# Alp Dener

COMPUTATIONAL SCIENCE · NUMERICAL OPTIMIZATION · HIGH-PERFORMANCE COMPUTING · AI / ML

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# Summary \_

Passionate computational scientist specializing on large-scale gradient-based optimization algorithms and their applications in scientific discovery, engineering design, artificial intelligence and machine learning problems. Extensive experience developing high-quality scientific software on heterogeneous high-performance computing systems, with significant contributions to large open source projects.

# Skills

Numerical Optimization
Machine Learning
Machine Learning
Software Development

PDE-constrained Problems, Gradient-based Algorithms, Multidisciplinary Design Optimization
Physics-Informed Neural Networks, Constrained Training Methods, Supervised Learning
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 \_\_\_\_

GraphCore Palo Alto, California

Al Applications Specialist Dec. 2021 - Present

- · Help GraphCore customers solve challenging artificial intelligence and machine learning problems using GraphCore IPUs.
- · Optimize the poplar SDK to improve GraphCore IPU performance on MLPerf benchmark problems.

#### **Argonne National Laboratory**

Lemont, Illinois

ASSISTANT COMPUTATIONAL SCIENTIST

Oct. 2021 - Nov. 2021

POSTDOCTORAL RESEARCHER

Feb. 2018 - Sep. 2021

- · 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.

#### **Rensselaer Polytechnic Institute**

Troy, New York

GRADUATE RESEARCH AND TEACHING ASSISTANT

Aug. 2012 - Dec. 2017

- $\bullet \ \ {\sf Researched\ simulation-driven\ multidisciplinary\ design\ optimization\ problems}.$
- 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

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**Projects** 

#### ML-Collision: Approximating the Fokker-Planck-Landau Collision Operator with a PINN

Python3

(gitlab.com/adener/ml-collision-python)

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 (gittab.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

ANSI C / Python3

(gitlab.com/adener/tscoupled-petsc)

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

C++11 / Python3

(github.com/OptimalDesignLab/ElasticNozzleMDO)

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

Python3

(github.com/OptimalDesignLab/Kona)

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.

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# **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. "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)* (2021). https://doi.org/10.1016/j.parco.2021.102831.
- **Dener**, **A.**, Miller, M. A., Churchill, R. M., Munson, T., and Chang, C.-S. "Training neural networks under physical constraints using a stochastic augmented Lagrangian approach (submitted)". *Journal of Computational Physics* (2021). arXiv: 2009.07330.
- Miller, M. A., Churchill, R. M., **Dener**, **A.**, Chang, C.-S., Munson, T., and Hager, R. "Encoder-decoder neural network for solving the nonlinear Fokker-Planck-Landau collision operator in XGC". *Journal of Plasma Physics* (2020). https://doi.org/10.1017/S0022377821000155.
- **Dener**, **A.** and Hicken, J. E. "Matrix-free algorithm for the optimization of multidisciplinary systems". *Structural and Multidisciplinary Optimization*, *Springer* (2017). https://doi.org/10.1007/s00158-017-1734-0.
- **Hicken**, **J. E.** and Dener, A. "A flexible iterative solver for nonconvex, equality-constrained quadratic subproblems". *Journal on Scientific Computing*, *SIAM* (2015). https://doi.org/10.1137/140994496.

#### REFEREED PROCEEDINGS

- **Dener**, **A.**, Munson, T., Miller, M. A., Churchill, R. M., and Chang, C.-S. "Toward Constrained Optimization in Machine Learning: An Error-Tolerant Multisecant Method for Training PINNs". In *SIAM Conference on Computational Science and Engineering*. Virtual, Mar. 2021.
- **Dener**, **A.** "Investigating quasi-Newton Outer Product Representations on GPUs". In SIAM Conference on Parallel Processing for Scientific Computing. Seattle, WA, USA, Feb. 2020.
- Suh, H., **Dener**, **A.**, Isaac, T., and Munson, T. "Using the PETSc/TAO ADMM Methods on GPUs". In *SIAM Conference on Parallel Processing for Scientific Computing*. Seattle, WA, USA, Feb. 2020.
- **Dener**, **A.**, Denchfield, A., and Munson, T. "Preconditioning nonlinear conjugate gradient with diagonalized quasi-Newton". In *Proceedings for the Platform for Advanced Scientific Computing Conference*. Zurich, Switzerland, June 2019. https://doi.org/10.1145/3324989.3325712.
- **Dener**, **A.** and Munson, T. "Accelerating limited-memory quasi-Newton convergence for large-scale optimization". In *International Conference on Computational Science*. Faro, Portugal, June 2019. https://doi.org/10.1007/978-3-030-22744-9\_39.
- **Dener**, **A.**, Denchfield, A., and Munson, T. "Acelerating Quasi-Newton and Conjugate Gradient Convergence for Large-Scale Optimization". In *SIAM Conference on Computational Science and Engineering*. Spokane, WA, USA, Feb. 2019.
- **Dener**, **A.**, Hicken, J. E., Kenway, G. K. W., and Martins, J. R. R. A. "Enabling modular aerostructural optimization: Individual discipline feasible without the Jacobians". In *2018 Multidisciplinary Analysis and Optimization Conference*, *AIAA AVIATION Forum*. Atlanta, GA, USA, June 2018. https://doi.org/10.2514/6.2018-3570.
- **Dener**, **A.**, Meng, P., Hicken, J. E., Kennedy, G. J., Hwang, J., and Gray, J. S. "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, Jan. 2016. https://doi.org/10.2514/6.2016-1422.
- **Dener**, **A.**, Kenway, G. K. W., Hicken, J. E., and Martins, J. R. R. A. "Comparison of inexact- and quasi-Newton algorithms for aerodynamic shape optimization". In *53rd AIAA Aerospace Sciences Meeting, AIAA SciTech Forum*. Kissimmee, FL, USA, Jan. 2015. https://doi.org/10.2514/6.2015-1945.
- **Dener**, **A.** and Hicken, J. E. "Revisiting individual discipline feasible with matrix-free inexact-Newton-Krylov". In *10th AIAA Multidisciplinary Design Optimization Conference*, *AIAA SciTech Forum*. National Harbor, MD, USA, Jan. 2014. https://doi.org/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. *TAO users manual*. Tech. rep. ANL/MCS-TM-322 Revision 3.14. Argonne National Laboratory, 2020.
- 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. *PETSc users manual*. Tech. rep. ANL-95/11 Revision 3.14. Argonne National Laboratory, 2020.

#### **PREPRINTS**

Hicken, J. E., Meng, P., and **Dener**, **A.** "Error-tolerant multisecant method for nonlinearly constrained optimization". *arXiv* preprint (2017). arXiv: 1709.06985.

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#### **Presentations**

#### **CONFERENCES**

- **Dener**, **A.**, Munson, T., Miller, M. A., Churchill, R. M., and Chang, C.-S. "Toward Constrained Optimization in Machine Learning: An Error-Tolerant Multisecant Method for Training PINNs". In *SIAM Conference on Computational Science and Engineering*. Virtual, Mar. 2021.
- **Dener**, **A.** "Investigating quasi-Newton Outer Product Representations on GPUs". In SIAM Conference on Parallel Processing for Scientific Computing. Seattle, WA, USA, Feb. 2020.
- Suh, H., **Dener**, **A.**, Isaac, T., and Munson, T. "Using the PETSc/TAO ADMM Methods on GPUs". In *SIAM Conference on Parallel Processing for Scientific Computing*. Seattle, WA, USA, Feb. 2020.
- **Dener**, **A.**, Denchfield, A., and Munson, T. "Preconditioning nonlinear conjugate gradient with diagonalized quasi-Newton". In *Proceedings for the Platform for Advanced Scientific Computing Conference*. Zurich, Switzerland, June 2019. https://doi.org/10.1145/3324989.3325712.
- **Dener**, **A.** and Munson, T. "Accelerating limited-memory quasi-Newton convergence for large-scale optimization". In *International Conference on Computational Science*. Faro, Portugal, June 2019. https://doi.org/10.1007/978-3-030-22744-9\_39.
- **Dener**, **A.**, Denchfield, A., and Munson, T. "Acelerating Quasi-Newton and Conjugate Gradient Convergence for Large-Scale Optimization". In *SIAM Conference on Computational Science and Engineering*. Spokane, WA, USA, Feb. 2019.
- **Dener**, **A.**, Hicken, J. E., Kenway, G. K. W., and Martins, J. R. R. A. "Enabling modular aerostructural optimization: Individual discipline feasible without the Jacobians". In *2018 Multidisciplinary Analysis and Optimization Conference, AIAA AVIATION Forum*. Atlanta, GA, USA, June 2018. https://doi.org/10.2514/6.2018-3570.
- **Dener**, **A.**, Meng, P., Hicken, J. E., Kennedy, G. J., Hwang, J., and Gray, J. S. "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, Jan. 2016. https://doi.org/10.2514/6.2016-1422.
- **Dener**, **A.**, Kenway, G. K. W., Hicken, J. E., and Martins, J. R. R. A. "Comparison of inexact- and quasi-Newton algorithms for aerodynamic shape optimization". In *53rd AIAA Aerospace Sciences Meeting, AIAA SciTech Forum*. Kissimmee, FL, USA, Jan. 2015. https://doi.org/10.2514/6.2015-1945.
- **Dener**, **A.** and Hicken, J. E. "Revisiting individual discipline feasible with matrix-free inexact-Newton-Krylov". In *10th AIAA Multidisciplinary Design Optimization Conference*, *AIAA SciTech Forum*. National Harbor, MD, USA, Jan. 2014. https://doi.org/10. 2514/6.2014-0110.

#### INVITED TALKS

- Dener, A. Numerical optimization using PETSc/TAO. ATPESC 2021, Aug. 2021.
- Dener, A. Large-scale optimization using PETSc/TAO. ATPESC 2020, Aug. 2020.
- Dener, A. PDE-constrained optimization using PETSc/TAO. ATPESC 2019, Aug. 2019.
- Mills, R. T., Knepley, M., Munson, T., **Dener**, **A.**, and Zhang, H. *PDEs*, *optimization*, *and eigenproblems with PETSc/TAO and SLEPc*. ECP Annual Meeting 2019, Jan. 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

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# Teaching Experience \_\_\_\_\_

ensselaer Polytechnic Institute	Troy, New York
JEST LECTURER	
MANE 4280/6963 Design Optimization	Fall 2016, Fall 2017
MANE 4060 Aerospace Structures & Materials	Fall 2012
aching Assistant	_ ,, _ , _ , _ , _ , _ , _ , _ , _ , _
MANE 4280/6963 Design Optimization ENGR 2530 Strength of Materials	Fall 2016, Fall 2017 Summer 2017
MANE 4920 Aerospace Structures & Control Laboratory	Spring 2013
MANE 4060 Aerospace Structures & Materials	Fall 2012
MANE 4070 Aerodynamics I	Fall 2012
rofessional Activities & Service	
EVIEW 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
ONFERENCES	
Minisymposium Organizer, SIAM Conference on Computational Science and Engineering	Mar. 2021
Minisymposium Organizer, SIAM Conference on Computational Science and Engineering	Feb. 2019
RGONNE 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
<b>Lecturer</b> , Numerical Algorithms & Software Track	2019 - Present
olunteering & Outreach	
Invited Panelist, University of Pittsburgh Graduate Student Career Q&A	2021
Questions Judge, DoE Science Bowl Illinois Regionals & Nationals	2021
rofessional Societies	
MOS, Mathematical Optimization Society	2018 - Present
INFORMS, Institute for Operations Research and the Management Sciences	2018 - Present
<b>SIAM</b> , Society of Industrial and Applied Mathematics	2012 - Present
AIAA, American Institute of Aeronautics and Astronautics	2012 - Present
UPERVISED STUDENTS	
Jamal Shabani, Lousiana State University	2021
Hansol Suh, Georgia Institute of Technology	2019, 2021

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