David M. Rogers, Curriculum Vitae

Computational Scientist
National Center for Computational Sciences
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(a) Professional Preparation

Univ. Cincinnati, OH	Chemistry (Biochem. Concentration)	BS 2001-2004
	Mathematics	Minor 2001-2004
Univ. Cincinnati, OH	Physical Chemistry	Ph.D. 2004-2009
Sandia National Labs, NM	Nanobiology & Materials Sci.	Postdoc 2009-2013

(b) Appointments

Computational Scientist, ORNL	2020-present
Assistant Professor, Univ. South Florida	2013-2020
Postdoctoral Appointee, Sandia National Labs	2009-2013
Computational Science Graduate Fellow, Univ. Cincinnati	2006-2009

(c) Synergistic Activities

- Better Scientific Software Tutorial and Productivity and Sustainability Planning - Software Development Ecosystems Team Outreach (https://bssw-tutorial.github.io)
- GPU Hackathon Mentor (https://www.gpuhackathons.org/)
- Organizing 'Family Science Night' outreach event series at Elementary and Middle schools in need of academic support, 2017-2018
- Created publicly available course outline and teaching material for modern, graduate-level courses in quantum mechanics and scientific computing (available at predictivestatmech.org).

(d) Publications (**bold** for corresp. author)

- Statistical Mechanics of Fluids
  1. Julián M. Delgado, Nalvi Duro, David M. Rogers, Alexandre Tkatchenko, Sagar A. Pandit, Sameer Varma. Molecular Basis for SARS-CoV-2 spike affinity for human ACE2 receptor. *Proteins: Structure, Function, Bioinfo.*, 2021.
  2. **David M. Rogers**. Protein Conformational States – A First Principles Bayesian Method. *Entropy*, 22(11):1242, 2020.
  3. **David M. Rogers**. Range separation: the divide between local structures and field theories *Substantia*, 3(1), 2019.
  4. Guy W. Dayhoff and **David M. Rogers**. Hydration and Dispersion Forces in Hydroxypropylcellulose Phase Behavior. *J. Phys. Chem. B*, 123(23):4976-4985, 2019.

5. Phillip S. Hudson, Stefan Boresch, David M. Rogers, and H. Lee Woodcock Accelerating QM/MM Free Energy Computations via Intramolecular Force Matching. *J. Chem. Theory Comput.*, 14 (12):6327–35, 2018.
6. **David M. Rogers**. Extension of Kirkwood-Buff Theory to the Canonical Ensemble. *J. Chem. Phys.* 148:054102, 2018.
7. Juan M. Vanegas, Frank Heinrich, David M.Rogers, Bryan D. Carson, Sadie La Bauve, Briana C. Vernon, Bulent Akgun, Sushil Satija, Aihua Zheng, Margaret Kielian, Susan B. Rempe, and Michael S. Kent. Insertion of Dengue E into lipid bilayers studied by neutron reflectivity and molecular dynamics simulations. *BBA* 1860(5):1216–1230, 2018.
8. **David M. Rogers**. Overcoming the Minimum Image Constraint Using the Closest Point Search. *J. Mol. Graph. Model* 68:197–205, 2016.
9. Marielle Soniat, David M. Rogers, and Susan Rempe. Dispersion- and Exchange-Corrected Density Functional Theory for Sodium Ion Hydration. *J. Chem. Theory. Comput.*, 142:074101, 2015.
10. Andriy Anishkin, Juan M. Vanegas, David M. Rogers, Philip L. Lorenzi, Wai Kin Chan, Preeti Purwaha, John N. Weinstein, Sergei Sukharev, and Susan B. Rempe. Catalytic Role of the Substrate Defines Specificity of Therapeutic L-Asparaginase. *J. Mol. Biol.* 427:2867-2885, 2015.
11. David M. Rogers, Michael S. Kent, and Susan B. Rempe. Molecular basis of endosomal-membrane association for the dengue virus envelope protein. *BBA Biomembranes* 1848(4):1041-52, 2015.
12. W. K. Chan, P. L. Lorenzi, A. Anishkin, P. Purwaha, D. M. Rogers, S. Sukharev, S.B. Rempe, and J. N. Weinstein. The glutaminase activity of L-asparaginase is not required for anticancer activity against ASNS-negative cells. *Blood*, 123(23):3596-606, 2014.
13. David M. Rogers, Dian Jiao, Lawrence R. Pratt, and Susan B. Rempe. Structural models and molecular thermodynamics of hydration of ions and small molecules. In Ralph A. Wheeler, editor, *Annu. Rep. Comp. Chem.*, volume 8, pages 71–127, 2012.
14. Sameer Varma, David M. Rogers, Lawrence R. Pratt, and Susan B. Rempe. Perspectives on Ion Selectivity: Design principles for K^+ selectivity in membrane transport. *J. Gen. Physiol.*, 137(6):479–488, 2011.
15. David M. Rogers and Susan B. Rempe. Probing the thermodynamics of competitive ion binding using minimum energy structures. *J. Phys. Chem. B*, 115(29):9116–9129, 2011.
16. David M. Rogers and Thomas L. Beck. Quasichemical and structural analysis of polarizable anion hydration. *J. Chem. Phys.*, 132(1):014505, 2010.
17. Zhen Zhao, David M. Rogers, and Thomas L. Beck. Polarization and charge transfer in the hydration of chloride ions. *J. Chem. Phys.*, 132(1):014502, 2010.
18. **David M. Rogers**. *Using Bayes' Theorem for Free Energy Calculations.* Ph.D. Dissertation, Univ. Cincinnati, 2009.
19. David M. Rogers and Thomas L. Beck. Modeling molecular and ionic absolute solvation free energies with quasichemical theory bounds. *J. Chem. Phys.*,

129(13):134505, 2008.

- Nonequilibrium Statistical Mechanics
  1. **David M. Rogers**. Unifying theories for nonequilibrium statistical mechanics. *J. Stat. Mech.*, 084010, 2019.
  2. Guy W. Dayhoff II and **David M. Rogers**. Driving forces in MD simulations of transition and 'free' flows. *Mol. Sim.*, 43(5-6):467–477, 2017.
  3. **David M. Rogers**. An information theory model for dissipation in open quantum systems. *J. Phys. Conf. Series*, 330(1):012039, 2017. 8th International Workshop DICE2016, Italy.
  4. **David M. Rogers**. The Einstein-Podolsky-Rosen paradox implies a minimum achievable temperature. *Phys. Rev. E*, 95:012149, 2017.
  5. Elisa La Bauve, Briana C. Vernon, Dongmei Ye, David M. Rogers, Cathryn M. Siegrist, Bryan Carson. Susan L. Rempe, Aihua Zheng, Margaret C. Kielian, Andrew P. Shreve, and Michael S. Kent Method for measuring the unbinding energy of strongly-bound membrane-associated proteins. *BBA Biomembranes* 1858(11): 2753–2762, 2016.
  6. Mathias B. Andersen, David M. Rogers, Junyu Mai, Benjamin Schudel, Anson V. Hatch, Susan B. Rempe and Ali Mani. Spatiotemporal pH dynamics in concentration polarization near ion-selective membranes. *Langmuir*, 30(26):7902–7912, 2014.
  7. David M Rogers and Susan B Rempe. Irreversible thermodynamics. *J. Phys., Conf. Ser.*, 402:012014, 2012.
  8. David M. Rogers, Thomas L. Beck, and Susan B. Rempe. Information theory perspective on nonlinear, nonequilibrium thermodynamics. *J. Stat. Phys.*, 145(2):385–409, 2011.
- Reproducible Computational Infrastructure
  1. **David M. Rogers**. Three Practical Workflow Schedulers for Easy Maximum Parallelism. *Software: Practice and Experience* (https://doi.org/10.1002/spe.3047), 2021.
  2. Diego Gomez, Lawrence R. Pratt, David M. Rogers, Susan B. Rempe. Free Energies of Hydrated Anions: High throughput Computations on Clusters to Treat Rough Energy-Landscapes. *Molecules*, 26(11):3087, 2021.
  3. Jens Glaser, Josh V. Vermaas, David M. Rogers, Jeff Larkin, Scott LeGrand, Swen Boehm, Matthew B. Baker, Aaron Scheinberg, Andreas F. Tillack, Mathialakan Thavappiragasam, Ada Sedova, Oscar Hernandez. High-throughput virtual laboratory for drug discovery using massive datasets. *Int. J. HPC Appl.*, 2021.
  4. Josh V. Vermaas, Ada Sedova, Matthew Baker, Swen Boehm, David M. Rogers, Jeff Larkin, Jens Glaser, Micholas Smith, Oscar Hernandez, Jeremy Smith. Supercomputing Pipelines Search for Therapeutics Against COVID-19. *Computing in Science & Engineering*, 23(1):7–16, 2021.
  5. Covid Computational Drug Discovery Collaboration. Supercompuer-based ensemble docking drug discovery pipeline with application to COVID-19. *J. Chem. Inf. Model*, 60(12): 5832-5852, 2020.

6. **David M. Rogers**. Efficient Primitives for Standard Tensor Linear Algebra. *Proc. XSEDE (ACM)*, 2016.
7. **David M. Rogers**. Real-space quadrature: a convenient, efficient representation for multipole expansions. *J. Chem. Phys.* 142:074101, 2015. *JCP Editor's choice award.*
8. David M. Rogers and Susan B. Rempe; et. al. *Computational and experimental platform for understanding and optimizing water flux and salt rejection in nanoporous membranes*. Sandia Technical Report, 2010. SAND2010-6735.

- Research Products
  1. **David M. Rogers**. *mpi_remote*, a remote control for mpi_list. DOE-CODE, 2022
  2. **David M. Rogers**. *aiowire*, an asynchronous event library for python. DOE-CODE, 2022
  3. **David M. Rogers**. *actor-api*, an actor-based communication library for python. DOE-CODE, 2022
  4. **David M. Rogers**and Kathryn Knight. *The challenge of capturing and converting primary to secondary and summary datasets*. Whitepaper published in proc. DOE-ASCR Workshop on the Management and Storage of Scientific Data, Jan. 2022.
  5. **David M. Rogers**. *Investigating Software Developer Roles Supporting Reproducibility*. Whitepaper published in proc. DOE-ASCR Workshop on the Science of Scientific-Software Development and Use, Dec. 2021.
  6. **David M. Rogers**. *DataTrails*, A collection of reproducible computational experiments at OLCF. ORNL Gitlab, 2021.
  7. **David M. Rogers***et. al.* SARS-CoV2 Docking Dataset, Small-molecule conformations and docking scores for 1.4 billion molecules docked against 6 protein targets. OLCF Constellation Portal, 2021
  8. **David M. Rogers**. *HPL/HPCG Tutorial*, A walkthrough and tutorial for optimizing HPL and HPCG benchmarks on new hardware. frobnitzem.github.io/hpl-hpcg.
  9. **David M. Rogers**. *DWork*, a scalable bag of tasks implementation for work distribution on HPC. Github, 2021.
  10. **David M. Rogers**. *mpi_list*, a python-mpi-spark-like library for parallel operation son distributed lists. pypi, 2021
  11. Micholas D. Smith, **David M. Rogers**, J. V. Vermaas, and Jeremy C. Smith. SARS-CoV2 Protein-Ligand Simulation Dataset: (layers 1-3) OLCF Constellation Portal, 2021
  12. **David M. Rogers**. *SciComp Recipes*, A collect of recipes for emerging HPC paradigms. frobnitzem.github.io/scicomp-recipes.
  13. **David M. Rogers**. *Classify*, implementation of a Bayesian bitvector classification algorithm. Github, 2020.
  14. **David M. Rogers**. *Launchad*, high-throughput toolkit for billion-molecule docking campaigns. code.ornl.gov, 2019.
  15. **David M. Rogers**. *PMake*, a parallel make build system for running computational experiments. code.ornl.gov, 2019.

16. **David M. Rogers**. *Parallel Science*, gateway for citable, extensible, and reproducible scientific computing. parallelscience.com, 2017-2019.
17. **David M. Rogers**. *Introduction to Scientific Computing*, comprehensive online course notes. predictivestatmech.org/CompSciSpring2018, 2014-2018 (352,355 cumulative page views).
18. **David M. Rogers**. *ChemParam*, software for automated parameterization of molecular energies for CHARMM and Gromacs. Github, 2018.
19. **David M. Rogers**. *LAMMPS Plug-In*, adaptor for running LAMMPS molecular simulation engine as a workflow component. parallelscience.com/projects/md.lammps, 2017.
20. **David M. Rogers**. *PocketView*, software for displaying JSON data. GitHub, 2017.
21. **David M. Rogers**. *EwaldCorrel*, software for computing correlation functions in Fourier-space. GitHub, 2017.
22. **David M. Rogers**. *LibDAG*, software for parallel scheduling of task graphs. GitHub, 2017.
23. **David M. Rogers**. *USF-Slack*, software for fast tensor contraction using domain-specific languages. GitHub, 2016.
24. **David M. Rogers**and Olaf Lenz. *PBCTools*, VMD plug-in wrapping molecular structures. VMD Package, UIUC, IL., 2015.
25. **David M. Rogers**. *SProtoc*, code generator for writing data to the cloud. GitHub, 2015.
26. **David M. Rogers**. *RealPole*, implementation of the 'Real Space Quadrature' paper, along with a fast multipole method in Python. GitHub, 2014.
27. **David M. Rogers**. *rbtree*, C-library for binary trees. GitHub, 2013.
28. **David M. Rogers**. *cmap*, C-library for maps. GitHub, 2013.
29. **David M. Rogers** and Thomas L. Beck. *Force Solve*, software for force matching method of molecular energy parameter computation. SourceForge, Chicago, IL, 2008 and GitHub, 2016.

(e) Honors and Awards

Finalist, Gordon Bell Prize for HPC on Covid-19	ACM	2020
Honorable Mention, Better Scientific Software Fellowship	BSSw.org	2020
Member of Founding Faculty for the New Phi Beta Kappa Chapter (Eta of Florida at USF)	Phi Beta Kappa Society	2018
Top Reviewer Award	J. Chem. Physics	2016
R&D100 Award, Biomimetic Membranes for Water Purification	R&D Magazine	2011
Award for Excellence	Sandia National Labs LDRD Program	2010
Hans H. Jaffé Award for Outstanding Scholarship in Physical Chemistry	Univ. Cincinnati	2009
Computational Science Graduate Fellowship	DOE	2006
Phi Beta Kappa		2004
Biochemistry Award	UC Department of Chemistry	2004
McMicken Achiever's Scholarship	Univ. Cincinnati	2003
Dean's List	Univ. Cincinnati	2001-2004

(f) Meetings and Workshops Organized

- Florida ACS Meeting and Exhibition, Computational Session Organizer, 2017 and 2018.

(g) Patents

- S. Rempe, C. J. Brinker, D. Rogers, Y-B. Jiang, and S. Yang. "Biomimetic membranes and methods of making biomimetic membranes." No. US9486742B1 filed by Sandia National Labs and UNM, October 2011.
- S. Rempe, D. Rogers, A. Anishkin, S. Sukharev, P. L. Lorenzi, W. K. Chan, and J. N. Weinstein. "Therapeutic asparaginases." No. US9486742B1 filed by Sandia National Labs and MDACC, September, 2014.

(h) Presentations

- May 2, 2022, "Developing a Testing and Continuous Integration Strategy for Your Team." ECP Annual Meeting tutorial with Greg Watson and David M. Rogers.
- Aug. 25, 2021, "New Tools for Billion-Molecule Analytics at Scale." ACS Fall 2021.
- Aug. 21, 2021, "Software Productivity and Sustainability Presentation Series." ATPESC 2021 with David E. Bernholdt, Anshu Dubey, Rinku Gupta, and David M. Rogers.
- June 24-25, 2021, "Better Scientific Software Tutorial." ISC 2021 with David E. Bernholdt, Anshu Dubey, Patricia A. Grubel, Rinku Gupta, and David M. Rogers.
- Apr. 13, 2021, "Hands-On with Progress Tracking Cards" and "The Exascale Compute Project as a Team of Teams." ECP Annual Meeting tutorial with R. Milewicz, E. Pourmal, D. M. Rogers, B. Sims, G. R. Watson, J. M. Willenbring, and E. M. Raybourn.
- Mar. 25, 2021, "Better Scientific Software Tutorial - Software Testing (part 4 and 6)." SEA's Improving Scientific Software Conference.

- Mar. 3, 2021, "Querying the Exascale Compute Project " SIAM CSE21.
- Nov 31, 2020, "High-Throughput Virtual Laboratory for Drug Discovery Using Massive Datasets." SC20.
- June 4, 2020, "Working Effectively with the HPC Software Ecosystem." OLCF User Meeting.
- March 31, 2019, "Fast, reliable computation of small-angle structure factors in Kirkwood-Buff Theory." ACS Spring Meeting.
- July. 18, 2018, "Fixing Nonlocality in the Primitive Model" TSRC Workshop on Ions in Biology.
- Mar. 22, 2018, "Finite size effects in simulations of molecular Joule-Thomson flow" ACS Spring Meeting.
- Mar. 8, 2018, "Quantum Nonequilibrium Statistical Mechanics Meets the Measurement Problem," APS March Meeting.
- Aug. 31, 2017, "Demystifying Nonequilibrium Statistical Mechanics," at U. Pittsburgh.
- May 6, 2017, "Quantum Thermodynamics by Repeated Measurement," at the Florida ACS Meeting & Exposition (FAME2017).
- Feb. 17, 2017, "Demystifying Nonequilibrium Statistical Mechanics," at the USF Physics Colloquium.
- Sep. 14, 2016, "A moment generating function for flows in open quantum systems," at the International Conference for Spacetime, Matter, and Quantum Mechanics.
- July 12-16, 2016, "A Molecular Approach to Dispersion Energy" at the TSRC Workshop on Ions in Solution: Biology, Energy, and Environment.
- July 7-8, 2016, "The quantum mechanics of Jaynes," at the LANL Quantum Lunch.
- Mar. 13-17, 2016, "The Quantum Andersen Thermostat," at the 2016 ACS Spring Meeting.
- Feb., 2016, "Angle-free methods for boundary element problems on the sphere: The quadrature basis for spherical harmonics," at the USF Mathematics Department Analysis Lecture Series.
- Dec. 15, 2015, "Maximum Transition Entropy - A Causal, Canonical Model for Nonequilibrium Statistical Mechanics," at the 114th Statistical Mechanics Conference at Rutgers, New Brunswick New Jersey.
- September 14, 2015, "Understanding the origins of irreversibility: electrical driving and the second law.," Tulane Department of Chemistry.
- May 13, 2015, "Spatiotemporal Concentration-Polarization Induced pH Changes at Ion-Selective Membranes." at the Chemical and Biological Defense Sci. & Tech. conference in St. Louis, MO.
- May 8, 2015, "Where do Quanta Come From?" at the Florida ACS Meeting and Exhibition (FAME).
- Mar. 4, 2015, "Thermodynamics of Maximum Transition Entropy for Quantum Assemblies." at the APS March Meeting in San Antonio, TX.

- Nov. 22 2014, "Liquid Structure With Gromacs" USF MRI, Scientific Computing Workshop.
- Oct. 16, 2014, "Real-space quadrature: A convenient, universal representation for multipole expansions." at the Southeast Regional Meeting of the ACS in Nashville, TN.
- Aug. 18 2014, "pH Dynamics During Concentration Polarization," to the CM4 Mathematics for Mesoscopic Materials Modeling Group.
- July 8 2014, "What's Holding Up Multiscale modeling?" Telluride Workshop for Ions in Aqueous Solutions and Molecular Biology.
- May 9 2014, "Jumping from atomistic to continuum simulation of electrochemical driving at interfaces," at the 2014 Florida FAME Conference.
- March 7, 2014, Invited Guest Speaker at Writing Center/USF Library's annual "Dissertation Forum."
- Jan. 31, 2014, "Mixing Molecular & Continuum Simulations, From Statistical Sampling to Nanoscale-response functions," at the USF Department of Chemical and Biomedical Engineering.
- January 29th, 2014, "Simulating at the molecular / continuum interface," as a Featured Researcher at the USF Research Computing User's Group Forum.
- ACS Spring National Meeting, "Solute Partitioning and Transport through Natural and Biomimetic Membranes," New Orleans, April, 2013.
- Biophysical Society Meeting, "Molecular Modeling of the Attachment of the Dengue II Envelope Protein into Host Endosomal Membranes," Pittsburgh, February, 2013.
- Invited Presentation, Materials Design in Chemical Compound Space, "Organizing Desalination Membrane Design Using Thermodynamic Cycles," Institute for Pure and Applied Mathematics, UCLA, May, 2011.
- American Physical Society March Meeting, "Thermodynamic Analysis of Nanoporous Membrane Separation Processes," Dallas, 2011.
- Invited Presentation, Telluride Science Research Center Workshop, "Probing the Thermodynamics of Ion Hydration Using Minimum Energy Structures," July, 2010.
- DOE CSGF Conference Presentation, "Improved force matching using Bayes' theorem and stretched string energy priors." July, 2008.
- Invited Presentation, Central Regional Meeting of the American Chemical Society. "Accurate Solvation Free Energy Computation." May, 2007.

(i) Journals Refereed

- Journal of Chemical Physics 2016 Top Reviewer Award
- Journal of Physical Chemistry B
- ACS Omega
- Entropy

(j) Grant Reviewer for

- DOE (Condensed Phase and Interfacial Molecular Science)
- French National Research Agency
- Czech Science Foundation

(k) Grants Funded

Computation of the Phase Diagram of Aqueous Hydroxypropyl Cellulose, NSF XSede Resource Allocation CHE180030	$1,056	2018
NSF MRI CHE 1531590, Co-applicant (PI Arjan van der Vaart)	$197,469	2015
USF ORI Matching Funds Program	$12,474	2015
Generalizing Parallel Analysis of Trajectory Data, NSF XSede Resource Allocation TG-ASC130043	101,500 RU + collaborative support	2013
Department of Energy Computational Science Graduate Fellowship DE-FG02-97ER25308	∼$200,000	2006-2009