Ada Sedova | R&D Associate Scientist
Molecular Biophysics Group, Biosciences Division
Computational Chemistry and Nanomaterials Sciences Group, Computational Sciences and Engineering Division
Oak Ridge National Laboratory
sedovaaa@ornl.gov

Professional Preparation and Education

University at Albany, State University of New York, Albany, N.Y.
PhD Biophysics and Structural Biology: May 2015, Department of Biomedical Sciences
Thesis supervised by Dr. Nilesh K. Banavali: *"The Structural Heterogeneity and Dynamics of Base Stacking and Unstacking in Nucleic Acids.*" ProQuest (open version: ResearchGate)

University at Albany, State University of New York, Albany, N.Y.
MA Mathematics: May 2015, Department of Mathematics and Statistics
Thesis supervised by Dr. Martin Hildebrand: *"Conditions for Deterministic Limits of Markov Jump Processes: The Kurtz Theorem in Chemistry."* ProQuest (open version: ResearchGate)

University of North Carolina at Asheville, Asheville, N.C.
BS Premedical Studies: May 2009; **BA Applied Mathematics:** May 2009. Mathematics senior thesis supervised by Dr. Samuel Kaplan: *"Mathematics of Computed Tomography."*

Postdoctoral Research:

High performance computing, molecular simulation, programming models, performance portability, neutron scattering, 2016-2019: ***National Center for Computational Sciences (NCCS), Oak Ridge National Laboratory, Oak Ridge, T.N***.
Computational fluid dynamics and analytical bioelectrochemistry, 2015-2016: ***Department of Chemistry, University at Albany, State University of New York, Albany, N.Y.***

Appointments:

2019-Current: R&D Associate Staff Scientist, Molecular Biophysics Group, Biosciences Division; Joint affiliation: Computational and Computer Sciences Directorate, Oak Ridge National Laboratory.
2016-2019: CSEEN Postdoctoral Research Associate, Scientific Computing Group, National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, T.N.
2015-2016: Postdoctoral Research Associate, Department of Chemistry, University at Albany, State University of New York, Albany, N.Y.
2010-2015: Graduate Research Assistant, Center for Medical Science, NY State Department of Health, and Department of Biomedical Sciences, University at Albany, State University of New York.

Programming Languages and Programming Models:

C++, C, Python, MATLAB, CUDA, Linux/shell, FORTRAN, OpenMP, OpenACC, MPI
Deep Learning Frameworks: TensorFlow, PyTorch

GitHub: https://github.com/BSDExabio, https://github.com/ExaMat
Google Scholar page: https://scholar.google.com/citations?user=A4p_R1MAAAAJ&hl=en
Website: https://www.ornl.gov/staff-profile/ada-sedova

Professional Affiliations:

Association for Computing Machinery (ACM), American Chemical Society (ACS), American Physical Society (APS)

Awards:

Excellence in Research at the Doctoral Level, Biomedical Sciences Department, University at Albany (2015); Significant Event Award, ORNL (2020): "First Successful Evaluation of the ARM+NVIDIA Accelerated Node Architecture in the World"; 2020 ACM Special COVID-19 Gordon Bell Finalist.

Recent community engagement:

Organizer, SC23, two sessions: SC23 presenter page
Programming committee/reviewer: 38th and 39th International Parallel and Distributed Processing Symposium (IPDPS 2024, 2025), Applications Track
Programming committee/reviewer: Intelligent Systems for Molecular Biology (ISMB) 2024, Proceedings, Macromolecular Sequence, Structure, and Function
Reviewer, Nature Communications

Publications:
**corresponding author*

Shanmugavelu S, Taillefumier M, Culver C, Ganesh V, Hernandez O, **Sedova A***. Robustness of deep learning classification to adversarial input on GPUs: asynchronous parallel accumulation is a source of vulnerability. In: European Conference on Parallel Processing 2025 Apr 25 (pp. 306-320). Cham: Springer Nature Switzerland.

Valentino HR, Qian L, Parks JM, Drufva EE, **Sedova A**, Mehta PS, Watson MP, Giannone RJ, Galanie SS, Michener JK. Engineered enzymatic cascade converts diols to amino alcohols. Green Chemistry. 2025;27(21):6283-92.

Shanmugavelu S, Taillefumier M, Culver C, Hernandez O, Coletti M, **Sedova A***. Impacts of floating-point non-associativity on reproducibility for HPC and deep learning applications. In: SC24-W: Workshops of the International Conference for High Performance Computing, Networking, Storage and Analysis 2024 Nov 17 (pp. 170-179). IEEE.

Chahal R, Toomey MD, Kearney LT, **Sedova A**, Damron JT, Naskar AK, Roy S. Deep-learning interatomic potential connects molecular structural ordering to the macroscale properties of polyacrylonitrile. ACS Applied Materials & Interfaces. 2024 Jul 3;16(28):36878-91.

Bradley VC, Manard BT, Hendriks L, Dunlap DR, Bible AN, **Sedova A**, Saint-Vincent P, Sanders B, Andrews HB. Quantifying platinum binding on protein-functionalized magnetic microparticles using single particle-ICP-TOF-MS. Analytical Methods. 2024.

Roy S, Khanal R, Gibson L, Chahal R, **Sedova A**, Bryantsev VS. Tracing Mechanistic Pathways and Reaction Kinetics Toward Equilibrium in Reactive Molten Salts. Chemical Science (RSC), 2024, DOI: 10.1039/D3SC06587A (Edge Article)

Davidson RB, Coletti M, Gao M, Piatkowski B, Sreedasyam A, Quadir F, Weston DJ, Schmutz J, Cheng J, Skolnick J, Parks JM, **Sedova A*.** Predicted structural proteome of *Sphagnum divinum* and proteome-scale annotation. Bioinformatics. **2023** Aug 1;39(8):btad511.

Coletti M*, **Sedova A***, Chahal R, Gibson L, Roy S, Bryantsev VS. Multiobjective Hyperparameter Optimization for Deep Learning Interatomic Potential Training Using NSGA-II. In: Proceedings of the 52nd International Conference on Parallel Processing (ICPP) Workshops 2023 Aug 7 (pp. 172-179).

Morehead A*, Chen C, **Sedova A**, Cheng J. DIPS-plus: The enhanced database of interacting protein structures for interface prediction. Scientific Data. **2023** Aug 3;10(1):509.

Hsu DJ, Davidson RB, **Sedova A**, Glaser J*. tinyIFD: A High-Throughput Binding Pose Refinement Workflow Through Induced-Fit Ligand Docking. Journal of Chemical Information and Modeling. **2023** May 19.

Rogers DM*, Agarwal R, Vermaas JV, Smith MD, Rajeshwar RT, Cooper C, **Sedova A**, Boehm S, Baker M, Glaser J, Smith JC*. SARS-CoV2 billion-compound docking. Scientific Data. 2023 Mar 28;10(1):173.

Coletti M*, Davidson R, **Sedova A***. Toward designing effective exascale scientific computing workflows: experiences and best practices. Proceedings of the 2022 Improving Scientific Software Conference, National Center for Atmospheric Research (NCAR) Technical Notes, NCAR/TN-574+PROC, 9/2022.

Sedova A*, Russell B. Davidson, Mathieu Taillefumier, Wael Elwasif**.** HPC Molecular Simulation Tries Out a New GPU: Experiences on Early AMD Test Systems for the Frontier Supercomputer. **2022** Proceedings of Cray User Group (CUG 2022), 2022.

Davidson RB, Woods J, Effler TC, Thavappiragasam M, Mitchell JC, Parks JM, **Sedova A*.** OpenMDlr: Parallel, Open-source Tools for General Protein Structure Modeling and Refinement from Pairwise Distances. Bioinformatics. **2022** Jun 15;38(12):3297-8.

Glaser J*, **Sedova A**, Galanie S, Kneller DW, Davidson RB, Maradzike E, Del Galdo S, Labbé A, Hsu DJ, Agarwal R, Bykov D, et. al. Hit expansion of a noncovalent SARS-CoV-2 main protease inhibitor. ACS Pharmacology & Translational Science. **2022** Apr 4;5(4):255-65.

Gao M, Coletti M, Davidson RB, Prout R, Abraham S, Hernandez B, **Sedova A***. Proteome-scale Deployment of Protein Structure Prediction Workflows on the Summit Supercomputer. **2022** In: 2022 IEEE International Parallel and Distributed Processing Symposium Workshops (IPDPSW) 2022 May 30 (pp. 206-215). IEEE.

Thavappiragasam M*, Elwasif W*, **Sedova A*.** Portability for GPU-accelerated molecular docking applications for cloud and HPC: can portable compiler directives provide performance across all platforms? In: 2022 22nd IEEE International Symposium on Cluster, Cloud and Internet Computing (CCGrid) **2022** May 16 (pp. 975-984). IEEE.

Thavappiragasam M, Kale V, Hernandez O, **Sedova A***. Addressing Load Imbalance in Bioinformatics and Biomedical Applications: Efficient Scheduling across Multiple GPUs. In: 2021 IEEE International Conference on Bioinformatics and Biomedicine (BIBM) **2021** Dec 9 (pp. 1992-1999). IEEE.

Gao M, Lund-Andersen P, Morehead A, Mahmud S, Chen C, Chen X, Giri N, Roy RS, Quadir F, Effler TC, Prout R., ... & **Sedova, A***. High-Performance Deep Learning Toolbox for Genome-Scale Prediction of Protein Structure and Function. In: 2021 IEEE/ACM Workshop on Machine Learning in High Performance Computing Environments (MLHPC) **2021** Nov 15 (pp. 46-57). IEEE.

Davidson RB, Thavappiragasam M, Effler TC, Woods J, Elias DA, Parks JM, **Sedova A*.** Modeling Protein Structures from Predicted Contacts with Modern Molecular Dynamics Potentials: Accuracy, Sensitivity, and Refinement. In: Proceedings of the 12th ACM Conference on Bioinformatics, Computational Biology, and Health Informatics **2021** Aug 1 (pp. 1-10).

Glaser J*, Vermaas JV, Rogers DM, Larkin J, LeGrand S, Boehm S, Baker MB, Scheinberg A, Tillack AF, Thavappiragasam M, **Sedova A,** Hernandez, O. High-throughput Virtual Laboratory for Drug Discovery Using Massive Datasets. The International Journal of High-Performance Computing Applications. **2021 Mar** 23:10943420211001565.

Acharya A, Agarwal R, Baker MB, Baudry J, Bhowmik D, Boehm S, Byler KG, Chen SY, Coates L, Cooper CJ, Demerdash O., …& Smith JC*. Supercomputer-based Ensemble Docking Drug Discovery Pipeline with Application to COVID-19. Journal of Chemical Information and Modeling. **2020** Dec 16;60(12):5832-52.

Vermaas JV*, **Sedova A,** Baker MB, Boehm S, Rogers DM, Larkin J, Glaser J, Smith MD, Hernandez O, Smith JC. Supercomputing Pipelines Search for Therapeutics Against COVID-19. Computing in Science & Engineering. **2020** Nov 6;23(1):7-16.

LeGrand S, Scheinberg A, Tillack AF, Thavappiragasam M, Vermaas JV, Agarwal R, Larkin J, Poole D, Santos-Martins D, Solis-Vasquez L, Koch A, Forli S, Hernandez O, Smith JC and **Sedova A***. GPU Accelerated Drug Discovery with Docking on the Summit Supercomputer: Porting, Optimization, and Application to COVID-19 Research. In: Proceedings of the 11th ACM International Conference on Bioinformatics, Computational Biology and Health Informatics **2020** Sep 21 (pp. 1-10).

Thavappiragasam M, Scheinberg A, Elwasif W, Hernandez O, **Sedova A***. Performance Portability of Molecular Docking Miniapp on Leadership Computing Platforms. In: 2020 IEEE/ACM International Workshop on Performance, Portability and Productivity in HPC (P3HPC) **2020** Nov 13 (pp. 36-44). IEEE.

Ossyra J, **Sedova A*,** Tharrington A, Noé F, Clementi C, Smith JC. Porting Adaptive Ensemble Molecular Dynamics Workflows to the Summit Supercomputer. In: International Conference on High Performance Computing **2019** Jun 16 (pp. 397-417). Springer, Cham.

Ossyra JR, **Sedova A*,** Baker MB, Smith JC. Highly Interactive, Steered Scientific Workflows on HPC Systems: Optimizing Design Solutions. In: International Conference on High Performance Computing **2019** Jun 16 (pp. 514-527). Springer, Cham.

Sedova A*, Tillack AF, Tharrington A. Using Compiler Directives for Performance Portability in Scientific Computing: Kernels from Molecular Simulation. In: International Workshop on Accelerator Programming Using Directives **2018** Nov 11 (pp. 22-47). Springer, Cham.

Sedova A*, Eblen JD, Budiardja R, Tharrington A, Smith JC. High-performance Molecular Dynamics Simulation for Biological and Materials Sciences: Challenges of Performance Portability. In: 2018 IEEE/ACM International Workshop on Performance, Portability and Productivity in HPC (P3HPC) **2018 Nov** 16 (pp. 1-13). IEEE.

Pandey A[†], **Sedova A[†]*,** Daemen LL, Cheng Y, Ramirez-Cuesta AJ. Exposing Key Vibrational Contributions to Properties of Organic Molecular Solids with High Signal, Low Frequency Neutron Spectroscopy and Ab Initio Simulations. Crystal Growth & Design. **2018** Aug 3;18(9):4815-21. [†]Co-first authors, listed alphabetically.

Biała K, **Sedova A***, Mix M, Bär K, Orsag P, Fojta M, Flechsig GU*. Amplified Detection of Single Base Mismatches with the Competing-strand Assay Reveals Complex Kinetic and Thermodynamic Behavior of Strand Displacement at the Electrode Surface. Electrochimica Acta. **2018** Sep 20; 285:272-83.

Sedova A, Banavali NK*. Geometric Patterns for Neighboring Bases Near the Stacked State in Nucleic Acid Strands. Biochemistry. **2017** Mar 14;56(10):1426-43.

Joda H[†], **Sedova A[†]*,** Awan W, Flechsig GU*. The Osmium Tetroxide Bipyridine-labeled DNA Probe: Hairpin Conformations and Characterization of Redox-label Behavior. Electroanalysis. **2017** Jan; 29(1):51-9. [†]Co-first authors, listed alphabetically.

Ni X, Joda H, **Sedova A*,** Biała K, Flechsig GU*. Sequence Detection of Unlabeled DNA Using the Sandwich Assay: Strand-displacement, Hybridization Efficiency, and Probe-conformation Considerations for the Tethered Surface. Electrochimica Acta**. 2016** Dec 1; 220:581-6.

Sedova A, Banavali NK*. RNA Approaches the B-form in Stacked Single Strand Dinucleotide Contexts. Biopolymers. **2016** Feb; 105(2):65-82. *Cover article*.

Biala K, **Sedova A,** Flechsig GU*. Sequence and Temperature Influence on Kinetics of DNA Strand Displacement at Gold Electrode Surfaces. ACS Applied Materials & Interfaces. **2015** Sep 16;7(36):19948-59.