Mikel Landajuela, Ph.D.

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Machine Learning, Optimization, HPC, Interpretable AI | US Green Card | Spanish Citizen

Summary

Senior Staff Scientist at Lawrence Livermore National Laboratory building AI and high-performance-computing capabilities for national mission-critical problems — accelerating drug development, enabling rapid response to emerging biothreats, advancing non-invasive medical diagnostics, and powering simulation-driven engineering. Develops scalable deep-learning, reinforcement-learning, and agentic LLM pipelines paired with deterministic backbones for auditable, production-grade scientific applications. Demonstrated impact through publications in first-tier venues (Nature, Science Advances, NeurIPS, ICML, AAAI), patents, and leadership of cross-functional teams.

Technical Skills

Programming & Software Engineering: Python, C/C++, MATLAB, Wolfram Mathematica; proficient with software development best practices, version control (Git), and modular design

Machine Learning & AI: Deep learning, Reinforcement Learning, Symbolic regression, NLP/Transformer models, Protein language models; frameworks: PyTorch, TensorFlow, HuggingFace, scikit-learn

Agentic AI & LLM Systems: LLM-as-prior / LLM-as-tool patterns, schema-enforced JSON / structured outputs, autoresearch loops (Claude Code), prompt-design ablation, few-shot calibration; hybrid LLM + solver / LLM + classifier pipelines

Algorithmic & Statistical Methods: Optimization algorithms, Genetic Programming, Linear Programming, Bayesian hyperparameter tuning, statistical modeling, experiment design

Scientific Computing & HPC: MPI, OpenMP, PETSc, Trilinos, CUDA, GPU-accelerated pipelines, AWS HPC, scalable data infrastructure

Data Engineering & Analysis: NumPy, Pandas, data preprocessing, big-data pipelines, experiment automation, visualization

Responsible AI & Interpretability: Symbolic methods, model explainability, fairness, reproducible scientific workflows

Experience

Senior Staff Scientist — Jul 2020 – Present
Lawrence Livermore National Laboratory — *Livermore, CA*

Developed deep-learning capabilities for mission-critical therapeutic design and biodefense preparedness, integrating reinforcement learning, protein language models, inverse-folding architectures, and model alignment (PPO, DPO, DRO) with downstream combinatorial and linear-programming optimization. Work published in *Nature* and *Science Advances*.

Designed agentic AI pipelines pairing LLM agents with deterministic backbones for auditable scientific applications: LLM-guided ILP for combinatorial library design (CIBB '26), autoresearch loop for interpretable rule discovery improving LOSO ROC-AUC from 0.64 to 0.81 (bioRxiv '26), and a prompt-design benchmark with structured confidence signals.

Developed ML/RL frameworks for scientific discovery: implemented symbolic-equation discovery models, transparent RL controller architectures, and decision-tree regression pipelines—enhancing interpretability and reproducibility in AI-for-Science workflows.

Awards: LLNL Director's S&T Award (2022), Interpretable Symbolic Regression for Data Science Competition 1st place (GECCO 2022), and LLNL Publication Excellence Award (2022).

Postdoctoral Fellow — Jul 2018 – Jul 2020
Lawrence Livermore National Laboratory — *Livermore, CA*

Built virtual electroscope using deep learning to reconstruct cardiac activation maps from ECG signals.

Patent: US Patent 2021/0193291 A1: Machine learning-based reconstruction of intracardiac electrical behavior from ECG.

Postdoctoral Fellow — Apr 2016 – Apr 2018
Politecnico di Milano — *Milan, Italy*

Developed high-performance PDE solvers for fluid-structure interaction, optimized on HPC clusters.

Selected Projects

Deep Learning for Therapeutic Design & Biodefense: Built HPC-ready deep-learning pipelines for drug-development acceleration and robustness against viral escape. Principal developer of `protein_tune_rl` for alignment of infilling language models and `protlib-designer` for constrained library design. Published in *Science Advances* and *Nature*.

Reinforcement Learning for Symbolic Mathematics and Optimization: Co-developed the `deep-symbolic-optimization` framework for interpretable ML, earning 1st place at GECCO 2022. Research published in *ICLR*, *ICML*, *NeurIPS*, and *AAAI*.

Machine Learning for Electrocardiography: Created `cardiac_ml` framework for reconstructing cardiac potentials from ECG signals, advancing non-invasive heart diagnostics.

Education

Ph.D. in Applied Mathematics 2012 – 2016
Sorbonne University & Inria *Paris, France*
Awarded SMAI-GAMNI Best Ph.D. Thesis in Mechanical and Engineering Sciences (2017).

M.S. in Scientific Computing (Erasmus) 2011 – 2012
Utrecht University *The Netherlands*

B.S. & M.S. in Mathematical Sciences 2007 – 2012
University of the Basque Country *Bilbao, Spain*
Graduated with highest honors (Premio extraordinario de carrera, 2012).

Selected Publications

F. Zhu, et al., **M. Landajuela**, "Preemptive optimization of a clinical antibody for broad neutralization of SARS-CoV-2 variants." *Science Advances, 2024.* [Link]

J. Pettit, et al., **M. Landajuela**, "DisCo-DSO: Coupling Discrete and Continuous Optimization for Efficient Generative Design." *AAAI, 2024.* [Link]

T. A. Desautels, et al, **M. Landajuela**, "Computationally restoring the potency of a clinical antibody against Omicron." *Nature, 2024.* [Link]

M. Landajuela, et al., "A Unified Framework for Deep Symbolic Regression." *NeurIPS, 2022.* [Link]

M. Landajuela, et al., "Discovering symbolic policies with deep reinforcement learning." *ICML (Spotlight), 2021.* [Link]

B. K. Petersen, et al., **M. Landajuela**, "Deep symbolic regression: Recovering mathematical expressions from data via risk-seeking policy gradients." *ICLR, 2021.* [Link]

M. Landajuela, et al., "Numerical approximation of the electromechanical coupling in the left ventricle with inclusion of the Purkinje network." *Int. J. Numer. Methods Biomed. Eng., 2018.* [Link]

M. Landajuela, M. Vidrascu, D. Chapelle, M. A. Fernández, "Coupling schemes for the FSI forward prediction challenge: comparative study and validation." *Int. J. Numer. Methods Biomed. Eng., 2016.* [Link]