ARIANA QUEK

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PERSONAL STATEMENT

Ph.D. candidate in Mechanical Engineering and Materials Science at Duke University, focusing on computational materials science and uncertainty quantification. At Boehringer Ingelheim, I gained experience developing mechanistic models for drug release kinetics with computer-vision, and designing regulated experimental setups. I'm passionate about applying scientific rigor to real-world challenges that advance human, animal, and environmental health.

EDUCATION

Duke University; Durham, NC Aug 2021 - Nov 2025 (Anticipated)
Ph.D. in Mechanical Engineering and Materials Science
Advisor: Dr. Johann Guilleminot
Computational Mechanics and Scientific Computing focus
aiM-NRT fellowship (AI and Materials Science)

University of Southampton; UK Sep 2015 - Jul 2019
MEng(Hons) Mechanical Engineering in Aerospace (First Class Honors)
High Achiever Scholarship for the MEng(Hons) Mechanical Engineering Degree

TECHNICAL STRENGTHS

Computer Languages	Python, MATLAB
Machine Learning	PyTorch, TensorFlow, Computer Vision
Software & Tools	LaTeX, Git, LAMMPS, FEniCS, OpenCV, ImageJ, Microsoft Office
Analytical Techniques	Dissolution

KEY INTERESTS

Uncertainty Quantification, Mathematical Modeling, Multi-scale Modeling, Stochastic Modeling, Statistical Analysis, Machine Learning, Data-driven Modeling, Optimization, Molecular Dynamics

RESEARCH & WORK EXPERIENCE

Internship - Boehringer Ingelheim; Ridgefield, CT May 2025 - Present

- Integrate USP-compliant dissolution assays with a high-speed imaging pipeline, developing computer-vision algorithms to extract real-time drug disintegration metrics under GMP conditions.
- Design and implement a mechanistic model to predict dissolution kinetics, integrating image-derived measurements for enhanced formulation insight.
- Perform data-driven analysis of API–excipient interactions, using model simulations and image analysis to assess how formulation and process variables influence release profiles.
- Automate an end-to-end workflow– from image acquisition and preprocessing through model prediction to accelerate formulation optimization and quality-control decision making.

Ph.D. Research - Duke University Aug 2021 - Present
Guilleminot Lab

- **Nonlinear Probabilistic Framework for Molecular Dynamics:**
  - Developed a stochastic reduced-order model augmented with nonlinear enrichment to improve error robustness in simulating complex mechanical systems.
  - Proposed a novel method to determine the optimal dimensions of the model by integrating multiple data sources, enhancing the accuracy and robustness of reduced-order simulations.

- **Multi-Model Probabilistic Framework for Machine-Learned Molecular Dynamics (J2):**
  - Unified multiple ML potentials in a single nonparametric probabilistic framework, enhancing reliability in high-energy MD simulations.
  - Introduced stabilizing techniques (e.g., momenta augmentation, frequency splitting) and validated on sodium thiophosphate, improving reliability of ionic diffusivity prediction for battery materials.
  - Established an automated and scalable workflow for large-scale, data-intensive simulations, required for robust and scalable predictive modeling.
- **Generative Modeling for Predicting Fracture Paths in Complex Materials (J1):**
  - Developed an efficient generative modeling approach to approximate fracture paths, enabling robust uncertainty estimates for fracture in random heterogeneous materials, improving risk assessment in engineering applications.
  - Achieved comparable predictive accuracy to state-of-the-art deep-learning operators without extensive hyperparameter tuning.

Internship - Mitsubishi Japan, UK Jun 2018 - Aug 2018

- Quantified microstructural variations in aerospace composites through CT scan, mechanical testing, and data analysis– correlating material distribution with fracture behavior to identify critical failure mechanisms.
- Applied statistical and image-analysis techniques, enabling precise tracking of damage progression and modeling of crack initiation and propagation in stiffened composites.

SELECTED JOURNAL PUBLICATIONS & CONFERENCE TALKS

J2. **A. Quek**, N. Ouyang, H. M. Lin, O. Delaire, & J. Guilleminot. Enhancing Robustness in Machine-Learning-Accelerated Molecular Dynamics: A Multi-Model Nonparametric Probabilistic Approach. *Mechanics of Materials*, 2024. doi: 10.1016/j.mechmat.2024.105237.

J1. **A. Quek**, J. Y. Yong, & J. Guilleminot. Approximating Fracture Paths in Random Heterogeneous Materials: A Probabilistic Learning Perspective. *Journal of Engineering Mechanics*, 150(8):04024051, 2024. doi: 10.1061/JENMDT.EMENG-7617.

T3. **A. Quek**, N. Ouyang, H. M. Lin, O. Delaire, & J. Guilleminot, Enhancing Predictiveness in Atomistic Simulations Accelerated by ML Potentials: A Stochastic Reduced-Order Modeling Approach, U.S. National Congress on Computational Mechanics, Chicago, IL, July 19–23 (2025).

T2. H. Zhang, **A. Quek**, S. Kounouho, and J. Guilleminot (invited talk), Riemannian probabilistic Representation of model ensembles, with applications in atomistic and continuum simulations, SIAM Conference on Mathematical Aspects of Materials Science, Pittsburgh, PA, May 19-23 (2024).

T1. **A. Quek** and J. Guilleminot (invited talk), Operator learning for predicting fracture paths in brittle random media, 2023 MRS Spring Meeting, San Francisco, CA, April 10–14 (2023).

TEACHING EXPERIENCE

Teaching Assistant, Duke University Jan 2024 - May 2024
ME 582/CS 582: Applications in Data and Materials Science

- Assisted in modules including boosted decision trees for discovering structural patterns controlling bandgaps in metamaterials, machine learning to predict dynamic heterogeneities in materials, and AI-assisted design of high entropy materials for catalysis.

Teaching Assistant, Duke University Aug 2023 - Dec 2023
CEE 421L: Matrix Structural Analysis

- Facilitated student understanding of stiffness matrix methods from first principles, superposition of loads and elements, and linear analysis of plane and space structures comprising one-dimensional truss and beam elements.