Wei Xing

School of Integrated Circuit Science and Engineering, Beihang University, China Email: wxing@buaa.edu.cn

Research Area

Machine learning in physical applications and solving PDE, Surrogate model, Nonparametric Bayesian, Bayesian optimization, Uncertainty quantification, Manifold learning, Model order reduction

Education

Ph. D. in Applied Math and Computer Science

2012-2016

- Warwick Centre for Predictive Modelling, University of Warwick, UK
- Supervisor: Akeel Shah
- Research Topic: Manifold learning for the emulations of computer models

Bachelor of Science in Engineering

2008-2012

- Shenzhen University, China
- Major: Automation Engineering Minor: Chinese Literature
- GPA: 3.8/4.0 (rank 2nd, outstanding graduates)

Research Experience

Assistant Professor 2020-present

School of Integrated Circuit Science and Engineering, Beihang University, China

- Bayesian optimization for circuit design and optimization.
- Circuit design and optimization under uncertainty
- EDA acceleration via machine learning and model order reduction
- Large scale and efficient Ab Initio simulation via nonparametric Bayesian models
- Automatic image processing for characterization of materials
- Research projects in 2020:
 - o Satellite cloud imagery analysis and cloud predictions.
 - o Global solar radiation analysis and predictions.
 - o Data mining for QAR data for China Aviation Administration

Visiting Scholar 2020

School of Energy and Power Engineering, Chongqing University, China

- Digital twins for real-time monitoring and maintenance for fuel cell battery
- Machine learning aided fuel cell design
- Multi-fidelity fusion algorithm for fast simulation in engineering
- Machine learning aided *Ab Initio* simulations

Postdoctoral researcher 2017-2020

Scientific Computing and Imaging Institute, University of Utah

- Main researcher for DARPA program: Transformative Design (TRADES). Work includes:
 - o Design space visualization for transformative design,
 - o Ultra-high dimensional (1 million) non-parametric Bayesian modeling (Gaussian process) for learning partial differential equation simulators,
 - o Non-Gaussian data structured embedding through Gaussian process and Dirichlet process.

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- o Efficient multi-fidelity surrogate model for physical systems,
- o Physics informed Bayesian model,
- o Automatic machine learning for deep learning,
- o Intrusive reduced order model for medical image processing.
- o Bayesian optimization for design optimization.
- Main mathematical model researcher for NSF project, CPS: Synergy: A Layered Framework of Sensors, Models, Land-Use In`formation and Citizens for Understanding Air Quality in Urban Environments (https://www.aqandu.org/airu_sensor)
 - o Spatial-temporal modelling for sensor network,
 - o Automatic calibration, fault detection and filtering for sensor network.

Postdoctoral Researcher

2016-2017

School of Engineering, University of Warwick

- Main researcher for EPSRC project, Real-Time H₂ Purification and Monitoring for Efficient/Durable Fuel Cell Power Systems
- Uncertainty quantification for heterogeneous PDEs problems by developing hybrid surrogates that combine data-driven and physical based reduced order model.
- Data analysis and experimental design for sensors design and develop for H₂S and H₂ gas.
- Machine learning method for sensor signal analysis.
- Data-driven surrogate for complex Fuel Cell Power Systems and its control.

Ph.D. Candidate 2012-2016

Warwick Centre for Predictive Modelling, University of Warwick

- Non-parametric Bayesian statistical modeling for parameterized PDE/ODE models of highdimensional outputs.
- Manifold learning methods (including kernel principal component analysis, Isomap, diffusion maps, local linear embedding and local tangent alignment) and its application to high-dimensional data structures and to multi-variate emulation problems.
- Developing numerical solver (based on finite element, finite volume and finite difference) for fluid flow and heat transfer problems (e.g., heat conduction, Navier Stoke's equation, Richard's equation and Burgers equations).
- Developing hybrid surrogates that combines physical base model order reduction (MOR) method and machine learning techniques.
- Uncertainty quantification for stochastic PDE through surrogate models (data-driven emulator, MOR and hybrid surrogates)

Research Assistant 2015-2016

School of Engineering, University of Warwick

- EU FP7 project "New Concept of Metal-Air Battery for Automotive Application based on Advanced Nanomaterials (NECOBAUT)",
 - Data analysis and data-driven surrogate model developing for metal-air battery models.
- Validation and analysis against experimental data.

Research Assistant 2013-2014

School of Engineering, University of Warwick

- EPSRC project "Improvements to Soluble Lead Redox Flow Battery Component (PBatt)".
- Data analysis and data-driven surrogates developing for soluble lead acid battery model

Undergraduate Projects

2008-2012

School of automation and control, Shenzhen University

- Investigating into robot self-balancing problem and real-time control algorithms design.
- Developed 3 different low-cost self-balancing prototypes including dynamic model, mechanical structure, control circuit, and communication interface.

Research Skills

- Programing and software: Matlab, Python, Pytorch, TensorFlow, LaTex, C, Git, Comsol, R and MS office.
- Research topics: nonparametric Bayesian model, statistical learning, manifold learning, computational physics, reduced order model, uncertainty quantification.

Publications

Journal Paper

- [1] W. W. Xing, M. Cheng, K. Cheng, W. Zhang, and P. Wang, "InfPolyn, a Nonparametric Bayesian Characterization for Composition-Dependent Interdiffusion Coefficients," *Materials*, vol. 14, no. 13, p. 3635, Jun. 2021, doi: 10.3390/ma14133635.
- [2] H. Wang, C. Li, W. Xing, Y. Ye, and P. Wang, "A machine learning approach to quantify dissolution kinetics of porous media," *J Mach Learn Model Comput*, 2021, doi: 10.1615/JMachLearnModelComput.2021038529.
- [3] W. I. Ibrahim, M. R. Mohamed, R. M. T. R. Ismail, P. K. Leung, W. W. Xing, and A. A. Shah, "Hydrokinetic energy harnessing technologies: A review," *Energy Reports*, vol. 7, pp. 2021–2042, Nov. 2021, doi: 10.1016/j.egyr.2021.04.003.
- [4] W. W. Xing, A. A. Shah, P. Wang, S. Zhe, Q. Fu, and R. M. Kirby, "Residual Gaussian process: A tractable nonparametric Bayesian emulator for multi-fidelity simulations," *Applied Mathematical Modelling*, vol. 97, pp. 36–56, Sep. 2021, doi: 10.1016/j.apm.2021.03.041.
- [5] **W. W. Xing**, R. M. Kirby, and S. Zhe, "Deep coregionalization for the emulation of simulation-based spatial-temporal fields," *Journal of Computational Physics*, vol. 428, p. 109984, Mar. 2021, doi: 10.1016/j.jcp.2020.109984.
- [6] Kerry E. Kelly*#, **Wei W. Xing**#, Tofigh Sayahi, Logan Mitchell, Tom Becnel, Pierre-Emmanuel Gaillardon, Miriah Meyer, and Ross T. Whitaker., "Community-Based Measurements Reveal Unseen Differences during Air Pollution Episodes," *Environmental Science & Technology*, vol. 55, no. 1, pp. 120–128, Jan. 2021, doi: 10.1021/acs.est.0c02341.
- [7] **W. W. Xing**, F. Yu, P. K. Leung, X. Li, P. Wang, and A. A. Shah, "A new multi-task learning framework for fuel cell model outputs in high-dimensional spaces," *Journal of Power Sources*, vol. 482, p. 228930, Jan. 2021, doi: 10.1016/j.jpowsour.2020.228930.
- [8] W. Xing, S. Y. Elhabian, V. Keshavarzzadeh, and R. M. Kirby, "Shared-Gaussian Process: Learning Interpretable Shared Hidden Structure Across Data Spaces for Design Space Analysis and Exploration," *Journal of Mechanical Design*, vol. 142, no. 8, Aug. 2020, doi: 10.1115/1.4046074.
- [9] **W. Xing,** M. Razi, R. M. Kirby, K. Sun, and A. A. Shah, "Greedy nonlinear autoregression for multifidelity computer models at different scales," *Energy and AI*, vol. 1, p. 100012, Aug. 2020, doi: 10.1016/j.egyai.2020.100012.
- [10] C. Mullen, T. Collins, W. Xing, R. Whitaker, T. Sayahi, T. Becnel, P. Goffin, P. Gaillardon, M. Meyer, K. Kelly, "Patterns of distributive environmental inequity under different PM2.5 air pollution scenarios for Salt Lake County public schools," *Environmental Research*, vol. 186, p. 109543, Jul. 2020, doi: 10.1016/j.envres.2020.109543.

- [11] D.V. Mallia, A.K. Kochanski, K.E. Kelly, R. Whitaker, **W. Xing**, L.E. Mitchell, A. Jacques, A. Farguell, J. Mandel, P.E. Gaillardon, and , T. Becnel. "Evaluating Wildfire Smoke Transport Within a Coupled Fire-Atmosphere Model Using a High-Density Observation Network for an Episodic Smoke Event Along Utah's Wasatch Front," Journal of Geophysical Research: Atmospheres, vol. 125, no. 20, p. e2020JD032712, 2020, doi: https://doi.org/10.1029/2020JD032712.
- [12] C. Gadd, **W. Xing**, M. M. Nezhad, and A. A. Shah, "A Surrogate Modelling Approach Based on Nonlinear Dimension Reduction for Uncertainty Quantification in Groundwater Flow Models," *Transport in Porous Media*, vol. 126, no. 1, pp. 39–77, Jan. 2019, doi: 10.1007/s11242-018-1065-7.
- [13] V. Triantafyllidiis, **W. W. Xing**, P. K. Leung, A. Rodchanarowan, and A. A. Shah, "Probabilistic sensitivity analysis for multivariate model outputs with applications to Li-ion batteries," *Journal of Physics: Conference Series*, vol. 1039, p. 012020, Jun. 2018, doi: 10.1088/1742-6596/1039/1/012020.
- [14] A. A. Shah, **W. W. Xing**, and V. Triantafyllidis, "Reduced-order modelling of parameter-dependent, linear and nonlinear dynamic partial differential equation models," *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 473, no. 2200, p. 20160809, Apr. 2017, doi: 10.1098/rspa.2016.0809.
- [15] W. W. Xing, V. Triantafyllidis, A. A. Shah, P. B. Nair, and N. Zabaras, "Manifold learning for the emulation of spatial fields from computational models," *Journal of Computational Physics*, vol. 326, pp. 666–690, Dec. 2016, doi: 10.1016/j.jcp.2016.07.040.
- [16] **W. Xing**, A. A. Shah, and P. B. Nair, "Reduced dimensional Gaussian process emulators of parametrized partial differential equations based on Isomap," *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 471, no. 2174, p. 20140697, Feb. 2015, doi: 10.1098/rspa.2014.0697.

Key Conference Paper

- [1] Z. Wang, **W. Xing**, R. Kirby, and S. Zhe, "Multi-Fidelity High-Order Gaussian Processes for Physical Simulation," in *International Conference on Artificial Intelligence and Statistics*, Mar. 2021, pp. 847–855, Accessed: Apr. 21, 2021. [Online]. Available: http://proceedings.mlr.press/v130/wang21c.html.
- [1] S. Li, **W. Xing**, R. M. Kirby, and S. Zhe, "Scalable Gaussian Process Regression Networks," Jul. 2020, vol. 3, pp. 2456–2462, doi: 10.24963/ijcai.2020/340.
- [2] S. Li, **W. Xing**, R. Kirby, and S. Zhe, "Multi-Fidelity Bayesian Optimization via Deep Neural Networks," *Advances in Neural Information Processing Systems*, vol. 33, pp. 8521–8531, 2020, Accessed: Apr. 21, 2021. [Online]. Available: https://papers.nips.cc/paper/2020/hash/60e1deb043af37db5ea4ce9ae8d2c9ea-Abstract.html.
- [3] S. Zhe, **W. Xing**, and R. M. Kirby, "Scalable High-Order Gaussian Process Regression," in *The 22nd International Conference on Artificial Intelligence and Statistics*, Apr. 2019, pp. 2611–2620, Accessed: Jan. 14, 2021. [Online]. Available: http://proceedings.mlr.press/v89/zhe19a.html.
- [4] W. Xing, S. Elhabian, R. Kirby, R. T. Whitaker, and S. Zhe, "Infinite ShapeOdds: Nonparametric Bayesian Models for Shape Representations," *Proceedings of the AAAI Conference on Artificial Intelligence*, vol. 34, no. 04, pp. 6462–6469, Apr. 2020, doi: 10.1609/aaai.v34i04.6118.
- [5] J. Wang, W. Xing, R. M. Kirby, and M. Zhang, "Data-Driven Model Order Reduction for Diffeomorphic Image Registration," in *Information Processing in Medical Imaging*, vol. 11492, A. C. S. Chung, J. C. Gee, P. A. Yushkevich, and S. Bao, Eds. Cham: Springer International Publishing, 2019, pp. 694–705.
- [6] **W. Xing**, A. A. Shah, B. Urasinska-Wojcik, and J. W. Gardner, "Prediction of impurities in hydrogen fuel supplies using a thermally-modulated CMOS gas sensor: Experiments and modelling," in *2017 IEEE SENSORS*, Glasgow, Oct. 2017, pp. 1–3, doi: 10.1109/ICSENS.2017.8233907.
- [7] V. Triantafyllidis, **W. Xing**, A. A. Shah, and P. B. Nair, "Neural Network Emulation of Spatiotemporal Data Using Linear and Nonlinear Dimensionality Reduction," in *Advanced Computer and Communication Engineering Technology*, Cham, 2016, pp. 1015–1029. 2015 2nd International

Conference on Communication and Computer Engineering (ICOCOE) Phuket, Thailand, 2015-06-09 - 2015-06-11

Other Conference Paper

- K. Kelly, **W. Xing**, P. Goffin, T. Sayahi, T. Becnel, P-E. Gaillardon, A.E. Butterfield, M. Meyer, R. Whitaker, Understanding how pollution episodes affect community-level air quality with a distributed sensor network, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.
- J. Moore, **W. Xing**, M. Dailey, K. Le, T. Becnel, P. Goffin, M. Meyer, P-E Gaillardon, R. Whitaker, J. Wiese, A.E. Butterfield, K.E. Kelly, Engaging middle and high school students in hypothesis generation using a citizen-scientist network of air quality sensors, AIChE Annual Meeting, Orlando, FL, November 10-15, 2019.
- T. Sayahi, P.-E. Gaillardon, R. Whitaker, M. Meyer, T. Butterfield, P. Goffin, T. Becnel, A. Biglari, D. Kaufman, T. Sayahi, **W. Xing**, K. Kelly, Platform: Long-term evaluation of the plantower PMS sensor. 10th International Aerosol Conference, September 2nd-7th, St. Louis, Mo, 2018.
- K.E. Kelly, P.-E. Gaillardon, R. Whitaker, M. Meyer, T. Butterfield, P. Goffin, T. Becnel, A. Biglari, D. Kaufman, T. Sayahi, **W. Xing**, Poster: A layered framework for integrating low-cost sensor data and for engaging citizens to understand PM2.5 exposure. 10th International Aerosol Conference, September 2nd-7th, St. Louis, Mo, 2018.

Awards

Distinguish youth scholar award of Beihang University 2021 National university innovation and entrepreneurship competition Third prize 2021 National university innovation and entrepreneurship competition first prize of North China 2021 EDA Elite Championship competition first prize 2020 EDA Elite Championship competition second prize 2020 Best poster award in IPMI2019 2019 School of Engineering PhD scholarship 2012-2015 Outstanding graduate award of Shenzhen University 2012 Assistant Electronic Design Engineer Qualification by China Electronic Institute 2012 Scholarship of academician Yan Shuzi (Top academic award in the University) 2012 Top award, first prize, third prize and special prize in the 2011 China Electronic Innovation Design Competition. 2011 First prize in the innovation projects of 2011 China Educational Robots Competition 2011 Commercial scholarship "Haorizi Scholarship" (first class award) 2011

2011

2011

2009&2008

2008-2011

Commercial scholarship "Metro Scholarship" (first class award)

Academic Scholarship of First Class of Shenzhen University, twice

Excellent Academic Students of Shenzhen University award, all semesters

Academic Innovation Award

Referees

Professor Akeel Shah School of Engineering University of Warwick

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Professor of Computing, Mathematics, and
Bioengineering
University of Utah

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Department of Aerospace and Mechanical
Engineering
University of Notre Dame
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