Adam Rupe

adamrupe@lanl.gov

Google Scholar
GitHub
Webpage
ORCiD: 0000-0003-0105-8987

Center for Nonlinear Studies
Computational Earth Science
Computer, Computational, and Statistical Sciences
Los Alamos National Laboratory
Los Alamos NM, USA.

Research Interests

Data-driven science, nonlinear dynamics, machine learning, symbolic dynamics, computational mechanics, spontaneous self-organization and pattern formation, climate informatics, coherent structures, nonequilibrium thermodynamics and statistical mechanics, Perron-Frobenius and Koopman operators, information theory, computation theory.

Education

Ph.D., Physics, University of California Davis September 2013 – September 2020

Advisor: James P. Crutchfield

Thesis:

"*A Behavior-Driven Theory of Emergent Pattern and Structure in Complex Spatiotemporal Systems*"

B.S., Physics, University of Texas Austin May 2013

Graduated with High Honors

Special Honors in Physics

Advisor: Michael P. Marder

Thesis: "*Molecular Dynamics Simulation of Coulomb Friction in a Simple 1-D System"*

Experience

Research

Postdoctoral Research: Los Alamos National Laboratory 2020 – present

Joint appointment with Center for Nonlinear Studies, Computational Earth Science (PI – Monty Vesselinov, EES-16), and Computer, Computational, and Statistical Sciences (PI – Aric Hagberg, CCS). Theory, development, and applications of physics-based machine learning methods for complex dynamical systems and Earth systems science.

Theory and Software Lead: Project DisCo 2016 - 2020

Intel Parallel Computing Center, Academic Partner with the Intel Big Data Center at NERSC, LBNL

https://www.nersc.gov/research-and-development/data-analytics/big-data-center/

Supervisor: Prabhat, Director of the Big Data Center, NERSC, LBNL

Unsupervised discovery of coherent structures in large-scale, high-resolution climate data. Develop theory based on the Computational Mechanics framework. Develop associated software implementation in Python. Work with Intel and NERSC teams on high-performance and scaling optimizations on Cori.

DisCo YouTube channel with segmentation result videos:

https://www.youtube.com/channel/UCjf1IsmPMytVv7A1fZ3PdAQ

Project DisCo was chosen for an HPC Innovation Excellence Award:

https://www.hpcwire.com/off-the-wire/hyperion-research-announces-new-winners-of-hpc-innovation-excellence-awards/

Ph.D. Research: Complexity Sciences Center, Department of Physics, UC Davis 2014 – 2020

Advisor: James P. Crutchfield, Professor of Physics, UC Davis

Extended the theory and application of computational mechanics in spatiotemporal systems using local causal states. Developed the topological reconstruction algorithm for local causal states. Developed a theory of coherent structures in cellular automata. Investigated mathematical properties of spacetime shift spaces using local causal states. Developed a high-performance computing implementation of local causal state reconstruction in Python (Project DisCo). Made connections with Lagrangian Coherent Structures by applying local causal states to fluid flows using HPC implementation.

Graduate Student Researcher Funding: U. S. Army Research Laboratory and the U. S. Army Research Office under contract W911NF-13- 1-0390 (2015-2016) and Intel funding of Project DisCo through the Intel Parallel Computing Center at UC Davis (2016-2020).

Research Assistant: Center for Nonlinear Dynamics, Department of Physics, UT Austin 2012-2013

Advisor: Michael P. Marder, Professor of Physics, UT Austin

Computational study of semi-classical models of atomistic friction and self-healing cracks to better understand Coulomb friction from first-principles, and the associated statistical mechanics.

Teaching

Instructor on Record, Phy. 7A, Physics Department, UC Davis 2019

Associate Instructor for introductory physics for bioscience majors. Taught the first Discussion Lab (DL) each week, coordinated DL TAs, modified DL material and format for first fully online quarter due to COVID-19, wrote exam questions.

Graduate Teaching Assistant, Physics Department, UC Davis 2013 – 2015

Four quarters of introductory physics for bioscience majors, three quarters of introductory physics for science and engineering majors.

Tutor, Sanger Learning Center, UT Austin 2012-2013

Three semesters of introductory physics and calculus.

Learning Assistant, Physics Department, UT Austin 2012

Two semesters of introductory physics for non-science majors.

Internships

Computing Sciences Summer Student Program, LBNL 2016, 2017, and 2018

Spent three summers (June – September each year) as a graduate student research intern at Lawrence Berkeley National Laboratory under the supervision of Prabhat in the Data and Analytics Services Group in NERSC, working with mentor Karthik Kashinath in the same group. The first summer, 2016, we showed proof-of-concept for the ideas and algorithms that would shortly become Project DisCo as part of the NERSC-Intel Big Data Center. The following two summers were dedicated to development and deployment of Project DisCo, culminating in a technical submission accepted to the MLHPC workshop at SC'19.

Development

Fellow in Residence, NSF Institute for Pure and Applied Mathematics at UCLA, Fall 2019 Long Program on Machine Learning for Physics and the Physics of Learning 2019

https://www.ipam.ucla.edu/programs/long-programs/machine-learning-for-physics-and-the-physics-of-learning/?tab=overview

Selected as a fully funded "core" member that is hosted in residence at IPAM for the three-month duration of the Long Program. Core members are automatically admitted to all four week-long Workshops of the Long Program, as well as the opening week Tutorials. Outside of the main Workshops, core members participate in weekly seminars and working groups, as well as in-person collaborations among members. I presented a research poster for the second workshop, gave a seminar talk on my current research, and gave an introductory lecture on symbolic dynamics, measurement theory, and Kolmogorov-Sinai (metric) entropy for the Dynamical Systems Working Group.

Peer-Reviewed Publications

Journals

- A. Salova, J. Emenheiser, **A. Rupe**, J.P. Crutchfield, and R.M. D'Souza, "Koopman Operator and its Approximations for Systems with Symmetries", *Chaos: An Interdisciplinary Journal of Nonlinear Science* 29, 093128 (2019) https://doi.org/10.1063/1.5099091
- **A. Rupe**, and J.P. Crutchfield, "Local Causal States and Discrete Coherent Structures", *Chaos: An Interdisciplinary Journal of Nonlinear Science* 28:7, 075312 (2018) https://doi.org/10.1063/1.5021130

In Proceedings

- **A. Rupe**, N. Kumar, V. Epifanov, K. Kashinath, O. Pavlyk, F. Schlimbach, M. Patwary, S. Maidanov, V. Lee, Prabhat, and J. P. Crutchfield,
  "DisCo: Physics-Based Unsupervised Discovery of Coherent Structures in Spatiotemporal Systems", In 2019 IEEE/ACM Workshop on Machine Learning in High Performance Computing Environments (MLHPC), pp. 75-87. IEEE, 2019. arXiv:1909.11822 [physics.comp-ph]
- **A. Rupe**, K. Kashinath, N. Kumar, V. Lee, Prabhat, and J.P. Crutchfield,
  "Towards Unsupervised Segmentation of Extreme Weather Events",
  Brajard, J., Charantonis, A., Chen, C., & Runge, J. (Eds.). (2019). Proceedings of the 9th International Workshop on Climate Informatics: CI 2019
  (No. NCAR/TN-561+PROC). doi:10.5065/y82j-f154. arXiv:1909.07520 [physics.comp-ph]
- **A. Rupe**, J.P. Crutchfield, K. Kashinath, and Prabhat,
  "A Physics-Based Approach to Unsupervised Discovery of Coherent Structures in Spatiotemporal Systems",

Lyubchich, V., N. C. Oza, A. Rhines, and E. Szekely, eds., 2017: Proceedings of the 7th International Workshop on Climate Informatics: CI 2017. NCAR Technical Note NCAR/TN-536+PROC, 132 pp, doi:10.5065/D6222SH7. arXiv:1709.03184 [physics.flu-dyn]

Under Review

- **A. Rupe** and J.P. Crutchfield, "Spacetime Autoencoders Using Local Causal States", Submitted to AAAI Fall 2020 Symposium on Physics-Guided AI to Accelerate Scientific Discovery
- Y. Liu, E. Agee, M. E. Craig, A. M. Jurgens, **A. Rupe**, A. P. Walker, S. Besnard, J. P. Crutchfield, F. M. Hoffman, A. W. King, B. Kraft, D. Lu, K. Ogle, D. Peltier, and J. M. Warren "Understanding Ecological Memory: Plants, Communities, and Ecosystems As Information Processors", Submitted to *TRENDS in Ecology and Evolution: Opinion*
- **A. Rupe**, and J.P. Crutchfield, "Spacetime Symmetries, Invariant Sets, and Additive Sub-Dynamics of Cellular Automata", Submitted to J. Stat. Phys. arXiv:1812.11597 [cond-mat.stat-mech]

In Preparation

- **A. Rupe**, and J.P. Crutchfield, "Intrinsic Computation and Physics-Based Representation Learning for Complex Dynamical Systems"
- **A. Rupe**, and J.P. Crutchfield, "Spatiotemporal Computational Mechanics"
- **A. Rupe**, and J.P. Crutchfield, "Contamination and the Structural Semantics of Local Causal States"

Honors and Awards

Fellow in Residence, NSF Institute for Pure and Applied Mathematics at UCLA, Fall 2019 Long Program on Machine Learning for Physics and the Physics of Learning 2019

https://www.ipam.ucla.edu/programs/long-programs/machine-learning-for-physics-and-the-physics-of-learning/?tab=overview

HPC Innovation Excellence Award, Hyperion Research and HPC Users Forum 2019

https://www.hpcwire.com/off-the-wire/hyperion-research-announces-new-winners-of-hpc-innovation-excellence-awards/

AGU Outstanding Student Presentation Award 2018

https://membership.agu.org/ospawinner/345087/

Ryan Couch Memorial Travel Award, Department of Physics, UC Davis 2017

http://physics.ucdavis.edu/academics/graduate-program/list-fellowships

Distinguished College Scholar, UT Austin 2011 and 2012

https://cns.utexas.edu/honors/academic-distinction/gpa-based-honors

Abel Family Scholarship, Physics Dept., UT Austin 2011 – 2013

https://ph.utexas.edu/current-undergraduate-students/scholarships

Invited Member: Phi Kappa Phi National Honors Society 2012

Presentations

Invited Talks

- A. Rupe, K. Kashinath, N. Kumar, V. Lee, Prabhat, J.P. Crutchfield, "Towards Data-Driven Discovery of Extreme Weather Events," Dec. 2019, AGU 100 Fall Meeting, Invitation Only Session - Student Engagement to Enhance Development: Outstanding Student Presentation Award Winners from 2018 Fall Meeting, San Francisco CA.

- A. Rupe, K. Kashinath, N. Kumar, V. Lee, Prabhat, J.P. Crutchfield, “Modeling Collective Spatiotemporal Organization Using Memory-Dependent Local Dynamics,” Sep. 2019, ORNL workshop - Emerging frameworks for understanding memory in ecological systems, Oak Ridge TN.
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Talks

- A. Rupe, K. Kashinath, Nalini Kumar, Victor Lee, Prabhat, and J.P. Crutchfield, “Intrinsic Computation and Physics-Based Representation Learning for Complex Dynamical Systems”, Oct. 1 2019, Seminar Series, IPAM Long Program on Machine Learning for Physics and the Physics of Learning, Los Angeles CA.
- A. Rupe, J.P. Crutchfield, “Discovering Unknown Physics: Models, Mechanism, and the Computation-Dynamics Duality”, Jul. 26 2019, Telluride Science Research Center Workshop – Information Engines at the Frontiers of Nanoscale Thermodynamics, Telluride CO.
- A. Rupe, N. Kumar, V. Epifanov, K. Kashinath, O. Pavlyk, F. Schlimbach, M. Patwary, S. Maidanov, V. Lee, Prabhat, and J. P. Crutchfield, "Project DisCo: Physics-Based Discovery of Coherent Structures in Spatiotemporal Systems," Jul. 9 2019, NERSC Big Data Summit, Berkeley CA. https://www.nersc.gov/research-and-development/data-analytics/big-data-center/big-data-summit-2019/
- A. Rupe, K. Kashinath, N. Kumar, J.P. Crutchfield, and Prabhat, "Project DisCo: Physics-Based Discovery of Coherent Structures in Spatiotemporal Systems," Dec. 11 2018, American Geophysical Union Fall Meeting, Washington D.C.

  Awarded AGU Outstanding Student Presentation Award
- A. Rupe, and J.P. Crutchfield, “Local Causal States: A Behavior-Driven Approach to Pattern and Structure in Spacetime”, Jul. 20 2018, Telluride Science Research Center Workshop – Information Engines at the Frontiers of Nanoscale Thermodynamics, Telluride CO.
- A. Rupe, K. Kashinath, Nalini Kumar, J.P. Crutchfield, R. G. James, and Prabhat, "Project DisCo: Physics-Based Discovery of Coherent Structures in Spatiotemporal Systems," Jul. 18 2018, NERSC Big Data Summit, Berkeley CA. https://www.nersc.gov/research-and-development/data-analytics/big-data-center/big-data-summit/
- A. Rupe, J.P. Crutchfield, K. Kashinath, and Prabhat, "Discovering Coherent Structures Using Local Causal States", Nov. 19 2017, 70th Annual Meeting of the American Physical Society Division of Fluid Dynamics, Denver CO.
- A. Rupe, K.Kashinath, J.P. Crutchfield, R. G. James, and Prabhat, “Computational Mechanics for Climate”, Apr. 19 2017, Intel Big Data Center Kickoff, LBNL, Berkeley CA.
- A. Rupe, and J.P. Crutchfield, “Computational Mechanics of Coherent Structures in Spatiotemporal Systems”, Jan. 12 2017, 7th Annual Davis Math Conference, Davis CA.
- A. Rupe, and J.P. Crutchfield, “Computational Mechanics of Coherent Structures in Spatiotemporal Systems,” Jan. 5 2017, Dynamics Days, Silver Springs MD.
- A. Rupe, and J.P. Crutchfield, “Computational Mechanics of Coherent Structures in Spatiotemporal Systems,” Oct. 28 2016, Annual Meeting of the American Physical Society Far West Section, Davis CA.
- A. Rupe, and J.P. Crutchfield, “Computational Mechanics of Coherent Structures in Spatiotemporal Systems,” Oct. 12 2016, UT Austin Center for Nonlinear Dynamics Seminar, Austin TX.

Posters

- A. Rupe, K. Kashinath, Nalini Kumar, Victor Lee, Prabhat, and J.P. Crutchfield, “Intrinsic Computation and Physics-Based Representation Learning for Complex Dynamical Systems”, October 14, 2019, Workshop II: Interpretable Learning in Physical Sciences, IPAM Long Program on Machine Learning for Physics and the Physics of Learning, Los Angeles CA.
- A. Rupe, K. Kashinath, Nalini Kumar, J.P. Crutchfield, and Prabhat, “A Physics- Based Approach to Unsupervised Discovery of Coherent Structures in Spatiotemporal Systems”, May 23 2018, Intel AI Developer Conference, San Francisco CA.

- A. Rupe and J.P. Crutchfield, “Spacetime Symmetries and Additive Dynamics: The Domains of Cellular Automata”, Jan. 5 2018, Dynamics Days, Denver CO.
- A. Rupe, J.P. Crutchfield, K. Kashinath, and Prabhat, “A Physics- Based Approach to Unsupervised Discovery of Coherent Structures in Spatiotemporal Systems”, Nov. 11 2017, Intel HPC Developer Conference, Denver CO.
- A. Rupe, J.P. Crutchfield, K. Kashinath, and Prabhat, “A Physics- Based Approach to Unsupervised Discovery of Coherent Structures in Spatiotemporal Systems”, Sept. 21 2017, 7th International Workshop on Climate Informatics Hosted by NCAR, Boulder CO.
- A. Rupe, J.P. Crutchfield, K. Kashinath, and Prabhat, “Unsupervised Discovery of Coherent Structures in Spatiotemporal Systems”, Dec. 12 2016, American Geophysical Union Fall Meeting, San Francisco CA.

Academic Service

Journal Referee

Chaos: An Interdisciplinary Journal of Nonlinear Science

Nature Communications

Tutorials

Scientific Programming in Python, Complexity Sciences Center, UC Davis July 2017

https://github.com/adamrupe/Scientific-Python-Tutorials

Diversity and Inclusion

Volunteer, UC Davis Conference for Undergraduate Women in Physics January 2019

Complexity Sciences Center Group Meetings

90-minute lectures given to students and faculty at the Complexity Sciences Center at UC Davis.

- “Complexity, Emergence, and the Breakdown of the Hypothesis-Driven Scientific Paradigm”, May 6 and May 21, 2019
- "Intro to Deep Learning", Jun. 13 2018
- "Koopman Operator and (Extended) Dynamic Mode Decomposition", Mar. 7 2018
- "Intro to Symbolic Dynamics and Shift Spaces," Dec. 13 2017
- "Lagrangian Coherent Structures," Oct. 25 2017
- “Pattern Formation Theory”
  - “Part II – Amplitude Equations”, Mar. 16 2017
  - “Part I – Linear Stability”, Mar. 23 2017
- “The Case for Computation – Exploring the Duality Between Complex Dynamical Systems and Computation Theory”, Dec. 2 2015
- “The Maximum Entropy Approach to Thermodynamics: A Theory of Energy and Information”
  - “Part II – Nonequilibrium”, Dec. 17 2014
  - “Part I – Equilibrium”, Dec. 10 2014

Computational Skills

Python (numpy, numba, daal4py, mpi4py, matplotlib, scikit-learn, argparse), Jupyter, Conda, Unix, git, Distributed Computing (SLURM, daal4py, mpi4py), LaTex