# Cosmin Safta

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# Summary

Cosmin is a computational research scientist with 20+ years of experience in computational science algorithms for a wide range of applications. Cosmin has excelled in developing technical solutions to bridge the gap between fundamental research and modeling challenges to engineering applications for a variety of DoD, DOE, Darpa, and NNSA mission areas. His research portfolio began with a focus in combustion research and has expanded to include a broad spectrum of uncertainty quantification and statistical learning techniques for large scale models with specific applications in combustion, earth system modeling, biosurveillance, power grids, and material science. He developed unsupervised and supervised learning techniques for large scale models leading to approximately 100x reduction in the computational cost and enabling design decisions with quantified uncertainty that were not otherwise possible. His work resulted in over 45 peer-reviewed journal articles and 140 presentations since 2010 and lead to the release of several software toolkits for scientific computing and statistical modeling.

# **Work Experience**

# 2021-present, Distinguished Member of Technical Staff 2013-2021, Principal Member of Technical Staff

Sandia National Laboratories, Livermore, CA

- Lead the development of Sandia Forecast Model for the Covid-19 Epidemic
  - **Challenge**: lack of models that could provide short-term forecasts of Covid-19 spread during early stages of epidemics generated by unknown pathogens.
  - Action: Designed and released a model that assimilates partially-observed epidemics and provides robust forecasts in less than 10 minutes. Assembled and lead a team of 10 scientists to provide nightly results for all 50 US States. This work was featured on ABC7 News (link)
  - *Results*: The New Mexico Department of Health used SNL forecasts to assess the epidemic trends and plan for health resource allocation within the state. The US Department of State has shared weekly forecasts with foreign partners.
- Lead the development of software tools for catalytic processes at scale
  - **Challenge**: The Department of Energy Basic Energy Sciences and SNL's Combustion Research Facility are having a renewed focus on fundamental research for catalysis processes. Nevertheless, there is lack of software tools to support design and analyze catalytic processes *at scale*.
  - Action: Led a team that overhauled the TChem software, previously released by Safta (lead author) in 2010, with new capabilities for catalysis simulations and the ability to execute on heterogenous computational platforms including many-core and GPU-based architectures.
  - *Results:* The new software version, recently released as open source, is the first software toolkit of this kind, enabled for catalysis simulations on next-generation computing platforms. It expands the range of models accessible in computational studies by an order of magnitude paving the way for the discovery of new fuel blends and design of novel catalysts at scale.
- Developed efficient tools for the calibration of computationally expensive models
  - **Challenge**: Lack of efficient tools for statistical calibration of highly non-linear, partially known, and computationally expensive models.
  - Action: I have combined statistical tools to allow a principled treatment of computational model deficiencies and further developed sampling algorithms to allow the exploration of multi-modal parameter spaces for computational expensive models that were previously outside the reach of

sampling tools available at SNL. These tools, including a transitional Markov Chain Monte Carlo algorithm, are now part of the UQTk library.

- *Results*: The new capability became the focus of a DOE SBIR project for use in geosteering models. This framework is now employed in a NA-22 project for calibration of network models leading to the first model inversion study in power line communication models that are expected to be a key component in smart-grids. These new capabilities also lead to a DOE ASCR project on modeling metallic alloys for long term energy storage.
- Developed algorithms and computational tools focused on reducing model complexity
  - **Challenge**: Computational models of interest to SNL are typically too expensive and span a large set of parameters, putting them out of range for typical UQ workflows
  - **Action**: Developed compressive sensing algorithms that enable the construction of surrogate models for high-dimensional and compute intensive applications.
  - *Results*: New global sensitivity analysis and model calibration workflows implemented in UQTk reduce the computational expense by *10-100x*. The library has over 1000 downloads from across the world.

### • Lead the SNL entry to the NASA UQ Challenge 2014-2015

- **Challenge**: NASA Langley assembled a set of black-box aircraft dynamics models to test the capabilities of current uncertainty quantification models from across the world.
- Action: Proposed an ensemble of algorithms to tackle the challenge components and lead a team of 5 to apply current tools and develop new capabilities when necessary to address the challenges posed by the NASA models.
- *Results*: This effort resulted in new uncertainty quantification workflows implemented in UQTk. The conference paper resulted from this effort was selected for a special issue of the AIAA Journal.

Broad Research Portfolio in Uncertainty Quantification and Machine Learning - Taking an active role in bridging the gap between fundamental research and modeling challenges posed by engineering systems of interest to SNL, DOE, and the nation

- *adversarial machine learning* algorithms to reverse-engineer black-box machine learning models novel data exfiltration from black-box models.
- functional tensor-train approximations & sampling techniques for discrete and mixed continuousdiscrete random variables – aiming to break current curse-of-dimensionality barriers and expand the range of engineering problems that can be tackled with accurate models.
- *unsupervised learning techniques*: low-dimensional manifolds in experimental and computational data via diffusion maps algorithms that can enable the design of hypersonic trajectories in real-time.
- generative models for synthetic data consistent with underlying physics models enable analysis of aging processes in NW components
- supervised learning techniques: tree-based Recurrent Neural Network models following a physicsinspired architecture – a novel approach to enable modeling of sequence data with reduced data requirements

# 2009 – 2013, Senior Member of Technical Staff

# Sandia National Laboratories, Livermore, CA

- Developed data assimilation models based on Kalman Filters and support vector machines for computational biosurveillance. The modeling framework was used to detect the onset of epidemics based on heterogeneous data streams.
- Developed a Bayesian framework to tackle discontinuous behavior in climate model outputs. This work resulted in peer-reviewed publications and subsequent DOE BER projects.
- Lead developer of *TChem*, a software library (written in C) that facilitates the analysis of detailed chemical models. It spans a comprehensive set of elementary chemical reaction types and implements modules for analytical Jacobian evaluations leading to efficient analysis of the reaction time scales.

# 2007 – 2009, Postdoctoral Researcher

#### Sandia National Laboratories, Livermore, CA

 Designed high-order adaptive mesh refinement algorithms for chemical reacting flows. Designed and published the first high-order discretization scheme for low-speed combustion applications.

#### 2004 – 2007, Postdoctoral Researcher & Research Engineer

#### SUNY Stony Brook and TTC Technologies, Long Island, NY

• Focused on algorithms for turbulence-combustion coupling in reacting flow simulations. Algorithm developments were transitioned to the Air Force Research Laboratory.

#### 1997 – 2004, PhD Researcher

#### University at Buffalo, Buffalo, NY

• Designed new analysis tools to explore flame-vortex interaction processes in computational simulations. The work revealed previously unknown extinction mechanism in hydrocarbon flames.

# Education

PhD Mechanical Engineering, University at Buffalo, Buffalo, NY

09/1997 - 01/2004

**MS Aerospace Engineering** (first in class), University POLITEHNICA of Bucharest, Romania 09/1995 - 07/1996

**BS Aerospace Engineering** (first in class), University POLITEHNICA of Bucharest, Romania 09/1990 - 07/1995

# **Professional Activities**

- Scientific minisymposia organizer
  - SIAM Conference on Uncertainty Quantification 2022
  - SIAM Computational Science and Engineering 2021
  - SIAM Mathematics on Data Science 2020: Inference and Control in Complex Systems
  - o SIAM UQ 2016: Stochastic Modeling and Optimization
  - SIAM CSE 2015: Uncertainty Quantification Algorithms for Power Grids
- New Idea LDRD Committee (joined February 2020). Contributor to standard committee activities including
  proposal selection, providing feedback to individual PIs on the progress of their work; shaping the call for
  proposals for the upcoming FY.
- Reviewer (at a rate of about 3-5 manuscripts/year) for AIAA Journal, Combustion Science & Technology, Combustion and Flame, Proceedings of the Combustion Institute, Computational Science & Discovery, Methodology and Computing in Applied Probability, IEEE Transactions on Power Systems, IEEE Transactions on Sustainable Energy, Geoscientific Model Development, Journal of Computational Physics, SIAM Journal on Scientific Computing, International Journal on Uncertainty Quantification
- Reviewer for DOE Small Business Innovation Research Program Modeling and Simulation, NSF Panel on Computational Fluid Dynamics, NSF Panel on Combustion and Fire Research, DOE Early Career Program (Applied Mathematics)
- Professional Memberships: Combustion Institute (past member), American Institute of Aeronautics and Astronautics, Society for Industrial and Applied Mathematics, International Society for Bayesian Analysis, American Geophysical Union

# Software

- 1. Lead developer of **PRIME** (link)
  - Software library that assimilates partially-observed epidemics data and provides robust forecasts at regional and national level in less than 10 minutes with limited computational resources
  - Sandia National Labs video: https://youtu.be/IMiNSziud6Y
- 2. Lead developer of TChem (link)
  - The current version of TChem is the first open source computational chemistry library designed for future heterogenous computing platforms
- 3. Lead developer of EGSim (link)
  - C++ software toolkit for solving static load flow problems in electric power grids
- 4. Key developer of UQ Toolkit (link)
  - collection of C++/Python libraries and tools for the quantification of uncertainty in computational models and experimental data
- 5. Key developer of graphMC
  - C++ toolkit designed to test the independence of graphs

# **Peer-reviewed Journal Papers**

# 2022

1. Frankel, **C. Safta**, C. Alleman, R. Jones, "*Mesh-based Graph Convolutional Networks for Modeling Materials with Microstructure*," Journal of Machine Learning for Modeling and Computing, doi: 10.1615/JMachLearnModelComput. 2021039688 (2022).

# 2021

- O. Díaz-Ibarra, K. Kim, C. Safta, J. Zádor, H.N. Najm, "Using Computational Singular Perturbation as a Diagnostic Tool in ODE and DAE Systems: A Case Study in Heterogeneous Catalysis," Combustion Theory and Modeling, doi: 10.1080/13647830.2021.2002417 (2021).
- 3. P. Blonigan, J. Ray, **C. Safta**, "*Forecasting Multi-Wave Epidemics Through Bayesian Inference*," Archives of Computational Methods in Engineering, doi: 10.1007/s11831-021-09603-9 (2021).
- 4. K. Lee, J. Ray, **C. Safta**, "*The predictive skill of convolutional neural networks models for disease forecasting*", PLOS One, doi: 10.1371/journal.pone.0254319 (2021).
- Y.T. Lin, J. Neumann, E.F. Miller, R.G. Posner, A. Mallela, C. Safta, J. Ray, G. Thakur, S. Chinthavali, W.S. Hlavacek, "Daily Forecasting of Regional Epidemics of Coronavirus Disease with Bayesian Uncertainty Quantification, United States," Emerging Infectious Diseases, doi: 10.3201/eid2703.203364 (2021).

- L. Swiler, M. Gulian, A. Frankel, C. Safta, J. Jakeman, "A Survey of Constrained Gaussian Process Regression: Approaches and Implementation Challenges," Journal of Machine Learning for Modeling and Computing, doi: 10.1615/JMachLearnModelComput.2020035155 (2020).
- 7. **C. Safta**, K. Sargsyan, J. Ray, "Characterization of Partially Observed Epidemics through Bayesian Inference Application to COVID-19", Computational Mechanics, doi: 10.1007/s00466-020-01897-z (2020).
- H. Lu, Q. Shen, J. Chen, X. Wu, X. Fu, M. Khalil, C. Safta, Y. Huang, "Bifidelity Gradient-Based Approach for Nonlinear Well-Logging Inverse Problems," IEEE Journal on Multiscale and Multiphysics Computational Techniques 5, pp 132-143, doi: 10.1109/JMMCT.2020.3007839 (2020).

 Z.J. Buras, C. Safta, J. Zador, L. Sheps, "Simulated Production of OH, HO2, CH2O, and CO2 During Dilute Fuel Oxidation Can Predict 1<sup>st</sup>-Stage Ignition Delays," Combustion and Flame 216, pp 472-484, doi: 10.1016/j.combustflame.2019.12.013 (2020).

#### 2019

- R.G. Ghanem, C. Soize, C. Safta, X. Huan, G. Lacaze, J.C. Oefelein, and H.N. Najm, "Design optimization of a scramjet under uncertainty using probabilistic learning on manifolds," Journal of Computational Physics 399, pp 108930, doi: 10.1016/j.jcp.2019.108930 (2019).
- M. Lucchesi, H.H. Alzahrani, C. Safta, O. M. Knio, "A hybrid, non-split, stiff/RKC, solver for advection-diffusionreaction equations and its application to low-Mach number combustion," Combustion Theory and Modelling 23, pp 935-955, doi: 10.1080/13647830.2019.1600723, (2019).
- C. Soize, R.G. Ghanem, C. Safta, X. Huan, Z.P. Vane, J.C. Oefelein, G. Lacaze, and H.N. Najm, Q. Tang, X. Chen, "*Entropy-based closure for probabilistic learning on manifolds*," Journal of Computational Physics 388, pp 518-533, doi: 10.1016/j.jcp.2018.12.029 (2019).
- P. Tsilifis, X. Huan, C. Safta, K. Sargsyan, G. Lacaze, J.C. Oefelein, H.N. Najm, R.G. Ghanem, "Compressive Sensing Adaptation for Polynomial Chaos Expansions," Journal of Computational Physics 380, pp 28-47, doi: 10.1016/j.jcp.2018.12.010 (2019).
- M. Vohra, A. Alexanderian, C. Safta, S. Mahadevan, "Sensitivity-Driven Adaptive Construction of Reducedspace Surrogates," Journal of Scientific Computing 79, pp 1335-1359, doi: 10.1007/s10915-018-0894-4 (2019).
- C. Soize, R.G. Ghanem, C. Safta, X. Huan, Z.P. Vane, J.C. Oefelein, G. Lacaze, and H.N. Najm, "Enhancing Model Predictability for a Scramjet Using Probabilistic Learning on Manifolds," AIAA Journal 57, pp. 365-378, doi: 10.2514/1.J057069 (2019).

#### 2018

- K. Chowdhary, C. Safta, and H.N. Najm, "Enhancing Statistical Moment Calculations for Stochastic Galerkin Solutions with Monte Carlo Techniques," Journal of Computational Physics 374, pp 1017-1030, doi: 10.1016/j.jcp.2018.07.004 (2018).
- X. Huan, C. Safta, K. Sargsyan, Z. Vane, G. Lacaze, J. Oefelein, and H.N. Najm, "Compressive Sensing with Cross-Validation and Stop-Sampling for Sparse Polynomial Chaos Expansions," SIAM/ASA Journal on Uncertainty Quantification 6, pp 907–936, doi: 10.1137/17M1141096 (2018).
- J. Cheng, R.L.-Y. Chen, H.N. Najm, A. Pinar, C. Safta, J.-P. Watson, "Distributionally Robust Optimization with Principal Component Analysis," SIAM Journal on Optimization 28, pp 1817-1841, doi: 10.1137/16M1075910 (2018).
- J. Cheng, R.L.-Y. Chen, H.N. Najm, A. Pinar, C. Safta, J.-P. Watson, "Chance-constrained economic dispatch with renewable energy and storage," Computational Optimization and Applications 70, pp. 479-502, doi: 10.1007/s10589-018-0006-2 (2018).
- X. Huan, C. Safta, K. Sargsyan, G. Geraci, M.S. Eldred, Z. Vane, G. Lacaze, J. Oefelein, and H.N. Najm, "Global Sensitivity Analysis and Estimation of Model Error, Toward Uncertainty Quantification in Scramjet Computations," AIAA Journal 50, pp 1170-1184, doi: 10.2514/1.J056278 (2018).

- D. Lu, D. Ricciuto, A. Walker, C. Safta, W. Munger, "Bayesian calibration of terrestrial ecosystem models: a study of advanced Markov chain Monte Carlo methods," Biogeosciences 14, pp 4295-4314, doi: 10.5194/bg-14-4295-2017 (2017).
- 22. R. Malpica Galassi, M. Valorani, H.N. Najm, **C. Safta**, M. Khalil, P.P. Ciottoli, "*Chemical model reduction under uncertainty*," Combustion and Flame 179, pp 242-252, doi: 10.1016/j.combustflame.2017.02.018 (2017).

- F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O. Le Maître, O. Knio, B. Debusschere, "Exploring the interplay of resilience and energy consumption for a task-based partial differential equations preconditioner," Parallel Computing 73, pp. 16-27, doi: 10.1016/j.parco.2017.05.005 (2017).
- P. Mycek, A. Contreras, O. Le Maître, K. Sargsyan, F. Rizzi, K. Morris, C. Safta, B. Debusschere, O. Knio, "A resilient domain decomposition polynomial chaos solver for uncertain elliptic PDEs," Computer Physics Communications 216, pp 18-34, doi: 10.1016/j.cpc.2017.02.015 (2017).
- P. Mycek, F. Rizzi, O. Le Maître, K. Sargsyan, K. Morris, C. Safta, B. Debusschere, O. Knio, "Discrete A Priori Bounds for the Detection of Corrupted PDE Solutions in Exascale Computations," SIAM Journal on Scientific Computing 39, pp C1-C28, doi: 10.1137/15M1051786 (2017).
- F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O. Le Maître, O. Knio, B. Debusschere, "Partial differential equations preconditioner resilient to soft and hard faults," The International Journal of High Performance Computing Applications 32, pp 658-673, doi: 10.1177/1094342016684975 (2017).

#### 2016

- M. Khalil, K. Chowdhary, C. Safta, K. Sargsyan, H.N. Najm, "Inference of reaction rate parameters based on summary statistics from experiments," Proceedings of the Combustion Institute 36, pp 699-708, doi: 10.1016/j.proci.2016.08.058 (2016).
- C. Safta, R.L.-Y. Chen, H.N. Najm, A. Pinar, J.-P. Watson, "Efficient Uncertainty Quantification in Stochastic Economic Dispatch," IEEE Transactions on Power Systems 32, pp 2535-2546, doi: 10.1109/TPWRS.2016.2615334 (2016).
- C. Safta, M. Blaylock, J.A. Templeton, S.P. Domino, K. Sargsyan, H.N. Najm, "Uncertainty Quantification in LES of Channel Flow", International Journal for Numerical Methods in Fluids 83, pp 376-401, doi: 10.1002/fld.4272 (2016).

#### 2015

- K. Sargsyan, F. Rizzi, P. Mycek, C. Safta, K. Morris, H.N. Najm, O. Le Maître, O. Knio, B. Debusschere, "Fault Resilient Domain Decomposition Preconditioner for PDEs," SIAM Journal on Scientific Computing 37, pp A2317-A2345, doi: 10.1137/15M1014474 (2015).
- C. Safta, D.M. Ricciuto, K. Sargsyan, B. Debusschere, H.N. Najm, M. Williams, and P.E. Thornton, "Global sensitivity analysis, probabilistic calibration, and predictive assessment for the data assimilation linked ecosystem carbon model," Geoscientific Model Development 8, pp 1899-1918, doi: 10.5194/gmd-8-1899-2015 (2015).
- 32. C. Safta, K. Sargsyan, B.J. Debusschere, H.N. Najm, "*Hybrid discrete/continuum algorithms for stochastic reaction networks*," Journal of Computational Physics **181**, pp 177-198, doi: 10.1016/j.jcp.2014.10.026 (2015).

- C. Safta, K. Sargsyan, H.N. Najm, K. Chowdhary, B.J. Debusschere, L. P. Swiler, and M. S. Eldred, "Probabilistic Methods for Sensitivity Analysis and Calibration of Computer Models in the NASA Challenge Problem," AIAA Journal of Aerospace Information Systems 12, pp 219-234, doi: 10.2514/1.1010256 (2014).
- H.N. Najm, R. D. Berry, C. Safta, K. Sargsyan, B.J. Debusschere, "Data-Free Inference of Uncertain Parameters in Chemical Models," International Journal for Uncertainty Quantification 4, pp 111-132, doi: 10.1615/Int.J.UncertaintyQuantification.2013005679 (2014).
- K. Kedia, C. Safta, J. Ray, H.N. Najm, A. F. Ghoniem, "A second-order coupled immersed boundary-SAMR construction for chemically reacting flow over a heat-conducting Cartesian grid-conforming solid," Journal of Computational Physics 272, pp 408-428, doi: 10.1016/j.jcp.2014.04.019 (2014).
- K. Sargsyan, C. Safta, H.N. Najm, B.J. Debusschere, D. Ricciuto, and P. Thornton, "Dimensionality Reduction for Complex Models via Bayesian Compressive Sensing," International Journal for Uncertainty Quantification 4, pp 63-93, doi: 10.1615/Int.J.UncertaintyQuantification.2013006821 (2014).

#### 2013

 J. Prager, H.N. Najm, C. Safta, K. Sargsyan and W. J. Pitz, "Uncertainty quantification of reaction mechanisms accounting for correlations introduced by rate rules and fitted Arrhenius parameters," Combustion and Flame 160, pp 1583-1593, doi: 10.1016/j.combustflame.2013.01.008 (2013).

#### 2012

- K. E. Cheng, D. J. Crary, J. Ray and C. Safta, "Structural models used in real-time biosurveillance outbreak detection and outbreak curve isolation from noisy background morbidity levels," Journal of the American Medical Informatics Association 20, pp 435-440, doi: 10.1136/amiajnl-2012-000945 (2012).
- K. Sargsyan, C. Safta, B.J. Debusschere and H.N. Najm, "Multiparameter Spectral Representation of Noiseinduced Competence in Bacillus Subtilis," IEEE/ACM Transactions on Computational Biology and Bioinformatics 9, pp 1709-1723, doi: 10.1109/TCBB.2012.107 (2012).

#### 2011

 K. Sargsyan, C. Safta, B.J. Debusschere and H.N. Najm, "Uncertainty Quantification given Discontinuous Model Response and a Limited Number of Model Runs," SIAM Journal on Scientific Computing 34, pp B44-B64, doi: 10.1137/100817899 (2011).

#### 2010 and before

- 41. **C. Safta**, J. Ray and H.N. Najm, "A high-order low-Mach AMR construction for chemically reacting flows," Journal of Computational Physics **229**, pp 9299-9322, doi: 10.1016/j.jcp.2010.09.002 (2010).
- 42. N. Bharadwaj, **C. Safta**, and C.K. Madnia, "*Characteristics of Flame Wall Interactions for a Nonpremixed Flame Propelled by a Vortex Ring*," Combustion Theory and Modelling **11**, pp 1-19, doi: 10.1080/13647830600739140 (2007).
- C. Safta and C.K. Madnia, "Autoignition and Structure of Non-Premixed Methane Flames: Detailed and Reduced Kinetic Models," Combustion and Flame 144, pp 64-73, doi: 10.1016/j.combustflame.2005.07.001 (2006).
- 44. **C. Safta** and C.K. Madnia, "*Characteristics of methane diffusion flame in a reacting vortex ring*," Combustion Theory and Modelling **8**, pp 449-474, doi: 10.1088/1364-7830/8/3/002 (2004).
- 45. **C. Safta**, S. Enachescu, and C.K. Madnia, "*Interaction of a vortex ring with a diffusion flame*," Physics of Fluids **14**, pp 668, doi: 10.1063/1.1429248 (2002).

# **Conference Proceedings, Reports, Book Chapters**

- 1. A. Jivani, X. Huan, **C. Safta**, B.Y. Zhou, N.R. Gauger, <u>"</u>Uncertainty Quantification for a Turbulent Round Jet Using Multifidelity Karhunen-Loeve Expansions," *AIAA Scitech 2021 Forum* (2021).
- J.B. Ortiz, K. McCoy, M.J. Grant, M. Sparapany, R. Ghanem, H.N. Najm, C. Safta, "Trajectory Optimization via Unsupervised Probabilistic Learning On Manifolds," *Sandia Technical Report*, SAND2021-11867 (2021).
- 3. O. Diaz-Ibarra, K. Kim, **C. Safta**, H.N. Najm, "CSPlib A Software Toolkit for the Analysis of Dynamical Systems and Chemical Kinetic Models", *Sandia Technical Report*, SAND2021-1212 (2021).
- 4. K. Sargsyan, **C. Safta**, K. Johnston, M. Khalil, K. Chowdhary, P. Rai, T.A. Casey, X. Zeng, B. Debusschere, "UQTk v3.1 User Manual", *Sandia Technical Report*, SAND2020-2879 (2020).
- 5. K. Lee, J. Ray, **C. Safta**, "Predictive Skill of Deep Learning Models Trained on Limited Sequence Data", *Sandia Technical Report*, SAND2020-10958 (2020).
- 6. L. Sheps, Z.J. Buras, K. Au, J. Zador, **C. Safta**, "Rapid Assessment of Autoignition Propensity in Novel Fuels and Blends", *Sandia Technical Report*, SAND2020-10342 (2020).

- T.L. Bauer, W.E. Beyeler, P.D. Finley, R.F. Jeffers, C.D. Laird, M. Makvandi, A.V. Outkin, C. Safta, and K.M. Simonson, "Sandia's Research in Support of COVID-19 Pandemic Response: Computing and Information Sciences", Sandia Technical Report, SAND2020-9261 (2020).
- C. Safta, J. Ray, E. Acquesta, T. Catanach, K. Chowdhary, B. Debusschere, E. Galvan, G. Geraci, M. Khalil, T. Portone, "Characterization of Partially Observed Epidemics - Application to COVID-19", Sandia Technical Report, SAND2020-6563 (2020).
- 9. M. Khalil, J. Lao, **C. Safta**, H.N. Najm, "Transitional Markov Chain Monte Carlo Sampler in UQTk", *Sandia Technical Report*, SAND2020-3166 (2020).
- 10. C. Safta, R. Bambha, H. Michelsen, "Estimating Regional Methane Emissions Through Atmospheric Measurements and Inverse Modeling," Sandia Technical Report, SAND2019-11190 (2019).
- C. Safta, H.N. Najm, "EGSim a C++ Toolkit for Analysis of Power Grid Systems," Sandia Technical Report, SAND2019-4485 (2019).
- M. Salloum, C. Safta, E. Galvan, A.M. Smith, A.C. Brownlow, C. Lam, "Quantification of Uncertainty due to Random Insults in a Transmission Line with Digital Signal Inputs," Sandia Technical Report, SAND2019-7485 (2019).
- X. Huan, C. Safta, Z.P. Vane, G. Lacaze, J.C. Oefelein, H.N. Najm, "Uncertainty Propagation Using Conditional Random Fields in Large-Eddy Simulations of Scramjet Computations," AIAA Scitech 2019 Forum, AIAA Paper 2019-0724, doi: 10.2514/6.2019-0724 (2019).
- G. Geraci, F. Menhorn, X. Huan, C. Safta, Y. Marzouk, H.N. Najm, M.S. Eldred, "Progress in Scramjet Design Optimization Under Uncertainty Using Simulations of the HIFiRE Configuration," AIAA Scitech 2019 Forum, AIAA Paper 2019-0725, doi: 10.2514/6.2019-0725 (2019).
- X. Huan, G. Geraci, C. Safta, M.S. Eldred, K. Sargsyan, Z.P. Vane, J.C. Oefelein, H.N. Najm, "Multifidelity Statistical Analysis of Large Eddy Simulations in Scramjet Computations," AIAA Scitech 2018 Forum, AIAA Paper 2018-1180, doi: 10.2514/6.2018-1180 (2018).
- X. Huan, C. Safta, K. Sargsyan, G. Geraci, M.S. Eldred, Z. Vane, G. Lacaze, J.C. Oefelein, H.N. Najm, "Global Sensitivity Analysis and Quantification of Model Error for Large Eddy Simulation in Scramjet Design," 19th AIAA Non-Deterministic Approaches Conference, AIAA Paper 2017-1089, doi: 10.2514/6.2017-1089 (2017).
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- 22. **C. Safta**, H.N. Najm, B.J. Debusschere, and R.D. Berry, "*EGSim a C++ toolkit for analysis of power grid systems*," Sandia Technical Report, SAND2013-2838 (2013).
- 23. G. Backus et al, "*Risk Assessment of Climate Systems for National Security*," Sandia Technical Report, SAND2012-10554 (2012).
- 24. **C. Safta**, J. Ray, K. Sargsyan, S. Lefantzi, K. Cheng, and D. Crary, "*Real-time characterization of partially observed epidemics using surrogate models*," Sandia Technical Report, SAND2011-6766 (2011).
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- K. Sargsyan, C. Safta, B.J. Debusschere, and H.N. Najm, "Uncertainty Quantification in the Presence of Limited Climate Model Data with Discontinuities," IEEE International Conference on Data Mining, pp 241-247, doi: 10.1109/ICDMW.2009.111 (2009).
- H.N. Najm, J. Ray, C. Safta, Y. Marzouk, M. Valorani, and D. Goussis, "High-order AMR computations of reacting flow with adaptive reduction of chemical stiffness," Journal of Physics: Conference Series 125, doi: 10.1088/1742-6596/125/1/012032 (2007).
- H.N. Najm, J. Ortega, C. Safta, M. Valorani, D. Goussis, and M. Frenklach, "Adaptive Explicit Integration of Stiff Chemical Systems," International Workshop on Model Reduction in Reacting Flow, SAND2007-5546C (2007).
- C. Safta, F. Ladeinde, X. Cai, and K. Alabi, "A Combined Level-Set/Mixture Fraction/Progress-Variable Approach for Partially-Premixed Turbulent Reacting Flows," 45th AIAA Aerospace Sciences Meeting and Exhibit, AIAA Paper 2007-1436, doi: 10.2514/6.2007-1436 (2007).
- C. Safta, F. Ladeinde, X. Cai, and K. Alabi, "A High-Fidelity Level-Set Approach for Predicting Turbulent Reacting Flows," 42nd AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, AIAA Paper 2006-5090, doi: 10.2514/6.2006-5090 (2006).
- C. Safta, K. Alabi, and F. Ladeinde, "Comparative advantages of high-order schemes for subsonic, transonic, and supersonic flows," 44th AIAA Aerospace Sciences Meeting and Exhibit, AIAA Paper 2006-299, doi: 10.2514/6.2006-299 (2006).
- C. Safta, K. Alabi, F. Ladeinde, X. Cai, B. Sekar, and B. Kiel, "Level-Set/Large-Eddy Simulation of a Premixed Augmentor Flame Holder," 44th AIAA Aerospace Sciences Meeting and Exhibit, AIAA Paper 2006-156, doi: 10.2514/6.2006-156 (2006).
- F. Ladeinde, K. Alabi, C. Safta, and X. Cai, "The First High-Order CFD Simulation of Aircraft: Challenges and Opportunities," 44th AIAA Aerospace Sciences Meeting and Exhibit, AIAA Paper 2006-1526, doi: 10.2514/6.2006-1526 (2006).
- 35. **C. Safta** and C.K. Madnia, "*Finite Rate Chemistry Effects in Non-Premixed CH4/H2 Flames*," 42nd AIAA Aerospace Sciences Meeting and Exhibit, AIAA Paper 2004-798, doi: 10.2514/6.2004-798 (2004).
- 36. **C. Safta** and C. K. Madnia, "Unsteady Non-Premixed CH4/H2 Flame Structure: Detailed and Reduced Kinetic Models," Proceedings of the Third Joint Meeting of the U.S. Sections of The Combustion Institute (2003).

# Presentations & Posters (since joining Sandia)

- 1. "Hit twice by the curse of dimensionality: spatio-temporal land model calibration using Karhunen-Loève and sparse polynomial chaos expansions," *American Geophysical Union Fall Meeting*, New Orleans, LA, Dec 2021.
- 2. "Functional Tensor Network Approximations for E3SM Land Model," *American Geophysical Union Fall Meeting*, New Orleans, LA, Dec 2021.
- 3. "Multifidelity Karhunen-Loeve Expansions for Uncertainty Propagation of Random Field Quantities," *SIAM Computational Science and Engineering*, Mar 2021.
- 4. "Polynomial Chaos Expansions for Discrete Random Variables in Cyber Security Emulytics Experiments," *SIAM Computational Science and Engineering*, Mar 2021.
- 5. "Manifold-Based Optimization for Constrained Trajectories," *SIAM Computational Science and Engineering*, Mar 2021.
- 6. "Dimensionality Reduction and Physics-Informed Neural Networks for Climate Land Models," *SIAM Computational Science and Engineering*, Mar 2021.

7. "Low-Rank Tensor Network Approximations for Earth System Models," SIAM Computational Science and Engineering, Mar 2021.

#### 2020 (1 invited)

- 8. "Low-rank tensor network approximations for Earth System Models," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2020.
- 9. "Dimensionality Reduction and Physics-Informed Recurrent Neural Networks for Climate Land Models", *American Geophysical Union Fall Meeting*, S an Francisco, CA, Dec 2020.
- 10. (invited) "Characterization of Partially Observed Epidemics," *Workshop on Modeling and Simulation of Infectious Diseases*, Berkeley, Aug 2020.

#### 2019 (3 invited)

- 11. "Physics-informed Recurrent Neural Network Surrogates for E3SM Land Model," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2019.
- 12. "Uncertainty Quantification for E3SM Land Component using Low-Rank Surrogate Models," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2019.
- 13. "Calibration and Propagation of Model Structural Error for E3SM Land Model," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2019.
- 14. (invited) "Uncertainty Quantification and Machine Learning Algorithms for Physical Models: Tackling Computational Expense and High-Dimensionality," *Scientific Computing and Data Science Seminar, University of California, Merced*, CA, Oct 2019.
- 15. "Uncertainty Quantification in Computational Models of Large-Scale Physical Systems," *15th U.S. National Congress on Computational Mechanics*, Austin, TX, July 2019.
- 16. "Bayesian Estimation of Random Field Biases in Pollutant Emissions Using Multiscale Data," 15th U.S. National Congress on Computational Mechanics, Austin, TX, July 2019.
- 17. "Physics-Informed Recurrent Neural Networks for Land Model Surrogate Construction," *Workshop on Research Challenges and Opportunities at the Interface of Machine Learning and Uncertainty Quantification*, University of Southern California, Los Angeles, CA, July 2019.
- 18. (invited) "Exploiting Spatio-Temporal Structure for Forward Propagation of Uncertainty in Large Scale Models," *International Congress on Industrial and Applied Mathematics*, Valencia, Spain, July 2019.
- 19. "Uncertainty Quantification in Large Scale Computational Models," *International Congress on Industrial and Applied Mathematics*, Valencia, Spain, July 2019.
- 20. "Surrogate-enabled sensitivity analysis and parameter inference of high-dimensional models," *International Congress on Industrial and Applied Mathematics*, Valencia, Spain, July 2019.
- 21. "Exploiting Model Structure for Forward Propagation of Uncertainty in Earth System Models," 3rd International Conference on Uncertainty Quantification in Computational Sciences and Engineering, Crete, Greece, June 2019.
- 22. "Modeling Computationally Intensive E3SM-ELM Components using Hierarchical Recurrent Neural Networks," Workshop on Machine Learning in Solid Earth Geoscience, Santa Fe, NM, Mar 2019.
- 23. "Exploiting Low-rank Structure for Sensitivity Analysis in Earth System Model," *SIAM Computational Science and Engineering*, Spokane, WA, Mar 2019.
- 24. "Global Sensitivity Analysis for Multilevel Scramjet Computations," *SIAM Computational Science and Engineering*, Spokane, WA, Mar 2019.
- 25. "UQTk, a FASTMath C++/Python Toolkit for Uncertainty Quantification: Overview and Applications," *SIAM Computational Science and Engineering*, Spokane, WA, Mar 2019.
- 26. (invited) "Workflows for Quantifying Uncertainty in Computational Model Predictions," *The Department of Electrical & Computer Engineering Speaker Series, University of Houston*, Houston, TX, Feb 2019.
- 27. "Uncertainty Propagation Using Conditional Random Fields in Large-Eddy Simulations of Scramjet Computations," *AIAA SciTech*, San Diego, CA, Jan 2019.

28. "Progress in Scramjet Design Optimization Under Uncertainty Using Simulations of the HIFiRE Direct Connect Rig," AIAA SciTech, San Diego, CA, Jan 2019.

### 2018

- 29. "Bayesian Framework for Structural Uncertainty Estimation of Land Models," *American Geophysical Union Fall Meeting*, Washington DC, Dec 2018.
- 30. "Estimating Biases for Regional Methane Fluxes Using Spatially/Temporally Varying Random-Field Representations of Biases," *American Geophysical Union Fall Meeting*, Washington DC, Dec 2018.
- 31. "Exploiting Model Structure for Global Sensitivity Analysis in E3SM Land Model," *American Geophysical Union Fall Meeting*, Washington DC, Dec 2018.
- 32. "Designing observation networks using Earth System Models to reduce uncertainty in regional carbon fluxes," *American Geophysical Union Fall Meeting*, Washington DC, Dec 2018.
- 33. "Bayesian Estimation of Pollutant Emissions Using Multiscale Data," *Joint Statistical Meetings*, Vancouver, British Columbia, Canada, July 2018.
- 34. "Adaptive Sparse Quadrature for Multifidelity Scramjet Flow Simulations," *SIAM Annual Meeting*, Portland, OR, July 2018.
- 35. "Bayesian Inference for Model Error Quantification and Propagation with UQTk," *SIAM Annual Meeting*, Portland, OR, July 2018.
- 36. "Bayesian Estimation of Spatio-Temporal Parameters for Atmospheric Transport Models," *International Society for Bayesian Analysis World Meeting*, Edinburgh, UK, June 2018.
- 37. "Machine Learning Techniques for Global Sensitivity Analysis in Earth System Models," 6th European Seminar on Computing, Pilsen, Czechia, June 2018.
- "Sparse Multifidelity Approximations for Forward UQ with Application to Scramjet Combustor Computations," SIAM Conference on Uncertainty Quantification, Garden Grove, CA, Apr 2018.
- 39. "Compressive Sensing with Cross-validation and Stop-sampling for Sparse Polynomial Chaos Expansions," *SIAM Conference on Uncertainty Quantification*, Garden Grove, CA, Apr 2018.
- 40. "A Flexible Python/C++ Toolkit for Uncertainty Quantification," *SIAM Conference on Uncertainty Quantification*, Garden Grove, CA, Apr 2018.
- 41. "Multifidelity Statistical Analysis of Large Eddy Simulations in Scramjet Computation," *AIAA SciTech*, Kissimmee, FL, Jan 2018.

- 42. "Embedded Model Error Representation and Propagation in Climate Models," *American Geophysical Union Fall Meeting*, New Orleans, LA, Dec 2017.
- 43. "Machine Learning Techniques for Global Sensitivity Analysis in Climate Models," *American Geophysical Union Fall Meeting*, New Orleans, LA, Dec 2017.
- 44. "Estimating Biases for Regional Methane Fluxes using Co-emitted Tracers," *American Geophysical Union Fall Meeting*, New Orleans, LA, Dec 2017.
- 45. "A Bayesian Framework for the Estimation of Regional Methane Fluxes," *14th U.S. National Congress on Computational Mechanics*, Montreal, Canada, July 2017.
- 46. "A Resilient Solver for 2D Uncertain Elliptic PDEs Via Fault-Tolerant MPI Server-Client-Based Implementation," *SIAM Computational Science and Engineering*, Atlanta, GA, Feb 2017.
- 47. "Partial Differential Equations Solver Resilient to Soft and Hard Faults," *SIAM Computational Science and Engineering*, Atlanta, GA, Feb 2017.
- 48. "Acceleration of Monte Carlo Methods for Stochastic Elliptic PDEs Using Domain Decomposition and PC Approximations of Local Dirichlet Maps," *SIAM Computational Science and Engineering*, Atlanta, GA, Feb 2017.
- 49. "Robust Compressive Sensing with Application to Multifidelity Analysis of Complex Turbulent Flows," *SIAM Computational Science and Engineering*, Atlanta, GA, Feb 2017.

- 50. "Intrusive UQ Algorithms for Emerging Computing Platforms," *SIAM Computational Science and Engineering*, Atlanta, GA, Feb 2017.
- 51. "Global Sensitivity Analysis and Quantification of Model Error for Large Eddy Simulation in Scramjet Design," *19th AIAA Non-Deterministic Approaches Conference*, Grapevine, TX, Jan 2017.

# 2016 (1 invited)

- 52. "Weighted Iterative Bayesian Compressive Sensing (WIBCS) for High Dimensional Polynomial Surrogate Construction," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2016.
- 53. "Global Sensitivity Analysis for Large Eddy Simulation Models," SIAM Annual Meeting, Boston, MA, July 2016.
- 54. (invited) "A Sparse Quadrature Approach for Stochastic Optimization in Power Grid Models," XIV International Conference on Stochastic Programming, Buzios, Brazil, June 2016.
- 55. "Distributionally Robust Optimization with Principal Component Analysis," XIV International Conference on Stochastic Programming, Buzios, Brazil, June 2016.
- 56. "Bayesian Estimation of Thermal Conductivity Parameters for a Polyurethane Foam," *ASME Verification and Validation Symposium*, Las Vegas, NV, May 2016.
- 57. "A soft and hard faults resilient solver for 2D elliptic PDEs via server-client-based implementation," *SIAM Parallel Processing*, Paris, France, April 2016.
- 58. "A Resilient Domain Decomposition Approach for Extreme Scale UQ Computations," *SIAM Parallel Processing*, Paris, France, April 2016.
- 59. "Quantifying Performance of a Resilient Elliptic PDE Solver on Uncertain Architectures Using SST/macro," *SIAM Parallel Processing*, Paris, France, April 2016.
- 60. "A soft and hard faults resilient solver for 2D uncertain elliptic PDEs via fault-tolerant MPI server-client-based implementation," *SIAM Uncertainty Quantification*, Lausanne, Switzerland, April 2016.
- 61. "A Hybrid Approach to Tackle Resiliency in Extreme Scale Computations Using a Domain Decom- position Solver for Uncertain Elliptic PDEs," *SIAM Uncertainty Quantification*, Lausanne, Switzerland, April 2016.
- 62. "UQTk: a C++/Python Toolkit for Uncertainty Quantification," *SIAM Uncertainty Quantification*, Lausanne, Switzerland, April 2016.
- 63. "Implementation of UQ workflows with the C++/Python UQTk toolkit," *SIAM Uncertainty Quantification*, Lausanne, Switzerland, April 2016.
- 64. "Probabilistic Inference of Model Parameters and Missing High-Dimensional Data Based on Summary Statistics," *SIAM Uncertainty Quantification*, Lausanne, Switzerland, April 2016.
- 65. "Reduction of Chemical Models under Uncertainty," *SIAM Uncertainty Quantification*, Lausanne, Switzerland, April 2016.
- 66. "Adaptive Sparse Quadrature for Stochastic Optimization," *SIAM Uncertainty Quantification*, Lausanne, Switzerland, April 2016.
- 67. "Surrogate-based Approach for Optimization Problems under Uncertainty," *SIAM Uncertainty Quantification*, Lausanne, Switzerland, April 2016.

- 68. "Sparse Polynomial Chaos Surrogate for ACME Land Model via Iterative Bayesian Compressive Sensing," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2015.
- 69. "PDE Preconditioner Resilient to Soft and Hard Faults," SuperComputing 2015, Austin, TX, Nov 2015.
- 70. "Partial Differential Equations Preconditioner Resilient to Soft and Hard Faults," *FTS 2015, First International Workshop on Fault Tolerant Systems, IEEE Cluster 2015,*, Chicago, IL, Sep 2015.
- 71. "An Efficient Approach for Stochastic Optimization of Electricity Grid Operations," 13th U.S. National Congress on Computational Mechanics, San Diego, CA, July 2015.
- 72. "Calibration and Forward Uncertainty Propagation of Turbulence Models for Coarse-Grid Large Eddy Simulation," *13th U.S. National Congress on Computational Mechanics*, San Diego, CA, July 2015.
- 73. "Sparse Surrogate Construction Via Bayesian Compressive Sensing," *International Conference on Uncertainty Quantification in Computational Sciences and Engineering*, Crete, Greece, May 2015.

- 74. "Bayesian Compressive Sensing Framework for High-Dimensional Surrogate Construction," *SIAM Computational Science and Engineering*, Salt Lake City, UT, March 2015.
- 75. "An Efficient Approach for Stochastic Optimization of Electricity Grid Operations," *SIAM Computational Science and Engineering*, Salt Lake City, UT, March 2015.
- 76. "Two-Stage Adaptive Robust Unit Commitment Using Scenarios Induced Uncertainty Set," *SIAM Computational Science and Engineering*, Salt Lake City, UT, March 2015.
- 77. "Spatial Decomposition for Resilient Extreme-Scale Scientific Simulations," *SIAM Computational Science and Engineering*, Salt Lake City, UT, March 2015.
- 78. "Model Calibration and Error Propagation for Large-Eddy Simulation of Turbulent Flows," *SIAM Computational Science and Engineering*, Salt Lake City, UT, March 2015.

# 2014

- 79. "Parameter Estimation in High-Dimensional Climate Models," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2014.
- 80. "Toward Using Surrogates to Accelerate Solution of Stochastic Electricity Grid Operations Problems," *North-American Power Symposium*, Pullman, WA, Sep 2014.
- 81. "Sandia Software Enabling Extreme-Scale Uncertainty Quantification," *DOE SciDAC Meeting*, Washington DC, July 2014.
- 82. "An Overview of Select UQ Algorithms and their Utility in Applications," *DOE SciDAC Meeting*, Washington DC, July 2014.
- 83. "Probabilistic methods for power grid networks," SIAM Annual Meeting, Chicago, IL, July 2014
- 84. "Towards a Probabilistic Approach to Extreme-Scale Simulations under Uncertainty and System Faults," *SIAM Annual Meeting*, Chicago, IL, July 2014.
- 85. "Bayesian Compressive Sensing Framework for High-Dimensional Surrogate Model Construction," International Conference on Spectral and Higher Order Methods, Salt Lake City, UT, June 2014.
- 86. "Rigorous LES Assessment for Predictive Simulations," *Predictive Engineering Science Panel Review*, Sandia National Labs, Livermore, CA, April 2014.
- 87. "Probabilistic Approaches for Fault-Tolerance and Scalability in Extreme-Scale Computing," *SIAM Uncertainty Quantification*, Savannah, GA, Mar 2014.
- 88. "Bayesian Discontinuity Detection and Surrogate Construction for Complex Computer Models," *SIAM Uncertainty Quantification*, Savannah, GA, Mar 2014.
- 89. "Bayesian Compressive Sensing Framework for Sparse Representations of High-Dimensional Models," *SIAM Uncertainty Quantification*, Savannah, GA, Mar 2014.
- 90. "Low-rank and sparse representation methods for uncertainty quantification," *SIAM Uncertainty Quantification*, Savannah, GA, Mar 2014.
- 91. "Probabilistic Approaches for Fault-Tolerance and Scalability in Extreme-Scale Computing," SIAM Conference on Parallel Processing for Scientific Computing, Portland, OR, Feb 2014.
- 92. "Uncertainty Quantification Methods for Model Calibration, Validation, and Risk Analysis," *AIAA Science and Technology Forum and Exposition*, National Harbor, MD, Jan 2014.

# 2013 (2 invited)

- 93. "Inference of Chemical Model Parameters given Partial Information," *33rd International Workshop on Bayesian Inference and Maximum Entropy Methods in Science and Engineering*, Canberra, Australia, Dec 2013.
- 94. "Global Sensitivity Analysis and Parameter Calibration for an Ecosystem Carbon Mode," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2013.
- 95. "Probabilistic Approaches for Communication Avoidance and Resilience in Exascale Simulations," *ExaMath13 Workshop*, Washington, DC, August 2013.
- 96. "Hybrid Discrete-Continuum Algorithms for Stochastic Reaction Networks," *DOE ASCR PI meeting*, Albuquerque, NM, Aug 2013.

- 97. "Probabilistic Schwarz Preconditioner for Fault Tolerance and Scalability," *DOE ASCR PI meeting*, Albuquerque, NM, Aug 2013.
- 98. "Algorithms for Sparse and Missing Data," DOE SciDAC Meeting, Washington DC, July 2013.
- 99. "Sandia Software Enabling Extreme-Scale Uncertainty Quantification," *DOE SciDAC Meeting*, Washington DC, July 2013.
- 100. "Surrogate Construction and Dimensionality Reduction via Bayesian Compressive Sensing," *12th US National Congress on Computational Mechanics*, Raleigh, NC, July 2013.
- 101. "Data Free Inference in Computational Models," SIAM Annual Meeting, San Diego, CA, July 2013.
- 102. "Sparse surrogate model construction via compressive sensing for high-dimensional complex models," *SIAM Annual Meeting*, San Diego, CA, July 2013.
- 103. "DALEC calibration with daily NEE Data at Harvard Forest," *DOE BER PI Meeting*, Washington, DC, May 2013.
- 104. "Parameter Estimation with Partial Information," *Workshop on Numerical Methods for Uncertainty Quantification*, Bonn, Germany, May 2013.
- 105. "Probabilistic Schwarz Coupling for Fault-Tolerance and Scalability," *SIAM Computational Science and Engineering*, Boston, MA, Feb 2013.
- 106. "Hybrid Discrete/Continuum Algorithms for Stochastic Reaction Networks," *SIAM Computational Science and Engineering*, Boston, MA, Feb 2013.
- 107. "High-dimensional Polynomial Chaos Basis Selection with Bayesian Compressive Sensing," *SIAM Computational Science and Engineering Meeting*, Boston, MA, Feb 2013.
- 108. (invited) "Surrogate construction via Bayesian compressive sensing for the Community Land Model," *Winter CESM Uncertainty Quantification and Analysis Interest Group Meeting*, Boulder, CO, Feb 2013.
- 109. (invited) "Dimensionality Reduction and Global Sensitivity Analysis for the Community Land Model," *Winter CESM Uncertainty Quantification and Analysis Interest Group Meeting*, Boulder, CO, Feb 2013.

#### 2012 (2 invited)

- 110. "Surrogate-Based Uncertainty Quantification in Climate Models in the Presence of High Dimensional, Dependent Inputs and Multimodal Outputs," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2012.
- 111. "Uncertainty analysis and Bayesian Inference of emissions and transport from urban areas," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2012.
- 112. (invited) "Algorithmic Developments for UQ in Extreme Scale Simulations," *SciDAC 3 PI meeting*, Rockville, MD, Sep 2012.
- 113. "Sparse Polynomial Representations of High Dimensional Models," *10th World Congress on Computational Mechanics*, Sao Paulo, Brazil, Jul 2012.
- 114. **(invited)** "Uncertainty Quantification in Community Land Model," *CESM Annual Workshop*, Breckenridge, CO, Jun 2012.
- 115. "Coupled Chemical Master Equation Fokker Planck solver for stochastic reaction networks," *SIAM Uncertainty Quantification*, Raleigh, NC, Apr 2012.
- 116. "Efficient Surrogate Construction for High-Dimensional Climate Models," *SIAM Uncertainty Quantification*, Raleigh, NC, Apr 2012.
- 117. "Adaptive Basis Selection and Dimensionality Reduction with Bayesian Compressive Sensing," *SIAM Uncertainty Quantification*, Raleigh, NC, Apr 2012.
- 118. "An Overview of Uncertainty Quantification in the Community Land Model," *SIAM Uncertainty Quantification*, Raleigh, NC, Apr 2012.

#### 2011

119. "Efficient Source Inversion Methodologies using Regional Transport Models," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2011.

- 120. "Uncertainty Quantification in Climate Modeling," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2011.
- 121. "Bayesian Quantification of Uncertainty in Systems with Intrinsic Noise," ASCR Applied Math PI Meeting, Washington, DC, Oct 2011.
- 122. "A high-order AMR algorithm for chemically reacting flows," 23rd ICDERS Conference, UC Irvine, July 2011.
- 123. "Dynamic casualty estimation from biosurveillance data," 79th Military Operations Research Society Symposium, NPS, Montetrey, CA.
- 124. "High-order AMR Computations of Chemically Reacting Flow," 7th US National Combustion Meeting, Atlanta, GA, March 2011.
- 125. "Uncertainty Quantification given Discontinuities, Long-tailed Distributions, and Computationally Intensive Models," *SIAM Computational Science and Engineering*, Reno, NV, March 2011.
- 126. "Uncertainty Quantification given Discontinuities, Long-tailed Distributions, and Computationally Intensive Models," *SIAM Computational Science and Engineering*, Reno, NV, Feb 2011.

#### 2010 and before

- 127. "Uncertainty Quantification given Discontinuous Climate Model Response and a Limited Number of Model Runs," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2010.
- 128. "Advanced Methods for Uncertainty Quantification in Tail Regions of Climate Model Predictions," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2010.
- 129. "Characterization of Communicable Disease Epidemics Using Bayesian Inversion," *International Society for Disease Surveillance 9th Annual Conference*, Park City, UT, Dec 2010.
- 130. "Accuracy of Tail Regions in Uncertain Climate Model Predictions," *SIAM Annual Meeting*, Pittsburgh, PA, Jul 2010.
- 131. "Uncertainty Quantification Methodologies for Climate Model Data with Discontinuities," *SIAM Annual Meeting*, Pittsburgh, PA, Jul 2010.
- 132. "Bayesian Methods for Discontinuity Detection in Climate Model Data," *ISBA 2010 World Meeting on Bayesian Statistics*, Benidorm, Spain, June 2010.
- 133. "Bayesian Classification of Partially Observed Outbreaks Using Time-series Data," *ISBA 2010 World Meeting on Bayesian Statistics*, Benidorm, Spain, June 2010.
- 134. "Uncertainty quantification in the presence of limited climate model data with discontinuities," *American Geophysical Union Fall Meeting*, San Francisco, CA, Dec 2009.
- 135. "Uncertainty quantification in the presence of limited climate model data with discontinuities," 2009 IEEE International Conference on Data Mining, Miami, FI, Dec 2009.
- 136. "Statistical methods for classification of partially observed outbreaks," *International Society for Disease Surveillance 8th Annual Conference*, Miami, FL, Dec 2009.
- 137. "Anomaly detection techniques for biosurveillance application," *International Society for Disease Surveillance 8th Annual Conference*, Miami, FL, Dec 2009.
- 138. "A high-order projection scheme for AMR computations of chemically reacting flows," 2009 Fall Meeting of the Western States Section of the Combustion Institute, Irvine, CA, October 2009.
- 139. "A High-Order Projection Scheme for AMR Computations of Chemically Reacting Flows," SIAM Conference on Computational Science and Engineering, Miami, FL, March 2009.
- 140. "Performance of a High-order Projection Scheme for AMR Computations of Chemically Reacting Flows," *SIAM 12th International Conference on Numerical Combustion*, Monterey, CA, March 2008.
- 141. "High-Order Computations of Reacting Flow with Adaptive Reduction of Chemical Stiffness," *Journal of Physics: Conference Series*, 2007.
- 142. "Adaptive Explicit Integration of Stiff Chemical Systems," *International Workshop on Model Reduction in Reacting Flow*, Rome, Italy, 2007.