

Anuj Kumar

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EDUCATION

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

MS in Mechanical Engineering | (GPA: 4.0/4.0) en-route to PhD
North Carolina State University *Raleigh, NC*

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

TECHNICAL SKILLS

Programming Languages: Python, Julia, C, Fortran, MATLAB
ML Developer Tools: JAX, TensorFlow, PyTorch, Git, CUDA, PETSc
ML Architectures: Transformers, GNN, Neural ODE, Autoencoder, CNN, DeepONet, PINNs
Software Packages/ Simulation Codes: ANSYS Fluent, CONVERGE, Tecplot, Cantera, S3D, US3D
Miscellaneous: MPI, OpenMP, HPC, Turbulence, CFD, ROM, Chemical Kinetics, Dynamical Systems

RESEARCH EXPERIENCE

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

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 100 for a highly complex turbulent combustion system of ECN Spray A

Graph-Transformer: A Robust Surrogate Model for Turbulent Combustion

- Encoded spatial information of snapshots in embeddings via Message Passing Graph Neural Network Autencoder
- Modeled temporal variation of encoded snapshots in embedding space via decoder type Transformer (GPT-2)
- Graph-Transformer model is trained in an auto-regressive manner to obtain accurate long-time horizon predictions

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 to 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 80 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 Still-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

Thermal Buckling in a Jet Engine Compressor Disk

- Modeled a solid disk and performed eigenbuckling analysis via Ansys, aligning results with theoretical predictions
- Predicted the compressor disk's factor of safety using the established solid disk analysis method

Suppression of the Vortex Shedding around a Square cylinder

- Numerically investigated flow around a square cylinder; discretizing Navier-Stokes equation by Marker and Cell Method
- Identified suppression region and obtained drag coefficient for various sizes of control cylinders and Reynolds numbers

PROJECTS

Linear Reduced Basis Extraction from Autoencoder

Oct. 2021 – Dec. 2021

- Identified differences in reduced-order basis and modes from linear Autoencoder and POD
- Customized hidden layers of the decoder and regularized the loss function to get same basis as POD

Reduced-Order Dynamics of Compressible Channel Flow

Oct. 2020 – Dec. 2020

- Obtained reduced order basis for the turbulent flow in form of dominant POD and DMD modes
- Identified similarities in dominant flow frequencies and structures from DMD and Resolvent analysis

Development of an FVM solver for Euler equations on unstructured grids

Feb. 2020 – Apr. 2020

- Developed a compressible Euler equation solver in Fortran for 2D unstructured meshes
- Evaluated Fluxes using the Van Leer flux vector splitting and reconstruction-evolution (MUSCL) methods
- Validated the solver for subsonic, transonic and supersonic flows past a circular cylinder, NACA0012 airfoil and circular bump

INVITED TALKS AND CONFERENCE PRESENTATIONS

1. The Crunch Group, Brown University (Invited Talk)

Feb. 2024

Efficient and Physically Consistent Surrogate Modeling of Chemical Kinetics Using Deep Operator Networks

2. NeurIPS 2023, Machine Learning and the Physical Sciences

Dec. 2023

Physics - Informed Machine Learning for Reduced Space Chemical Kinetics

3. Multi-Physics Computations, Argonne National Lab.

Dec. 2023

Development of a Neural ODE-based Scientific Machine Learning Framework Towards Acceleration of Combustion CFD Simulations

4. 76th Annual Meeting of the APS Division of Fluid Dynamics

Nov. 2023

A Framework for Combustion Chemistry Acceleration with DeepONets

5. The 13th U.S. National Combustion Meeting

Mar. 2023

Acceleration of Stiff Chemistry Integration with DeepONets

6. Multi-Physics Computations, Argonne National Lab. (Invited Talk)

Mar. 2023

Combustion Simulation Acceleration via Principal Component (PC) Transport and Deep Operator Networks (DeepONets)

7. 75th Annual Meeting of the APS Division of Fluid Dynamics

Nov. 2022

Acceleration of Turbulent Combustion Simulation through Principal Components Transport and Machine Learning

8. 18th International conference on Numerical Combustion

May. 2022

Reduced Order Modeling of Turbulent Combustion via Principal Component Transport

LEADERSHIP

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

Manager, Mechanical Division of Sinter Plant, Tata Steel India

July 2017 – July 2019

- Efficiently managed planned shutdowns and breakdowns, minimizing operational disruptions
- Formulated and executed annual budgets, optimizing inventory management and cost efficiency
- Led and developed a team of 25 junior engineers, enhancing team performance and skillset

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 Echehki. Combustion Chemistry Acceleration with DeepONets. *Fuel*, 365:131212, 2024.
- [2] Ki Sung Jung, **Anuj Kumar**, Tarek Echehki, 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.
- [3] **Anuj Kumar** and Tarek Echehki. Physics - Informed Machine Learning for Reduced Space Chemical Kinetics. 2023. NeurIPS 2023 Workshop: Machine Learning and the Physical Sciences.
- [4] 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.
- [5] **Anuj Kumar**, Martin Rieth, Opeoluwa Owoyele, Jacqueline H. Chen, and Tarek Echehki. Acceleration of turbulent combustion DNS via principal component transport. *Combustion and Flame*, 255:112903, 2023.
- [6] **Anuj Kumar** and Tarek Echehki. A Framework for Combustion Chemistry Acceleration with DeepONets. *arXiv preprint arXiv:2304.12188*, 2023.