LUMI

Rozstrzygnięcie konkursu PLL/2024/07 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	***Relativistic MHD simulations of merging and collapsing stars***
	Wnioskodawca	Agnieszka Janiuk (Centrum Fizyki Teoretycznej PAN)
	Ocena	116
	Streszczenie projektu	*The project aims to explore the compact object mergers and massive star collapse leading to bright transients in high energy range. Electromagnetic gamma ray bursts and radioactivity of kilonovae may be accompanied by gravitational waves, To simulate collapsing stars and compact merger remnants., we use numerical scheme HARM (High Accuracy Relativistic MHD). Current code branches developed by our team are HARM-EOS, with tabulated equation of state, and HARM-SELFG, with evolving Kerr metric and self-gravity. We focus on configurations of magnetic field important for powering electromagnetic jets. We also explore the nuclear heating in the post-merger ejecta and calculate synthetic lightcurves to be compared with observed kilonovae. Code performance and grid settlements have been already tested and optimized on LUMI during development grant, so now it is ready to be launched in high-resolution 3D setups. These endeavors require substantial resources, available at the LUMI supercomputer.*
2.	Tytuł projektu	***Superfluid dynamics in inhomogeneous Fermi systems***

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	Wnioskodawca	Gabriel Wlazlowski (Politechnika Warszawska / Wydział Fizyki)
	Suma punktów	113
	Streszczenie projektu	*The most remarkable property of a superfluid, mass transport without energy losses, can be significantly affected or even destroyed by impurities. In this project, we will investigate the impact of inhomogeneities on superfluid dynamics. The research will focus on two physical systems: spin-imbalanced ultracold atomic gases under conditions that can be realized in a laboratory, and nuclear matter under conditions as expected in the crust of neutron stars. For these systems, we will explore the superfluid fraction dependence and quantum vortex dynamics with respect to inhomogeneities that create spontaneously. We will apply the very accurate method of density functional theory extended to superfluid systems. The result obtained for cold atoms will benchmark ongoing experiments, while results for the nuclear matter will provide benchmarks for effective models of neutron stars. The project will contribute to a deep understanding of superfluidity properties in Fermi systems.*
3.	Tytuł projektu	***Temperature and nonlinear effects in the spectroscopy of rare earths in glass***
	Wnioskodawca	Małgorzata Wierzbowska (Instytut Wysokich Ciśnień PAN)
	Ocena	107
	Streszczenie projektu	*Aim of the proposal is to perform calculations for a project submitted to National Science Center, titled: "Jumping over the transverse mode instability in the high-power fiber lasers". Problem to be solved is a laser beam splitting and its chaotic fluctuations in time when the strong laser pumping causes an increase of the average output power above the critical value characteristic for doped glass used in the fiber. It is known since 2010 and remains not solved. Experiments and theoretical models showed that a beam destruction is caused by the increased temperature in a fiber and nonlinear optical effects, leading to a generation of the laser modes additional to the fundamental mode. Modeling will start from a generation of atomic clusters,*

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		followed by the calculation of spectroscopic properties and finished with a simulation of the device operation.
4.	Tytuł projektu	***Inverse design of materials for metal-ion batteries***
	Wnioskodawca	Oleksandr Malyi (ENSEMBLE3 spółka z ograniczoną odpowiedzialnością)
	Ocena	106
	Streszczenie projektu	*The project aims to design low-cost, high-energy-density, long-cycle-life sodium-ion batteries by developing a comprehensive model for hard carbon anodes, using electronic structure theory and molecular dynamics learning to guide synthesis and performance optimization.*
5.	Tytuł projektu	***Zero Waste Machine Learning in Computer Vision***
	Wnioskodawca	Tomasz Trzciński (Politechnika Warszawska / Wydział Elektroniki i Technik Informacyjnych)
	Ocena	106
	Streszczenie projektu	*In science and industry, machine learning models play a pivotal role, yet they demands substantial computational resources. While the issue of computational complexity is recognized within the computer science community, conventional solutions primarily involve shrinking models. Although these techniques offer notable speed enhancements, they predominantly limit model access to resources. 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, and knowledge gained during past training sessions. Our research endeavors to establish a new trajectory of zero-waste machine learning, aimed at conserving computations and reducing their resource consumption.*

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6.	Tytuł projektu	***The study of protein dynamics important in neurobiology***
	Wnioskodawca	Katarzyna Walczewska-Szewc (Uniwersytet Mikołaja Kopernika w Toruniu)
	Ocena	105
	Streszczenie projektu	*This project aims to explore the role of prolyl oligopeptidase (PREP) in neurodegenerative diseases, such as Alzheimer's (AD) and Parkinson's (PD), where the accumulation of protein aggregates contributes to disease progression. Building on previous work, which successfully identified binding pathways for key ligands, this project will expand the analysis to new PREP inhibitors with distinct mechanisms of action. In collaboration with international experts, we will investigate how these inhibitors influence non-catalytic functions of PREP, especially its interactions with drivers of pathological aggregation in AD and PD.* *The project will also explore the binding potential of cyclopeptides to PREP, with the ultimate goal of uncovering novel compounds that could disrupt harmful protein aggregation. By utilizing advanced molecular modeling techniques, we hope to contribute to the development of new therapeutic strategies targeting early-stage neurodegeneration.*

Projekty niezakwalifikowane do realizacji:

Lp.	Projekt	
1.	Tytuł projektu	***Modelling of phase diagram of gallium nitride (GaN) at high temperatures and high pressures***
	Wnioskodawca	Jacek Piechota (Instytut Wysokich Ciśnień PAN)
	Ocena	94

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	Streszczenie projektu	*The technology of gallium nitride (GaN) is very advanced due to excellent figures of merit relevant for key applications like LEDs or high-power–high-frequency transistors. Nevertheless, some fundamental physical properties, including the phase diagram, of this so important semiconductor, are still not determined. In this project, we will perform a series of simulations of the GaN crystal behavior at heating to extremely high temperatures in a high pressure range (above 50GPa). Ab initio density functional theory (DFT) molecular dynamics extensive calculations will be used to obtain the temporal change of the system.*
2.	Tytuł projektu	***Role of glycosphingolipids in membrane bending and clathrin-independent endocytosis biogenesis through galectin-3***
	Wnioskodawca	Paweł Rogowski (Instytut Fizyki PAN)
	Ocena	91
	Streszczenie projektu	*Galectin-3 is a chimeric galectin comprising two domains: intrinsically disordered N-terminal (NTD) and folded, structured, carbohydrate binding (CRD). Recently it has been shown experimentally that galectin-3 undergoes liquid-liquid phase separation and drives glycosphingolipid - dependent biogenesis of clathrin-independent carriers, but the function of biomolecular condensates of galectin-3 in endocytic pit formation is unknown. The aim of our project is to use molecular dynamics (MD) methods to simulate a system of condensated galectin-3 which will be interacting with the glycosphingolipids membrane. Simulations will be performed at coarse-grained level of detail to achieve reduction of computational cost. We expect that analysis of trajectories will elucidate the mechanisms of membrane deformations by galectin-3 condensates. Our study may significantly contribute to explaining the causes behind these diseases in which galectin-3 participates (cancer and Alzheimer's diseases).*
3.	Tytuł projektu	***Large scale numerical model of composites including interphase properties***

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	Wnioskodawca	Eligiusz Postek (Instytut Podstawowych Problemów Techniki Polskiej Akademii Nauk)
	Ocena	90
	Streszczenie projektu	*In multiphase composite the important role play the interfaces between the phases, porosity of their skeletons and matrices and he other imperfections. The modern CT-scanning technologies allow for observations of detailed internal structure of the composites. It is posiible to observe the porosities, inclusions and he initial cracks. Using the CAD programs the CT scans are converted into geometrical models in which the internal structure of the composites is discretized with tetrahedrals. The the models are converted into peridynamics and finite element method formats.*
4.	Tytuł projektu	***From denoising to segmentation: multi-task optimization of temporal neural networks***
	Wnioskodawca	Daniel Węsierski (Politechnika Gdańska / Wydział Elektroniki, Telekomunikacji i Informatyki)
	Ocena	88
	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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