

Andrey Alekseenko

Postdoctoral Researcher at KTH Royal Institute of Technology
and Science for Life Laboratory

Summary

PhD in Applied Mathematics with 4 years of post-doctoral experience.

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Education

Ph.D. in Mathematical modeling, numerical methods and software complexes, 2013–2017

Moscow Institute of Physics and Technology, Department of Computational Mathematics.
Thesis topic: Modeling and adaptive control of transportation flow dynamics in urban setting.
Advisor: Yaroslav Kholodov.

M.S. in Applied Mathematics and Physics, 2011–2013

Moscow Institute of Physics and Technology, Department of Control and Applied Mathematics.
Thesis topic: The reconstruction of protein–protein interaction energy landscapes.
Advisor: Yaroslav Kholodov.

B.S. in Applied Mathematics and Physics, 2007–2011

Moscow Institute of Physics and Technology, Department of Control and Applied Mathematics.
Thesis topic: Advanced methods and algorithms for computational modeling of protein–protein interaction dynamics.
Advisor: Yaroslav Kholodov.

Publications

Journal Publications

- M.F. Lensink, ..., A. Alekseenko *et. al.*, "Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment," *Proteins Struct. Funct. Bioinforma.*, vol. 89, no. 12, pp. 1800–1823, 2021.
- Y. Kholodov, A. Alekseenko, V. Kazorin, A. Kurzhanskiy, "Generalization Second Order Macroscopic Traffic Models via Relative Velocity of the Congestion Propagation," *Mathematics*, vol. 9, no. 16, 2021.
- D. Padhorny, ..., A. Alekseenko *et. al.*, "ClusPro in rounds 38 to 45 of CAPRI: Toward combining template-based methods with free docking," *Proteins Struct. Funct. Bioinforma.*, vol. 88, no. 8, pp. 1082–1090, 2020.

- A. Alekseenko, S. Kotelnikov, M. Ignatov *et al.*, "ClusPro LigTBM: Automated Template-Based Small Molecule Docking," *J. Mol. Biol.*, vol. 432, no. 11, pp. 3404–3410, 2020.
- S. Kotelnikov, A. Alekseenko, *et al.*, "Sampling and refinement protocols for template-based macrocycle docking: 2018 D3R Grand Challenge 4," *J. Comput. Aided Mol. Des.*, vol. 34, no. 2, pp. 179–189, 2020.
- K.A. Porter, . . . , A. Alekseenko, *et al.*, "Template-based modeling by ClusPro in CASP13 and the potential for using co-evolutionary information in docking," *Proteins Struct. Funct. Bioinforma.*, vol. 87, no. 12, pp. 1241–1248, 2019.
- A. Alekseenko, *et al.*, "ITS+DM Hackathon (ITSC 2017): Lane Departure Prediction With Naturalistic Driving Data," *IEEE Intell. Transp. Syst. Mag.*, vol. 11, no. 4, pp. 78–93, 2019.
- J. Wang, A. Alekseenko, D. Kozakov, and Y. Miao, "Improved Modeling of Peptide-Protein Binding Through Global Docking and Accelerated Molecular Dynamics Simulations," *Front. Mol. Biosci.*, vol. 6, 2019.
- C. Yueh, . . . , A. Alekseenko, *et al.*, "Kinase Atlas: Druggability Analysis of Potential Allosteric Sites in Kinases," *J. Med. Chem.*, vol. 62, no. 14, pp. 6512–6524, 2019.
- M. Ignatov, C. Liu, A. Alekseenko, *et al.*, "Monte Carlo on the manifold and MD refinement for binding pose prediction of protein–ligand complexes: 2017 D3R Grand Challenge," *J. Comput. Aided Mol. Des.*, vol. 33, no. 1, pp. 119–127, 2019.
- M.D. West, . . . , A. Alekseenko, *et al.*, "Use of deep neural network ensembles to identify embryonic-fetal transition markers: repression of COX7A1 in embryonic and cancer cells," *Oncotarget*, vol. 9, no. 8, pp. 7796–7811, 2018.
- D. Padhorny, . . . , A. Alekseenko, D. Beglov, D. Kozakov, "Protein–ligand docking using FFT based sampling: D3R case study," *J. Comput. Aided Mol. Des.*, vol. 32, no. 1, pp. 225–230, 2018.
- A.E. Alekseenko, A.S. Kholodov, and Y.A. Kholodov "Boundary control problems for quasilinear systems of hyperbolic equations," *Comput. Math. Math. Phys.*, vol. 56, no. 6, pp. 916–931, 2016.
- A. Alekseenko, O. Kononova, Y. Kholodov, K.A. Marx, and V. Barsegov "SOP-GPU: influence of solvent-induced hydrodynamic interactions on dynamic structural transitions in protein assemblies," *J. Comput. Chem.*, vol. 37, no. 17, pp. 1537–1551, 2016. (cover article)
- A.M. Kazennov, A.E. Alekseenko, D. Kozakov, D.N. Padhorny, and Y.A. Kholodov "Efficient search for the possible mutual arrangements of two rigid bodies with the use of the generalized five-dimensional Fourier transform," *Math. Model. Comput. Simulations*, vol. 7, no. 4, pp. 315–322, 2015.
- A. Kazennov, A. Alekseenko, V. Bozhenko, T. Kulinich, N. Shuvalov, and Y. Kholodov "Evaluation of CDK6 and p16/INK4a-derived peptides interaction," *Comput. Mol. Biosci.*, vol. 3, no. 3, pp. 53–57, 2013.
- O. Kononova, R.I. Litvinov, A. Zhmurov, A. Alekseenko, *et al.* "Molecular mechanisms, thermodynamics, and dissociation kinetics of knob-hole interactions in fibrin," *J. Biol. Chem.*, vol. 288, no. 31, pp. 22681–22692, 2013.

Conference Proceedings

- A. Alekseenko, "Adding SYCL Support to GROMACS Molecular Dynamics Package" Intel DevHub at International Conference for High Performance Computing, Networking, Storage, and Analysis (SC'21), online, November 14–19, 2021.

A. Alekseenko, S. Páll, E. Lindahl “Experiences With Adding SYCL Support to GROMACS,” International Workshop on OpenCL (IWOCCL’21), online, April 26–27, 2021.

S. Verentsov, E. Magerramov, V. Vinogradov, R. Gizatullin, A. Alekseenko, Y. Kholodov, E. Nikolskiy “Bayesian Framework for Vehicle Localization Using Crowdsourced Data,” 2018 IEEE Intelligent Vehicles Symposium (IV’18), Chang Shu, China, June 26–29, 2018.

S. Verentsov, E. Magerramov, V. Vinogradov, R. Gizatullin, A. Alekseenko, Y. Kholodov, E. Nikolskiy “Bayesian Localization for Autonomous Vehicle using Sensor Fusion and Traffic Signs,” 2017 International Conference on Robotics and Artificial Intelligence, Shanghai, China, December 29–31, 2017.

A. Alekseenko, Y. Kholodov, A. Kholodov, Y. Chekhovich, and V. Starozhilets “Adaptive Traffic Light Control on Highway Entrances,” IEEE 20th International Conference on Intelligent Transportation Systems (ITSC), Yokohama, Japan, October 16–19, 2017.

A. Alekseenko “The optimal traffic light control for highway on-ramps,” 12th World Congress on Computational Mechanics (WCCM XII) and 6th Asia-Pacific Congress on Computational Mechanics (APCOM VI), Seoul, Korea, July 24–29, 2016.

Y.A. Kholodov, A.E. Alekseenko “Optimal traffic signalization at entrances to highways,” The IV International Research and Practice Conference “Modern Problems of Life Safety: Intelligent Transport Systems”, Kazan, Russia, February 24–26, 2016.

A.E. Alekseenko, O.G. Kononova, Y.A. Kholodov, and V. Barsegov “Accounting for hydrodynamic interactions in coarse-grained protein model,” The XXII International Conference “Mathematics. Computing. Education”, Puschino, Russia, January 27–29, 2015.

A. Alekseenko, O. Kononova, Y. Kholodov, V. Barsegov “Effects of hydrodynamic interactions on biological matter,” International workshop “Computational and Theoretical Modeling of Biomolecular Interactions”, Dubna, Russia, June 3–8, 2013.

Book chapters

A. Alekseenko, M. Ignatov, G. Jones, M. Sabitova, D. Kozakov, “Protein-protein and protein-peptide docking with ClusPro server”, in *Methods in Molecular Biology*, vol. 2165. pp.157–174.

Awards & Certifications

Winner of IEEE ITS+DM Hackathon on Naturalistic Driving, 2017.

Employee of the year at Innopolis University, 2017.

Amazon Web Services (AWS) Certified Security - Specialty, 2020.

Grants

PI of the Russian Scientific Foundation Grant 19-74-00090 “Affinity prediction for MHC-peptide interactions for the development of personalized immunotherapeutic agents” (2019–2020)

Professional Experience

Postdoctoral Researcher, KTH Royal Institute of Technology, Sep 2020–current

Adapting GROMACS molecular dynamics package for the new generations of supercomputers.
Optimizing core molecular dynamics algorithms for GPUs.

Postdoctoral Associate, Stony Brook University, Sep 2018–Aug 2020

Developing methodology for template-based protein-ligand docking and refinement.
Research into applications of metagenomic data for protein-protein docking.
Developing code for Monte-Carlo-based refinement of peptides and small molecules.

Assistant, Innopolis University, Aug 2016–Sep 2018

Researching numerical models for road traffic modeling using macroscopic (fluid-like) models.
Supervising undergraduate students developing sensor-fusion methods for vehicle localization.
Optimizing code for Monte-Carlo-based refinement of protein-ligand poses from rigid-body docking.

Computer Vision Engineer, Innosoft, LLC., Sep 2016–May 2017

Developing computer vision algorithms (OpenCV, Tensorflow) for video analysis on embedded (Raspberry Pi) systems, including continuous testing pipeline.

System Administrator, Moscow Institute of Physics and Technology, Jun 2010–Aug 2016

Technical support of the HPC clusters and private cloud (VmWare ESXi, Cisco IOS).

Research Associate, InSilico Medicine, Inc, May 2015–Apr 2016

Using deep neural networks (Keras) for analysis of large transcriptomic datasets.

co-PI, Moscow Institute of Physics and Technology CUDA Research Center, May 2012–Jan 2015

Teaching introductory courses on GPGPU (CUDA, OpenCL) programming.

Visiting Research Scholar, University of Massachusetts Lowell, Jul 2012–Oct 2012

Developing GPU-accelerated code (SOP-GPU) for coarse-grained simulations of protein-protein interaction and analysis of mechanical properties of proteins.

Teaching Experience

Assistant, SYCL Workshop by ENCCS, 2021.

Assistant, Core course “High performance computing” in Innopolis University, 2018.

Trainee, Instructional Skills Workshop in Innopolis University, 2017.

Assistant, Core course “Calculus I” in Innopolis University, 2016, 2017.

Assistant, Introductory course for future students “Introduction to programming” in Innopolis University, 2017.

Assistant, Elective course “Transport Modeling” in Innopolis University, 2017.

Assistant, Core course “Linear Algebra I” in Innopolis University, 2017.

Lecturer, Summer School on High-Performance Computing for Computer Vision in Innopolis University, 2016.

Assistant, Winter School on High-Performance Computing in Kabardino–Balkarian State University, 2012.

Assistant, Elective course “Multithread computing with CUDA and OpenCL” in Moscow Institute of Physics and Technology, 2011.

Assistant, Summer School on High-Performance Computing in Moscow Institute of Physics and Technology, 2010, 2011.

Assistant, Elective course “Modeling of biological systems on GPU” in Moscow Institute of Physics and Technology, 2012, 2013.

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