Anuj Kumar

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Google Scholar | GitHub

Education

PhD in Mechanical Engineering, Minor in Applied Mathematics | (GPA: 4.0/4.0) Aug. 2019 – Jul. 2024
North Carolina State University *Raleigh, NC*

MS in Mechanical Engineering | (GPA: 4.0/4.0) Aug. 2019 – Sep. 2024
North Carolina State University *Raleigh, NC*

Bachelor of Technology in Mechanical Engineering | (GPA: 8.4/10.0) Jul. 2012 – May 2016
Indian Institute of Technology Kanpur *Kanpur, India*

Technical Skills

Programming Languages: Python, Julia, C, Fortran, MATLAB
Developer Tools: JAX, PyTorch, Git, VS Code, Azure ML, CI/CD
ML Architectures: Transformers, GNN, Neural ODE, CNN-based, Operator-learning-based, Neural Fields, PINNs
Software Packages/ Simulation Codes: ANSYS Fluent, CONVERGE, Tecplot, Cantera, S3D, US3D
Miscellaneous: MPI, HPC, PETSc, Turbulence, CFD, ROM, Chemical Kinetics, Dynamical Systems

Work Experience

Simulation Intelligence Scientist, Pasteur Labs Inc. Jul. 2024 – Present

- Design and implement production-ready graph/point-cloud surrogates in JAX and PyTorch; built ML-ready data pipelines and preprocessing for reliable training, testing, and deployment.
- Researched geometry encoding, global-interaction designs in MGNs and enforcing physical symmetries for steady-state surrogacy, enabling strong generalization on real-world CAD/CAE geometries.
- Design and implement subsampling and subgraph partitioning strategies to scale surrogacy to arbitrarily large CAE datasets, enabling training/inference without memory bottlenecks.
- Collaborate with cross-functional teams and external research partners to drive innovation, validate methodologies, and align Simulation Intelligence (SI) advancements with real-world constraints.

Research Assistant, Computational Combustion and Energy Sciences Lab, NCSU Jan. 2021 – Jul. 2024

React-DeepONet: An Efficient Deep Learning Chemical Kinetics Solver

- Developed an efficient and robust surrogate model for stiff chemical kinetics based on Deep Operator Networks
- Devised novel DeepONet architecture and training mechanism for robustness and physical constraints compliance
- Efficiently integrated Python(JAX) based surrogate ML model with C based CFD simulation code(Converge)
- Achieved speed-up of 100x for a highly complex turbulent combustion system of ECN Spray A

Turbulent Combustion Closure with Physics-Informed DeepONet *In collaboration with a lab-mate*

- Modeled physics-informed DeepONet and formulated its training mechanism in JAX
- Modified the architecture to isolate training for turbulence and combustion and extract the source terms for species
- Obtained species source terms and high-fidelity scalar values from sparse experimental observations

Reduced-Order Modeling of Turbulent Combustion *In collaboration with Sandia National Lab.*

- Formulated low-dimensional reacting flow Navier-Stokes equations in form of Principal Components (PCs)
- Modified S3D simulation code and obtained robust and accurate mapping for PC source terms via ML models
- Achieved speed-up of 80x with high accuracy on a laboratory-scale Bunsen flame

Research Aide - PhD, Multi-Physics Computations, Argonne National Lab. May 2023 – Dec. 2023

Neural ODE Surrogate Model for Stiff Chemical Kinetics

- Implemented second-order optimizer (Levenberg–Marquardt) for efficient model training and robust predictions
- Deployed physics-informed formulation for faster training and physically compliant and robust predictions
- Devised Latent Space Kinetics Identification framework through Neural ODE for large and complex fuels

Research Assistant, NCSU Aug. 2019 – Dec. 2020

Stability and Resolvent Analysis of Turbulent Boundary Flows

- Identified the unstable Reynolds number through eigenvalue analysis of the linearized flow operator
- Formulated reduced order dynamics through Resolvent Analysis on time averaged mean flow data
- Captured low-frequency unsteadiness and identified most-energetic turbulent eddies after flow separation in the shock-wave turbulent boundary layer interaction

Invited Talks and Conference Presentations

1. **Summer Geometry Initiative, MIT**(Guest Lecture) Jul. 2025
   Level-of-Detail Thinking of Scientific ML Surrogates
2. **The Crunch Group, Brown University**(Invited Talk) Feb. 2024
   Efficient and Physically Consistent Surrogate Modeling of Chemical Kinetics Using Deep Operator Networks
3. **NeurIPS 2023, Machine Learning and the Physical Sciences** Dec. 2023
   Physics - Informed Machine Learning for Reduced Space Chemical Kinetics
4. **Multi-Physics Computations, Argonne National Lab.** Dec. 2023
   Development of a Neural ODE-based Scientific Machine Learning Framework Towards Acceleration of Combustion CFD Simulations
5. **76th Annual Meeting of the APS Division of Fluid Dynamics** Nov. 2023
   A Framework for Combustion Chemistry Acceleration with DeepONets
6. **The 13th U.S. National Combustion Meeting** Mar. 2023
   Acceleration of Stiff Chemistry Integration with DeepONets
7. **Multi-Physics Computations, Argonne National Lab.**(Invited Talk) Mar. 2023
   Combustion Simulation Acceleration via Principal Component (PC) Transport and Deep Operator Networks (DeepONets)
8. **75th Annual Meeting of the APS Division of Fluid Dynamics** Nov. 2022
   Acceleration of Turbulent Combustion Simulation through Principal Components Transport and Machine Learning
9. **18th International conference on Numerical Combustion** May. 2022
   Reduced Order Modeling of Turbulent Combustion via Principal Component Transport

Leadership

Manager Mechanical Maintenance, Sinter Plant, Tata Steel India July 2016 – July 2019

- Ensured availability of Sinter Plant Mechanical equipment as per set target
- Led a team of 25 members and trained them on various training modules

Vice-President, MAE Graduate Student Association June 2022 – May 2023

- Led the organization of key social and professional departmental events, enhancing community engagement
- Chaired weekly GSA committee meetings, ensuring leadership continuity and decision-making efficacy

National Cadet Corps Cadet, 2 UP Composite Technical Regiment July. 2012 – May. 2013

- Actively engaged in adventurous activities including parasailing and target shooting, and contributed to awareness rallies

Publications

[1] **Anuj Kumar** and Tarek Echekki. Combustion Chemistry Acceleration with DeepONets. *Fuel*, 365:131212, 2024.

[2] Arsalan Taassob, **Anuj Kumar**, Kevin M. Gitushi, Rishikesh Ranade, and Tarek Echekki. A PINN-DeepONet framework for extracting turbulent combustion closure from multiscalar measurements. *CMAME*, 429:117163, 2024.

[3] Ki Sung Jung, **Anuj Kumar**, Tarek Echekki, and Jacqueline H. Chen. On the application of principal component transport for compression ignition of lean fuel/air mixtures under engine relevant conditions. *Combustion and Flame*, 260:113204, 2024.

[4] **Anuj Kumar** and Tarek Echekki. Physics - Informed Machine Learning for Reduced Space Chemical Kinetics. 2023. NeurIPS 2023 Workshop: Machine Learning and the Physical Sciences.

[5] Tadbhagya Kumar, **Anuj Kumar**, and Pinaki Pal. A Physics-Constrained NeuralODE Approach for Robust Learning of Stiff Chemical Kinetics. 2023. NeurIPS 2023 Workshop: Machine Learning and the Physical Sciences.

[6] **Anuj Kumar**, Martin Rieth, Opeoluwa Owoyele, Jacqueline H. Chen, and Tarek Echekki. Acceleration of turbulent combustion DNS via principal component transport. *Combustion and Flame*, 255:112903, 2023.

[7] **Anuj Kumar** and Tarek Echekki. A Framework for Combustion Chemistry Acceleration with DeepONets. *arXiv preprint arXiv:2304.12188*, 2023.