

Madeleine S. Gastonguay

Biomedical Engineering and Institute for Computational Medicine at Johns Hopkins University

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PhD candidate in Biomedical Engineering (focus area: Computational Medicine) with expertise in mechanistic modeling, viral dynamics, QSP, and Bayesian inference. Skilled in building ODE, stochastic, and nonlinear mixed effects models to gain mechanistic insights and support therapeutic design. Seeking an industry internship applying mathematical and statistical modeling to drug development and clinical translation for novel therapeutic modalities.

Skills & Certifications

Modeling: ODE, DDE, stochastic modeling, QSP, PK/PD, PBPK, NLME, structural and practical identifiability analysis, sensitivity analysis and parameter optimization, Bayesian inference

Programming: Bash, R (*tidyverse, mrgsolve, Shiny, plotly, brms*), Python, MATLAB, HPC/SLURM, SQL, Monolix, Stan, JAGS

Teaching: Certified Instructor with The Carpentries

Education

Johns Hopkins School of Medicine, Baltimore, MD

August 2022 - present

PhD in Biomedical Engineering

GPA: 4.0/4.0

Advisors: Dr. Alison L. Hill & Dr. Feilim Mac Gabhann

University of Connecticut, Storrs, CT

August 2016 - May 2020

Bachelor of Science, Applied Mathematics

Summa Cum Laude with Honors; GPA: 3.98/4.00

Minor: Bioinformatics

Thesis: A Quantitative Pipeline for The Identification of Combinations of Targets

for Claudin-Low Triple Negative Breast Cancer Reversion

Advisor: Dr. Paola Vera-Licona

Experience

Johns Hopkins Institute for Computational Medicine, Baltimore, MD

August 2022 – present

Biomedical Engineering PhD Candidate

Topic: Integrating mathematical models and statistical methods for within-host viral dynamics of persistent infection with quantitative systems pharmacology models of novel immunotherapies

- Building mechanistic mathematical models of persistent viral infections and evaluating their dynamic properties
- Developing Bayesian methods for parameter estimation and uncertainty quantification
- Designing stochastic and deterministic simulations to evaluate efficacy of therapeutic interventions for persistent viral infections
- Developing a pipeline for assessing practical identifiability of nonlinear mixed-effects models and reducing overfitting in data-driven model building approaches
- Implementing nonlinear-mixed effects modeling to understand mechanisms of action of novel HIV immunotherapies
- Collaborating with experimentalists in the field of infectious diseases
- Outcomes: 5 contributed talks, 2 poster presentations, 2 manuscripts in preparation

The Jackson Laboratory (JAX), Bar Harbor, ME

June 2020 – July 2022

Research Data Analyst

Topic: A Bayesian approach to mediation analysis of complex traits with measurement noise

- Contributed to the development and validation of an R package implementation of a Bayesian model selection approach to mediation analysis (*bmediatR*) that is flexible in both data inputs and potential inferences
- Diagnosed the effect of measurement noise on the inference of mediation using synthetic data and derived guidelines to avoid incorrect causal interpretation of spurious correlations in real-world genetic association examples
- Applied these tools to better understand the mechanisms underlying the effects of sex and diet on protein and gene expression in the livers of genetically diverse mice
- Outcomes: 2 papers, 1 R package

UConn Health Center for Quantitative Medicine, Farmington, CT

Sept. 2018 - May 2020

Undergraduate Research Assistant

Topic: A quantitative pipeline for cancer reversion analysis in triple negative breast cancer

- Constructed a static intracellular signaling network for a claudin-low triple negative breast cancer (CL TNBC) cell line with multi-omics data using bioinformatics techniques

- Applied a structure-based control method for nonlinear systems, implemented in python, to identify putative targets that steer the system to any desired attractor
- Conducted virtual screenings using a network-based approach and a signal propagation algorithm to estimate long term behaviors
- Implemented machine learning methods to analyze virtual screenings and identify concerted perturbations of control nodes resulting in reversion of the CL TNBC phenotype
- Outcomes: 1 contributed talk, 2 poster presentations, foundational pipeline for the Vera-Licona lab

Metrum Research Group, Tariffville, CT

June 2018 - Aug. 2018

Summer Intern

Topic: A maternal-fetal physiologically based pharmacokinetic model for drugs metabolized by cytochrome P450 isoenzymes

- Modeled maternal and fetal drug exposures at varying gestational ages by incorporating anatomical, biochemical, and physiological changes associated with pregnancy as a system of ordinary differential equations using R and *mrgsolve*
- Performed local sensitivity analysis, optimized model parameters, and validated the model by comparing model predictions to external published data
- Outcomes: 1 paper, 2 contributed talks, 2 poster presentations

University of Connecticut, Department of Molecular and Cellular Biology, Storrs, CT

Jan. 2017 - Sept. 2017

Undergraduate Research Assistant/Holster Scholar

Topic: The effect of host genetic variability on Epstein Barr Virus (EBV)-associated cancer susceptibility

- Reviewed relevant literature to identify genes that may impact EBV-associated cancer susceptibility
- Used wet lab techniques such as Polymerase Chain Reactions, Gel Electrophoresis, and Sanger Sequencing to sequence the genes of interest in several EBV-associated cancer cell lines and a non-cancerous EBV+ control cell line
- Aligned the genetic sequence of target genes to identify common and distinct single nucleotide polymorphisms (SNPs) across EBV-associated cancer cell lines using the software Geneious and BLAST
- Outcomes: 1 contributed talk

Children's Hospital of Philadelphia, Philadelphia, PA, **Metrum Research Group**, Tariffville, CT

Sept. 2015 - Aug. 2016

High School Independent Study

Topic: A pharmacogenomic study of midazolam and morphine clearance in critically ill pediatric patients

- Analyzed variability of SNPs in the sample dataset for inclusion in the analysis
- Estimated the effect of pediatric risk of mortality score on drug clearance using population pharmacokinetic modeling
- Identified a SNP in UGT2B7 whose minor allele frequency is associated with increased midazolam clearance
- Outcomes: 2 papers

Manuscripts in Preparation

Juillard F⁺, Gastonguay MS⁺, Szymula A⁺, Gerold J, Li S, Lomonte P, Simas JP, Hill AL, & Kaye KM (2025+). KSHV episomal DNA replicates and partitions to progeny cell nuclei at similar, imperfect efficiencies.

Gastonguay MS⁺, Gerold J⁺, Balelli I, Pasin C, Li JZ, Barouch DH, Whitney JB, Hill AL⁺, & Prague M⁺ (2025+). Viral rebound kinetics following single and combination immunotherapy for HIV/SIV.

⁺These authors contributed equally to the work

Publications

Liu, T. Y. A., Liu, Y., Gastonguay, M. S., Midgett, D., Kuo, N., Zhao, Y., Ullah, K., Alexander, G., Hartman, T., Koseoglu, N., Jones, C. (2025). Predicting imminent conversion to exudative age-related macular degeneration using multimodal data and ensemble machine learning. *Ophthalmology Science*, <https://doi.org/10.1016/j.xops.2025.100785>.

Gastonguay, M. S., Keele, G. R., & Churchill, G. A. (2023). The trouble with triples: Examining the impact of measurement error in mediation analysis. *Genetics*, 224(1), iyad045. <https://doi.org/10.1093/genetics/iyad045>

Crouse, W. L., Keele, G. R., Gastonguay, M. S., Churchill, G. A., & Valdar, W. (2022). A Bayesian model selection approach to mediation analysis. *PLOS Genetics*, 18(5), e1010184. <https://doi.org/10.1371/journal.pgen.1010184>

Utsey, K., Gastonguay, M. S., Russell, S., Freling, R., Riggs, M. M., & Elmokadem, A. (2020). Quantification of the Impact of Partition Coefficient Prediction Methods on Physiologically Based Pharmacokinetic Model Output Using a Standardized Tissue Composition. *Drug Metabolism and Disposition*, 48(10), 903 LP – 916. <https://doi.org/10.1124/dmd.120.090498>

Zuppa, A. F., Benitez, G. R., Zane, N. R., Curley, M. A. Q., Bradfield, J., Hakonarson, H., Gastonguay, M. S., Moorthy, G., Prodell, J., & Gastonguay, M. R. (2019). Morphine Dose Optimization in Critically Ill Pediatric Patients With Acute Respiratory Failure. *Critical Care Medicine*, 47(6), e485–e494. <https://doi.org/10.1097/CCM.0000000000003741>

Zuppa, A. F., Conrado, D. J., Zane, N. R., Curley, M. A. Q., Bradfield, J., Hakonarson, H., Gastonguay, M. S., Moorthy, G., Prodell, J., & Gastonguay, M. R. (2019). Midazolam Dose Optimization in Critically Ill Pediatric Patients With Acute Respiratory Failure. *Critical Care Medicine*, 47(4), e301–e309. <https://doi.org/10.1097/CCM.0000000000003638>

Contributed Talks

Viral rebound kinetics following single and combination immunotherapy for HIV/SIV, Epidemics, December 1st, 2025

Using mixed effects models to quantify the effects of single and combination immunotherapy on HIV/SIV rebound kinetics, Society of Mathematical Biology Annual Meeting, July 15th, 2025

Quantifying the dynamics of Kaposi's sarcoma-associated herpesvirus persistence, Society of Mathematical Biology Annual Meeting, July 17th, 2025

Quantifying the dynamics of Kaposi's sarcoma-associated herpesvirus persistence, Dynamics & Evolution of Human Viruses, Paris, France, May 9th, 2025

Quantifying the dynamics of Kaposi's sarcoma-associated herpesvirus persistence, Epidemics, Bologna, Italy, November 27th, 2023

Prediction of maternal-fetal exposures of CYP450-metabolized drugs using physiologic pharmacokinetic modeling implemented in R and mrgsolve, R/Pharma Conference, Cambridge, MA, August 23rd, 2019

Identification of Combinations of Targets for Claudin-Low Triple Negative Breast Cancer Reversion, UConn Center for Cell Analysis and Modeling Summer Seminar, July 26th, 2019

Development of an Open and General Physiologically Based Pharmacokinetic Model to Predict Maternal-Fetal Exposures for Drugs Metabolized by CYP Isoenzymes, R/Medicine Conference, New Haven, CT, September 8th, 2018

The Effect of Host Genetic Variability on Epstein Barr Virus-associated cancer susceptibility, UConn Holster Scholar Symposium, October 2017

Poster Presentations

Quantifying the dynamics of Kaposi's sarcoma-associated herpesvirus persistence, MIDAS Network Annual Meeting, Bethesda, MD, November 18th, 2024

Quantifying the dynamics of Kaposi's sarcoma-associated herpesvirus persistence, International Workshop on Kaposi's Sarcoma Herpesvirus & Related Agents, Boston, MA, July 7th, 2024

Identification of Combinations of Pharmacologic Targets for Claudin-Low Triple Negative Breast Cancer Reversion, International Society of Pharmacometrics Quantitative Systems Pharmacology Student Symposium, Virtual, April 28th, 2021

Identification of Combinations of Targets for Claudin-Low Triple Negative Breast Cancer Reversion, Joint Meeting in Mathematics, Denver, CO, January 15th – 18th, 2020

Development of an Open-source Physiologically-Based Pharmacokinetic Model to Predict Maternal-Fetal Exposures of CYP450-Metabolized Drugs, International Society of Pharmacometrics Regional Quantitative Systems Pharmacology Day, Princeton, NJ, July 16th, 2019

Open-Source Contributions

bmediatR, an open-source R package implementing a Bayesian model selection approach to mediation analysis. May 2022

Available to install from github <https://github.com/wesleycrouse/bmediatR>

- Contributed to methods development and validation in both synthetic and real data
- Designed and built package vignettes

Fellowships

Summer Undergraduate Research Fund, University of Connecticut Office of Undergraduate Research May 2019

- Awarded funding for a 9-week summer research project

Holster Scholar, University of Connecticut Honors Program May 2017

- Offered enrollment in a semester-long course to learn how to develop and write a project proposal
- Selected as one of 8 students awarded funding for a 10-week summer research project

Honors and Awards

Blue Ribbon Poster Award, ISoP Quantitative Systems Pharmacology Student Symposium April 2021

Dean's List, The University of Connecticut Sept. 2016 - May 2020

Academic Excellence Scholarship, The University of Connecticut Sept. 2016 - May 2020

Babbidge Scholar, The University of Connecticut Dec. 2017, 2019

New England Scholar, The University of Connecticut Dec. 2018

Teaching Experience

Dynamic modeling of infectious diseases in patients and populations , Johns Hopkins University (TA)	Oct. - Dec. 2024
Systems pharmacology and personalized medicine , Johns Hopkins University (TA)	Feb. - May 2024
Data carpentry ecology with R workshop , Bioinformatics Training Program at JAX (Instructor)	Dec. 2021
Data carpentry genomics workshop , Bioinformatics Training Program at JAX (Instructor)	Nov. 2021
Introductory statistics with R , Bioinformatics Training Program at JAX (TA)	Sept. 2021
Introduction to R and RStudio , Bioinformatics Training Program at JAX (TA)	June 2021

Professional Development

Society for Mathematical Biology Member	2025-Present
Summer Institute in Statistics and Modeling in Infectious Diseases , Emory University	July 2024
Simulation Modeling in Immunology by Andreas Handel and Paul Thomas	2023
Building Tidy R Packages , R/pharma 2021	Oct. 2021
Julia Language for R Programmers , R/pharma 2021	Oct. 2021
Advanced Shiny , RStudio	Sept. 2021
Introduction to Bayesian Data Analysis , Juliacon	July 2021
Carpentries Instructor Training , The Carpentries	Mar. 2021
Shiny, RMarkdown, and RStudio Connect , RStudio	Mar. 2021
Quantitative Trait Mapping in the Diversity Outbred , University of Wisconsin-Madison	Dec. 2020
Containerization with Singularity , JAX	Oct. 2020
Introduction to HPC , JAX	Sept. 2020
Human and Mammalian Genetics and Genomics: The 61st McKusick Short Course , JAX	July 2020
Shiny Reproducibility , R/pharma 2019	Aug. 2019
Machine Learning , R/pharma 2019	Aug. 2019

Service & Involvement

Student Mentor , Johns Hopkins University Women Mentoring Women Program	2025 - Present
Member of Synaptic Clefs A Cappella , Johns Hopkins School of Medicine	2023 - Present
BME Application Assistance Program , Johns Hopkins University	2022 - Present
Math Motivators High School Tutoring , The University of Connecticut	2017 - 2019
iGEM Genetic Engineering Team , The University of Connecticut	2016-2017
President & Treasurer of Rubyfruit A Cappella , The University of Connecticut	2016-2020