Ongoing postdoc – Ecole nationale des ponts et chaussées / CNRS

PhD in physics, master in statistics, C1 English

Lune Maillard ✉ lune.maillard@enpc.fr

Professional experience

2026	**Post-doc**, laboratory: Centre d'Enseignement et de Recherche en MathématIques et Calcul Scientifique (CERMICS), 1 year Titre: *Computing transition rates: models and algorithms* Transition rates, adaptive multilevel splitting, importance sampling
2024-2025	**Postdoc**, laboratory: Institut des NanoSciences de Paris (INSP), 1 year Subject: « *Complex Phases in Ammonia-Water Mixtures Under Extreme Conditions: Disorder, Plasticity, and Super-Ionicity* » Plasticity, hydrogen bonds (frustration, dissociation), disorder, quantum effects, machine learning, experience-theory, high pressure

Education

2021-2024	**PhD**, doctoral school: Physique en Île-de-France, laboratory: Institut des NanoSciences de Paris (INSP), doctoral scholarship Sorbonne Center for Artificial Intelligence (SCAI) Subject: « *Bayesian methods for studying Nuclear Quantum Effects in Material Science* » Machine learning, nested sampling, nuclear quantum effects, co-developer of nested_fit program Teaching mission in the mathematics' department of Sorbonne Université
2019-2021	**Master 2 in Statistics**, Sorbonne Université Average master 2: 81,97%; Average master 1: 87,65%
2020	MOOC *« Elements of AI »* (University of Helsinki)
2016 - 2019	**Double bachelor mathematics and physics**, Sorbonne Université Mathematics' average: 77,36%, Physics' average: 75,73%
-2016	Secondary school, European School Brussels III in the French section. European Baccalaureate

Publications / Program

Articles	L. Maillard, F. Finocchi and M. Trassinelli. *Assessing Search and Unsupervised Clustering Algorithms in Nested Sampling*. Entropy, 25(2):347, Feb. 2023. L. Maillard, F. Finocchi, C. Godinho, and M. Trassinelli. *Nested Sampling for Exploring Lennard-Jones Clusters*. In The 43rd International Workshop on Bayesian Inference and Maximum Entropy Methods in Science and Engineering; MDPI, p 8, Oct. 2025 L. Maillard., P. Depondt, F. Finocchi, S. Huppert, T. Plé, J. Salomon and M. Trassinelli. *Probing the Partition Function for Temperature-Dependent Potentials with Nested Sampling*. The Journal of Chemical Physics, 163(18):184109, Nov. 2025
Program	M. Trassinelli, L. Maillard. and C. Godinho (September 2025). nested_fit (Version 5.5). Github. https://github.com/martinit18/nested_fit

Conferences / workshops

2025	Workshop *Uncertainty quantification in atomistic modeling: From uncertainty-aware density functional theory to machine learning* workshop – poster *John Skilling's 80th birthday meeting* – oral presentation
2022-2024	MaxEnt conference – oral presentation (2022, 2024) and poster (2023). Member of local organisation committee of MaxEnt'22 conference
2024	*Atoms, Molecules and cluster in Motion* conference – oral presentation
2023	*Deep Modeling for Molecular Simulations 2023* workshop (Princeton University, Chemistry department) – best poster
2022	*GDR IAMAT* – oral presentation

Other professional experiences

2021	**Five-month internship at INSP** (CNRS/Sorbonne Université) for Master 2 Subject: « *Nested Sampling for Nuclear Quantum Effects* »
2018	**Four-week internship**, CNRS, « Bioénergétique et Ingénierie des Protéines » laboratory, team « Biophysique des métalloprotéines »

Skills

Languages	-French, mother tongue -**English**, CLES **certification C1** -Spanish, B1-B2
Computer	-Python, Fortran (OpenMP), R, C++ -git/GitHub -Bases in Mathematica -Microsoft Office suite, QtiPlot, LaTeX
Teaching	French qualification to teaching function: sections 26 (Applied mathematics and applications of mathematics), 28 (Dense media and materials) et 30 (Diluted media and optic)
Other	BVA driving licence (automatic car)