Alexander D. Greenhalgh

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Educational Background

Georgia Institute of Technology, M.S. in Computer Science — Aug. 2023 - May 2025
Machine Learning Concentration — GPA: **4.00/4.00**

- *Coursework: Machine Learning, Deep Learning, Graduate Algorithms.*
- *Academic Integrity TA: Machine Learning for Trading, Software Development/Architecture Processes.*

New Mexico State University, M.Eng. in Industrial Engineering — Aug. 2023 - Dec. 2024
Department of Industrial Engineering — GPA: **4.00/4.00**

- *Coursework: Linear Programming, Stochastic Simulation, Optimization.*
- *ORSA Military Applications Course: 14 Week Operations Research Training at Army Logistics University.*

The University of Tennessee, B.S. Materials Science and Engineering — Aug. 2019 - May 2023
Minors: Computer Science and Mathematics — GPA: **3.88/4.00**

- *Coursework: Materials, Thermodynamics, Algorithms, Scientific Computing, Machine Learning.*
- *Additional: Summa Cum Laude, Distinction in Undergraduate Research, Cook Grand Challenge Honors.*

Honors and Awards

- Presidential PhD Fellowship, Georgia Institute of Technology, August 2025
- Civilian Service Commendation Medal, Department of the Army, April 2025
- OMSCS Project Showcase Student's Choice Award Winner, April 2025
- Undergraduate Researcher of the Year, University of Tennessee, May 2023
- Goldwater Scholar, Barry Goldwater Scholarship Foundation, March 2022
- ASM International Oak Ridge Chapter Undergraduate Poster Contest Finalist, February 2022
- DOD Science, Mathematics, and Research for Transformation (SMART) Scholarship, April 2021
- Consortium for Enabling Technologies & Innovation (ETI) Undergraduate Fellowship Award, Georgia Institute of Technology, March 2021
- Eagle Scout, Boy Scouts of America, March 2018

Professional Experience

Operations Research Analyst — June 2022 - August 2022, July 2023-September 2025
Maneuver Division – The Research and Analysis Center - Army Futures Command

- Developed operational combat models for simulation in Python with Apache SVN version control in Linux environment.
- Designed and built a large language model chatbot in Python for tactical Q&A using LangChain for vector embeddings and OpenAI API. Model trained on Army Doctrine Manuals scraped with BeautifulSoup.
- Performed Design of Experiments to compare the effectiveness of several combat vehicle platforms through combat modeling. Results presented to Army leadership and used to inform Pentagon G-8 billion-dollar yearly acquisition budget.
- Built interactive visualization dashboards in Bokeh package in Python to convey operational modeling results to Army Senior Leaders.

Computational Material Science Research October 2019 – May 2023

Advisor: Prof. David Keffer and Dr. Dayton Kizzire at UT-MSE

- Research project #1: Developed method to statistically characterize chemical ordering in Atom Probe Tomography (APT) data sets of high entropy alloys.
  - Created MATLAB program to visualize and quantify atomic ordering through manipulation of Radial Distribution function.
  - Generated Radial Distribution Functions for APT and synthetic data sets using FORTRAN
  - Analyzed APT data from ORNL with new visualization technique to display presence of nanoprecipitates in a High Entropy Alloy.
- Research project #2: Classical Molecular Dynamics simulations and minimizations to attain mechanical and thermodynamic properties of Aluminum alloys in preparation for testing Cerium interatomic potential
  - Scientific Computing through ISAAC (Infrastructure for Scientific Applications and Advanced Computing), running simulations in a Linux environment with LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) software
  - Generated thermodynamic, mechanical, structural, and transport properties for aluminum and aluminum alloy $Mg_{12}Al_{17}$ (cohesive energy, thermal expansivity, elastic constants, thermal conductivity, etc.)
- Research project #3: Automation of interatomic potential property calculations with Python for development of optimized Cerium potential.
  - Designed high performance computing Molecular Dynamics automation workflow with Bash, LAMMPS, and Python (NumPy, matplotlib), enabling Molecular Dynamics calculation of thermodynamic, mechanical, and transport properties of a new interatomic potentials.
  - Developed novel Machine Learning optimization algorithm to parameterize interatomic potentials.
  - Implemented parallelized novel optimization algorithm through mpi4py, VASP to discover interatomic potential of Cerium.

DOE Science Undergraduate Laboratory Internship June 2021 - August 2021

Advisor: Dr. Yuanpeng Zhang at Oak Ridge National Laboratory

- Continued development of the ADvanced DIffraction Environment, a GUI to integrate the NOMAD Diffractometer into the Manipulation and Analysis Toolkit for Instrument Data (Mantid) framework at the Spallation Neutron Source.
- Enabled access of raw neutron data to scientific community of 1000 yearly experimental SNS users with open-source project.
- Integrated **PyQt** GUI data with backend Neutron Diffraction Fourier Transform codes for data reduction.

Projects

High-Entropy Alloy Strength Prediction: Spring 2023

- XGBoost model for joint optimization of yield strength and ductility. Testing accuracy of **90.1%.**
- Trained on High-Entropy Alloy Database extracted from experimental literature.

Language Translation Task: Fall 2023

- Implementation of LSTM, Seq2Seq, and Transformer Architectures with PyTorch for English to German Translation Task.
- Transformer Attention mechanism from Vaswani et al.'s "*Attention Is All You Need".*
- Trained on dataset of 31014 sentences with testing perplexity of 4.81.

Autonomous AI Algorithms: Spring 2024

- A-star, PID control, Particle/Kalman Filters, Simultaneous Localization and Mapping (SLAM).

Trainings

Army Logistics University, ORSA Military Applications Course Fall 2023

- 14 Week Training covering foundations of military operations research.
- Operational combat modeling, stochastic simulation, data analysis, probability/statistics.

Skills

Languages and Software

- Python (PyTorch, NumPy, Pandas, sklearn), C++, R, MATLAB, Linux, Bash, JavaScript, FORTRAN, Git.
- LAMMPS Classical Molecular Dynamics Software.
- OVITO Molecular visualization software.

Publications

Archived journal articles

- Kizzire, D.G., Greenhalgh, A.D., Neveau, M.L., Pekol, C.M., Thompson, M.J., Rios, O., Keffer, D.J., "Modified Embedded Atom Method Interatomic Potential for FCC γ-Cerium", *Computational Materials Science* 230, article # 112454, 2023, pp. 1-9. doi: 10.1016/j.commatsci.2023.112454.
- Greenhalgh, A.D., Sanjeewa, L.D., Luszczek, P., Maroulas, V., Rios, O, Keffer, D.J., "Assessment of Local Observation of Atomic Ordering in Alloys via the Radial Distribution Function: A Computational and Experimental Approach", *Frontiers in Materials*, December, 2021.†
- Biewer, T., Smith, C., Gebhart, T., Greenhalgh, A.D., Ren, X., & Thomas, C. "Considerations for in situ, real time measurement of plasma-material interactions using Digital Holographic imaging," *Journal of Instrumentation*, 15(2), C02017–C02017, February, 2020.

Presentations

Oral

- Sanjeewa, L.D., Greenhalgh, A., Rios, O., Luszczek, P., Maroulas, V., Keffer, D.J., "Local Observation of Atomic ordering in Alloys via the Radial Distribution Function: A Computational and Experimental Approach", SIAM Conference on Mathematical Aspects of Materials Science - MS 21, May, 2021, Madrid (virtual).
- Keffer, D.J., Spannaus, A., Greenhalgh, A., Maroulas, V., Luszczek, P., Liaw, P.K., "Generating Intermolecular Potentials from Atom Probe Tomography Experiments", AIChE Annual Meeting, Nov. 2020, San Francisco, CA.

Poster

- Alex Greenhalgh, Kylie Berry, Makenna Curcuru, Jonathan Landry, Baldur Steingrimsson, Peter Liaw, "Optimization of Refractory High-Entropy Alloy Strength and Ductility through a Predictive Development Process," International Conference on High-Entropy Materials, Knoxville TN, June 2023.
- Alex Greenhalgh, Dayton Kizzire, David Keffer, "Modified embedded atom method atomic potential for pure Cerium to facilitate AlCe characterization," Exhibition of Undergraduate Research and Creative Achievement (EUReCA), Research Poster Contest, Knoxville TN, April 2023.
- Alex Greenhalgh, Dayton Kizzire, David Keffer, "Modified embedded atom method atomic potential for pure Cerium to facilitate AlCe characterization," Exhibition of Undergraduate Research and Creative Achievement (EUReCA), Research Poster Contest, Knoxville TN, April 2023.
- Alex Greenhalgh, Dayton Kizzire, David Keffer, "Modified embedded atom method atomic potential for pure Cerium to facilitate AlCe characterization," Center for Materials Processing Student Poster Night, Knoxville, TN, February 2023.

- Alex Greenhalgh, David Keffer, “Assessment of Atomic Ordering in Alloys,” ASM International Oak Ridge Chapter Student Poster Night, Knoxville, TN, April 2022.
- Alex Greenhalgh, David Keffer, “Assessment of Atomic Ordering in Alloys,” ASM International Oak Ridge Chapter Student Poster Night, Knoxville, TN, February 2022.
- Alex Greenhalgh, Yuanpeng Zhang, “A New Data Reduction Environment for Neutron Diffraction Data,” ORNL SULI Poster Session, Oak Ridge, TN, August 2021.
- Alex Greenhalgh, David Keffer, “Energy and Entropy of Defect Formation in Crystalline Solids,” Exhibition of Undergraduate Research and Creative Achievement (EUReCA), Research Poster Contest, Knoxville TN, April 2021.
- Alex Greenhalgh, David Keffer, “Material Properties through LAMMPS Molecular Dynamics Simulation,” ASM International Oak Ridge Chapter Student Poster Night, Knoxville, TN, October 2020.
- Alex Greenhalgh, David Keffer, “Visualization and Metrics of Atomic Ordering,” Exhibition of Undergraduate Research and Creative Achievement (EUReCA), Research Poster Contest, Knoxville TN, April 2020.
- Alex Greenhalgh, Theodore Biewer, “Simulation of Surface Damage by Laser Ablation to Material Targets as Proxy for Plasma Exposure Erosion,” ORNL Undergraduate Poster Session, Oak Ridge, TN, August 2019.

Extracurricular Activities

- Eagle Scout Project, Chapel on the Hill Nursery School, August 2017
    - Designed detailed schematics leading to creation of functional play kitchen and drainage system for nonprofit organization
    - Organized supply drive from group of 150 individuals for necessary materials.
    - Led group of 30 volunteers in the creation of kitchen from collected supplies.
- Trek Backpacking: Tour du Mont Blanc, Sections of Appalachian Trail.
- Certified Open Water Diver, PADI International