Arpan Biswas

Phone: (541)908-7528 Email: biswasa@ornl.gov / arpanbiswas52@gmail.com

Address: 401 S Gallaher View Rd APT 3, Knoxville, TN 37919, Citizenship – Indian

PROFESSIONAL SUMMARY

Completed PhD in Dec 2020, specializing in **Mechanical engineering** -**Design and Minor: Statistics.** (Major Advisor – Dr Christopher Hoyle, Minor Advisor – Dr Claudio Fuentes)

Current: Postdoc at Center for Nanophase Material Science, Oak Ridge National Lab under supervision of Dr Sergei Kalinin and Dr Rama Vasudevan

EDUCATION

| Ph.D. in Mechanical Engineering, Minor in Statistics (3.92/4) | Oregon State University, 2016 - 2020 |
|---|---|
| MS in Mechanical Engineering (3.93/4) | Oregon State University, 2015 - 2017 |
| BTECH in Mechanical Engineering (8.2/10-Scale) | West Bengal University of Technology, 2008 - 2012 |
| RESEARCH SKILLS/EXPERIENCE | |

- Broad domain in design problem formulation (computational) from problem statement (scratch), appropriate optimization algorithm selection, enhancement, and development to solve for large scale real-world problems.
 - Design problem optimization algorithm development with global trade-off between solution accuracy (reliability) vs cost (practical applicability).
- Unsupervised deep learning-based feature engineering from large scale complex data.
- Combined approach: Efficient design/optimization algorithm + ML/statistical applications + physics/domain knowledge attempt to learn faster and better with lesser data (expensive evaluations/sampling/experiments).
- Model Development/ Practical Application:
 - Simulation-based Design (Probabilistic) and Nested Robust Optimization: Renewable Hydro-Energy System (Multi-Reservoir Columbia River System)
 - Data-driven (ML), domain knowledge driven, Nested, Meta-model-based design (Probabilistic) of Rapid Structural Assessment and Optimization: diffusion bonded Compact Heat Exchanger
 - Nested Optimization: Integrated Resilience based Complex System- Multirotor Drone model
 - Data-driven (ML), Physics-driven, meta-model-based optimization, automated experiments, and deep learning-based feature analysis (Probabilistic): Material Systems Ferroelectric (BTO), Antiferroelectric (PZO), multi-ferroic (BFO), Oxide Samples, Graphene, Plasmonic Nanoparticles, thin films

| Design/Optimization | Statistics | Machine Learning |
|--|--|---|
| Multi-objective/ multi-disciplinary optimization Black-box design optimization Design of Experiments – Bayesian Optimization Nested Design Reliability/ Probabilistic design Robust Optimization Non-linear, Mixed-Integer Programming Classical and Heuristic Optimization Methods Simulation -based optimization | Statistical data analysis/modelling – Classical and Bayesian regression, Gaussian Process Statistical Meta-modelling-based optimization – Bayesian Optimization Dimension reduction - PCA Uncertainty propagation and quantification- Monte Carlo, Stochastic collocation, stratified sampling, adaptive sampling Model Validation – Cross-Validation, Bootstrapping Bayesian Network (Fundamental) | Data-driven sequential, adaptive meta-learning – Bayesian optimization, Physics augmented BO Supervised/unsupervised classification/regression – SVM, Random Forest, Bagging, Boosting, Clustering, PCA Deep-learning/ Computer Vision – Variational Autoencoders, Physics Augmented VAEs |
| Soft skills: Ability to work in diverse environments, multi-disciplinary projects, problem-solver, pro-active, willingness to learn outside comfort zone, good leadership, communication, mentoring and presentation skills. | | |

COMPUTER SKILLS

Python (Numpy, PyTorch, AtomAI, PyroVED), Matlab, Google Colab, RStudio, RMarkdown, SolidWork, MS Office (MS Excel, MS outlook, MS PowerPoint, MS OneNote), GPU platform (SDGX box), Linux

PHD DISSERTATION

Title: Hybrid Statistical and Engineering Optimization Architectures in Early Multidisciplinary Designs of Resilience and Expensive Black-box Complex Systems (**Citation Link: https://ir.library.oregonstate.edu/concern/graduate_thesis_or_dissertations/cc08hp06m**)

MS THESIS

Title:Bi-levelFlexible-RobustOptimizationforEnergyAllocationProblems(CitationLink:https://ir.library.oregonstate.edu/concern/graduate_thesis_or_dissertations/fn107371n)

WORK EXPERIENCE

Postdoctoral Research Associate

UT-Battelle, LLC (Oak Ridge National Lab), April 2021 – Present

- Overall research on physics-informed computational design of experiments, optimization, metamodeling and uncertainty quantification, and application of Machine Learning (deep learning) in reducing the effort/time of expensive and/or black box experiments towards rapid discoveries.
- Build simulation models (in python) of different material systems (eg. PZO, BTO).
- Automated Experiments: Design a dynamic, human-guided, physics-driven Bayesian optimized Spectral recommendation system in Python for accelerated learning of desired spectral domain phases of complex microscopic images. (Manuscript in prep)
- Design physics driven VAEs in pyroVED for better complex microscopic image analysis. (Manuscript in prep)
- Developed Latent Bayesian Optimization framework in pyroVED to tackle high dimensional (hyper)parameter optimization of computationally expensive ML (eg. Autoencoder models), in optimal pattern and feature extractions from large-scale microscopic data.
- Design automated experiments (Bayesian Optimization framework) in PyTorch for synthesis of WSE2 monolayer films.
- Developed **physics-driven Multi-objective Bayesian optimization architecture (MOBO) in PyTorch** to extend the rapid exploration in more complex multi-parameter and multi-function space (high dimensional), attempting to reduce time and cost of experiments or expensive simulations.
- Methodology implemented/researched on Automated Experiments, Bayesian Optimization, Multi-Objective Bayesian Optimization, Metamodeling and uncertainty quantification, kernel functions, Genetic Algorithm, Variational Autoencoders, Physics augmented modelling.
- Software/Platform Used: Python (Numpy, PyTorch, AtomAI, PyroVED), MATLAB, Google Colab, GPU (SDGX box), Linux environment.

ORISE Postdoctoral Fellow

National Center for Toxicological Research, Feb 2021 – April 2021

- Working in the division of Biostatistician and Bioinformatics
- Review of existing Adverse Outcome pathways (AOP) network related to drug induced liver injury (DILI).
- Configure combined complex AOP networks for modelling, from mechanistic knowledge of several sources.
- Methodology researched on AOP wiki, Bayesian network.
- Software Used: R.

Research Assistant – funded by Department of Energy

- Overall research focus on developing a design strategy for rapid structural assessment for manufacturing diffusion-bonded Hybrid Compact Heat Exchangers.
- Developed a data-driven (ML) based meta-model sequential Two-Stage Multi-Objective Bayesian Optimization (MOBO) framework in classifying safe and unsafe design in terms of Creep-Fatigue failure and then finding an optimal design geometry as a trade-off between risk of failure and cost in manufacturing.
- The Proof of Concept (thin tube design) model validation performs better than existing ML methods with an <1% classification error rate and cost of average 100 training data.
- Developed an algorithm of **Nested Weighted Tchebycheff MOBO** for better pareto solutions and minimize the multi-functional space complexity.

Oregon State University, 2018 - 2020

- Methodology implemented/researched on Bayesian Optimization, Gaussian Process, Classical & Bayesian Regression, Simulation, Uncertainty Propagation and Quantification, Probabilistic Constraints, Inverse Reliability, Latin Hypercube Sampling, SVM, RF, Boosting, Weighted Tchebycheff Multi-Objective Global Criteria, Model Calibration and Validation.
- Software Used: MATLAB, R, RStan (MCMC), SolidWork

Research Assistant – funded by NASA Ames

- <u>Overall research focus on developing mathematical non-linear Mixed Integer Bi-level programming in optimizing functionbased fault propagation model resilience in large scale dynamic Complex engineered system designs.</u>
- Implementation of **reliability based hierarchical Bi-level design in Python** to complex design problems (drone model) which optimizes the trade-off among design **architecture cost**, **operation cost and resilience** cost under hazardous events, where the sub-systems are added or dropped with different design concepts, minimizing the overall risk of the design.
- Methodology implemented/researched on Co-Design, Bi-level Optimization, Evolutionary, Penalty & Gradient based algorithms.
- Software Used: MATLAB, Python

Summer Internship (12 weeks)

Proctor & Gamble, June 2019 - Sep 2019

Oregon State University, 2015 - 2018

- Worked as Statistician in Data & Modelling Science Dept. where I was involved in Sequential Design, developing Bayesian
 Optimization models in R, MATLAB (DACE) in an efficient sample selection to maximize learning of location of true optimal
 regions with conducting minimum expensive black-box experiments from an unknown, complex, data driven design space in early
 experimental phase.
- Integration of experimental uncertainties into the design framework for robust learning.
- The results show better performance (accuracy) than existing frequentist approaches in finding true optimal solution, with lot lesser number of samplings for experiments.
- **Methodology implemented/researched** on Bayesian Optimization, Gaussian Process, Latin Hypercube Sampling, PCA, KL-Expansion, Stochastic Collocation, Uncertainty Propagation and Quantification.
- **Software Used**: MATLAB, R Markdown JMP, Comsol.

Research Assistant – funded by Bonneville Power Administration

- Developed a reliability based non-linear bi-level Flexible-Robust optimization model (Probabilistic design in MATLAB) for optimum allocation of hydro-energy of dynamic Complex River systems, considering probabilistic constraints of multi-reservoir systems, thereby provided better optimal decisions with increased revenue, and minimizing risk of future shortages of energy.
- Developed a multi-reservoir system simulation model with inflow and price uncertainty.
- Applied **KL-expansions, stochastic collocation methods** for quantification and propagation of inflows and price uncertainty in the system, reducing dimensions of large-scale problem, thereby increasing computational efficiency of the model.
- Integrate an efficient economic model (Real Options) in optimization framework to ensure risk-averse future prediction and robust design.
- The performance of the Bi-level Flexible-Robust optimization model performed better than existing model, and gave 1% (\$30764) increase in Revenue of 14 day-period.
- Methodology implemented/researched on Bi-Level Optimization, Utility Function (Robust Objective), Simulation, Uncertainty Propagation and Quantification, Probabilistic Constraints, Inverse Reliability, Evolutionary, Penalty & Gradient based algorithms, KL-Expansion, Stochastic Collocation, Monte Carlo, Real Option.
- Software Used: MATLAB.

Teaching Assistant

- Teaching Assistant in both undergraduate classes like Introduction in Design (3 terms), Mechanical Component Design (2 terms) and graduate class like Optimization in Design (1 term)
- Mentored groups of 28-40 students together in a single class, provided regular monitoring of their theoretical and practical work, grading and feedback in labs, conducted weekly meeting with students

Software Engineer

- Worked as UAT tester, automation tester and test lead in Microsoft project. Created test plans as leads and executed more than 1000 test cases as tester.
- Had led a team of 9 members, provided daily project status updates to clients with 100% project completion rate.

Oregon State University, 2016 – 2020

Accenture, 2012 - 2015

Oregon State University, 2019 - 2020

PUBLICATIONS

Journal Papers:

- 1. Biswas, A., Rama Vasudevan, Maxim Ziatdinov, Sergei V. Kalinin " Optimizing Training Trajectories in Variational Autoencoders via Latent Bayesian Optimization Approach" 2023 Mach. Learn.: Sci. Technol. 4 015011 https://doi.org/10.1088/2632-2153/acb316
- Biswas, A., Fuentes, C., and Hoyle, C. (May 4, 2022). "A Nested Weighted Tchebycheff Multi-Objective Bayesian Optimization Approach for Flexibility of Unknown Utopia Estimation in Expensive Black-box Design Problems." ASME. J. Comput. Inf. Sci. Eng. doi: https://doi.org/10.1115/1.4054480
- Anna N. Morozovska, Eugene A. Eliseev, Arpan Biswas, Hanna V. Shevliakova, Nicholas V. Morozovsky, Sergei V. Kalinin "Chemical control of polarization in thin strained films of a multiaxial ferroelectric: phase diagrams and polarization rotation" Phys. Rev. B 105, 094112 Published 23 March 2022; https://doi.org/10.1103/PhysRevB.105.094112
- 4. Arpan Biswas, Anna N. Morozovska, Maxim Ziatdinov, Eugene A. Eliseev, and Sergei V. Kalinin "Multi-objective Bayesian optimization of ferroelectric materials with interfacial control for memory and energy storage applications" Journal of Applied Physics 130, 204102 (2021); <u>https://doi.org/10.1063/5.0068903</u>
- Anna N. Morozovska, Eugene A. Eliseev, Arpan Biswas, Nicholas V. Morozovsky, and Sergei V. Kalinin "Effect of Surface Ionic Screening on Polarization Reversal and Phase Diagrams in Thin Antiferroelectric Films for Information and Energy Storage" Phys. Rev. Applied 16, 044053 – Published 27 October 2021; https://doi.org/10.1103/PhysRevApplied.16.044053
- 6. Biswas, Arpan; Fuentes, C.; Hoyle, C. A MO-BAYESIAN OPTIMIZATION APPROACH USING THE WEIGHTED TCHEBYCHEFF METHOD. Journal of Mechanical Design 2021, 1–30. <u>https://doi.org/10.1115/1.4051787</u>.
- 7. Hulse, D, Biswas, Arpan, Hoyle, C, Tumer, Irem Y., Kulkarni, C, Goebel, K," Exploring Architectures for Integrated Resilience Optimization", Journal of Aerospace Information Systems, AIAA 2021. https://doi.org/10.2514/1.1010942.
- 8. Biswas, Arpan, and Hoyle, C. (February 8, 2021). "An Approach to Bayesian Optimization for Design Feasibility Check on Discontinuous Black-Box Functions." ASME. J. Mech. Des. March 2021; 143(3): 031716. https://doi.org/10.1115/1.4049742
- 9. Biswas, Arpan, Chen, Y., Gibson, N., and Hoyle, C. "Bi-Level Flexible-Robust Optimization for Energy Allocation Problems." ASME. ASME J. Risk Uncertainty Part B. doi: https://doi.org/10.1115/1.4046269

Conference Papers:

- Biswas, Arpan, Fuentes, C, & Hoyle, C. "An Approach to Bayesian Optimization in Optimizing Weighted Tchebycheff Multi-Objective Black-Box Functions." Proceedings of the ASME 2020 International Mechanical Engineering Congress and Exposition. Volume 6: Design, Systems, and Complexity. Virtual, Online. November 16–19, 2020. V006T06A030. ASME. https://doi.org/10.1115/IMECE2020-23414
- Biswas, Arpan, & Hoyle, C. "An Approach to Bayesian Optimization for Design Feasibility Check on Discontinuous Black-Box Functions." Proceedings of the ASME 2020 International Design Engineering Technical Conferences and Computers and Information in Engineering Conference. Volume 11B: 46th Design Automation Conference (DAC). Virtual, Online. August 17–19, 2020. V11BT11A017. ASME. https://doi.org/10.1115/DETC2020-22116 (Selected among top papers of IDETC 2020 for journal submissions)
- Biswas, Arpan, and Hoyle, Christopher. "A Literature Review: Solving Constrained Non-Linear Bi-Level Optimization Problems With Classical Methods." Proceedings of the ASME 2019 IDETC Conference. Volume 2B: 45th Design Automation Conference. V02BT03A025. ASME. https://doi.org/10.1115/DETC2019-97192
- Biswas, Arpan, Chen, Yong, and Hoyle, Christopher. "A Bi-Level Optimization Approach for Energy Allocation Problems." Proceedings of the ASME 2018 IDETC Conference. Volume 2B: 44th Design Automation Conference. V02BT03A041. ASME. https://doi.org/10.1115/DETC2018-85139
- 14. Biswas, Arpan, Chen, Yong, and Hoyle, Christopher. "An Approach to Flexible-Robust Optimization of Large-Scale Systems." Proceedings of the ASME 2017 IDETC Conference. Volume 2B: 43rd Design Automation Conference. V02BT03A045. ASME. <u>https://doi.org/10.1115/DETC2017-67221</u>

Abstract Talks (To be published in journals):

- **15.** A Biswas, Y Liu, R Vasudevan, M Ziatdinov Bulletin of the American Physical Society, 2023. "A Bayesian optimized spectral recommender system with dynamic human-guided targets for physics discovery"
- **16.** A Biswas, S Kalinin, M Ziatdinov Bulletin of the American Physical Society, 2023- Bulletin of the American Physical Society, 2023. "Towards better physics extraction in images via unsupervised custom loss shift-variational autoencoders"

RESEARCH PROPOSAL – as Principal Investigator

CNMS, ORNL User Proposal (2022-2023): Project title, "Towards scientific discovery from experiments via data driven optimization and machine learning approaches."

AWARDS and HONORS

Academic Excellence- Dean's Honor List for Winter 2020 by maintaining GPA above 3.75 with course load of 12+ credits

SOCIAL ACTIVITIES

- Member of ASME, APS.
- Program Committee member of Smoky Mountain Computational Science and Engineering Conferences (SMC 2021, 2022) in Data Challenge Seminar.
- Session chair at IMECE 2022, APS March meeting 2023 conferences.
- Invited reviewer at Journal of Applied Physics and npj Computaional Materials.
- Reviewer at Journal of Mechanical Design, ASME, (SMC 2021, 2022).
- Invited talk ORNL ML Workshop Conference
- Contributed talks in several conferences (such as EMA, March Meeting APS, IDETC, IMECE, IMRC etc)
- Outreach Programs:
 - o Seminar as mentorship to ORNL Interns
 - In-depth engagement as career representative with the students at the outreach program: Karns High School Technology and Innovation Day.

LIST OF CONTACTS FOR RECOMMENDATION

- Dr Sergei Kalinin (Project lead during most part of my ORNL tenure, Ex- ORNL manager), University of Tennessee, sergei2@utk.edu, Ph: 8652077885
- Dr Rama Vasudevan (Current ORNL manager), Group Leader, Data Nano Analytics, Center for Nanophase Material Science, ORNL, vasudevanrk@ornl.gov, Ph: 8652426552
- Dr Christopher Hoyle (Major Advisor), Associate Professor of Mechanical Engineering, Oregon State University, chris.hoyle@oregonstate.edu, Ph: 8472042204