

Ada Sedova | R&D Associate Scientist
Molecular Biophysics Group, Biosciences Division
Computational Chemistry and Nanomaterials Sciences Group, Computational Sciences and
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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.*”

<https://www.proquest.com/docview/1690900217/9D6608284AC54FA6PQ/1?accountid=26379>

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.*”

<https://www.proquest.com/docview/1682043212/7464572F47E74CAEPQ/1?accountid=26379>

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 Chemistry and Nanomaterials Sciences Group, Computational Sciences and Engineering Division, 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.

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.

Programming Languages and Programming Models:

C++, C, Python, MATLAB, CUDA, Linux/shell, FORTRAN, OpenMP, OpenACC, MPI

Google Scholar page: https://scholar.google.com/citations?user=A4p_R1MAAAAJ&hl=en

Website: <https://www.ornl.gov/staff-profile/ada-sedova>

Publications:

**corresponding author*

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. The Third International Workshop on Parallel and Distributed Algorithms for Decision Sciences (PDADS), in print.

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.

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.