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github | linkedin

SUMMARY

Results-driven data scientist with 6+ years post-PhD across **India, Japan, Germany** in AI, scientific ML (differentiable physics, reduced-order modeling, CFD, time-series forecasting, optimization). Led research interns and collaborated with **JAXA, KAIST, NVIDIA, ISRO**. **15 journal papers** (3 featured) and **16 conference papers** on AI/ML/CFD/optimization; focus on turning models into measurable business impact (rNPV projections across use-cases).

EDUCATION

INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI, IITG *2013-2019*

PH.D IN FLUIDS AND THERMAL ENGINEERING, MECHANICAL ENGINEERING

- Finite Volume/Immersed Boundary Methods for Compressible Flows: Development and Applications

GAUHATI UNIVERSITY, GIMT *2008-2012*

B.E. IN MECHANICAL ENGINEERING

- 2^{nd} position in the merit list of the Gauhati University

PROGRAMMING LANGUAGES	Python | C | MATLAB
ML LIBRARIES	PyTorch | PhiFlow | NVIDIA Modulus | DeepXDE | TensorFlow
DL STACK	Differentiable physics | ANN | CNN | Fourier Neural Operator (FNO) | DeepONet
LLM/NLP STACK	ChatGPT-3.5-turbo-16k | Llama-3.1-70B | LangChain
UNSUPERVISED ML	K-means | Hierarchical clustering | DBSCAN | PCA
SUPERVISED ML	Multiple Linear Regression | Logistic Regression | Random Forest
PYTHON/DATA STACK	Jupyter | Matplotlib | NumPy | pandas | scikit-learn | seaborn
MODELING	Finite Volume | Finite Difference
OPERATING SYSTEMS	Linux | macOS | Windows
OPEN-SOURCE OPTIMIZATION TOOLS	NSGA (KANGAL) | SAEA (MDOLab)

EXPERIENCE

SCIML RESEARCHER, SHELL PLC *Sept. 2023 - Present / India*

- AI-Agents assisted robust framework for end-to-end multi-physics fluid simulations using OpenFoam. Framework utilises RAG and state-of-the-art reasoning models such as GPT-4o, DeepSeek-R1, Llama-4-Scout-17B, O3, etc. Projected impact: **$14 million USD** rNPV.
- ML-based molecular discovery framework with multiple conflicting objectives. Projected impact: **$19 million USD** rNPV.
- Machine learning-based shape optimisation framework for Catalytic Partial Oxidation Reactor design. Projected impact: **$8.5 million USD** rNPV.
- Machine learning-based framework for novel gas-liquid contactor design for efficient CO_2 capture using amine-based solvents. Projected impact: **$9 million USD** rNPV.
- Spatio temporal prediction of full wave inversion (FWI) process to map earth's subsurface properties using Fourier Neural Operators (FNO). Paper accept for publication in EAGE HPC workshop 2025. Projected impact: **$50 million USD** rNPV.
- Hierarchical Physics informed neural network as fast proxy for steady state prediction of temperature profile inside MCHE, potentially impacting upto **$5 million**/LNG train
- DeepONet-based neural operator for time series forecast of auto cool down sequence of an MCHE for fault detection. Projected impact: **$19.5 million USD** rNPV.
- LLM based agentic AI framework (LEO) for complex single and multi-objective optimisation problems.
- Article on "On Scientific Foundation Models: Rigorous Definitions, Key Applications, and a Survey", as project lead. Presently under review.
- Language model based evolutionary optimisation (LEO) published in Neurocomputing Journal. (link)

• Hierarchical clustering for semantically similar images in hardhat dataset based on ResNet 50 encodings.

RESEARCH SCIENTIST, TECHNICAL UNIVERSITY OF MUNICH *Jan. 2022 - Sept. 2023 / Germany*

• Built a differentiable-physics ML framework for spatio-temporal flowfield prediction (incompressible flows). (link)

• Delivered 5 lectures (IN2298) on advanced deep learning for physical simulations (optimization, convergence, differentiable physics). (link)

• Co-organized a seminar and mentored Master's students (Deep Learning in Physics). (link)

RESEARCH SCIENTIST, KYUSHU UNIVERSITY *Sept. 2019 - Sept. 2021 / Japan*

• Developed surrogate assisted evolutionary algorithm (SAEA) pipelines for aerodynamic shape optimization of high-speed vehicles. (link)

• Developed a ROM-assisted NN for scramjet intake & combustor flowfields; Additional collaborations with JAXA and KAIST. (link) (link) (link)

• Led a team of research interns at Kyushu University with successful publiction in Journal (link)

PHD SCHOLAR, IITG *Jan. 2013 - June. 2019 / India*

• Developed an inhouse immersed boundary based finite volume (IB-FV) solver for high-speed compressible flows. The overarching aim of the thesis was to develop, validate and apply the IB-FV solver for aerodynamic shape optimisation in collaboration with ISRO. (link)

• Collaborated to University of Rennes to optimise an nozzle configuration for minimum radial velocity which was later experimentally examined. (link)

SUBJECT MATTER EXPERT, NANOBIZ PVT. LTD. *Jan. 2019-Apr. 2019 / India*

• Led a team while working as a subject matter expert to deliver the project titled "Technology landscape on artificial intelligence in the field of computational fluid dynamics" for Diamler, India

ASSISTANT PROJECT ENGINEER *Sept. 2012- Dec. 2012 / India*

• Worked as an asisstant project engineer for 3D design of a shock tube for its inhouse fabrication and setup at IITG

TRAINING AND CERTIFICATIONS

- Machine Learning in Production by deeplearning.ai (website)
- Generative AI with Large Language Models by deeplearning.ai (website)
- Data Driven Engineering (DDE), Isaac Newton Institute for Mathematical Science, Workshops 2023 (website)
- Institute for Computational and Mathematical Engineering (ICME), Stanford University, Summer Workshops 2021 | Fundamentals of Data Science: Machine learning, Deep learning, High Performance Computing (website)
- Large Language Model Agents by UC Berkeley (ongoing) (website)
- Langchain for LLM application development (website)
- R & D valuation and basic economics for technology by Shell, Plc

SELECTED PUBLICATIONS

- Brahmachary, S., Thuerey, N.,*"Unsteady Cylinder Wakes from Arbitrary Bodies with Differentiable Physics-Assisted Neural Network"* (**Physical Review E**, 2024) Link
- Brahmachary, S., Bhagyarajan, A., and Ogawa, H.,*"Fast Estimation of Internal Flowfields in Scramjet Intakes via Reduced-Order Modeling and Machine Learning"* (**Physics of Fluids**, 2021, Selected as featured article) Link
- Brahmachary, S., Joshi, S., Panda, A., Konerapalli, K., Sagotra, A., Patel, H., Sharma, A., Jagtap, A., Kalyanaraman, K. "Large Language Model-Based Evolutionary Optimizer: Reasoning with Elitism" (**Neurocomputing**, 2024) Link

OTHERS

- Invites talks at Paral-Intelligence seminar series, Worcester Polytechnic Institute WPI, Karlsruhe Institute of technology (KIT, Germany) and Space Transportation Systems Engineering Laboratory, Kyushu University (STSEL, Japan)
- Blogs on topics "When Kolmogorov-Arnold network meet PiNNs: Good, Bad and the Ugly Link", "Differentiable Physics for Unsteady Fluid Dynamics Link", "Principal component analysis in aerodynamic shape optimisation Link"
- Life member: Society for Shock Wave Research (SSWR) and Member of the Soft Computing Research Society (SCRS)