Guillem Simeon, PhD

Physicist & AI Research Scientist
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Skills

Programming & Tools: Python, PyTorch, Linux, Git
Expertise: Graph neural networks, Geometric deep learning, Machine learning for physics, Machine learning interatomic potentials, Machine learning for molecules and materials

Professional Experience

Research Scientist - PhysicsX Nov 2025 – Present
PhysicsX - London, UK
- Research on AI-based surrogate physics models

Machine Learning Scientist - Microsoft Quantum Jun 2024 – Jun 2025
Microsoft - Remote, contract
- Developed and benchmarked new methods for machine learning interatomic potentials (MLIPs)
- MLIP training and deployment library development in collaboration with Microsoft Research
- Collaborated with quantum chemists and materials scientists to meet their needs with MLIPs

PhD Researcher - Computational Science Laboratory Jul 2021 – May 2024
Universitat Pompeu Fabra - Barcelona
- Researched, developed and optimized equivariant graph neural network interatomic potentials (TensorNet).
- Co-developed an open-source MLIP library (TorchMD-Net).
- Focus on geometric deep learning for molecular systems.

Research Intern - Neuroradiology Group, Dept. of Radiology Oct 2020 – Jun 2021
Vall d'Hebron Hospital Institute of Research (VHIR) - Barcelona
- Analysis of brain fMRI time-series.
- Conducted Master's thesis on resting-state brain functional connectivity.

Education

PhD in Machine Learning for Molecular Systems, Universitat Pompeu Fabra (2021 – 2025)
Thesis: *Novel Geometric Representations and Optimized Frameworks for Deep Learning Models of Interatomic Potentials*. Supervisor: Prof. Gianni de Fabritiis.

Master's degree in Computational Biomedical Engineering, Universitat Pompeu Fabra (2020 – 2021) Focus: Machine learning, Cognitive systems, Computational neuroscience

Bachelor's degree in Physics, Universitat de Barcelona (2014–2018)

Publications

Full list: Google Scholar

Selected Publications

TensorNet: Cartesian Tensor Representations for Efficient Learning of Molecular Potentials. G. Simeon, G. de Fabritiis (2023). *NeurIPS 2023.*

TorchMD-Net 2.0: Fast Neural Network Potentials for Molecular Simulations. R. P. Pelaez*, G. Simeon*, R. Galvelis, A. Mirarchi, P. Eastman, S. Doerr, P. Thölke, T. E. Markland, G. de Fabritiis (2024). *Journal of Chemical Theory and Computation.*

SimPoly: Simulation of Polymers with Machine Learning Force Fields Derived from First

Principles. G. N. C. Simm, J. Hélie, H. Schulz, Y. Chen, G. Simeon, A. Kuzina, E. Martinez-Baez, P. Gasparotto, G. Tocci, C. Chen, Y. Li, L. Cheng, Z. Wang, B. H Nguyen, J. A Smith, L. Sun (2025). *Preprint, under review.*

Other Publications

Broadening the Scope of Neural Network Potentials through Direct Inclusion of Additional Molecular Attributes. G. Simeon, A. Mirarchi, R. P. Pelaez, R. Galvelis, G. de Fabritiis (2025). *J. Chem. Theory Comput.*

AMARO: All Heavy-Atom Transferable Neural Network Potentials of Protein Thermodynamics. A. Mirarchi, R. P. Pelaez, G. Simeon, G. de Fabritiis (2024). *Journal of Chemical Theory and Computation.*

Riemannian geometry of functional connectivity matrices for multi-site attention-deficit hyperactivity disorder data harmonization. G. Simeon, G. Piella, O. Camara, D. Pareto (2022). *Frontiers in Neuroinformatics.*

Geometric deep learning for the assessment of thrombosis risk in the left atrial appendage. X. Morales, J. Mill, G. Simeon, K. Juhl, O. De Backer, O. Camara, R. R. Paulsen (2021). *International Conference on Functional Imaging and Modelling of the Heart.*

Scalar-tensor extension of natural inflation. G. Simeon (2020). *Journal of Cosmology and Astroparticle Physics.*

Natural inflation with a periodic non-minimal coupling. R. Z. Ferreira, A. Notari, G. Simeon (2018). *Journal of Cosmology and Astroparticle Physics.*

Invited Talks

- Cohere For AI, ML Theory group, Apr 2024. *TensorNet: Cartesian tensor representations for efficient learning of molecular potentials.*
- Deep Learning Barcelona Symposium, Dec 2023. *Symmetries and equivariance in neural network molecular potentials.*
- CECAM - Psi-k Research Conference, Berlin, Jun 2023. *Enhancing ML potentials for molecular dynamics simulations.*
- Workshop on Methods in Molecular Simulations and ML, Barcelona, Jul 2022. *Forward differentiation for physics-informed neural networks.*

Additional Activity

- Organizer of Workshop: *Machine Learning for Life and Material Science: From Theory to Industry Applications*, ICML 2024.
- Reviewer for JCAP, NeurIPS, ICLR, Artificial Intelligence in Medicine.

Fellowships & Awards

- FI-AGAUR grant from Generalitat de Catalunya, PhD funding (Apr 2022 – May 2024).
- IFAE Summer Fellowship 2017 for undergraduate students, Theory Division, Barcelona.
- Silver Medal, Spanish Chemistry Olympiad 2014.
- Honour Mention, Spanish Physics Olympiad 2014.