Computational Science Division Argonne National Laboratory 9700 Cass Avenue, Lemont, IL 60439

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Professional experience

Assistant Computational Scientist, Argonne National Laboratory, Aug, 2021 - Present.

Postdoctoral Researcher - Cosmological Physics and Advanced Computing Group, High Energy Physics Division, Argonne National Laboratory, **Aug**, **2018** - **Aug**, **2021**.

Associate Fellow - Kavli Institute for Cosmological Physics, University of Chicago, March, 2019 - January, 2024.

Fellow - Kavli Summer Program on Astrophysics, University of California, Santa Cruz, **June**, **2019** - **Aug**, **2019**.

Graduate researcher - Cosmological Physics and Advanced Computing (CPAC) Group, Argonne National Laboratory, Jan, 2018 - Aug, 2018.

HEP-Center for Computational Excellence Fellow - High Energy Physics Division, Argonne National Laboratory, **June**, **2017 - Aug**, **2017.**

Head Teaching Assistant, Department of Physics and Astronomy, University of Kansas, Aug, 2015 - May, 2016.

Graduate Research Assistant - Department of Physics and Astronomy, University of Kansas, **Aug, 2013** - **June, 2017**.

Research Scholar - Tata Institute of Fundamental Research Centre for Interdisciplinary Science, Hyderabad, India, Jan, 2013 - July, 2013.

Research scholar - Indian Institute of Astrophysics, Bangalore, India, Jan 2012 - Jan 2013.

Academic background

1. Ph.D. (Hons.) Physics, University of Kansas, 2018.

Dissertation title: Topology, Geometry and Morphology of the Dark Matter web.

Adviser: Professor Sergei Shandarin

2. Integrated M.S. (Hons.) Physics, Birla Institute of Technology and Science (BITS) Pilani, India, 2012.

Thesis title: Dynamics of ellipsoidal collapse in a cosmological setting.

Adviser: Professor Arun Mangalam, Indian Institute of Astrophysics.

Research interests and experience

Techniques: Scientific machine learning and foundation models, high-performance computing, numerical methods, Bayesian inference, topological and geometrical techniques.

Domains: Astrophysics, Nuclear and Particle physics, Data analysis experience in Climate science, and aero-structure manufacturing.

Teaching experience

1. *Head Teaching Assistant*, Department of Physics and Astronomy, University of Kansas (2015-2016): Implemented, oversaw and evaluated new teaching strategies for 12 undergraduate courses.

- 2. *Graduate Teaching Assistant*, Department of Physics and Astronomy, University of Kansas (2014-2015): General Physics II Honors, General Physics I, College Physics I.
- 3. Undergraduate Teaching Assistant, Department of Physics, BITS-Pilani (2011): Theory of Relativity.

Mentorship

- 1. Postdoc researchers: Arkaprabha Ganguli (Argonne), Anirban Samaddar (Argonne)
- 2. Summer internship students: Claire Guilloteau (IRAP), Ting-Yun Cheng (University of Nottingham), Kate Storey-Fisher (NYU), Madeline Lucey (University of Texas Austin), Aurora Cossairt (Argonne National Lab).
- 3. Longer term students: James Butler (University of Chicago), Xiaofeng Dong (University of Chicago), Xin Liu (University of Chicago).

Publications

Under review

- A. Ganguli, N. Ramachandra, J. Bessac, E. Constantinescu: Enhancing Interpretability in Generative Modeling: Disentangled Latent Spaces Guided by Generative Factors in Scientific Datasets, Submitted to the NeurIPS-2024 Main Conference.
- M. Michael Rau, F. Kéruzoré, N. Ramachandra, L. Bleem: Reducing Model Error Using Optimised Galaxy Selection: Weak Lensing Cluster Mass Estimation, Submitted to the Monthly Notices of the Royal Astronomical Society, arxiv:2406.11950.
- 3. Anirban Samaddar, S. K. Ravi, **N. Ramachandra**, L. Luan, S. Madireddy, A. Bhaduri, P. Pandita, C. Sun, L. Wang: Data-Efficient Dimensionality Reduction and Surrogate Modeling of High-Dimensional Stress Fields, Submitted to the The ASME Journal of Mechanical Design.
- 4. D. Huppenkothen *et al.* (incl. **N. Ramachandra**): Constructing Impactful Machine Learning Research for Astronomy: Best Practices for Researchers and Reviewers, Submitted, Bulletin of the American Astronomical Society, *arxiv*:2310.12528
- 5. A. Bhaduri, N. Ramachandra, S. K. Ravi, L. Luan, P. Pandita, P. Balaprakash, M. Anitescu, C. Sun, L. Wang: Efficient mapping between void shapes and stress fields using Deep Convolutional Neural Networks with sparse data, Submitted, ASME Selected Papers from CIE2023, ASME Journal of Computing and Information Science in Engineering (JCISE) special issue.
- 6. T. Y. Chen, B. Dey, A. Ghosh, M. Kagan, B. Nord, N. Ramachandra: Interpretable Uncertainty Quantification in AI for HEP, Submitted to the Proceedings of the US Community Study on the Future of Particle Physics (Snowmass 2021), arxiv:2208.03284.
- 7. S. Madireddy, **N. Ramachandra**, N. Li, , P. Balaprakash, S. Habib: A Modular Deep Learning Pipeline for Galaxy-Scale Strong Gravitational Lens Detection and Modeling, Submitted to the Open Journal of Astrophysics, *arxiv*:1911.03867v3.

Refereed journal articles

1. H. Wang, S. Sreejith, Y. Lin, **N. Ramachandra**, A. Slosar, S. Yoo: Neural Network Based Point Spread Function Deconvolution For Astronomical Applications, *Open Journal of Astrophysics*, 2023.

- 2. M. Lucey, N. A. Kharusi, K. Hawkins, Y. Ting, N. Ramachandra, A. M. Price-Whelan, T. C. Beers, Y. S. Lee, J. Yoon: Carbon-enhanced metal-poor star candidates from BP/RP spectra in Gaia DR₃, *Monthly Notices of the Royal Astronomical Society*, 2023.
- 3. **N. Ramachandra**, J. Chaves-Montero, A. Alarcon, A. Fadikar, S. Habib, K. Heitmann: Machine learning synthetic spectra for probabilistic redshift estimation: SYTH-Z, *Monthly Notices of the Royal Astronomical Society*, 2022.
- 4. A. Hearin, **N. Ramachandra**, M. Becker, J. DeRose: Differentiable Predictions for Large Scale Structure with SHAMNet, *Open Journal of Astrophysics*, 2021.
- 5. K. Fukami, R. Maulik, **N. Ramachandra**, K. Fukagata, K. Taira: Global field reconstruction from sparse sensors with Voronoi tessellation-assisted deep learning, *Nature Machine Intelligence*, 2021.
- 6. L. Vazsonyi, P. Taylor, G. Valogiannis, **N. Ramachandra**, A. Ferte, J. Rhodes: Constraining f(R) Gravity with a k-cut Cosmic Shear Analysis of the Hyper Suprime-Cam First-Year Data, *Physical Review D*, 2021.
- 7. K. Storey-Fisher, M. Huertas-Company, N. Ramachandra, F. Lanusse, A. Leauthaud, Y. Luo, S. Huang, X. Prochaska: Anomaly detection in Hyper Suprime-Cam galaxy images with generative adversarial networks, *Monthly Notices of the Royal Astronomical Society*, 2021.
- 8. Y. Wang, N. Ramachandra, E. Salazar-Canizales, H. Feldman, R. Watkins, K. Dolag: Peculiar Velocity Estimation from Kinetic SZ Effect using Deep Neural Networks, Accepted, *Monthly Notices of the Royal Astronomical Society*, 2021.
- 9. **N. Ramachandra**, G. Valogiannis, M. Ishak, K. Heitmann (for the LSST Dark Energy Science Collaboration): Matter Power Spectrum Emulator for f(R) Modified Gravity Cosmologies, Accepted, *Physical Review D*, 2021.
- 10. T. Cheng, M. Huertas-Company, C. Conselice, A. Aragón-Salamanca, B. Robertson, N. Ramachandra: Beyond the Hubble Sequence Exploring Galaxy Morphology with Unsupervised Machine Learning, *Monthly Notices of the Royal Astronomical Society*, Volume 503, Issue 3, May 2021, Pages 4446–4465.
- 11. R. Maulik, T. Botsas, N. Ramachandra, M. Lachlan, I. Pan: Latent-space time evolution of non-intrusive reduced-order models using Gaussian process emulation, Accepted, *Physica D: Nonlinear Phenomena*, 2020.
- 12. R. Maulik, K. Fukami, **N. Ramachandra**, K. Fukagata, K. Taira: Probabilistic neural networks for fluid flow model-order reduction and data recovery, *Physical Review Fluids*, 5, 104401, 2020.
- 13. M. Lucey, Y. Ting, **N. Ramachandra**, K. Hawkins: From the Inner to Outer Milky Way: A Photometric Sample of 2.6 Million Red Clump Stars, *Monthly Notices of the Royal Astronomical Society*, Volume 495, Issue 3, Pages 3087–3103.
- 14. L. Bleem et al. (incl. N. Ramachandra): The SPTpol Extended Cluster Survey, The Astrophysical Journal Supplement Series, Volume 247, Number 1.
- 15. **N. Ramachandra**: Topology, Geometry and Morphology of the Dark Matter Web (Doctoral Dissertation), *ProQuest Dissertations & Theses Global database*, Publication Number: 10845180.

16. N. Libeskind *et al.* (incl. **N. Ramachandra**): Tracing the cosmic web, *Monthly Notices of the Royal Astronomical Society*, Volume 473, Issue 1, Pages 1195-1217.

- 17. **N. Ramachandra**, S. Shandarin: Dark matter haloes: a multistream view, *Monthly Notices of the Royal Astronomical Society*, Volume 470, Issue 3, p. 3359-3373.
- 18. **N. Ramachandra**, S. Shandarin: Topology and geometry of the dark matter web: a multistream view, *Monthly Notices of the Royal Astronomical Society*, Volume 467, Issue 2, p.1748-1762.
- 19. **N. Ramachandra**, S. Shandarin: Multi-stream portrait of the Cosmic web, *Monthly Notices of the Royal Astronomical Society*, Volume 452, Issue 2, p.1643-1653.

Papers in technical conference proceedings – refereed

- 1. L. Luan, S. Krishnan Ravi, A. Bhaduri, P. Pandita, L. Wang, N. Ramachandra, S. Madireddy: High-dimensional Surrogate Modeling for Image Data with Nonlinear Dimension Reduction, Accepted at *American Institute of Aeronautics and Astronautics SciTech Forum* 2024
- 2. L. Luan, **N. Ramachandra**, S. K. Ravi, A. Bhaduri, P. Pandita, P. Balaprakash, M. Anitescu, C. Sun, L. Wang: Application of probabilistic modeling and automated machine learning framework for high-dimensional stress field, Accepted at *ASME-IDETC Conference* 2023, arxiv:2303.16869.
- 3. A. Bhaduri, **N. Ramachandra**, S. K. Ravi, L. Luan, P. Pandita, P. Balaprakash, M. Anitescu, C. Sun, L. Wang: Efficient mapping between void shapes and stress fields using Deep Convolutional Neural Networks with sparse data, Accepted at *ASME-IDETC Conference* 2023.
- 4. H. Wang, S. Sreejith, Y. Lin, **N. Ramachandra**, A. Slosar, S. Yoo: Deconvolution of Astronomical Images with Deep Neural Networks, Accepted at *NeurIPS workshop on AI for Science*, 2022.
- 5. X. Dong, **N. Ramachandra**, S. Habib, K. Heitmann, M. Buehlmann, S. Madireddy: Physical Benchmarking for AI-Generated Cosmic Web, Accepted at *NeurIPS workshop on AI for Science*, 2021.
- 6. K. Storey-Fisher, M. Huertas-Company, N. Ramachandra, F. Lanusse, A. Leauthaud, Y. Luo, S. Huang: Anomaly Detection in Astronomical Images with Generative Adversarial Networks, Accepted at NeurIPS workshop on Machine Learning and the Physical Sciences, 2020.
- 7. K. Fukami, R. Maulik, **N. Ramachandra**, K. Fukagata, K. Taira: Probabilistic neural network-based reduced-order surrogate for fluid flows, Accepted at *NeurIPS workshop on Machine Learning and the Physical Sciences*, 2020.
- 8. S. Madireddy, N. Li, **N. Ramachandra**, P. Balaprakash, S. Habib: Modular Deep Learning Analysis of Galaxy-Scale Strong Lensing Images, *Machine Learning and the Physical Sciences Workshop at the 33rd Conference on Neural Information Processing Systems* (2019).

External software developed

- 1. MGemu: The Modified Gravity Emulator, N. Ramachandra, G. Valogiannis, M. Ishak, K. Heitmann (for the LSST Dark Energy Science Collaboration).
- 2. SYTH-Z: The galactic redshift estimator, **N. Ramachandra**, J. Chaves-Montero, A. Alarcon, A. Fadikar, S. Habib, K. Heitmann.

Talks

Major Conferences and Symposia

1. **N. Ramachandra**, A. Ganguli, J. Bessac, E. Constantinescu, Foundation models for physical sciences, QCD at the Femtoscale in the Era of Big Data, 2024.

- 2. **N. Ramachandra**, A. Ganguli, J. Bessac, E. Constantinescu, Latent spaces in generative models, QCD at the Femtoscale in the Era of Big Data, 2024.
- 3. **N. Ramachandra**, Physics Benchmarking strategies for Large Language Models, AuroraGPT Evaluation strategy, 2024.
- 4. **N. Ramachandra**, M. Buehlmann, S. Habib, P. Larsen: Cosmology and EBL simulations, SPHEREX Science L4 SIR Peer Review and Science Team Meeting, Pasadena, 2023.
- 5. **N. Ramachandra**, K. Moran, N. Frontiere, K. Heitmann, S. Habib: Calibrating sub-grid hydrodynamical parameters using cosmic emulators, 2023 SciDAC Principal Investigator (PI) Meeting, Washington DC, 2023.
- 6. **N. Ramachandra**, H. Wang, S. Sreejith, Y. Lin, A. Slosar, S. Yoo: Deconvolution of Astronomical Images with Deep Neural Networks, NeurIPS, 2023.
- 7. **N. Ramachandra**: Estimation of Galaxy Redshift with Probabilistic Neural Networks, SIAM Conference on Parallel Processing for Scientific Computing, Seattle, 2022 (remote).
- 8. **N. Ramachandra**: Astrophysical AI: Issues and lessons learned, Exascale Astronomy AI and benchmarking workshop, Edinburgh, 2020 (remote).
- 9. **N. Ramachandra**, G. Valogiannis, M. Ishak, K. Heitmann: Matter Power Spectrum Emulator for f(R) Modified Gravity Cosmologies, Science Highlight Plenary talk, LSST-DESC July Meeting, 2020.
- 10. **N. Ramachandra**: Scientific Machine Learning using Astrophysical Simulations, Conference on Data Analysis, Santa Fe, 2020.
- 11. **N. Ramachandra**: Scientific machine learning with synthetic astrophysical data, Machine Learning Tools for Research in Astronomy Ringberg, Germany, 2019.
- 12. **N. Ramachandra**, S. Habib, K. Heitmann: Cosmological analysis pipelines through Neural Networks, American Physical Society April Meeting, Columbus, Ohio 2018.
- 13. **N. Ramachandra**, S. Shandarin: Topology and geometry of the dark matter web, American Physical Society April Meeting, Washington D.C, 2017
- 14. **N. Ramachandra**, S. Shandarin: The Multi-stream portrait of the cosmic web, American Physical Society April Meeting, Salt Lake City, Utah, 2016.
- 15. **N. Ramachandra**, S. Shandarin: The Multi-stream structures of the cosmic web, Canadian-American-Mexican Graduate Students Physics Conference at Oaxaca, Mexico, 2015.

Seminars and Colloquia

- 1. **N. Ramachandra**, S. Habib: Synthetic sky catalogs, NASA-SPHEREx meeting, California Institute of Technology, Pasadena, 2023.
- 2. **N. Ramachandra**, P. Balaprakash: DeepHyper at scale: NERSC Perlmutter, ALCF DeepHyper Automated Machine Learning Workshop, Lemont, 2022

3. **N. Ramachandra**: Cosmology using Scientific Machine Learning, AI & HPC Seminar, Argonne National Laboratory, 2020.

- 4. **N. Ramachandra**, S. Madireddy, N. Li, P. Balaprakash, S. Habib: Probabilistic Deep Learning for Galaxy-Scale Strong Lensing Studies, University of Chicago, 2020.
- 5. **N. Ramachandra**: Deep Generative models and Astrophysical Image emulation, Machine Learning in the Era of Large Astronomical Surveys, Santa Cruz, 2019.
- 6. **N. Ramachandra**, G. Valogiannis, M. Ishak, K. Heitmann: Gaussian Process Emulators for Modified Gravity Summary Statistics, LSST-DESC meeting, Paris, France, 2019 (remote).
- 7. **N. Ramachandra**, M. Binois, S. Habib, K. Heitmann: Suite of Gaussian Process emulators for cosmological inference problems, Likelihood-free inference workshop, Flatiron Institute, New York, 2019.
- 8. **N. Ramachandra**, M. Binois, S. Habib, K. Heitmann: Cosmology meets Machine learning: Emulation of CMB Power Spectra, Astro seminar, University of Kansas, Lawrence, 2019.
- 9. **N. Ramachandra**, M. Binois, S. Habib, K. Heitmann: Variational autoencoders for the emulation of cosmological functions, KICP Postdoc Symposium, University of Chicago, 2019.
- 10. **N. Ramachandra**, P. Larsen: Cosmic Emulators for next generation surveys, Accurate lensing in the era of precision Cosmology, University of California, Berkeley, 2019.
- 11. **N. Ramachandra**, S. Madireddy, N. Li, P. Balaprakash, S. Habib: Deep learning pipelines for lensing analysis, Astrophysics Seminar, University of Kansas, 2017.
- 12. **N. Ramachandra**, S. Madireddy, N. Li, P. Balaprakash, S. Habib: Strong Lensing analysis using Deep Neural Networks, Young Scientists Symposium, Argonne National Laboratory, 2017.
- 13. **N. Ramachandra**: Emulation of the halo mass function, SAMSI Research Triangle Park, North Carolina, 2017
- 14. **N. Ramachandra**, S. Shandarin: The dynamical structure of the cosmic web, MidAmerican Regional Astrophysics Conference at The University of Missouri, 2015.

General-interest lectures

- 1. **N. Ramachandra**: Artificial Intelligence assisted understanding of the Universe, Art of Science Public lecture, Chicago, 2023.
- 2. **N. Ramachandra**: Cosmology in the era of Artificial Intelligence, Lifelong Learning Outreach Series, Chicago, 2021.

Organization

- 1. Co-organizer: ALCF DeepHyper Automated Machine Learning Workshop, 2022
- 2. Co-organizer: AI, Statistics and Machine Learning Journal Club, Argonne National Laboratory, 2019.
- 3. Co-organizer: Workshop on Advanced Statistical Methods Meet Machine Learning, Argonne National Laboratory, 2018-2019

Major projects

- 1. Member, AuroraGPT A large-scale AI models for Science, Argonne National Laboratory, 2024.
- 2. Principal Investigator, Laboratory Computing Resource Center (LCRC) AI-modeling of cosmic fields and dark matter halos, Argonne National Laboratory, 2020-2024.
- 3. Principal Investigator, Laboratory Directed Research and Development (LDRD) Pushing the mapping limits of the cosmological evolution, Argonne National Laboratory, 2023.
- 4. Co-Principal Investigator, SciDAC-5 Femtoscale Imaging of Nuclei using Exascale Platforms, DOE-NP, 2022.
- 5. Co-Principal Investigator, Probabilistic Machine Learning for Rapid Large-Scale and High-Rate Aerostructure Manufacturing, with Argonne, GE Research, Edison Welding Institute and GKN Aerospace, DOE-EERE, 2021.
- 6. Member: SciDAC-5 Enabling Cosmic Discoveries in the Exascale Era, DOE-HEP, 2022.
- 7. Principal Investigator, Laboratory Directed Research and Development (LDRD) Artificial Intelligence (AI)-enabled analytics for Cosmology, Argonne National Laboratory, 2022-2024.
- 8. Principal Investigator, Argonne Laboratory Computing Resource Center allocation AI-modeling of cosmic fields and dark matter halos, 2022-2023.
- 9. Co-Principal Investigator, Swift LDRD: Deep-Learning Inference for Nuclear Femtography on Exascale Platforms, Argonne National Laboratory, 2022.
- 10. Member, NASA-SPHEREx mission L4 Science Team, 2020-2024
- 11. Co-Principal Investigator, Laboratory Directed Research and Development (LDRD) Expedition Project: Deep Learning-Based Scalable and Robust Strong Gravitational Lensing Characterization Pipeline Using SambaNova, Argonne National Laboratory, 2021.
- 12. Co-Principal Investigator, Laboratory Directed Research and Development (LDRD): Automated Model Inference for Cosmological Structure Formation using Reinforcement Learning, Argonne National Laboratory, 2021.
- 13. Co-lead, Strong Lensing Working group project, LSST-DESC: Deep Learning to Identify and Deblend Strong Lenses for LSST.
- 14. Co-lead, Photometric Redshifts Working group project, LSST-DESC: Synthetic-spectra for sample redshift inference
- 15. Co-lead: Modeling and Combined Probes (MCP) Working group project, LSST-DESC, Power spectra emulators for f(R) Modified Gravity Cosmologies.
- 16. Member: SciDAC-4 Inference and Machine Learning at Extreme Scales, DOE-HEP.

Professional service

- 1. Journal referee, Monthly Notices of Royal Astronomical Society Oxford University Press, 2018, 2023.
- 2. International Journal of Intelligent Systems The Wiley Hindawi publishing, 2023.

3. Conference proceedings referee, NeurIPS workshop on Machine Learning and the Physical Sciences, 2021, 2023.

- 4. Journal referee, The Astrophysical Journal IOPscience, 2021.
- 5. Journal referee, Astronomy and Computing Elsevier Publishing, 2019.
- 6. Journal Referee, Journal of Cosmology and Astroparticle Physics IOP Publishing, 2015.
- 7. Grant reviewer: Future Investigators in NASA Earth and Space Science and Technology (FINESST) program, 2019-2020.

Honors, grants & awards

- 1. Kavli Summer Program fellowship grant, 2019.
- 2. Physics and Astronomy Department Scholarship, University of Kansas, 2018.
- 3. Division of Astrophysics Travel grant, American Physical Society, 2018.
- 4. Graduate Research travel award, University of Kansas, 2017.
- 5. High Energy Physics Center for Computational Excellence summer fellowship, 2017.
- 6. SAMSI Travel grant, Astrophysical population emulation workshop, 2016, 2017.
- 7. Division of Astrophysics Travel grant, American Physical Society, 2016.
- 8. Graduate Research Competition Award, University of Kansas, 2016.
- 9. National Science Foundation, the American Physical Society and the Sociedad Mexicana de Fisica travel grant, CAM conference, 2015.
- 10. Junior research fellowship, Council for Scientific and Industrial Research, Government of India, 2012.
- 11. Innovation in Science Pursuit for Inspired Research (INSPIRE) fellowship, Department of Science and Technology, Government of India, 2008 2012.

Outreach

- 1. Judge: Illinois Junior Academy of Science Region 6 Fair, Skokie, IL 2023.
- 2. Member: Rubin Observatory Legacy Survey of Space and Time (LSST)- Dark Energy Science Collaboration (DESC), 2018.
- 3. President: Society of Physics Students, The University of Kansas chapter, 2015 2018.
- 4. Founding Member: KUbeSat team a University of Kansas miniature satellite Mission that won the SPS Chapter Research Award by American Institute of Physics, 2016-2018.
- 5. Member: American Physical Society (APS), 2014.
- Mentor: Afro-Academic, Cultural, Technological and Scientific Olympics (ACT-SO) initiative by National Association for the Advancement of Colored People (NAACP), 2020-2021.
- 7. Chief Organizer: TEDxBITSGoa conference, India, 2011.