Gaurav Khanal

Saint-Étienne, France   gaurav.khanal@etu.univ-cotedazur.fr   +33 7 45 94 71 00

Website   LinkedIn   GitHub

PERSONAL SUMMARY

Final-year MSc Data Science & AI candidate focused on scientific machine learning for physical systems, particularly physics-informed inverse problems, geometry/topology-aware representation learning, material behavior, and equivariant neural networks. Research experience spans continuum mechanics, structured 3D data, multiscale topology, wave-based reconstruction, and graph signal processing.

EDUCATION

MSc in Data Science and Artificial Intelligence *Sep. 2024—Aug. 2026*
Université Côte d'Azur, Sophia Antipolis, France
EFELIA Bourse d'Excellence 2025 *(Scholarship of Excellence)*

BA in Economics and Accounting *Aug. 2009—May 2013*
Westminster College, Fulton, Missouri, USA

PROFESSIONAL EXPERIENCE

Research Intern, *Predictive Constitutive Modeling of Atrial Appendage Tissue* *Apr. 2026—Present*
Mines Saint-Étienne | Centre Ingénierie et Santé | SAINBIOSE Lab Inserm U1059

- Developing mechanics-informed ML models to infer specimen-specific force response and constitutive behavior of atrial appendage (AA) tissue from projected 2D thickness maps and 3D surface mesh scans.
- Engineering 3D morphology and anisotropy descriptors from tissue meshes, including loading-relative geometry, curvature morphology, Laplace–Beltrami spectral signatures, principal-curvature ridge/saddle/cap-cup features, and fabric-tensor anisotropy.
- Extending the framework with point-cloud and mesh representation learning, including PointNet++, DGCNN, and mesh GNN baselines, to predict mechanical properties and constitutive parameters from 3D atrial tissue morphology.
- Investigating topology-aware descriptors for 3D tissue scans using topological data analysis, including persistent-homology-based summaries of multiscale shape, fold, ridge, and cycle structure, to assess whether topological features improve prediction of mechanical properties and constitutive parameters beyond geometric and graph-based baselines.
- Developing hybrid mechanics-informed models that map learned 2D/3D tissue representations to constitutive-law parameters, with force-response curves generated through differentiable Veronda–Westmann (isotropic) and/or Holzapfel–Gasser–Ogden (anisotropic) constitutive layers.
- Formulating hybrid energy-based models in which learned geometry representations predict constitutive parameters or specimen-specific strain-energy functions, with force–stretch responses generated through differentiable constitutive laws and energy derivatives.

RESEARCH EXPERIENCE

PERSIST: Topology-Guided Multiscale Domain Identification in Spatial Transcriptomics *Sep.—Dec. 2025*

- Developed PERSIST, an unsupervised topology-guided framework for spatial transcriptomics domain identification, addressing resolution sensitivity by inferring intrinsic tissue scales rather than relying on fixed clustering resolutions, smoothing radii, or neighborhood parameters.
- Constructed alpha-complex filtrations over tissue coordinates and used H_1 persistent homology birth-time distributions to identify topology-informed spatial scales associated with compartmentalization and boundary structure.
- Designed a Discrete Exterior Calculus-based multiscale stability field using 0-form smoothing, discrete gradients, topology-weighted local variation, bootstrap robust-core estimation, and Morse-like basin decomposition to separate stable domains, transition regions, and high-gradient boundaries.
- Applied PERSIST to breast cancer, human lymph node, and mouse brain spatial transcriptomics datasets, recovering biologically interpretable tissue organization supported by marker enrichment and H&E histology overlays.

Beyond Energy MAE: Input-Gradient Geometry in Molecular GNNs *(In progress)* *May 2026–Present*

- Designing a controlled energy-only comparison of SchNet and NequIP on 50,500 QM7-X molecular families, using a within-family low-to-high displacement split and held-out reference forces to test whether comparable energy MAE conceals differences in learned energy-surface geometry.
- Developing numerical $SE(3)$ symmetry audits and Wilson B-matrix/Shapley attribution of model energy gradients across bond, angle, and torsional subspaces for interpretable analysis of molecular energy models.

Graph Signal Processing for Characterization of Multipolar Electrograms in AF *Oct. 2025—Mar. 2026*

- Developed a geometry-aware graph signal processing framework for multipolar intracardiac electrograms (EGMs) in Atrial Fibrillation (AF), modeling PentaRay catheter electrodes as graph nodes and EGM recordings as graph signals over catheter geometry.
- Applied joint Short-Term Fourier Transform and Graph Fourier Transform analysis and graph total variation to detect rotor-proximal spatial discordance, showing that AF-band graph-time variation captured intermittent wavefront-collision patterns missed by per-channel temporal features.
- Proposed edge-flow extensions of catheter graph signals, enabling propagation dynamics to be interpreted through discrete differential operators and motivating Helmoltz-Hodge-style separation of planar/focal activation, rotor-like circulation and obstacle-related harmonic flow, providing a mechanistic route toward rotor-proximity indicators for AF ablation guidance.

Physics-Informed Image Registration for Hyperelastic Material Identification *Jan.—Apr. 2026*

- Developed a unified PINN framework for soft-tissue characterization that couples differentiable image registration with hyperelastic material-parameter identification, replacing the classical sequential digital image correlation (DIC) → displacement extraction → constitutive fitting pipeline.
- Integrated Ogden-model equilibrium constraints, explicit gravity loading, boundary-condition penalties, and multi-step reaction-force losses to regularize deformation fields and improve identifiability of material parameters.
- Generated synthetic tissue image sequences replicating the Gao–Desai porcine liver experiment, including gravity-induced pre-compression, tensile loading, natural-texture synthesis, and realistic imaging noise.
- Recovered Ogden parameters on synthetic validation with relative errors of 0.02% for μ and 0.006% for α, while implicitly resolving the zero-strain reference-state ambiguity that classical DIC pipelines estimate heuristically.

Deep Learning for Full Waveform Inversion: Seismic Waveforms to Velocity Fields *May—Aug. 2025*

- Developed a data-driven FWI framework to learn the inverse map from multisource seismic shot gathers to subsurface velocity fields, targeting key limitations of conventional FWI: high computational cost, ill-posedness, and cycle skipping.
- Designed a hybrid Swin V2 Transformer + enhanced U-Net architecture combining long-range wavefield dependency modeling with high-fidelity spatial reconstruction of geological layers, faults, and heterogeneous structures.
- Built a scalable HPC OpenFWI training pipeline for 470,000 Vel/Fault/Style samples using memory-mapped data loading, GPU augmentations, PyTorch DDP/AMP, EMA checkpointing, and H100 GPUs.
- Formulated a custom loss with inverse frequency weighting, and achieved best validation MAE of 63.27 m/s, with SSIM 0.8725–0.9188 across OpenFWI families; errors were concentrated mainly near sharp interfaces and fault boundaries.

SKILLS

Computer Languages: Python, R, MATLAB

Machine / Deep Learning Frameworks: PyTorch, JAX, Equinox, Flax, TensorFlow, scikit-learn

Scientific Computing & Geometry: NumPy, pandas, SciPy, CuPy, Gudhi, Trimesh, PyVista, ParaView

HPC, MLOps & Development: Grid5000, OAR, CUDA, PyTorch DDP, Git, Docker, MLflow, TensorBoard

Languages: English (C2—*fluent*), French (B1—*intermediate*), Spanish (A2—*elementary*)

CONTRIBUTIONS & COMPETITIONS

TopoBench Topological Deep Learning (TDL) Challenge 2026

- Implemented and benchmarked a TopoBench-native E(n)-equivariant topological neural network, integrating graph-to-combinatorial-complex lifting, rank-wise message passing, geometric invariants, equivariant coordinate updates, coordinate policies, unit tests, and GraphUniverse + QM9 evaluation.

OTHER PROFESSIONAL EXPERIENCE

Senior Consultant, **Ernst & Young** *(Melbourne, Australia)* Jul. 2021 – Apr. 2024

Senior Consultant, **Protiviti** *(USA & Australia)* Jul. 2017 – Jun. 2021

Experienced Consultant, **PricewaterhouseCoopers** *(Kansas City, Missouri, USA)* Sep. 2013 – Jul. 2017