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| CONTACT INFORMATION | 4410, William E. Kirwan Hall 4176 Campus Drive 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 deep learning-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 |
| JOURNAL PUBLICATIONS | Bayesian inference using generative machine learning: <ol style="list-style-type: none"> 1. A dimension-reduced variational approach for solving physics-based inverse problems using generative adversarial network priors and normalizing flows. A. Dasgupta, D. V. Patel, D. Ray, E. A. Johnson, A. A. Oberai. <i>Computer Methods in Applied Mechanics and Engineering</i>, Vol. 420, 2024. 2. Conditional generative learning for medical image imputation. R. Raad, D. Ray, B. Varghese, D. Hwang, I. Gill, V. Duddalwar, A. A. Oberai. <i>Nature Scientific Reports</i> 14, 171, 2024. 3. The efficacy and generalizability of conditional GANs for posterior inference in physics-based inverse problems. | |

- D. Ray, H. Ramaswamy, D. Patel, A. A. Oberai. *Numerical Algebra, Control and Optimization, Vol. 14(1), 160-189, 2024.*
4. Probabilistic Brain Extraction in MR Images via Conditional Generative Adversarial Networks.
S. Moazami, D. Ray, D. Pelletier, A. A. Oberai. *IEEE Transactions on Medical Imaging, 43(3), 1071-1088, 2024.*
 5. Solution of physics-based inverse problems using conditional generative adversarial networks with full gradient penalty.
D. Ray, J. Murgoitio-Esandi, A. Dasgupta, A. A. Oberai. *Computer Methods in Applied Mechanics and Engineering, Vol. 417, 2023.*
 6. Solution of Physics-based Bayesian Inverse Problems with Deep Generative Priors.
D. Patel, D. Ray, A. A. Oberai. *Computer Methods in Applied Mechanics and Engineering, Vol. 400, 2022.*
 7. 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, 38, 3975–3986, 2022*

Learning surrogates and reduced order models:

8. Variationally Mimetic Operator Networks.
D. Patel, D. Ray, M. R. A. Abdelmalik, T. J. R. Hughes, A. A. Oberai. *Computer Methods in Applied Mechanics and Engineering, Vol. 419, 2024.*
9. Fourier Collocation and Reduced Basis Methods for Fast Modeling of Compressible Flows.
J. Yu, D. Ray, J. S. Hesthaven. *Communications in Computational Physics, 32 (3), 595-637, 2022.*
10. 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.*
11. Deep learning observables in computational fluid dynamics.
K. O. Lye, S. Mishra, D. Ray. *Journal of Computational Physics, Vol. 410, 2020.*
12. 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.*

Deep learning-guided shock capturing for high-order algorithms:

13. On the approximation of rough functions with deep neural networks.
T. De Ryck, S. Mishra, D. Ray. *SeMA Journal, 79, 399–440, 2022.*
14. 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.*
15. 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.*
16. Constraint-Aware Neural Networks for Riemann Problems.
J. Magiera, D. Ray, J. S. Hesthaven, C. Rohde. *Journal of Computational Physics, Vol. 409, 2020.*

17. Detecting troubled-cells on two-dimensional unstructured grids using a neural network.
D. Ray, J. S. Hesthaven. *Journal of Computational Physics*, Vol. 384, 2019.
18. An artificial neural network as a troubled-cell indicator.
D. Ray, J. S. Hesthaven. *Journal of Computational Physics*, Vol. 367(15), 2018.

High-order solvers for conservation laws:

19. 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.
20. 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.
21. 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.
22. 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.
23. A sign preserving WENO reconstruction method.
U. S. Fjordholm, D. Ray. *Journal of Scientific Computing*, Vol. 68(1), 2015.

Multi-phase flow through porous structures:

24. 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.
25. 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*, 25, 1775–1792, 2021.

CONFERENCE PROCEEDINGS & WORKSHOPS

1. Conditional score-based generative models for solving physics-based inverse problems.
A. Dasgupta, J. Murgioito-Esandi, D. Ray, A. A. Oberai.
NeurIPS Workshop on Deep Learning and Inverse Problems, 2023.
2. GAN-Flow: A dimension-reduced variational framework for physics-based inverse problems.
A. Dasgupta, D. Patel, D. Ray, E. Johnson, A. A. Oberai.
NeurIPS Workshop on Machine Learning and the Physical Sciences, 2022.
3. Efficient posterior inference & generalization in physics-based Bayesian inference with conditional GANs.
D. Ray, D. Patel, H. Ramaswamy, A. A. Oberai.
NeurIPS Workshop on Deep Learning and Inverse Problems, 2021.
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.

5. 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.*
6. Entropy stable schemes for compressible Euler equations.
D. Ray, P. Chandrashekar. *Int. J. Numer. Anal. Model. Ser. B, no. 4, 2013.*
7. 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
1. Generative Algorithms for Fusion of Physics-Based Wildfire Spread Models with Satellite Data for Initializing Wildfire Forecasts.
B. Shaddy, D. Ray, A. Farguell, V. Calaza, J. Mandel, J. Haley, K. Hilburn, D. V. Mallia, A. Kochanski, A. Oberai. *Submitted 2023.*
 2. Lecture notes on Deep Learning and Computational Physics.
D. Ray, O. Pinti, A. A. Oberai. *Preprint 2023.*
 3. Learning end-to-end inversion of circular Radon transforms in the partial radial setup.
D. Ray, S. Roy. *Submitted 2023.*

TEACHING
EXPERIENCE

Instructor:

- AMSC-460: Undergraduate course on Computational Methods, at UMD (Spring 2024)
- STAT-426: Undergraduate course on Introduction to Data Science and Machine Learning, at UMD (Fall 2023)
- AME-508: Course on Machine Learning and Computational Physics, at USC (co-instructor, Fall 2021 & Fall 2022)
- MATH-459: Graduate course on Numerical Methods for Conservation Laws, at EPFL (Fall 2020)

Course development:

- AME-599: Course on Machine Learning and Computational Physics, at USC (Fall 2020)

Mini-courses and workshops:

- Lectures on Deep Learning and Computational Physics, at the Workshop On Scientific Computing, Modeling And Deep Learning, SRM IST (January 2024)
- Mini-course on Deep Learning Approaches for Inverse Problems, at the Workshop on Inverse Problems and Related Topics, ICTS Bangalore (October 2021).
- Mini-course on the Application and Implementation of Deep Learning, at TIFR-CAM (January, 2019).

Teaching assistant:

- MATH-459: Graduate course on Numerical Methods for Conservation Laws, at EPFL (Fall 2017 & Fall 2018)
- Graduate course on Computational Partial Differential Equations, at TIFR-CAM (Spring 2015)
- Graduate course on Numerical Analysis, at TIFR-CAM (Fall 2012 & Fall 2013)

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| RESEARCH MENTORSHIP | PhD thesis supervision: | | |
| | Philip Charles | UMD | Ongoing |
| | 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 |
| | Short term supervision: | | |
| PROFESSIONAL SERVICE & OUTREACH | <ul style="list-style-type: none"> • Co-mentored 3 summer students interning with the Research for Intelligence & Security Challenges Initiative internship program. UMD, June-August, 2023. • Mentored undergraduate students working on data-driven predictions for COVID-19 severity. USC, 2021. • Senior mentor for the Center for Undergraduate Research in Viterbi Engineering (CURVE) program. USC, 2021. | | |
| | Board member of the Burgers Program at University of Maryland (January 2024 – present). | | |
| | Thesis committee: | | |
| | - PhD thesis committee: 2 students (2023) | | |
| | - Doctoral candidacy committee: 4 students (2023), 1 student (2024). | | |
| | - External expert for the oral exam of a Master's project at EPFL (2021). | | |
| | Organizer/session chair: | | |
| | <ul style="list-style-type: none"> • Minisymposium on <i>Generative Models for Physics-Based Forward and Inverse Problems</i> at SIAM UQ (February 2024). • Minisymposium on <i>Recent Developments in Operator Networks</i> at USNCCM17 (July 2023). • Discussion sessions on benchmarks for data-driven methods at USC (April 2023) • Minisymposium on <i>Advances in data-enhanced predictive modeling in simulation science</i> at SIAM-CSE (March 2021). | | |
| | Co-organizer: | | |
| | <ul style="list-style-type: none"> - Numerical Analysis Seminar at University of Maryland (August 2023 – present). - Numerical sessions for optimal control at the IFCAM Summer School on Numerics and Control of PDEs, IISc Bangalore (2013). - Students Seminar Series at TIFR-CAM (2012 – 2013). | | |
| | Volunteer: | | |
| | <ul style="list-style-type: none"> • Judge at the Science and Engineering Fair of Houston (2020 & 2021). • 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 –2014). | | |

Conferences (invited)

- A variationally mimetic operator network (April, 2024)
AMS Sectional Meeting at Howard University, Washington DC.
- A variationally mimetic operator network (March, 2024)
AMS Sectional Meeting at Florida State University.
- A Novel Conditional Wasserstein GAN for Bayesian Inference (27th February, 2024)
SIAM-UQ, Trieste.
- Learning WENO for entropy stable schemes to solve conservation laws (23rd February, 2024)
Brin Workshop in Scientific Machine Learning, UMD.
- A deep learning strategy for solving physics-based Bayesian inference problems (February, 2024)
Data Science Symposium at South Dakota State University.
- A variationally mimetic operator network (20th January, 2024)
International symposium on Complete Flux Scheme for Convection Diffusion Reaction Models, Fluid Flow and Allied Topics, IIT Kanpur.
- A variationally mimetic operator network (3rd January, 2024)
5th International Conference on Mathematical Techniques and Applications, Institute of Science and Technology, Kattankulathur.
- 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 leaning-based posterior inference for inverse problems (26th March, 2022)
Annual Math Symposium, IISER Bhopal.
- Bayesian inference using generative adversarial networks (7th Dec, 2021)
87th Annual Conference of the Indian Mathematical Society, Aurangabad, India.
- Discontinuous Galerkin discretization of phase-field models for pore-scale flows (24th June, 2021)
SIAM-GS 2021, Milan, Italy.
- Using deep learning to overcome algorithmic bottlenecks (18th June, 2019)
NumHyp 2019, Malaga.
- 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.
- An artificial neural network for detecting discontinuities (11th March, 2018)
7th International Conference on High Performance Scientific Computing, Hanoi, Vietnam.
- 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.

Conferences (other)

- A variationally mimetic operator network (6th April, 2023)
USACM Data-Driven Benchmarks Workshop, USC, California.
- Conditional GANs and their generalizability in physics-based inverse problems (18th August,

2022)

USACM Thematic Conference UQ-MLIP, Arlington, Virginia.

- A Deep Learning Framework for p-adaptation (5th March, 2021)
SIAM-CSE 2021, Fort Worth, Texas.
- 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.
- 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 (14th Aug, 2015)
International Conference on Industrial and Applied Mathematics, Beijing, China.
- 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.

Colloquia and seminars

- A deep learning strategy for solving physics-based Bayesian inference problems (16th February, 2024)
Seminar talk, CMAI, George Mason University
- A deep learning strategy for solving physics-based Bayesian inference problems (13th October, 2023)
Seminar talk, Department of Mathematics, Brigham Young University
- A variationally mimetic operator network (17th April, 2023)
Seminar talk, Department of Mathematics, Iowa State University
- Bayesian inference using GANS (31st March, 2023)
RIT on Machine Learning for Rare Events, University of Maryland
- A variationally mimetic operator network (21st March, 2023)
Seminar talk, Department of Mathematics, North Carolina State University
- A variationally mimetic operator network (25th Jan, 2023)
LANS seminar, Argonne National Laboratory.
- A variationally mimetic operator network (16th Nov, 2022)
CMX Seminar, Caltech.
- Deep learning-based enhancements in numerical analysis (14th Dec, 2021)
Seminar talk, Department of Mathematics, University of Maryland.
- Deep learning-based enhancements in computational physics (10th Dec, 2021)
Seminar talk, Department of Artificial Intelligence, IIT Hyderabad.
- 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.
- A data-driven approach to predict artificial viscosity in high-order solvers (14th May, 2021)
Department of Mathematics, University of Würzburg, Germany.
- 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.
- Detecting discontinuities using deep learning (12th April, 2019)
Deep Learning Meetup, Zürich, Switzerland.
- Controlling spurious oscillations in high-order methods through deep neural networks (9th Jan, 2019)
TIFR-CAM Colloquium, Bangalore, India.
- Using neural nets to detect discontinuities (19th June, 2018)
MATHICSE Retreat, St. Croix, Switzerland.
- An artificial neural network for detecting discontinuities (3rd Jan, 2018)
TIFR-CAM Colloquium, Bangalore, India.
- A sign preserving WENO reconstruction (23rd Nov, 2015)
Department of Mathematics, University of Würzburg, Germany.
- A sign preserving WENO reconstruction (11th June, 2015)
Department of Applied Mathematics, University of Washington, Seattle, Washington.
- Entropy stable schemes for compressible flows (9th July, 2014)
Department of Mathematics, University of Würzburg, Germany.

Posters

- Bayesian Inference in Physics-Driven Problems with Adversarial Priors (11th Dec, 2020)
NeurIPS 2020 Workshop on Deep Learning and Inverse Problems.
- Entropy stable schemes for compressible flows on unstructured meshes (9th Sep, 2014)
Analysis and Numerical Approximation of PDEs, ETH Zürich, Switzerland.

EDITORIAL SERVICE

Journal article reviews:

Computer Methods in Applied Mechanics and Engineering • Journal of Computational Physics
• SIAM Journal on Numerical Analysis • SIAM Journal on Scientific Computing • Journal
of Machine Learning Research • 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 • Computers and Mathematics with Applications • Numerical
Algorithms • BIT Numerical Mathematics • Indian Journal of Pure and Applied Mathematics.

Book chapter reviews:

De Gruyter publication

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

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

Last updated on March 16, 2024.