Aurelien Pelissier, Ph.D.

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S Google Scholar   Github
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Current positions:
- Postdoctoral Scientist in Generative AI & Foundation Models, **Yale University** (Swiss-funded) (2023–Present)
- ML Research Collaborator in Organoid Profiling, **University of British Columbia** (2023–Present)
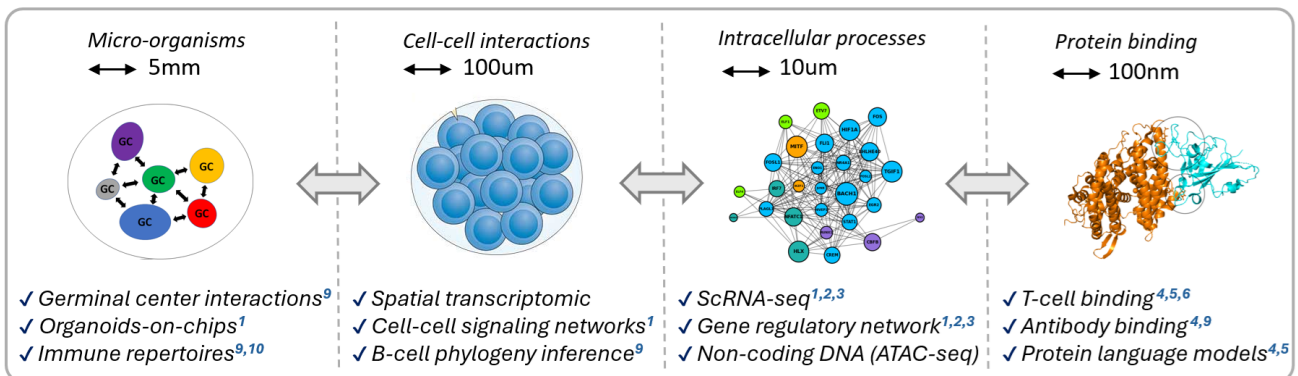
Background & Education:
- AI Researcher at **IBM Research Europe** (2019–2023) | AI for Scientific Discovery
- PhD in AI & Computational Biology, **ETH Zurich** (2019–2023) [Thesis]
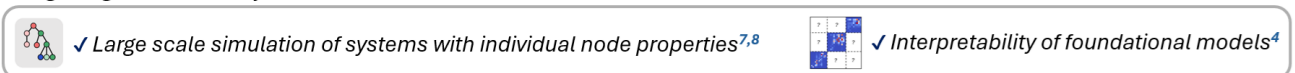- MSc in Quantum Physics, **ENS Paris-Saclay** (2018)

Notable work:
- Publications in **Nature Computational Science** [6], *Analytical Chemistry* [10, 11]
- Conference proceedings in **SDM 2019** [12]
- Conference talks at **ISMB 2022** [2], **ISMB 2021** [6], *the leading conference in computational biology* (A/A*)
- Participation in **AIntibody** (Generative AI competition) and **IMMREP 2023** [4] (TCR-epitope binding challenge)
- Co-Founder of **Peer2Panel** [13], a blockchain startup bridging NFTs and solar energy

My current research bridges artificial intelligence and mathematical modeling frameworks to advance our understanding of immunology, with a particular focus on **Foundation Models** in the context of B-cell and T-cell dynamics. I combine together interpretability methods, diffusion models, and graph neural networks to achieve efficient and flexible feature representations for **Generative AI** tasks in immunology.

Micro-organisms ↔ 5mm	Cell-cell interactions ↔ 100um	Intracellular processes ↔ 10um	Protein binding ↔ 100nm
✓ Germinal center interactions[9]	✓ Spatial transcriptomic	✓ ScRNA-seq[1,2,3]	✓ T-cell binding[4,5,6]
✓ Organoids-on-chips[1]	✓ Cell-cell signaling networks[1]	✓ Gene regulatory network[1,2,3]	✓ Antibody binding[4,9]
✓ Immune repertoires[9,10]	✓ B-cell phylogeny inference[9]	✓ Non-coding DNA (ATAC-seq)	✓ Protein language models[4,5]

Integrating multi-scale layers into a unified framework

✓ *Large scale simulation of systems with individual node properties*[7,8]   ✓ *Interpretability of foundational models*[4]

Ultimately, my goal is to integrate together biological processes **spanning multiple scales**, such as cell population dynamics, cell-cell interactions, intracellular mechanisms, and protein binding, to construct a realistic *in-silico model* of the immune response.

Selected Publications and Preprints

* Indicates co-first authors

ScRNA-seq, Gene regulatory networks and Cell-cell signaling networks

1 **Pelissier, A.***, Laragione, T.*, Harris, C., Martínez, M. R., & Gulko, P. S. (2025). BACH1 as a key driver in rheumatoid arthritis fibroblast-like synoviocytes identified through gene network analysis. *Life Science Alliance*, 8(1). 🔗 doi:10.26508/lsa.202402808

→ Identified computationally BACH1 inhibition as a promising therapeutic strategy for RA, currently undergoing in vivo testing

2 **Pelissier**, **A.**, Laragione, T., Gulko, P. S., & Martinez, M. R. (2024). Cell-specific gene networks and drivers in rheumatoid arthritis synovial tissues. *Frontier in Immunology*, 2024–12.

🔗 doi:`10.3389/fimmu.2024.1428773`

→ Oral presentation at ISMB2022 (Leading conference in computational biology, ranked A/A).*

Protein Language Models

3 Deutschmann, N.*, **Pelissier, A.***, Weber, A., Gao, S., Bogojeska, J., & Martínez, M. R. (2024). Do domain-specific protein language models outperform general models on immunology-related tasks? *ImmunoInformatics*, 100036. 🔗 doi:`10.1016/j.immuno.2024.100036`

4 Nielsen, M., Eugster, A., Jensen, M. F., Goel, M., Tiffeau-Mayer, A., **Pelissier**, A., … Greiff, V. et al. (2024). Lessons learned from the IMMREP23 TCR-epitope prediction challenge. *ImmunoInformatics*, *16*, 100045.

🔗 doi:`10.1016/j.immuno.2024.100045`

→ Demonstrated the potential of protein language models to generalize TCR binding to "unseen" epitopes.

5 Weber, A., **Pelissier, A.**, & Martinez, M. R. (2024). T-cell receptor binding prediction: A machine learning revolution. *ImmunoInformatics*, 100040. 🔗 doi:`10.1016/j.immuno.2024.100040`

Multi-scale stochastic models & Non-Markovian processes

6 **Pelissier**, **A.**, Phan, M., Beerenwinkel, N., & Rodriguez Martinez, M. (2025). Practical and scalable simulations of non-Markovian stochastic processes and temporal networks with individual node properties. *Nature Computational Science (in revision).* 🔗 doi:`10.48550/arXiv.2212.05059`

→ Oral presentation at ISMB2021 (Leading conference in computational biology, ranked A/A).*

7 **Pelissier**, **A.**, Akrout, Y., Jahn, K., Kuipers, J., Klein, U., Beerenwinkel, N., & Rodriguez Martinez, M. (2020). Computational model reveals a stochastic mechanism behind germinal center clonal bursts. *Cells*, *9*(6), 1448. 🔗 doi:`10.3390/cells9061448`

→ Third best poster award at ISMB2020.

Immune repertoires & B-cell phylogeny

8 **Pelissier, A.***, Stratigopoulou, M.*, Dimitriadis, E., Bende, R., van Noesel, C., Rodriguez Martinez, M., & EJ Guikema, J. (2023). Convergent evolution and B-cell recirculation in germinal centers in a human lymph node. *Life Science Alliance.* 🔗 doi:`10.26508/lsa.202301959`

9 **Pelissier, A.***, Luo, S.*, Stratigopoulou, M., EJ Guikema, J., & Rodriguez Martinez, M. (2023). Exploring the impact of clonal definition on B-cell diversity: Implications for the analysis of immune repertoires. *Frontier in immunology.* 🔗 doi:`10.3389/fimmu.2023.1123968`

Raman spectroscopy

10 **Pelissier, A.***, Hashimoto, K.*, Mochizuki, K.*, Kumamoto, Y., Taylor, J., Fujita, K., … Komatsuzaki, T. (2025). Beyond the nucleus: Cytoplasmic dominance in follicular thyroid carcinoma detection using single-cell Raman imaging across multiple devices. *Analytical Chemistry (under review).*

🔗 doi:`10.48550/arXiv.1904.05675`

11 Taylor, J. N., **Pelissier**, **A.**, Mochizuki, K., Hashimoto, K., Kumamoto, Y., Harada, Y., … Komatsuzaki, T. (2023). Correction for extrinsic background in Raman hyperspectral images. *Analytical Chemistry*, *95*(33), 12298–12305. 🔗 doi:`10.1021/acs.analchem.3c01406`

Others

12 **Pelissier**, **A.**, Nakamura, A., & Tabata, K. (2019). Feature selection as monte-carlo search in growing single rooted directed acyclic graph by best leaf identification. In *Proceedings of the 2019 SIAM International*

Conference on Data Mining (pp. 450–458). SIAM. 🔗 doi:`10.1137/1.9781611975673.51`

13 Lehner, J., & **Pelissier**, A. (2022). Peer2Panel: Democratizing renewable energy investment with liquid and verifiable tokenized solar panels. *Whitepaper.* 🔗 doi: 10.13140/RG.2.2.11113.06247

Work Experience

Academic

2023 – Present 🔖 **Postdoctoral Research Associate - AI & Computational Biology**
Yale School of Medicine, United States
Interpretable AI for personalized medicine - Prof. Maria Rodrigez Martinez.
Utilized protein language models (PLM) to study antibody and T-cell binding to antigens [3, 5], and demonstrated their effectiveness at the IMMREP23 T-cell prediction challenge [4] as well as the AIntibody challenge.
→ *Currently developing interpretable transformer models for rational antibody and TCR design, utilizing PLM likelihood dependency maps to capture residue co-dependencies and sequence-function relationships.*

Life Sciences Institute, University of British Columbia, Canada
Organoid-on-chips for disease modeling - Prof. Josef Penninger.
Characterizing the benefit of high flux environments for the growth of vascularized organoids and the organ-specificity of their vascular networks using scRNA analysis, spatial transcriptomics, and cell-cell communication networks [**??**].

2019 – 2023 🔖 **Ph.D. Fellowship - AI & Computational Biology**
IBM Research Zurich & ETH Zurich, Switzerland
AI for Scientific Discovery – Prof. Maria Rodriguez Martinez.
Stochastic Modeling of the Humoral Immune Response: A Multi-scale Challenge.
→ *Nominated for the 2023 ETH Silver Medal awarded to outstanding doctoral theses.*
(Thesis)

2018 – 2019 🔖 **Research Scientist - AI & Raman Spectroscopy**
Imperial University of Hokkaido, Japan
Molecule & Life nonlinear science laboratory – Prof. Tamiki Komatsuzaki.
Accelerated cancer diagnosis measurement technologies by integrating single-cell Raman imaging with machine learning [10, 11].

Feb. – July 2018 🔖 **Master Thesis - Reinforcement Learning**
Imperial University of Hokkaido, Japan
Laboratory for Pattern recognition & Machine Learning - Prof. Atsuyoshi Nakamura.
Feature Selection as Reinforcement Learning by Bandit strategies and Monte Carlo tree search [12].
(Thesis) (Code) (Poster)

2016 – 2017 🔖 **Visiting International Student - Experimental Physics & Modeling**
University of British Columbia, Vancouver, Canada
Ultrafast Spectroscopy Laboratory – Prof. David Jones.
Study of High Harmonic Generation (HHG) in high repetition rate systems.
(A one year research program as part of my ENS degree).
(Thesis) (Code) (Poster)

Work Experience (continued)

Apr. – July 2016   **Research Internship - Experimental Physics & Modeling**
Ecole Polytechnique federale de Lausanne, Switzerland
Advanced Semiconductors for Photonics & Electronic (LASPE) - Prof. Nicolas Grandjean.
Impact of piezoelectric effects on Nitride-III Nanobeam optical properties.
(Thesis) (Code)

Blockchain

2022 – Present   **Co-Founder - Peer2Panel**
The company aims at making investment in renewable energy secured, transparent and accessible to customers with capital of any size. With the acquisition of tokens backed by physical solar panels, clients can grow a renewable energy portfolio easily and affordably through the Ethereum blockchain [13]. (https://www.peer2panel.com)

Education

2019 – 2023   **Ph.D. Fellowship - AI & Computational biology**
ETH Zurich, Switzerland
Joint program with IBM Research.
Germinal center B cell evolution, Antigen-Antibody binding, Gene regulatory networks, Single cell transcriptomic, non-Markovian processes, Interpretable AI, Drug discovery.
$\rightarrow$ *Nominated for the 2023 ETH Silver Medal awarded to outstanding doctoral theses.*
(Thesis)

2017 – 2018   **M.Sc. Quantum physics, Nanophysics**
University Grenoble - Alpes, France
Double degree with ENS Paris-Salclay.
Quantum information theory, Nanoelectronics, Nanomagnetism, Nanophotonics.

2014 – 2018   **Grande École Degree - Fundamental physics & Applications**
Ecole Normale Superieure (ENS), Paris-Saclay, France
PHYTEM (PHYsics, Theory, Experiment, Modeling).
Statistical physics, Solid state physics, Astrophysics, Particle physics, Semiconductors.

2012 – 2014   **Scientific CPGE**
Classe Préparatoire aux Grandes Écoles, Grenoble, France
Two years preparation to highly selective national competitive exam.

Skills & Interests

ML & Coding   Python, R, C++, Matlab, Fortran,
TensorFlow, PyTorch,
Diffusion model, Generative AI,
Graph neural network, Geometric deep learning,
Stochastic processes, Bayesian statistics, Interpretable ML,
Transformers, LSTM, Reinforcement learning,
Quantum machine learning (See my article on Qiskit).

Skills & Interests (continued)

Bioinformatics   📑 Protein language models (PLMs), T-cell and Antibody binding,
ScRNA-seq, RNA velocity, Spatial transcriptomic,
ScATAC-seq, Non-coding DNA,
Gene regulatory networks, Cell-cell communication networks,
Immune repertoires, B-cell phylogeny inference,
Non-Markovian processes, Mechanistic models.

Awards, Trainings & Certifications

2023   📑 **Nominated for the ETH Silver Medal awarded to outstanding doctoral theses.**
Zurich, Switzerland

2020   📑 **Innosuisse Entrepreneurship Program**
Zurich, Switzerland
From Idea to Market, Business model development, Financial planning & Pitching.