LUMI

Rozstrzygnięcie konkursu PLL/2024/06 na granty obliczeniowe dla naukowców z Polski realizowane na superkomputerze LUMI

Zgodnie z *Regulaminem konkursu na granty obliczeniowe dla naukowców z Polski realizowane na superkomputerze LUMI* na podstawie przedstawionych recenzji Panel Ekspertów zakwalifikował do realizacji następujące projekty:

Lp.	Projekt	
1.	Tytuł projektu	***Computational spectroscopy of OPV materials at the interface***
	Wnioskodawca	dr Iulia Brumboiu, Uniwersytet Mikołaja Kopernika w Toruniu
	Ocena	4,79
	Streszczenie projektu	*With the development of organic co-polymers with tunable band gaps, as well as small molecule and non-fullerene electron acceptors, organic photovoltaics (OPVs) have recently achieved excellent power conversion efficiencies [1]. However, OPVs suffer from a lack of stability of the organic layer and organic/inorganic interfaces due to photodegradation [2, 3]. The aim of our project is to identify possible photodegradation products of a series of organic molecules used in photovoltaics, as well as to determine the influence of photodegradation on their adsorption on various surfaces, as well as on their optical and electron transport properties. By further performing spectroscopy calculations, we aim to identify the fingerprints of photodegradation in the X-ray and Raman spectra of these molecules. The project is related to a 3-year Poland-Taiwan NCBR-NSTC grant, and in the following, we will focus on the computations planed for the first year of the project, in the context of the entire research plan.*
2.	Tytuł projektu	***Particle acceleration at oblique mildly relativistic shocks***
	Wnioskodawca	prof. Jacek Niemiec, Instytut Fizyki Jądrowej PAN

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	Suma punktów	4,58
	Streszczenie projektu	*The proposed research aims to explore particle acceleration in magnetized oblique mildly relativistic shock waves in collisionless astrophysical plasma in the jets of active galactic nuclei (AGN), known for their intense nonthermal emissions in high-energy X-ray and gamma-ray ranges, linked to high-energy neutrino events and considered potential sources of ultra-high-energy cosmic rays. The studies will use Particle-in-cell (PIC) simulation technique and modern proprietary PIC code THATMPI. A series of large-scale, high-resolution two-dimensional simulations will be conducted, evolving the shock systems to their strongly nonlinear, close-to-steady-state, long-time evolution stages. Our studies aim to explore novel electron and proton acceleration mechanisms in shock and plasma parameter regimes that have not been previously investigated. These endeavors require substantial computational resources, available at the LUMI supercomputing facility.*
3.	Tytuł projektu	***Foundational models for sequential decision making***
	Wnioskodawca	prof. Piotr Miłoś, Uniwersytet Warszawski
	Ocena	4,54
	Streszczenie projektu	*Foundation models, such as large language models (LLMs), have gained immense popularity in recent years, due to their impressive capabilities. In this proposal, we focus on using foundation models in sequential decision-making (SDM) scenarios, where the agent needs to execute a deliberate sequence of actions to achieve a specific goal.* *We aim to address the following fundamental questions:* • ***Research Question A** (RQ A): how to use existing LLMs for decision-making and leverage text instructions?*

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		• ***Research Question B*** *(RQ B): how to create new foundation models specifically for the SDM task?* *We will use the complex NetHack game as our main testbed. To answer RQ A we seek to assess the performance of existing LLMs in SDM scenarios across various settings, including zero-shot learning, in-context learning (ICL), and fine-tuning. To answer RQ B, we aim to develop novel multi-task SDM models utilizing diverse sequential architectures such as Transformers and State Space Models (SSMs).*
4.	Tytuł projektu	**Co3O4|CeO2 heterostructure electronic structure role in small gaseous molecules catalysis**
	Wnioskodawca	prof. Filip Zasada, Uniwersytet Jagielloński
	Ocena	4,46
	Streszczenie projektu	*The purpose of the project is to understand how the molecular and electronic structure of the n-p heterojunctions based on cobalt spinel and ceria [Co3O4|CeO2] control their catalytic activity in redox processes. Extensive quantum chemical modeling is planned to provide an in-depth insight into the band alignment, charge transfer characteristics at the interface, and the associated formation of the built-in electric field, as well as in detail evaluation of the electronic structure of the active centers in the interfacial region. The results will provide the basis for establishing the structure-reactivity relationship for the redox behavior of the Co3O4|CeO2 interface and identification of the key factors controlling the catalytic activity with small inorganic molecules such as N2O and O2.*
5.	Tytuł projektu	***4MOST Hemisphere Galaxy Cosmic Web***
	Wnioskodawca	dr hab. Wojciech Hellwing, Centrum Fizyki Teoretycznej Polskiej Akademii Nauk
	Ocena	4,42
	Streszczenie projektu	*The 4MOST Hemisphere Survey (4HS) aims to revolutionize our understanding of the universe by mapping approximately six million galaxies across 2π steradians with the ESO-operated 4MOST telescope. Key objectives include: 1) Mapping mass and*

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		motion in the Cosmic Local Volume, 2) Analyzing environmental influences on galaxy evolution, and 3) Creating a reference dataset for future astronomical research with LSST, Euclid, and SKA. Essential to 4HS's success are high-quality mock data and simulations, critical for interpreting survey results and ensuring its legacy as a foundational resource for astronomy.
6.	Tytuł projektu	**Alignment Of Large Language Models Via Debate And Reinforcement Learning**
	Wnioskodawca	dr Łukasz Kuciński, Instytut Matematyczny PAN
	Ocena	4,42
	Streszczenie projektu	*The goal is to develop a debate-based training pipeline that is useful for aligning. LLMs. The main hypothesis of this proposal is that the teacher-student framework for debates will allow an autonomous discovery of diverse debate rules and help align LLMs. This is supported by the fact that model interaction often leads to high-performance systems, debates can obviate the necessity for explicitly defining alignment criteria, and curriculum learning is an efficient exploration technique. The work is split into three work packages:* • *In-context learning: all models are frozen and learning happens in the teacher-student setup via iterative prompting, retrieval, and skill repository.* • *A setup where debate participants (LLMs) have their weights updated via fine-tuning or preference optimization, while the teacher's LLM remains frozen.* • *A full teacher-student setup: the teacher and student LLMs are trained, with the teacher's objective based on measures of student progress.*
7.	Tytuł projektu	***Transport of plastic upcycling reactants through bacterial cell envelopes***
	Wnioskodawca	dr Anna Stachowicz, Uniwersytet Jagielloński
	Ocena	4,38
	Streszczenie projektu	*Microbial upcycling has recently emerged as a promising method to deal with the plastic pollution problem. In this*

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		approach, the first step involves polymer degradation by microbial, enzymatic, or chemical methods. In the second step, microorganisms which are able to use degradation products as carbon source, are used as whole cell catalyst to transform them into valuable products. In whole cell catalysis one of the key aspects is the substrate entry into the cell, as it influences the rate and yield of the process. Spontaneous passage of products out of the cell is also desirable, since it simplifies product isolation. *The proposed project aims at exploring the interactions between reactants taking part in the upcycling process with components of bacterial cell envelope by means of classical MD simulations. Reactants derived from the most popular commodity plastics as well as selected bioplastics will be studied. Membrane systems will correspond to the outer and inner cell membranes of Gram-negative bacteria. Energy barriers for diffusion of reactants through the membranes will be determined, and the role of individual lipids in this process will be studied.*
8.	Tytuł projektu	***Understanding of liquid SIMS through molecular dynamics simulations - sputtering of frozen and liquid systems***
	Wnioskodawca	dr Michał Kański, Uniwersytet Jagielloński
	Ocena	4,33
	Streszczenie projektu	*The aim of this project is to gain insight into the processes occurring when a surface of water or ice is bombarded by atomic or cluster projectiles possessing high kinetic energy. Such phenomena occur when biological or liquid systems are analysed by secondary ion mass spectrometry (SIMS), which can detect femtomole amounts of molecules with spatial resolution better than 100 nanometres. It is achieved by bombardment of the sample by a scanning beam of atoms or atom clusters and subsequent detection of molecules and fragments ejected from the surface after the impact. Molecular dynamics (MD) simulations will be used to identify and analyse mechanisms present in such conditions, leading to an understanding of what happens when SIMS is employed to study biological or liquid systems.*
9.	Tytuł projektu	***ML potentials for computational design of magnetic MOFs***

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	Wnioskodawca	dr hab. Mihails Arhangelskis, Uniwersytet Warszawski
	Ocena	4,29
	Streszczenie projektu	*This project will develop methods for ab initio computational design of magnetic metal-organic framework (MOF) materials. MOFs offer an excellent platform for magnetic materials, as their compositional, structural and topological diversity provides ample opportunities for tuning long-range ordering of metal centers and control the strength of magnetic coupling.* *Our group is developing a method for ab initio crystal structure prediction (CSP) of MOFs, which allows us to systematically explore the structural landscape of MOFs constructed from a given combination of nodes and linkers, without prior assumptions on metal-linker connectivity and structure topology.* *To achieve this aim in the fastest possible way, we will now utilize machine learning (ML) methods for fast and accurate minimization of the predicted structures, and evaluation of magnetic properties. This will allow us to rapidly identify experimentally-relevant structures with interesting properties among our prediction.* *Finally, our long-term aim is to make the CSP methodology into a recognized and widely used tool by the MOF community as a support and, potentially, replacement for experimental screening methods.*

Projekty niezakwalifikowane do realizacji:

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Lp.	Projekt	
1.	Tytuł projektu	***Descriptors of electronically excited states of large molecules***
	Wnioskodawca	prof. Tatiana Korona, Uniwersytet Warszawski
	Ocena	4,04
	Streszczenie projektu	*The purpose of our research is to explore the descriptors of electronically excited states in large molecules using advanced quantum chemistry methods. Excited states play a crucial role in various chemical and physical processes, with applications ranging from renewable energy to biomedicine. We will utilize state-of-the-art computational techniques like time-dependent density functional theory (TD-DFT) and high-level ab initio electronic structure methods to characterize the electronic structure, energies, and properties of these molecules. The obtained quantum chemical descriptors, including charge density and bond critical point properties, will be essential for predicting and rationalizing the behavior of molecules in excited states. We have developed a standard operation protocol with combinations of advanced quantum chemistry packages and versatile postprocessing tools to extract meaningful information about the excited state. With access to LUMI, we are one step closer to unlocking the full potential of computational research.*
2.	Tytuł projektu	***Zero Waste Machine Learning in Computer Vision***
	Wnioskodawca	prof. Tomasz Trzciński, Politechnika Warszawska
	Ocena	3,92
	Streszczenie projektu	*In contemporary science and industry, machine learning models, particularly artificial neural networks, play a pivotal role, yet their growing complexity demands substantial computational resources. This trend spans various domains, from medical imaging to robotics. The computational burden incurred by these models—processing vast amounts of data—comes at a steep cost: prolonged processing times, heightened energy consumption, and a substantial carbon footprint. While the issue of computational complexity is recognized within the computer science community, conventional solutions primarily*

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		involve shrinking models through pruning or weight compression. Alternatively, newer methods draw inspiration from biological neural networks, employing simple heuristics to expedite decision-making processes. Although these techniques offer notable speed enhancements, they predominantly limit model access to resources, rather than exploring avenues for resource reuse or recycling. Our project proposes a holistic approach to machine learning model efficiency, drawing inspiration from principles of green and sustainable economics. Rather than restricting computations or memory usage, our focus is on maximizing resource reuse. This entails leveraging computations from previous processing steps, information acquired from prior exploration of the model's environment, and knowledge gained during past training sessions in continual learning systems. We hypothesize that recycling resources used by machine learning models can significantly bolster their efficiency. Thus, our research endeavors to establish a new trajectory of zero-waste machine learning, aimed at conserving computations and reducing their resource consumption (for a more detailed description please visit this website).
3.	Tytuł projektu	***From denoising to segmentation: multi-task optimization of temporal neural networks***
	Wnioskodawca	dr inż. Daniel Węsierski, Politechnika Gdańska
	Ocena	3,83
	Streszczenie projektu	*The project aims to develop a novel machine learning technology that will leverage redundancy in long videos to contribute to creating sustainable vision-first machines and systems with a cross-pollination of fundamental visual capabilities. To this end, we will conduct foundational research on neural-like, multi-task temporal architectures and data-driven temporal, self-supervised learning algorithms that train the temporal models basic seeing capabilities from vast numbers of video frames. The tangible project's results will include open-sourced implementations of algorithms and datasets for free use and the associated publications, potentially in top journals and conferences in computer vision and machine learning. Our systematic basic study of temporal multi-task networks will advance the development of robust Embodied AI, such as robotic and monitoring systems, that are expected to process, analyze, and reason from long videos.*

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4.	Tytuł projektu	***Simulations of nanoporous materials wetting/dewetting.***
	Wnioskodawca	prof. Yuriy Bushuev, Uniwersytet Śląski
	Ocena	3,79
	Streszczenie projektu	*The economic development of countries is determined by their ability to use scientific discoveries, technical achievements, and new materials effectively. The proposed research project is based on studying the behavior of new porous materials using a combination of unique experiments and computer simulations.* *The proposed project is devoted to investigating the behavior of systems consisting of porous solids immersed in a non-wetting liquid. We are going to study molecular mechanisms of water and aqueous solutions intrusion/extrusion by hydrophobic porous materials. One of the achievements of modern science is the synthesis of new porous materials with unique properties, such as pure silica zeolites, metal-organic frameworks, and mesoporous silica.* *Hydrophobic porous systems with intruded water demonstrate the three types of behavior when external pressure drops. They are called "molecular springs" if extrusion and intrusion pressures are equal, "shock absorbers" when extrusion pressure is lower than an intrusion, and "bumpers" when water stays in the pores at atmospheric pressure. The "molecular springs" can be used for the storage and recuperation of energy. Systems that can absorb or totally dissipate mechanical energy are essential too. The other practical problem is using porous materials for water purification. Reverse osmosis has been widely used to increase clean water supply by purifying nontraditional water sources. If ions do not penetrate porous materials, they can be used for water desalination.* *The project will focus on hydrophobic porous materials, water, and aqueous solutions. It was established recently that the topology of the zeolite pore system is a controlling parameter. Intrusion pressure depends not only on the hydrophobicity of material and geometry of pores but the dimensionality of the pore system. We are going to extend a number of systems by including hydrophobic mesoporous materials with different topologies and aqueous solutions.* *The energetic characteristics of the systems, including heat effects, and the structure of aqueous solutions in porous materials will be investigated. We believe that the obtained*

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		results will not only give new knowledge about molecular mechanisms controlling the systems' behavior but will help design the actual materials, which can be used in industry to improve the current technology for energy/heat recovery, purification, and desalination of water.
5.	Tytuł projektu	***Radiation Damage in Complex Alloys Using Molecular Dynamics***
	Wnioskodawca	dr Amin Esfandiarpour, Narodowe Centrum Badań Jądrowych
	Ocena	3,71
	Streszczenie projektu	*Our project seeks to understand the response of complex alloys, specifically Inconel 615 and CoNiFeCr high entropy alloys, to radiation damage through advanced molecular dynamics simulations. By investigating defect creation, evolution, and the effects of grain boundary segregation under irradiation, we aim to evaluate these materials' suitability for radiation-intensive applications. This research is pivotal for enhancing the durability and safety of materials used in nuclear reactors and aerospace. Utilizing the LUMI supercomputer will enable us to perform comprehensive cascade overlap simulations, offering insights into material behaviors at an atomic level and guiding the development of radiation-resistant alloys.*

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