

CONTACT INFORMATION	Department of Mathematics 4410 William E. Kirwan Hall University of Maryland, College Park	Email: deepray@umd.edu Website: deepray.github.io Phone: (301) 405-2054
RESEARCH INTERESTS	Scientific machine learning • Numerical methods for conservation laws • Uncertainty quantification • Bayesian inference.	
EMPLOYMENT HISTORY	Assistant Professor Joint appointment at the <i>Department of Mathematics</i> and <i>Institute for Physical Science & Technology, University of Maryland, College Park</i>	January 2023 - present
	Postdoctoral Research Associate <i>Aerospace and Mechanical Engineering, University of Southern California (USC), Los Angeles</i> Developed machine learning tools for uncertainty quantification; investigated strategies to embed physical constraints in DL-based prediction models.	July 2020 - December 2022
	Postdoctoral Research Associate <i>Computational and Applied Mathematics, Rice University, Houston</i> Developed high-resolution numerical methods to simulate multiphase flows through real rock structures at the pore scale.	July 2019 – June 2020
	Postdoctoral Researcher <i>Computational Mathematics and Simulation Science, EPFL, Switzerland</i> Developed deep learning strategies to resolve computational bottlenecks in numerical methods for PDEs.	July 2017 – June 2019
EDUCATION	Ph.D., Mathematics <i>Tata Institute of Fundamental Research - Center For Applicable Mathematics (TIFR-CAM), Bangalore, India</i> Dissertation: Entropy-stable finite difference and finite volume schemes for compressible flows Advisors: Praveen Chandrashekar (TIFR-CAM) and Siddhartha Mishra (ETH Zürich). <i>Awarded the Harish Chandra Memorial Award for the best Ph.D. thesis.</i>	May 2017
	M.Sc. in Mathematics <i>TIFR-CAM, Bangalore, India</i>	May 2012
	B.Sc (Honours) in Mathematics Hindu College, University of Delhi, India	June 2010
PUBLICATIONS	Journals:	
	20. The efficacy and generalizability of conditional GANs for posterior inference in physics-based inverse problems. D. Ray, H. Ramaswamy, D. Patel, A. A. Oberai. <i>Numerical Algebra, Control and Optimization</i> , 2022.	
	19. Fourier Collocation and Reduced Basis Methods for Fast Modeling of Compressible Flows. J. Yu, D. Ray, J. S. Hesthaven. <i>Communications in Computational Physics</i> , 32 (3), 595-637, 2022.	
	18. Solution of Physics-based Bayesian Inverse Problems with Deep Generative Priors. D. Patel, D. Ray, A. A. Oberai. <i>Computer Methods in Applied Mechanics and Engineering</i> , Vol. 400, 2022.	

17. Probabilistic Medical Image Imputation via Deep Adversarial Learning.
R. Raad, D. Patel, C.-C. Hsu, V. Kothapalli, D. Ray, B. Varghese, D. Hwang, I. Gill, V. Duddalwar, A. A. Oberai. *Engineering with Computers*, 2022
16. On the approximation of rough functions with deep neural networks.
T. De Ryck, S. Mishra, D. Ray. *SeMA Journal*, 2022.
15. A pressure-correction and bound-preserving discretization of the phase-field method for variable density two-phase flows.
C. Liu, D. Ray, C. Thiele, L. Lin, B. Riviere. *Journal of Computational Physics*, Vol. 449, 2022.
14. A discontinuous Galerkin method for a diffuse-interface model of immiscible two-phase flows with soluble surfactant.
D. Ray, C. Liu, B. Riviere. *Computational Geosciences*, 2021.
13. Controlling oscillations in spectral methods by local artificial viscosity governed by neural networks.
L. Schwander, D. Ray, J.S. Hesthaven. *Journal of Computational Physics*, Vol. 431, 2021.
12. Multi-level Monte Carlo finite difference methods for fractional conservation laws with random data.
U. Koley, D. Ray, T. Sarkar. *SIAM/ASA Journal on Uncertainty Quantification*, Vol. 9(1), 2021.
11. Iterative Surrogate Model Optimization (ISMO): An active learning algorithm for PDE constrained optimization with deep neural networks.
K. O. Lye, S. Mishra, D. Ray, P. Chandrashekar. *Computer Methods in Applied Mechanics and Engineering*, Vol. 374, 2021.
10. Deep learning observables in computational fluid dynamics.
K. O. Lye, S. Mishra, D. Ray. *Journal of Computational Physics*, Vol. 410, 2020.
9. Constraint-Aware Neural Networks for Riemann Problems.
J. Magiera, D. Ray, J. S. Hesthaven, C. Rohde. *Journal of Computational Physics*, Vol. 409, 2020.
8. Controlling oscillations in high-order Discontinuous Galerkin schemes using artificial viscosity tuned by neural networks.
N. Discacciati, J. S. Hesthaven, D. Ray. *Journal of Computational Physics*, Vol. 409, 2020.
7. Detecting troubled-cells on two-dimensional unstructured grids using a neural network.
D. Ray, J. S. Hesthaven. *Journal of Computational Physics*, Vol. 384, 2019.
6. Non-intrusive reduced order modelling of unsteady flows using artificial neural networks with application to a combustion problem.
Q. Wang, J. S. Hesthaven, D. Ray. *Journal of Computational Physics*, Vol. 384, 2019.
5. An artificial neural network as a troubled-cell indicator.
D. Ray, J. S. Hesthaven. *Journal of Computational Physics*, Vol. 367(15), 2018.
4. An entropy stable finite volume scheme for the two dimensional Navier-Stokes equations on triangular grids.
D. Ray, P. Chandrashekar. *Applied Mathematics and Computation*, Vol. 314, 2017.
3. Convergence of fully discrete schemes for diffusive-dispersive conservation laws with discontinuous flux.
U. Koley, R. Dutta, D. Ray. *ESAIM: Mathematical Modelling and Numerical Analysis*, Vol. 50(5), 2016.

2. Entropy stable schemes on two-dimensional unstructured grids for Euler equations.
D. Ray, P. Chandrashekar, U. S. Fjordholm, S. Mishra. *Communications in Computational Physics*, Vol. 19(5), 2016.
1. A sign preserving WENO reconstruction method.
U. S. Fjordholm, D. Ray. *Journal of Scientific Computing*, Vol. 68(1), 2015.

Conference Proceedings:

4. Bayesian Inference in Physics-Driven Problems with Adversarial Priors.
D. Patel, D. Ray, H. Ramaswamy, A. A. Oberai. *NeurIPS Workshop on Deep Learning and Inverse Problems*, 2020.
3. A Third-Order Entropy Stable Scheme for the Compressible Euler Equations.
D. Ray. *Theory, Numerics and Applications of Hyperbolic Problems II. HYP 2016. Springer Proceedings in Mathematics and Statistics*, Vol. 237, 2018.
2. Entropy stable schemes for compressible Euler equations.
D. Ray, P. Chandrashekar. *Int. J. Numer. Anal. Model. Ser. B*, no. 4, 2013.
1. Kinetic energy preserving and entropy stable finite volume schemes for compressible Euler and Navier-Stokes equations.
D. Ray, P. Chandrashekar. *14th Annual CFD Symposium - Aeronautical Society of India, IISc, Bangalore, 10-11 August, 2012*.

Preprints and submissions

2. Variationally Mimetic Operator Networks. (*preprint*, 2022)
D. Patel, D. Ray, M. R. A. Abdelmalik, T. J. R. Hughes, A. A. Oberai.
1. Probabilistic Brain Extraction in MR Images via Conditional Generative Adversarial Networks. (*submitted*, 2022)
S. Moazami, D. Ray, D. Pelletier, A. A. Oberai.

TEACHING EXPERIENCE

Instructor/co-instructor:

- AME-508: Course on Machine Learning and Computational Physics, at USC (August - December, 2022)
- AME-508: Course on Machine Learning and Computational Physics, at USC (August - December, 2021)
- MATH-459: Graduate course on Numerical Methods for Conservation Laws, at EPFL (September - December, 2020)
- Mini-course on the Application and Implementation of Deep Learning, at TIFR-CAM (January, 2019).
- Workshop on Inverse Problems and Related Topics, at ICTS Bangalore (October 2021).

Course development:

- AME-599 (special topics): Course on Machine Learning and Computational Physics, at USC (August - December, 2020)

Teaching assistant:

- MATH-459: Graduate course on Numerical Methods for Conservation Laws, at EPFL (September - December, 2018)
- MATH-459: Graduate course on Numerical Methods for Conservation Laws, at EPFL (September - December, 2017)

- Graduate course on Computational Partial Differential Equations, at TIFR-CAM (January - May, 2015)
- Graduate course on Numerical Analysis, at TIFR-CAM (August - December, 2013)
- Graduate course on Numerical Analysis, at TIFR-CAM (August - December, 2012)

MENTORING
EXPERIENCE

Master thesis co-supervision:

Niccolò Discacciati	EPFL/Politecnico di Milano	2018
Andrea Romani	EPFL/Politecnico di Milano	2019
Lukas Schwander	ETH	2019
Tim De Ryck	ETH	2019

Bachelors thesis co-supervision:

Moritz Reinders	ETH	2019
-----------------	-----	------

Undergraduate project co-supervision:

- Data-driven predictions for COVID-19 severity. USC, 2021.
- Data-driven predictions for bladder cancer recurrence. USC, 2021.
- Senior mentor for the Center for Undergraduate Research in Viterbi Engineering (CURVE) program. USC, 2021.

PROFESSIONAL
SERVICE &
OUTREACH

- Served as external expert for the oral exam of a Master's project at EPFL (July 2021).
- Session chair and organizer for the minisymposium *Advances in data-enhanced predictive modeling in simulation science* at SIAM-CSE, 2021.
- Judged at the Science and Engineering Fair of Houston (February 2021).
- Judged at the Science and Engineering Fair of Houston (February 2020).
- Led an interactive session on applied mathematics for high-school students visiting Rice University (July 2019).
- Led an initiative to systematically overhaul the waste management and recycling system at TIFR-CAM (2013-14).
- Organised numerical sessions for optimal control at the IFCAM Summer School on Numerics and Control of PDEs-2013, at the Indian Institute of Science, Bangalore.
- Organiser of the Students Seminar Series at TIFR-CAM (2012-13). The purpose of this committee was to organise and oversee talks by motivated students, on mathematical or other science oriented topics.
- General Secretary of the mathematics society ALPHA at Hindu College (2008-09).
- Founding member of *Science Forum* at Hindu College (2008-10).
- Founding member of the model UN society *Caucus* at Hindu College (2009-10).

TALKS AND
POSTERS

- A variationally mimetic operator network (16th November, 2022)
CMX Seminar, Caltech.
- Conditional GANs and their generalizability in physics-based inverse problems (18th August, 2022)
USACM Thematic Conference UQ-MLIP, Arlington, Virginia.
- Deep leaning-based posterior inference for inverse problems (28th April, 2022)
Conference on PDE and numerical analysis, TIFR-CAM, Bangalore.
- A data-driven approach to predict artificial viscosity in high-order solvers (27th March, 2022)
AMS Spring Central Sectional Meeting.

- Deep learning-based posterior inference for inverse problems (26th March, 2022)
Annual Math Symposium, IISER Bhopal.
- Deep learning-based enhancements in computational physics (10th Dec, 2021)
Seminar talk, Department of Artificial Intelligence, IIT Hyderabad.
- Bayesian inference using generative adversarial networks (7th Dec, 2021)
87th Annual Conference of the Indian Mathematical Society, Aurangabad, India.
- Deep learning-based enhancements in computational physics (29th Nov, 2021)
Seminar talk, Department of Mathematics and Statistics, Auburn University.
- Solving physics-based inverse problems using generative adversarial networks (8th Oct, 2021)
Seminar talk, Department of Mathematics and Statistics, UNC Charlotte.
- Discontinuous Galerkin discretization of phase-field models for pore-scale flows (24th June, 2021)
SIAM-GS 2021, Milan, Italy.
- A data-driven approach to predict artificial viscosity in high-order solvers (14th May, 2021)
Department of Mathematics, University of Würzburg, Germany.
- A Deep Learning Framework for p-adaptation (5th March, 2021)
SIAM-CSE 2021, Fort Worth, Texas.
- Poster: Bayesian Inference in Physics-Driven Problems with Adversarial Priors (11th Dec, 2020)
NeurIPS 2020 Workshop on Deep Learning and Inverse Problems.
- Data-driven enhancements of numerical methods. (2nd March, 2020)
Colloquium Talk, Department of Mathematical Sciences, Michigan Technological University.
- Deep learning enhancements of numerical methods (12th Feb, 2020)
Colloquium Talk, Department of Mathematics, University of Florida.
- Deep learning enhancements of numerical methods (9th Sep, 2019)
CAAM Colloquium, Rice University, Houston, Texas.
- Using deep learning to overcome algorithmic bottlenecks (18th June, 2019)
Invited speaker at NumHyp 2019, Malaga.
- Detecting discontinuities using deep learning (12th April, 2019)
Deep Learning Meetup, Zürich, Switzerland.
- Controlling oscillations in high-order accurate methods through artificial neural networks (28th Feb, 2019)
SIAM-CSE 2019, Spokane, Washington.
- A fully-discrete kinetic energy preserving and entropy conservative scheme for compressible flows (27th Feb, 2019)
SIAM-CSE 2019, Spokane, Washington.
- Controlling spurious oscillations in high-order methods through deep neural networks (9th Jan, 2019)
TIFR-CAM Colloquium, Bangalore, India.
- Controlling spurious oscillations in high-order methods through deep neural networks (15th Nov, 2018)
High-Fidelity Industrial LES/DNS symposium, Brussels, Belgium.
- An artificial neural network as a troubled-cell indicator (10th July, 2018)
SIAM Annual Meeting 2018, Portland, Oregon.
- Using neural nets to detect discontinuities (19th June, 2018)
MATHICSE Retreat, St. Croix, Switzerland.

- An artificial neural network for detecting discontinuities (11th March, 2018)
7th International Conference on High Performance Scientific Computing, Hanoi, Vietnam.
- An artificial neural network for detecting discontinuities (3rd Jan, 2018)
TIFR-CAM Colloquium, Bangalore, India.
- A high-resolution energy preserving method for the rotating shallow water equation (27th Sep, 2017)
European Conference on Numerical Mathematics and Advanced Applications, Voss, Norway.
- A third order entropy stable scheme for the compressible Euler equations (4th Aug, 2016)
XVI International Conference on Hyperbolic Problems (HYP2016), Aachen, Germany.
- A sign preserving WENO reconstruction (23rd Nov, 2015)
Department of Mathematics, University of Würzburg, Germany.
- A sign preserving WENO reconstruction (14th Aug, 2015)
International Conference on Industrial and Applied Mathematics, Beijing, China.
- A sign preserving WENO reconstruction (11th June, 2015)
Department of Applied Mathematics, University of Washington, Seattle, Washington.
- Entropy stable schemes for compressible flows on unstructured meshes (20th Dec, 2014)
Conference on Computational PDEs, Finite Element Meet, TIFR-CAM, Bangalore, India.
- Entropy stable schemes for compressible flows on unstructured meshes (9th Nov, 2014)
The 5th International Conference on Scientific Computing and Partial Differential Equations, HKBU, Hong Kong.
- Poster: Entropy stable schemes for compressible flows on unstructured meshes (9th Sep, 2014)
Analysis and Numerical Approximation of PDEs, ETH Zürich, Switzerland.

REVIEW FOR
JOURNALS

Computer Methods in Applied Mechanics and Engineering • Journal of Computational Physics • SIAM Journal on Numerical Analysis • SIAM Journal on Scientific Computing • Communications in Computational Physics • Journal of Scientific Computing • Proceedings of the Royal Society A • Computers & Fluids • SN Partial Differential Equations and Applications • Combustion Theory and Modelling • Boundary Value Problems • Communications in Nonlinear Science and Numerical Simulation • Applied Numerical Mathematics • Numerical Algorithms • BIT Numerical Mathematics • Indian Journal of Pure and Applied Mathematics.

WORKSHOPS &
VISITS

- Academic Industry Modelling Week, University of Zürich (9th-13th November, 2015)
- Workshop on the Analysis and Numerical Approximation of PDEs, ETH Zürich (8th - 10th September, 2014)
- CIME-CIRM Workshop on Mathematical Models and Methods for Living Systems, Levico Terme, Italy (1st - 5th September, 2014)
- Workshop on Optimization with PDE constraints, TIFR-CAM (25th November - 6th December, 2013)
- Compact course on Discontinuous Galerkin method for time-dependent convection-dominant PDEs, by Prof. Chi-Wang Shu, TIFR-CAM (4th - 5th July, 2013)
- IFCAM Summer School on Numerics and Control of PDEs, IISc, Bangalore (22nd July - 2nd August, 2013)
- CIMPA Summer Research School on Current Trends in Computational Methods for PDEs, IISc, Bangalore (24th June - 19th July, 2013)
- Workshop on Theoretical and Computational Aspects of Nonlinear Waves, NPDE-TCA, IIT-Bombay (27th - 31st May, 2013)

- Advanced Workshop on Non-Standard Finite Element Methods, NPDE-TCA, IIT Bombay (11th - 15th February, 2013)
- Data Assimilation Research Program, TIFR-CAM (4th - 23rd July, 2011)
- Visiting Students' Research Programme, TIFR Mumbai (15th June - 10th July, 2009)

COMPUTING
SKILLS

Languages: Python, C++, Fortran
Programming Software: MATLAB
Visualisation Software: Paraview, Gnuplot, VisIt, Paraview, Gmsh
Machine-Learning Software: TensorFlow, PyTorch