Alp Dener

Computational Science · Numerical Optimization · High-Performance Computing · AI / ML

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Summary

I am a computational scientist specializing on gradient-based and constrained numerical optimization methods and their parallel implementations, with large-scale applications in engineering design, scientific discovery and machine learning. I am also a member of the core development team for PETSc/TAO, one of the premiere research libraries in the US Department of Energy software portfolio.

Skills

Numerical Optimization	PDE-constrained Problems, Gradient-based Algorithms, Multidisciplinary Design Optimization
Machine Learning	Physics-Informed Neural Networks, Constrained Training Methods, Supervised Learning
Software Development	Parallel Programming, Heterogeneous Architectures, Test-based Development, CI/CD
Tools & Languages	Python3, PyTorch, Cython, F2Py, ANSI C, C++11, Boost, MPI, CUDA, Fortran77/90/95, MATLAB, LaTeX

Experience

Argonne National Laboratory — *Lemont, Illinois*

Assistant Computational Scientist — *Oct. 2021 - PRESENT*

- Research and develop large-scale optimization methods for engineering design and scientific machine learning.
- Collaborate with domain experts on challenging applications in plasma physics and Earth systems modeling.
- Maintain the Toolkit for Advanced Optimization (TAO) package in the PETSc library.
- Prepare the PETSc library for next-generation exascale supercomputer architectures.

Postdoctoral Researcher — *Feb. 2018 - Sep. 2021*

- Developed novel stochastic optimization methods for training deep neural networks under physics constraints.
- Extended conjugate gradient, quasi-Newton and Newton optimization methods in the PETSc/TAO library with active-set bound constraints.
- Implemented a Python interface for using PETSc/TAO optimization algorithms in PyTorch training workflows.
- Spearheaded the transition of PETSc/TAO development to a full CI/CD workflow with a Jenkins prototype.

Rensselaer Polytechnic Institute — *Troy, New York*

Graduate Research and Teaching Assistant — *Aug. 2012 - Dec. 2017*

- Researched simulation-driven multidisciplinary design optimization problems.
- Developed matrix-free optimization library for large-scale engineering design applications.
- Integrated parallel, high-fidelity, coupled aero-structural solvers with optimization algorithms via adjoint-based sensitivity analysis.
- Served as a grader, proctor, tutor and substitute lecturer for undergraduate-level mechanical and aeronautical engineering courses.

University of Maryland, Baltimore County — *Maryland, Baltimore*

Undergraduate Research Assistant & Machinist — *Oct. 2010 - May 2011*

- Developed an optical aerosol measurement instrument for deployment on ground and air vehicles.
- Designed and manufactured micrometer-tolerance aluminum mounts for optical components.

Turkish Aerospace Industries — *Ankara, Turkey*

Aerodynamic Analysis and Design Intern — *Jun. 2009 - Sep. 2009*

- Modeled geometry and generated meshes for A129 hardpoints.
- Analyzed effects of rotor downwash on fired ordnance using CFD tools.

Education

Rensselaer Polytechnic Institute — *Troy, New York*

Ph.D. in Aeronautical Engineering — *Aug. 2012 - Dec. 2017*

- Thesis: A Modular Matrix-Free Approach to Multidisciplinary Design Optimization

University of Maryland, Baltimore County — *Baltimore, Maryland*

B.S. in Mechanical Engineering — *Jan. 2008 - May. 2012*

Honors & Awards

2021 **Impact Award,** Enhancement of Argonne's Reputation (NSF Science Bowl Volunteer) — *Lemont, Illinois*

2018 **1st Place,** AIAA AVIATION 2018 Student Paper Competition (Category: Multidisciplinary Design Optimization) — *Atlanta, Georgia*

Publications

Journal Articles

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. 2021. "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)*. doi:10.1016/j.parco.2021.102831.

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

Hang, Shinhoo, Emil M Constantinescu, Alp Dener, and Robert L Jacob. 2021. "Implicit-Explicit and Multirate methods for a Coupled Navier-Stokes Equations". In *American Geophysical Union Fall Meeting*. New Orleans, LA, USA.

Dener, Alp, Todd Munson, Marco Andres Miller, R Michael Churchill, and Choong-Seock Chang. 2021. "Toward Constrained Optimization in Machine Learning: An Error-Tolerant Multisecant Method for Training PINNs". In *SIAM Conference on Computational Science and Engineering (CSE21)*. Virtual.

Dener, Alp. 2020. "Investigating quasi-Newton Outer Product Representations on GPUs". In *SIAM Conference on Parallel Processing for Scientific Computing (PP20)*. Seattle, WA, USA.

Suh, Hansol, Alp Dener, Tobin Isaac, and Todd Munson. 2020. "Using the PETSc/TAO ADMM Methods on GPUs". In *SIAM Conference on Parallel Processing for Scientific Computing (PP20)*. Seattle, WA, USA.

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, Adam Denchfield, and Todd Munson. 2019. "Acelerating Quasi-Newton and Conjugate Gradient Convergence for Large-Scale Optimization". In *SIAM Conference on Computational Science and Engineering (CSE19)*. Spokane, WA, USA.

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.

Presentations

Conferences

Hang, Shinhoo, Emil M Constantinescu, Alp Dener, and Robert L Jacob. 2021. "Implicit-Explicit and Multirate methods for a Coupled Navier-Stokes Equations". In *American Geophysical Union Fall Meeting*. New Orleans, LA, USA.

Dener, Alp, Todd Munson, Marco Andres Miller, R Michael Churchill, and Choong-Seock Chang. 2021. "Toward Constrained Optimization in Machine Learning: An Error-Tolerant Multisecant Method for Training PINNs". In *SIAM Conference on Computational Science and Engineering (CSE21)*. Virtual.

Dener, Alp. 2020. "Investigating quasi-Newton Outer Product Representations on GPUs". In *SIAM Conference on Parallel Processing for Scientific Computing (PP20)*. Seattle, WA, USA.

Suh, Hansol, Alp Dener, Tobin Isaac, and Todd Munson. 2020. "Using the PETSc/TAO ADMM Methods on GPUs". In *SIAM Conference on Parallel Processing for Scientific Computing (PP20)*. Seattle, WA, USA.

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, Adam Denchfield, and Todd Munson. 2019. "Acelerating Quasi-Newton and Conjugate Gradient Convergence for Large-Scale Optimization". In *SIAM Conference on Computational Science and Engineering (CSE19)*. Spokane, WA, USA.

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.

Invited Talks

Dener, Alp. *Numerical optimization using PETSc/TAO*. ATPESC 2021.

Dener, Alp. *Large-scale optimization using PETSc/TAO*. ATPESC 2020.

Dener, Alp. *PDE-constrained optimization using PETSc/TAO*. ATPESC 2019.

Mills, Richard Tran, Matthew Knepley, Todd Munson, Alp Dener, and Hong Zhang. *PDEs, optimization, and eigenproblems with PETSc/TAO and SLEPc*. ECP Annual Meeting 2019.

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:** Scott Klasky (ORNL), **Role:** Senior Personnel, **Sponsor:** DOE-ASCR, DE-FOE-0002482, 2021, **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

Projects

ML-Collision: Approximating the Fokker-Planck-Landau Collision Operator with a PINN (gitlab.com/adener/ml-collision-python)

Python3

Creator, Maintainer, Developer — *Mar. 2020 - PRESENT*

- Using nuclear fusion simulation data to train an encoder-decoder DNN under physical conservation and entropy constraints to approximate the FPL operator.
- Developing a stochastic extension of the augmented Lagrangian method to train NNs with nonlinear constraints.
- Integrating trained model into the XGC1 nuclear fusion simulation to improve scaling and performance of particle collisions.

MADtorch: Multisecant Accelerated Descent Optimizer for PyTorch (gitlab.com/adener/madtorch)

Python3

Creator, Maintainer, Developer — *Feb. 2021 - PRESENT*

- Lead architect of a novel PyTorch optimizer for stochastic mini-batch training under general nonlinear constraints.
- Currently used in research efforts to accelerate large-scale nuclear fusion simulations using a physics-informed neural network.

TScoupled: Scalable Parallel Navier-Stokes Solver for Ocean-Atmosphere Interaction (gitlab.com/adener/tscoupled-petsc)

ANSI C / Python3

Creator, Maintainer, Developer — *Nov. 2020 - PRESENT*

- Ported a serial 2D N-S solver implemented in Julia to an equivalent scalable parallel implementation in ANSI C using PETSc/TAO.
- Solved an ocean-atmosphere interaction problem with velocity and temperature couplings at the boundary using the 4-stage Range-Kutta integrator in PETSc/TS.
- Currently extending the solver to handle 3D cases, and investigating multi-rate time integrators to iterate ocean and atmosphere sides at different rates.

TAOster & CUTEst: Framework for Testing TAO Optimization Solvers on Canonical CUTEst Benchmark Problems (gitlab.com/adener/TAOster & gitlab.com/adener/CUTEst)

Python3 / Fortran77

Creator, Maintainer, Developer — *Mar. 2019 - PRESENT*

- Defined interfaces for connecting TAO solvers to CUTEst problems via FORTRAN.
- Created Python scripts to control the execution flow of bulk test runs on CUTEst problems.

TAO: Toolkit for Advanced Optimization (gitlab.com/petsc/petsc)

ANSI C / Fortran90

Maintainer, Developer — *Feb. 2018 - PRESENT*

- 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.
- 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: Parallel Extensible Toolkit for Scientific Computing (gitlab.com/petsc/petsc)

ANSI C / Fortran90

Developer — *Feb. 2018 - PRESENT*

- Member of the core development team. Contributor and maintainer for new features required by TAO solvers.
- Implemented quasi-Newton Jacobian/Hessian approximations as abstract matrix objects used in both optimization and nonlinear solvers.
- 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.

MACH: MDO for Aircraft Configurations with High Fidelity (github.com/mdolab/MACH-Aero)

Python3 / C++11 / Fortran95

External Contributor — *Jun. 2014 - Dec. 2017*

- 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.

ElasticNozzleMDO: 2D Multidisciplinary Analysis and Optimization for an Elastic Nozzle (github.com/OptimalDesignLab/ElasticNozzleMDO)

C++11 / Python3

Developer — *Jan. 2013 - Dec. 2017*

- Developed a 2D linear elasticity model with finite-element analysis and coupled to a solver for quasi-1D Euler equations via fluid pressure force transfer.
- Implemented Python interfaces for the C++ solver using Boost.Python bindings to integrate solver into an optimization workflow.

Kona: A Parallel Optimization Framework for Engineering Design Problems (github.com/OptimalDesignLab/Kona)

Python3

Creator, Maintainer, Developer — *Jan. 2013 - Dec. 2017*

- Lead architect of the core optimization research library for Optimal Design Lab at RPI.
- Designed parallel-agnostic implementations of SQP methods using abstract data structured and reverse-communication-based linear algebra.

Teaching Experience

Rensselaer Polytechnic Institute *Troy, New York*

Guest Lecturer

- MANE 4280/6963 Design Optimization — Fall 2016, Fall 2017
- MANE 4060 Aerospace Structures & Materials — Fall 2012

Teaching Assistant

- MANE 4280/6963 Design Optimization — Fall 2016, Fall 2017
- ENGR 2530 Strength of Materials — Summer 2017
- MANE 4920 Aerospace Structures & Control Laboratory — Spring 2013
- MANE 4060 Aerospace Structures & Materials — Fall 2012
- MANE 4070 Aerodynamics I — Fall 2012

Professional Activities & Service

Review Committees

INFORMS, Mathematics of Optimization Research *2018 - PRESENT*
SIAM, Journal of Scientific Computing *2018 - PRESENT*
Springer, Optimization and Engineering *2018 - PRESENT*
AIAA, AIAA Journal *2018 - PRESENT*
US Dept. of Energy, SBIR Phase I Review Panel *2019*

Conferences

Minisymposium Organizer, SIAM Conference on Computational Science and Engineering *Mar. 2021*
Minisymposium Organizer, SIAM Conference on Computational Science and Engineering *Feb. 2019*

Argonne Training Program on Extereme Scale Computing

Member, ATPESC Program Committee *2021*
Lead Organizer, Numerical Algorithms & Software Track *2021*
Co-organizer & Lecturer, Numerical Algorithms & Software Track *2020*
Lecturer, Numerical Algorithms & Software Track *2019 - PRESENT*

Volunteering & Outreach

Invited Panelist, University of Pittsburgh Graduate Student Career Q&A *2021*
Questions Judge, NSF Science Bowl Illinois Regionals & Nationals *2021*

Professional Societies

MoS, Mathematical Optimization Society *2018 - PRESENT*
INFORMS, Institute for Operations Research and the Management Sciences *2018 - PRESENT*
SIAM, Society of Industrial and Applied Mathematics *2012 - PRESENT*
AIAA, American Institute of Aeronautics and Astronautics *2012 - PRESENT*

Supervised Students

Jamal Shabani, Lousiana State University *2021*
Hansol Suh, Georgia Institute of Technology *2019, 2021*