

Advanced Computational Science



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**Master's
theses**

Full Name	Advisor / Co-adviser	Thesis Title	
Nikolay Kotoyants	Phan Anh / Oleg Rogov	Cross-Channel Activation Function for Deep Neural Network	
Artem Chuprov	Nikolay Brilliantov	Development of Hybrid Models for Simulating Large Particle Collisions	
Danil Ivanov	Nikolay Brilliantov	Quantum Theory of Diffusive Memristors	
Maryush Soroka	Aslan Kasimov	Classical and Data-driven Modelling of Dynamics of Gaseous Flames in Nonuniform Media	
Oleg Shepelin	Pavel Osinenko / Dmitry Dobriborsci	Reinforcement Learning in Executing and Trading Strategy	
Oluwafemi Adejumobi	Vladimir Palyulin	Diffusion Properties in Systems with Slow and Fast Diffusion with an Exchange	
Vsevolod Avilkin	Vladimir Palyulin	Data-driven Prediction of Porous Media Transport Properties from 2D Images	
Viacheslav Naumov	Vladimir Palyulin	Random Search with Home Range	

Full Name	Advisor / Co-adviser	Thesis Title	
Ekaterina Andreichuk	Petr Popov	Prediction of Protein Stability Change Upon Point Mutation Using Molecular Dynamics and Machine Learning	
Alexander Ganibaev	Sergey Rykovanov	Efficient Real-Time Path Tracing with Neural Radiance Caching and Dedicated Temporal Adaptation	
Olga Gorbunova	Sergey Rykovanov / Alexey Artemov	3D Polygonal Mesh Generation with Diffusion Models	
Antonina Timoshenko	Sergey Rykovanov	Modeling of a High-energy Radiation Source on Modern Computational Architectures (CPU and GPU)	
Ivan Gurev	Natallia Strushkevich	De Novo Design Of Heme-coordinating Ligands of Cytochrome P450 Using Methods of Machine Learning	
Koffivi Gbagbe	Dzmitry Tsetserukou	Robotic Skill Synthesis for Bimanual Dexterous Manipulation based on Vision-Language-Action Model	