Curriculum Vitae: Sergii Domanskyi

E-mail: sergii.domanskyi@jax.org
Phone: (315) 212-6041
Web: `www.domanskyi.com`

600 Main Street
The Jackson Laboratory
Bar Harbor, ME 04609

Education

May 2012–August 2018 **PhD in Physics,** Clarkson University, Potsdam, NY. *Thesis Advisor:* Prof. Dipankar Roy. *Former Thesis Advisor:* Prof. Vladimir Privman.

September 2010–May 2012 **Master of Science in Physics,** National Technical University of Ukraine, Kyiv, Ukraine. *Thesis Advisor:* Prof. Vyacheslav Gorshkov.

September 2006–June 2010 **Bachelor of Science in Physics,** National Technical University of Ukraine, Kyiv, Ukraine.

Honors, Awards, Professional Accomplishments and Affiliations

The Physics Department **Distinguished Graduate Student Award**, Clarkson University, Potsdam, NY. *Awarded in Spring 2016.*

Outstanding Teaching Assistant Award, Physics Department, Clarkson University, Potsdam, NY. *Awarded for teaching Freshmen Physics during the period Jan 2013–May 2015.*

Invited to coauthor a chapter in a book of invited reviews (*Publ. 8 below).*

Results of my work have been showcased by the Editors as **Journal Issue Covers** *(Publ. 3, 5, 7 below).*

Selected as a graduate student **visiting researcher at Los Alamos National Laboratory**, *Fall 2015, invited again in Summer 2016.*

American Physical Society *member since 2016*; **American Chemical Society**: *member 2016-2018.*

2^{nd} **place in the Tumor Deconvolution DREAM Challenge 2020**, a machine learning competition for computational methods to deconvolve bulk RNA expression data into individual immune components.

Research Experience

July 2021–present **Assistant Computational Scientist**, The Jackson Laboratory, Bar Harbor, ME; *Supervisor:* Anuj Srivastava, Ph.D.

Research Topic: Development of novel computational, statistical and mathematical approaches for the analysis of Next Generation Sequencing (NGS) data, specifically, in the area of single-cell genomics.

August 2018–July 2021 **Research Associate**, Michigan State University, East Lansing, MI; *Advisor:* Prof. Carlo Piermarocchi.

Research Topic: Data-driven models of hematological cell fate decision and differentiation. Development of novel statistical and mathematical approaches for analysis of time-series and single cell RNA sequencing data and other modalities of Next Generation Sequencing (NGS) data.

During *June–July 2019* I also worked on the research topic: Integrative personalized omics profiling next steps: detection and classification of deviations from wellness. *Advisors:* Prof. Carlo Piermarocchi and Prof. George I. Mias.

May 2012–August 2018 **Research Assistant, Ph.D. Thesis Research in theoretical and computational modelling**, Clarkson University, Potsdam, NY; *Thesis Advisor:* Prof. Dipankar Roy. *Former Thesis Advisor:* Prof. Vladimir Privman.

Research Topic: Statistical Mechanical and Physiochemical Kinetics Modeling of Bio-Inspired, Biomolecular, and Biotechnology Systems and Materials.

Modelling of several types of materials and biochemical systems with statistical mechanical and physiochemical kinetics approaches and techniques. The topics included models for multi-input biomolecular signals processes for actuation, drug delivery, release and other applications; percolation-type modeling of autonomous self-damaging in "smart" composite materials; Monte Carlo and mean-field simulation of certain polymerization processes; reaction-diffusion equations modelling of surface erosion of highly crosslinked polymers; analytical modeling of diffusion of oligonucleotides and other large molecules from hydrogel beads; modeling of progression of viral infection in cell culture resulting in cell apoptosis and necrosis; and cell culture dynamics under stress.

May–August 2016, September–December 2015 **Visiting Graduate Student Researcher**, Los Alamos National Laboratory, Center for Nonlinear Studies, Los Alamos, NM; *Supervisor:* Dr. Dmitry Mozyrsky.

Research Topic: Quantum Chemistry Methods. Computational Techniques in Non-Adiabatic Molecular Dynamics. Thawed Gaussian Propagation with Recurrent Basis Expansions and Matching-Pursuit Basis Reduction for Simulations of Quantum Dynamics.

Non-adiabatic molecular dynamics is important in the study of many photophysical and photochemical reactions. We applied the accelerated Semi-classical Monte Carlo technique that has features of Surface hopping methods but accounts for quantum coherence effects to problems where common approximations break down, comparing the solution to that of existing approaches such as the Ehrenfest method, the Fewest Switches Surface Hopping method, and exact quantum solution. Also we utilized the thawed Gaussian approximation and a recurrent basis expansions to avoid rapid growth of the basis, making computations feasible. The latter is based on the Batista group's Matching-Pursuit method, along with a Split-operator Fourier-transform (MP/SOFT), applied to an arbitrary wavefunction for propagation along energy surfaces of arbitrary adiabatic potentials, e.g. Morse potential, double-well potential and Tully's test problems, for the desired time duration.

May 2011–May 2012 **Software Designer**, Consulting and Information Technology, LLC, Kyiv, Ukraine, *Supervisor:* Evgeny Fedorin.

Project: Development and automation of specialized accounting and management systems for companies.

September 2010–May 2012 **Research Assistant, Master's Thesis Research in theoretical and computational modelling**, National Technical University of Ukraine, Kyiv, Ukraine; *Advisor:* Prof. Vyacheslav Gorshkov.

Research Topic: Biomolecular Logic Gates in Biochemical Information Processing.

The research objective was the characterization of biochemical signal processing, optimization of biomolecular logic gates, formulation of the concepts of suppression of analogue and digital noise in biochemical logic networks. These mathematical models can be used to select parameters in biochemical experiments.

Collaborative Institutional Training Initiative (CITI) Certification

August 2012, *August 2016*, *April 2021* Responsible Conduct of Research (RCR).
April 2021 Human Subjects Research (HSR) for Biomedical Researchers.

Information Technology Qualifications

Programming languages: Python, JavaScript, R, C/C++ and Fortran 77/90, including OpenMP and OpenACC, experience of usage of LAPACK, BLAS and ScaLAPACK libraries, Visual Basic, Delphi (by Borland); Object Pascal; SQL (MySQL, IBM DB2); HTML.

Software: Microsoft Visual Studio IDE, RStudio, Wolfram Mathematica, MathWorks MATLAB, MapleSoft Maple, PTC Mathcad, OriginLab (LabTalk and Origin C), Mtplotlib, GPlot/gnuplot, Refworks, Zotero (+ CSL Editor), SciFinder, LaTeX (MiKTeX, Overleaf), Adobe Dreamweaver/Photoshop/Acrobat Pro, Autodesk AutoCAD, MatrixTSL Flowcode, Proteus PCB Design, PASCO Capstone, Cytoscape, Git, RNAseq data processing tools (CellRanger, Kallisto/Kallisto-Bustools, Sleuth).

Other: Microsoft Windows Server deployment and management; Sun Grid Engine; fluent in use of High-performance computing clusters (HPCC).

Publications

Total number of publications: 23; Total citations: 170 (Google Scholar); h-number: 8.

23. Naturally occurring combinations of receptors from single cell transcriptomics in endothelial cells. *S. Domanskyi*, A. Hakansson, M. Meng, J. S. Graff Zivin, C. Piermarocchi, G. Paternostro, N. Ferrara, *in review* (2021).

22. Visibility Graph Based Community Detection for Biological Time Series. M. Zheng, *S. Domanskyi*, C. Piermarocchi, G. I. Mias, *Scientific Reports*, **11**, 5623 (2021).

21. Digital Cell Sorter (DCS): a cell type identification, anomaly detection, and Hopfield landscapes toolkit for single-cell transcriptomics. *S. Domanskyi*, A. Hakansson, T. Bertus, G. Paternostro, C. Piermarocchi, *PeerJ*, **9:e10670** (2021).

20. Longitudinal Saliva Omics Responses to Immune Perturbation: A Case Study. G. I. Mias, V. V. Singh, L. R. K. Rogers, S. Xue, M. Zheng, *S. Domanskyi*, M. Kanada, C. Piermarocchi, J. He, *Scientific Reports*, **11**, 710 (2021).

19. Modeling drug combination sensitivity with Hopfield networks and transcriptomics data. C. Piermarocchi, *S. Domanskyi*, A. Hakansson, G. Paternostro, *CANCER RESEARCH* **80** (11), 41-41 (2020).

18. PyIOmica: Longitudinal Omics Analysis and Classification, *S. Domanskyi*, C. Piermarocchi, G. I. Mias, *Bioinformatics* **36** (7), 2306-2307 (2020).

17. Modeling disease progression in Multiple Myeloma with Hopfield networks and single-cell RNA-seq, *S. Domanskyi*, A. Hakansson, G. Paternostro, C. Piermarocchi, *IEEE International Conference on Bioinformatics and Biomedicine*, 2129-2136 (2019).

16. Polled Digital Cell Sorter (p-DCS): Automatic identification of hematological cell types from single cell RNA-sequencing clusters, *S. Domanskyi*, A. Szedlak, N. T. Hawkins, J. Wang, G. Paternostro, C. Piermarocchi, *BMC Bioinformatics* **20**, Article number: 369 (2019).

15. Predictive Design of Polymer Molecular Weight Distributions from Living Anionic Polymerization with Controlled Temporal Supply of Initiator, *S. Domanskyi*, D. T. Gentekos, V. Privman, B. P. Fors, *Polym. Chem.* **11**, 326-336 (2019).

14. Biomolecular Release from Alginate Triggered by Chemical Inputs Processed Through a Biocatalytic Cascade – Integration of Biomolecular Computing and Actuation, A. V. Okhokhonin, *S. Domanskyi*, Y. Filipov, M. Gamella, A. N. Kozitsina, V. Privman, E. Katz, *Electroanalysis*, **30** (3), 426-435 (2017).

13. Experimental Realization of High Quality Biochemical XOR Gate, Y. Filipov, *S. Domanskyi*, M. L. Wood, M. Gamella, V. Privman, E. Katz, *ChemPhysChem*, **18** (20), 2908–2915 (2017).

12. SIRT6 Knockout Cells Resist Apoptosis Initiation but not Progression after Nutrient Stress, *S. Domanskyi*, J. Nicholatos, J. Schilling, V. Privman, S. Libert, *Apoptosis*, **22** (11), 1336—1343 (2017).

11. Glucose-triggered Insulin Release from Fe^{3+}-cross-linked Alginate Hydrogel: Experimental Study and Theoretical Modeling, S. Scheja, *S. Domanskyi*, M. Gamella, K. L. Wormwood, C. C. Darie, A. Poghossian, M. J. Schöning, A. Melman, V. Privman, and E. Katz, *ChemPhysChem*, **18** (12), 1541-1551 (2017).

10. Design of High Quality Chemical XOR Gates with Noise Reduction, M. L. Wood, *S. Domanskyi*, and V. Privman, *ChemPhysChem* **18** (13), 1773-1781 (2017).

9. Rate-Equation Modelling and Ensemble Approach to Extraction of Parameters for Viral Infection-Induced Cell Apoptosis and Necrosis, *S. Domanskyi*, J. E. Schilling, V. Gorshkov, S. Libert, and V. Privman, *J. Chem. Phys.* **145** (9), Article 094103, 8 pages (2016).

8. *Invited Review:* Modeling and Modifying Response of Biochemical Processes for Biocomputing and Biosensing Signal Processing, *S. Domanskyi*, and V. Privman, Ch. 3 in *Advances in Unconventional Computing, Vol. 2: Prototypes, Models and Algorithms*, pages 61-83, edited by A. Adamatzky, Vol. **23** of *Emergence, Complexity and Computation* (Springer Nature, Basel, Switzerland, 2017).

7. Diffusion of Oligonucleotides from within Iron-Crosslinked Polyelectrolyte-Modified Alginate Beads: a Model System for Drug Release, V. Privman, *S. Domanskyi*, R. A. S. Luz, N. Guz, M. L. Glasser, and E. Katz, *ChemPhysChem* **17** (7), 976-984 (2016).
Journal Issue Cover: Results of this work have been highlighted by the Editors of *ChemPhysChem*, by using a compilation of images for a cover of Issue 7 of Volume **17.**

6. *Refereed Conference Proceeding Article:* Challenges in Modeling Delayed Erosion Due to Degradation of Novel Polyanhydride Biomaterials, V. Privman, *S. Domanskyi*, K. L. Poetz, and D. A. Shipp, in: Proc. Conf. ICQNM 2015 (ThinkMind Digital Publishing: thinkmind.org, Wilmington, DE, 2015), pages 10-15.

5. Reaction-Diffusion Degradation Model for Delayed Erosion of Cross-Linked Polyanhydride Biomaterials, *S. Domanskyi*, K. L. Poetz, D. A. Shipp, and V. Privman, *Phys. Chem. Chem. Phys.* **17** (20), 13215-13222 (2015).
Journal Issue Cover: Results of this work have been highlighted by the Editors of *Phys. Chem. Chem. Phys.*, by using a compilation of images for a cover of Issue 20 of Volume **17.**

4. Percolation Modeling of Self-Damaging of Composite Materials, *S. Domanskyi* and V. Privman, *Physica A* **405**, 1-9 (2014).

3. Kinetic Model for a Threshold Filter in an Enzymatic System for Bioanalytical and Biocomputing Applications, V. Privman, *S. Domanskyi*, S. Mailloux, Y. Holade, and E. Katz, *J. Phys. Chem. B* **118** (43), 12435-12443 (2014).
Journal Issue Cover: Results of this work have been highlighted by the Editors of *J. Phys. Chem. B*, by using a compilation of images for a cover of Issue 43 of Volume **118.**

2. *Refereed Conference Proceeding Article:* Design of Biosensors with Extended Linear Response and Binary-Type Sigmoid Output Using Multiple Enzymes, O. Zavalov, *S. Domanskyi*, V. Privman, and A. Simonian, in: Proc. Conf. ICQNM 2013 (ThinkMind Digital Publishing: thinkmind.org, Wilmington, DE, 2013), pages 54-59.

1. Design of Digital Response in Enzyme-Based Bioanalytical Systems for Information Processing Applications, *S. Domanskyi* and V. Privman, *J. Phys. Chem. B* **116** (46), 13690-13695 (2012).

Presentations & Conference Attendance

Computational Biology Forum at Michigan State University:

- Applications of the Digital Cell Sorter (DCS) platform to the analysis of single-cell RNA-seq data from immune and endothelial cells. *April 2021.*

Systems Approaches to Cancer Biology Conference:

- *Poster:* Cell anomaly quantification method for single-cell transcriptomics. *November 2020.*

IEEE International Conference on Bioinformatics and Biomedicine San Diego, CA. *November 2019*:

- Modeling disease progression in Multiple Myeloma with Hopfield networks and single-cell RNA-seq. *November 2019.*

Conference on Computational Health: CoCoH, Grand Rapids, MI. *August 2019*:

- *Poster:* PyIOmica: Longitudinal Omics Analysis and Classification.

- *Poster:* Modeling disease progression in Multiple Myeloma with Hopfield networks and single-cell RNA-seq.

Oncogenomics Tenets of Precision Oncology, East Lansing, MI. *November 2018.*

APS March Meeting New Orleans, LA. *March 2017*:

- Diffusion of oligonucleotides from within Iron-Cross-Linked, Polyelectrolyte-Modified Alginate Beads: A Model System for Drug Release.
- Reaction-diffusion degradation model for delayed erosion of cross-linked polyanhydride biomaterials.
- *Posters:* Percolation Modeling of Self-Damaging of Composite Materials.Poster: Percolation Modeling of Self-Damaging of Composite Materials.; Rate-Equation Modelling and Ensemble Approach to Extraction of Parameters for Viral Infection-Induced Cell Apoptosis and Necrosis.

Seminar at Los Alamos National Laboratory:

- Non-Adiabatic Molecular Dynamics in Multi-Crossing Systems. *November 2015.*

Excited State Processes at Electronic and Bio Nanomaterials, Santa Fe, NM. *June 2016.*

Polymer Nanostructures for Emerging Science and Technology symposium, Clarkson University, *March 2018.*

Clarkson University Symposium presentations: *Poster:* Design of Digital Response in Enzyme-Based Bioanalytical Systems for Information Processing Applications. *October 2012. Poster:* Percolation Modeling of Self-Damaging of Composite Materials. *October 2013. Poster:* Rate-Equation Modelling and Ensemble Approach to Extraction of Parameters for Viral Infection-Induced Cell Apoptosis and Necrosis. *November 2016.* This poster was recognized as the **best presentation** in the category of Computational Science. *Poster:* Dynamics of Apoptosis in SIRT6 Knockout versus Wild Type Cells under Stress: Flow Cytometry Distribution Data and Their Numerical Modeling. *April 2017.*

Clarkson University Physics Department Seminars: Design of Digital Response in Enzyme-Based Bioanalytical Systems for Information Processing Applications. *November 2012.* Percolation Modeling of Self-Damaging of Composite Materials. *December 2013.* Reaction-Diffusion Degradation Model for Photopolymerized Crosslinked Polyanhydrides. *March 2014.* Modeling of Bio-Inspired, Biomolecular, and Biotechnology Systems and Materials. *April 2015.* Non-Adiabatic Molecular Dynamics in Multi-Crossing Systems. *March 2016.* Towards a Better Understanding and Simulation of Nonadiabatic Quantum Dynamics. *September 2016.* Physiochemical Modeling of Bio-Inspired Systems and Materials. *December 2016.*