

# Xinyue (Leslie) Xu

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## INTRODUCTION

Researcher specializing in Physics-informed Machine Learning (PIML) and Bayesian inference for uncertainty-aware simulations of complex physical systems. Experienced in developing scalable ML and LLM agent frameworks and integrating physics constraints/priors into AI models for engineering applications. Proven publication record in model calibration, uncertainty quantification, and physics-guided neural networks.

## EDUCATION

<b>Pennsylvania State University</b> Ph.D. in Architectural Engineering; Ph.D. Minor in Computational Science	Aug. 2019 - May. 2026
<b>Arizona State University</b> M.S. in Computer Science; concentration on Machine Learning	Aug. 2022 - Dec. 2024
<b>Tongji University</b> B.S. in Mechanical Engineering	Jul. 2015 - May. 2019

## SKILLS

<b>Languages:</b>	Python, C/C++, MATLAB, Java, SQL, C#, R
<b>Framework:</b>	Pytorch, TensorFlow, Keras, Scikit-learn, PyMC3P, Pyro, Pandas, AWS, Azure, Jax
<b>Software:</b>	Abaqus, COMSOL Multiphysics, Ansys, Solidworks, SAP2000, ETABS
<b>Technical Skills:</b>	Physics-informed ML, Bayesian Inference, Uncertainty Quantification, Bayesian Inference, Stochastic Optimization, Model Calibration, Model Selection, Structural/FEA Analysis

## RESEARCH EXPERIENCE

<b>Large Language Model Framework for Climate-Specific Retrofit Strategies</b>   <i>Python</i>	Feb. 2025 – Present
<ul style="list-style-type: none"><li>Developed ResStock-LLM, an LLM-assisted framework to automate residential retrofit decision-making.</li><li>Used Jensen–Shannon Divergence to identify feature disparity in low-efficiency homes across 140,000 homes.</li><li>Automated climate-specific retrofit recommendations aligned with IECC standards.</li><li>Advanced LLM reasoning for building energy efficiency, enabling automated and climate-aware retrofit strategies.</li></ul>	
<b>A Review of UQ in ML-based Building Energy Modeling</b>   <i>Python</i>	Aug. 2023 – Jan. 2025
<ul style="list-style-type: none"><li>Conducted a comprehensive review of 141 papers on ten UQ methods in ML-based BEM.</li><li>Demonstrated modeling principles and ML-based BEM applications in deterministic and stochastic contexts.</li><li>Identified research gaps and proposed strategies to integrate UQ into ML-based engineering simulations.</li></ul>	
<b>Parameter Enrichment for Building Envelope using Gaussian Naïve Bayes</b>   <i>Python</i>	Feb. 2024 – Dec. 2024
<ul style="list-style-type: none"><li>Developed a Gaussian Naïve Bayes classifier to probabilistically infer missing insulation wall features.</li><li>Optimized classification using grid search to enhance accuracy, precision, and F1-score.</li><li>Quantified predictive confidence via probabilistic entropy, supporting thermal vulnerability assessments.</li></ul>	
<b>UQ in Physics-guided Bayesian Neural Networks for Vibration Dynamics</b>   <i>Python</i>	Aug. 2023 – Present
<ul style="list-style-type: none"><li>Designed Physics-Guided Bayesian Neural Networks (PG-BNNs) combining physical laws into ML models.</li><li>Compared Monte Carlo dropout ANNs, BNNs, and PG-BNNs for modeling a 1-DOF vibration isolation system.</li><li>Assessed model accuracy and uncertainty performance using statistical metrics.</li><li>Demonstrated that PG-BNNs outperformed data-driven models in accuracy, uncertainty, and generalization.</li></ul>	
<b>Model Selection in Balancing Fit, Complexity, and Generalization</b>   <i>MATLAB</i>	May. 2020 – Aug. 2025
<ul style="list-style-type: none"><li>Proposed a Bayesian criterion <i>Indicator of Calibration Flexibility (ICaF)</i> to balance fit and generalization.</li><li>Reviewed state-of-the-art model selection criteria in information-theoretic and Bayesian paradigms.</li><li>Evaluated sensitivity of model selection criteria to five calibration factors in polynomial regressions.</li><li>Developed and calibrated a hierarchy of physics-based thermal models for double-pane windows.</li><li>Revealed limitations of classical criteria in distinguishing effective fidelity from redundant complexity, highlighting Bayesian criteria for model robustness.</li></ul>	

## WORK EXPERIENCE

<b>Machine Learning Engineer Intern</b> Computer Vision for Automated Construction Cost Estimation   <i>Python, YOLOv8</i>	Builder Supply Link LLC, NJ, USA Aug. 2025 – Present
<ul style="list-style-type: none"><li>Built YOLO-based computer vision pipeline to recognize construction elements from floor plans.</li><li>Integrated recognition with cost database for real-time quotation, reducing estimation time from 3 hours → 30 seconds with 95% accuracy.</li><li>Demonstrated scalability for early-stage project bidding and pricing transparency.</li></ul>	

- J1. X. Xu, J. Wang.** Information-theoretic and Bayesian Model Selection for Physics-based Model Calibration: Balancing Fit, Complexity, and Generalization. *Information Sciences*, Volume 726, 2026, 122743, ISSN 0020-0255, <https://doi.org/10.1016/j.ins.2025.122743>, (Impact factor: 6.8)
- J2. X. Xu, Y. Hu, S. Atamturktur, L. Chen, J. Wang.** Systematic review on uncertainty quantification in machine learning-based building energy modeling. *Renewable and Sustainable Energy Reviews*, Volume 218, 2025, 115817, ISSN 1364-0321, <https://doi.org/10.1016/j.rser.2025.115817>, (Impact factor: 16.3)
- J3. X. Xu, J. Wang.** Comparative Analysis of Physics-Guided Bayesian Neural Networks for Uncertainty Quantification in Dynamic Systems. *Forecasting* 2025, 7(1), 9; <https://doi.org/10.3390/forecast7010009>, (Impact factor: 3.2)
- J4. S. Paneru, X. Xu, J. Wang, G. Chi, Y. Hu, 2024.** Assessing building thermal resilience in response to heat-waves through integrating a social vulnerability lens, *Journal of Building Engineering*, <https://doi.org/10.1016/j.jobbe.2024.111219>, (Impact factor: 7.4)
- J5. C. Chen, J. Wang, H. Zhang, X. Xu, E. Hinkle, X. Chao, Q. Shi, 2024.** Dual impacts of solar-reflective façades in high-density urban areas on building energy use and outdoor thermal environments, *Energy and Buildings*, <https://doi.org/10.1016/j.enbuild.2024.114926>, (Impact factor: 7.1)
- J6. C. Ehrett, A. Brown, C. Kitchens, X. Xu, R. Platz, S. Atamturktur, 2023.** Simultaneous Bayesian calibration and engineering design with an application to a vibration isolation system. *Journal of Verification, Validation and Uncertainty Quantification*. <https://doi.org/10.1115/1.4050075>
- C1. X. Xu, Y. Wang, R. Platz, S. Atamturktur, 2024.** Analyzing the Influential Factors on ICaF Performance in Bayesian Model Calibration and Forecasting, *IMAC, A Conference and Exposition on Structural Dynamics*. [https://doi.org/10.1007/978-3-031-68893-5\\_11](https://doi.org/10.1007/978-3-031-68893-5_11),
- C2. X. Xu, S. Paneru, S. Atamturktur, J. Wang, 2024.** Physics-guided Bayesian Neural Networks and their applications in ODE problems, *Verification and Validation*, <https://doi.org/10.1115/VVUQ2024-122961>
- C3. X. Xu, Y. Yu, R. Platz, S. Atamturktur, 2023.** An Uncertainty-Aware Measure of Model Calibration Flexibility, *Society for Experimental Mechanics Annual Conference and Exposition*, [https://doi.org/10.1007/978-3-031-37003-8\\_2](https://doi.org/10.1007/978-3-031-37003-8_2)
- C4. R. Platz, X. Xu, S. Atamturktur, 2023.** Introducing a Round-Robin Challenge to Quantify Model Form Uncertainty in Passive and Active Vibration Isolation, *Model Validation and Uncertainty Quantification, Volume 3. SEM 2023*, [https://doi.org/10.1007/978-3-031-37003-8\\_1](https://doi.org/10.1007/978-3-031-37003-8_1)
- C5. Y. Wang, Y. Yu, X. Xu, S. Atamturktur, 2023.** Predicting Nonlinear Structural Dynamic Response of ODE Systems Using Constrained Gaussian Process Regression, *Society for Experimental Mechanics Annual Conference and Exposition*, [https://doi.org/10.1007/978-3-031-37003-8\\_18](https://doi.org/10.1007/978-3-031-37003-8_18)
- C6. X. Xu, Z. Li, J. Zhao, 2019.** The optimization of personalized ventilation based on a jogger's unsteady breathing cycle, *IOP Conference Series: Earth and Environmental Science*, <https://doi.org/10.1088/1755-1315/238/1/012040>
- C7. W. Zhao, X. Zhang, X. Xu, C. Wu, W. Ye, 2019.** CFD simulations on the cooling effect of air supply velocity for high heat flux surfaces, *IOP Conference Series: Earth and Environmental Science*, <https://doi.org/10.1088/1755-1315/238/1/012044>

## ON-SITE CONFERENCE PRESENTATIONS

<b>ASME Verification, Validation, and Uncertainty Quantification Symposium</b>	College Station, TX
Presenter	May 2024
<b>IMAC-XLII, Society for Experimental Mechanics</b>	Orlando, FL
Presenter	Jan. 2024
<b>IMAC-XLI, Society for Experimental Mechanics</b>	Austin, TX
Presenter	Feb. 2023
<b>4th Asia Conference of International Building Performance Simulation Association</b>	Hong Kong
Presenter	Dec. 2018

## HONORS AND AWARDS

The Kissinger Scholarship	Dec. 2024
The Wormley Family Graduate Fellowship	Jun. 2023
Louis S. And Sara S. Michael Endowed Graduate Fellowship In Engineering	Jun. 2022
University Graduate Fellowship	Aug. 2019 - May. 2024
Glenn E. Singley Memorial Graduate Fellowship	Aug. 2019
Outstanding Graduates of Tongji University	May. 2019
Student Scholarship of Tongji University	May. 2015 - May. 2019