Georgios (Yorgos) Psarellis

Postdoctoral Researcher| Machine Learning Scientist, Chemical Engineer

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Early career researcher interested in the intersection between Machine Learning, Chemical Engineering and Biology. Experience in designing and implementing algorithms that (i) learn, (ii) explore, (iii) understand complex systems in Chemistry and Biology.

Education

2017-2022 **Johns Hopkins University, PhD**, Chemical and Biomolecular Engineering [GPA : 4/4]
Thesis title : "Data-assisted modeling of complex chemical and biological systems".

2017-2021 **Johns Hopkins University, MSE** Applied Mathematics and Statistics [GPA : 3.81/4] **(dual degree)**
Focus on probability theory, stochastic simulations and dynamical systems.

2012-2017 **National Technical University of Athens, Bachelor's**, Chemical Engineering [9.26/10]
Graduated one semester earlier, on the top 2% of my class.

Experience

10/2022-present **Postdoctoral Researcher, Massachusetts Institute of Technology, Boston, MA**
Research on Active Learning (Bayesian Optimization, Bayesian Experimental Design) for predicting extreme events in biological systems. PI : Prof. T.Sapsis

05/2018-01/2019 **Technology Fellow, Center of Education Resources, JHU, Baltimore, MD**
Fellowship/contract position to develop educational material for an Applied Mathematics class. Collaboration was extended to training new Teaching Assistants for two years.

Publications

2023 Y.M. Psarellis,M. Kavousanakis, P.J. Dauenhauer, I.G. Kevrekidis, "Computing, Optimizing, Rationalizing the Programs of Programmable Catalysis" doi.org/10.1021/acscatal.3c00864.

2023 C.P. Martin-Linares, **Y.M. Psarellis**, G. Karapetsas, E.D. Koronaki, I.G. Kevrekidis, "Physics-agnostic and Physics-infused machine learning for thin films flows : modeling, and predictions from small data" (under review).

2023 E.D. Koronaki, N. Evangelou, **Y.M. Psarellis**, A.G. Boudouvis, I.G. Kevrekidis, "From partial data to out-of-sample parameter and observation estimation with Diffusion Maps and Geometric Harmonics" (under review).

2022 R.J. Lovelett, **Y.M. Psarellis**, I.G. Kevrekidis, M.Morari, "A Note on the Control of Processes Exhibiting Input Multiplicity", Industrial & Engineering Chemistry Research, doi.org/10.1021/acs.iecr.2c03515.

2022 Y.M Psarellis, S. Lee, S. Datta, J.M. Bello-Rivas, I.G. Kevrekidis, "Data-driven Discovery of Chemotactic Migration of Bacteria via Machine Learning" (under review).

2022 Y.M Psarellis, M. Kavousanakis, M.A. Henson, I.G. Kevrekidis, "Limits of Entrainment of Circadian Neuronal Networks", AIP Chaos, doi.org/10.1063/5.0122744.

2022 S. Lee, Y.M. Psarellis, C.I. Siettos, I.G. Kevrekidis, "Learning black- and gray-box chemotactic PDEs/closures from agent based Monte Carlo simulation data" doi.org/10.1007/s00285-023-01946-0.

2020 M.O. Williams, **Y.M. Psarellis**, D. Pozharskiy, C. Chong, F. Li, J. Yang, P.G. Kevrekidis, I.G. Kevrekidis, "Equation-Free Computations as DDDAS Protocols for Bifurcation Studies : A Granular Chain Example, Chapter in DDDAS Volume", F. Darema, E. Blasch (in press).

2018 G.M. Psarellis, I.G. Aviziotis, T. Duguet, C. Vahlas, E.D. Koronaki, A.G. Boudouvis, "Investigation of reaction mechanisms in the chemical vapor deposition of Al from DMEAA", Chemical Engineering Science,doi.org/10.1016/j.ces.2017.12.006.

Selected Conference Presentations [9/16]

2022 **Y.M. Psarellis**, M. Kavousanakis, M.A. Henson, I.G. Kevrekidis, "Limits of Entrainment of Circadian Neuronal Networks", AIChE Annual Meeting, Phoenix AZ (poster presentation).

2022 N. Wichrowski, **Y.M. Psarellis**, A. Georgiou, I.G. Kevrekidis, "Accelerating Global Optimization through Reduced Bayesian Optimization", AIChE Annual Meeting, Phoenix AZ.

2022 **Y.M. Psarellis**, P.J. Dauenhauer, M. Kavousanakis, I.G. Kevrekidis, "Computations and Optimization for Catalysts under Dynamic Operation", Advanced Manufacturing and Processing AIChE Conference, Bethesda MD (oral presentation).

2021 **Y.M. Psarellis**, S. Lee, S. Datta, I.G. Kevrekidis, "Learning Partial Differential Equations from Multiscale or Experimental Data : A Showcase on Bacterial Chemotaxis", AIChE Annual Meeting, Boston MA (poster presentation).

2021 **Y.M. Psarellis**, P.J. Dauenhauer, M. Kavousanakis, I.G. Kevrekidis, "Computations and Optimization for Catalysts Under Dynamic Operation", AIChE Annual Meeting, Boston MA (oral presentation).

2020 **Y.M. Psarellis**, M.A. Ardagh, P.J. Dauenhauer, I.G. Kevrekidis, "Assessing the Response of Dynamic Catalyic Surfaces", AIChE Annual Meeting, virtual (poster presentation).

2020 T. Cui, T.S. Bertalan, **Y.M. Psarellis**, I.G. Kevrekidis, "Connections between Residual Networks and Explicit Numerical Integrators, with Applications to Identification of Noninvertible Dynamical Systems", AIChE Annual Meeting, virtual.

2019 **Y.M. Psarellis**, N.J. Wichrowski, I.G. Kevrekidis, "Exploring Energy Landscapes using the Directed Graph Laplacian", Applied mathematics – The Next 50 Years, University of Washington, Seattle, WA (poster presentation).

2017 **G.M. Psarellis**, I.G. Aviziotis, T. Duguet, C. Vahlas, E.D. Koronaki, A.G. Boudouvis, "Chemical Vapor Deposition with the precursor DMEAA : Investigation of novel reaction mechanisms", 11th Panhellenic Scientific Conference of Chemical Engineering, Thessaloniki, Greece (oral presentation).

Teaching and Mentoring

Fall 2022 | **Nonlinear Dynamics and Chaos, JHU, Applied Mathematics and Statistics**
- Delivered 1/3 of semester's lectures as a co-instructor.
- Prepared material and software/code demonstrations.
- Mentored students on their semester proejcts.

Fall 2020 | **Nonlinear Dynamics and Chaos, JHU, Applied Mathematics and Statistics**
- Served as a Teaching Assistant.
- Prepared and taught software exercises.
- Mentored students on their semester projects.

Fall 2018 | **Advanced Transport Phenomena, JHU, Chemical and Biomolecular Engineering**
- Served as a Teaching Assistant.
- Graded homeworks and exams.
- Offered office hours and sessions.

Certifications

2021 Justice, Equity, Diversity and Inclusion training series, JHU.

2021 Johns Hopkins Teaching Academy, Center of Educational Resources, JHU.

2016 English Language certifications : TOEFL, GRE.

2000 German Language certification : C1 fluency level.

Selected Awards [7/13]

2022 MINDS Summer Fellowship, Johns Hopkins University (recognizing outstanding graduate students working broadly in data science, and particularly in the foundations of deep learning and graph learning)

2021 AIChE Compuing and Systems Technology Division director's award, for an outstanding poster presentation at the AIChE Annual meeting.

2019 Thomaidion Award for an original publication of an alumnus of National Technical University of Athens.

2018 Jay D. Samstag Engineering Fellowship in memory of his parents, Helen and Phil Samstag (renewed fellow).

2018 Onassis Scholarship, Onassis Foundation, for outstanding Greek doctoral students in the USA.

2018 Best Thesis Award, Sector II, School of Chemical Engineering, National Technical University of Athens, Greece.

2017 Jay D. Samstag Engineering Fellowship in memory of his parents, Helen and Phil Samstag, for outstanding incoming doctoral students accepted to the graduate programs of the Johns Hopkins University.

Outreach and Volunteering

2019-2022 | **Member, PhD Education Committee, JHU, Baltimore, Maryland**
- Selected to serve as one out of three representatives from the Whiting School of Engineering.
- Contributed to policies about Advisor-Advisee Mentorship Requirements, Diversity and Inclusion, Graduate Student Mental Health.

2019-2020 | **Vice President, GSLC, JHU, Baltimore, Maryland**
- Represented my research group to the Graduate Student Liaison Committee (GSLC).
- Organized social, professional and networking events for over 40 graduate students.
- Oversaw the registration of GSLC as a student organization.

2015-2017 | **Cofounder, General Coordinator, CHEMECON, Athens, Greece**
- Cofounded and served as General Coordinator at Chemecon, the first Association of Young Chemical Engineers in Greece.
- Increased the size of the organization by 150%.
- Organized and supervised 8 field visits to industrial plants.
- Organized and supervised 4 workshops and 4 seminars.