

# Mikel Landajuela

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AI for Science, Machine Learning, and Scientific  
Computing  
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## PROFESSIONAL EXPERIENCE

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**Staff Scientist / Senior Staff Scientist** Jul. 2020 - Present  
AI for science, antibody engineering, symbolic optimization, and  
scientific computing

Computational Engineering Directorate,  
Lawrence Livermore National Laboratory,  
Livermore, CA, USA

**Postdoctoral Fellow** Jul. 2018 - Jul. 2020  
Machine learning for intracardiac electrical imaging and  
synthetic-data generation

Biochemical and Biophysical Systems Group,  
Lawrence Livermore National Laboratory,  
Livermore, CA, USA

**Postdoctoral Fellow** Apr. 2016 - Apr. 2018  
Cardiac electromechanics, Purkinje-network modeling, and  
scientific computing

MOX - Dipartimento di Matematica,  
Politecnico di Milano, Milan, Italy

## EDUCATION

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**PhD in Applied Mathematics** Oct. 2012 - Mar. 2016  
Coupling schemes and unfitted mesh methods for fluid-structure  
interaction - Thesis defended on 29th March 2016 (mention *très*  
*honorable*)

Université Pierre et Marie Curie (Paris VI) and  
INRIA, Paris, France

**Master program in Scientific Computing** 2011 - 2012  
Erasmus Exchange Program

Utrecht University,  
Utrecht, The Netherlands

**B.S. and M.S in Mathematical Sciences** 2007 - 2012

University of the Basque Country (UPV/EHU),  
Bilbao, Spain

## RESEARCH INTERESTS

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AI for science, antibody engineering, reinforcement learning, symbolic regression and interpretable machine learning, discrete and combinatorial optimization, computational biology, computational cardiology, scientific computing, finite element methods, fluid-structure interaction, and high-performance computing.

## AWARDS

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**2022 Director's Science and Technology Award**, Tue 27 Sep 2022, LLNL, Livermore, US

**2022 DDS&T Excellence in Publication Award**, Tue 27 Sep 2022, LLNL, Livermore, US

**1st Place (Real-world Track) - Interpretable Symbolic Regression for Data Science Competition**, July 9-13, 2022, Genetic and Evolutionary Computation Conference (GECCO) 2022, Boston, US

**SMAI-GAMNI award 2017**, French Society of Industrial and Applied Mathematics, Annual award for the best thesis in numerical methods for mechanics and engineering sciences, France.

**Premio extraordinario de carrera award 2012**, University of the Basque Country (UPV/EHU), Prize awarded to the most outstanding graduate in Mathematics of the 2011/2012 class, Bilbao, Spain

## PUBLICATIONS

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### Journal and Conference Papers

C. F. Hayes, S. A. Magana-Zook, A. Goncalves, A. Can Solak, D. Faissol, **M. Landajuela**. **Combinatorial Optimization of Antibody Libraries via Constrained Integer Programming**. *25th International Conference on Autonomous Agents and Multiagent Systems (AAMAS)*, 2026. PDF — BioRxiv

F. Leno da Silva, **M. Landajuela**, E. A. Saada, P. Karande, S. Sarma, I. D'Angelo, S. Conti, D. Faissol. **Machine Learning Models Assisting the Development of Antibody Therapeutics and Vaccines – an Emerging Trend**. *Proceedings of the AAAI Conference on Artificial Intelligence (AAAI Emerging Trends in AI)*, 2026. PDF — Paper

F. Zhu, S. Rajan, C. F. Hayes, K. Y. Kwong, A. R. Goncalves, A. T. Zemla, E. Y. Lau, Y. Zhang, Y. Cai, J. W. Goforth, **M. Landajuela**, et al. **Preemptive Optimization of a Clinical Antibody for Broad Neutralization of SARS-CoV-2 Variants and Robustness Against Viral Escape**. *Science Advances*, 2025. PDF — Journal

J. Pettit, C. S. Lee, J. Yang, A. Ho, D. Faissol, B. K. Petersen, **M. Landajuela**. **DisCo-DSO: Coupling Discrete and Continuous Optimization for Efficient Generative Design in Hybrid Spaces**. *Thirty-Ninth AAAI Conference on Artificial Intelligence*, 2025. PDF — Paper

F. O. de Franca, M. Virgolin, M. Kommenda, M. S. Majumder, M. Cranmer, G. Espada, L. Ingelse, A. Fonseca, **M. Landajuella**, et al. **SRBench++: Principled Benchmarking of Symbolic Regression With Domain-Expert Interpretation**. *IEEE Transactions on Evolutionary Computation*, 2024. PDF

T. A. Desautels, K. T. Arrildt, A. T. Zemla, E. Y. Lau, F. Zhu, D. Ricci, S. Cronin, S. J. Zost, E. Binshtein, S. M. Scheaffer, **M. Landajuella**, et al. **Computationally Restoring the Potency of a Clinical Antibody Against Omicron**. *Nature*, 2024. PDF

F. Leno da Silva, A. Goncalves, S. Nguyen, D. Vashchenko, R. Glatt, T. Desautels, **M. Landajuella**, B. Petersen, D. Faissol. **Language Model-Accelerated Deep Symbolic Optimization**. *Neural Computing and Applications*, 2023. PDF

**M. Landajuella**, C. S. Lee, J. Yang, R. Glatt, C. Santiago, T. N. Mundhenk, I. Aravena, G. Mulcahy, B. K. Petersen. **A Unified Framework for Deep Symbolic Regression**. *36th Conference on Neural Information Processing Systems (NeurIPS)*, 2022. Proceedings — OpenReview

**M. Landajuella**, R. Anirudh, J. Loscazo, and R. Blake. **Intracardiac Electrical Imaging Using the 12-Lead ECG: A Machine Learning Approach Using Synthetic Data**. *Computing in Cardiology (CinC)*, 2022. IEEE Xplore — PDF

T. N. Mundhenk, **M. Landajuella**, R. Glatt, C. P. Santiago, D. Faissol, B. K. Petersen. **Symbolic Regression via Deep Reinforcement Learning Enhanced Genetic Programming Seeding**. *35th Conference on Neural Information Processing Systems (NeurIPS)*, 2021. OpenReview — ArXiv

**M. Landajuella**, B. K. Petersen, S. K. Kim, C. Santiago, R. Glatt, N. Mundhenk, J. Pettit, D. Faissol. **Discovering Symbolic Policies with Deep Reinforcement Learning**. *38th International Conference on Machine Learning (ICML)*, 2021. **Spotlight**. Proceedings — Spotlight — PDF

B. K. Petersen, **M. Landajuella**, T. N. Mundhenk, C. Prata Santiago, S. Kyung Kim, J. Taery Kim. **Deep Symbolic Regression: Recovering Mathematical Expressions From Data via Risk-Seeking Policy Gradients**. *9th International Conference on Learning Representations (ICLR)*, 2021. **Oral**. OpenReview — ArXiv — Talk

M. A. Fernández, **M. Landajuella**. **Splitting Schemes and Unfitted-Mesh Methods for the Coupling of an Incompressible Fluid With a Thin-Walled Structure**. *IMA Journal of Numerical Analysis*, 2019. PDF

**M. Landajuella**, C. Vergara, A. Gerbi, L. Dede', L. Formaggia, A. Quarteroni. **Numerical Approximation of the Electromechanical Coupling in the Left Ventricle With Inclusion of the Purkinje Network**. *International Journal for Numerical Methods in Biomedical Engineering*, 2018. PDF

**M. Landajuella**, M. Vidrascu, D. Chapelle, M. A. Fernández. **Coupling Schemes for the FSI Forward Prediction Challenge: Comparative Study and Validation**. *International Journal for Numerical Methods in Biomedical Engineering*, 2016. PDF

F. Alauzet, B. Fabrèges, M. A. Fernández, **M. Landajuella**. **Nitsche-XFEM for the Coupling of an Incompressible Fluid With Immersed Thin-Walled Structures**. *Computer Methods in Applied Mechanics and Engineering*, 2016. PDF

M. A. Fernández, **M. Landajuella**, M. Vidrascu. **Fully Decoupled Time-Marching Schemes for Incompressible Fluid/Thin-Walled Structure Interaction**. *Journal of Computational Physics*, 2015. PDF

M. A. Fernández, **M. Landajuella**. **Splitting Schemes for Incompressible Fluid/Thin-Walled Structure Interaction With Unfitted Meshes**. *Comptes Rendus Mathématique*, 2015. PDF

M. A. Fernández, **M. Landajuella**. **A Fully Decoupled Scheme for the Interaction of a Thin-Walled Structure With an Incompressible Fluid**. *Comptes Rendus Mathématique*, 2013. PDF

### Book Chapters and Edited Volumes

C. F. Hayes, F. Leno da Silva, J. Yang, T. N. Mundhenk, C. S. Lee, J. F. Pettit, C. Santiago, S. Kim, J. T. Kim, I. Aravena Solis, R. Glatt, A. R. Goncalves, A. Ladd, A. C. Solak, T. Desautels, D. Faissol, B. K. Petersen, **M. Landajuella**. **Deep Symbolic Optimization: Reinforcement Learning for Symbolic Mathematics**. *Under review in LNCS Computational Approaches to Scientific Discovery*, 2025. ArXiv

A. Quarteroni, C. Vergara, **M. Landajuella**. **Mathematical and Numerical Description of the Heart Function**. *Imagine Math 6: Between Culture and Mathematics*, 2018. Chapter

M. A. Fernández, **M. Landajuella**, J. Mullaert, M. Vidrascu. **Robin-Neumann Schemes for Incompressible Fluid-Structure Interaction**. *In Domain Decomposition Methods in Science and Engineering XXII*, 2015. Chapter

### Preprints

C. S. Lee, C. F. Hayes, D. Vashchenko, **M. Landajuella**. **Reinforcement Learning for Antibody Sequence Infilling**. *BioRxiv*, 2025. PDF — BioRxiv

### WORKSHOP PUBLICATIONS

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C. F. Hayes, S. A. Magana-Zook, A. Goncalves, A. Can Solak, D. Faissol, **M. Landajuela**. **Antibody Library Design by Seeding Linear Programming with Inverse Folding and Protein Language Models**. *NeurIPS 2024 Workshop on Machine Learning for Structural Biology*, 2024. PDF — BioRxiv

J. G. Faris, **M. Landajuela**, K. G. Sprenger, D. Faissol, F. Leno da Silva. **Computational Antigen Optimization Through Symbolic Optimization and Affinity Maturation Simulation**. *NeurIPS 2024 Workshop on AI for New Drug Modalities*, 2024. OpenReview

J. Pettit, C. S. Lee, J. Yang, A. Ho, D. Faissol, B. K. Petersen, **M. Landajuela**. **Generative Design of Decision Tree Policies for Reinforcement Learning**. *ICML 2024 Workshop on Structured Probabilistic Inference & Generative Modeling*, 2024. PDF

J. G. Faris, C. F. Hayes, A. R. Goncalves, K. G. Sprenger, D. Faissol, B. K. Petersen, **M. Landajuela**, F. Leno da Silva. **Pareto Front Training for Multi-Objective Symbolic Optimization**. *Adaptive and Learning Agents Workshop (ALA)*, 2024. PDF

F. Leno da Silva, A. Goncalves, S. Nguyen, D. Vashchenko, R. Glatt, T. Desautels, **M. Landajuela**, B. Petersen, D. Faissol. **Leveraging Language Models to Efficiently Learn Symbolic Optimization Solutions**. *Adaptive and Learning Agents Workshop (ALA)*, 2022. PDF

B. K. Petersen, C. Santiago, **M. Landajuela**. **Incorporating Domain Knowledge Into Neural-Guided Search via In Situ Priors and Constraints**. *8th ICML Workshop on Automated Machine Learning*, 2021. OpenReview — ArXiv

**M. Landajuela**, B. K. Petersen, S. Kim, C. Santiago, R. Glatt, N. Mundhenk, J. Pettit, D. Faissol. **Improving Exploration in Policy Gradient Search: Application to Symbolic Optimization**. *ICLR Math-AI Workshop*, 2021. Workshop PDF — ArXiv — Poster

J. Taery Kim, **M. Landajuela**, B. K. Petersen. **Distilling Wikipedia Mathematical Knowledge Into Neural Network Models**. *ICLR Math-AI Workshop*, 2021. Workshop PDF — ArXiv — Poster

## PATENTS

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**Machine learning based reconstruction of intracardiac electrical behavior based on electrocardiograms**. *US20210193291A1* · Filed Nov 24, 2020  
<https://patentimages.storage.googleapis.com/e5/54/e3/8ed424340a5f7a/US20210193291A1.pdf>

## DATASETS

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**M. Landajuela**, Rushil Anirudh, Robert Blake **Dataset of Simulated Intracardiac Transmembrane Voltage Recordings and ECG Signals**. *Lawrence Livermore National Laboratory (LLNL) Open Data Initiative*. UC San Diego Library Digital Collections. 2022 <https://library.ucsd.edu/dc/object/bb29449106>

## TALKS AND CONFERENCES

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**AI for SCIENCE 2025**, Ljubljana, Slovenia, Sep. 22-26, 2025. *Deep Symbolic Optimization: Reinforcement Learning for Equation Discovery*. **Keynote**.

**AAAI Spring Symposium on Computational Approaches to Scientific Discovery**, Hyatt Regency / San Francisco Airport, CA, USA, Mar. 27-29, 2023. *Deep Symbolic Optimization for Scientific Discovery*.

**36th Conference on Neural Information Processing Systems (NeurIPS 2022)**, New Orleans, LA, USA, Dec. 5-10, 2022. *A Unified Framework for Deep Symbolic Regression*.

**IEEE San Francisco and Oakland East Bay Computer Society**, San Francisco, CA, USA, Oct. 19, 2022. *Deep Symbolic Optimization: A Framework for Symbolic Optimization Using Deep Learning*.

**49th Computing in Cardiology Conference**, Virtual, Sep. 4-7, 2022. *Intracardiac Electrical Imaging Using the 12-Lead ECG: A Machine Learning Approach Using Synthetic Data*.

**Center for Advanced Signal and Image Sciences (CASIS) 25th Annual Workshop**, Virtual, Aug. 4, 2021. *Deep Symbolic Optimization: A Framework for Symbolic Optimization Using Deep Learning*.

**38th International Conference on Machine Learning (ICML 2021)**, Virtual, Jul. 18-24, 2021. *Discovering Symbolic Policies with Deep Reinforcement Learning*.

**1st Mathematical Reasoning in General Artificial Intelligence Workshop (ICLR 2021)**, Virtual, May 3-7, 2021. *Improving Exploration in Policy Gradient Search*.

**INdAM Workshop – Mathematical and Numerical Modeling of the Cardiovascular System**, Rome, Italy, Apr. 16-19, 2018. *Numerical Approximation of the Electromechanical Coupling in the Left Ventricle With Inclusion of the Purkinje Network*.

**ECCOMAS Young Investigators Conference 2017**, Milan, Italy, Sep. 13-15, 2017. *Coupling Schemes and Unfitted Mesh Methods for Fluid-Structure Interaction*. Participant in the **ECCOMAS PhD Olympiad 2017**.

**VII International Conference on Coupled Problems in Science and Engineering**, Rhodes, Greece, Jun. 12-14, 2017. *Coupling Schemes for the FSI Forward Prediction Challenge: Comparative Study and Validation*.

**XIII SIMAI Biannual Congress (SIMAI 2016)**, Milan, Italy, Sep. 13-16, 2016. *Nitsche-XFEM Formulations and Splitting Schemes for the Coupling of an Incompressible Fluid With Immersed Thin-Walled Structures.*

**Séminaire d'Analyse Numérique**, Université de Genève, Geneva, Switzerland, Mar. 8, 2016. *Nitsche-XFEM for the Coupling of an Incompressible Fluid With Immersed Thin-Walled Structures.*

**13th U.S. National Congress on Computational Mechanics (USNCCM13)**, San Diego, CA, USA, Jul. 22-25, 2015. *Nitsche-XFEM for the Coupling of an Incompressible Fluid With Immersed Thin-Walled Structures.*

**International Workshop on Numerical Methods and Applications in Fluid-Structure Interactions**, Laboratoire Jean Kuntzmann, Grenoble, France, Nov. 24-25, 2014. *Poster: Splitting Schemes for Fluid/Thin-Walled Structure Interaction Using Unfitted Meshes.*

**WCCM-ECCM-ECFD 2014**, Barcelona, Spain, Jul. 21-25, 2014. *Recent Developments in Explicit Robin-Neumann Schemes for Fluid-Structure Interaction.*

**12th U.S. National Congress on Computational Mechanics (USNCCM12)**, Raleigh, NC, USA, Jul. 22-25, 2013. *Fully Decoupled Time-Marching Schemes for Incompressible Fluid/Thin-Walled Structure Interaction.*

## PROJECT LEADERSHIP

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**Principal Investigator, LDRD Exploratory Research (\$2M over 3 years)**, Oct. 2023 - Oct. 2026. Principal Investigator for *Generative Transformers for Optimization* (LDRD ER 2023-2026).

**GUIDE DSO Team Lead**, Apr. 2023 - Sep. 2023. Led the Deep Symbolic Optimization thrust within GUIDE, coordinating a team of 9 researchers. Program website

**Data Science Challenge Lead Mentor**, Jan. 2023 - Jun. 2023. Lead organizer and mentor for LLNL's Data Science Challenge. Program website

**ML Training Pilot Program Lead**, Apr. 2022 - Sep. 2022. Led development of a deep reinforcement learning curriculum for the DSI and CASC divisions.

## ACADEMIC SERVICE

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**Reviewer** *International Journal for Numerical Methods in Biomedical Engineering, Artificial Intelligence Review, Neural Computing and Applications, Neural Information Processing Systems, International Conference on Learning Representations, International Conference on Autonomous Agents and Multiagent Systems*

**Editorial Work** *Guest Associate Editor in Coronary Artery Disease in Frontiers in Cardiovascular Medicine, Editorial board member of the American Journal of Computer Science and Technology*

## GRANTS

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**Programa Estatal Juan de la Cierva Formación 2017**, REF.: FJCI-2017-34535, Declined

**Campagne de recrutement des doctorants Inria 2012**, 1st selected candidate of the 2012 PhD Inria Paris-Rocquencourt recruitment campaign

**Subprograma de Formación del Personal Investigador 2012**, REF.: BES-2012-056511, Declined

**Beca de movilidad universitaria internacional curso 2011-2012**, Grant given by Basque Government and the BBK (Bilbao Bizkaia Kutxa) bank for international studies.

## TEACHING

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**Mentoring Garrett Mulcahy - "Monte Carlo Tree Search and Language Models for Antibody Design"**, Jul. 2023 - Sep. 2023, LLNL, California, USA

**Mentoring Wayne Mitchell - "Reinforcement Learning"**, Mar. 2021 - Oct. 2022, LLNL, California, USA

**Mentoring Garrett Mulcahy - "Supervised learning of first token of a dataset"**, May. 2021 - Aug. 2021, LLNL, California, USA

**Mentoring Haoyu Niu - "High scores in Atari"**, May. 2021 - Aug. 2021, LLNL, California, USA

**Calcolo numerico ed elementi di analisi**, Mar. 2017 - Jul. 2017, Aerospace Engineering, Politecnico di Milano, Milano, Italy

## TECHNICAL SKILLS

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Languages : English (proficient), Spanish (native), French (fluent), Italian (fluent), Basque (basic).

Programming Languages : PYTHON, C/C++, MATLAB, WOLFRAM LANGUAGE, LATEX

Operating Systems : LINUX, MACOS, WINDOWS

Machine Learning and Data : PYTORCH, TENSORFLOW, KERAS, SCIKIT-LEARN, PANDAS, HUGGING FACE

Version Control : GIT, GITHUB, SVN

Scientific Computing : MPI, PETSC, TRILINOS, FreeFem++, Gmsh, VMTK, ParaView, Enight

Tools : JUPYTER, MATHEMATICA, VISUAL STUDIO CODE, MATLAB, MICROSOFT OFFICE

## SOFTWARE AND OPEN-SOURCE PROJECTS

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**ProteinTuneRL.** Framework for antibody and protein sequence optimization with infilling language models and reinforcement learning. [GitHub](#)

**ProtLib-Designer.** Toolkit for combinatorial antibody-library design using constrained optimization and protein-language-model priors. [GitHub](#) — [PyPI](#)

**Deep Symbolic Optimization (DSO).** Research framework for symbolic regression, symbolic control, and interpretable optimization. [GitHub](#)

**Cardiac ML Tools.** Repositories for intracardiac electrical imaging, synthetic-data generation, and the CinC cardiac challenge. [cardiac.ml](#) — [cardiac\\_challenge](#)

**Cardioid.** Cardiac multiscale simulation suite for large-scale electrophysiology and mechanics. [GitHub](#)

**EXIFSI.** Project website for explicit coupling schemes for incompressible fluid-structure interaction. [Project website](#)

**FELiScE.** Finite Elements for Life SCiences and Engineering. [Project website](#)

**LifeV.** Parallel finite-element library for the numerical solution of PDEs. [Project website](#)