CONFERENCE PROGRAMME

Zakopane, 19-21 April 2023

Wednesday, 19th April 2023		
15:00 – 19:30		**Training: Effective Use of HPC in Research Utilizing Machine Learning** *Szymon Mazurek, Michał Karwatowski, Marcin Pietroń, Klemens Noga*
Thursday, 20th April 2023		
9:00 – 10:50		**Session 1** — **Chair: Robert Pająk**
	9:00	Conference opening
	9:10	Cyfronet - Moc dla polskiej nauki, *prof. Kazimierz Wiatr, ACC Cyfronet AGH*
	9:50	*Invited speech*: Artificial Intelligence and Intensive Numerical Simulations for Heavy Industry by Using High-Performance Computing, *prof. Łukasz Rauch, AGH UST*
	10:20	*Invited speech*: Artificial Intelligence, Health Science and Case of Predicting Orthostatic Intolerance in Older Persons, *prof. Matej Mertik, Alma Mater Europea ECMe*
10:50 – 11:15		**Coffee break**
11:15 – 13:00		**Session 2** — **Chair: Grzegorz Mazur**
	11:15	Ab Initio Molecular Dynamics Studies of Hydrogen Bonding and IR Spectra in EMIM-TFSI/H_2O Systems, *P. Wróbel, P. Kubisiak, A. Eilmes*
	11:30	Vibrational Spectra from Molecular Dynamics: Seeking for an Efficient Computational Method, *A. Eilmes, P. Wróbel, P. Kubisiak*
	11:45	Computational Modeling of Intermolecular Interactions in Supramolecular Crystals: Towards Automated Explorations of Chemical Spaces, *G. Niedzielski, R. Podgajny, J. Hooper*
	12:00	Molecular Modeling of Cisplatin Derivatives: the Relationship Between Structure and Potential Bioactivity, *W. M. Łach, M. M. Solarek, M. Nowakowska, K. Szczubiałka, M. Z. Brela*
	12:15	Solvent Molecules Impact on the Nylon 6 Thermal Degradation Process: the Ab Initio Molecular Dynamics and DFT Study, *Y. Didovets, M. Z. Brela*
	12:30	Molecular Modeling of Selected Perovskites with Possible Application in Photovoltaics, *A. Mikłas, M. Z. Brela*
	12:45	Computational Studies on Structural and Photophysical Properties of a 2,4-Dihydroxyphenyl-Substituted 1,3,4-Thiadiazole, *D. Kaczmarczyk, A. Matwijczuk, M. Srebro-Hooper*
13:00 – 14:00		**Lunch**
14:00 – 15:45		**Session 3** — **Chair: Klemens Noga**
	14:00	The Strategy of a Living Organism – the Simulation Model, *I. Roterman, L. Konieczny*
	14:15	Molecular Dynamics Simulations for the Michaelis Complex of Ectoine Synthase (EctC), *J. Andrys-Olek, J. Heider, T. Borowski*
	14:30	Advances in the System for the Automatic Dogs' Skin Cancer Detection, *R. Frączek, M. Karwatowski, J. Grzeszczyk, J. Caputa, P. Pindel, D. Łukasik, M. Wielgosz, P. Russek, A. Dąbrowska-Boruch, E. Jamro, M. Pietroń, S. Koryciak, K. Wiatr*
	14:45	Sonochemical Formation of Fluorouracil Nanoparticles: Toward Controlled Drug Delivery from Polymeric Surfaces, *P. Chytrosz-Wróbel, M. Gołda-Cępa, P. Kubisiak, W. Kulig, Ł. Ćwiklik, A. Kotarba*
	15:00	Computational Studies of Potential Mechanisms for Inhibiting the Toxicity of Amphotericin B via Molecular Association, *M. Gurba, A. Matwijczuk, J. Hooper*
	15:15	Hybrid-Kinetic Simulations of Quasi-perpendicular Shocks in High Beta Cosmic Plasmas, *S. Boula, J. Niemiec, T. Amano*
	15:30	Particle-In-Cell Simulation of the Leptons Acceleration in the Precursor of Young Supernova Remnant Shock, *O. Kobzar*
15:45 – 16:05		**Coffee break**
16:05 – 17:35		**Session 4** — **Chair: Patryk Lasoń** Panel discussion: Cyfronet's computing infrastructure - current status and plans for the future
19:30 – 22:00		**Conference Dinner** Karczma Regionalna "Przy Młynie", ul. Bulwary Słowackiego 23, Zakopane

Friday, 21st April 2023		
9:00 – 10:10		**Session 5** — **Chair: Marek Magryś**
	9:00	HPC&AI; trends and strategy @ HPE, *Marc Simon, HPE*
	9:30	Procesory i akceleratory AMD do superkomputerów, *Krzysztof Łuka, Robert Gorajek, AMD*
	9:50	Accelerated High Performance Computing in the Exascale Era, *Jean-Pierre Panziera, Atos*
10:10 – 10:30		**Coffee break**
10:30 – 12:15		**Session 6** — **Chair: Jacek Kitowski**
	10:30	Differences Between Vibrational Wavepackets Generated via Singlet Fission and Those Shaped by Direct Raman Pumping, *G. Mazur, M. Andrzejak, T. Skóra, P. Petelenz*
	10:45	Particle Transport Simulation for the Personalized Radiotherapy, *L. Grzanka, S. Kania, J. Niechaj, Ł. Pitrus*
	11:00	Improving Hip Dysplasia Diagnosis in Dogs through Augmented 3D Video Simulation, *K. Strzałka, S. Mazurek, M. Wielgosz, J. Caputa, R. Frączek, M. Karwatowski, J. Grzeszczyk, J. Krupiński, D. Łukasik, A. Śmiech, P. Russek, A. Dąbrowska-Boruch, E. Jamro, M. Pietroń, S. Koryciak, K. Wiatr*
	11:15	Development of the Machine Learning Based Track Reconstruction in the MUonE Experiment, *M. Zdybał, M. Kucharczyk, M. Wolter*
	11:30	Deep Neural Networks for the Calibration of Timing Detectors, *M. Kocot, K. Misan, V. Avati, E. Bossini, L. Grzanka, N. Minafra*
	11:45	Neural Networks for the Analysis of Particle Tracing in PIC Simulations, *G. Torralba Paz, A. Bohdan, J. Niemiec*
	12:00	Dog Gait Assessment Using Temporal Graph Neural Networks, *S. Mazurek, K. Strzałka, M. Wielgosz, J. Caputa, R. Frączek, M. Karwatowski, J. Grzeszczyk, D. Łukasik, A. Śmiech, P. Russek, A. Dąbrowska-Boruch, E. Jamro, M. Pietroń, S. Koryciak, K. Wiatr*
12:15 – 12:35		**Coffee break**
12:35 – 14:20		**Session 7** — **Chair: Andrzej Eilmes**
	12:35	Do Cohort Studies in Diffusion MRI Require a Marriage of Convenience with High-Performance Computing? A Case Study, *D. Ciupek, J. Machnio, M. Malawski, T. Pięciak*
	12:50	Classification of Images of Cytological Samples for the Purposes of Initial Analysis, *J. Krupiński, S. Mazurek, K. Strzałka, M. Wielgosz, J. Caputa, R. Frączek, M. Karwatowski, J. Grzeszczyk, D. Łukasik, A. Śmiech, P. Russek, A. Dąbrowska-Boruch, E. Jamro, M. Pietroń, S. Koryciak, K. Wiatr*
	13:05	Leveraging ACC Resources for Medical Research, *P. Nowakowski, M. Bubak, K. Gądek, M. Kasztelnik, M. Malawski, J. Meizner, A. Nowak, P. Połeć, K. Zając, T. Zhyulin*
	13:20	Towards Observability in Scientific Computing, *B. Baliś, A. Kuźma, Ł. Wroński*
	13:35	UWLCM - Eulerian-Lagrangian Cloud Model for Heterogeneous Computing Clusters, *P. Dziekan, P. Żmijewski*
	13:50	Unsupervised Detection of Decoupled Subspaces in the Quantum Hilbert Space, *T. Szołdra, P. Sierant, M. Lewenstein, J. Zakrzewski*
	14:05	Scalability of a Neuroevolutionary Based Framework for Anomaly Detection, *M. Pietroń, D. Żurek, K. Faber*
14:20 – 14:30		**Conference closing**
14:30 – 15:30		**Lunch**