

Shobhan Roy, PhD

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SUMMARY

Computational physicist and scientific machine learning researcher building physics-aware neural operators (PARC, D-PARC) and high-fidelity multi-physics simulators for materials under extreme loading. 7 peer-reviewed journal papers across Shock Waves, J. Fluid Mechanics, J. Applied Physics, and APL Machine Learning. Production HPC track record — 140M-cell, 7,000-core, ~2.8M CPU-hour campaigns on DoD clusters. Translates first-principles physics into ML surrogates that respect conservation laws, causality, and entropy constraints of the governing PDEs.

CORE SKILLS

- Scientific ML: Physics-informed neural networks, neural operators (PARC, D-PARC, FNO, DeepONet), differentiable simulation, physics-aware evaluation, surrogate modeling, uncertainty quantification, diffusion models, U-Net, CycleGAN
- Scientific Computing & HPC: Python, Fortran 90, C++, R, Bash; MPI, domain decomposition, Slurm/PBS, parallel I/O; sharp-interface / level-set / WENO finite-volume methods; multi-thousand-core campaigns on DoD HPC clusters
- ML Frameworks & Tooling: PyTorch, PARCtorch, TensorFlow; Git, LaTeX, Jupyter; LLM-assisted research workflows (Copilot CLI, VS Code agent mode) for code review, scheme prototyping, and reproducible build pipelines
- Domains: Shock physics, energetic materials, detonation, equation-of-state and reactive-burn modeling, multi-material interface dynamics, microstructure-resolved simulation, materials informatics

EXPERIENCE

Postdoctoral Research Scholar — IIHR–Hydroscience & Engineering, University of Iowa

May 2025 – Present · Iowa City, IA

- Co-shaped the architectural design of D-PARC — a deformable-convolution neural operator encoding differential operators for physics-aware emulation of nonlinear transport — providing physics-derived design constraints, curating ground-truth DNS datasets, and defining the evaluation criteria that decide whether learned models respect conservation, interface, and entropy structure (Beerman, Roy, et al., arXiv 2026).
- Designed and executed high-resolution simulations of pore collapse, hotspot formation, and shock propagation to benchmark physics-aware deep learning surrogates against physically critical quantities (peak pressure, temperature localization, reaction-front velocity).
- Architected novel numerical interfacial treatments for materials undergoing solid-with-strength → gaseous (hydrodynamic) phase change, extending the multi-material solver to chemically decomposing systems; augmented JWL and Mie-Grüneisen equations of state to handle the full tensile-to-high-compression pressure range required for macroscale shock-to-detonation simulations.
- Built data-driven surrogate models and closure relations linking mesoscale hotspot metrics to macroscale continuum predictions, enabling design-loop use of expensive first-principles simulations.
- Interfaced with University of Virginia's ML research group (Baek lab) as the simulation-side lead — curating ground-truth DNS databases across canonical flow problems and energetic-material regimes, selecting simulation parameters to maximize physical coverage, and defining validation benchmarks for training PARC and D-PARC neural architectures.
- Mentoring 2 PhD students on simulation methodology, HPC workflows, and SCIMITAR3D adoption; serving as simulation-side technical reference for junior researchers at IIT Delhi and IIT Madras on a co-developed multi-physics solver. Contributing to a newly awarded ONR-MURI on non-equilibrium reactive dynamics in energetic materials.

Graduate Research Assistant (PhD) — University of Iowa

Aug 2019 – Apr 2025 · Iowa City, IA

- Extended SCIMITAR3D, an in-house multi-material reactive simulation code, into a sharp-interface framework for shock-to-detonation transition in heterogeneous energetic materials; integrated full 5th-order WENO reconstruction and Riemann-based ghost-fluid coupling, eliminating the 2.5–3× grid-refinement overhead otherwise required for equivalent accuracy at lower order.

- Designed and managed production-scale simulation campaigns on DoD HPC clusters — 140M grid cells, 7,000 CPU cores, ~2.8M CPU-hours — resolving sub-micron hotspot features at the grid-convergence threshold for energetic-material initiation studies.
- Validated mesoscale shock-initiation predictions against experimental data from collaborators at UIUC (Dlott lab) and Los Alamos National Laboratory, selecting constitutive models and resolution criteria for head-to-head comparison at sub-grain fidelity.
- Led simulation and physics-validation components of the HEDS framework (Heterogeneous Energetic Material Damage Simulator) — a deep learning + computational mechanics pipeline learning microstructure-to-sensitivity mappings while respecting conservation and damage-mechanics constraints; contributed physics-aware evaluation criteria, simulation integration, and interpretation of learned representations (APL Machine Learning, 2025).
- Bridged simulation contributions across a 7-university AFOSR-MURI ('Microstructurally-Aware Continuum Models for Energetic Materials,' 2019–2024) — planning and executing mesoscale shock-initiation simulations in coordination with the UIUC experimental group and the consortium's broader computational/ML teams.

Graduate Research Scholar (MS) — IIT Madras, India

Jul 2015 – Jun 2019 · Chennai, India

- Characterized normal-shock/boundary-layer interaction (SBLI) and porous-medium flow control through combined CFD simulations and transonic wind-tunnel experiments; designed finite-volume RANS campaigns to evaluate shock-control effectiveness and validated against experimental data from a novel nozzle configuration (Shock Waves 2021; AIAA Journal 2019).
- Formulated an analytical model for asymmetric wedge-induced Mach reflection in 2-D steady supersonic flows (parallel research with Prof. G. Rajesh; Journal of Fluid Mechanics 2019). Subsequently contributed to DRDO's Variable Camber Morphing Wing project (2018–2019) at IIT Madras's Center for Propulsion Technologies through immersed-boundary implementation and preliminary aerodynamic analysis.

SELECTED PUBLICATIONS

Reverse chronological. Full list at [Google Scholar](#).

1. Beerman, J.T., Roy, S., Udaykumar, H.S., Baek, S.S. — Size is Not the Solution: Deformable Convolutions for Effective Physics-Aware Deep Learning, arXiv preprint (2026).
2. Roy, S., Seshadri, P.K., Okafor, C., Johnson, B.P., & Udaykumar, H.S. — High-Fidelity Simulations of Shock Initiation of an Energetic Crystal–Binder System Due to Flyer Impact, Shock Waves 36(2), 2026.
3. Fang, I., Roy, S., Nguyen, P.C.H., Baek, S.S., Udaykumar, H.S. — Heterogeneous Energetic Material Damage Simulator (HEDS): A Deep Learning Approach to Simulate Damage–Sensitivity Linkages, APL Machine Learning 3(2), 2025.
4. Roy, S., Johnson, B.P., Zhou, X., Nguyen, Y.T.H., Dlott, D.D., & Udaykumar, H.S. — Hot Spot Ignition and Growth from Tandem Micro-Scale Simulations and Experiments on Plastic-Bonded Explosives, Journal of Applied Physics 131(20), 2022.
5. Roy, S., Gopalapillai, R. — An Analytical Model for Asymmetric Mach Reflection Configuration in Steady Flows, Journal of Fluid Mechanics 863, 242–268, 2019.

AWARDS

- Ballard & Seashore Dissertation Fellowship, University of Iowa (2025)
- 1st Place (Graduate Category, Mechanical Engineering), Research Open House Poster Competition, College of Engineering, University of Iowa (2025)
- Dean's Graduate Fellowship, College of Engineering, University of Iowa (2019)

EDUCATION

PhD, Mechanical Engineering — University of Iowa, 2025 · Advisor: Prof. H.S. Udaykumar

Dissertation: A versatile framework for high-fidelity computations of high-speed reactive multi-material dynamics.

MS (Research), Aerospace Engineering — IIT Madras, India, 2019 · Advisors: Prof. Santanu Ghosh & Prof. G. Rajesh

BTech, Mechanical Engineering — NIT Durgapur, India, 2015