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, 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

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

Summer Research Intern, GE Aviation, General Electric India May 2015 – July 2015

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

Undergraduate Research Assistant, IIT Kanpur May 2014 – July 2014

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. **76th 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 2022 – 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 Echekki. Combustion chemistry acceleration with deeponets. *Fuel*, 365:131212, 2024.

[2] 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.

[3] **Anuj Kumar** and Tarek Echekki. 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 Echekki. Acceleration of turbulent combustion dns via principal component transport. *Combustion and Flame*, 255:112903, 2023.

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