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 — ***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 Mangusta attack helicopter 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 – 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.

Publications

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). "Acelerating 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). "Acelerating 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 — 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 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, Lousiana State University *2021*
Hansol Suh, Georgia Institute of Technology *2019, 2021*