Manoja Rajalakshmi Aravindakshan

Postdoctoral Research Associate | Computational Modeling & Digital Twins

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Profile

- Computational scientist with a PhD in Computer Science and 7+ years building **physics-based digital twins and PBPK/PK-PD models** that accelerate drug development and reduce reliance on animal and clinical studies.
- Track record of translating complex physiology - *cardiovascular, lymphatic, central nervous system (CNS), and metabolic systems* - into predictive ODE-based simulators, with validated industry collaborations (Eli Lilly, esqLABS, Metflux Research) and peer-reviewed publications.
- Bridges rigorous mathematical modeling (lumped-parameter networks, IVIVE) with **model calibration and inference** - variational inference, Bayesian and gradient-based parameter estimation, sensitivity analysis - and scientific computing in Python/JAX (differentiable simulation, AI agents for model authoring).

Research & Professional Experience

Purdue University
West Lafayette, IN, USA

Postdoctoral Research Associate, School of Mechanical Engineering
Oct 2025 - Present

Vlachos Research Group, Predictive Science Lab · Lilly–Purdue Research Collaboration

- **Developing predictive models for clinical success**—a reduced-order framework for whole-body circulatory and lymphatic transport that more effectively predicts the outcome of new therapies in humans across cardiovascular and interstitial routes of administration, de-risking drug-development investment
- Researching tools, methodologies, and physiology of drug-delivery routes—including **intrathecal delivery of genetic medicines to the central nervous system**—to develop technologies that improve the pace of getting therapies to patients who need them
- Designing a **domain-specific language for compartmental PK models** that integrates a hierarchy of AI agents into the Design-Make-Test-Analyze (DMTA) cycle, accelerating the discovery, development, and commercialization of innovative therapeutics

Purdue University
West Lafayette, IN, USA

SERB Overseas Visiting Doctoral Fellow, Department of Computer Science
Aug 2023 - Aug 2025

Awarded India's prestigious SERB OVDF fellowship (USD 38,000)

- Developed a **closed-loop lumped-parameter whole-body cardiovascular model** (RCR network analogy for resistance, compliance, and inertance) for pressure/flow analysis under disease conditions
- Built **DigiLoCS**—a digital liver-on-chip simulator predicting drug distribution across organ-on-chip platforms (published in *PLOS ONE*, 2025)
- Extended modeling to a coupled cranial-spinal CSF / Circle-of-Willis lumped-parameter system capturing intracranial pulsatility and cerebrovascular regulation

Indian Institute of Technology Kharagpur
West Bengal, India

Doctoral Research Scholar
Aug 2019 - Aug 2023

Department of Computer Science and Engineering

- **PBPK modeling of drug distribution in liver-on-chip devices:** built compartmental ODE models integrating biology, device hardware, and physicochemical drug properties; differentiated active vs. passive hepatic processes; applied *in vitro*-to-*in vivo* extrapolation (IVIVE) to improve human clearance prediction
- **Insulin-glucose modeling for type 2 diabetes:** extended the oral minimal model with adipokine (leptin) and BMI coupling; identified three distinct patho-clinical clusters in uncontrolled T2D patients using rural community-clinic data (published in *BMJ Open Diab Res Care*)
- **Sponsored research, IIT Kharagpur:** delivered commercial-grade route-control-chart software for Indian Railways under MHRD/SERB IMPRINT-2 (IMP/2018/000471); deployed across zonal signaling sections

- **Teaching Assistant:** Foundations of Computing Science (CS60005), Algorithm Design & Analysis (CS60007), Computer Organization & Architecture (CS31001), Algorithms (CS21003)

Embedon Global Energy Pvt Ltd *Pune, India*
Software Engineer *Nov 2016 - June 2018*

- Developed embedded firmware and Linux/Windows tooling for (i) a sensor-driven cardio-rehab game using interactive light patterns and (ii) a high-precision 3D industrial marking machine for component traceability

Industry Internships

esqLABS GmbH *Saterland, Germany*
Computational Research Intern *June 2023 - Dec 2023*
Industry collaboration in physiologically-based pharmacokinetic modeling

- Built digital-twin scripts and simulation workflows in **PK-Sim / MoBi** for *in vitro* systems (organ-on-chip, 3D spheroids), enabling mechanistic interpretation of preclinical readouts
- Improved *in vitro*-to-clinical translation accuracy to support reductions in animal testing, trial cost, and patient burden during drug development

Metflux Research Pvt Ltd *Mumbai, India*
Computational Biology Intern *Aug 2021 - Dec 2021*
Selected via competitive Metflux Research Internship 2021

- Calibrated a whole-body adult-metabolism model under diet perturbation; simulated body-weight trajectories to characterize macronutrient-level metabolic regulation
- Delivered physiologically grounded insights informing downstream nutrition and metabolic-disease modeling efforts

AAIC Technologies Pvt Ltd *Hyderabad, India*
Software Developer Intern *Mar 2020 - July 2020*

- Developed GATE-prep and applied machine-learning course software; mentored students and authored course content

Education

Indian Institute of Technology Kharagpur *West Bengal, India*
Ph.D. in Computer Science | GPA: 9.52/10.0 *Jan 2020 - Dec 2024*
Department of Computer Science and Engineering

- **Thesis:** *Application of computational modeling towards digital twinning of human physiological and biochemical processes*
- **Coursework:** Systems Biology, Computational Structural Biology, Applied Multivariate Statistical Modelling, Machine Learning, Deep Learning

Government Engineering College, Palakkad *Palakkad, India*
B.Tech. in Computer Science | GPA: 8.54/10.0 (University Rank Holder) *Aug 2012 - May 2016*
University of Calicut

Publications & Patents

- **Aravindakshan MR**, Mandal C, Pothen A, Schaller S, Maass C. *DigiLoCS: A leap forward in predictive organ-on-chip simulations.* PLoS ONE 20(1): e0314083 (2025). doi:10.1371/journal.pone.0314083
- **Aravindakshan MR**, et al. *Parameter estimation for the oral minimal model and parameter distinctions between obese and non-obese type 2 diabetes.* DNA and Cell Biology Reports (2024). doi:10.1089/dcbr.2024.0018
- **Aravindakshan MR**, et al. *Distinct patho-clinical clusters among uncontrolled type 2 diabetes patients: results from a prospective study in rural India.* BMJ Open Diab Res Care (2022). doi:10.1136/bmjdrc-2021-002654
- **Aravindakshan MR**, et al. *A closed-loop lumped parameter model for whole-body cardiovascular simulation* (under review)

- **Aravindakshan MR**, et al. *A comprehensive computational framework for whole-body lymphatic transport simulation* (submission-ready)
- **Aravindakshan MR**, et al. *A coupled cranial-spinal CSF and Circle-of-Willis lumped-parameter model: Monro–Kellie volume coupling shapes intracranial pulsatility and cerebrovascular regulation* (in preparation)
- **Patent:** System for design of Route Control Chart (RCC) and application logic for interlocked signaling, Indian Patent App. No. 202431029893, filed Apr 2024

Skills & Certifications

- **Languages:** Python (JAX, NumPy, SciPy, scikit-learn), R, MATLAB, Java, C
- **Modeling:** PBPK / PK-PD, lumped-parameter ODE systems, IVIVE, digital twins; PK-Sim, MoBi
- **Calibration & Inference:** Variational inference, Bayesian and gradient-based parameter estimation, sensitivity analysis, differentiable simulation
- **Domains:** Cardiovascular hemodynamics, hepatic clearance, CSF/CNS transport, glucose-insulin dynamics, organ-on-chip
- **Certifications:** Professional Development (Purdue); NPTEL Deep Learning (Top 1%)
- **Other:** Trained Carnatic vocalist; yoga and strength training; Treasurer, Purdue Postdoctoral Association (PPDA)

Talks & Conference Presentations

- "A whole-body digital twin for fluid transport using a 0D lumped parameter model", *Lilly Deep Dive*, Purdue University, IN, USA (Mar 2026)
- "Lumped parameter model for simulating brain-body fluid dynamics: integration of CNS and whole-body circulatory systems", 10^{th} International Biofluid Mechanics and Mechanobiology Symposium (IBMS 10), UC Irvine, CA, USA (Sep 2025)
- "A whole-body lumped parameter model for cardiovascular simulation", 18^{th} U.S. Association for Computational Mechanics Congress, Chicago, IL, USA (Jul 2025)
- Invited talk: "Application of computational modeling towards digital twinning for human physiological systems", *OVDF Symposium*, Purdue University, IN, USA (Dec 2024)
- Invited talk: "Digital twins for liver-on-chip devices", *Data-Driven Mechanistic Models of Complex Biomedical Systems* workshop, University of Birmingham, UK (Dec 2023)
- "Parameter estimation for the oral minimal model and parameter distinctions between obese and non-obese type 2 diabetes", *Bioinformatics and Computational Biology Conference (BBCC)* (Dec 2022)

Awards & Honors

- **SERB Overseas Visiting Doctoral Fellowship** (OVDF), Government of India — competitive national fellowship for doctoral research at Purdue University, total grant USD 38,000 (Aug 2023)
- **Metflux Research Internship 2021** — selected for competitive industry internship for aspiring computational biologists
- Contributed to *Online Despatch System for Fabrication and T&E of AVN Packages* at **Vikram Sarabhai Space Centre (ISRO)**, Trivandrum
- **University Rank Holder** and **Batch Topper**, Computer Science, Calicut University (2016)

References

Pavlos Vlachos
Senior Vice President, DDCS, Eli Lilly
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