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-on-Chip Profiling, **University of British Columbia** (2023–Present)
- Co-Founder of **Peer2Panel** [17], a blockchain startup integrating NFTs into the solar energy market

BACKGROUND & EDUCATION:
- ML Researcher at **IBM Research Europe** (2019–2023) | AI for Scientific Discovery
- PhD in AI & Computational Biology, **ETH Zurich** (2019–2023) [Thesis]
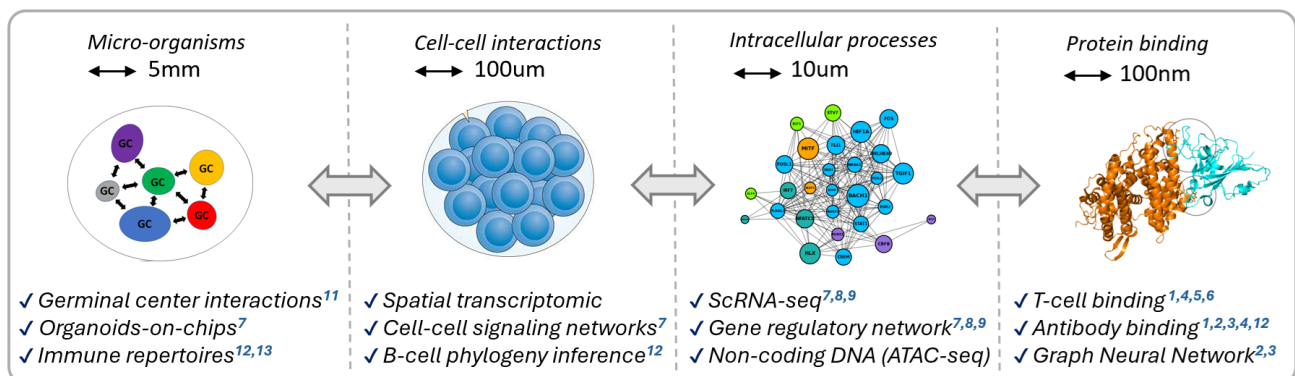- MSc in Quantum Physics, **ENS Paris-Saclay** (2018)

NOTABLE WORK (MACHINE LEARNING):
- Multiple contributions under review for top venues *Neurips 2025* [2] and *ICML 2025 GenBio workshop* [1, 3]
  (*Conditional fine-tuning of generative PLMs & Graph-based metric-learning for TCR and antibody design*)
- Manuscript under review in *PNAS* [10]
- Participant in **AIntibody** [2] (Generative AI competition) and **IMMREP** [5] (TCR-epitope binding challenge)
- Publications in *Analytical Chemistry* [14, 15]
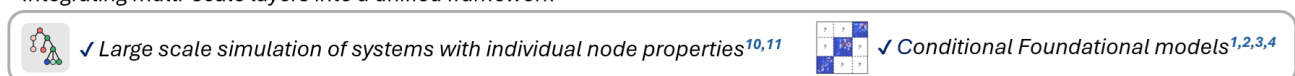- Conference paper at *SDM 2019* [16]

NOTABLE WORK (COMPUTATIONAL BIOLOGY):
- Manuscript under review in *Nature Biotechnology* [7]
- Contributed talks at top venues: *ISMB (2021, 2022)* [9, 10]
- Manuscript *"Modeling Heart Attacks on a Chip"* in preparation for *Nature*
- Identified **BACH1** as a promising therapeutic target for rheumatoid arthritis, validated experimentally [8].
- Published work on B-cell phylogenies and gene regulatory networks [4, 8, 9, 12, 13, 11]

My current research bridges machine learning, bioinformatics 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-inspired 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*[11]   ✓ *Spatial transcriptomic*   ✓ *ScRNA-seq*[7,8,9]   ✓ *T-cell binding*[1,4,5,6]
✓ *Organoids-on-chips*[7]   ✓ *Cell-cell signaling networks*[7]   ✓ *Gene regulatory network*[7,8,9]   ✓ *Antibody binding*[1,2,3,4,12]
✓ *Immune repertoires*[12,13]   ✓ *B-cell phylogeny inference*[12]   ✓ *Non-coding DNA (ATAC-seq)*   ✓ *Graph Neural Network*[2,3]

Integrating multi-scale layers into a unified framework

✓ *Large scale simulation of systems with individual node properties*[10,11]   ✓ *Conditional Foundational models*[1,2,3,4]

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; author order may be adjusted for CV.

Generative AI | Masked Language Models | Graph Neural Networks

1 **Pelissier, A.***, Shao, Y.*, & Martinez, M. R. (2025). Logit-preserving contrastive fine-tuning for generative and interpretable conditional masked language models. *In preparation for ICLR / ICML GenBio workshop.* 🔗 [Poster] [Draft]

2 **Pelissier, A.***, Lui, C.*, Denzle, L., Shao, Y., Martin C.R., A., Paige, B., & Rodriguez Martinez, M. (2025). Abrank: A benchmark dataset and metric-learning framework for antibody-antigen affinity ranking. *Under review for NeurIPS 2025 Datasets & Benchmarks Track.* 🔗 [Submission]

3 **Pelissier, A.***, Denzler, L.*, Lui, C., Shao, Y., Paige, B., & Martinez, M. R. (2025). Functional convergence in antibody repertoires via graph-based binding mode representation. *In preparation for ICML 2025 GenBio workshop.* 🔗 [Draft]

4 **Pelissier, A.***, Deutschmann, N.*, 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

5 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.*

6 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

ScRNA-seq | Gene Regulatory Networks | Cell-Cell Signaling Networks

7 Quintard, C., Wang, J., **Pelissier, A.**, Ren, J., Sebastien, R., Lee, J., … Penninger, J. (2025). Engineering perfusable vascular network organoids-on-chip and modeling cardiac-specific vasculature under flow. *Nature Biotechnology (under review)*
→ *Led the computational biology analysis, including scRNA-seq, cell-cell signaling network inference, RNA velocity, and gene regulatory network inference. Identified key transcription factors and pathways driving heart organogenesis, offering critical insights into developmental biology* [Figures].

8 **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, validated in vitro and currently undergoing in vivo testing*

9 **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
→ *Contributed talk at ISMB2022 (Leading conference in computational biology, ranked A/A*).*

Multi-Scale Stochastic Models & Non-Markovian Processes

10 **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. *Proceedings of the National Academy of Sciences (under review).* 🔗 doi:10.48550/arXiv.2212.05059
→ *Contributed talk at ISMB2021 (Leading conference in computational biology, ranked A/A*).*

11 **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

12 **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

13 **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 & Hyperspectral Imaging

(14) **Pelissier, A.***, Hashimoto, K.*, Mochizuki, K.*, Kumamoto, Y., Taylor, J., ..., & Komatsuzaki, T. (2025). Beyond the nucleus: Cytoplasmic dominance in follicular thyroid carcinoma detection using single-cell Raman imaging across multiple devices. *Analytical Chemistry (in press)*. 🔗 doi:`10.48550/arXiv.1904.05675`

(15) 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

(16) **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`

(17) 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

(18) Sammut, R., Fenwarth, L., **Pelissier**, **A.**, Marceau, A., Duployez, N., Benachour, S., ... Loschi, M. (2025). Clonal evolution of myeloid malignancies treated with microtransplantation: A single-centre experience. *Journal of Cellular and Molecular Medicine*, *29*(6), e70520. 🔗 doi:`10.1111/jcmm.70520`

Invited Talks & Presentations

- **Keynote Speaker** — Representing IBM Research at the Biotechnet Meet-Up 2023.
  Presented: *AI-Driven Engineering of the Immune System*.

- Contributed talk, ISMB 2022, *Cell-type Specific Gene Regulation in Rheumatoid Arthritis*.

- Contributed talk, ISMB 2021, *A Rejection Gillespie Algorithm for Non-Markovian Stochastic Processes*.

- **Best Poster Award** (Third Place), ISMB 2020, *Computational Model Reveals a Stochastic Mechanism Behind Germinal Center Clonal Bursts* [Poster].

- Contributed poster, ISMB 2022, *Characterization of Antibody Specificity Leads to the Identification of Convergent Evolution in Germinal Centers* [Poster].

Skills & Interests

ML & Coding	🔖 Python, R, `C++`, Matlab, Fortran, TensorFlow, PyTorch, Masked Language Models, 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).
Computational Biology	🔖 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.

Work Experience

Academic

2023 – Present

Postdoctoral Research Associate - Generative AI & Foundation Models
Yale School of Medicine, United States
Leading the fine-tuning of masked language models (MLMs) for diverse downstream tasks across DNA and protein sequences, with an emphasis on retaining interpretability [1]. Demonstrated the benefits of representing antigen complexes as graphs, rather than relying solely on sequence-based approaches [2, 3].
→ Coordinating contributions from multiple students within the group.
→ Organized team participation in the IMMREP25 T-cell prediction challenge and the AIntibody generative antibody design competition.

Life Sciences Institute, University of British Columbia, Canada
Organoid-on-chips for disease modeling - Prof. Josef Penninger.
Characterizing the benefits of high-flux environments for the growth of vascularized organoids and the organ specificity of their vascular networks using scRNA-seq, spatial transcriptomics, and cell–cell communication network analysis [7].
→ Contributed rigorous, in-depth computational analyses for multiple high-impact studies forthcoming in *Cell Stem Cell*, *Nature*, and *Nature Biotechnology* [Figures].

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 [Thesis].
→ *Nominated for the 2023 ETH Silver Medal awarded to outstanding doctoral theses.*

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 [14, 15].

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 [16]. [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]

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 [17]. [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.
→ *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.

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.