

# Noah J. Wichrowski

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## Education

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JOHNS HOPKINS UNIVERSITY, BALTIMORE, MD

- **Ph.D. Candidate, Applied Mathematics and Statistics**
- **M.S.E., Applied Mathematics and Statistics**, May 2020
- Dissertation: *Data-Driven Dimensionality Reduction: Manifold Learning for Optimization*
- Adviser: Dr. Ioannis G. “Yannis” Kevrekidis
- Research Interests: Data Science, Optimization, Stochastic Processes, Machine Learning

UNIVERSITY OF MARYLAND, COLLEGE PARK, MD

- **B.S., Chemical Engineering**, *summa cum laude*, May 2017
- **B.S., Mathematics**, *summa cum laude*, May 2017

## Research Experience

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JOHNS HOPKINS UNIVERSITY, BALTIMORE, MD

**Graduate Research Assistant**, May 2018–Present

- *Parameter Nonidentifiability*: data-driven model order reduction, parameter estimation, prediction
  - Discovered reduced sets of effective parameters with which to describe dynamic models.
  - Confirmed equivalence of data-driven parameters to analytical expressions proposed by experts.
  - Used reduced representations to predict unseen system behaviors and parameter values.
  - Implemented conformal autoencoders to disentangle effective from redundant parameters.
- *Machine Learning for Materials Science*: parameterizing structure-process-property relations in data
  - Constructed machine learning models of zeolite catalyst properties from small data set.
  - Used models to propose new synthesis conditions that improved catalytic performance.
  - Co-developed an active learning scheme for exploration of high-entropy alloy lattice space.
  - Including dimensionality reduction and comparing performance to composition-based approach.
- *Data-Driven Optimization*: manifold learning for accelerated solution of high-dimensional problems
  - Analyzed trajectories of simulated annealing as time series from Langevin dynamics.
  - Combined diffusion maps with SDE parameter inference to inform larger, coarse-grained steps.
  - Achieved convergence with fewer objective evaluations than standard simulated annealing.
  - Extending approach to Bayesian optimization on reduced space of diffusion coordinates.

UNIVERSITY OF MARYLAND, COLLEGE PARK, MD

**Gemstone Honors Research Program**, September 2013–May 2017

- Team MagNET: Magnetic Non-mechanical Energy Transfer
- Thesis: Magnetic Field Manipulation as a Means of Stabilization
  - Contributed to design and construction of prototype device for levitating, moving, and rotating magnetic payload without physical contact, via an electromagnetically-based control system.
  - Aided development of control structure for microcontroller implementation of device.
  - Developed mathematical model to describe experimental magnetic field data.

## Work Experience

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JOHNS HOPKINS UNIVERSITY, BALTIMORE, MD

**AMS Teaching Fellow**, January 2020–Present

**Apprentice Teaching Fellow**, January 2019–January 2020

**Graduate Teaching Assistant**, August 2017–January 2019

- Lead weekly recitation sections and office hours; respond to students’ emails.
- Interview candidates for grader positions; coordinate grading duties.
- Write problems and solutions for homework and exams; proctor exams.
- Create and present material for review sessions and coding tutorials.

U.S. FOOD AND DRUG ADMINISTRATION, SILVER SPRING, MD

**ORISE Research Intern**, May 2017–August 2017

- Conducted quantitative characterization of methods and operations of drug substance manufacturing processes in recently FDA-approved drug applications.
- Contributed to published technical report about drug substance manufacturing project.
- Collaborated on internal report assessing the drug quality review of orphan drug applications.

NAVAL AIR WARFARE CENTER, PATUXENT RIVER, MD

**Pathways Intern**, June 2014–August 2016

- Applied chemical kinetic theory to derive mathematical model describing electrochemical impedance spectroscopy and galvanic corrosion.
- Performed and implemented model evaluation on basis of experimental data.
- Conducted data analysis to predict metal corrosion rate from environmental conditions.
- Collected and analyzed data for experiments investigating chloride diffusion in metals.
- Designed improvement of experimental apparatus for chloride diffusion experiments.
- Contributed to declassified technical report on ionic transport through organic coatings.

## Technical Skills

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### PROGRAMMING LANGUAGES

- Python: Autograd/Jax, Jupyter, Matplotlib, NumPy, Pandas, Pyomo, PyTorch, Scikit-learn, SciPy
- MATLAB/Octave
- Some experience with C++, Fortran, Java

### COMPUTATIONAL TECHNIQUES

- Dimensionality reduction: autoencoders, diffusion maps, principal component analysis
- Optimization: simulated annealing, Bayesian optimization, stochastic approximation, recursive least squares, line search, trust region
- Regression: Gaussian processes, geometric harmonics, heteroscedastic GPR, neural networks
- Classification: nearest neighbors, random forest, support vector machines

### SOFTWARE

- Typesetting: L<sup>A</sup>T<sub>E</sub>X, Beamer, TikZ
- MS Office: Excel, Word, PowerPoint
- Dynamical Systems: AUTO, Scigma
- Development: Git, Markdown

## Publications

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- X. Li\*, H. Han\*, N. Evangelou\*, **N. J. Wichrowski\***, and nine others, “Machine-Learning Assisted Crystal Engineering of a Zeolite,” **2022**. [Under review]
- N. Evangelou\*, **N. J. Wichrowski\***, and five others, “On the Parameter Combinations That Matter and on Those That do Not: Data-Driven Studies of Parameter (Non)identifiability,” *arXiv preprint arXiv:2110.06717*, **2022**. [To appear in PNAS Nexus]
- D. Pozharskiy, **N. J. Wichrowski**, and three others, “Manifold Learning for Accelerating Coarse-Grained Optimization”, *J. Comput. Dyn.*, **2020**, 7(2), 511–536.
- **N. J. Wichrowski**, A. C. Fisher, N. S. Arden, X. Yang, “An Overview of Drug Substance Manufacturing Processes,” *AAPS PharmSciTech*, **2020**, 21(7), 1–6.
- B. Mobley, **N. Wichrowski**, and four others, “Ionic Transport Through Metal-Rich Organic Coatings,” *Report No. NAWCADPAX/TIM-2016/54*, Patuxent River, MD: U.S. Department of the Navy, Naval Air Warfare Center Aircraft Division, **2016**.

\* Equal contribution

## Affiliations

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Graduate Student Member, Society for Industrial and Applied Mathematics  
Knights of Columbus, Ss. Philip and James Council, #14102  
Omega Chi Epsilon ( $\Omega$ XE) Chemical Engineering Honor Society  
Pi Mu Epsilon ( $\Pi$ ME) Mathematics Honor Society