Kartikey Singh

Undergraduate Researcher | Scientific Machine Learning, Geometric DL & Computational Mathematics

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Research Profile

Undergraduate mathematical researcher investigating the intersection of **Scientific Machine Learning (SciML)**, **Symplectic Geometry**, **Inverse Problems**, and **High-Dimensional Stochastic PDEs**. Author of **8 research manuscripts** and **2 open-source scientific computing packages**. Architect of the **"Adaptive Subspace (AS) Paradigm"**—a cohesive three-act theoretical lineage resolving destructive gradient interference across parameter manifolds, progressing from static algebraic null-space direct-sum decomposition (Act I: *null-space-pinn*), to autonomous parameter-space Adaptive Mesh Refinement in physical PDEs (Act II: *as-pinn*), to dynamic Mixture-of-Experts in transformer latent feature manifolds (Act III: *as-vit-multitask*). Primary methodology emphasizes **structural geometric invariants** (exact symplectic 2-form conservation, Arnold extended contact phase spaces, and B-spline sensitivity projections) over black-box heuristics.

Education

2023–2027 **B.Sc. (Honours) Mathematics**, *University of Delhi*, Delhi, India

- **Degree Structure:** 4-Year Undergraduate Research Degree with advanced research specialization.
- **Undergraduate Dissertation Supervisor: Prof. Vinay Kumar** (Department of Mathematics).
- **Relevant Core Coursework:** Real Analysis, Multivariable Calculus, Ordinary & Partial Differential Equations, Complex Analysis, Abstract Algebra, Linear Algebra, Numerical Analysis, Probability & Statistics.
- **Independent Scholarly Trajectory:** Rigorous, self-directed specialization in geometric deep learning, symplectic mechanics, nonlinear PDEs, and high-performance scientific computing developed alongside the formal undergraduate program.

Research Manuscripts & Preprints

Pillar I: Inverse Problems, Symplectic Astrodynamics & Fluid Mechanics

Under Review **Shape Inversion in Electrical Impedance Tomography**, *IEEE Transactions on Computational Imaging (TCI)*

"Derivative-Informed Neural Forward Surrogates with Directional Sensitivity Supervision for Shape Inversion in Electrical Impedance Tomography"

- **Authors:** Kartikey Singh (Sole Author / Lead Investigator).
- **Mathematical Formulation:** Parameterized closed inclusion boundaries via 64-dimensional periodic cubic B-splines coupled to mollified boundary-integral winding indicators. Verified analytic sensitivities $\mathbf{J}_{\mathrm{FEM}} = \mathbf{J}_\sigma \frac{\partial \boldsymbol{\Sigma}}{\partial \boldsymbol{\theta}}$ against directional finite differences ($< 3.2 \times 10^{-4}$ discrepancy).
- **Algorithmic Novelty:** Introduced **Stochastic Directional JVP Supervision** on $\mathbb{S}^{63}$, reducing retained tangent autograd branches from 64 to 1 per sample and bounding peak VRAM to $342.8\,\mathrm{MB}$.
- **Empirical Results:** Zero-online-FEM inversion delivers a $\mathbf{56.8}\times$ wall-clock speedup ($35.6\,\mathrm{ms}$ vs $2.02\,\mathrm{s}$/step) with a consensus IoU of 0.8235 and a 99.57% noise robustness rate across 234 trials.
- **Codebase:** `https://github.com/KartikeyaGangwar/eit-neural-surrogate-inversion`
  Preprint DOI: 10.5281/zenodo.22096368

Working Paper **CPA-SHNN: Symplectic Neural Networks for Celestial Mechanics**, *Target: Astronomy & Computing / New Astronomy*

"Causality-Preserving Adaptive Symplectic Hamiltonian Neural Networks (CPA-SHNN) for Autonomous and Non-Autonomous Multi-Body Celestial Gravitational Dynamics"

- **Authors:** **Kartikey Singh** (Lead Author), **Prof. Vinay Kumar** (Supervisor & Senior Author).
- **Mathematical Formulation:** Proved *Theorem 1* (Separable Symplectic Kinetic-Coriolis Decomposition, $\nabla_{\mathbf{z}} \cdot \mathbf{f}_\theta \equiv 0$) and *Theorem 2* (Arnold Extended Contact Phase Space $\mathbf{Z}_{\text{ext}} = (\mathbf{q}, t, \mathbf{p}, p_t)$, $\mathcal{K}_\theta \equiv 0$).
- **Empirical Benchmarks:** Benchmarked across 6 chaotic multi-body celestial systems from Prof. Vinay Kumar's research portfolio (Binary Quasars, Restricted 6-Body, Sitnikov 5-Body, Magnetic Yukawa, Variable-Mass Binaries), preserving energy to machine precision ($\Delta\mathcal{H} \leq 10^{-4}\%$).
- **Ablation Discoveries:** Multi-scale Fourier features achieved up to a $\mathbf{126.40}\times$ error collapse on gravitational saddle singularities. Poincaré generating function ablations demonstrated the necessity of continuous vector fields.
- **Codebase:** `https://github.com/KartikeyaGangwar/cpa-shnn`

Working Paper **Formulation Failure Modes in High-Re Fluid Dynamics**, *Target: CMAME / Physics of Fluids*

"Formulation-Induced Failure Modes in Physics-Informed Neural Networks for High-Reynolds-Number Incompressible Flows: Operator Conditioning and False Convergence"

- **Authors:** **Kartikey Singh** (Sole Author / Lead Investigator).
- **Scientific Investigation:** Conducted controlled formulation-level study on 2D lid-driven cavity flow at $\mathrm{Re} = 1000$, contrasting Streamfunction-Pressure ($\psi - p$) against Streamfunction-Vorticity ($\psi - \omega$).
- **Theoretical Discovery:** Discovered that $\psi - \omega$ PINNs suffer from **False Convergence and Operator Diffusion** because continuous mesh-free networks lack discrete spatial stencils for **Thom's wall-vorticity formula**, attenuating secondary corner eddies by $> 50\%$.
- **Hodge Projection:** Proved that retaining pressure p in $\psi - p$ serves as an elliptic Lagrange multiplier (Helmholtz-Hodge projection), successfully capturing primary and secondary vortex cores. Benchmarked against Ghia et al. (1982) and Botella & Peyret (1998).
- **Codebase:** `https://github.com/KartikeyaGangwar/pinn-fluid-formulations`

Pillar II: The Adaptive Subspace (AS) Optimization Paradigm

Preprint **Null-Space Gradient Conflict Decoupling in PINNs**, *Target: Journal of Computational Physics (JCP)*

"Decoupling Gradient Conflicts in Physics-Informed Neural Networks via Null-Space Parameter Subspaces"

- **Authors:** **Kartikey Singh** (Lead Author), **Samarjeet Malik** (Co-Author).
- **Mathematical Formulation:** Algebraically decomposed the parameter manifold into orthogonal direct-sum subspaces ($\Theta = \Theta_0 \oplus \Theta_1$ with $\mathcal{W}_0 \mathcal{W}_1^T = \mathbf{0}$) blended via a C^2 **Quintic Hermite operator** ($\psi(\xi) = 6\xi^5 - 15\xi^4 + 10\xi^3$).
- **Theoretical Guarantee:** Proved structural gradient orthogonality ($\langle \nabla\mathcal{L}_{\text{if}}, \nabla\mathcal{L}_{\text{des}} \rangle \equiv 0$) on saturated domains, eliminating boundary clash without sacrificing second-order PDE regularity ($\nabla^2 u$).
- **Benchmarks:** Evaluated across 6 physical benchmarks, including 3D Linear Paul Ion Traps with harmonic multipole analysis and CAD coordinate bivariate quadratic polynomial distillation ($R^2 > 0.95$).
- **Codebase:** `https://github.com/KartikeyaGangwar/null-space-pinn` **Preprint DOI:** 10.5281/zenodo.22132799

Working Paper **Adaptive N-Subspace PINN (AS-PINN)**, *Target: SIAM Journal on Scientific Computing (SISC)*

"Adaptive N-Subspace Physics-Informed Neural Networks (AS-PINN): Autonomous Domain Decomposition via Parameter-Space Adaptive Mesh Refinement"

- **Authors: Kartikey Singh** (Lead Author / Principal Investigator).
- **Algorithmic Novelty:** Developed an autonomous parameter-space AMR engine using vectorized per-sample Gram alignment profiling ($\mathcal{G}_{ij} = \cos\angle(\mathbf{g}_i, \mathbf{g}_j)$) via `torch.func.vmap`) with exact zero-disruption cleavage invariance ($\|u^{(N+1)} - u^{(N)}\| = 0$).
- **Empirical Verification:** Validated across 9 canonical PDEs (Burgers, Convection 2D, Quantum NLS, 4D Diffusion, Bratu 2D, Kovasznay, Cavity NS, Klein-Gordon), achieving a $\mathbf{725.6}\times$ loss reduction over standard PINNs, PCGrad, and CAGrad on high-frequency Helmholtz ($k = 4\pi$).
- **Codebase:** `https://github.com/KartikeyaGangwar/as-pinn`

Working Paper **AS-ViT: Adaptive Subspace Vision Transformers**, *Target: IEEE TPAMI / CVPR*

"AS-ViT: Adaptive Subspace Vision Transformers with Autonomous Gradient-Clash Routing for Multi-Task Learning"

- **Authors: Kartikey Singh** (Lead Author / Principal Investigator).
- **Architectural Innovation:** Resolved negative transfer in dense multi-task vision backbones (segmentation, depth, normals, edges) by continuously tracking inter-task Gram matrix eigenvalues ($\lambda_{\min}(\mathcal{G}) < -\tau_{\text{conflict}}$) and cleaving dedicated latent expert subspaces using Partition of Unity (PoU) gating.
- **Empirical Results:** Outperformed monolithic ViTs, PCGrad, CAGrad, and fixed MoEs on NYUv2, Cityscapes, and Taskonomy benchmarks, achieving $+5.84\%$ mean multi-task gain (ΔM) with zero manual expert tuning.
- **Codebase:** `https://github.com/KartikeyaGangwar/as-vit-multitask`

Pillar III: High-Dimensional Stochastic Systems & Uncertainty Quantification

Working Paper **High-Dimensional American Basket Options (Deep-EEP-PINN)**, *Target: Quantitative Finance*

"Deep Early Exercise Premium Physics-Informed Neural Network for High-Dimensional Free-Boundary Obstacle Problems"

- **Authors: Kartikey Singh** (Lead Author / Principal Investigator).
- **Mathematical Formulation:** Embedded the analytical Kim (1990) / Carr-Jarrow-Myneni (1992) Early Exercise Premium decomposition into a hard-constrained boundary ansatz: $V_{\text{Amer}} = V_{\text{Euro}}^{\text{exact}} + e_\theta(\mathbf{S}, t)$ with $e_\theta(\mathbf{S}, T) \equiv 0$.
- **High-Dimensional Breakthrough:** Priced correlated American basket options up to $\mathbf{d = 50}$ **assets (1,225 correlations)**, breaking Bellman's Curse of Dimensionality (N^d) via Directional Autograd Hessian Trace Contraction in $\mathcal{O}(d)$ linear complexity ($< 3\,\text{GB}$ VRAM). Validated against 100,000-path Longstaff-Schwartz Monte Carlo and Crank-Nicolson PSOR (0.37% relative error).
- **Codebase:** `https://github.com/KartikeyaGangwar/Deep-EEP-PINN`

Working Paper **Bayesian PINN Fidelity & Posterior Distortion**, *Target: Reliability Engineering & System Safety / Inverse Problems*

"Bayesian PINN Fidelity & Parameter-Resolved Error Localization Framework"

- **Authors: Kartikey Singh** (Lead Author / Principal Investigator).
- **Epistemological Investigation:** Formally investigated how PINN forward surrogate approximation errors distort Bayesian inverse posteriors.
- **Proposed Diagnostic Metric:** Formulated the **Bayesian Fidelity Ratio (BFR)**: $\text{BFR} = \mathcal{W}_1(\pi_E, \pi_A)/\mathcal{W}_1(\pi_{E,1}, \pi_{E,2})$ based on 1-Wasserstein optimal transport distance normalized by empirical MCMC stochastic noise floors under paired control chains.
- **Codebase:** `https://github.com/KartikeyaGangwar/PINN-Bayesian-Posterior-Fidelity`

Scientific Software & Computational Infrastructure

Open-Source **High-Performance 2D Navier–Stokes FDM Solver**, *C++ / Vectorized NumPy*

- **Lead Developer: Kartikey Singh**.
- **Purpose:** Engineered from first principles to serve as the high-fidelity numerical ground truth generator for SciML fluid benchmark validation.
- **Numerical Methods:** Coupled Streamfunction–Vorticity (ψ–ω) formulation employing the **Alternating Direction Implicit (ADI)** scheme for parabolic vorticity transport and **Red-Black Successive Over-Relaxation (SOR)** with Chebyshev acceleration for the elliptic streamfunction Poisson equation.
- **Benchmark Validation:** Validated rigorously up to $\mathrm{Re} = \mathbf{1000}$ on dense 251×251 spatial grids ($63{,}001$ degrees of freedom), achieving strict alignment with benchmark spectral data from Ghia et al. (1982) and Botella & Peyret (1998).
- **Open-Source Dissemination:** `https://github.com/KartikeyaGangwar/Lid-Driven-Cavity-FDM-Solver` **DOI:** 10.5281/zenodo.18312938

Open-Source **BeamNG Research SDK (BRSDK)**, *Lua / Python / Systems Programming*

- **Architect & Lead Developer: Kartikey Singh**.
- **System Architecture:** High-frequency, deterministic telemetry extraction and autonomous driving simulation framework operating inside the **2000 Hz Vehicle Lua physics thread** of BeamNG.drive and BeamNG.tech.
- **Near-Zero-Allocation Hot Path:** Eliminates Lua garbage collection spikes during telemetry streaming, logging thousands of physical signals per second (kinematics, powertrain, multi-body suspension, tire friction) without physics stepping disruption.
- **Scientific Interface:** Integrates RFC 8259 JSON metadata sidecars for vehicle constraint immutability, dynamic schema layouts, and Python bindings for reinforcement learning and system identification.
- **Open-Source Dissemination:** `https://github.com/KartikeyaGangwar/BRSDK` **DOI:** 10.5281/zenodo.21729606

Technical Expertise & Methodologies

Scientific Machine Learning Physics-Informed Neural Networks (PINNs), Hamiltonian Neural Networks (HNNs), Symplectic Neural ODEs, Deep Surrogate Inversion, Boundary-Encoded Neural Ansätze, Fourier Positional Encodings, Neural Operators.

Theoretical Mathematics Symplectic Geometry & Differential Forms, Canonical Phase Space Topologies, Contact Hamiltonian Mechanics, Nonlinear Parabolic & Elliptic PDEs, Free-Boundary Obstacle Problems, Optimal Transport & Wasserstein Metrics, Functional Analysis, Operator Theory.

Autograd & Deep Learning Engineering PyTorch (low-level custom autograd engines, `torch.func.vmap`, forward-mode automatic differentiation, Jacobian-Vector Products (JVP), Hessian-vector contractions), CUDA acceleration, GPU memory profiling, mixed-precision arithmetic.

Numerical Analysis & Optimization Finite Element Method (FEM), Finite Difference Schemes (ADI, Red-Black SOR, Crank-Nicolson), Symplectic Runge-Kutta (RK4), L-BFGS (Strong-Wolfe curvature line search), AdamW, Gradient Surgery (PCGrad, CAGrad), Markov Chain Monte Carlo (MCMC, Metropolis-Hastings).

Languages & Developer Toolchain Python (NumPy, SciPy, Matplotlib, PyTorch), C++, Git/GitHub, Linux/Bash, LaTeX, VS Code, Kaggle GPU Environments.

Scholarly Philosophy

Open Science & Rigor Firm conviction in reproducible computational science. Every research framework is accompanied by self-contained automated benchmark runners, zero-redundancy unit testing, full ablation matrices, and permissive open-source licensing (MIT / Apache 2.0).