

BÁLINT Á. MÁTÉ

PHD STUDENT IN MACHINE LEARNING AND PHYSICS

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I am a PhD student in the Computer Science and Physics departments of the University of Geneva under the supervision of François Fleuret. Before this, I studied theoretical physics and differential geometry in Hamburg and mechanical engineering in Budapest. I am interested in ML-enhanced science, generative modelling and statistical physics.

EDUCATION

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| Ph.D. in Computer Science and Physics , Université de Genève, Geneva, Switzerland | 12/2020 - |
| M.Sc. in Mathematical Physics , Universität Hamburg, Hamburg, Germany | 10/2018 - 10/2020 |
| M.Sc. in Mathematics , Central European University, Budapest, Hungary | 09/2016 - 05/2018 |
| B.Sc. in Mechanical Engineering , Technical University of Budapest, Budapest, Hungary | 09/2012 - 01/2016 |

SELECTED PAPERS

- Bálint Máté, François Fleuret, and Tristan Berreau. *Solvation free energies from neural thermodynamic integration*. The Journal of Chemical Physics 162.12 (Mar. 2025), p. 124107. ISSN: 0021-9606. DOI: [10.1063/5.0251736](https://doi.org/10.1063/5.0251736). eprint: https://pubs.aip.org/aip/jcp/article-pdf/doi/10.1063/5.0251736/20452824/124107_1_5.0251736.pdf. URL: <https://doi.org/10.1063/5.0251736>
- Bálint Máté, François Fleuret, and Tristan Berreau. *Neural Thermodynamic Integration: Free Energies from Energy-Based Diffusion Models*. The Journal of Physical Chemistry Letters 15.45 (2024), pp. 11395–11404. DOI: [10.1021/acs.jpcllett.4c01958](https://doi.org/10.1021/acs.jpcllett.4c01958). eprint: <https://arxiv.org/abs/2406.02313>
- Bálint Máté and François Fleuret. *Learning Interpolations between Boltzmann Densities*. Transactions on Machine Learning Research (2023). ISSN: 2835-8856. URL: <https://openreview.net/forum?id=TH6YrEcbth>
- Bálint Máté, Samuel Klein, Tobias Golling, and François Fleuret. *Flowification: Everything is a Normalizing Flow*. Advances in Neural Information Processing Systems 35 (2022), pp. 35478–35489. URL: https://proceedings.neurips.cc/paper_files/paper/2022/hash/e6c5195dac675f03d0fcf3955bcdd3c9-Abstract-Conference.html

RESEARCH AND WORK EXPERIENCE

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| Fundamental AI Research @ Meta , San Francisco, US Research Intern in the Chemistry team with Ben Miller | 05/2025 - 10/2025 |
| University of Heidelberg , Heidelberg, Germany Visited the group of Tristan Berreau | 01/2024 - 06/2024 |
| AI4Science @ Microsoft Research , Amsterdam, Netherlands Research Intern in the Electronic Structure team with Chin-Wei Huang | 07/2023 - 10/2023 |

AWARDS AND SCHOLARSHIPS

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| Mobility Grant from the Swiss National Science Foundation for visiting the University of Heidelberg | 2024 |
| NeurIPS Scholar Award | 2022 |
| Ph.D funding from the Swiss National Science Foundation | 2020 |

INVITED TALKS

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| Lennard-Jones Center, University of Cambridge, UK (online) | 02/2025 |
| ML-Based Sampling in Lattice Field Theory and Quantum Chemistry, University of Bonn, Germany | 10/2024 |
| Chalmers University of Technology, Gothenburg, Sweden (online) | 07/2024 |
| NEC Laboratories Europe, Heidelberg, Germany | 06/2024 |
| Particle Phenomenology Seminar, University of Heidelberg, Germany | 03/2024 |
| Machine Learning Galore, University of Heidelberg, Germany | 01/2024 |
| Seminar of the Control & Inference group, Donders Institute, Netherlands (online) | 04/2023 |

TEACHING EXPERIENCE

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| Logiciels et réseaux informatiques B.Sc. in Computer Science | University of Geneva springs of 2022, 2023 |
| Deep Learning M.Sc. in Computer Science | University of Geneva falls of 2021, 2022 |

COMPLETE LIST OF PAPERS

- [1] Bálint Máté, François Fleuret, and Tristan Berreau. *Solvation free energies from neural thermodynamic integration*. The Journal of Chemical Physics 162.12 (Mar. 2025), p. 124107. ISSN: 0021-9606. DOI: [10.1063/5.0251736](https://doi.org/10.1063/5.0251736). eprint: https://pubs.aip.org/aip/jcp/article-pdf/doi/10.1063/5.0251736/20452824/124107_1_5.0251736.pdf. URL: <https://doi.org/10.1063/5.0251736>.
- [2] Bálint Máté and François Fleuret. *Multi-lattice Sampling of Quantum Field Theories via Neural Operator-based Flows*. Machine Learning: Science and Technology 5.4 (Dec. 2024), p. 045053. DOI: [10.1088/2632-2153/ad9707](https://doi.org/10.1088/2632-2153/ad9707).
- [3] Bálint Máté, François Fleuret, and Tristan Berreau. *Neural Thermodynamic Integration: Free Energies from Energy-Based Diffusion Models*. The Journal of Physical Chemistry Letters 15.45 (2024), pp. 11395–11404. DOI: [10.1021/acs.jpcllett.4c01958](https://doi.org/10.1021/acs.jpcllett.4c01958). eprint: <https://arxiv.org/abs/2406.02313>.
- [4] Atul Kumar Sinha, Daniele Paliotta, Bálint Máté, John Raine, Tobias Golling, and François Fleuret. *SUPA: A Lightweight Diagnostic Simulator for Machine Learning in Particle Physics*. Advances in Neural Information Processing Systems 36 (2024). URL: https://proceedings.neurips.cc/paper_files/paper/2023/hash/cca79c22037280d066fbd8bc35ac2e72-Abstract-Datasets_and_Benchmarks.html.
- [5] Bálint Máté and François Fleuret. *Learning Interpolations between Boltzmann Densities*. Transactions on Machine Learning Research (2023). ISSN: 2835-8856. URL: <https://openreview.net/forum?id=TH6YrEcbth>.
- [6] Daniele Paliotta, Mathieu Alain, Bálint Máté, and François Fleuret. *Graph Neural Networks Go Forward-Forward*. NeurIPS 2023 Workshop: New Frontiers in Graph Learning (2023). URL: <https://openreview.net/forum?id=P1qQ8V5BfC>.
- [7] Bálint Máté and François Fleuret. *Deformations of Boltzmann Distributions*. NeurIPS 2022 Workshop: Machine Learning and the Physical Sciences (2022). URL: https://ml4physicalsciences.github.io/2022/files/NeurIPS_ML4PS_2022_48.pdf.
- [8] Bálint Máté, Samuel Klein, Tobias Golling, and François Fleuret. *Flowification: Everything is a Normalizing Flow*. Advances in Neural Information Processing Systems 35 (2022), pp. 35478–35489. URL: https://proceedings.neurips.cc/paper_files/paper/2022/hash/e6c5195dac675f03d0fcf3955bcdd3c9-Abstract-Conference.html.