Samuel Leventhal

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Summary

Machine learning engineer and researcher (Ph.D. Computer Science; B.Sc. Physics & Mathematics) who builds graph learning systems and deploys them at scale. I design reusable, modular architectures for message passing on graphs and higher-order complexes—including production APIs, test suites, and operator-learning modules built on PyTorch Geometric and DGL—and have shipped ML pipelines across national laboratories (ORNL, LLNL), government programs (ARPA-H), and multi-institution research teams where I served as ML technical lead. My research extends graph neural networks and neural operators to richer relational and topological structures, with publications in IEEE TVCG, NeurIPS, ICIP, and the American Journal of Clinical Pathology (NeurIPS 2026 and JMLR submissions under review). I am particularly interested in making foundation models on relational and graph-structured data accessible through elegant tooling, scalable infrastructure, topological and geometric insights, and human-in-the-loop workflows.

Core Competencies: Graph Neural Networks · Topological Data Analysis · Neural Operators · Scientific Visualization (VTK-m) · HPC (CUDA/MPI) · PyTorch/PyG · Geometric Deep Learning · CUDA · MPI · OpenMP · SLURM · C++ · Generative Models · Biomedical Image Analysis · In Situ ML–Simulation Coupling

Technical Profile

- **Geometric & Topological ML:** Graph neural networks & architectures, topological deep learning, architectures or learning based on cochain- and simplicial/combinatorial complexes, PyTorch Geometric, DGL; message passing on meshes, hierarchical graph learning and architectures.
- **PDEs & Neural Operators:** Topologically informed neural operators for operator learning on simplicial/combinatorial complexes, physics-informed ML, surrogate modeling for PDE-based simulators.
- **Generative Models:** Conditional GANs, 3D geometries / volumetric and mesh data, simulation-conditioned generation, physics-aware generative pipelines
- **3D Geometry & Meshing:** Large unstructured meshes, Morse–Smale complexes, ridge/valley graphs, mesh-based feature extraction, hierarchical topological representations (University Utah, LLNL, ORNL).
- **High-Performance Computing:** CUDA, MPI, OpenMP, SLURM; multi-GPU distributed training, large scale simulation; deployed at ORNL, LLNL, ARPA-H
- **Topological Data Analysis & Computational Topology:** Morse–Smale complexes, persistence filtrations, discrete Morse theory, TTK, topological simplification
- **Scientific Visualization & In Situ Computing:** VTK-m, ParaView, in situ ML–simulation coupling (PAVE), path tracing, feature tracking
- **PDE Surrogate Modeling & Operator Learning:** Neural operators extended to topological and relational domains; surrogate models that generalize across discretizations. Research bridging deep learning on graphs with structured physical and relational data.
- **Human-in-the-Loop & Interpretability:** Interactive labeling tools, active learning loops, and explainability workflows for iterative model refinement on graph-structured data.
- **Biomedical Image Analysis:** Histopathology classification (DenseNet), topology-based segmentation, clinical dataset curation.
- **Software Engineering:** Python, C++, PyTorch, TensorFlow, PyTorch Geometric, DGL, TensorFlow; numerical libraries and scientific visualization tools (VTK, ParaView); Linux/HPC environments.

Education

Ph.D. in Computer Science **2024**
University of Utah, School of Computing & Scientific Computing and Imaging Institute

Dissertation: Leveraging Topology to Advance Machine Learning Models and Methods
Advisor: Dr. Valerio Pascucci

B.Sc. in Physics, Minor in Philosophy **2013**
University of Utah, Department of Physics and Astronomy & Department of Philosophy

B.Sc. in Mathematics, Minor in Computer Science **2013**
University of Utah, Department of Mathematics & Kahlert School of Computing

Experience

Postdoctoral Researcher, University of San Francisco **2025–Present**

Topological Deep Learning, Neural Operators, & Physics-Aware ML

- Designed reusable topologically based neural operator modules (APIs, tests) supporting geometry-conditioning and mesh-invariant operator learning.
- Built cochain-level architectures grounded in Hodge theory for diffusion/transport processes on meshes and higher-order cell complexes.
- Developed prototype surrogate models for PDE behavior that generalize across mesh resolutions and topological refinements.
- Designed copresheaf-based neural network architectures that generalize message passing to higher-order cells, enabling discretization-invariant operator learning for PDEs and geometric data.
- Implemented cochain-level neural operators grounded in Hodge theory to model diffusion- and transport-like dynamics on meshes and complex topologies, and developed prototype PDE surrogates that generalize across mesh resolutions.

Graduate Research Assistant, University of Utah, Scientific Computing & Imaging Institute **2017–2024**

Topological Deep Learning, Geometry, and HPC

- Developed topology-aware graph learning methods for scientific images, using Morse–Smale complexes and hierarchical training schemes for GNNs to improve segmentation and classification on complex structures.
- Built large-scale topological and segmentation tools for 3D volumes and meshes (open-cell foams, medical and neuroscience data), scaling to large unstructured grid datasets.
- Co-designed **PAVE**, an in situ scientific visualization + ML pipelines for HPC simulations, coupling conditional GANs with path tracing to accelerate physically based rendering and light transport.
- Collaborated with LLNL and ORNL on geometry/topology-driven ML and HPC deployment; mentored students contributing to geometric ML and scientific computing tools.

AI Research Engineer, University of Utah **2023–2024**

ARPA-H: High-Resolution Tissue Scanning with ML + HPC

- Served as ML technical lead, defining imaging requirements, model milestones, and task breakdowns for a multi-institution team.
- Designed topology- and graph-based pipelines for large 3D datasets using discrete Morse theory to create sparse geometric representations.
- Integrated ML with high-throughput imaging systems and HPC workflows for large-scale inference and segmentation.

AI & Scientific Visualization Research Engineer, WiFIRE Lab, UC San Diego **2022–2024**

BurnPro3D: Geometry and Physics Informed Wildfire Modeling and Prediction

- Developed ML components integrating terrain geometry, fuels, and simulation outputs into predictive models.
- Built visualization and design-space exploration tools enabling physics-informed evaluation of wildfire behavior.
- Implemented explainability and active learning workflows for spatial simulation data.

Research Scientist, **Lawrence Livermore National Laboratory** **2018**

Spectral Sampling & Surrogate Modeling

- Co-designed spectral sampling frameworks for surrogate modeling and high-dimensional experimental design within a laboratory research program.

Machine Learning & Scientific Visualization Research Engineer, **Oak Ridge National Laboratory** **2019**

Scientific Visualization, Generative ML, and HPC

- Co-developed **PAVE**, an in situ framework coupling scientific visualization with ML in HPC environments.
- Implemented conditional GANs trained on path-traced images to produce high-quality renderings with reduced simulation effort, demonstrating ML-driven acceleration of visualization workflows on large-scale GPU resources.

AI Research Engineer, **Lawrence Livermore National Laboratory** **2022**

Topological GNNs and Geometry-Aware Graph Learning

- Developed topology- and geometry-aware graph neural networks for node and edge classification on graphs derived from topological complexes and scientific images.
- Designed homophily/heterophily-aware graph filtrations and hierarchical training schemes for learning on complex scientific data.

AI Research Engineer, **ARUP Laboratories & Mayo Clinic** **2017–2020**

Deep Learning for Hematopathology Diagnostics

- Built and trained DenseNet-based models on large histopathology datasets; produced two peer-reviewed publications.
- Standardized imaging and preprocessing pipelines and optimized model architectures for high-resolution scientific data.

Teaching Mentorship, **University of Utah** **2020, 2021**

Advanced Algorithms & Programming for Engineers (mentored student projects and provided guidance on algorithms and scientific programming).

Technical Skills

- **Languages:** Python, C++.
- **ML / DL Frameworks:** PyTorch, PyTorch Geometric, DGL, TensorFlow
- **Geometry & Visualization:** VTK, ParaView, discrete Morse/Morse–Smale tooling
- **HPC & Systems:** CUDA, MPI, OpenMP, SLURM; GPU clusters, in situ pipelines
- **Methods:** Generative models (GANs, simulation-conditioned learning), Topological ML, Operator learning, PDE surrogates, Mesh-based modeling, Graph Neural Networks, In Situ Scientific Visualization, Active Learning

Selected Systems & Projects

- **PAVE** (U of U & ORNL): In situ ML + scientific visualization framework; couples generative models with rendering and HPC simulations to accelerate physically based analysis.
- **Topological Segmentation Tools**: Hierarchical Morse–Smale-based segmentation, geometric feature extraction, topology-preserving mesh/volume processing, feature tracking, and visualization for 2D/3D scientific, medical, and materials data.
- **Interactive Labeling & Active Learning Tool**: GUI system for labeling topological priors and iteratively retraining geometric ML models on graphs derived from images.
- **BurnPro3D** (WiFIRE): ML-driven tools and visualization pipelines for 3D wildfire spread modeling on complex terrain.
- **Quantum Structuring in Keplerian Systems** (U of U): Theoretical and numerical study of quantum-like structuring in Keplerian systems.

Selected Publications

Peer Reviewed Journal Articles

- (*In submission*) Leventhal, S., Gyulassy, A., Heimann, M., Pascucci, V. *Homophily-based Filtration Learning for Graph Neural Networks.*
- Leventhal, S., Gyulassy, A., Heimann, M., Pascucci, V. *Exploring Classification of Topological Priors with Machine Learning for Feature Extraction.* IEEE Transactions on Visualization and Computer Graphics, 2023.
- Mohlman, J.S., Leventhal, S., Hansen, T., Kohan, J., Pascucci, V., Salama, M.E. *Improving Augmented Human Intelligence to Distinguish Burkitt Lymphoma from Diffuse Large B-Cell Lymphoma Cases.* American Journal of Clinical Pathology, 2020.
- Petruzza, S., Gyulassy, A., Leventhal, S., Baglino, J.J., Czabaj, M., Spear, A.D., Pascucci, V. *High-Throughput Feature Extraction for Measuring Attributes of Deforming Open-Cell Foams.* IEEE Transactions on Visualization and Computer Graphics, 2019.
- Mohlman, J., Leventhal, S., Venkat, A, Gyulassy, A., Pascucci, V., Salama, M.E. *Application of a Convolutional Neural Network to Distinguish Burkitt Lymphoma from Diffuse Large B-Cell Lymphoma.* American Journal of Clinical Pathology, 2018.

Peer Reviewed Conference Papers

- L. Bastian, S. Leventhal, M. Hajij, T. Birdal. *Topological Neural Operators.* NeurIPS, 2026 (under review) arXiv:2606.09806, 2026.
- Leventhal, S., Gyulassy, A., Pascucci, V., Heimann, M. *Modeling Hierarchical Topological Structure in Scientific Images with Graph Neural Networks.* International Conference on Image Processing, 2023.

Peer Reviewed Workshop Papers

- Leventhal, S., Gyulassy, A., Pascucci, V., Heimann, M. *Modeling Hierarchical Topological Structure in Scientific Images with Graph Neural Networks.* NeurIPS Workshop: New Frontiers in Graph Learning, 2022.
- Leventhal, S., Kim, M., Pugmire, D. *PAVE: An In Situ Framework for Scientific Visualization and Machine Learning Coupling.* IEEE/ACM 5th International Workshop on Data Analysis and Reduction for Big Scientific Data, 2019.

Other Peer Reviewed Papers

- Leventhal, S., LeBohec, S. *A Search for Quantum Like Structuring in Keplerian Systems.* University of Utah Undergraduate Research Abstracts Journal, 2013.
- Leventhal, S. *Entropy Is Not Our Anomie.* The Sponge, 2011.

Selected Coursework

Graduate work in ML, computational geometry/topology, scientific computing, and high-performance ML; undergraduate work in advanced math and physics (PDEs, linear & abstract algebra, numerical analysis, quantum mechanics).