

Gabriel A. Terejanu

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Department of Computer Science

College of Computing and Informatics

University of North Carolina at Charlotte

Research Interests

Causal Inference, Explainable Modeling, Deep Learning, Uncertainty Quantification, Bayesian Inference

Education

Ph.D. in Computer Science and Engineering

University at Buffalo, State University of New York

Jun 2010

M.S. in Computer Science and Engineering

University at Buffalo, State University of New York

Sep 2007

Eng.Diploma (B.Eng./M.Eng.) in Robotics

University of Craiova, Romania

Jun 2004

Valedictorian

First prize for the undergraduate thesis nationally awarded by the Romanian Society of Automation and Technical Informatics

Professional Experience

Associate Professor, University of North Carolina at Charlotte

Department of Computer Science

Aug 2018 - present

Assistant Professor, University of South Carolina

Department of Computer Science and Engineering

2017 Breakthrough Star Award

Jun 2012 - Jul 2018

Postdoctoral Fellow, University of Texas at Austin

Institute for Computational Engineering and Sciences (ICES)

May 2010 - May 2012

Quantitative Research Analyst, Maple Securities USA, Buffalo, New York

Statistical Arbitrage Trading Group

May 2008 - May 2009

Research Grants

PI: TOXIMAP: Computational Framework for Prediction of Geographical and Temporal Incidence of Mycotoxins in US Crop Fields, USDA-NIFA, \$500,000, 02/2017 - 02/2020, PI: Gabriel Terejanu, Co-PIs: Sourav Banerjee, Anindya Chanda.

Co-PI: RII Track-2 FEC: Center for a Sustainable Water, Energy, and Food Nexus (SusWEF), NSF, \$2,000,000, 08/15/2016 - 08/14/2020, PI: Nelson Cardona-Martinez, Co-PIs: Juan Lopez-Garriga, Maria Curet-Arana, Andreas Heyden, Gabriel Terejanu

PI: SciLAF: Scientific-based Learning Assessment Framework for Student Knowledge Tracking, NSF-IUSE, \$250,000, 08/2015 - 08/2017, PI: Gabriel Terejanu, Co-PIs: Juan Caicedo, Charles Pierce.

Co-PI/advisor: MAGELLAN: Noemi Glaeser: Generating Geographic and Temporal Heat Maps of Afla-

toxin Incidence using Regularized Linear Models, Office of Undergraduate Research, University of South Carolina, \$2,500, 2017, PI: Noemi Glaeser, Co-PI/advisor: Gabriel Terejanu

Co-PI/advisor: MAGELLAN: Jonathan Senn: Validating in Vitro Models for Aflatoxin Production in Maize using a New Open Field Sample Database, Office of Undergraduate Research, University of South Carolina, \$2,500, 2017, PI: Jonathan Senn, Co-PI/advisor: Gabriel Terejanu

PI: Demonstration of Model using Cover Crops to Improve Soil Health and Reduce Crop Stress and Aflatoxin Contamination, USDA-NRCS, \$75,000, 01/2016 - 12/2018, PI: Gabriel Terejanu, Co-PIs: Sourav Banerjee, Anindya Chanda, Buz Kloot.

Co-PI: DMREF: Collaborative Research: Design and Discovery of Multimetallic Heterogeneous Catalysts for a Future Biorefining Industry, NSF-DMREF, \$840,000, 09/2015 - 09/2019, PI: Andreas Heyden, Co-PIs: Gabriel Terejanu (share \$270,000), Ammal Salai.

Co-PI/advisor: SPARC: Xiao Lin: Computational Tool for Identifying Branching Types in Hyphal Growth Models, Office of the Vice President for Research, University of South Carolina, \$5,000, 2016, PI: Xiao Lin, Co-PI/advisor: Gabriel Terejanu

PI: ASPIRE II: Uncertainty Quantification driven Multi-scale Model Development for Aflatoxin Prediction, Office of the Vice President for Research, University of South Carolina, \$100,000, 05/2014 - 08/2015, PI: Gabriel Terejanu, Co-PIs: Sourav Banerjee, Anindya Chanda.

Co-PI: ASPIRE III: A Platform for Basic and Applied Research in Personal Robotics, Office of the Vice President for Research, University of South Carolina, \$50,000, PI: Jason M. OKane, Co-PIs: Jenay M. Beer, Gabriel Terejanu, Michael Huhns.

Selected Professional Services

Reviewer: Statistical Analysis and Data Mining, ACS Catalysis, Computers and Geosciences, Computers and Geosciences, Information Fusion, Scientific Reports, Journal of Computers & Mathematics with Applications, SIAM Journal on Scientific Computing, Journal of Uncertainty Quantification, Computer Methods in Applied Mechanics and Engineering, Environmental Modeling & Software, Journal of Applied Stochastic Models in Business and Industry, IEEE Signal Processing Letters, Reliable Computing, Entropy, Elsevier Journal of Signal Processing, IEEE Transaction on Automatic Control, American Control Conference (2010, 2011, 2012), IEEE Conference on Decision and Control 2012, International Conference on Information Fusion 2012, IEEE 9th Sensor Array and Multichannel Signal Processing Workshop (SAM 2016)

Minisymposia Co-organizer: SIAM Conference on Uncertainty Quantification: 2016 (Lausanne, Switzerland) “Data Assimilation Techniques for High Dimensional and Nonlinear Problems” - 8 talks, 2014 (Savannah, Georgia) “Advances in Optimal Experimental Design” - 14 talks, 2012 (Raleigh, North Carolina) “From Model Calibration and Validation to Reliable Extrapolations” - 12 talks and “UQ for Model Calibration, Validation and Predictions” - 8 talks.

Review Panels: NSF-DMREF, NSF-IUSE, DOE-CSGB, USC-VPR ASPIRE II & SPARC

Thesis and Dissertation

[1] Gabriel Terejanu. *Towards a decision-centric framework for uncertainty propagation and data assimilation*. PhD thesis, State University of New York at Buffalo, Buffalo, NY, 2010.

[2] Gabriel Terejanu. *Software Architecture for Remote Monitoring and Controlling of Mechatronic Systems*. Bachelor’s thesis, University of Craiova, Romania, 2004.

- [3] Asif J. Chowdhury, Wenqiang Yang, Kareem E. Abdelfatah, Mehdi Zare, Andreas Heyden, and Gabriel A. Terejanu. A multiple filter based neural network approach to the extrapolation of adsorption energies on metal surfaces for catalysis applications. *Journal of Chemical Theory and Computation*, 16(2):1105–1114, 2020. PMID: 31962041.
- [4] Gabriel Terejanu, Jawad Chowdhury, Rezaur Rashid, and Asif Chowdhury. Explainable deep modeling of tabular data using TableGraphNet, 2020. <http://arxiv.org/abs/2002.05205>.
- [5] Kareem Abdelfatah, Jonathan Senn, Noemi Glaeser, and Gabriel Terejanu. Prediction and Measurement Update of Fungal Toxin Geospatial Uncertainty using a Stacked Gaussian Process. *Agricultural Systems*, 176:102662, 2019.
- [6] Kareem Abdelfatah, Wenqiang Yang, Rajadurai Vijay Solomon, Biplab Rajbanshi, Asif Chowdhury, Mehdi Zare, Subrata Kumar Kundu, Adam Yonge, Andreas Heyden, and Gabriel Terejanu. Prediction of transition-state energies of hydrodeoxygenation reactions on transition-metal surfaces based on machine learning. *The Journal of Physical Chemistry C*, 123(49):29804–29810, 2019.
- [7] Xiao Lin, Asif Chowdhury, Xiaofan Wang, and Gabriel Terejanu. Approximate Computational Approaches for Bayesian Sensor Placement in High Dimensions. *Information Fusion*, 46:193 – 205, 2019.
- [8] Kareem Abdelfatah, Junshu Bao, and Gabriel Terejanu. Geospatial uncertainty modeling using Stacked Gaussian Processes. *Environmental Modelling & Software*, 109:293 – 305, 2018.
- [9] Asif J. Chowdhury, Wenqiang Yang, Eric Walker, Osman Mamun, Andreas Heyden, and Gabriel A. Terejanu. Prediction of Adsorption Energies for Chemical Species on Metal Catalyst Surfaces Using Machine Learning. *The Journal of Physical Chemistry C*, 122(49):28142–28150, 2018.
- [10] Eric A Walker, Donald Mitchell, Gabriel A Terejanu, and Andreas Heyden. Identifying Active Sites of the Water–Gas Shift Reaction over Titania Supported Platinum Catalysts under Uncertainty. *ACS Catalysis*, pages 3990–3998, 2018.
- [11] Wei Chen, George Kesidis, Tina Morrison, J Tinsley Oden, Jitesh H Panchal, Christiaan Paredis, Michael Pennock, Sez Atamturktur, Gabriel Terejanu, and Michael Yukish. *Research Challenges in Modeling and Simulation for Engineering Complex Systems*, chapter Uncertainty in Modeling and Simulation, pages 75–86. Springer International Publishing, 2017.
- [12] Xiao Lin, Gabriel Terejanu, Sajan Shrestha, Sourav Banerjee, and Anindya Chanda. Bayesian Model Selection Framework for Identifying Growth Patterns in Filamentous Fungi. *Journal of Theoretical Biology*, 398:85–95, 2016.
- [13] Eric Walker, Salai Cheettu Ammal, Gabriel Terejanu, and Andreas Heyden. Uncertainty Quantification Framework Applied to the Water-Gas Shift Reaction over Pt-Based Catalysts. *J. Phys. Chem. C*, 120(19):10328–10339, 2016.
- [14] Todd A. Oliver, Gabriel Terejanu, Christopher S. Simmons, and Robert D. Moser. Validating Predictions of Unobserved Quantities. *Computer Methods in Applied Mechanics and Engineering*, 283(0):1310 – 1335, 2015.
- [15] Subir Patra, Sourav Banerjee, Gabriel Terejanu, and Anindya Chanda. Subsurface Pressure Profiling: A Novel Mathematical Paradigm for Computing Colony Pressures on Substrate during Fungal Infections. *Nature Scientific Reports*, 5:12928, 2015.

- [16] Sourav Banerjee, Phani M. Gummadidala, Rowshan A. Rima, Riaz U. Ahmed, Gabriel J. Kenne, Chandrani Mitra, Ola M. Goma, Jasmine Hill, Sandra McFadden, Nora Banaszek, Raja Fayad, Gabriel Terejanu, and Anindya Chanda. Quantitative acoustic contrast tomography reveals unique multiscale physical fluctuations during aflatoxin synthesis in *Aspergillus parasiticus*. *Fungal Genetics and Biology*, 73(0):61 – 68, 2014.
- [17] Sourav Banerjee, Gabriel Terejanu, and Anindya Chanda. Uncertainty Quantification Driven Predictive Multi-Scale Model for Synthesis of Mycotoxins. *Computational Biology and Bioinformatics*, 2(1):7–12, 2014.
- [18] E. Walker, S. C. Ammal, S. Suthirakun, F. Chen, G. Terejanu, and A. Heyden. Mechanism of Sulfur Poisoning of $\text{Sr}_2\text{Fe}_{1.5}\text{Mo}_{0.5}\text{O}_{6-\delta}$ Perovskite Anode under Solid Oxide Fuel Cell Conditions. *J. Phys. Chem.*, C 118:23545–23552, 2014.
- [19] Kenji Miki, Ernesto E. Prudencio, Sai Hung Cheung, and Gabriel Terejanu. Using Bayesian Analysis to Quantify Uncertainties in the $\text{H}+\text{O}_2 \rightarrow \text{OH}+\text{O}$ Reaction. *Combustion and Flame*, 160(5):861 – 869, 2013.
- [20] Rebecca E. Morrison, Corey M. Bryant, Gabriel Terejanu, Serge Prudhomme, and Kenji Miki. Data partition methodology for validation of predictive models. *Computers & Mathematics with Applications*, 66(10):2114–2125, 2013.
- [21] Gabriel Terejanu, Rochan R. Upadhyay, and Kenji Miki. Bayesian Experimental Design for the Active Nitridation of Graphite by Atomic Nitrogen. *Experimental Thermal and Fluid Science*, 36:178–193, Jan. 2012.
- [22] Gabriel Terejanu, Puneet Singla, Tarunraj Singh, and Peter D. Scott. Adaptive Gaussian Sum Filter for Nonlinear Bayesian Estimation. *Automatic Control, IEEE Transactions on*, 56(9):2151–2156, Sept. 2011.
- [23] Gabriel Terejanu, Puneet Singla, Tarunraj Singh, and Peter D. Scott. A Decision-Centric Framework for Density Forecasting. *Journal of Advances in Information Fusion*, 5(2):73–87, Dec. 2010.
- [24] Jemin George, Gabriel Terejanu, and Puneet Singla. Spacecraft Attitude Estimation Using Adaptive Gaussian Sum Filter. *Journal of the Astronautical Sciences, Special Issue: Markley Symposium*, 57(1):31–45, 2009.
- [25] Gabriel Terejanu, Puneet Singla, Tarunraj Singh, and Peter D. Scott. Uncertainty Propagation for Nonlinear Dynamical Systems using Gaussian Mixture Models. *Journal of Guidance, Control, and Dynamics*, 31(6):1622–1633, Nov. 2008.
- [26] Ionut Dinulescu, Dorin Popescu, Gabriel Terejanu, and Andras Marinescu. Software Architecture of a Web-based PLC Laboratory. *Annals of the University of Craiova, Automation, Computers, Electronics and Mechatronics*, 3(30)(1):30–35, 2006.

Peer-Reviewed Conference Publications & Conference Proceedings

- [27] Chao Chen, Lin Xiao, Yuan Huang, and Gabriel Terejanu. Approximate Bayesian Neural Network Trained with Ensemble Kalman Filter. In *International Joint Conference on Neural Networks (IJCNN)*, Budapest, Hungary, July 2019.
- [28] Xiao Lin and Gabriel Terejanu. EnLLVM: Ensemble based Nonlinear Bayesian Filtering using Linear Latent Variable Models. In *International Conference on Acoustics, Speech, and Signal Processing (ICASSP)*, Brighton, UK, May 2019.

- [29] Chao Chen, Xiao Lin, and Gabriel Terejanu. An Approximate Bayesian Long Short-Term Memory Algorithm for Outlier Detection. In *International Conference on Pattern recognition (ICPR), Beijing, China*, August 2018.
- [30] Chao Chen and Gabriel Terejanu. Sub-Event Detection on Twitter Network. In *14th International Conference on Artificial Intelligence Applications and Innovations (AIAI), Rhodes, Greece*, May 2018.
- [31] Seyedramin Madarshahian, Chao Chen, Juan Caicedo, Charles Pierce, and Gabriel Terejanu. Using Multiple Choice Responses to Assess Uncertainty in Student Understanding of Vector Concepts. In *ASEE Annual Conference and Exposition, Columbus OH*, June 2017.
- [32] Kareem Abdelfatah, Junshu Bao, and Gabriel Terejanu. Unsupervised Detection of Violent Content in Arabic Social Media. In *Fourth International Conference on Computer Science and Information Technology (CoSIT-2017)*, March 2017.
- [33] Chao Chen, Seyedramin Madarshahian, Juan Caicedo, Charles Pierce, and Gabriel Terejanu. Bayesian network models for student knowledge tracking in large classes. In *ASEE Annual Conference and Exposition, New Orleans LA*, June 2016.
- [34] Gabriel Terejanu, Juan Caicedo, and Charles Pierce. SciLAF: Scientific-based Learning Assessment Framework for Student Knowledge Tracking. In *Envisioning the Future of Undergraduate STEM Education: Research and Practice, Washington DC*, April 2016.
- [35] Asif Chowdhury and Gabriel Terejanu. Enhanced Metropolis-Hastings Algorithm Based on Gaussian Processes. In *IMAC-XXXIV Conference and Exposition on Structural Dynamics, Orlando, Florida*, January 2016.
- [36] Gabriel Terejanu. From Model Calibration and Validation to Reliable Extrapolations. In *IMAC-XXXIV Conference and Exposition on Structural Dynamics, Orlando, Florida*, January 2016.
- [37] Hui Li, Asif Chowdhury, Gabriel Terejanu, Anindya Chanda, and Sourav Banerjee. A Stacked Gaussian Process for Predicting Geographical Incidence of Aflatoxin with Quantified Uncertainties . In *International Conference on Advances in Geographic Information Systems ACM SIGSPATIAL, Seattle, Washington*, November 2015.
- [38] Gabriel Terejanu. Active Data Collection for Inadequate Models. In *Information Fusion (Fusion), 2015 18th International Conference on*, pages 421–427, July 2015.
- [39] Gabriel Terejanu. Predictive Validation of Dispersion Models Using a Data Partitioning Methodology. In *IMAC-XXXII Conference and Exposition on Structural Dynamics, Orlando, Florida*, pages 151–156, February 2015.
- [40] Xiao Lin and Gabriel Terejanu. Model-driven data collection for biological systems. In *American Control Conference (ACC), 2014*, pages 2524–2529, June 2014.
- [41] Jiting Xu and Gabriel Terejanu. Approximate Bayesian Computation based on Progressive Correction of Gaussian Components. In *American Control Conference (ACC), 2014*, pages 2023–2028, June 2014.
- [42] Corey Bryant and Gabriel Terejanu. An Information-Theoretic Approach to Optimally Calibrate Approximate Models. In *The 50th AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition, Nashville, Tennessee, 9-12 January, 2012*. AIAA 2012-0153.
- [43] Gabriel Terejanu, Corey Bryant, and Kenji Miki. Bayesian optimal experimental design for a Shock-tube experiment. In *The International Conference on Mathematical Modeling in Physical Sciences, IC-MSQUARE, Budapest, Hungary, September 3-7, 2012*.

- [44] Rebecca Morrison, Corey Bryant, Gabriel Terejanu, Kenji Miki, and Serge Prudhomme. Optimal Data Split Methodology for Model Validation. In *Proceedings of the World Congress on Engineering and Computer Science 2011 Vol II, WCECS 2011*, pages 1038–1043, October 19-21 2011.
- [45] Gabriel Terejanu, Todd Oliver, and Chris Simmons. Application of Predictive Model Selection to Coupled Models. In *Proceedings of the World Congress on Engineering and Computer Science 2011 Vol II, WCECS 2011*, pages 927–932, October 19-21 2011.
- [46] Gabriel Terejanu. An Adaptive Split-Merge Scheme for Uncertainty Propagation using Gaussian Mixture Models. In *49th AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition, Orlando, Florida, January 2011*. AIAA-2011-890.
- [47] Gabriel Terejanu, Puneet Singla, Tarunraj Singh, and Peter D. Scott. Approximate propagation of both epistemic and aleatory uncertainty through dynamic systems. In *13th International Conference on Information Fusion, Edinburgh, UK, July 2010*.
- [48] Gabriel Terejanu, Puneet Singla, Tarunraj Singh, and Peter D. Scott. Approximate Interval Method for Epistemic Uncertainty Propagation using Polynomial Chaos and Evidence Theory. In *Proceedings of the American Control Conference (ACC)*, pages 349 – 354, June 2010.
- [49] Gabriel Terejanu, Puneet Singla, Tarunraj Singh, and Peter D. Scott. Decision Based Uncertainty Propagation Using Adaptive Gaussian Mixtures. In *12th International Conference on Information Fusion, Seattle, Washington, July 2009*.
- [50] Gabriel Terejanu, Puneet Singla, Tarunraj Singh, and Peter D. Scott. Application of the Decision-Centric Uncertainty Propagation in CBRN incidents. In *22nd Annual CSE Graduate Research Conference at Buffalo, Buffalo, New York, April 2009*.
- [51] Gabriel Terejanu, Yang Cheng, Tarunraj Singh, and Peter D. Scott. Comparison of SCIPUFF Plume Prediction with Particle Filter Assimilated Prediction for Dipole 26 Data. In *Chemical and Biological Defense Physical Science and Technology Conference, New Orleans, November 2008*.
- [52] Gabriel Terejanu, Puneet Singla, Tarunraj Singh, and Peter D. Scott. Uncertainty Propagation for Nonlinear Dynamical Systems using Gaussian Mixture Models. In *AIAA Guidance, Navigation and Control Conference and Exhibit, Honolulu, Hawaii, August 2008*. AIAA-2008-7472.
- [53] Gabriel Terejanu, Jemin George, and Puneet Singla. An Adaptive Gaussian Sum Filter for the Spacecraft Attitude Estimation Problem. In *Proceedings of the American Astronautical Society F. Landis Markley Astronautics Symposium*, pages 35–50, June 2008. AAS 08-262.
- [54] Gabriel Terejanu, Puneet Singla, Tarunraj Singh, and Peter D. Scott. A Novel Gaussian Sum Filter Method for Accurate Solution to Nonlinear Filtering Problem. In *11th International Conference on Information Fusion, Cologne, Germany, June 2008*.
- [55] Tarunraj Singh, Puneet Singla, Peter Scott, Umamaheswara Reddy, Gabriel Terejanu, and Yang Cheng. Data Assimilation for Forecasting Plume Dispersion. In *First Annual Conference of Center for GeoHazards Studies, Natural Disasters in Small Communities: How Can We Help?, Buffalo, New York, March 2008*.
- [56] Puneet Singla, Tarunraj Singh, Peter Scott, Gabriel Terejanu, Yang Cheng, and Umamaheswara Reddy. Accurate Uncertainty Propagation through Nonlinear Systems. In *First Annual Conference of Center for GeoHazards Studies, Natural Disasters in Small Communities: How Can We Help?, Buffalo, New York, March 2008*.

- [57] Gabriel Terejanu, Tarunraj Singh, and Peter D. Scott. Unscented Kalman Filter/Smoother for a CBRN Puff-Based Dispersion Model. In *11th International Conference on Information Fusion, Quebec City, Canada*, July 2007.
- [58] Ionut Dinulescu, Dorin Popescu, and Gabriel Terejanu. Web based Telematics Application using Open-Source technologies. In *Proceedings of the 12th International Symposium on Systems Theory, SINTES 12, Vol.3*, pages 267–272, October 2005. ISBN 973-742-148-5.
- [59] Dorin Popescu, Gabriel Terejanu, Ionut Dinulescu, and Mihnea Leoveanu. PLC based Telemanipulation via Internet. In *Proceedings of the 14th International Workshop on Robotics in Alpe-Adria-Danube Region*, pages 441–447, May 2005. ISBN 973-718-241-3.
- [60] Dorian Cojocaru and Gabriel Terejanu. Remote System for Mobile Robots. In *Proceedings of the 2nd International Conference on Robotics*, pages 43–45, October 2004. ISBN 973-97258-3-X.

Technical Reports

- [61] Robert D. Moser, Gabriel Terejanu, Todd A. Oliver, , and Christopher S. Simmons. Validating the Prediction of Unobserved Quantities. Technical Report 12-32, The Institute for Computational Engineering and Sciences, The University of Texas at Austin, Austin, Texas 78712, Aug. 2012.
- [62] Tarunraj Singh, Peter Scott, Puneet Singla, Yang Cheng, Uma Konda, Gabriel Terejanu, Alex James, Sue E. Haupt, George Young, Anke Beyer-Lout, and Kerrie Long. Blending Chem-Bio Dispersion Forecasts and Sensor Data. Technical Report Contract No. W911NF-06-C-0162, Defense Threat Reduction Agency, Joint Science & Technology Office for Chemical & Biological Defense, Fort Belvoir, Virginia, Dec. 2008.
- [63] Gabriel Terejanu. Crib Sheet: Linear Kalman Smoothing. Web-tutorial, Department of Computer Science and Engineering, University at Buffalo, Buffalo, New York, 2008.
- [64] Gabriel Terejanu. Discrete Kalman Filter Tutorial. Web-tutorial, Department of Computer Science and Engineering, University at Buffalo, Buffalo, New York, 2008.
- [65] Gabriel Terejanu. Extended Kalman Filter Tutorial. Web-tutorial, Department of Computer Science and Engineering, University at Buffalo, Buffalo, New York, 2008.
- [66] Gabriel Terejanu. Tutorial on Monte Carlo Techniques. Web-tutorial, Department of Computer Science and Engineering, University at Buffalo, Buffalo, New York, 2008.
- [67] Gabriel Terejanu. Unscented Kalman Filter Tutorial. Web-tutorial, Department of Computer Science and Engineering, University at Buffalo, Buffalo, New York, 2008.

Talks

- (1) *Automated Machine Learning (AutoML) - the Hype, the Limitations, the Opportunities*, Lowe’s Home Improvement Corporate Office, Mooresville, NC, January 16, 2020
- (2) *An Information Theoretic Approach to Guiding Model Development*, The Applied Inverse Problems (AIP) Conference, Grenoble, France, July 8-12, 2019

- (3) *Approximate Bayesian Neural Network Trained with Ensemble Kalman Filter*, Eastern European Machine Learning Summer School, Bucharest, Romania, July 1-6, 2019
- (4) *Geospatial Uncertainty Modeling using Stacked Gaussian Processes*, SAMSI Workshop on Coupling Uncertain Geophysical Hazards, Raleigh, NC, March 24-26, 2019
- (5) *Mutual Information Estimation in High Dimensions*, SIAM Conference on Uncertainty Quantification, Garden Grove, CA, April 16, 2018
- (6) *Bayesian Optimization using Stacked Gaussian Processes*, SIAM Conference on Uncertainty Quantification, Garden Grove, CA, April 16, 2018
- (7) *Accelerated MCMC using Bayesian Optimization*, SIAM Conference on Uncertainty Quantification, Garden Grove, CA, April 16, 2018
- (8) *Acceleration of Science and Decision-Making using Uncertainty Quantification*, Department of Computer Science, University of North Carolina at Charlotte, February, 2018
- (9) *Fast Active Learning for High Dimensional Nonlinear Dynamical Systems*, InfoSymbiotics/DDDAS Conference, Cambridge, MA, August 7-9, 2017
- (10) *Approximate Bayesian Inference for Intractable Likelihood Functions*, SIAM Conference on Computational Science and Engineering, Atlanta, GA, February 27, 2017
- (11) *Approximate Experimental Design in High Dimensional Spaces*, SIAM Conference on Computational Science and Engineering, Atlanta, GA, February 27, 2017
- (12) *Stacked Gaussian Processes with Applications in Environmental Sciences*, SIAM Conference on Computational Science and Engineering, Atlanta, GA, February 27, 2017
- (13) *Uncertainty Quantification in Computational Catalysis*, The Center for Rational Catalyst Synthesis (CeRCaS), 2016 Fall Meeting, December 2016
- (14) *Uncertainty Quantification of the Water-Gas Shift Reaction over Pt-Based Catalysts*, AIChE 2015 Annual Meeting, Salt Lake, UT, November 8-13, 2015
- (15) *How Can We Ever Trust Extrapolative Predictions?* Department of Civil and Environmental Engineering (September 25, 2015), Department of Mathematics (March 21, 2016), Department of Statistics (April 14, 2016), University of South Carolina
- (16) *Fast Data Assimilation for High Dimensional Nonlinear Dynamical Systems* SIAM Conference on Uncertainty Quantification, Lausanne, Switzerland, April 5 - 8, 2016
- (17) *Fast Approximate Bayesian Inference in High Dimensional Spaces using Latent Variable Models*, ICERM workshop on Mathematics in Data Science, Brown University, July 28-30, 2015
- (18) *Towards Experimental Design Strategies for Inadequate Models*, SIAM Conference on Computational Science and Engineering, Salt Lake, UT, March 14-18, 2015
- (19) *Uncertainty Quantification of a Computational Study of the Water-Gas Shift Reaction Catalyzed by Platinum Clusters Supported on Titanium Oxide (Pt/TiO₂)*, AIChE 2014 Annual Meeting, Atlanta GA, November 16-21, 2014
- (20) *An integrated approach to pathogen growth modeling*, IMAG 2014 Multiscale Modeling (MSM) Consortium, Bethesda, MD, September 3-4, 2014

- (21) *Bayesian Experimental Design in the Presence of Model Error*, SIAM Conference on Uncertainty Quantification, Savannah, GA, March 31 - April 3, 2014
- (22) *Sequential Bayesian Experimental Design with Applications to Biological Systems*, 12th US National Congress on Computational Mechanics Raleigh, North Carolina July 22-25, 2013
- (23) *High Performance Embedded Tracking*, Boeing SBIR/STTR Summit, SCRA Technology Ventures, Charleston, SC, February 19, 2013
- (24) *The Building Blocks of Reliable Extrapolations*, PSAAP 2012 V&V UQ Workshop, University of Michigan, Ann Arbor, August 8-10, 2012
- (25) *On Data Splitting for Model Validation*, 2012 Joint Statistical Meetings, San Diego, July 28 - August 2, 2012
- (26) *Towards a Comprehensive Framework for Building Confidence in Predictive Simulations*, Brookhaven National Laboratory, Environmental Sciences Department, July 11, 2012
- (27) *From Model Calibration and Validation to Reliable Extrapolations*, SAMSI/ORNL Uncertainty Quantification in High Performance Computing Workshop, Oak Ridge, TN, May 2-4, 2012
- (28) *Towards Finding the Necessary Conditions for Justifying Extrapolations*, SIAM Conference on Uncertainty Quantification, Raleigh, North Carolina, April 2-5, 2012
- (29) *On Data Partitioning for Model Validation*, SIAM Conference on Uncertainty Quantification, Raleigh, North Carolina, April 2-5, 2012
- (30) *Optimal Data Collection under Model Error*, SIAM Conference on Uncertainty Quantification, Raleigh, North Carolina, April 2-5, 2012
- (31) *Challenges on Incorporating Uncertainty in Computational Model Predictions*, SIAM Conference on Uncertainty Quantification, Raleigh, North Carolina, April 2-5, 2012
- (32) *Predictive Capability Assessment via Cross-Validation or Model Selection*, Winter Simulation Conference, Phoenix, Arizona, December 11-14, 2011
- (33) *Integrated Methodology for Building Confidence in the Predictive Capability of Computational Models*, Seminar in the Department of Computer Science and Engineering, University of South Carolina, November 4, 2011
- (34) *Confidence Building in the Predictive Capability of Physical Models*, PECOS Center 2011 Review Meeting, University of Texas at Austin, Austin, Texas, October 12-13, 2011
- (35) *An Information Theoretic Approach to Model Calibration and Validation*, SAMSI Uncertainty Quantification: Engineering and Renewable Energy Opening Workshop, Research Triangle Park, NC, September 19-21, 2011
- (36) *Reliable Predictions of QoIs in Coupled Multiphysics Problems Using an Efficient Decision-Centric Validation Framework*, The 11th U.S. National Congress on Computational Mechanics, Minneapolis, Minnesota, July 25-28, 2011
- (37) *Data Assimilation Algorithms Applied to Short Term Ground Motion Stochastic Forecasts*, The 11th U.S. National Congress on Computational Mechanics, Minneapolis, Minnesota, July 25-28, 2011
- (38) *Information-Theoretic Experimental Design for the Active Nitridation of Graphite*, ICiS Workshop on Verification, Validation and Uncertainty Quantification Across Disciplines Park City, Utah, August 6-13, 2011

- (39) *An Information Theoretic Approach to Model Calibration and Validation using QUESO*, IMA Hot Topics Workshop: Uncertainty Quantification in Industrial and Energy Applications: Experiences and Challenges, University of Minnesota, Minneapolis, Minnesota, June 2-4, 2011
- (40) *Predictive Model Selection for Coupled Multiphysics*, Trilab Sponsor Team (TST) Meeting, University of Texas at Austin, Austin, Texas, April 27-28, 2011
- (41) *Information-Theoretic Experimental Design for the Active Nitridation of Graphite*, Uncertainty Quantification for Multiphysics and Multiscale Systems Workshop, University of Southern California, Los Angeles, California, March 7-8, 2011
- (42) *Validation Framework for Coupled Multiphysics Models using Predictive Model Selection*, Uncertainty Quantification for Multiphysics and Multiscale Systems Workshop, University of Southern California, Los Angeles, California, March 7-8, 2011
- (43) *Application of the Decision-Centric Uncertainty Propagation in CBRN incidents*, The Chemical and Biological Defense Physical Science and Technology Conference, Dallas, TX, Nov 2009
- (44) *Decision-based Uncertainty Propagation*, School of Engineering and Applied Sciences, Graduate Student Poster Competition at University at Buffalo, Buffalo, New York, April 2009
- (45) *Source Estimation for CBRN Incidents Based On Field Data*, School of Engineering and Applied Sciences, Graduate Student Poster Competition at University at Buffalo, Buffalo, New York, April 2009
- (46) *A Novel Gaussian Sum Filter Method for Accurate Solution to Nonlinear Filtering Problem*, The 21st Annual CSE Graduate Research Conference at University at Buffalo, Buffalo, New York, March 2008
- (47) *Source Estimation in CBRN Incidents*, First Annual Conference of Center for GeoHazards Studies, Natural Disasters in Small Communities: How Can We Help?, Buffalo, New York, March 2008
- (48) *Predicting the Evolution of Toxic Plumes for Casualty Mitigation in Chem-Bio Incidents*, School of Engineering and Applied Sciences, Graduate Student Poster Competition at University at Buffalo, Buffalo, New York, April 2007

Research Supervision (Students and Postdocs)

Jawad Chowdhury, PhD expected December 2021, “Causal Inference for Tabular Data”

Rezaur Rashid, PhD expected December 2021, “Self-Supervising Learning for Tabular Data”

Asif Chowdhury, PhD March 2020, “A Machine Learning based Approach to Faster Catalyst Discovery”

Kareem Abdelfatah, PhD October 2020, “Stacked Modeling Framework”

Chao Chen, PhD December 2018, “Uncertainty Estimation of Deep Neural Networks”

Xiao Lin, PhD February 2018, “Inference Framework for Model Update and Development” (USC SPARC awardee)

Eric Walker, PhD August 2016, “Bayesian Method for Identifying the Mechanism of Water-Gas Shift Reaction on Noble Metal Catalysts”

Sourav Das, MS November 2016, “Blind Change Point Detection and Regime Segmentation using Gaussian Processes Regression”

Jiting Xu, MS July 2014, “Approximate Bayesian Computation based on Progressive Selection of Gaussian Components”

Xiaofan Wang, visiting scholar November 2012 - November 2013, Department of Computer Science, Xian University of Technology, Shaanxi Province, PR China, “Optimal Sensor Placement for Monitoring Chemical Release Incidents”

Noemi Glaeser, BSc May 2017, “Generating Geographic and Temporal Heat Maps of Aflatoxin Incidence using Regularized Linear Models” (USC MAGELLAN awardee)

Jonathan Senn, BSc December 2018, “Validating in Vitro Models for Aflatoxin Production in Maize using a New Open Field Sample Database” (USC MAGELLAN awardee)

Service

CS PhD Recruitment, Admission and Review Committee Chair (2018 - 2020)

University of North Carolina at Charlotte

Search Committee Member (2018-2020)

University of North Carolina at Charlotte

Qualifying Exam Committee Chair (2018)

University of South Carolina

Program Director of Minor in Data Science (2017 - 2018)

University of South Carolina

Graduate Studies Committee Member (2012 - 2018)

University of South Carolina

Search Committee Member

University of South Carolina

QE Committee member, Yuehua Duan (Computer Science), “Sentiment Analysis in Recommender System”, January 2019

QE Committee member, Ashutosh Dutta (Software and Information Systems), “Adaptive Cyber Defense using POMDP”, December 2018

PhD Committee member, Mark Daniels (Computer Science and Engineering), “Ontology-Guided Pre-Release Inference Disruption”, proposal: December 2017, defense: April 2018

PhD Committee member, Leydy Mejia Cruz (Civil Engineering), “Construction of a Probabilistic Multi-dimensional Constitutive Model (PMCM) of the Compressive Strength of Hardened Cement Paste (HCP) reinforced with MWCNTs”, proposal: December 2017, defense: December 2018

PhD Committee member, Beidi Qiang (Statistics), “Improved Simultaneous Estimation of Location and System Reliability Via Shrinkage Ideas”, proposal: October 2016, defense: May 2017

MS Committee member, Lacie Cochran (Computer Science and Engineering), “Hardware Accelerated Spiking Neural Network”, proposal: August 2017, defense: October 2018

PhD Committee member, Wenqiang Yang (Chemical Engineering), “Rational Design of Heterogeneous Catalysts for Hydrodeoxygenation of Succinic Acid”, proposal: May 2017

PhD Committee member, Yan Zhang (Computer Science and Engineering), “Deep Learning in Computa-

tional Biology”, proposal: April 2017 , defense: November 2017

External evaluation member - qualifying exam, Christopher Edgar (Mathematics), August 2016

External evaluation member - qualifying exam, Sajan Shrestha (Mechanical Engineering), Nov 2015

PhD Committee member, Albert Ortiz Lasprilla (Civil and Environmental Engineering), “Modeling Human-Structure Interaction using a Controller System”, proposal: November 2015, defense: March 2016.

PhD Committee member, Zizhen Wu (Statistics), “Methods for Registration and Clustering of Functional Observations”, proposal: October 2015, defense: May 2016.

PhD Committee member, Mohammad Saleheen (Chemical Engineering), “Developing an Artificial Neural Network (ANN) Potential for Describing Metal- Water Interactions Applications of Machine Learning Techniques”, proposal: September 2015

PhD Committee member, Ramin Madarshahian (Civil and Environmental Engineering), “Reducing Computational Cost in Bayesian Model Updating Using a Two Layered Approach”, proposal: February 2015, defense: July, 2017

PhD Committee member, Arjang Fahim (Computer Science and Engineering), “nD-PDPA: n-Dimensional Probability Density Profile Analysis”, proposal: October 2014, defense: November 2015

PhD Committee member, Osman Mamun (Chemical Engineering), “Rational Design of Bifunctional Catalysts for the Conversion of Levulinic Acid to γ -Valerolactone”, proposal: September 2014, defense: July, 2017

MS Committee member, Ahmed AL-Qurri (Computer Science and Engineering), “Incorporating Amino Acid Bonds to Improve Peptides Identification Accuracy”, proposal: September 2016, defense: April 2017

MS Committee member, Chandrahas Gurram Venkat (Computer Science and Engineering), “Hidden Markov Model for State Estimation using Underground Sensor Data”, proposal: September 2016, defense: November 2016

MS Committee member, Eric Walker (Chemical Engineering), “Comparison of a Particle Filter and other State Estimation Methods for Prognostics of Lithium-ion Batteries”, defense: August 2013

Judge at Dutch Fork High School Research Symposium, October 2016

Student Representative in the Computer Science Graduate Studies Committee, Sep 2007 - May 2008

Vice-President & IT Coordinator, European Student Association AEGEE Craiova, Jan 2000 - Oct 2003

Teaching

DSBA 6100 Big Data Analytics for Competitive Advantage (graduate) (Spring 2019, Fall 2019, Spring 2020)

ITCS 5122 Visual Analytics (undergraduate/graduate) (Fall 2018)

CSCE 582 Bayesian Networks and Decision Graphs (undergraduate/graduate) (Spring 2018)

CSCE 590/576 Data Visualization (undergraduate/graduate) (Spring 2016, Spring 2017)

CSCE 883 Machine Learning (graduate) (Fall 2014, Fall 2015, Fall 2016)

CSCE 758 Probabilistic System Analysis (graduate) (Fall 2012, Fall 2013)

CSCE 350 Data Structures and Algorithms (undergraduate), (Spring 2013, Spring 2015, Fall 2017)

CSCE 791 Seminar Advances in Computing (graduate), (Fall 2015, Fall 2016)

Software Skills

Skills: Python, JavaScript, D3, C++, SQL, Linux, LaTeX, Git

GitHub: <https://bitbucket.org/uqlab>

Software (releases & contributions)

1. Contribution to **QUESO** (Quantification of Uncertainty for Estimation, Simulation, Optimization) added information-theoretic estimators to be used in model validation and calibration projects (<https://github.com/libqueso/queso>).
2. **Predictive Selection of Coupled Models** C++ application framework developed on top of QUESO for solving the problem of predictive model selection of coupled models (<https://bitbucket.org/uqlab/predictiveselectioncoupleddmodels>).
3. **Adaptive Gaussian Sum Filter**. Matlab code for adapting the weights of a Gaussian sum in the context of nonlinear filtering (<https://bitbucket.org/uqlab/adaptivegaussiansumfilter>).
4. **SciLAF** Learning Assessment Framework. Scientific based Learning Assessment Framework for student knowledge tracking. The main functionalities of this framework are to construct Bayesian student models, optimize the models, and generate individualized student models for student knowledge estimation, student misconception identification, and evaluation of questions design (<https://bitbucket.org/uqlab/scilaf>).
5. **StackedGP**. Python library that implements the StackedGP modeling framework. The main applications for StackedGP framework are to integrate different datasets through model composition, enhance predictions of quantities of interest through a cascade of intermediate predictions, and to propagate uncertainties through emulated dynamical systems driven by uncertain forcing variables, (<https://bitbucket.org/uqlab/stackedgp>).