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

- Productivity and Sustainability Planning - Software Development Ecosystems Team Outreach
- 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 predictives-tatmech.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. 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*, 2021.
  2. 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.
  3. 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.
  4. 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.
  5. **David M. Rogers**. Efficient Primitives for Standard Tensor Linear Algebra. *Proc. XSEDE (ACM)*, 2016.

6. **David M. Rogers**. Real-space quadrature: a convenient, efficient representation for multipole expansions. *J. Chem. Phys.* 142:074101, 2015. *JCP Editor's choice award.*
7. 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**. *DWork*, a scalable bag of tasks implementation for work distribution on HPC. Github, 2021.
2. **David M. Rogers**. *mpi_list*, a python-mpi-spark-like library for parallel operation son distributed lists. pypi, 2021
3. 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
4. **David M. Rogers**. *Classify*, implementation of a Bayesian bitvector classification algorithm. Github, 2020.
5. **David M. Rogers**. *Launchad*, high-throughput toolkit for billion-molecule docking campaigns. code.ornl.gov, 2019.
6. **David M. Rogers**. *PMake*, a parallel make build system for running computational experiments. code.ornl.gov, 2019.
7. **David M. Rogers**. *Parallel Science*, gateway for citable, extensible, and reproducible scientific computing. parallelscience.com, 2017-2019.
8. **David M. Rogers**. *Introduction to Scientific Computing*, comprehensive online course notes. predictivestatmech.org/CompSciSpring2018, 2014-2018 (352,355 cumulative page views).
9. **David M. Rogers**. *ChemParam*, software for automated parameterization of molecular energies for CHARMM and Gromacs. Github, 2018.
10. **David M. Rogers**. *LAMMPS Plug-In*, adaptor for running LAMMPS molecular simulation engine as a workflow component. parallelscience.com/projects/md.lammps, 2017.
11. **David M. Rogers**. *PocketView*, software for displaying JSON data. GitHub, 2017.
12. **David M. Rogers**. *EwaldCorrel*, software for computing correlation functions in Fourier-space. GitHub, 2017.
13. **David M. Rogers**. *LibDAG*, software for parallel scheduling of task graphs. GitHub, 2017.
14. **David M. Rogers**. *USF-Slack*, software for fast tensor contraction using domain-specific languages. GitHub, 2016.
15. **David M. Rogers**and Olaf Lenz. *PBCTools*, VMD plug-in wrapping molecular structures. VMD Package, UIUC, IL., 2015.
16. **David M. Rogers**. *SProtoc*, code generator for writing data to the cloud. GitHub, 2015.

17. **David M. Rogers**. *RealPole*, implementation of the 'Real Space Quadrature' paper, along with a fast multipole method in Python. GitHub, 2014.
18. **David M. Rogers**. *rbtree*, C-library for binary trees. GitHub, 2013.
19. **David M. Rogers**. *cmap*, C-library for maps. GitHub, 2013.
20. **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.