Ravinder

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Nationality: Indian
Date of birth: 29 January, 1994
Gender: Male
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Research Interests

Machine learning aided structural design, physics informed machine learning, graph neural networks, material modelling, dynamic fracture and crack propagation on ballistic impact, molecular dynamics and peridynamics.

Experience

Postdoctoral Scholar April 2023 – Present
Civil and Environmental Engineering
University of Wisconsin–Madison, Madison

EarlyDoc Scholar January 2023 – March 2023
Civil Engineering
Indian Institute of Technology Delhi, Delhi

Structural Bridge Design Engineer September 2015 – May 2016
ASC Infratech Pvt Ltd
Noida, Uttarpradesh, India

Education

Ph. D., Civil Engineering July 2017 – January 2023
Indian Institute of Technology Delhi, Delhi
CGPA: 9.50/10

B. Tech., Civil Engineering July 2011 – June 2015
Indian Institute of Technology Roorkee, Roorkee
CGPA: 7.92/10

CURRENT RESEARCH Postdoctoral Research, University of Wisconsin–Madison

Advisor: Prof. Bu Wang
At University of Wisconsin–Madison, I am working in an interdisciplinary research group that focuses on material research. I am working on response modelling of materials under indentation loading. A mesoscale material model will be developed that can reproduce the deformation behavior of materials under indentation loading. The work involves atomistic simulation and machine learning for up-scaling of material properties from nanoscale to mesoscale.

PH.D. THESIS Civil Engineering, Indian Institute of Technology Delhi

Advisor: Prof. N. M. Anoop Krishnan
Title: Data-driven Modeling and Physics-informed Machine Learning for Glass Discovery
Description: The research work explores the use of machine learning methods in modeling inorganic glass properties, revealing composition–property relationships through explainable ML, understanding mechanisms at the atomic scale, and up-scaling of material properties using MD and DFT simulation trajectory. The research work uses the graph neural network-based interatomic potential for reproducing features at the atomic scale for complex systems and uses ML material models (peridynamics nonlocal operators) for reproducing material behavior at mesoscale with MD and DFT simulation trajectories.

RESEARCH ACHIEVEMENTS AND AWARDS

PyGGi (Python for Glass Genomics)
It is an indigenous industry-relevant software package that uses trained Machine Learning algorithms to predict/optimize composition-property relationships in inorganic glasses. It will make the tedious process of designing tailored glasses economical in terms of time, effort, and money.
The software package is launched through FITT IITD and is available at www.pyggi.iitd.ac.in.

Awards:

- Prime Ministers Research Fellowship (PMRF)
- SERB Travel grant (2022)
- SITARE/SRISTI Gandhian Young Technological Innovation (GYTI) Awards/Appreciations (2020)
- ICG-GOMD 2019 registration grant (2019).

Teaching Experience

Teaching Assistant

- Structural Analysis (UG Lab), 2018,2019
- Structural Analysis I (UG Course), 2018
- Finite Element Method (PG Course), 2018
- Atomistic and Multiscale Modelling of Materials (PG Course), 2019

Workshop Instructor

- Molecular dynamics workshop 2, Advanced Simulation Methods: DFT, MD and Beyond, Delhi, 2019
- Introduction to Machine Learning: Machine Learning For Engineering Applications (TEQIP Course) IIT Delhi, 2019
- Introduction to Machine Learning Tools, Artificial Intelligence Concepts and Multi-disciplinary Applications in Modern Biology, ICGEB, Delhi, 2019

Books and Contributed Chapters

Machine Learning for Materials Discovery: Numerical Recipes and Practical Applications (In Draft)
N. M. Anoop Krishnan, Hariprasad Kodamana and Ravinder Bhattoo

Journal Publications

1. **Bhattoo, Ravinder**; Ranu, Sayan; Krishnan, N. M. Anoop; Learning the dynamics of particle-based systems with lagrangian graph neural networks. *Machine Learning: Science and Technology* (2023)
https://doi.org/10.1088/2632-2153/acb03e
2. **Ravinder, R**; Bishnoi, Suresh; Zaki, Mohd; Krishnan, N. M. Anoop; Understanding the compositional control on electrical, mechanical, optical, and physical properties of inorganic glasses with interpretable machine learning. *Acta Materialia* (2022)
https://doi.org/10.1016/j.actamat.2022.118439
3. Zaki, Mohd; Venugopal, Vineeth; **Bhattoo, Ravinder**; Bishnoi, Suresh; Singh, Sourabh Kumar; Allu, Amarnath R; Krishnan, N. M. Anoop; Interpreting the optical properties of oxide glasses with machine learning and Shapely additive explanations. *Journal of the American Ceramic Society* (2022)
https://doi.org/10.1111/jace.18345

4. **Ravinder, R**; Venugopal, Vineeth; Bishnoi, Suresh; Singh, Sourabh; Zaki, Mohd; Grover, Hargun Singh; Bauchy, Mathieu; Agarwal, Manish; Krishnan, N. M. Anoop; Artificial intelligence and machine learning in glass science and technology: 21 challenges for the 21st century. *International Journal of Applied Glass Science* (2021) https://doi.org/10.1111/ijag.15881

5. Bishnoi, Suresh; **Ravinder, R**; Grover, Hargun Singh; Kodamana, Hariprasad; Krishnan, N. M. Anoop; Scalable Gaussian processes for predicting the optical, physical, thermal, and mechanical properties of inorganic glasses with large datasets. *Materials Advances* (2021) https://doi.org/10.1039/D0MA00764A

6. **Ravinder, R**; Sridhara, Karthikeya H; Bishnoi, Suresh; Grover, Hargun Singh; Bauchy, Mathieu; Jayadeva, J; Kodamana, Hariprasad; Krishnan, N. M. Anoop; Deep learning aided rational design of oxide glasses. *Materials Horizons* (2020) https://doi.org/10.1039/D0MH00162G

7. **Ravinder, R**; Kumar, Abhishek; Kumar, Rajesh; Vangla, Prashanth; Krishnan, N. M. Anoop; Irradiation-induced brittle-to-ductile transition in α-quartz. *Journal of the American Ceramic Society* (2020) https://doi.org/10.1111/jace.16951

8. **Ravinder, R**; Singh, Sourabh; Bishnoi, Suresh; Jan, Amreen; Sharma, Amit; Kodamana, Hariprasad; Krishnan, N. M. Anoop; An adaptive, interacting, cluster-based model for predicting the transmission dynamics of COVID-19. *Heliyon* (2020) https://doi.org/10.1016/j.heliyon.2020.e05722

9. Nayak, Sumeru; **Ravinder, R**; Krishnan, N. M.; Das, Sumanta; A peridynamics-Based micromechanical modeling approach for random heterogeneous structural materials. *Materials* (2020) https://doi.org/10.3390/ma13061298

10. Bhaskar, Pratik; Kumar, Rajesh; Maurya, Yashasvi; **Ravinder, R**; Allu, Amarnath R; Das, Sumanta; Gosvami, Nitya Nand; Youngman, Randall E; Bødker, Mikkel S; Mascaraque, Nerea; Cooling rate effects on the structure of 45S5 bioglass: Insights from experiments and simulations. *Journal of Non-Crystalline Solids* (2020) https://doi.org/10.1016/j.jnoncrysol.2020.119952

11. Krishnan, N. M. Anoop; **Ravinder, R**; Kumar, Rajesh; Le Pape, Yann; Sant, Gaurav; Bauchy, Mathieu; Density-stiffness scaling in minerals upon disordering: Irradiation vs. vitrification. *Acta Materialia* (2019) https://doi.org/10.1016/j.actamat.2019.01.015

12. Bishnoi, Suresh; Singh, Sourabh; **Ravinder, R**; Bauchy, Mathieu; Gosvami, Nitya Nand; Kodamana, Hariprasad; Krishnan, N. M. Anoop; Predicting Young's modulus of oxide glasses with sparse datasets using machine learning. *Journal of Non-Crystalline Solids* (2019) https://doi.org/10.1016/j.jnoncrysol.2019.119643

13. Dhawan, Sameer; Ghosh, Sukanya; **Ravinder, R**; Bais, Sachendra S; Basak, Soumen; Krishnan, N. M. Anoop; Agarwal, Manish; Banerjee, Manidipa; Haridas, V; Redox sensitive self-assembling dipeptide for sustained intracellular drug delivery. *Bioconjugate chemistry* (2019)
https://doi.org/10.1021/acs.bioconjchem.9b00532

14. Rivera, Jared; Berjikian, Jonathan; **Ravinder, R**; Kodamana, Hariprasad; Das, Sumanta; Bhatnagar, Naresh; Bauchy, Mathieu; Krishnan, N. M. Anoop; Glass fracture upon ballistic impact: new insights from peridynamics simulations. *Frontiers in Materials* (2019)
https://doi.org/10.3389/fmats.2019.00239

15. **Ravinder, R**; Kumar, Rajesh; Agarwal, Manish; Krishnan, NM; Evidence of a two-dimensional glass transition in graphene: Insights from molecular simulations. *Scientific reports* (2019)
https://doi.org/10.1038/s41598-019-41231-z

16. **Ravinder, R**; Garg, Prateet; Krishnan, N. M. Anoop; Glass transition and crystallization in hexagonal boron nitride: Crucial role of orientational order. *Advanced Theory and Simulations* (2019)
https://doi.org/10.1002/adts.201900174

17. **Bhattoo, Ravinder**; Ranu, Sayan; Krishnan, NM; Lagrangian neural network with differentiable symmetries and relational inductive bias. *arXiv preprint (**pre-print**)* (2021)
https://doi.org/10.48550/arXiv.2110.03266

    Please go to https://scholar.google.com/citations?user=lPTdGRMAAAAJ&hl=en for an updated list of publications.

Conference Publications

1. Bishnoi, Suresh; **Bhattoo, Ravinder**; Jayadeva, Jayadeva; Ranu, Sayan; Krishnan, N. M. Anoop; Learning the Dynamics of Physical Systems with Hamiltonian Graph Neural Networks. *ICLR 2023 Workshop on Physics for Machine Learning* (2023)
https://openreview.net/forum?id=Ugl-B_at5n

2. Bishnoi, Suresh; **Bhattoo, Ravinder**; Krishnan, Ranu, Sayan; N. M. Anoop; Enhancing the Inductive Biases of Graph Neural ODE for Modeling Dynamical Systems. *The Eleventh International Conference on Learning Representations* (2023)
https://openreview.net/forum?id=ATLEl_izD87

3. **Bhattoo, Ravinder**; Ranu, Sayan; Krishnan, NM; Learning Articulated Rigid Body Dynamics with Lagrangian Graph Neural Network. *Advances in Neural Information Processing Systems 35* (2022)
https://openreview.net/forum?id=nOdfIbo3A-F

4. Thangamuthu, Abishek; Kumar, Gunjan; Bishnoi, Suresh; **Bhattoo, Ravinder**; Krishnan, N. M. Anoop; Ranu, Sayan; Unravelling the Performance of Physics-informed Graph Neural Networks for Dynamical Systems. *Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track* (2022) https://openreview.net/forum?id=tXEe-Ew_ikh

Conference Talks and Posters

Talk: Understanding the Compositional Control on Electrical, Mechanical, Optical, And Physical Properties of Inorganic Glasses with Interpretable Machine Learning
Ravinder Bhattoo, N. M. Anoop Krishnan*
XXX International Materials Research Congress (IMRC2022) and International Conference on Advanced Materials (ICAM2021)
Cancun, Mexico, August 2022

Talk: Lagrangian and Hamiltonian Graph Neural Networks for Robust Molecular Simulations
Ravinder Bhattoo, N. M. Anoop Krishnan*
XXX International Materials Research Congress (IMRC2022) and International Conference on Advanced Materials (ICAM2021)
Cancun, Mexico, August 2022

Talk: PeriDyn: A Peridynamics Package Written in Julia Programming Language
Ravinder Bhattoo, N. M. Anoop Krishnan*
11th European Solid Mechanics Conference
NUI, Galway, Ireland, July 2022

Talk: Learning Quantum-accuracy Interatomic Potential for Silica Using Lagrangian Graph Neural Networks
Ravinder Bhattoo, N. M. Anoop Krishnan*
2022 Glass and Optical Materials Division Annual Meeting
Hyatt Regency Baltimore, Baltimore, MD, United States, May 2022

Talk: Learning Interaction Laws in Atomistic System using Lagrangian Graph Neural Networks
Ravinder Bhattoo, N. M. Anoop Krishnan*
2022 Glass and Optical Materials Division Annual Meeting
Hyatt Regency Baltimore, Baltimore, MD, United States, May 2022

Talk: Decoding the Genome of Inorganic Glasses using Interpretable Machine Learning
Ravinder Bhattoo, Suresh Bishnoi, M. Zaki, N. M. Anoop Krishnan*
14th Pacific Rim Conference on Ceramic and Glass Technology and GOMD 2021 Division Meeting
Vancouver, British Columbia, Canada (Virtual), December 2021

Talk: Molecular Dynamics Simulation Using Graph Neural Networks
Ravinder Bhattoo, N. M. Anoop Krishnan*
MRS Fall Meeting 2021
Boston, Massachusetts, USA (Virtual), December 2021

Talk: Understanding the Composition-property Relationship of Glasses Using Interpretable Machine Learning
Ravinder Bhattoo, Suresh Bishnoi, M. Zaki, N. M. Anoop Krishnan*
Materials Science and Technology (MS&T) 2021
Columbus, Ohio, USA (Virtual), October 2021

Talk: Machine Learning to Predict the Elastic Properties of Glasses.
Sourabh Singh, Suresh Bishnoi, R. Ravinder, Hariprasad Kodamana, N. M. Anoop Krishnan*
Material Science and Technology (MS&T) 2019
Oregon Convocation Center, Portland, USA, October 2019

Poster: Designing Functional Glasses using Machine Learning.
R. Ravinder, Suresh Bishnoi, Sourabh Kumar Singh, Hargun Singh, Hariprasad Kodamana, N M Anoop Krishnan*
IIT Delhi Industry Day 2019
Indian Institute of Technology Delhi, New Delhi, September 2019

Poster: Two-dimensional Glass Transition in Graphene: Insights from Molecular Simulations.
R. Ravinder, Rajesh Kumar, Manish Agarwal, N. M. Anoop Krishnan*
Advanced Simulation Methods: DFT, MD and Beyond
Indian Institute of Technology Delhi, New Delhi, March 2019

Poster: Role of Topological Defects on the Rigidity of Glassy Graphene.
R. Ravinder, N. M. Anoop Krishnan*
COMPFLU-2018: 12th International Conference on Complex Fluids and Soft Matter
Indian Institute of Technology Roorkee, Roorkee, December 2018

Workshops

Tutor: Introduction to Machine Learning Tools.
Artificial Intelligence Concepts and Multidisciplinary Applications in Modern Biology
International Center for Genetic Engineering and Biotechnology, New Delhi, September 2019

Tutor: Introduction to Machine Learning.
Machine Learning For Engineering Applications (TEQIP Course)
Indian Institute of Technology Delhi, New Delhi, June 2019

Tutor: Molecular Dynamics Workshop 2
Advanced Simulation Methods: DFT, MD and Beyond
Indian Institute of Technology Delhi, New Delhi, March 2019

Membership and Affiliation

- **Professional Memberships**
  1. Structural Engineering Institute (SEI)
  2. Engineering Mechanics Institute (EMI)
  3. The Institution of Engineers (India)
  4. The American Ceramic Society
- **Reviewer for the following journals**
  1. Journal of materials in civil engineering
  2. Journal of Non-Crystalline Solids

Software and Programming Languages

- **Packages Developed:**

  Peridynamics: *PeriDyn.jl, PDMaterialPoints.jl and PDBenchmark.jl*

  Molecular Dynamics: *MDSimulator.jl and MDBase.jl*

  Others: *GlassConversionPy, MLPipeline, MixModelsPytorch*

  Contribution to other packages: *jax-md*

  All packages can be accessed at the github repository.
- **Operating Systems:** Linux, MacOS and Windows
- **Softwares:** LAMMPS, NAMD, Peridigm, R.I.N.G.S, Ovito, VMD, Abaqus and STAADPRO
- **Languages:** Julia, Python, C++ and Matlab