EVANGELOS-MARIOS NIKOLADOS

MACHINE LEARNING & COMPUTATIONAL SCIENTIST · AI FOR BIOLOGY

DETAILS

BASED IN
Edinburgh, UK

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LINKS

emnikolados.dev
github.com/evanniko1
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SKILLS

Languages: Python, Julia, C, MATLAB, SQL

ML / Modelling: Deep learning, mechanistic & dynamical modelling, whole-cell simulation, active learning / DoE

Frameworks: PyTorch, TensorFlow, scikit-learn, Dash, FastAPI, SQLAlchemy

LLMs & Agents: MCP, tool-calling agents, Claude Code, Codex, Ollama, OpenRouter

Tools: Git, Bash, Docker

DOMAINS

AI for biology
Sequence-to-function modelling
Whole-cell modelling
Synthetic biology
Autonomous experimentation

LANGUAGES

Greek (native)
English (fluent)

I build the models and platforms that make living cells predictable — and, ultimately, programmable. My work spans the two halves of biological modelling that rarely meet: **mechanistic, mathematical models** of how cells actually work — whole-cell simulation, dynamical systems, resource allocation — and **machine learning** that predicts biological function directly from sequence and data. I believe the next advance in AI-for-biology comes from fusing the two, wrapped in autonomous agents that design and run their own experiments, turning biological engineering from trial-and-error into **simulation and inference**. My goal is to help build the AI-driven **virtual cell**: a model of a living system you can query, steer, and trust well enough to design new biology on.

EXPERIENCE

Head of AI — Myria Biosciences AG

Edinburgh, UK · Basel HQ

Nov 2024 – Present · Full-time

Engineering macrocyclic-peptide therapeutics at scale from non-ribosomal peptide synthetases (NRPS).

- Built **MyriaLoop**, an end-to-end closed-loop data platform (Python, Dash) that unifies LC-MS peptide discovery with NRPS combinatorial-biosynthesis design — replacing a fragmented MZmine-and-spreadsheets process with a single design–build–test–learn system.
- Built the platform's ML engine for predicting NRPS construct functionality and used it to guide the wet lab: the first model-guided round reached a **~47% functional hit rate** — roughly a **7× enrichment** over the ~7% unguided combinatorial baseline.
- Turned experiment planning into an **active-learning loop**, so each wet-lab round is selected to be maximally informative and the platform's predictions sharpen as data accrues.

Research Assistant — Weiße Group, University of Edinburgh

Edinburgh, UK

Jun 2023 – Nov 2023

- Developed and validated mechanistic bacterial-growth models in Julia, linking ribosome allocation and nutrient uptake to whole-cell physiology.

Project Supervisor — University of Edinburgh

Edinburgh, UK

2020–2023

- Supervised undergraduate and PhD students on ML-for-biology projects — from data preparation and dimensionality reduction to image-analysis pipelines for classifying neural stem cells.

SELECTED PROJECTS

Independent of my role at Myria Biosciences — academic, open-source & hackathon work.

seq2yield-agent IN DEVELOPMENT

github.com/evanniko1/seq2yield-agent

Autonomous, "self-driving" ML for sequence-to-yield prediction.

- A system that **automatically builds, critiques, and improves ML models predicting expression or yield from short biological sequences** — for any such dataset, not one hand-tuned model. An LLM "council" proposes approaches, reviewers challenge them, and a bounded ML-engineer loop implements and validates each under fixed metrics and protected-data guards. Already spans **five public datasets — ~1.12M sequences across *E. coli*, yeast, and human**; validated by autonomously reproducing and beating a published deep-learning baseline (the 227k-sequence *E. coli* set).

wcEcoli Platform & "Coli Agent" IN DEVELOPMENT

feature/wcecoli-platform

Making a genome-scale whole-cell simulator explorable by conversation (primary contributor).

- Primary contributor to a platform that opens up a **molecular-resolution whole-cell *E. coli* model** — all **~1,592 genes**, ~9 min of compute per simulated generation — through a browser and a natural-language **agent** that designs knockout and media-shift experiments, launches batch simulations, and analyses results conversationally, with human approval gating any state change — putting a genome-scale whole-cell model in the hands of **experimental biologists — and students learning systems biology** — not just computational specialists. Roadmap: layer in **Vivarium's agent-based, multi-cell capabilities to extend to antimicrobial-resistance (AMR) studies.**

The Well, for the Cell IN DEVELOPMENT

Hugging Face corpus + benchmark

A public ML benchmark of whole-cell dynamics — the biology counterpart to Polymathic AI's The Well.

- Co-designing a large, standardized Hugging Face corpus of whole-cell *E. coli* simulation trajectories — fully observable, causally perturbed, and dynamic (every modelled molecule and flux over time) — with benchmark tasks, leakage-free splits, and baselines: model-derived data that **complements** the sparse, noisy, partial snapshots of experimental omics rather than competing with them. The wcEcoli platform generates the corpus and the **Coli agent** is its grounded query interface.

Cellarium HACKATHON · THROUGH 12 JUL 2026

github.com/evanniko1/cellarium

Grounded, guardrailed Claude copilot over a whole-cell E. coli simulation.

- Building for the **Built with Claude: Life Sciences** hackathon (finishing 12 July 2026): an agentic Claude copilot (Anthropic Messages API, tool-using loop) that answers only from real simulation data and enforces **biosecurity and scientific guardrails** — refusing experiments outside the model's validated envelope and withholding non-viable results rather than laundering them into clean-looking numbers.

RECOGNITION

Selected participant (1 of 500) — **Built with Claude: Life Sciences**, Cerebral Valley (in progress, through 12 Jul 2026); building **Cellarium**

Principal's Career Development Scholarship, University of Edinburgh

Darwin Trust PhD Studentship in Biology & Biomedical Sciences

DDE Venture Builder Incubator grant (£2,000) — **KOIOS**, a cause-and-effect discovery NLP pipeline for advanced materials

Centenary Prize for MSc, Imperial College London

Alpha Sigma Lambda (ΑΣΛ) Honor Society; Dean's List (Harvard Extension)

State Scholarship Foundation excellence award (Greece)

SELECTED COURSEWORK

Applied Data Science — Columbia Engineering Executive Education / EMERITUS (2018–2019)

PUBLICATIONS

Citation metrics on Google Scholar.

Nagdi M., **Nikolados E.-M.**, Yermakov A., Gao M., Kutz N., Menolascina F. "Learning the Koopman Operator using Attention-Free Transformers." *arXiv*, **2026**. arxiv.org/abs/2606.23957

Baranowski C., Martin H. G., Oyarzún D. A., … **Nikolados E.-M.**, et al. "Can protein expression be 'solved'?" *Trends in Biotechnology*, **2025**. link

Bonfá G., Martino G., Sellitto A., … **Nikolados E.**, et al. "Design of novel synthetic promoters to tune gene expression in T cells." *bioRxiv*, **2025**. link

Nikolados E.-M., Oyarzún D. A. "Deep learning for optimization of protein expression." *Current Opinion in Biotechnology*, **2023**; 81:102941. link

Nikolados E.-M., Wongprommoon A., Mac Aodha Ó., Cambray G., Oyarzún D. A. "Accuracy and data efficiency in deep learning models of protein expression." *Nature Communications*, **2022**; 13(1):7755. link

Nikolados E.-M., Weiße A. Y., Oyarzún D. A. "Prediction of cellular burden with host–circuit models." *Synthetic Gene Circuits: Methods and Protocols* (Springer), **2021**; pp. 267–291. link

Nikolados E.-M., Weiße A. Y., Ceroni F., Oyarzún D. A. "Growth defects and loss-of-function in synthetic gene circuits." *ACS Synthetic Biology*, **2019**; 8(6):1231–1240. link

TALKS & PRESENTATIONS

Talks — "Deep learning models of protein expression":

- Darwin Trust Symposium, Edinburgh (2023)
- Turing Workshop on AI, Engineering Biology & Beyond, Edinburgh (2023)
- ICSB Satellite — "Synthetic Biology in the Age of Machine Learning", Berlin (2022)
- Synthetic Biology UK, Nottingham (2021)

Posters:

- Microbes22 — Emerging Applications of Microbes, Leuven, Belgium (2022) — flash talk & poster
- MOMI22 — World of Industrial Mathematics, INRIA Sophia Antipolis (2022) — *Best Poster Award*
- EMBO Workshop on Codon Usage, Edinburgh (2022)
- Control Engineering & Synthetic Biology, University of Oxford (2019) — "Growth defects & loss-of-function in synthetic gene circuits"
- Synthetic Biology UK, Bristol (2018) — "Growth defects & loss-of-function in synthetic gene circuits"

EDUCATION

PhD, Quantitative Biology, Biochemistry & Biotechnology

Edinburgh, UK

University of Edinburgh · 2019–2024

- Thesis: "Next-generation computational optimization of protein expression systems." Supervisors: Dr Diego Oyarzún, Prof. Meriem El Karoui.

Master of Research (MRes), Systems & Synthetic Biology

London, UK

Imperial College London · 2017–2018 · Distinction

- Thesis: "Growth defects and loss-of-function in synthetic gene circuits." Supervisors: Dr Diego Oyarzún, Dr John Heap.

Bachelor of Liberal Arts (ALB), Biology

Cambridge, MA

Harvard University, Extension School · 2015–2017 · GPA 3.87

- Thesis: "Intrusion Prevention & Detection Models for DNA Data Storage Systems." Supervisor: Edward G. Freedman.

BSc studies, Molecular Biology & Genetics

Alexandroupolis, GR

Democritus University of Thrace · 2011–2013 · transferred to Harvard

EARLIER ROLES

- **Tutor, Quickhelp Inc.** (Boston, 2016–2017) — online instruction in study, note-taking, and test strategies.
- **Teaching Assistant & Class President**, Democritus University of Thrace (2011–2013) — Computational & Structural Biology; organised research trips to EMBL and DKFZ (Heidelberg).