

Alp Dener

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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 Supervisor: Todd Munson

- Principal developer on Toolkit for Advanced Optimization (TAO) and contributor to PETSc.
- Research large-scale optimization algorithms with efficient treatment of nonlinear constraints.
- 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

- 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
Joint Center for Earth Systems Technology Supervisor: Gergely Dolgos

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

Honors & Awards

- Impact Argonne Award - Enhancement of Argonne's Reputation 2021
 - Volunteering for the NSF Science Bowl regional and national competitions
- AIAA Student Paper Competition - 1st Place 2018
 - Category: Multidisciplinary Analysis and Optimization

Publications

Journal Articles.....

- Miller, M Andres, R Michael Churchill, Alp Dener, Choong-Seock Chang, Todd Munson, and R Hager. 2020. "Encoder-decoder neural network for solving the nonlinear Fokker-Planck-Landau collision operator in XGC". *Journal of Plasma Physics*. doi:10.1017/S0022377821000155.
- Dener, Alp, and Jason E Hicken. 2017. "Matrix-free algorithm for the optimization of multidisciplinary systems". *Structural and Multidisciplinary Optimization, Springer*. doi:10.1007/s00158-017-1734-0.
- Hicken, Jason E, and Alp Dener. 2015. "A flexible iterative solver for nonconvex, equality-constrained quadratic subproblems". *Journal on Scientific Computing, SIAM*. doi:10.1137/140994496.

Refereed Proceedings.....

- Dener, Alp, Adam Denchfield, and Todd Munson. 2019. "Preconditioning nonlinear conjugate gradient with diagonalized quasi-Newton". In *Proceedings for the Platform for Advanced Scientific Computing Conference*. Zurich, Switzerland. doi:10.1145/3324989.3325712.
- Dener, Alp, and Todd Munson. 2019. "Accelerating limited-memory quasi-Newton convergence for large-scale optimization". In *International Conference on Computational Science*. Faro, Portugal. doi:10.1007/978-3-030-22744-9_39.
- Dener, Alp, Jason E Hicken, Gaetan K W Kenway, and Joaquim R R A Martins. 2018. "Enabling modular aerostructural optimization: Individual discipline feasible without the Jacobians". In *2018 Multidisciplinary Analysis and Optimization Conference, AIAA AVIATION Forum*. Atlanta, GA, USA. doi:10.2514/6.2018-3570.
- Dener, Alp, Pengfei Meng, Jason E Hicken, Graeme J Kennedy, John Hwang, and Justin S Gray. 2016. "Kona: A parallel optimization library for engineering-design problems". In *57th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, AIAA SciTech Forum*. San Diego, CA, USA. doi:10.2514/6.2016-1422.
- Dener, Alp, Gaetan K W Kenway, Jason E Hicken, and Joaquim R R A Martins. 2015. "Comparison of inexact- and quasi-Newton algorithms for aerodynamic shape optimization". In *53rd AIAA Aerospace Sciences Meeting, AIAA SciTech Forum*. Kissimmee, FL, USA. doi:10.2514/6.2015-1945.
- Dener, Alp, and Jason E Hicken. 2014. "Revisiting individual discipline feasible with matrix-free inexact-Newton-Krylov". In *10th AIAA Multidisciplinary Design Optimization Conference, AIAA SciTech Forum*. National Harbor, MD, USA. doi:10.2514/6.2014-0110.

Technical Reports.....

- Balay, Satish, Shrirang Abhyankar, Mark F Adams, Jed Brown, Peter Brune, Kris Buschelman, Lisandro Dalcin, Alp Dener, Victor Eijkhout, William D Gropp, Dmitry Karpeyev, Dinesh Kaushik, Matthew G Knepley, Dave A May, Lois Curfman McInnes, Richard Tran Mills, Todd Munson, Karl Rupp, Patrick Sanan, Barry F Smith, Stefano Zampini, Hong Zhang, and Hong Zhang. 2020. *PETSc users manual*. Tech. rep. ANL-95/11 - Revision 3.14. Argonne National Laboratory.
- Dener, Alp, Adam Denchfield, Hansol Suh, Todd Munson, Jason Sarich, Stefan Wild, Steven Benson, and Lois Curfman McInnes. 2020. *TAO users manual*. Tech. rep. ANL/MCS-TM-322 - Revision 3.14. Argonne National Laboratory.

Doctoral Thesis.....

- Dener, Alp. 2017. "A modular matrix-free approach to multidisciplinary design optimization". PhD thesis, Rensselaer Polytechnic Institute.

Preprints / Working Papers.....

- Kang, Shinhoo, Emil M Constantinescu, Alp Dener, Hong Zhang, and Robert L Jacob. 2021. "Implicit-Explicit and Multirate methods for a Coupled Navier-Stokes Equations (submitted)". In *American Geophysical Union Fall Meeting 2021*. New Orleans, LA, USA.
- Dener, Alp, Todd Munson, M Andres Miller, R Michael Churchill, and Choong-Seock Chang. 2021. "Toward constrained optimization in machine learning: An error-tolerant multiseant method for training PINNs (in preparation)".
- Dener, Alp, Adam Denchfield, and Todd Munson. 2021. "The TAO nonlinear conjugate gradient and quasi-Newton laboratory (in preparation)".
- Dener, Alp, M Andres Miller, R Michael Churchill, Todd Munson, and Choong-Seock Chang. 2020. "Training neural networks under physical constraints using a stochastic augmented Lagrangian approach (submitted)". *Journal of Computational Physics*. arXiv: 2009.07330.

Mills, Richard Tran, Mark F Adams, Satish Balay, Jed Brown, Alp Dener, Matthew Knepley, Scott E. Kruger, Hannah Morgan, Todd S Munson, Karl Rupp, Barry F Smith, Stefano Zampini, Hong Zhang, and Junchao Zhang. 2020. "Toward performance-portable PETSc for GPU-based exascale systems (accepted)". *IEEE Transactions on Parallel and Distributed Systems (Special Section on Innovative R&D toward the Exascale Era)*. arXiv: 2011.00715.

Hicken, Jason E, Pengfei Meng, and Alp Dener. 2017. "Error-tolerant multiseccant method for nonlinearly constrained optimization". *arXiv preprint*. arXiv: 1709.06985.

Presentations

Conference Presentations.....

Dener, Alp, Todd Munson, M Andres Miller, R Michael Churchill, and Choong-Seock Chang. 2021. *Toward Constrained Optimization in Machine Learning: An Error-Tolerant Multiseccant Method for Training PINNs*. SIAM Conference on Computational Science and Engineering.

Dener, Alp. 2020. *Investigating quasi-Newton outer product representations on GPUs*. SIAM Conference on Parallel Processing for Scientific Computing.

Dener, Alp, Adam Denchfield, and Todd Munson. 2019. *Accelerating quasi-Newton and conjugate gradient convergence for large-scale optimization*. SIAM Conference on Computational Science and Engineering.

Dener, Alp, Jason E Hicken, Gaetan K W Kenway, and Joaquim R R A Martins. 2018. *Enabling modular aerostuctural optimization: Individual discipline feasible without the Jacobians*. 2018 Multidisciplinary Analysis and Optimization Conference, AIAA AVIATION Forum.

Dener, Alp, Pengfei Meng, Jason E Hicken, Graeme J Kennedy, John Hwang, and Justin S Gray. 2016. *Kona: A parallel optimization library for engineering-design problems*. 57th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, AIAA SciTech Forum.

Dener, Alp, Gaetan K W Kenway, Jason E Hicken, and Joaquim R R A Martins. 2015. *Comparison of inexact- and quasi-Newton algorithms for aerodynamic shape optimization*. 53rd AIAA Aerospace Sciences Meeting, AIAA SciTech Forum.

Dener, Alp, and Jason E Hicken. 2014. *Revisiting individual discipline feasible with matrix-free inexact-Newton-Krylov*. 10th AIAA Multidisciplinary Design Optimization Conference, AIAA SciTech Forum.

Invited Talks.....

Dener, Alp. 2020. *Large-scale optimization using PETSc/TAO*. Argonne Training Program for Extreme-Scale Computing.

Dener, Alp. 2019. *PDE-constrained optimization using PETSc/TAO*. Argonne Training Program for Extreme-Scale Computing.

Proposal Contributions

"Distributed Workflows and Infrastructure to Couple Experiments and AI Services for Scientific Discovery", **PI:** Scott Klasky (ORNL), **Role:** Senior Personnel, **Sponsor:** DOE-ASCR, DE-FOE-0002482, 2021, **Status:** Not Funded

"Quantum Dynamics in Systems with Strong Electron-Phonon and Electron-Electron Interactions", **PI:** Ivar Martin (ANL), **Role:** Senior Personnel, **Sponsor:** DOE-BES/ASCR, DE-FOA-0002441, 2021, **Status:** Not Funded

"Development of a Machine Learning Toolkit in PETSc", **PI:** Richard Tran Mills (ANL), **Role:** Senior Personnel, **Sponsor:** LDRD Prime - Future Computing, 2021-0177, 2021, **Status:** Funded, \$295K

"Frameworks, Algorithms and Scalable Technologies for Mathematics (FASTMath) SciDAC Institute", **PI:** Esmond G. Ng (LBNL), **Role:** Senior Personnel, **Sponsor:** DOE-ASCR, LAB 20-2223, 2020, **Status:** Funded, \$4.05M

"Machine Learning and Artificial Intelligence for Simulation Acceleration and Real-Time Scientific Discovery of Fusion Science on Exascale Computers (MASS)", **PI:** Choong-Seock Chang (PPPL), **Role:** Senior Personnel, **Sponsor:** DOE-FES/ASCR, LAB 20-2224, 2020, **Status:** Not Funded

"Machine learning enhanced sampling methods for the stochastic multi-fidelity optimization of complex systems", **PI:** Marc Day (LBNL), **Role:** Senior Personnel, **Sponsor:** DOE-ASCR, LAB 20-2321, 2020, **Status:** Not Funded

Software Projects

TAO: Toolkit for Advanced Optimization
Maintainer, Developer

ANSI C / Fortran
Feb 2018–Present

🔗 <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.
- Developed new quasi-Newton-based preconditioner and sparse Hessian initialization for NCG and QN methods.
- Implemented a bound-constrained Gauss-Newton method with built-in support for commonly used regularization terms.
- 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.
- Currently developing new error-tolerant constrained optimization algorithm for solving problems with inaccurate gradients.
- Currently developing Python interfaces linking TAO with pyTorch for ML training problems (funded by LDRD Prime).

PETSc: Portable Extendable Toolkit for Scientific Computing
Developer

ANSI C / Fortran
Feb 2018–Present

🔗 <https://gitlab.com/petsc/petsc>

- 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.
- 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
Creator, Maintainer, Developer

Python3
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
External Contributor

Python3 / C++ / Fortran
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
Creator, Maintainer, Developer

Python3
Jan 2013–Dec 2017

🔗 <https://github.com/OptimalDesignLab/Kona>

- 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.
- Implemented a novel matrix-free preconditioner for efficient multidisciplinary design optimization.
- Library still in use by current doctoral students.

Teaching Experience

Guest Lecturer – Rensselaer Polytechnic Institute

Mechanical, Aerospace and Nuclear Engineering Department

- o Design Optimization (MANE 4280/6963) Fall 2016, Fall 2017
- o Aerospace Structures and Materials (MANE 4060) Fall 2012

Teaching Assistant – Rensselaer Polytechnic Institute

Mechanical, Aerospace and Nuclear Engineering Department

- o Design Optimization (MANE 4280/6963) Fall 2016, Fall 2017
- o Strength of Materials (ENGR 2530) Summer 2017
- o Aerospace Structures and Controls Laboratory (MANE 4920) Spring 2013
- o Aerospace Structures and Materials (MANE 4060) Fall 2012
- o Aerodynamics I (MANE 4070) Fall 2012

Professional Activities and Service

Referee/Reviewer

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

Conference Service

- o Session Organizer: SIAM CSE19, SIAM CSE21

Argonne Training Program for Extreme-Scale Computing

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

Volunteer Work/Outreach

- o University of Pittsburgh, Graduate Student Career Q&A, Invited Panelist (2021)
- o National Science Bowl, Illinois Regionals & Nationals, Volunteer (2021)

Society Memberships

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

Supervised Students

- o Jamal Shabani, Louisiana State University, lead mentor (2021)
- o Hansol Suh, Georgia Institute of Technology, lead mentor (2019, 2021)