

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 for large-scale applications in artificial intelligence, machine learning, simulation-based design and scientific discovery. I am also a member of the core development team for PETSc/TAO, one of the premiere numerical libraries in the US Department of Energy research software portfolio. In this capacity, I develop and maintain parallel implementations of optimization algorithms using test-based development and CI/CD workflows on heterogeneous high-performance computing systems.

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

ASSISTANT COMPUTATIONAL SCIENTIST

Lemont, Illinois

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

GRADUATE RESEARCH AND TEACHING ASSISTANT

Troy, New York

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

UNDERGRADUATE RESEARCH ASSISTANT & MACHINIST

Maryland, Baltimore

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

AERODYNAMIC ANALYSIS AND DESIGN INTERN

Ankara, Turkey

Jun. 2009 - Sep. 2009

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

Education

Rensselaer Polytechnic Institute

PH.D. IN AERONAUTICAL ENGINEERING

Troy, New York

Aug. 2012 - Dec. 2017

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

University of Maryland, Baltimore County

B.S. IN MECHANICAL ENGINEERING

Baltimore, Maryland

Jan. 2008 - May. 2012

Honors & Awards

- 2021 **Impact Award**, Enhancement of Argonne's Reputation – DoE National Science Bowl Volunteer
- 2018 **1st Place**, AIAA AVIATION 2018 Student Paper Competition – Multidisciplinary Design Optimization

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

- Developing stochastic extension of constrained optimization methods for training PINNs.
- Training an encoder-decoder DNN under physical conservation and entropy constraints using nuclear fusion simulation data.
- Integrating trained model into the XGC1 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

- Novel PyTorch optimizer based on Anderson mixing for stochastic mini-batch training with general nonlinear constraints.
- Currently used for training PINNs under physics-based constraints.

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 to PETSc code from a serial 2D N-S solver implemented in Julia.
- Solved an ocean-atmosphere interaction problem with velocity and temperature couplings at the boundary.
- Currently extending the solver to 3D and investigating solutions with multi-rate time integrators.

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

- Refactored existing NCG, QN and NEwton methods with active-set bound projections.
- Developed a diagonalized-QN preconditioner and sparse Hessian initialization for NCG and QN methods.
- Implemented a bound-constrained Gauss-Newton method with dictionary-based approximate L1 regularization.
- Supervised a summer student for developing an ADMM algorithm with closed-form solutions for common regularization terms.
- Currently developing new error-tolerant constrained optimization algorithms for solving problems with inaccurate/noisy gradients.
- Currently developing Python interfaces linking TAO with pyTorch for ML training problems.

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 optimization solvers.
- Unified QN methods in TAO and SNES with abstractions for QN Jacobian and Hessian approximations.
- Developed efficient parallel vector projection tools to support bound-constraint optimization methods.
- Spearheaded PETSc's transition to a CI/CD workflow with a Jenkins prototype.

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 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.

JOURNAL ARTICLES

- Mills, R. T., Adams, M. F., Balay, S., Brown, J., **Dener, A.**, Knepley, M., Kruger, S. E., Morgan, H., Munson, T., Rupp, K., Smith, B. F., Zampini, S., Zhang, H., and Zhang, J. (2021). “Toward performance-portable PETSc for GPU-based exascale systems (accepted)”. In: *IEEE Transactions on Parallel and Distributed Systems (Special Section on Innovative R&D toward the Exascale Era)*. doi: 10.1016/j.parco.2021.102831.
- Dener, A.**, Miller, M. A., Churchill, R. M., Munson, T., and Chang, C.-S. (2020). “Training neural networks under physical constraints using a stochastic augmented Lagrangian approach (submitted)”. In: *Journal of Computational Physics*. arXiv: 2009.07330.
- Miller, M. A., Churchill, R. M., **Dener, A.**, Chang, C.-S., Munson, T., and Hager, R. (2020). “Encoder-decoder neural network for solving the nonlinear Fokker-Planck-Landau collision operator in XGC”. In: *Journal of Plasma Physics*. doi: 10.1017/S0022377821000155.
- Dener, A.** and Hicken, J. E. (2017). “Matrix-free algorithm for the optimization of multidisciplinary systems”. In: *Structural and Multidisciplinary Optimization, Springer*. doi: 10.1007/s00158-017-1734-0.
- Hicken, J. E. and **Dener, A.** (2015). “A flexible iterative solver for nonconvex, equality-constrained quadratic subproblems”. In: *Journal on Scientific Computing, SIAM*. doi: 10.1137/140994496.

REFEREED PROCEEDINGS

- Dener, A.**, Munson, T., Miller, M. A., Churchill, R. M., and Chang, C.-S. (Mar. 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, A.** (Feb. 2020). “Investigating quasi-Newton Outer Product Representations on GPUs”. In: *SIAM Conference on Parallel Processing for Scientific Computing (PP20)*. Seattle, WA, USA.
- Suh, H., **Dener, A.**, Isaac, T., and Munson, T. (Feb. 2020). “Using the PETSc/TAO ADMM Methods on GPUs”. In: *SIAM Conference on Parallel Processing for Scientific Computing (PP20)*. Seattle, WA, USA.
- Dener, A.**, Denchfield, A., and Munson, T. (June 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, A.** and Munson, T. (June 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, A.**, Denchfield, A., and Munson, T. (Feb. 2019). “Accelerating Quasi-Newton and Conjugate Gradient Convergence for Large-Scale Optimization”. In: *SIAM Conference on Computational Science and Engineering (CSE19)*. Spokane, WA, USA.
- Dener, A.**, Hicken, J. E., Kenway, G. K. W., and Martins, J. R. R. A. (June 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, A.**, Meng, P., Hicken, J. E., Kennedy, G. J., Hwang, J., and Gray, J. S. (Jan. 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, A.**, Kenway, G. K. W., Hicken, J. E., and Martins, J. R. R. A. (Jan. 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, A.** and Hicken, J. E. (Jan. 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

- Dener, A.**, Denchfield, A., Suh, H., Munson, T., Sarich, J., Wild, S., Benson, B., and Curfman-McInnes, L. (2020). *TAO users manual*. ANL/MCS-TM-322 - Revision 3.14. Argonne National Laboratory.
- Balay, S.**, Abhyankar, S., Adams, M. F., Brown, J., Brune, P., Buschelman, K., Dalcin, L., Dener, A., Eijkhout, V., Gropp, W. D., Karpeyev, D., Kaushik, D., Knepley, M. G., May, D. A., Curfman-McInnes, L., Mills, Todd Munson, R. T., Rupp, K., Sanan, P., Smith, B. F., Zampini, S., Zhang, H., and Zhang, H. (2020). *PETSc users manual*. ANL-95/11 - Revision 3.14. Argonne National Laboratory.

Presentations

CONFERENCES

- Dener, A.**, Munson, T., Miller, M. A., Churchill, R. M., and Chang, C.-S. (Mar. 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, A.** (Feb. 2020). “Investigating quasi-Newton Outer Product Representations on GPUs”. In: *SIAM Conference on Parallel Processing for Scientific Computing (PP20)*. Seattle, WA, USA.
- Suh, H., **Dener, A.**, Isaac, T., and Munson, T. (Feb. 2020). “Using the PETSc/TAO ADMM Methods on GPUs”. In: *SIAM Conference on Parallel Processing for Scientific Computing (PP20)*. Seattle, WA, USA.
- Dener, A.**, Denchfield, A., and Munson, T. (June 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, A.** and Munson, T. (June 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, A.**, Denchfield, A., and Munson, T. (Feb. 2019). “Accelerating Quasi-Newton and Conjugate Gradient Convergence for Large-Scale Optimization”. In: *SIAM Conference on Computational Science and Engineering (CSE19)*. Spokane, WA, USA.
- Dener, A.**, Hicken, J. E., Kenway, G. K. W., and Martins, J. R. R. A. (June 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, A.**, Meng, P., Hicken, J. E., Kennedy, G. J., Hwang, J., and Gray, J. S. (Jan. 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, A.**, Kenway, G. K. W., Hicken, J. E., and Martins, J. R. R. A. (Jan. 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, A.** and Hicken, J. E. (Jan. 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, A.** (n.d.). *Numerical optimization using PETSc/TAO*. ATPESC 2021.
- Dener, A.** (n.d.). *Large-scale optimization using PETSc/TAO*. ATPESC 2020.
- Dener, A.** (n.d.). *PDE-constrained optimization using PETSc/TAO*. ATPESC 2019.
- Mills, R. T., Knepley, M., Munson, T., **Dener, A.**, and Zhang, H. (n.d.). *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

Teaching Experience

Rensselaer Polytechnic Institute

Troy, New York

GUEST LECTURER

- MANE 4280/6963 Design Optimization
- MANE 4060 Aerospace Structures & Materials

Fall 2016, Fall 2017
Fall 2012

TEACHING ASSISTANT

- MANE 4280/6963 Design Optimization
- ENGR 2530 Strength of Materials
- MANE 4920 Aerospace Structures & Control Laboratory
- MANE 4060 Aerospace Structures & Materials
- MANE 4070 Aerodynamics I

Fall 2016, Fall 2017
Summer 2017
Spring 2013
Fall 2012
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 EXTREME SCALE COMPUTING

Member, ATPESC Program Committee

2021

Lead Organizer, Numerical Algorithms & Software Track

2021

Co-organizer, 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, DoE 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, Louisiana State University

2021

Hansol Suh, Georgia Institute of Technology

2019, 2021