Tyler Joseph Grear

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Education

Ph.D. Bioinformatics and Computational Biology, Concentration: Molecular Biophysics — Sept. 2021 – May 2026
The University of North Carolina at Charlotte | GPA 3.84 — *Charlotte, NC*

Master of Science in Applied Physics — Sept. 2019 – Dec. 2021
The University of North Carolina at Charlotte | GPA 3.74 — *Charlotte, NC*

Bachelor of Science in Physics with Honors, Minor: Mathematics — June 2016 – May 2020
The University of North Carolina at Charlotte | GPA 3.29 — *Charlotte, NC*

12B Combat Engineer — Jan. 2009 – May 2009
United States Army, Advanced Individual Training (AIT) — *Fort Leonard Wood, MO*

Publications

- T. Grear, D. Jacobs (2026). "Quantifying the Peripheral Surface Information Entropy from Conformational Ensembles of Globular Protein-Peptide Complexes", *Biophysical Journal*. DOI: 10.1016/j.bpj.2026.06.036.
- T. Grear (2026). "Harnessing Peripheral Surface Information Entropy to Characterize Biomolecular Recognition and Osmotic Stress Response", *Ph.D. Dissertation*. The University of North Carolina at Charlotte. DOI: 10.13140/RG.2.2.32813.65765.
- J. Patterson, C. Avery, T. Grear, T. Frater, D. Jacobs (2024). "Leveraging the Twilight Zone of Protein Homology to Design Novel Binding Peptides", *Biophysical Journal*. Vol. 123(3): 472a. DOI: 10.1016/j.bpj.2023.11.2869.
- C. Avery[†], J. Patterson[†], T. Grear[†], T. Frater, D. Jacobs (2022). "Protein Function Analysis through Machine Learning", *Biomolecules*. Vol. 12(9): 1246. DOI: 10.3390/biom12091246. † These authors contributed equally to this work.
- J. Patterson[†], C. Avery[†], T. Grear, D. Jacobs (2021). "Biased Hypothesis Formation From Projection Pursuit", *Advances in Artificial Intelligence and Machine Learning*. Vol. 1(3): 221–233. DOI: 10.54364/AAIML.2021.1114.
- T. Grear (2021). "Supervised Projective Learning for Electroencephalography Analysis", *Master's Thesis*. The University of North Carolina at Charlotte. DOI: 10.13140/RG.2.2.25666.30404.
- T. Grear, D. Jacobs (2021). "Classifying EEG Motor Imagery Signals Using Supervised Projection Pursuit for Artefact Removal", *IEEE Systems, Man, and Cybernetics 2021 Conference*. Melbourne, Australia. DOI: 10.1109/SMC52423.2021.9659169.
- T. Grear, C. Avery, J. Patterson, D. Jacobs (2021). "Molecular Function Recognition by Supervised Projection Pursuit Machine Learning", *Nature Publishing Group: Scientific Reports*. DOI: 10.1038/s41598-021-83269-y.

Presentations

- T. Grear*, D. Jacobs (2026). "On the Peripheral Surface Information Entropy of Globular Protein-Peptide Complexes", *70th Biophysical Society Annual Meeting*. San Francisco, CA. *Speaker.
- J. Patterson, C. Avery, T. Grear, T. Frater*, D. Jacobs (2024). "Leveraging the Twilight Zone of Protein Homology to Design Novel Binding Peptides", *68th Biophysical Society Annual Meeting*. Philadelphia, PA. DOI: 10.13140/RG.2.2.28067.57128. *Speaker.
- C. Avery*, T. Grear, J. Patterson, N. Mauney, D. Jacobs (2023). "Toward Turn-Key Inhibitor Peptide Predictions for TEM Beta-Lactamases", *67th Biophysical Society Annual Meeting*. San Diego, CA. DOI: 10.13140/RG.2.2.21214.72007. *Speaker.
- D. Jacobs*, T. Grear, C. Avery (2022). "Supervised Projection Pursuit for Discriminant Analysis Through Machine Learning", *15th International Conference of the European Research Consortium for Informatics and Mathematics Working Group on Computational and Methodological Statistics (CMStatistics 2022)*. London, UK. DOI: 10.13140/RG.2.2.12470.00327. *Speaker.
- T. Grear*, D. Jacobs (2021). "Classifying EEG Motor Imagery Signals Using Supervised Projection Pursuit for Artefact Removal", *IEEE Systems, Man, and Cybernetics 2021 Conference - Brain-Machine Interface Workshop*. Presentation. URL: https://www.youtube.com/watchv=gLc3mF2rSxk. *Speaker.
- T. Grear*, C. Avery, D. Jacobs (2019). "Functional Dynamics Recognition by Machine Learning with Applications to Drug Discovery", *TechConnect World Innovation Conference*. Boston, MA. Presentation. DOI: 10.13140/RG.2.2.16160.53761. *Speaker.

Experience

Research Associate – The University of North Carolina at Charlotte — Nov. 2018 – Present
BioMolecular Physics Group (Lab Director: Professor Donald J. Jacobs) — *Charlotte, NC*

- Ran GPU-accelerated molecular dynamics simulations using OpenMM, GROMACS, CHARMM, and AMBER.
- Applied molecular docking tools (HADDOCK, RosettaDock, AutoDock Vina, DiffDock) to model protein-ligand interactions.
- Parameterized OpenFF forcefields for non-standard amino acids, small molecules, protein-DNA complexes, and fluorophores.
- Developed a projection pursuit machine learning framework to predict functional protein dynamics.
- Performed free-energy calculations, including MM(PB/GB)SA, free-energy perturbation (FEP), and alchemical replica exchange.
- Modeled and predicted peptide binding for intrinsically disordered regions of the p53 and MDM2 proteins.

Research Intern – Lawrence Livermore National Laboratory June 2025 – Sept. 2025

Computing Directorate – Computing Scholar Program *Livermore, CA*

- Performed research tasks in accordance with the Generative Unconstrained Intelligent Drug Engineering (GUIDE) mission directives, including molecular docking, free-energy calculations, and molecular dynamics simulations.
- Introduced a new metric derived from geometrically constrained spatial entropy, Distance-Dependent Entropy (DDE).
- Performed feature engineering to construct a Structural Interaction Fingerprint (SIF) library for machine learning models.

Physics Laboratory Instructor – The University of North Carolina at Charlotte Sept. 2020 – May 2022

Department of Physics and Optical Science *Charlotte, NC*

- Assisted with the construction of the undergraduate physics laboratory manual under the supervision of the dept. coordinator.
- Delivered lectures introducing lab-related theory and held office hours for problem-solving sessions.

Research Intern – National Aeronautics and Space Administration May 2021 – Aug. 2021

Goddard Space Flight Center - Global Modeling and Assimilation Office *Greenbelt, MD*

- Developed algorithms which reduced the time-complexity of radiative transfer calculations for atmospheric modeling/prediction.

Combat Engineer – United States Army Feb. 2009 – May 2012

572nd Mobility Augmentation Company, 8th Engineer Battalion, 36th Engineer Brigade *Fort Hood, TX*

- Authorized with a Secret security clearance. Provided countermobility, dismounted/mounted route clearance, and reconnaissance in support of Operation Enduring Freedom (OEF) within Logar, Paktika, Ghazni, and Kandahar Provinces, Afghanistan.
- Performed controlled demolition, mine warfare, and combat construction operations.
- Responsible for the maintenance and accountability of equipment valued in excess of $1,800,000.
- Conducted software and hardware updates for encrypted communications of platoon equipment and vehicles.

Technical Skills

- **Operating Systems** – Windows and Unix/Linux-based systems.
- **Programming Languages** – Python, Bash, MATLAB, GNU Octave, R, and C++.
- **Developer Tools** – OpenMM, OpenFF Toolkit, Tensorflow, Keras, Scipy, Scikit-Learn, Qiskit, GitHub, GitLab, tLEaP, ChemDraw, PyMOL, Chimera, Singularity, Podman, Docker, Cursor, AlphaFold/ColabFold, Jupyter Notebook, CUDA, and OpenCL.
- **HPC** – Experienced with high-performance computing and three workload management systems: TORQUE, SLURM, and FLUX.
- **Experimental** – Bruker Avance-III NMR spectroscopy; microscale thermophoresis (MST) via NanoTemper Monolith NT.115 Series; time-resolved fluorescence spectroscopy and FRET; circular dichroism (CD) spectroscopy via JASCO J-1500 spectrophotometer.

Honors/Awards

- Graduate Research Assistantship – National Institutes of Health (NIH) R15 grant, PI Professor Donald Jacobs – 2022–2026.
- Graduate Teaching Assistantship – University of North Carolina at Charlotte, Dept. of Physics and Optical Science – 2020–2022.
- Honors in Physics – University of North Carolina at Charlotte, Department of Physics and Optical Science – 2020.
- Chancellor's List – University of North Carolina at Charlotte – 2019.
- Dean's List – University of North Carolina at Charlotte – 2018.
- Dean's List – Central Piedmont Community College – 2015.

Military Service:

- NATO Medal, US Army (2012).
- Army Commendation Medal, US Army (2012).
- Army Good Conduct Medal, US Army (2012).
- National Defense Service Medal, US Army (2011).
- Afghanistan Campaign Medal with two campaign stars (2nd Award), US Army (2011).
- Overseas Service Ribbon, US Army (2011).
- Combat Action Badge, US Army (2011).
- Global War on Terrorism Service Medal, US Army (2011).
- Battlefield promotion to Specialist, FOB Frontenac, Afghanistan, US Army (ERB-03Feb2011).
- Soldier of the Month - 572nd MAC, Ghazni Province, Afghanistan, US Army (2011).
- Inducted into the Order of the Combat Spur, 2nd Stryker Cavalry Regiment, US Army (2011).
- Army Service Ribbon, US Army (2009).

Societies

Biophysical Society, Bioengineering Subgroup – Student Member, ID 127253 Jan. 2025 – Present

IEEE Computational Intelligence Society – Affiliate Member #96524465, R3 Southeastern USA Oct. 2021 – Present

Physics Undergraduate Mentorship Program (PUMP) – Coordinator Sept. 2019 – Jan. 2024

Journal Reviews

click here for certificates

NPJ Computational Materials June 2026 – Present

Discover Nano Oct. 2025 – Present

Scientific Reports (Nature Publishing Group) Apr. 2024 – Present