practical introduction to the PCJ. Participants will write and execute parallel applications starting from the “Hello world”, trough different communications schemas up to the parallelization
4. of the selected computational kernels.
5. Part 3 (1 hour) will focus on more advanced applications including problems suggested by the participants.

Presenters:

- prof. Piotr Bała, *Interdisciplinary Centre for Mathematical and Computational Modelling University of Warsaw, Poland*
- dr Marek Nowicki, *Nicolaus Copernicus University, Poland*
- dr Łukasz Górski, *Interdisciplinary Centre for Mathematical and Computational Modelling University of Warsaw, Poland*

Abstract:

The goal of the tutorial is the presentation of the PCJ library and its application for parallelization of example programs (computational kernels). The attendees will get familiar with the PGAS programming models used by the PCJ library. The tutorial will focus on the practical development of the parallel codes using Java, therefore, the main part of the tutorial will be in the form of hands-on. The PCJ library runs on any HPC system equipped with Java runtine environment. It shows good performance and scalability up to 100k+ cores. The PCJ library has been already used to parallelize different benchmarks as well as large scale parallel applications such as raytracing, FFT, MapReduce, BFS or Genetic Algorithm. The PCJ library (http://pcj.icm.edu.pl) implements partitioned global address space (PGAS) model. The PCJ does not extend nor modify language syntax. The PCJ library put emphasis on compliance with Java standards. The programmer does not have to use additional libraries, which are not part of the standard Java distribution. Compared to the other solutions PCJ does not need a dedicated compiler to preprocess
code.

WORKSHOPS
DAY 4

TUTORIAL 5:
MAXELER TECHNOLOGIES: PRACTICAL DATAFLOW COMPUTING: FROM HPC TO CLOUD

Time:
9:00 am – 12:30 pm

Presenter:
Tobias BECKER, *Maxeler Technologies*

Abstract:

Maxeler Technologies pioneers a new Multiscale Dataflow Computing model that centres on maximal performance and efficiency. By offloading computations to dedicated Data Flow Engines (DFEs), the typical bottlenecks of the conventional Von Neumann architecture are avoided, resulting in 20-50x higher performance and energy efficiency. This has been demonstrated across many application domains including machine learning, finance, security and scientific computations.

The workshop introduces the Maxeler Dataflow compute model and its associated high-level programming paradigm. We cover practical application development and dedicated optimisations across various layers of abstraction. Furthermore, we cover the practical deployment of Dataflow technology from conventional on-premise HCP to public Cloud. Amazon EC2 F1 Instances are compatible to the latest generation MAX5 DFEs and open up new exciting opportunities to perform Dataflow computing in the Cloud. We illustrate how developers can scale elastically from an on-premise Dataflow system into the Cloud to cover peak demand. Dataflow computing in the Cloud also allows academics to carry out research without investing into specialised compute infrastructure.

WORKSHOPS
DAY 4

TUTORIAL 6:
NUMERICAL ALGORITHMS GROUP LTD.: PERFORMANCE ANALYSIS: AN INTRODUCTION TO THE TOOLS AND PERFORMANCE ANALYSIS METHODOLOGY USED IN POP COE

Time:
1:30 pm – 5:00 pm

Brief agenda:

1. Introduction to performance analysis and POP CoE methodology.
2. Performance analysis with Paraver and Scalasca for parallel codes.
3. Parallel I/O Profiling and Darshan profiling tool.
4. Hands-on session with profiling tools.

Presenters:

- Jon Gibson, *Numerical Algorithms Group Ltd., Great Britain*
- Wadud Miah, *Numerical Algorithms Group Ltd., Great Britain*

Abstract:

POP CoE (Performance Optimisation and Productivity Centre of Excellence) is funded by the Horizon 2020 programme to help people write more efficient parallel. We will present the systematic approach used to analyse and optimise parallel codes and an introduction to some open source profiling tools used within the project. Measuring application performance often results in large amounts of data that is difficult to handle or interpret beyond some simple first observations. The methodology used within POP CoE provides a quantitative way of measuring the relative impact of the different factors inherent in parallelisation, each metric reflecting a common cause of inefficiency. This provides the knowledge necessary to decide the best course of action to get performance via reproducible and comparable measurements of the performance. POP CoE is a collaboration between Barcelona Supercomputing Center, High Performance Computing Center Stuttgart, Jülich Supercomputing Centre, Numerical Algorithms Group Ltd, RWTH Aachen and TERATEC.

WORKSHOPS
DAY 4

TUTORIAL 7:
MICROSOFT AZURE — THE BEST PUBLIC CLOUD FOR HPC

Time:
9:00 am – 12:30 pm

Brief agenda:

1. Introduction to HPC on Azure and lab environment (1 hour)
2. Hands-on lab session (3 hours)
    - Deploying Linux RDMA Infiniband cluster with Azure CLI,
    - Deploying SLURM cluster from ARM template,
    - Deploying HPC cluster from CycleCloud template,
    - Image processing with Azure Batch service,
    - Running TCFD simulation in Ubercloud container.

Presenters:

- Tomasz Józefiak, *Microsoft Poland*
- Mike Kiernan, *Microsoft*
- Reha Senturk, *The Ubercloud*

Abstract:

Microsoft Azure offers the best and the most highly-optimized infrastructure for HPC among all public cloud providers:

- high-end multicore CPUs for compute-intensive calculations,
- NVIDIA GPUs for accelerated computing and visualization,
- RDMA InfiniBand interconnect for real scalability of MPI jobs,
- bare-metal Cray supercomputer infrastructure for the most demanding HPC workloads.

Azure also offers platform services like Azure Batch, VM scalesets and CycleCloud which assist in easy deployment, management and scaling of HPC workloads in the cloud environment.
This workshop aims to demonstrate different ways of using Azure for running HPC jobs. We'll start with an introductory presentation of HPC services on Azure and the workshop environment, followed by a hands-on lab session. Our instructors will walk step-by-step through the lab content. Participants will receive free Azure passes and will be able to execute the labs following the instructor guidance or at their own pace.
Prerequisites:

- Please bring your own laptop with any OS – Windows, Linux, MacOS
- In order to use Azure pass that you will receive during the workshop, please create your Microsoft Account: https://account.microsoft.com/
- In case of any questions please contact us via email: azurepl@microsoft.com

WORKSHOPS
DAY 4

TUTORIAL 8:
BASICS OF HIGH PERFORMANCE COMPUTING SYSTEMS AT ICM

Time:
1:30 pm – 5:00 pm
Presenters:

- Maciej Marchwiany, *Interdisciplinary Centre for Mathematical and Computational Modelling University of Warsaw, Poland*
- Maciej Szpindler, *Interdisciplinary Centre for Mathematical and Computational Modelling University of Warsaw, Poland*

Abstract:
This tutorial aims at basic usage scenarios of High Performance Computing systems available at ICM. Agenda covers system access, creating and submitting user jobs, user environment, custom application codes enabling. Common scenarios will be discussed with step-by-step approach. Hands-on session is included. Registered users are the target audience of the tutorial.
Important Notes:
Tutorial language is Polish.

TUTORIAL 9:
INTEL CORPORATION: INTEL SOFTWARE TOOLS FOR HPC AND DATA ANALYSIS – PRACTICAL SESSION

Time:
1:30 pm – 5:00 pm
Presenters:

- Dmitry Sivkov, *Technical Consulting Engineer, Intel*
- Olga Andrianova, *Business Development Manager, Intel*
- Robert Adamski, *HPC AE – EMEA Territory, Intel*

Abstract:
Intel Software helps developers and end users to get a full performance of their HPC and Data Analytic applications. Intel provides a wide range of tools and libraries that can be used for numerous scientific and industry applications.
This practical training is targeted to give an overview of tools and aspects of usage, basic practices of optimizing Python* application, starting with Intel® Distribution for Python, performance profiling with Intel® VTune™ Amplifier, speedup code with Intel® Advisor, and distributed HPC/AI usage. *Live demo on HPC/AI cluster!*
Important Notes
Training audience: software developers, Data Analytics, Data Scientists, Researchers.
Attendees will get personal license for Intel® Software used in the training.

ACKNOWLEDGEMENT

Honorary Patronage

Ministerstwo Cyfryzacji

MINISTERSTWO PRZEDSIĘBIORCZOŚCI I TECHNOLOGII

UNIWERSYTET WARSZAWSKI

Media Partners

CIO FROM IDG

COMPUTERWORLD FROM IDG

ENTERPRISETECH INSIDE ADVANCED SCALE CHALLENGES

HPCwire

KLUB CIO

TOP500 News

SUPERCOMPUTING FRONTIERS EUROPE 2018

SPONSORS

Platinum Sponsor

golem

Gold Sponsor

DDN STORAGE

IBM

Silver Sponsors

arm

Atos

comtegra

CRAY THE SUPERCOMPUTER COMPANY

Hewlett Packard Enterprise

intel

Microsoft

MooseFS

PGNiG

Bronze Sponsor

FCA

infinera

Symkom