ERDEM CALISKAN (U.S. PERSON)

GRO Intern, Oak Ridge National Laboratory
Ph.D. Candidate, Mechanical Engineering, The University of Tennessee, Knoxville
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SUMMARY

Ph.D. Candidate specializing in high-rate dynamics, failure of ceramics/metals, and resonant metamaterials under impact/blast. Expertise in numerical PDE solvers and scalable HPC workflows. Developing robust graph neural networks for microstructure-to-property prediction with uncertainty quantification, achieving state-of-the-art accuracy. Proficient with open-source scientific software and in-house code development.

RESEARCH INTERESTS

- Graph neural networks for microstructure-to-property prediction in polycrystalline alloys and fiber composites
- High-strain-rate dynamics and failure of heterogeneous materials (metals, ceramics, composites)
- Design and dynamic response analysis of locally resonant metamaterials under impact and blast loading
- Uncertainty quantification in machine-learning surrogates for elastic-plastic and fatigue indicator parameters
- Multiscale computational mechanics using finite-element, discontinuous Galerkin, and phase-field methods
- Scalable high-performance computing workflows for materials simulations

EXPERIENCE

GRO Intern, Oak Ridge National Laboratory May 2024 – Dec 2024; May 2025 – present
Computational Coupled Physics, CSED, CCSD *Mentor: Massimiliano Lupo Pasini*

- Building microstructure-to-property workflows using graph neural networks for composites and polycrystals.
- Developing elastic/plastic multitask GNN surrogates incorporating aleatoric uncertainty for fatigue.
- Enhanced accuracy for stiffness tensor, while using 160x fewer parameters than CNNs.
- Improved accuracy 3x with microstructure feature engineering.
- Outperforms CNN peak-strength predictions, achieving 2x better accuracy with 12x fewer parameters.
- Improved robustness for extreme material contrasts via physics-based normalization.
- Developed multitask GNNs for polycrystals to predict 12 elastic-plastic QoIs & stress–strain curves.
- The model is used to construct statistically consistent random fields for mesoscale fatigue/damage studies.
- Carried out code reviews for HydraGNN and contributed to maintenance and quality improvements.

Graduate Research Assistant, The University of Tennessee, Knoxville Jan 2022 – present
Department of Mechanical and Aerospace Engineering *Advisor: Prof. Reza Abedi*

- Conducted nonlinear high-strain-rate simulations of locally resonant metamaterials (MM) under impact/blast.
- Studied a ceramic MM with local resonance that slows down the wave by 5x vs. conventional materials.
- Designed a graded MM that can reduce energy transfer by 6x compared to a uniform MM.
- Incorporated material damping, which amplifies MM performance up to 4x vs. monolithic slabs.
- Implemented UMAT & postprocessing workflows supporting parametric studies with hundreds of simulations.
- Incorporated residual eigenstrain into an Abaqus UEL phase-field subroutine to incorporate thermal effects.
- Studied a 1D discontinuous Galerkin solver in C++ for formulation comparison.
- Delivered arbitrary Lagrangian-Eulerian (ALE) simulations to investigate fluid–microstructure.
- Trained my PhD group on HPC, maintained an HPC environment(compiling, benchmarking, troubleshooting).

Mechanical Engineer, ITUNOVA Technologies Mar 2020 – Feb 2021

· Managed multiphysics CAE workflows for a high-performance turbopump, spanning structural, thermal, fatigue, and dynamics, resulting in an optimized turbopump design meeting structural requirements.

Intern, Baykar Technologies Aug – Sep 2019

· Performed structural analysis for composite control surfaces; modeled and analyzed structural components.

Intern, Turkish Aerospace Industries - ITU Very Light Aircraft Project Aug 2018 – Aug 2019

· Set up global FEM models and studied sizing for composite structures in a very light aircraft (VLA).
· Carried out buckling, crippling, and stability checks (Bruhn, Niu, Roark; EASA CS-23, FAA FAR 23).

Student Organization Member, ITU Facilis Vehicle Team Sep 2016 – Mar 2020

· Led structural analyses for a composite monocoque and subsystems, and CFD for the body; carried out composite manufacturing in the workshop; conducted structural tests. The vehicle achieved 1000 mpg.
· Team manager in 2020 Season, management of finances, project time plans, and headcount.
· Participating in the race events of Shell Eco-marathon Europe 2018 and 2019 in London, UK

EDUCATION

Ph.D., Mechanical Engineering *University of Tennessee, Knoxville*, Jan 2022 – Jul 2026 (Expected)
Minor: Interdisciplinary Graduate Minor in Computational Science (IGMCS) GPA: 4.00/4.00
Thesis: Microstructure as a Graph: Surrogates for Elastic and Failure Responses
Committee: Professors Reza Abedi, Stephanie TerMaath, Sergei Kalinin, and Dr. Massimiliano Lupo Pasini
Selected courses: Nonlinear FEM (Timothy Truster), DG (Reza Abedi), ML for Materials (Sergei Kalinin)

M.Sc., Solid Mechanics *Istanbul Technical University*, Feb 2020 – Nov 2021
Thesis: Mechanical Properties of Boron Nanotubes GPA: 3.56/4.00
Advisor: Prof. Mesut Kirca

B.Sc., Mechanical Engineering *Istanbul Technical University*, Aug 2015 – Feb 2020
Thesis: Design of Composite Monocoque Body for Lightweight Gasoline Vehicles
Advisor: Prof. Atakan Altinkaynak

SKILLS

Simulation/CAE	LS-DYNA, Abaqus, Ansys, COMSOL, SolidWorks, Siemens NX, nCode, NASGRO
User subroutines	LS-DYNA UMAT, Abaqus UEL (FORTRAN), MATLAB
In-house coding	DG/FEM/FV solvers (C++/Python), phase-field implementations
ML/AI	HydraGNN, PyTorch, PyTorch Geometric; uncertainty modeling
HPC	Linux, Slurm, MPI, OpenMP; build systems (CMake)
Open source	deal.II, OpenFOAM, LAMMPS; scientific stack (NumPy, pandas, scikit-learn)

RESEARCH PROJECTS

· Innovative Material Systems for Engaging Ballistic Energy
Jan 2022 – Jan 2025, *PIs:* Alireza Amirkhizi (UML) and Reza Abedi, *Funding Agency:* ARL
· Graph Neural Networks for Material Property Prediction
May 2024 – present, *PI:* Massimiliano Lupo Pasini, *Funding Agency:* ORNL, ORISE
· A microstructure-informed and statistical analysis of plasticity and fatigue crack nucleation and propagation
Jan 2025 – present, *PIs:* Reza Abedi and Stephanie TerMaath, *Funding Agency:* AFOSR
· Acoustical Investigation of Nanoporous Materials by Using Molecular Dynamics Method
May 2018 – Mar 2020, *PI:* Mesut Kirca, *Funding Agency:* TUBITAK

AWARDS & SCHOLARSHIPS

- UTK Graduate Student Senate Travel Award: Spring 2023, Summer 2024, Fall 2025
- Graduate School Fellowship, Summer 2023
- **2nd place**, 5 Minute Thesis Competition - BASARIM 2022 - 7^{th} High-Performance Computing Conference, 2022, organized with the cooperation of Turkish Academic Network and Information Center (ULAKBIM), Sabanci University, Middle East Technical University (METU), and the support of the EuroCC@Turkey.
  - Masters and PhD combined thesis competition in the largest HPC conference in Turkiye. Presented benchmarks for distributed and shared memory parallelism for different architectures. *Presentation*
- High-Performance Computing (HPC) resource scholar at UHeM and TRUBA (2020 – 2022)

AWARDS & SERVICE

- UTK Graduate Student Senate Travel Award: 2023, 2024, 2025, Graduate School Fellowship, Summer 2023
- **2nd place**, 5-Minute Thesis Competition - BASARIM 2022 - 7th High-Performance Computing Conference
- **Reviewer:** Mechanics of Materials; **Member:** Tau Beta Pi, USACM, ASME

PUBLICATIONS

Caliskan, E., Abedi, R. & Lupo Pasini, M. (2025). *Graph Neural Networks for Mechanical Property Prediction of 2D Fiber Composites. Materials & Design*, 114500. | *Link* | **IF: 7.9**

Caliskan, E., Cheney, W., Wang, W., Plaisted, T., Amirkhizi, A. V., & Abedi, R. (2026). *Time domain analysis of locally resonant elastic metamaterials under impact. Mechanics of Advanced Materials and Structures*, 33(1), 2619034. | *Link* | **IF: 3.6**

Abedi, R., Furey, C., Pourkamali-Anaraki, F., Huynh, G., **Caliskan, E.**, & Amirkhizi, A. V. (2025). *Analyzing fragmentation response of heterogeneous ring using the method of characteristics and machine learning techniques. Computer Methods in Applied Mechanics and Engineering*, 436, 117709. | *Link* | **IF: 7.3**

Caliskan, E., & Kirca, M. (2022). *Tensile characteristics of boron nanotubes by using reactive molecular dynamics simulations. Computational Materials Science*, 209, 111368. | *Link* | **IF: 3.3**

Under preparation

Cheney, W., Wang, W., Abedi, R., **Caliskan, E.**, & Amirkhizi, A. V. (under preparation, will be submitted by May) *Time Domain Parameter Extraction for High-Efficiency Reduced Order Models of Resonant Microstructured Media*

Caliskan, E., *et al., Multitask Graph Neural Networks for Elastic–Plastic Response Prediction in 2D Polycrystals* (under preparation, will be submitted by March)

CONFERENCES (SELECTED)

Presented 7; contributor on 20+. Presented at SES, IMECE, WCCM, USNCCM, and EMI.

(†) presenter

Erdem Caliskan†, Anik Das Anto, Reza Abedi, and Massimiliano Lupo Pasini. *Probabilistic multi-task graph neural network surrogates for elastic-plastic behavior and fatigue indicator prediction in polycrystalline alloys.* In SES Conference 2025, Atlanta, Georgia, USA, October 12-15, 2025.

Erdem Caliskan†, Weidi Wang, Willoughby Cheney, Alireza V. Amirkhizi, and Reza Abedi. *Transient nonlinear response of resonant metamaterial arrays under impact loading.* In 16th World Congress on Computational Mechanics and 4th Pan American Congress on Computational Mechanics, Vancouver, British Columbia, Canada, July 21-26, 2024