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Research Interests

Optimization: PDE-constrained Problems, Gradient-based Algorithms, Multidisciplinary Design Optimization **Machine Learning**: Physics Informed Neural Networks, Constrained Training Methods, Supervised Learning **Scientific Computing**: High-Performance Computing for Optimization, Reusable Scientific Software

Education

Rensselaer Polytechnic Institute

December 2017

Aeronautical Engineering, Ph.D.

University of Maryland, Baltimore County

May 2012

Mechanical Engineering, B.S.

Work Experience

Postdoctoral Appointee - Argonne National Laboratory

Feb 2018-Present

Mathematics and Computer Science Division

o Principal developer on Toolkit for Advanced Optimization (TAO) and contributor to PETSc.

- o Research large-scale optimization algorithms with efficient treatment of nonlinear constraints.
- o Promote TAO, expand its user base, and provide software support for external researchers.

Graduate Research Assistant - Rensselaer Polytechnic Institute

Feb 2013-Dec 2017

Optimal Design Lab

Supervisor: Jason E. Hicken

Supervisor: Todd Munson

- o Investigate PDE-constrained multidisciplinary design optimization problems.
- Research gradient-based, reduced-space, matrix-free optimization algorithms.
- Develop a parallel-agnostic optimization library tailored for large-scale engineering systems.

Undergraduate Research Assistant – University of Maryland, Baltimore County

Oct 2010-May 2011

Supervisor: Gergely Dolgos

Joint Center for Earth Systems Technology

Construction of an optical aerosol measurement instrument.

- o Design and manufacture of high-precision optical component mounts.
- Propose instrument mounting solutions for the NASA GSFC science fleet aircraft.

Honors & Awards

o AIAA Student Paper Competition - 1st Place

2018

- Category: Multidisciplinary Analysis and Optimization

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Refereed Proceedings
echnical Reports.
Ooctoral Thesis
reprints / Working Papers.

Presentations
Conference Presentations
Invited Talks

Proposal Contributions

- "Development of a Machine Learning Toolkit in PETSc", co-investigator, LDRD Prime Future Computing, 2021-0177, 2021, funding: \$295K
- "Frameworks, Algorithms and Scalable Technologies for Mathematics (FASTMath) SciDAC Institute", numerical optimizations expert, DOE-ASCR, LAB 20-2223, 2020, funding: \$4.05M
- "Machine Learning and Artificial Intelligence for Simulation Acceleration and Real-Time Scientific Discovery of Fusion Science on Exascale Computers (MASS)", numerical optimization expert, DOE-FES, LAB 20-2224, 2020, not funded
- "Machine learning enhanced sampling methods for the stochastic multi-fidelity optimization of complex systems", numerical optimization expert, DOE-ASCR, LAB 20-2321, 2020, not funded

Software Projects

TAO: Toolkit for Advanced Optimization

ANSI C / Fortran Feb 2018-Present

Maintainer, Developer

https://gitlab.com/petsc/petsc

- Principal maintainer and code reviewer, point-of-contact for users and contributors, and lead developer for constrained optimization methods.
- Refactored existing nonlinear conjugate gradient (NCG), quasi-Newton (QN) and truncated-Newton methods with active-set bound projections.
- o Developed new quasi-Newton-based preconditioner and sparse Hessian initialization for NCG and QN methods.
- o Implemented a bound-constrained Gauss-Newton method with built-in support for commonly used regularization terms.
- o Implemented the augmented Lagrangian method of multipliers for generally constrained problems.
- Supervised a summer student for implementing the alternating direction method of multipliers with closed-form solutions for commonly used regularization terms.
- o Currently developing new error-tolerant constrained optimization algorithm for solving problems with inaccurate gradients.
- o Currently developing Python interfaces linking TAO with pyTorch for ML training problems (funded by LDRD Prime).

PETSc: Portable Extendable Toolkit for Scientific Computing

ANSI C / Fortran Feb 2018-Present

Developer

https://gitlab.com/petsc/petsc

- o Member of the core development team. Contributor and maintainer for new features required by TAO solvers.
- Implemented quasi-Newton Jacobian/Hessian approximations as new Mat objects that can be used in both TAO and SNES.
- Contributed vector projection tools to support bound-constraint projections, and vector subspace manipulation tools to support primal-dual algorithms in TAO.
- o Lead architect for Jenkins CI/CD prototype, leading up to PETSc's eventual migration to GitLab.
- Currently assisting in the development of an ML toolkit for PETSc (funded by LDRD Prime).

MADtorch: Multisecant Accelerated Descent Optimizer for pyTorch

Python3

Creator, Maintainer, Developer

Feb 2021-Present

https://gitlab.com/adener/madtorch

- Lead architect of a novel pyTorch optimizer for mini-batch training under general nonlinear constraints.
- Currently used in research efforts to accelerate XGC fusion simulation using a physics-informed neural network.

MACH: MDO for Aircraft Configurations with High Fidelity

Python3 / C++ / Fortran

External Contributor

Jun 2014-Dec 2017

- https://github.com/mdolab/MACH-Aero
- Software suite for aerodynamic and aero-structural shape optimization, developed and maintained by MDOLab at University of Michigan, Ann Arbor.
- Implemented a new MDO coupling architecture and related second-order adjoint-based matrix-free Hessian-vector products.

Kona: A Parallel Optimization Framework for Engineering-design Problems

Python3

Creator, Maintainer, Developer

Jan 2013-Dec 2017

☑ https://github.com/OptimalDesignLab/Kona

- o Lead architect of the core optimization research library for Optimal Design Lab at Rensselaer Polytechnic Institute.
- Designed parallel-agnostic implementations of SQP methods using vector algebra abstractions.
- o Implemented a novel matrix-free preconditioner for efficient multidisciplinary design optimization.
- o Library still in use by current doctoral students.

Teaching Experience

Guest Lecturer - Rensselaer Polytechnic Institute

Mechanical, Aerospace and Nuclear Engineering Department

Design Optimization (MANE 4280/6963)

Aerospace Structures and Materials (MANE 4060)

Fall 2016, Fall 2017

Fall 2012

Teaching Assistant - Rensselaer Polytechnic Institute

Mechanical, Aerospace and Nuclear Engineering Department

Design Optimization (MANE 4280/6963)
Strength of Materials (ENGR 2530)
Fall 2016, Fall 2017
Summer 2017

Aerospace Structures and Controls Laboratory (MANE 4920)

o Aerospace Structures and Materials (MANE 4060)

Aerodynamics I (MANE 4070)

Spring 2013 Fall 2012

Fall 2012

Professional Activities and Service

Referee/Reviewer

- o Mathematics of Optimization Research (2018-)
- o SIAM Journal on Scientific Computing (2018-)
- Optimization and Engineering (2018-)
- o AIAA Journal (2018-)
- DOE SBIR Phase I Review Panel (2019)

Conference Service

Session Organizer: SIAM CSE19, SIAM CSE21

Argonne Training Program for Extreme-Scale Computing

- o Program Committee, Member (2021-)
- Lead Organizer, Numerical Software Track (2021-)
- o Organizer, Numerical Software Track (2020)

Volunteer Work/Outreach

- University of Pittsburg, Graduate Student Career Q&A, Invited Panelist (2021)
- o National Science Bowl, Illinois Regionals, Questions Judge (2021)

Society Memberships

- Mathematical Optimization Society (2018-)
- o Institute for Operations Research and the Management Sciences (2018-)
- Society of Industrial and Applied Mathematics (2012-)
- o American Institute of Aeronautics and Astronautics (2012-)

Supervised Students

- o Jamal Shabani, Louisiana State University (2021), lead mentor
- o Sam Reynolds, Portland State University (2021), backup mentor
- o Han Sol Suh, Georgia Institute of Technology (2019, 2021), lead mentor