



CONFERENCE PROGRAMME

Zakopane, 13-15 March 2024

Wednesday, 13 th March 2024		
15:00 – 19:30	Using HPC Infrastructure in Machine Learning of Large Language Models, Szymon Mazurek, Krzysztof Wróbel, Aleksander Smywiński-Pohl, Klemens Noga	
Thursday, 14 th March 2024		
9:00 – 10:50	Session 1	Chair: Robert Pająk
	9:00	Conference opening
	9:10	Cyfronet – jaka moc dla Polskiej Nauki, prof. Kazimierz Wiatr , ACC Cyfronet AGH
	9:50	Infrastruktura PLGrid – ewolucja, Andrzej Zemła, PhD , ACC Cyfronet AGH
	10:20	<i>Invited speech:</i> Stepping along the Stabilization Pathways in Hybrid Perovskites: Insights from Neutron Spectroscopy & Materials Modeling, Kacper Drużbicki, PhD DSc , Centre of Molecular and Macromolecular Studies Polish Academy of Sciences and Materials Physics Center, CSIC-UPV/EHU
10:50 – 11:20	Coffee break	
11:20 – 13:20	Session 2	Chair: Andrzej Eilmes
	11:20	Theoretical Studies of the Propylene Oxide Opening Reaction Mechanism in the Copolymerization of CO ₂ with Epoxides Process Catalyzed by a Cobalt(III) Complex with Salen Ligand: Unraveling the Computational Complexity, Olga Żurowska, A. Michalak
	11:35	A Study of the Properties of Unsymmetrically Substituted 4,5-dialkoxy-2-nitroanilines by Spectroscopic and Theoretical Methods, Karina Synowiec, M. Boczar, J. Grolik
	11:50	Investigating the Mechanical Characteristics of Al ₂ O ₃ through Density Functional Theory and Molecular Dynamics, Mostafa Fathalian, E. Postek, M. Tahani, T. Sadowski
	12:05	Multi-scale Modeling of Texture Evolution in Deformed Metals, Bartosz Sułkowski
	12:20	Studies on the Interaction of Nanoplastics with Lipid Systems, Franciszek Włodek, W. Kulig, J. Korchowiec, A. Stachowicz-Kuśnierz
	12:35	Theoretical Study of Copper Complexes in Artificial Photosynthesis, Alicja Mikłas, M. Z. Brela
	12:50	Hydrolysis as an Alternative Path of Nylon 6 and PHB Degradation: a Computational Study, Yuliia Didovets, M. Z. Brela
	13:05	A Detail that Matters? Rotational Isomerism in Some Ortho-substituted Benzophenones, Andrzej J. Kałka, M. Z. Brela, A. M. Turek
13:20 – 14:20	Lunch	
14:20 – 16:20	Session 3	Chair: Andrzej Zemła
	14:20	The System for Automatic Skin Cancer Detection – Achievements and Challenges, Rafał 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
	14:35	Transcriptomics Atlas Pipeline: HTC with Salmon, Piotr Kica, S. Lichotaj, M. Malawski
	14:50	Simulation of Neurotransmitter Flow in a Presynaptic Bouton of a Neuron with Cellular Automaton, A. Bielecki, Maciej Gierdziewicz
	15:05	Magnetic Resonance T ₁ - and T ₂ -weighted Data Synthesis from Heterogeneous Sources: a Federated Learning Approach, J. Fiszer, Dominika Ciupek, M. Malawski, T. Pięciak
	15:20	Comparison of One and Two-Step Deep Learning Models for Cytology Image Classification, Jan Krupiński, S. Mazurek, K. Strzałka, M. Wielgosz, J. Caputa, R. Frączek, M. Karwatowski, J. Grzeszczyk, P. Russek, A. Dąbrowska-Boruch, Ernest Jamro, M. Pietroń, S. Koryciak, K. Wiatr
	15:35	Deep Learning Classification of Cytology Images with Uncertain Training Data, Jan Krupiński, S. Mazurek, K. Strzałka, M. Wielgosz, J. Caputa, R. Frączek, M. Karwatowski, J. Grzeszczyk, D. Łukasik, P. Russek, A. Dąbrowska-Boruch, E. Jamro, M. Pietroń, S. Koryciak, K. Wiatr
	15:50	Integrating Data Repositories with HPC Resources for Execution of Simulation Models, Taras Zhyhulin, K. Zajqc, P. Nowakowski, M. Malawski, M. Kasztelnik, P. Połec, M. Bubak
	16:05	Research towards Virtual Human Twins, Marian Bubak, M. Kasztelnik, M. Malawski, J. Meizner, P. Nowakowski, P. Połec
16:20 – 16:35	Coffee break	

16:35 – 18:00	Session 4 Panel discussion: Cyfronet's computing infrastructure - current status and plans for the future, <i>Marek Magryś, Łukasz Flis, Patryk Lasoń, ACC Cyfronet AGH</i>	Chair: Patryk Lasoń
19:30 – 22:00	Conference Dinner Restauracja Javorina, ul. Strążyska 1, Zakopane	

Friday, 15 th March 2024		
8:40 – 10:20	Session 5	Chair: Marek Magryś
	8:40	HPC&AI Hybrid supercomputing architectures, Marc Simon , HPE
	9:10	How to boost AI and HPC with Intel technologies, Nikolay Mester , Intel
	9:30	Akcelerator AMD Instinct serii MI300, Samuel Antão , AMD
	9:50	<i>Invited speech: Stationary States in Fixed Potentials, prof. Bartłomiej Dybiec, Institute of Theoretical Physics, Jagiellonian University</i>
10:20 – 10:35	Coffee break	
10:35 – 12:35	Session 6	Chair: Jacek Niemiec
	10:35	LUMI, the Elder Brother of Helios, Maciej Szpindler , ACC Cyfronet AGH
	10:50	Numerical Simulations of Short and Long Gamma-Ray Bursts on the Ares Supercomputer, Gerardo Urrutia , A. Janiuk
	11:05	Viscous Torque in Turbulent Magnetized AGN Accretion Disks and Its Effects on EMRI's Gravitational Waves, Agnieszka Janiuk , F. H. Nouri
	11:20	Analysis of Accelerated Particles in PIC Simulations by Using Neural Networks, Gabriel Torralba Paz , A. Bohdan, J. Niemiec
	11:35	Particle-In-Cell Simulations of Merger Shocks in Galaxy Clusters, Oleh Kobzar , J. Niemiec, T. Amano, M. Hoshino, S. Matsukiyo, Y. Matsumoto, M. Pohl
	11:50	Performance of LLAMA Large Language Model in Argument Detection, M. Karwatowski, M. Pietroń, Kamil Faber , D. Żurek
	12:05	Performance of Benchmarking Continual Curriculum Learning, D. Żurek, M. Pietroń, Kamil Faber , M. Karwatowski
	12:20	Comparison of GPU and CPU Implementations of New Variants of SDLS Algorithms for LABS Problem, D. Żurek, M. Pietroń, Kamil Faber , M. Karwatowski, K. Pięta
12:35 – 12:50	Coffee break	
12:50 – 14:50	Session 7	Chair: Klemens Noga
	12:50	Ab Initio Molecular Dynamics Simulations of Aqueous LiTFSI Solutions – Structure, Hydrogen Bonding, and IR Spectra, Andrzej Eilmes , P. Wróbel, P. Kubisiak
	13:05	Interaction Spheres for Molecular Interactions – Application in Drug Design, Rafał Kurczab
	13:20	Dynamic Disulfide Bonds in Molecular Dynamics Simulation, Pamela Smardz , P. Krupa
	13:35	Application of Fragment Molecular Orbital Method to Investigate G Protein Coupled Receptors, Paweł Śliwa
	13:50	Theoretical Description of Peptide Bonds in Selected Systems Based on the ETS-NOCV Method, Maria Rózga , A. Michalak
	14:05	Analytical Inversion Regional Modeling System for Estimation of National-Scale CO ₂ Fluxes – Results of the CoCO ₂ Project, M. Gałkowski, P. Sekuła, Mirosław Zimnoch
	14:20	Big Data in Proton Beam Monitoring: LGAD Detectors Study, Leszek Grzanka , N. Minafra, R. McNulty, T. Nowak, J. Swakoń, P. Rzeźnik
	14:35	Pedestrian Crossing Intention Detection within Challenging Road Conditions, Szymon Mazurek , M. Sakhai, M. Wielgosz
14:50 – 14:55	Conference closing	
14:55 – 16:00	Lunch	