Daniel O'Malley (omalled@gmail.com)

Experience

Team Leader 2022–present
Scientist 2016–present
Acting Deputy Group Leader 2023
Director's Postdoctoral Fellow 2014–2016
Postdoctoral Research Associate 2013–2014
Subsurface Flow and Transport Team,
Energy and Natural Resources Security Group,
Earth and Environmental Sciences Division,
Los Alamos National Laboratory
Co-founder & CTO 2016–present
Fill Education, LLC
Visiting Research Assistant Professor 2018–2020
Department of Computer Science and Electrical Engineering,
University of Maryland, Baltimore County
Postdoctoral Research Associate 2011–2013
Department of Earth, Atmospheric, and Planetary Sciences,
Purdue University

Education

Purdue University, West Lafayette, Indiana USA
Ph.D., Mathematics, May 2011
M.S., Mathematics, December 2006
B.S., Computer Science & Mathematics, May 2004

Honors & Awards

DOE Early Career Research Program Award (2024)

Awarded to support "the individual research programs of outstanding scientists early in their careers"

Outstanding Poster Award (2022)

Awarded at the Gordon Research Conference on Flow and Transport in Permeable Media for our poster on "Physics-informed machine learning with differentiable programming for heterogeneous underground reservoir pressure management"

R&D 100 Award (2021)

Awarded as part of the SmartTensors team. R&D Magazine honors the top 100 proven technological advances of the year. SmartTensors won in the Information Technology category and received special recognition as a market disruptor.

Outstanding Paper Award (2021)

Awarded at the IEEE High Performance Extreme Computing Conference for our paper on "Interrogating the performance of quantum annealing for the solution of steady-state subsurface flow"

Best Conference Paper Award (2021)

Awarded at the Large-Scale Scientific Computing Conference for our paper on "Boolean hierarchical Tucker networks on quantum annealers"

LAAP Award (2020)

$1,000 Los Alamos Awards Program award "in recognition of exceptional mentoring"

LANL Early Career Research Award (2019)

"designed to strengthen the Laboratory's scientific workforce by providing support to exceptional researchers during their crucial early career years"

LANL Large Team Distinguished Performance Award (2019)

"The multidisciplinary Subsurface Hydrology, Geology, and Geochemistry Science Team provided essential science through lab, field, and computer modeling contributions to characterize and assess subsurface geochemical and hydrological processes critical for decisions on how to remediate contamination at LANL."

LAAP Award (2019)

$500 Los Alamos Awards Program award "in recognition of excellence in the area of scientific publications"

LAAP Award (2018)

$500 Los Alamos Awards Program award "in recognition of outstanding publication record of first authored papers"

LAAP Award (2016)

$500 Los Alamos Awards Program award "in recognition of excellence in the area of scientific publications"

Orlob Foundation Travel Grant (2016)

All expenses paid for travel to the Second Orlob Symposium on Theoretical Hydrology

NSF/AGU Travel Grant (2015)

$2,000 to travel to the AGU Chapman Conference on highly heterogeneous aquifers

LANL Director's Postdoctoral Fellowship (2014)

Two year fellowship awarded four times a year in a fierce laboratory-wide competition

InterPore Fraunhofer Award for Young Researchers (2012)

5,000€ award from the International Society for Porous Media and funded by the Fraunhofer Institute for Industrial Mathematics (ITWM) for outstanding contributions to porous and composite materials modelling and computer simulation by a recent Ph.D. graduate

Charles C. Chappelle Fellowship (2004)

Awarded annually by Purdue University to outstanding seniors who continue their graduate studies at Purdue

Meyer E. Jerison Memorial Award in Analysis (2004)

Awarded annually by the mathematics department at Purdue University to an outstanding student in analysis

Funded Proposals

Quantum Computing and Machine Learning for Enhanced Understanding of Fracture Flow

DOE: Office of Science Basic Energy Sciences
2025-2029, $2,750,000
My role: Principal Investigator

Towards Federated Learning of a NNSA Trilabs Generative AI Model

NNSA: Advanced Simulation and Computing
2025-2026, $2,666,000 (LANL Budget)
My role: LANL Principal Investigator

Learning reduced models under extreme data conditions for design and rapid decision-making in complex systems

DOE: Office of Science Advanced Scientific Computing Research
2024-2026, $833,000 (LANL budget)
My role: LANL Principal Investigator

Large Language Models for Code

NNSA: Advanced Simulation and Computing
2024-2025, $4,000,000
My role: Principal Investigator

Emergent Flow Phenomena from Fracture Coalescence, Branching and Network Geometry

DOE: Basic Energy Sciences
2023-2025, $1,600,000
My role: Co-Principal Investigator (PI: Hari Viswanathan)

Consortium Advancing Technology for Assessment of Lost Oil & Gas Wells

DOE: Fossil Energy & Carbon Management
2023-2027, $9,000,000 (LANL budget)
My role: LANL Lead, Data Extraction Co-Lead

A Machine Learning Screening Tool for Rare Earth Elements and Critical Minerals at the Mine Scale

DOE: Fossil Energy & Carbon Management
2023-2025, $1,200,000
My role: Principal Investigator

Quantum Computing for Flow in Complex Fracture Networks

LANL: Laboratory Directed Research & Development
2022-2024, $975,000
My role: Principal Investigator

Scale-bridging for materials

NNSA: Advanced Simulation and Computing
2020-2022, $3,750,000
My role: Co-Principal Investigator (PI: Gowri Srinivasan)

Emergent Flow Phenomena from Fracture Coalescence, Branching and Network Geometry

DOE Office of Science: Basic Energy Sciences
2020-2022, $1,400,000
My role: Quantum Computing Lead (PI: Hari Viswanathan)

Accelerating Combinatorial Optimization with Noisy Analog Hardware

LANL: Laboratory Directed Research & Development
2021-2023, $945,000
My role: Co-Investigator (PI: Carleton Coffrin)

Differentiable Programming: Bridging the Gap between Numerical Models and Machine Learning Models

LANL: Laboratory Directed Research & Development
2020-2022, $436,000
My role: Principal Investigator

Machine Learning-based Well Design to Enhance Unconventional Energy Production

DOE: ARPA-E
2020-2022, $3,000,000 (+$500,000 cost share)
My role: LANL Principal Investigator

Machine Learning at the Marcellus Shale Energy and Environment Laboratory

DOE: Fossil Energy
2019-2020, $1,800,000
My role: Machine Learning Lead (PI: Hari Viswanathan)

Accelerating Brittle Fracture Simulations with Machine Learning

NNSA: Advanced Simulation and Computing
2019-2020, $400,000
My role: Principal Investigator

Reverse Annealing for Matrix Factorization

LANL: Laboratory Directed Research & Development
2019, $13,000
My role: Principal Investigator

Machine Learning-based Well Design to Enhance Unconventional Energy Production

DOE: EERE Geothermal Technologies Office
2019-2020, $500,000 (+$739,000 cost share)
My role: Co-Investigator (PI: Monty Vesslinov)

Tensor Networks: Robust Unsupervised Machine Learning for Big-Data Analytics

LANL: Laboratory Directed Research & Development
2019-2021, $4,710,000
My role: Co-Investigator

Coupling HPC with D-Wave

NNSA: Advanced Simulation and Computing
2018-2021, $1,130,000
My role: Principal Investigator

Machine Learning for Tight Rock Unconventional Reservoirs

CRADA between LANL and Chevron
2018-2020, $900,000
My role: Co-Investigator (PI: Monty Vesselinov)

Machine Learning Through Adiabatic Quantum Annealing

CRADA between LANL and Booz Allen Hamilton
2018-2020, $160,000
My role: LANL Principal Investigator

Leveraging quantum annealing to design additively manufactured products

LANL: Laboratory Directed Research & Development
2018, $50,000
My role: Principal Investigator

Implementing Grover's algorithm on an IBM quantum computer

LANL: Information Science and Technology Institute
2017-2018, $20,000
My role: Principal Investigator

Finding a needle in a haystack: Physics-constrained discrete optimization by coupling HPC and quantum annealing

LANL: Laboratory Directed Research & Development
2017-2018, $250,000
My role: Principal Investigator

Combinatorial Blind Source Separation using LANL's D-Wave 2X Ising

LANL: Laboratory Directed Research & Development
2016, $50,000
My role: Principal Investigator

Quantum uncertainty quantification for physical models using ToQ.jl

LANL: Information Science and Technology Institute
2016, $22,000
My role: Principal Investigator

Data Driven Multiscale Model Identification and Scaling via Random Renormalization Group Operators for Subsurface Transport

NSF-EAR: Hydrologic Sciences
2013-2016, $400,000
My role: Principal Author (PI: John H. Cushman)

Journal Papers

1. Kim, A., T. Kadeethum, C. Downs, H.S. Viswanathan, and **D. O'Malley**. Aerial imagery dataset of lost oil wells. *Scientific Data*. 2024. doi:10.1038/s41597-024-03820-0

2. Kadeethum, T., **D. O'Malley**, Y. Choi, H.S. Viswanthan, and H. Yoon. Progressive transfer learning for advancing machine learning-based reduced-order modeling. *Scientific Reports*. 2024. doi:10.1038/s41598-024-64778-y

3. Marcato, A., E. Guiltinan, H. Viswanathan, **D. O'Malley**, N. Lubbers, and J.E. Santos. Journey over destination: dynamic sensor placement enhances generalization. *Machine Learning: Science and Technology*. 2024. doi:10.1088/2632-2153/ad4e06

4. Henderson, J.M., J. Kath, J.K. Golden, A.G. Percus, and **D. O'Malley**. Addressing quantum's "fine print" with efficient state preparation and information extraction for quantum algorithms and geologic fracture networks. 3592. 2024. doi:10.1038/s41598-024-52759-0

5. Sweeney, M.R., J.D. Hyman, **D. O'Malley**, J.E. Santos, J.W. Carey, P.H. Stauffer, and H.S. Viswanathan. Characterizing the impacts of multi-scale heterogeneity on solute transport in fracture networks. *Geophysical Research Letters*. 50. 2023. doi:10.1029/2023GL104958

6. Santos, J.E., Z.R. Fox, A. Mohan, **D. O'Malley**, H. Viswanathan, and N. Lubbers. Development of the Senseiver for efficient field reconstruction from sparse observations. *Nature Machine Intelligence*. 5. 2023. doi:10.1038/s42256-023-00746-x

7. Santos, J.E., A. Marcato, Q. Kang, M. Mehana, **D. O'Malley**, H. Viswanathan, and N. Lubbers. Learning a general model of single phase flow in complex 3D porous media. *Machine Learning: Science and Technology*. 5. 2023. doi:10.1088/2632-2153/ad45af

8. **O'Malley, D.**, S.Y. Greer, A. Pachalieva, W. Hao, D. Harp, and V.V. Vesselinov. DPFEHM: a differentiable subsurface physics simulator. *Journal of Open Source Software*. 8. 2023. doi:10.21105/joss.04560

9. Greer, S.Y. and **D. O'Malley**. Early steps toward practical subsurface computations with quantum computing. *Frontiers in Computer Science*. 5. 2023.
doi:10.3389/fcomp.2023.1235784

10. Bello, K., D. Vikara, A. Sheriff, H. Viswanathan, T. Carr, M. Sweeney, **D. O'Malley**, M. Marquis, R.T. Vactor, and L. Cunha. Evaluation of the economic implications of varied pressure drawdown strategies generated using a real-time, rapid predictive, multi-fidelity model for unconventional oil and gas wells. *Gas Science and Engineering*. 2023
doi:10.1016/j.jgsce.2023.204972

11. Henderson, J.M., M. Podzorova, M. Cerezo, J.K. Golden, L. Gleyzer, H.S. Viswanathan, and **D. O'Malley**. Quantum algorithms for geologic fracture networks. *Scientific Reports*. 13. 2023.
doi:10.1038/s41598-023-29643-4

12. Wu, H., S.Y. Greer, and **D. O'Malley**. Physics-embedded inverse analysis with algorithmic differentiation for the earth's subsurface. *Scientific Reports*. 13. 2023.
doi:10.1038/s41598-022-26898-1

13. Mehana, M., A. Pachalieva, A. Kumar, J. Santos, **D. O'Malley**, J. Carey, M. Sharma, and H. Viswanathan. Prediction and uncertainty quantification of shale well performance using multifidelity Monte Carlo. *Journal of Natural Gas Science and Engineering*. 110. 2023. doi:10.1016/j.jgsce.2023.204877

14. Golden, J.K., **D. O'Malley**, and H.S. Viswanathan. Quantum preconditioners and hydrological linear systems. *Scientific Reports*. 12. 2023.
doi:10.1038/s41598-022-25727-9

15. Kadeethum, T., F. Ballarin, **D. O'Malley**, Y. Choi, N. Bouklas, and H. Yoon. Reduced order modeling with Barlow Twins self-supervised learning: Navigating the space between linear and nonlinear solution manifolds. *Scientific Reports*. 12. 2022.
doi:10.1038/s41598-022-24545-3

16. Kadeethum, T., **D. O'Malley**, F. Ballarin, I. Ang, J.N. Fuhg, N. Bouklas, V.L.S. Silva, P. Salinas, C.E. Heaney, C.C. Pain, S. Lee, H.S. Viswanathan, and H. Yoon. Enhancing high-fidelity nonlinear solver with reduced order model. *Scientific Reports*. 12. 2022.
doi:10.1038/s41598-022-22407-6

17. Pachalieva, A., **D. O'Malley**, D.R. Harp, and H.S. Viswanathan. Physics-informed machine learning with differentiable programming for heterogeneous underground reservoir pressure management. *Scientific Reports*. 12. 2022.
doi:10.1038/s41598-022-22832-7

18. Kadeethum, T., **D. O'Malley**, Y. Choi, H.S. Viswanathan, N. Bouklas, and H. Yoon. Continuous conditional generative adversarial networks for data-driven solutions of poroelasticity with heterogeneous material

properties. *Computers & Geosciences*. 167. 2022.
doi:j.cageo.2022.105212

19. Abhijith, J., A. Adedoyin, J. Ambrosiano, P. Anisimov, A. Baertschi, W. Casper, G. Chennupati, C. Coffrin, H. Djidjev, D. Gunter, S. Karra, N. Lemons, S. Lin, A. Malyzhenkov, D. Mascarenas, S. Mniszewski, B. Nadiga, **D. O'Malley**, D. Oyen, S. Pakin, L. Prasad, R. Roberts, P. Romero, N. Santhi, N. Sinitsyn, P.J. Swart, J.G. Wendelberger, B. Yoon, R. Zamora, W. Zhu, S. Eidenbenz, A. Bärtschi, P.J. Coles, M. Vuffray, A.Y. Lokhov. Quantum algorithm implementations for beginners. *ACM Transactions on Quantum Computing*. 2022.
doi:10.1145/3517340

20. Pelofske, E., G. Hahn, **D. O'Malley**, H.N. Djidjev, and B.S. Alexandrov. Quantum Annealing Algorithms for Boolean Tensor Networks. *Scientific Reports*. 12. 2022.
doi:10.1038/s41598-022-12611-9

21. Greer, S.Y., J.D. Hyman, and **D. O'Malley**. A comparison of linear solvers for resolving flow in three-dimensional discrete fracture networks. *Water Resources Research*. 58. 2022.
doi:10.1029/2021WR031188

22. Hao, W. **D. O'Malley**, J.K. Golden, and V.V. Vesselinov. Inverse analysis with variational autoencoders: a comparison of shallow and deep networks. *Journal of Machine Learning for Modeling and Computing*. 3:47. 2022.
doi:10.1615/JMachLearnModelComput.2022042093

23. Golden, J.K., A. Baertschi, **D. O'Malley**, and S. Eidenbenz. Fair sampling error analysis on NISQ devices. *ACM Transactions on Quantum Computing*. 3. 2022.
doi:10.1145/3510857

24. Kadeethum, T., F. Ballarin, Y. Choi, **D. O'Malley**, H. Yoon, and N. Bouklas. Non-intrusive reduced order modeling of natural convection in porous media using convolutional autoencoders: comparison with linear subspace techniques. *Advances in Water Resources*. 2022.
doi:10.1016/j.advwatres.2021.104098

25. Garcia-Cardona, C., M.G. Fernández-Godino, **D. O'Malley**, and T. Bhattacharya. Uncertainty bounds for multivariate machine learning predictions on high-strain brittle fracture. *Computational Materials Science*. 201:110883. 2022.
doi:10.1016/j.commatsci.2021.110883

26. Kadeethum, T., **D. O'Malley**, J.N. Fuhg, Y. Choi, J. Lee, H.S. Viswanathan, and N. Bouklas. A framework for data-driven solution and parameter estimation of PDEs using conditional generative adversarial networks. *Nature Computational Science*. 1:819. 2021
doi:10.1038/s43588-021-00171-3

27. Srinivasan, S., **D. O'Malley**, M.K. Maruti, M.R. Sweeney, J.D. Hyman, S. Karra, L. Frash, J.W. Carey, M.R. Gross, G.D. Guthrie, T. Carr, L. Li, and H.S. Viswanathan, A machine learning framework for rapid forecasting and history matching in unconventional reservoirs. *Scientific Reports*. 11:1. 2021
doi:10.1038/s41598-021-01023-w

28. Golden, J.K. and **D. O'Malley**. Pre- and post-processing in quantum-computational hydrologic inverse analysis. *Quantum Information Processing*. 20:176. 2021.
doi:10.1007/s11128-021-03115-y

29. Harp, D.R., **D. O'Malley**, B. Yan, and R. Pawar. On the feasibility of using physics-informed machine learning for underground reservoir pressure management. *Expert Systems with Applications*. 115006. 2021.
doi:10.1016/j.eswa.2021.115006

30. Golden, J.K., **D. O'Malley**. Reverse annealing for nonnegative/binary matrix factorization. *PLoS ONE*. 16:e0244026. 2021.
doi:10.1371/journal.pone.0244026

31. Fernández-Godino, M.G., N. Panda, **D. O'Malley**, K. Larkin, A. Hunter, R.T. Haftka, and G. Srinivasan. Accelerating High-Strain Continuum-Scale Brittle Fracture Simulations with Machine Learning. *Computational Materials Science*. 186:109959. 2021.
doi:10.1016/j.commatsci.2020.109959

32. Srinivasan, S., **D. O'Malley**, J.D. Hyman, S. Karra, H.S. Viswanathan, and G. Srinivasan. Transient flow modeling in fractured media using graphs. *Physical Review E*. 102:052310. 2020.
doi:10.1103/PhysRevE.102.052310

33. Dana, S., S. Srinivasan, S. Karra, N. Makedonska, J.D. Hyman, **D. O'Malley**, H. Viswanathan, and G. Srinivasan. Towards real-time forecasting of natural gas production by harnessing graph theory for stochastic discrete fracture networks. *Journal of Petroleum Science and Engineering*. 195:107791. 2020.
doi:10.1016/j.petrol.2020.107791

34. Sweeney, M.R., J.D. Hyman, S. Karra, N. Makedonska, **D. O'Malley**, S. Srinivasan, and H. Viswanathan. Advances in Discrete Fracture Network Modeling: A Review. *American Rock Mechanics Association Letters*. 29:35. 2020.

35. Panda, N., D. Osthus, G. Srinivasan, **D. O'Malley**, V. Chau, D. Oyen, and H. Godinez. Mesoscale informed parameter estimation through machine learning: A case-study in fracture modeling. *Journal of Computational Physics*. 109719. 2020.
doi:10.1016/j.jcp.2020.109719

36. Vesselinov, V.V., M.K. Mudunuru, S. Karra, **D. O'Malley**, and B.S. Alexandrov. Unsupervised machine learning based on non-negative tensor factorization for analyzing reactive-mixing. *Journal of Computational Physics*. 395:85. 2019.
doi:10.1016/j.jcp.2019.05.039

37. Battiato, I., P.T. Ferrero, **D. O'Malley**, C.T. Miller, P.S. Takhar, F.J. Valdés-Parada, and B.D. Wood. Theory and Applications of Macroscale Models in Porous Media. *Transport in Porous Media*. 2019.
doi:10.1007/s11242-019-01282-2

38. Vesselinov, V.V., B.S. Alexandrov, and **D. O'Malley**. Nonnegative tensor factorization for contaminant source identification. *Journal of Contaminant Hydrology*. 220:66. 2019.
doi:10.1016/j.jconhyd.2018.11.010

39. Hunter, A., B.A. Moore, M. Mudunuru, V. Chau, R. Tchoua, C. Nyshadham, S. Karra, **D. O'Malley**, E. Rougier, H. Viswanathan, and G. Srinivasan. Reduced-order modeling through machine learning and graph-theoretic approaches for brittle fracture applications. *Computational Materials Science*. 157:87. 2019.
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40. **O'Malley, D.**, V.V. Vesselinov, B.S. Alexandrov, and L.B. Alexandrov. Nonnegative/binary matrix factorization with a D-Wave quantum annealer. *PLoS ONE*. 13:e0206653. 2018.
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41. Srinivasan, S., J.D. Hyman, S. Karra, **D. O'Malley**, H. Viswanathan, and G. Srinivasan. Robust system size reduction of discrete fracture networks: a multi-fidelity method that preserves transport characteristics. *Computational Geosciences*. 22:1515. 2018.
doi:10.1007/s10596-018-9770-4

42. Viswanathan, H.S., J.D. Hyman, S. Karra, **D. O'Malley**, S. Srinivasan, A. Hagberg, and G. Srinivasan. Advancing graph-based algorithms for predicting flow and transport in fractured rock. *Water Resources Research*. 54:6085. 2018.
doi:10.1029/2017WR022368

43. Srinivasan, G., J.D. Hyman, D.A. Osthus, B.A. Moore, **D. O'Malley**, S. Karra, E. Rougier, A.A. Hagberg, A. Hunter, and H.S. Viswanathan. Quantifying topological uncertainty in fractured systems using graph theory and machine learning. *Scientific Reports*. 8:11665. 2018.
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44. **O'Malley, D.**, S. Karra, J.D. Hyman, H.S. Viswanathan, and G. Srinivasan. Efficient Monte Carlo with graph-based subsurface flow and transport models. *Water Resources Research*. 54:3758. 2018.
doi:10.1029/2017WR022073

45. Lovell, A.E., S. Srinivasan, S. Karra, **D. O'Malley**, N. Makedonska, H.S. Viswanathan, G. Srinivasan, J.W. Carey, and L.P. Frash. Extracting hydrocarbon from shale: an investigation of the factors that influence the decline and the tail of the production curve. *Water Resources Research*. 54:3748. 2018.
doi:10.1029/2017WR022180

46. Qian, E., B. Peherstorfer, **D. O'Malley**, V.V. Vesselinov, and K. Willcox. Multifidelity Monte Carlo estimation of variance and sensitivity indices. *SIAM/ASA Journal on Uncertainty Quantification*. 6:683. 2018. (**SIAM Student Paper Prize Winner**)
doi:10.1137/17M1151006

47. **O'Malley, D**. An approach to quantum-computational hydrologic inverse analysis. *Scientific Reports*. 8:6919. 2018.
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48. Karra, S., **D. O'Malley**, J.D. Hyman, H. Viswanathan, and G. Srinivasan. Modeling flow and transport in fracture networks using graphs. *Physical Review E*. 97:033304. 2018.
doi:10.1103/PhysRevE.97.033304

49. Moore, B.A., E. Rougier, **D. O'Malley**, G. Srinivasan, A. Hunter, and H. Viswanathan. Predictive modeling of dynamic fracture growth in brittle materials with machine learning. *Computational Materials Science*. 148:46. 2018.
doi:10.1016/j.commatsci.2018.01.056

50. Vesselinov, V.V., B.S. Alexandrov, and **D. O'Malley**. Contaminant source identification using semi-supervised machine learning. *Journal of Contaminant Hydrology*. 212:134. 2018.
doi:10.1016/j.jconhyd.2017.11.002

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doi:10.1002/2016WR020299

53. Bakarji, J., **D. O'Malley**, and V.V. Vesselinov. Agent-based socio-hydrological hybrid modeling for water resource management. *Water Resources Management*. 31:3881. 2017.
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56. Lin, Y., **D. O'Malley**, and V.V. Vesselinov. A computationally efficient parallel Levenberg-Marquardt algorithm for highly parameterized inverse model analyses. *Water Resources Research*. 52:6948. 2016.
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57. Throckmorton, H.M., B.D. Newman, J.M. Heikoop, G.B. Perkins, X. Feng, D.E. Graham, **D. O'Malley**, V.V. Vesselinov, J. Young, S.D. Wullschleger, and C.J. Wilson. Active layer hydrology in an Arctic tundra ecosystem: quantifying water sources and cycling using water stable isotopes. *Hydrologic Processes*. 30:26. 2016.
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58. Grasinger, M., **D. O'Malley**, V.V. Vesselinov, and S. Karra. Decision Analysis for Robust CO2 Injection: Application of Bayesian-Information-Gap Decision Theory. *International Journal of Greenhouse Gas Control*. 49:73. 2016.
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doi:10.1002/2015WR017413

61. Cushman, J.H. and **D. O'Malley**. Fickian dispersion is anomalous. *Journal of Hydrology*. 531:161. 2015.
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International Journal of Greenhouse Gas Control. 37:24. 2015.
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75. **O'Malley, D.** and J.H. Cushman. Two-scale renormalization-group classification of diffusive processes. *Physical Review E*. 86:011126. 2012.
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doi:10.1103/PhysRevE.78.052101

Conference Papers

1. Keller, C.M., S. Eidenbenz, A. Baertschi, **D. O'Malley**, J. Golden, and S. Misra. Hierarchical multigrid ansatz for variational quantum algorithms. *ISC High Performance 2024 Research Paper Proceedings (39th International Conference)*. 2024.
   doi:10.23919/ISC.2024.10528934

2. Marcato, A., **D. O'Malley**, H.S. Viswanathan, E. Guiltinan, and J.Santos. Reconstruction of fields from sparse sensing: differentiable sensor placement enhances generalization. *NeurIPS Workshop on Machine Learning and the Physics Sciences*. 2023.
   Link

3. Golden, J., A. Baertschi, **D. O'Malley**, E. Pelofske, and S. Eidenbenz. JuliQAOA: fast, flexible QAOA simulation. *Proceedings of the SC'23 Workshops of The International Conference on High Performance Computing, Network, Storage, and Analysis*. 2023.
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4. Golden, J., A. Baertschi, **D. O'Malley**, and S. Eidenbenz. Numerical evidence for exponential speed-up of QAOA over unstructured search for approximate constrained optimization. *IEEE International Conference on Quantum Computing and Engineering*. 2023.
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5. Jahan, I., M. Mehana, B. Ahmmed, J.E. Santos, **D. O'Malley**, and H.S. Viswanathan. Deep learning models for methane emissions identification and quantification. *SPE/AAPG/SEG Unconventional Resources Technology Conference*. 2023.
   doi:10.15530/urtec-2023-3866049

6. **O'Malley, D.**, J.E. Santos, and N. Lubbers. Interlingual automatic differentiation: Software 2.0 between PyTorch and Julia. *AAAI Symposium on Knowledge Guided Machine Learning*. 2022.

7. Santos, J.E., **O'Malley, D.**, M. Mehana, and H.S. Viswanathan. Upscaling microscale flow effects using differentiable programming. *CouFrac Conference*. 2022.

8. Golden, J.K., A. Baertschi, **D. O'Malley**, and S. Eidenbenz. Threshold-based quantum optimization. *IEEE International Conference on Quantum Computing and Engineering*. 2021.
   doi:10.1109/QCE52317.2021.00030

9. Pelofske, E., Golden, J.K., A. Baertschi, **D. O'Malley**, and S. Eidenbenz. Sampling on NISQ devices: "Who's the fairest one of all?". *IEEE International Conference on Quantum Computing and Engineering*. 2021.
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10. Henderson, J.M., **D. O'Malley**, and H.S. Viswanathan. Interrogating the performance of quantum annealing for the solution of steady-state

subsurface flow. *IEEE High Performance Extreme Computing*. 2021. (**Outstanding Paper Award**)

11. Pelofske, E., G. Hahn, **D. O'Malley**, H.N. Djidjev, and B.S. Alexandrov. Boolean hierarchical Tucker networks on quantum annealers. *Large-Scale Scientific Computing*. 2021. (**Best Conference Paper Award**) doi:10.1007/978-3-030-97549-4_40

12. **O'Malley, D.**, H.N. Djidjev, and B.S. Alexandrov. Tucker-1 Boolean tensor factorization with quantum annealers. *IEEE International Conference on Rebooting Computing*. 2020. doi:10.1109/ICRC2020.2020.00002

13. **O'Malley, D.** and J.K. Golden. Homomorphic encryption for quantum annealing with spin reversal transformations. *IEEE High Performance Extreme Computing*. 2020. doi:10.1109/HPEC43674.2020.9286176

14. Greer, S. and **D. O'Malley**. An approach to seismic inversion with quantum annealing. *Society of Exploration Geophysicists*. 2020. doi:10.1190/segam2020-3424413.1

15. Mudunuru, M.K., **D. O'Malley**, S. Srinivasan, J.D. Hyman, M.R. Sweeney, L. Frash, B. Carey, M.R. Gross, N.J. Welch, S. Karra, V.V. Vesselinov, Q. Kang, H. Xu, R.J. Pawar, T. Carr, L. Li, G.D. Guthrie, and H.S. Viswanathan. Physics-informed Machine Learning for Real-time Unconventional Reservoir Management. *Proceedings of the AAAI 2020 Spring Symposium on Combining Artificial Intelligence and Machine Learning with Physical Sciences*. 2020. Link

16. Fernandez-Godino, M.G., N. Panda, **D. O'Malley**, K.S. Hickmann, D.A. Oyen, R.T. Haftka, and G. Srinivasan. Flyer plate continuum simulations informed with machine learning crack evolution. *AIAA SciTech 2020 Forum*. 2020. doi:10.2514/6.2020-1410

17. Djidjev, H., **D. O'Malley**, H. Viswanathan, J.D. Hyman, S. Karra, and G. Srinivasan. Learning on graphs for predictions of fracture propagation, flow and transport. *IEEE Parallel and Distributed Symposium Workshops*. 2017. doi:10.1109/IPDPSW.2017.11

18. **O'Malley, D.** and V.V. Vesselinov. ToQ.jl: A high-level programming language for D-Wave machines based on Julia. *IEEE High Performance Extreme Computing*. 2016. doi:10.1109/HPEC.2016.7761616

19. Vesselinov, V.V, **D. O'Malley** and D. Katzman. Robust Decision Analysis for Environmental Management of Groundwater Contamination Sites. *Second International Conference on Vulnerability and Risk Analysis and Management*

(ICVRAM) and the Sixth International Symposium on Uncertainty, Modeling, and Analysis (ISUMA). 2014.
doi:10.1061/9780784413609.197

Book Chapters

1. Vesselinov, V.V., M.K. Mudunuru, B. Ahmmed, S. Karra, **D. O'Malley**. Machine Learning to Discover, Characterize, and Produce Geothermal Energy. *Machine Learning Applications in Subsurface Energy Resource Management*. S. Misra ed. 2022. ISBN 9781003207009.

2. Srinivasan, S., J.D. Hyman, **D. O'Malley**, S. Karra, H.S. Viswanathan, and G. Srinivasan. Machine learning techniques for fractured media. *Machine Learning in Geosciences*. Moseley and Krischer eds. 2020. ISBN 9780128216699.

3. **O'Malley, D.** and J.H. Cushman. Fractional Fokker-Planck equations. *Fractals: Concepts and Applications in Geosciences*. A. Hunt and B. Ghanbarian eds. 2017. ISBN 9781498748711.

4. **O'Malley, D.** and J.H. Cushman. Anomalous dispersion. *The Handbook of Groundwater Engineering*. J.H. Cushman and D.M. Tartakovsky eds. 2016. ISBN 9781498703048.

Other Publications

1. Li, Y.E., **D. O'Malley**, G. Beroza, A. Curtis, and P. Johnson. Machine learning developments and applications in solid-earth geosciences: Fad or future? *Journal of Geophysical Research: Solid Earth*. 2023.
doi:10.1029/2022JB026310

2. **O'Malley, D.**. Reconstructing Rocks with Machine Learning. *EOS*. July 2021.

3. Srinivasan, G., **D. O'Malley**, M.G. Fernandez. Scale-bridging with Machine Learning to Characterize Brittle Damage and Failure. *SIAM News*. 53:10. December 2020.

4. Curtis, A., **D. O'Malley**, G.C. Beroza, P.A. Johnson, E. Li, and E. Haber. Tackling 21st Century Geoscience Problems with Machine Learning. *Eos*. 101. October 2020.
doi:10.1029/2020EO150184

5. Dorn, M.F., **D. O'Malley**, H. Nagarajan, N. Ray, and A. Sornborger. Early Career Paths at Los Alamos National Laboratory. *Notices of the American Mathematical Society*. April 2020.

6. Lin, Y., **D. O'Malley**, V.V. Vesselinov, G.D. Guthrie, and D. Coblentz. Randomization in characterizing the subsurface. *SIAM News*. 51:1. January/February 2018.

ORAL PRESENTATIONS

1. Large Language Models for Code. LANL Information Science & Technology Capability Review (2024); Los Alamos, NM USA.
2. Large Language Models for Code. Advanced Simulation & Computing PI Meeting (2024); Los Alamos, NM USA.
3. Differentiable programming: bridging the gap between numerical models and machine learning models. Center for Nonlinear Studies (2023); Los Alamos, NM USA.
4. Differentiable programming: bridging the gap between numerical models and machine learning models. Boston University (2023); Boston, MA USA.
5. A machine learning screening tool for rare earth elements and critical minerals at the mine scale. National Energy Technology Laboratory (2023); Pittsburgh, PA USA.
6. IS&T for locating and characterizing undocumented orphan oil & gas wells. LANL Information Science & Technology Capability Pillar Review (2023); Los Alamos, NM USA.
7. Parallel differentiable programming for large-scale, sparse, distributed Jacobians. US National Congress on Computational Mechanics (2023); Albuquerque, NM USA.
8. Nonnegative/binary matrix factorization with a D-Wave quantum annealer. LANL Machine Learning Summer School (2023); Los Alamos, NM USA.
9. Subsurface Flow and Transport with Differentiable Programming and Quantum Computing. SIAM Computational Science and Engineering (2023); Amsterdam, The Netherlands.
10. Interlingual automatic differentiation: Software 2.0 between PyTorch and Julia. AAAI Symposium on Knowledge Guided Machine Learning (2022); Arlington, VA USA.
11. LANL Experimental and modeling studies to explore the feasibility of CO2-EOR/storage in unconventional reservoirs, CO2-EOR/Storage in Shales Workshop (2022); Pittsburgh, PA USA and online.
12. Differentiable programming: Bridging the gap between numerical models and machine learning models, Georgia Tech University (2022); Atlanta, Georgia USA.
13. Differentiable programming: Bridging the gap between numerical models and machine learning models, UC San Diego (2022); online.
14. Differentiable programming: Bridging the gap between numerical models and machine learning models, DOE's Fossil Energy and Carbon Management SMART Seminar (2022); online.

15. Differentiable programming: Bridging the gap between numerical models and machine learning models, US Naval Research Laboratory Machine Learning Seminar (2021); online.

16. Differentiable programming: Bridging the gap between numerical models and machine learning models, Machine Learning in Solid Earth Geoscience Lecture Series (2021); online.

17. Differentiable programming: Bridging the gap between numerical models and machine learning models, SIAM Conference on Mathematical & Computational Issues in the Geosciences (2021); online.

18. Subsurface inverse analysis with quantum annealing, Ben-Gurion University of the Negev (2021); online.

19. Differentiable programming: Bridging the gap between numerical models and machine learning models, Computational Methods in Water Resources (2020); online.

20. Adventures in quantum computing, Montana State University (2020); online.

21. Homomorphic encryption for quantum annealing with spin reversal transformations, Qubits (2020); online.

22. Homomorphic encryption for quantum annealing with spin reversal transformations, IEEE High Performance Extreme Computing Conference (2020); online.

23. Modeling flow and transport in fracture networks using machine learning and graphs, Computational Methods in Water Resources (2020); Stanford, CA USA. (conference postponed due to COVID-19)

24. Learning to regularize with a variational autoencoder for hydrologic inverse analysis, SIAM Conference on Uncertainty Quantification (2020); Munich, Germany. (conference cancelled due to COVID-19)

25. Bridging the gap between numerical models and machine learning models, Machine Learning in Solid Earth Geoscience (2020); Santa Fe, NM USA. (conference cancelled due to COVID-19)

26. Modeling flow and transport in fracture networks using machine learning and graphs, AGU Fall Meeting (2019); San Francisco, CA USA.

27. Tensor factorization with quantum annealing, AI and Tensor Factorization in Physics, Chemistry, and Biology (2019); Santa Fe, NM USA.

28. Learning to regularize with a variational autoencoder for hydrologic inverse analysis, EES-16 Science Café, Los Alamos National Laboratory (2019); Los Alamos, New Mexico USA.

29. Variations on a theme: solving linear systems with D-Wave, LANL/D-Wave Technical Exchange (2019); Los Alamos, NM USA.

30. Modeling flow and transport in fracture networks using machine learning and graphs, SIAM Conference on Mathematical & Computational Issues in the Geosciences (2019); Houston, Texas USA.

31. Decision analyses for groundwater remediation, SIAM Conference on Mathematical & Computational Issues in the Geosciences (2019); Houston, TX USA.

32. Dimensionality reduction for subsurface flow models, SIAM Conference on Computational Science & Engineering (2019); Spokane, WA USA.

33. An approach to quantum-computational hydrologic inverse analysis, AGU Fall Meeting (2018); Washington, DC USA.

34. Efficient Monte Carlo with graph-based subsurface flow and transport models, AGU Fall Meeting (2018); Washington, DC USA.

35. An approach to quantum-computational hydrologic inverse analysis, Qubits North America (2018); Knoxville, Tennessee USA.

36. Unsupervised machine learning via matrix factorization with a quantum annealer, LANL Applied Machine Learning Summer School (2018); Los Alamos, New Mexico USA.

37. Quantum-computational approach to discrete tomography for porous media, InterPore (2018); New Orleans, Louisianna USA.

38. Unsupervised machine learning based on tensor factorization, InterPore (2018); New Orleans, Louisianna USA.

39. Characterizing the subsurface with randomized matrix algorithms, Technical University of Munich (2018); Munich, Germany.

40. Quantum computational hydrology 101, Qubits Europe (2018); Munich, Germany.

41. Los Alamos National Laboratory site report, Qubits Europe (2018); Munich, Germany.

42. Hydrologic model analyses for decision support at the Los Alamos National Laboratory site, Waste Management Symposia (2018); Phoenix, Arizona USA.

43. An approach to quantum-computational hydrologic inverse analysis, NASA Goddard Space Flight Center (2018); Remotely.

44. Nonnegative/binary matrix factorization with a D-Wave quantum annealer, CHMPR Distinguished Lecture, University of Maryland (2018); Baltimore County, Maryland USA.

45. Quantum computational hydrology 101, Booz Allen Hamilton (2018); Remotely.

46. Nonnegative/binary matrix factorization with a D-Wave quantum annealer, Qubits (2017); National Harbor, Maryland USA.

47. D-Wave programming tools panel, Qubits (2017); National Harbor, Maryland USA.

48. Quantum computational hydrology 101, SIAM Conference on Mathematical & Computational Issues in the Geosciences (2017); Erlangen, Germany.

49. Uncertainty quantification with graph-based flow/transport models, SIAM Conference on Mathematical & Computational Issues in the Geosciences (2017); Erlangen, Germany.

50. Nonnegative/binary matrix factorization with a D-Wave quantum annealer, Oak Ridge National Laboratory (2017); Remotely.

51. Quantum-computational hydrology 101, EES-16 Science Café, Los Alamos National Laboratory (2017); Los Alamos, New Mexico USA.

52. Nonnegative/binary matrix factorization with a D-Wave quantum annealer, Information Science & Technology Institute, Los Alamos National Laboratory (2017); Los Alamos, New Mexico USA.

53. Experiences using LANL's D-Wave quantum annealer, EES-16 Science Café, Los Alamos National Laboratory (2017); Los Alamos, New Mexico USA.

54. LANL D-Wave quick-start guide, Information Science & Technology Institute, Los Alamos National Laboratory (2017); Los Alamos, New Mexico USA.

55. Quantum uncertainty quantification for physical models using ToQ.jl, Information Science & Technology Institute, Los Alamos National Laboratory (2016); Los Alamos, New Mexico USA.

56. Groundwater remediation using Bayesian information-gap decision theory, AGU Fall Meeting (2016); San Francisco, California USA.

57. Reduced order models for decision analysis and upscaling of aquifer heterogeneity, AGU Fall Meeting (2016); San Francisco, California USA.

58. ToQ.jl: A high-level programming language for D-Wave machines based on Julia, IEEE High Performance Extreme Computing Conference (2016); Waltham, Massachusetts USA.

59. ToQ.jl: A high-level programming language for D-Wave machines based on Julia, US Navy Space and Naval Warfare Systems Command (2016); Remotely.

60. Fickian dispersion is anomalous, Orlob Symposium on Theoretical Hydrology (2016); Davis, California USA.

61. Taming parameter unidentifiability of ill-posed inverse problems in porous media, InterPore (2016); Cincinnati, Ohio USA.

62. Robust CO_2 Injection: Application of Bayesian-Information-Gap Decision Theory, AGU Fall Meeting (2015); San Francisco, California USA.

63. Decision-oriented optimal-experimental design, AGU Fall Meeting (2015); San Francisco, California USA.

64. Fast Geostatistical Inversion using Randomized Matrix Decompositions and Sketchings for Heterogeneous Aquifer Characterization, AGU Fall Meeting (2015); San Francisco, California USA.

65. Adventures in inverse analysis: hydrogeology edition, Center for Nonlinear Studies, Los Alamos National Laboratory (2015); Los Alamos, New Mexico USA.

66. Decision-oriented optimal-experimental design, Postdoc Research Day, Los Alamos National Laboratory (2015); Los Alamos, New Mexico USA.

67. Science, uncertainty and decisions, Center for Nonlinear Studies, Los Alamos National Laboratory (2015); Los Alamos, New Mexico USA.

68. How long is this going to take & Science, uncertainty and decisions, Applied Mathematics and Statistics, Colorado School of Mines (2015); Golden, Colorado USA.

69. Science, uncertainty and decisions, Computational Earth Science Group, Earth and Environmental Sciences Division, Los Alamos National Laboratory (2015); Los Alamos, New Mexico USA.

70. Science, uncertainty and decisions. University of Colorado Denver (2015); Denver, Colorado USA.

71. Random dispersion coefficients and Tsallis entropy. Joint Mathematics Meeting (2015); San Antonio, Texas USA.

72. Decision support for groundwater remediation. University at Buffalo (2014); Buffalo, New York USA.

73. Science, uncertainty and decisions. New Mexico Institute of Mining and Technology (2014); Socorro, New Mexico USA.

74. Bayesian Information-Gap Uncertainty Quantification. The Climate Corporation (2014); San Francisco, California USA.

75. Pore-scale reactions combined with field-scale subsurface contaminant transport. Computational Methods in Water Resources XX (2014); Stuttgart, Germany.

76. Combining Bayes analysis with info-gap decision theory for environmental management. Computational Methods in Water Resources XX (2014); Stuttgart, Germany.

77. A method for identifying diffusive trajectories with stochastic models. 6th International Conference on Porous Media & Annual Meeting of the International Society for Porous media (2014); Milwaukee, Wisconsin USA.

78. Statistics applied to fracking, human-computer interaction, and groundwater remediation. Department of Mathematical Sciences, Binghamton University (2014); Binghamton, New York, USA.

79. Anomalous dispersion, Computational Earth Science Group, Earth and Environmental Sciences Division, Los Alamos National Laboratory (2013); Los Alamos, New Mexico USA.

80. The sound of diffusion, Department of Civil & Environmental Engineering & Earth Sciences, University of Notre Dame (2013); South Bend, Indiana USA.

81. Anomalous diffusion and nonstationary increments, Department of Bioengineering, University of Illinois, Chicago (2012); Chicago, Illinois USA.

82. Two scale renormalization group classification of diffusive processes, 4th International Conference on Porous Media & Annual Meeting of the International Society for Porous Media (2012); West Lafayette, Indiana USA.

83. Anomalous relaxation in diffusive processes with non-linear clocks, 4th International Conference on Porous Media & Annual Meeting of the International Society for Porous Media (2012); West Lafayette, Indiana USA.

84. Adaptive renormalization of stochastic dynamics with application to data assimilation and numerical modeling, European Geosciences Union General Assembly (2012); Vienna, Austria.

85. Fractional Brownian motion run with a non-linear clock, SIAM Conference on Mathematical & Computational Issues in the Geosciences (2011); Long Beach, California USA.

86. Diffusive processes run with non-linear clocks, INFORMS Annual Meeting (2010); Austin, Texas USA.

87. The chaotic dynamics of anomalous diffusion as modeled by a nonstationary extension of Brownian motion, SIAM Conference on Mathematical & Computational Issues in the Geosciences (2009); Leipzig, Germany.

88. Data compression and energy consumption on a wireless-networked handheld computing device, Department of Computer Science, Purdue University (2003); West Lafayette, Indiana USA.

Poster Presentations

1. Machine learning for rare earth elements and critical minerals at the mine scale. DOE Program Visit (2023); Los Alamos, NM USA.

2. Identifying and characterizing undocumented orphaned wells to mitigate methane missions and groundwater impacts. LANL Science of Signatures Capability Review (2023); Los Alamos, NM USA.

3. Physics-informed machine learning with differentiable programming for heterogeneous underground reservoir pressure management. Gordon Research Conference on Flow and Transport in Permeable Media (2022); Les Diablerets, Switzerland. (**Outstanding Poster Award Winner**)

4. An approach to quantum-computational hydrologic inverse analysis. Adiabatic Quantum Computing (2018); NASA Ames, Moffett Field, California USA.

5. Nonnegative/binary matrix factorization with a D-Wave quantum annealer. Physics Informed Machine Learning (2018); Santa Fe, New Mexico USA.

6. Quo vadis: Hydrologic inverse analyses using high-performance computing and a D-Wave quantum annealer. AGU Fall Meeting (2017); New Orleans, Louisiana USA.

7. Where does water go during hydraulic fracturing? (2016); DOE-FE-NETL Shale Collaboration Meeting, Los Alamos, New Mexico USA.

8. Stochastic inverse tomography of highly heterogeneous aquifers. AGU Chapman Conference (2015); Valencia Spain.

9. Decision-oriented optimal-experimental design, Postdoc Research Day, Los Alamos National Laboratory (2015); Los Alamos, New Mexico USA.

10. Bayesian Information-Gap (BIG) Decision Analysis Applied to a Geologic CO_2 Sequestration Problem. AGU Fall Meeting (2014); San Francisco, California USA.

11. Random dispersion coefficients and Tsallis entropy. AGU Fall Meeting (2014); San Francisco, California USA.

12. A Social Dynamics Dependent Water Supply Well Contamination Model. LANL Student Symposium (2014); Los Alamos National Laboratory, Los Alamos, New Mexico USA. (**Outstanding Student Poster Award Winner**)

13. Residual Analysis and Optimization of Well Pressure Data for Interpretation of Aquifer Tests. LANL Student Symposium (2014); Los Alamos National Laboratory, Los Alamos, New Mexico USA.

14. A combined probabilistic/non-probabilistic decision analysis for contaminant remediation. Postdoc Research Day (2014); Los Alamos National Laboratory, Los Alamos, New Mexico USA.

15. Information Gap Decision Theory for Monitoring Network Design. Computational Methods in Water Resources XX (2014); Stuttgart, Germany.

16. Groundwater remediation using the information gap decision theory. Conference on Data Analysis (2014); Santa Fe, New Mexico USA.

17. What matters when and where for anomalous dispersion/diffusion, AGU Fall Meeting (2013); San Francisco, California USA.

18. Two-scale renormalization group classification of stochastic processes in geophysics, AGU Fall Meeting (2012); San Francisco, California USA.

19. A geostatistical tool for stochastic processes with nonstationary increments, AGU Fall Meeting (2012); San Francisco, California USA.

Reports

1. D'Elia, M., H. Deng, C. Fraces, K. Garikipati, L. Graham-Brady, A. Howard, G. Karniadakis, V. Keshavarzzadeh, R.M. Kirby, N. Kutz, C. Li, X. Liu, H. Lu, P. Newell, **D. O'Malley**, M. Prodanovic, G. Srinivasan, A. Tartakovsky, D.M. Tartakovsky, H. Tchelepi, B. Vazic, H. Viswanathan, H. Yoon, P. Zarzycki. Machine learning in heterogeneous porous materials. Report from the National Academies AmeriMech Symposium Series. arXiv:2202.04137.
2. Quantum Computing CRADA Year 1 Report. CRADA between LANL and Booz Allen Hamilton. 2018.
3. Compendium of Technical Reports Related to the Deep Groundwater Investigation for the RDX Project at Los Alamos National Laboratory, LA-UR-18-21326, EP2018-0006, 2018.
4. Compendium of Technical Reports Conducted Under the Work Plan for Chromium Plume Center Characterization, LA-UR-18-21450, EP2018-0026, 2018.
5. Model-Assisted Decision Analyses Related to the Chromium Plume at LANL. 2016.
6. Interim Measures Work Plan for the Chromium Plume Control. 2015.
7. Completion Report for Groundwater Extraction Well CrEX-1. ESHID-600170-02. 2014.
8. Interim Measures Report for Source-Removal Testing at Well CdV-16-4ip. ERID-262526. 2014.
9. Interim Measures Work Plan For Source Removal Testing at Well CdV-16-4ip. ERID-239235. 2013.
10. Interim Measures Work Plan For The Evaluation of Chromium Mass Removal. ERID-241096, 2013.
11. Summary Report for the 2013 Chromium Groundwater Aquifer Tests at R-42, R-28, and SCI-2. ERID-255110. 2013.

Engagement and Service

Mentor

Postdocs mentored: Harun Ur Rashid (current postdoc), Agnese Marcato (current postdoc), Aleksandra Pachalieva (LANL staff), Wu Hao (Cella Mineral Storage), Bulbul Ahmmed (LANL staff), Adam Rupe (PNNL), John Golden (LANL staff)

Students working with me have published numerous papers. This has resulted in multiple awards including an Oustanding Paper Award from IEEE HPEC (Jessie Henderson), the Student Paper Prize from SIAM (Elizabeth Qian), an Outstanding Poster Award at the Gordon Research Conference on Flow and Transport in Permeable Media (Aleksandra Pachalieva), and an Outstanding Student Poster Award at the LANL Student Symposium (Joseph Bakarji).

Educator

EdTech co-founder and CTO

Fill Education
Developed and implemented a product to "fill" learning gaps. Key features of the product include: 1) an easy-to-use, teacher-facing quiz editor with advanced functionality such as image uploading, a point-and-click equation editor, and a LaTeX equaiton editor; 2) Student-facing software for taking quizzes; and 3) Software that intergrates students' quiz results with their schedules to find an opportunity for additional instruction if needed (i.e., if they have failed the quiz)

Primary Instructor

Department of Mathematics,
Purdue University
Taught an introductory algebra class to college freshman. Was the sole instructor for the course.

Teaching Assistant

Department of Mathematics,
Purdue University
Conducted recitation sessions for a variety of Calculus courses. Wrote and graded quizzes.

Artificial Intelligence Council 2024–present
Los Alamos National Laboratory
The goals of the AI Council are to (1) help the Lab wisely navigate the new era of AI, (2) garner support for new institutional investments, (3) build deeper partnerships with industry and academia, and (4) act as AI ambassadors for the rest of the Lab.

GUIDE Member 2020–2022
Geoscientists United for Inclusion, Diversity, and Equity,
Earth and Environmental Sciences Los Alamos National Laboratory
Our mission is to work with the Earth and Environmental Sciences (EES) Division Office, management, and staff to promote diversity, equity, and inclusion and to support the development of a multicultural workforce that attracts and retains the most qualified people at EES. GUIDE seeks to provide resources to EES employees to help them create a more inclusive, diverse, and equitable workplace.

Science Advisory Council Member 2018–2021
Information Science & Technology Institute,
Los Alamos National Laboratory
Advise the institute's leadership with respect to scientific directions as well as the selection of new and assessment of existing institutional activities.

Guest Editor 2020–2022
Special collection on "Machine learning for Solid Earth observation, modeling and understanding"
Journal of Geophysical Research: Solid Earth

Make acceptance/rejection recommendations for manuscripts, identify reviewers, and coordinate the review process.

Assistant Editor 2012–2016

InterPore Newsletter,
International Society for Porous Media
Edit and compose text for the newsletter. Recruit others to compose text for the newsletter.

Organizer

Organizing Committee, Machine Learning in Solid Earth Geoscience Conference, 2019-2025
Session Organizer, European Community on Computational Methods in Applied Sciences, 2024
Session Organizer, U.S National Congress on Computational Mechanics, 2023
Session Organizer, SIAM Conference on Computational Science and Engineering, 2023
Program Committee, IEEE Conference on Quantum Computing and Engineering, 2023
Session Organizer, International Association for Mathematical Geosciences, 2022
Workshop Organizer, American Rock Mechanics Association 2022
Session Organizer, SIAM Conference on Mathematical & Computational Issues in the Geosciences, 2018, 2021
Program Committee, First International Workshop on Architectures and Paradigms for Engineering Quantum Software, 2020
Program Committee, Workshop on Quantum Technology and Optimization, 2018
Session Organizer, AGU Fall Meeting, 2014-2017
Session Organizer, Interpore, 2016

Reviewer

Advances in Water Resources
DOE Office of Science
Energy & Fuels
Geophysical Research Letters
Journal of Applied Physics
Journal of Computational Physics
Journal of Contaminant Hydrology
LANL Laboratory Directed Research & Development
Nature Computational Materials
Nature Scientific Reports
Nature Sustainability
Physical Review Letters
Physical Review E
Quantum Information Processing
SIAM Journal on Scientific Computing
SIAM/ASA Journal on Uncertainty Quantification
Stochastic Environmental Research and Risk Assessment
Transport in Porous Media
Water Resources Research

Programmer Summer 2008
Google Summer of Code
Center for the Study of Complex Systems,
University of Michigan
Developed agent-based models for the Scientific Paper with Open Communication project. Funded by Google.

Skills

Expertise: Applied mathematics, Computational science, Machine learning, Multiphysics simulation, Quantum Computing, Subsurface flow and transport

Programming Languages: Julia (expert), C/C++, Java, Python, Scheme

Contact Information

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