# PRAKHAR SHARMA

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Area of interest: Physics-informed machine learning, Inverse modelling, Python development, Container technology (Docker/ Apptainer)

## Education

**Zienkiewicz Institute, Swansea University** — Swansea, United Kingdom
*PhD in Mechanical Engineering* — *Sep 2021 – Sep 2024*

- Fully-funded by Engineering and Physical Sciences Research Council (EPSRC) Doctoral Training Partnership (DTP) and UK Atomic Energy Authority (UKAEA).
- Received the NVIDIA academic hardware grant 2022, which included a NVIDIA RTX A5000 24GB.

**Zienkiewicz Institute, Swansea University** — Swansea, United Kingdom
*MSc in Computational Mechanics (Formerly Eramus Mundus)* — *Sep 2019 – Aug 2021*

- Fully-funded by Centre Internacional de Mètodes Numèrics a l'Enginyeria (CIMNE).
- Grade: 81.95% (Distinction)

**Dr. A.P.J. Abdul Kalam Technical University** — Lucknow, India
*B.Tech in Civil Engineering* — *Aug 2015 – May 2019*

- Partially funded by Ashoka merit studentship and AKTU university topper merit award.
- Grade: 84.88%, 1st division honors, gold medallist, and university topper.

## Work Experience

**Faculty of Science and Engineering, Swansea University** — Swansea, United Kingdom
*Teaching Assistant* — *Sep 2021 – Jan 2024*

- Industry 4.0 and Data Analytics Labs: Facilitated practical projects on predictive maintenance using clustering techniques and human activity classification with sensor data.
- Advanced Computational Methods: Guided numerical mathematics exercises in MATLAB, covering ODEs and convection-diffusion problems.
- Kinematics and Programming for Robot: Aided in robotics simulations covering kinematics, trajectory planning, and control systems.
- Mechanical Engineering Design: Mentored in the design and analysis of a remote-controlled car in SolidWorks, evaluating crash structures and vehicle dynamics.
- Mechanical Engineering Practice: Instructed on stress analysis in bolted joints, fluid dynamics, and stress concentration in ANSYS.

**Research Intern- ASTUTE Wales, Swansea University** — Jun – Aug 2020
*Computational Modelling & Topology Optimisation of Car Door Hinge* — *Remote*

- Explored the feasibility of using Additive layer manufacturing technique to manufacture the car door hinge of Titanium and Aluminium for Riversimple RASA.
- Conducted the structural analysis of a door hinge in three different positions for five different load cases and the topology optimisation of combined upstream system in ANSYS Mechanical.
- The mass of Titanium and Aluminium hinge was reduced by 83.20% and 56.51% of their original masses.

**Intern - Indian Institute of Technology (IIT BHU), India** — Jun – Jul 2018
*Analysis of Structural Elements and Plate Using Finite Element Method* — *In-campus*

- Developed MATLAB script for the finite element analysis of thin and thick plate. This includes coding of Gauss quadrature, Gauss elimination, Newton-Raphson, and isoparametric elements.
- Verified the accuracy of finite element simulations of rectangular and skew plates in ANSYS Mechanical by comparing the results to their corresponding analytical solutions.
- Developed a user-friendly GUI for Gauss quadrature and other integration techniques

## Dissertation

### PhD Dissertation
Sep 2021 – Sep 2024

*Supervisors: Perumal Nithiarasu , Llion Evans, Michelle Tindall* — *Swansea University*

- Initiated the foundational development of a digital twin (DT) for the sample under test (SUT), providing a theoretical framework focusing on ensuring safety of both the SUT and the testing facility CHIMERA.
- Explored the capabilities of PINNs to address challenges in modelling problems with discontinuous solutions, leveraging physics-informed ML tools such as DeepXDE and NVIDIA Modulus.
- Explored various inverse PINN approaches to assess their effectiveness in delivering a basic DT model.
- Developed a PINN based workflow for the reconstruction of solution to PDEs with limited experimental or simulation data.

### Masters Dissertation
Sep 2020 – Sep 2021

*Supervisor: Dunhui Xiao* — *Swansea University*

- Extended the SINDy and PDE-FIND framework for parameter estimation of differential equation from unstructured sparse measurements using radial basis functions (RBF) and fully-connected neural network for computing the derivatives.
- Discovered governing differential equation for 2D Burgers equation and flow past a cylinder from sparse simulation data with Gaussian noise.
- Developed a predictive data assimilation framework using an auto-encoder and LSTM to project high-dimensional fluid dynamics into a latent space, with subsequent state assimilation performed via an ensemble Kalman filter.

### Bachelors Dissertation
Jun 2018 – Apr 2019

*Supervisor: Rahul Singh* — *APJAKTU*

- Developed a set of MATLAB script to analyse skeletal structures using planar frames elements with 3 degrees of freedom per node to analyse beams, frames and truss.
- Developed GUI frontend in MATLAB GUIDE for data input and post-processing.

## Publications

- Sharma, P., Evans, L., Tindall, M., Nithiarasu, P. Hyperparameter selection for physics-informed neural networks (PINNs) – Application to discontinuous heat conduction problems. Numerical Heat Transfer, Part B: Fundamentals, 2023. DOI: 10.1080/10407790.2023.2264489
- Sharma, P., Evans, L., Tindall, M., Nithiarasu, P. Stiff-PDEs and Physics-Informed Neural Networks. Archives of Computational Methods in Engineering, 2023. DOI: 10.1007/s11831-023-09890-4
- Liu C, Fu R, Xiao D, Stefanescu R, Sharma P, Zhu C, et al. EnKF data-driven reduced order assimilation system. Engineering Analysis with Boundary Elements. 2022, Jun 1;139:46-55. DOI: 10.1016/j.enganabound.2022.02.016
- (Under review) Sparse measurements to solution reconstruction using Physics-informed neural networks (PINNs). Computer Methods in Applied Mechanics and Engineering (CMAME).
- (Contribution submitted) Physics-informed neural networks for solving partial differential equations. Artificial Intelligence in Heat Transfer: Advances in Numerical Heat Transfer Volume 6. Taylor & Francis.
- (Contribution submitted) Machine learning for modelling unstructured meshes in computational physics: A survey. Computer Physics Communications. (Co-authored with 11 Authors)

## Conference

- Physics-informed neural networks (PINNs) for solving forward and inverse thermal problems. Conference on Artificial Intelligence, Machine Learning and Advanced Computing (AIMLAC), Swansea University. 7-9 Jun 2023
- Hyperparameter Tuning of Physics-Informed Neural Networks (PINNs): Application to Discontinuous Heat Transfer Problems. Annual Conference of UK Association for Computational Mechanics (UKACM), University of Warwick. 19-21 Apr 2023

## Peer Reviews

- Archives of Computational Methods in Engineering, Springer Nature (3)
- International Journal for Numerical Methods in Biomedical Engineering, Wiley (1)
- Numerical heat transfer. Part B. Fundamentals, Taylor & Francis (2)

## Technical Skills

- **Machine Learning**: PyTorch, Hydra/ Hydra-zen, MLflow, Weights & Biases (W&B), NVIDIA Modulus
- **Programming Languages**: Python, Bash scripting, MATLAB, C++
- **Documentation**: LaTeX, LyX, Markdown, Sphinx, Jupyter book
- **Simulation**: ANSYS Mechanical and Fluent, SolidWorks, FEniCS, MATLAB PDE Toolbox and Simulink
- **Others**: Docker, Apptainer, Git, CI/CD, Github actions, Linux server setup

## Open source projects and contributions:

- **DeepINN**: Developed a Pytorch-based deep learning framework for solving PDEs using PINNs, featuring a geometry module wrapper, custom boundary condition and PDE modules, autograd capabilities, and an integrated training interface supporting both CPU and GPU with visualisation capabilities. Hosted a comprehensive documentation via Jupyter book on GitHub pages, along with automated Docker image deployment on Docker Hub, and PyPI package deployment for seamless installation.
- **HPC Helper**: Authored a comprehensive guide for machine learning on SLURM-based HPC clusters. This extensive documentation, covers a wide array of topics, including SSH automation, VNC and X2Go forwarding, Jupyter Lab setup, Python virtual environments, multi-instance (MIG) GPU job submission, parallel GPU usage with mpirun, GNOME Nautilus integration via proxy jump-based SFTP, Docker-to-Apptainer conversion, NVIDIA NGC Apptainer builds, and advanced container management.
- **DeepXDE**: Contributed to the DeepXDE library, dedicated to physics-informed machine learning, by resolving over 50 community queries and issues, and enhancing the project's documentation.
- **Dockerised LyX**: Developed a dockerised environment for the LyX document processor; utilised GitHub actions to build and deploy multiple container images with varying TeX Live configurations to Docker Hub; enabled X11 forwarding for GUI access from headless servers.
- **Image-Based Simulation (IBSim)**: Engaged in the development and documentation of the IBSim project, with a focus on the VirtualLab module. It enables users to conduct virtual simulations of physical laboratory experiments through image-based simulation techniques.
- **DeepXDE-frontend**: A beta project aims to develop a GUI frontend for DeepXDE in PyQt5. Focused on integrating CSG Geometry support and code optimisation.