Khachik Sargsyan

CONTACT INFORMATION

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INTRO

Computational scientist with a background in applied mathematics and over 20 years of experience in uncertainty quantification, machine learning, statistical analysis, reduced order modeling and numerical methods, applied to complex computational models in a range of disciplines including climate science, statistical physics, materials science, fluid dynamics.

EDUCATION

University of Michigan, Ann Arbor, MI, USA

- GPA: 4.05/4.00,
- Thesis: "Mean First Passage Times in the Near-Continuum Limit of Birth-Death Processes",
- Ph.D., Applied and Interdisciplinary Mathematics, August, 2007.

Moscow Institute of Physics and Technology, Moscow, Russian Federation

- GPA: 4.86/5.00,
- B.S., Applied Physics and Mathematics, June, 2001.

PROFESSIONAL EXPERIENCE

Sandia National Laboratories, Livermore, CA, USA

Member or lead of research projects on uncertainty quantification and machine learning applied to computational models of complex physical phenomena.

- *Principal Member of Technical Staff* **2015 - present**
- *Senior Member of Technical Staff* **2010 - 2015**
- *Postdoctoral Fellow* **2007 - 2010**

University of Michigan, Ann Arbor, MI, USA

- *Graduate Student Research Assistant* **2003 - 2006**
  Supported by NSF and Michigan Center for Theoretical Physics. Member of the 3-year NSF research project group "Fronts, Fluctuations and Growth".

Moscow Institute of Physics and Technology, Moscow, Russian Federation

- *Research Assistant* **1999 - 2002**
  Institute for Computer Aided Design of RAS and Institute for System Programming of RAS.

SUMMARY

- Over 70 publications in peer-reviewed journals,
- Over 100 research presentations in academic conferences and workshops,
- Estimated ∼500K lines of scientific programming in Python, C/C++, Matlab, Mathematica,
- Key or lead developer in 4 open-source software products,
- Mentoring over 25 graduate students, postdoctoral fellows and early career researchers,
- Teaching and tutoring of a wide range of undergraduate/graduate level math and engineering classes,
- Bronze medal at the International Math Olympiad in 1997,
- Fluent in English, Russian, Armenian. Reading knowledge of French.

Research Projects

Principal Investigator

- SNL LDRD, Analysis of Neural Networks as Random Dynamical Systems, 2020-2023:
  Developed state-of-the-art methods for improved training and generalization of neural networks. Demonstrated impact on materials science and climate modeling applications.

Co-PI

- DOE ASCR, Uncertainty of Physics-Aware Neural Networks, 2023-2024:
  Exploratory analysis of visualization and uncertainty estimation of neural networks.

- DOE BER, Land Model UQ lead for Energy Exascale Earth System Model, 2018-2025: `e3sm.org`.
  Developed and deployed automated surrogate modeling and calibration tools for a range of E3SM-based studies, including carbon release, crop modeling, vegetation growth, quasi-biennial oscillation.

- DOE BER-ASCR SciDAC, Sensor Networks for Climate Model Predictions, 2018-2020:
  Implemented physics-driven machine learning methods for land model surrogate construction and global sensitivity analysis.

- DOE FES SciDAC, Adaptive Quadrature Methods for Fast Evaluation of MP2 Integrals, 2014-2017:
  Developed and deployed low-rank integration methods for potential energy integration problems.

Contributor

- DOE BER SciDAC, Quasi-biennial oscillation through surrogate-accelerated parameter optimization, 2022-2026: `jjbenedict.github.io/scidac-qbo-e3sm`
  Construction of surrogate models to help parameter calibration for quasi-biennal oscillation.

- DOE FES SciDAC, Integrated Thermomechanical Model of First Wall Components During Fusion Reactor Operation, 2023-2027: `thermchem-fw.github.io`
  Uncertainty quantification and proagation between components.

- DOE BES, Exascale Catalytic Chemistry, 2017-2025: `ecc-project.org`
  Leading of UQ and ML components. Developed state-of-the-art methods for combining parametric and intrinsic uncertainties for Kinetic Monte-Carlo models. Developed a new machine learning method, minima-preserving neural network, to approximate potential energies in catalytic systems.

- DOE ASCR SciDAC, FASTMath Institute, 2017-2024: `fastmath-scidac.llnl.gov`
  Developed state-of-the art methods for model error estimation in physical models. The work has been applied across a range of applications.

- DOE FES-ASCR Fusion Materials and ML, 2020-2024:
  Developed and deployed methods and software for augmenting machine-learned potential energy approximations with uncertainty quantification.

- DOE FES-ASCR SciDAC, Plasma Surface Interactions, 2017-2023:
  Developed UQ methods for global impurity transport models.

- DOE NE-ASCR SciDAC, Simulation of Fission Gas in Uranium Oxide Nuclear Fuel, 2017-2023:
  Development of UQ methods for surrogate construction and global sensitivity analysis.

- NNSA ASC, Artificial Machine Intelligence, 2020-2021:
  Developed methods for classification of time series for aging detection.

- SNL LDRD, Sandia Forecast Model for the COVID-19 Epidemic, 2020-2021:
  Advised on development of calibration methods. SNL forecasts are now used in NM Department of Health to assess the epidemic trends and plan for health resource allocation.

- SNL LDRD, Subsystem Reduced-Order Modeling and Network UQ, 2017-2019:
  Developed network uncertainty quantification strategies for multi-component systems.

- DOD DARPA, UQ in LES Computations of Turbulent Combustion in SCRAMJET, 2016-2018:
  Developed and deployed embedded model error estimation techniques.

- DOE ASCR SciDAC, Quantification of Uncertainty in Extreme Scale Computations, 2011-2017:
  UQ method development and deployment for large scale applications.

- SNL ASC, Stochastic Simulation Toolkit, 2011–2016:
  UQ method development for SST targeting discrete event simulations.

- DOE ASCR, Probabilistic Approach for Extreme-Scale Simulations under System Faults, 2012-2015:
  Developed probabilsitic coupling algorithms for domain-decomposition methods.

- DOE BER, Climate Science for a Sustainable Energy Future, 2011-2014:
  Deployed UQ methods for climate models targeting phase transitions and extreme events.

- SNL LDRD, Regional inversion for Green House Gas Sources, 2011-2014:
  Developed inverse modeling techniques for GHG source inference.

- DOE ASCR, Uncertainty Quantification in Multiscale Modeling, 2009–2012:
  Advisory role - UQ method development for multiscale stochastic systems.

- SNL LDRD, Uncertainty Quantification in Climate Modeling, 2009–2010:
  UQ method development targeting tail event probabilities.

- DOE ASCR, Uncertainty Quantification in Stochastic Dynamical Systems, 2007-2010:
  Developed and deployed domain-decomposition UQ methods for stochastic models.

Professional Activities

- Maintaining active direct collaborations with *Brown U, Northeastern U, Emory U, U of Michigan, USC, UCLA, NOAA, LANL, ANL, ORNL, LBNL, PNNL LLNL.*
- Editorial Board:
  - Journal of Discrete & Continuous Dynamical Systems – S (DCDS-S)
  - Journal of Machine Learning for Modeling and Computing (JMLMC).
- Professional memberships:
  - Society of Industrial and Applied Mathematics (SIAM),
  - American Geophysical Union (AGU),
  - International Society of Bayesian Analysis (ISBA),
  - American Statistical Association (ASA).
- Organized sessions at recognized national and international conferences with over 100 speakers total:
  - SIAM UQ
  - SIAM AN
  - ISBA
  - SIAM CSE
  - AGU
  - USNCCM

- Co-organized Bay Area Scientific Computing Day Workshop, 2018.
- Led a SIAM CSE 2023 Affinity Group on Scientific Machine Learning.
- Invited participation in the US-Norway bilateral AI forum, 2022.
- Invited co-chair at the series of workshops on Artificial Intelligence for Earth System Processes, AI4ESP (`ai4esp.org`): Neural Networks and Surrogate Modeling, 2021.
- Co-chair of Foreign National Networking Group (FNNG) at Sandia, 2020-present.
- Participated or lead over 50 interview panels since 2020. Active participation in WDTS and SULI student intern hiring programs.
- Invited judge for Outstanding Student Participation Award at AGU Fall Meeting 2019.
- Invited reviewer of multiple proposals to funding agencies:
  - National Science Foundation (NSF),
  - Sandia Laboratory Directed Research and Development,
  - DOE Office of Science Advanced Scientific Computing Research (ASCR).
- Invited referee for *Environmental Modelling and Software; Geophysical Research Letters; Scientific Reports; International Journal for Uncertainty Quantification; Computer Methods in Applied Mechanics and Engineering; Structural and Multidisciplinary Optimization; SIAM Journal on Scientific Computing; Journal of Computational Chemistry; International Journal on Chemical Kinetics; SIAM Journal on Uncertainty Quantification; Reliability Engineering and System Safety; Probabilistic Engineering Mechanics; Combustion and Flame; Journal of Computational Science; Mathematics of Climate and Weather Forecasting; Water Resources Research; AIChE Journal; Physics Letters A; Journal of Computational Physics; Journal of Physical Chemistry; Journal of Guidance, Control, and Dynamics; Mathematical Biosciences; AIAA Journal; Multiscale Modeling and Simulation; Physica D; The European Physical Journal B; Computational Geosciences.*

Mentorship

- *Postdoctoral (lead advisor):* Joy Mueller (2022-present), Joshua Hudson (2020-2023), Logan Williams (2022-2023), Varuni Dantanarayana (2020-2021), Vishagan Ratnaswamy (2019-2020), Prashant Rai (2017-2020), Martin Drohmann (2013-2015).
- *Postdoctoral (co-advisor):* Luis Damiano (2023-present), Pieterjan Robbe (2020-2023), Eric Hermes (2018-2022), Xun Huan (2016-2018), Zhen Liu (2012-2014), Thomas Catanach (2017-2018).
- *Sandia Early-Career Mentorship:* Cristian Lacey, Pieterjan Robbe, Moe Khalil, Oscar Diaz-Ibarra, Francesco Rizzi, Tiernan Casey.
- *Graduate Students:* Javier Murgoitio Esandi (2023-present, U of Southern California), Chase Dwelle (2016-2019, U of Michigan, Ph.D. thesis committee member), Katherine Johnston (2020-2022, U of Washington), Haley Rosso (2021-present, Emory U), Sofia Guzzetti (2018, Emory U).
- *Undergraduate Students:* Jonathan Vo (2018-2019, U of California, Irvine), Sarah Teichman (2016, U of Massachusetts), Joseph Heindel (2016, Seattle Pacific Univ.), Cagan Ozen (2016, Columbia U), Jason Bender (2014-2015, U of Minnesota), Chi Feng (2015, MIT).

Software

- Uncertainty Quantification Toolkit (UQTk): a Python/C++ software kit for uncertainty quantification, `sandia.gov/UQToolkit`. Key developer: implemented most of the advanced algorithms present in the library.
- Minima-Preserving Neural Networks (MPNN): a Python library for neural network approximations to chemistry potentials preserving minima, `github.com/sandialabs/mpnn`. Sole developer.
- Quantifying Uncertainties in Neural Networks (QUiNN): a Python library centered around various probabilistic wrappers over PyTorch modules in order to provide uncertainty estimation in neural network predictions, `github.com/sandialabs/quinn`. Sole developer.

- FitSNAP: a Python library for building machine learning (ML) potentials based on LAMMPS, `github.com/FitSNAP/FitSNAP`. Developed and implemented uncertainty quantification methods for constructing the ML potentials.

Invited Recent Presentations

- "Visualizing and Quantifying Uncertainty of Physics-aware Neural Networks", FASTMath All-Hands, Denver, CO, November, 2023.
- "Quantifying Uncertainties in Residual Neural Networks and Neural ODEs", UNCECOMP, 5th International Conference on Uncertainty Quantification in Computational Science and Engineering, Athens, Greece, June, 2023.
- "Climate Model Parameterization with Probabilistic Neural Networks", Bilateral AI US-Norway Forum, Oslo, Norway, October, 2022.
- "Training and Generalization of Residual Neural Networks as Discrete Analogues of Neural ODEs", MLDL Workshop, SNL, July, 2022.
- "Model Error Estimation and Uncertainty Quantification of Machine Learning Interatomic Potentials", Error control in first-principles modelling CECAM-EPFL, Lausanne, Switzerland, June, 2022.
- "Bayesian Inference of Interatomic Potentials: Model Errors and Active Learning", MIT CESMIX-UQ, March, 2022.
- "Quantifying and Reducing Uncertainty in the E3SM Land Model Using Surrogate Modeling", E3SM All Hands Monthly Seminar Series, May, 2021.
- "Probabilistic Methods for Forward and Inverse Uncertainty Quantification", Joint BYU/Utah State Department of Mathematics Seminar, October, 2020.
- "Embedded Model Error Methods", Summer School, Department of Mechanical and Aerospace Engineering University of Rome La Sapienza, September, 2020.
- "Overview of Uncertainty Quantification Methods for Complex Models", DOE Climate Modeling PI meeting, November, 2018.
- "Bayesian Framework for Embedded Model Error Representation and Quantification", Joint Statistical Meetings, Vancouver, Canada, August, 2018.
- "Embedded Model Error Representation for Bayesian Model Calibration", Radcliffe Institute for Advanced Study, Harvard University, May, 2018.
- "Probabilistic Methods for Uncertainty Quantification in Computational Models", MICDE Seminar, University of Michigan, Ann Arbor, April, 2018.

Publications

An up-to-date publication list: `https://scholar.google.com/citations?user=S9st9uEAAAAJ`

[as of 01/10/2024]	All	Since 2019
Citations	2295	1368
h-index	25	21
i10-index	41	28

- J. Mueller, K. Sargsyan, C. Daniels, H. N. Najm, "Polynomial Chaos Surrogate Construction for Random Fields with Parametric Uncertainty", Submitted, *SIAM J for Uncert. Quant.*, December, 2023.
- J. Hudson, M. D'Elia, H. Najm, K. Sargsyan, "The Role of Stiffness in Training and Generalization of ResNets", *Journal of Machine Learning for Modeling and Computing*, 4:2, 2023.
- M. Johnson, M. Gierada, E. Hermes, D. Bross, K. Sargsyan, H. Najm, J. Zádor, "Pynta - An automated workflow for calculation of surface and gas-surface kinetics", *Journal of Chemical Information and Modeling*, 63, 16, pp. 5153-5168, 2023.

- F. Ghahari, K. Sargsyan, G. Parker, D. Swensen, M. Celebi, H. Haddadi, E. Taciroglu, "Performance-Based Earthquake Early Warning for Tall Buildings", Submitted, *Earthquake Spectra*, September, 2023.
- W. Zhou, L. Zhang, A. Sheshukov, J. Wang, M. Zhu, K. Sargsyan, D. Xu, D. Liu, T. Zhang, V. Mazepa, A. Sokolov, V. Valdayskikh, V. Ivanov, "Ground Heat Flux Reconstruction Using Bayesian Uncertainty Quantification Machinery and Surrogate Modeling", *Journal of Geophysical Research - Earth Surface*, Submitted, February, 2023.
- W. Pringle, Z. Burnett, K. Sargsyan, S. Moghimi, E. Myers, "Efficient Probabilistic Prediction and Uncertainty Quantification of Tropical Cyclone–Driven Storm Tides and Inundation", *Artificial Intelligence for the Earth Systems*, 2, e220040, 2023.
- K. Blöndal, K. Sargsyan, David H. Bross, B. Ruscic, C. Goldsmith, "Configuration Space Integration for Adsorbate Partition Functions: The Effect of Anharmonicity on the Thermophysical Properties of CO–Pt(111) and CH3OH–Cu(111)", *ACS Catalysis*, 13:1, pp.19–32, 2023.
- E. Sinha, Katherine V. Calvin, B. Bond-Lamberty, B. Drewniak, D. Ricciuto, K. Sargsyan, Y. Cheng, C. Bernacchi, C. Moore, "Modeling Perennial Bioenergy Crops in the E3SM Land Model (ELMv2)", *Journal of Advances in Modeling Earth Systems*, 15:1, p.e2022MS003171, 2023.
- A. Rohskopf, C. Sievers, N. Lubbers, M. A. Cusentino, J. Goff, J. Janssen, M. McCarthy, D. Montes de Oca Zapiain, S. Nikolov, K. Sargsyan, E. Sikorski, L. Williams, D. Sema, A. P. Thompson, M. A. Wood, "FitSNAP: Atomistic machine learning in LAMMPS", *Journal of Open Source Software*, 8(84), 5118, 2023.
- J. N. Mueller, K. Sargsyan, H. N. Najm, "Polynomial Chaos Surrogate Construction for Stochastic Models with Parametric Uncertainty", *ICASP14: Proceedings of the 14th International Conference on Application of Statistics and Probability in Civil Engineering*, June, 2023.
- P. Robbe, S. Blondel, T. Casey, A. Lasa, K. Sargsyan, B. Wirth, H. Najm, "Global sensitivity analysis of a coupled multiphysics model to predict surface evolution in fusion plasma–surface interactions", *Computational Materials Science*, 226, 112229, 2023.
- P. Robbe, D. Andersson, L. Bonnet, T. Casey, M. Cooper, C. Matthews, K. Sargsyan, H. Najm, "Bayesian calibration with summary statistics for the prediction of xenon diffusion in UO2 nuclear fuel", *Computational Materials Science*, 225, 112184, 2023.
- J. Hudson, M. D'Elia, H. N. Najm, K. Sargsyan, "Measuring Stiffness in Residual Neural Networks", *Proceedings of RAMSES: Reduced order models; Approximation theory; Machine learning; Surrogates, Emulators and Simulators*, December, 2022.
- E. Hermes, K. Sargsyan, H. N. Najm, J. Zádor, "Sella, an Open-Source Automation-Friendly Molecular Saddle Point Optimizer", *Journal of Chemical Theory and Computation*, 18:11, pp.6974–6988, 2022.
- F. Ghahari, K. Sargsyan, M. Çelebi, E. Taciroglu, "Quantifying modeling uncertainty in simplified beam models for building response prediction", *Structural Control and Health Monitoring*, 29:11, p.e3078, 2022.
- D. Xu, G. Bisht, K. Sargsyan, C. Liao, L. R. Leung, "Using a surrogate-assisted Bayesian framework to calibrate the runoff-generation scheme in the Energy Exascale Earth System Model (E3SM) v1", *Geoscientific Model Development*, 15:12, pp.5021–5043, 2022.
- T.R. Younkin, K. Sargsyan, T. Casey, H.N. Najm, J.M. Canik, D.L. Green, R.P. Doerner, D. Nishijima, M. Baldwin, J. Drobny, D. Curreli, B.D. Wirth, "Quantification of the effect of uncertainty on impurity migration in PISCES-A simulated with GITR", *Nuclear Fusion*, 62:5, p.056007, 2022.
- K. Blöndal, K. Sargsyan, D. Bross, B. Ruscic, C. Goldsmith, "Adsorbate Partition Functions via

Phase Space Integration: Quantifying the Effect of Translational Anharmonicity on Thermodynamic Properties", *Journal of Physical Chemistry C*, 125:37, pp.20249–20260, 2021.

- V. Y. Ivanov, D. Xu, M. Dwelle, K. Sargsyan, D. B. Wright, N. Katopodes, J. Kim, V. Tran, A. Warnock, S. Fatichi, P. Burlando, E. Caporali, P. Restrepo, B. F. Sanders, M. M. Chaney, A. M. B. Nunes, F. Nardi, E. R. Vivoni, E. Istanbulluoglu, G. Bisht, R. L. Bras, "Breaking Down the Computational Barriers to Real-Time Urban Flood Forecasting", *Geophysical Research Letters*, 48:20, p.e2021GL093585, 2021.
- B. Kreitz, K. Sargsyan, K. Blöndal, E. J. Mazeau, R. H. West, G. D. Wehinger, T. Turek, C. Goldsmith, "Quantifying the Impact of Parametric Uncertainty on Automatic Mechanism Generation for CO2 Hydrogenation on Ni(111)", *JACS Au*, 1:10, pp.1656–1673, 2021.
- E. D. Hermes, K. Sargsyan, H. N. Najm, J. Zádor, "Geometry optimization speedup through a geodesic approach to internal coordinates", *The Journal of Chemical Physics*, 155:9, p.094105, 2021.
- C. Safta, J. Ray, K. Sargsyan, "Characterization of partially observed epidemics through Bayesian inference: application to COVID-19", *Computational Mechanics*, 66:5, pp.1109–1129, october, 2020.
- V. N. Tran, M. S. Dwelle, K. Sargsyan, V. Ivanov, J. Kim, "A novel modeling framework to secure efficiency and accuracy in real-time ensemble flood forecasting", *Water Resources Research*, 56:3, p. e2019WR025727, 2020.
- E. Hermes, K. Sargsyan, H. N. Najm, J. Zador, "Accelerated Saddle Point Refinement through Full Exploitation of Partial Hessian Diagonalization", *Journal of Chemical Theory and Computation*, 15:11, pp.6536–6549, 2019.
- M. C. Dwelle, J. Kim, K. Sargsyan, V. Ivanov, "Streamflow, stomata, and soil pits: sources of inference for complex models with fast, robust uncertainty quantification", *Advances in Water Resources*, 125, pp.13–31, 2019.
- P. Rai, K. Sargsyan, H. Najm, S. Hirata, "Sparse Low Rank Approximation of Potential Energy Surfaces with Applications in Estimation of AnharmonicZero Point Energies and Frequencies", *Journal of Mathematical Chemistry*, 57, pp.1732–1754, 2019.
- P. 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.29–47, 2019.
- K. Sargsyan, X. Huan, H. N. Najm. "Embedded Model Error Representation for Bayesian Model Calibration", *International Journal of Uncertainty Quantification*, 9:4, pp. 365–394, 2019.
- D. Ricciuto, K. Sargsyan, P. Thornton, "The Impact of Parametric Uncertainties on Biogeochemistry in the E3SM Land Model", *Journal of Advances in Modeling Earth Systems*, 10:2, pp.297–319, 2018.
- F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O. Le Maître, O.M. Knio, B.J. Debusschere, "Exploring the interplay of resilience and energy consumption for a task-based partial differential equations preconditioner", *Parallel Computing*, 73, p.16–27, 2018.
- O. Cekmer, K. Sargsyan, S. Blondel, H. Najm, D. Bernholdt,, B.D. Wirth, "Uncertainty quantification for incident helium flux in plasma-exposed tungsten", *International Journal for Uncertainty Quantification*, 8:5, pp.429–446, 2018.
- P. Rai, K. Sargsyan, H. Najm, "Compressed sparse tensor based quadrature for vibrational quantum mechanics integrals", *Computer Methods in Applied Mechanics and Engineering*, 336, pp.471–484, 2018.
- L. Hakim, G. Lacaze, M. Khalil, K. Sargsyan, H. Najm, J. Oefelein, "Probabilistic parameter estimation in a 2-step chemical kinetics model for n-dodecane jet autoignition", *Combustion Theory and Modeling*, 22:3, pp.446–466, 2018.

- J. Kenny, K. Sargsyan, S. Knight, G. Michelogiannakis, J. Wilke, "The Pitfalls of Provisioning Exascale Networks: A Trace Replay Analysis for Understanding Communication Performance", *High Performance Computing*, p.269–288, 2018.
- X. Huan, C. Safta, K. Sargsyan, G. Geraci, M. S. Eldred, Z. P. Vane, G. Lacaze, J. C. Oefelein, Habib N. Najm, "Global Sensitivity Analysis and Estimation of Model Error, toward Uncertainty Quantification in Scramjet Computations", *AIAA Journal*, 56:3, pp.1170–1184, 2018.
- X. Huan, C. Safta, K. Sargsyan, Z. P. Vane, G. Lacaze, J. C. Oefelein, H. N. Najm, "Compressive sensing with cross-validation and stop-sampling for sparse polynomial chaos expansions", *SIAM/ASA Journal of Uncertainty Quantification*, 6:2, pp.907–936, 2018.
- F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O. Le Maitre, O. Knio, B. Debusschere, "Partial differential equations preconditioner resilient to soft and hard faults", *The International Journal of High Performance Computing Applications*, 32:5, pp.658–673, 2018.
- 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 Forum*, No. AIAA-2018-1180, 2018.
- N. Griffiths, P. Hanson, C. Iversen, A. Malhotra, K. McFarlane, R. Norby, D. Ricciuto, K. Sargsyan, S. Sebestyen, X. Shi, A. Walker, E. Ward, J. Warren, D. Weston, "Temporal and spatial variation in peatland carbon cycling and implications for interpreting responses of an ecosystem-scale warming experiment", *Soil Science Society of America*, 81:6, pp.1668–1688, 2017.
- K. Sargsyan, "Surrogate Models for Uncertainty Propagation and Sensitivity Analysis", "Forward Problems" section, Handbook of Uncertainty Quantification, Springer, 2017.
- B. Debusschere, K. Sargsyan, C. Safta, K. Chowdhary, "The Uncertainty Quantification Toolkit (UQTk)", "Software" section, Handbook of Uncertainty Quantification, 2017.
- P. Mycek, A. Contreras, O. Le Maitre, 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, 2017.
- P. Mycek, F. Rizzi, O. Le Maitre, 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*, 39:1, pp.C1–C28, 2017.
- P. Rai, K. Sargsyan, H. Najm, M.R. Hermes, S. Hirata, "Low-rank canonical-tensor decomposition of potential energy surfaces: application to grid-based diagrammatic vibrational Green's function theory", *Molecular Physics*, 115:17-18, pp.2120–2134, 2017.
- M. Khalil, K. Chowdhary, C. Safta, K. Sargsyan, H. N. Najm, "Inference of Reaction Rate Parameters based on Summary Statistics from Experiments", *Proc. Comb. Inst.*, 36:1, pp.699–708, 2017.
- X. Huan, C. Safta, K. Sargsyan, G. Geraci, M. Eldred, Z. Vane, G. Lacaze, J. Oefelein, H. Najm, "Global Sensitivity Analysis and Quantification of Model Error for Large Eddy Simulation in Scramjet Design", *19th AIAA Non-Deterministic Approaches Conference*, No. 2017-1089, 2017.
- K. Morris, F. Rizzi, B. Cook, P. Mycek, O. Le Maitre, O. Knio, K. Sargsyan, K. Dahlgren, B. Debusschere, "Performance scaling variability and energy analysis for a resilient ULFM-based PDE solver", *7th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems (ScalA)*, pp.41–48, 2016.
- C. Safta, M. Blaylock, J. Templeton, S. Domino, K. Sargsyan, H. Najm, "Uncertainty Quantification in LES of Channel Flow", *International Journal for Numerical Methods in Fluids*, 83, pp.376–401, 2016.
- K. Morris, F. Rizzi, K. Sargsyan, K. Dahlgren, P. Mycek, C. Safta, O. Le Maitre, O. Knio, B.

Debusschere, "Scalability of Partial Differential Equations Preconditioner Resilient to Soft and Hard Faults", *Proceedings of High Performance Computing: 31st International Conference, ISC High Performance 2016*, Frankfurt, Germany, p.469–485, June 19-23, 2016.

- F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, B. Debusschere, O. Le Maitre, O. Knio, "ULFM-MPI implementation of a resilient task-based partial differential equations preconditioner", *Proceedings of the ACM Workshop on Fault-Tolerance for HPC at Extreme Scale*, pp.19–26, 2016.
- J. Ray, Z. Hou, M. Huang, K. Sargsyan, L. Swiler, "Bayesian calibration of the Community Land Model using surrogates", *SIAM/ASA Journal on Uncertainty Quantification*, 3:1, pp.199–233, 2015.
- K. Sargsyan, H. N. Najm, R. Ghanem, "On the Statistical Calibration of Physical Models", *International Journal for Chemical Kinetics*, 47:4, pp. 246–276, 2015.
- F. Rizzi, K. Morris, K. Sargsyan, P. Mycek, C. Safta, O. LeMaitre, O. Knio, B. Debusschere, "Partial differential equations preconditioner resilient to soft and hard faults", *2015 IEEE International Conference on Cluster Computing (CLUSTER)*, pp.552–562, 2015.
- C. Safta, D. Ricciuto, K. Sargsyan, B. Debusschere, H.N. Najm, M. Williams, P. Thornton, "Global Sensitivity Analysis, Probabilistic Calibration, and Predictive Assessment for the Data Assimilation Linked Ecosystem Carbon Model", *Geosci. Model Dev.*, 8, pp.1899–1918, 2015.
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