Daniel C. Elton, Ph.D.

www.moreisdifferent.com
www.github.com/delton137

Skills

- Machine learning, physics, scientific writing and presentation
- My primary programming language is Python. I have extensive experience with Matlab and Fortran and some experience with C++.
- Python libraries I am proficient with include pytorch, keras, scikit-learn, pandas, numpy, and matplotlib.
- git, LaTeX, MS Office, 3D Slicer, GNU/Linux, MacOS, MS Windows
- I have experience doing research in HPC environments and with server installation and maintenance.

Experience

Jan 2019 - **Staff Scientist**, *National Institutes of Health, Bethesda, Maryland*

Contractor working for Dr. Ronald Summers in the Computer-Aided Diagnosis lab at the NIH Clinical Center, Department of Radiology and Imaging Sciences.

- Trained a deep learning system (3D U-Net) to segment and identify the L1 vertebra with 88% accuracy, and wrote an iterative instance segmentation algorithm for full spine segmentation.
- Helped develop a CycleGAN method for novel CT data augmentation for deep learning.
- Compared a 3D mask R-CNN and a 3D U-Net for detection and segmentation of plaque in the aorta.
- Made improvements to NIH C++ codes for performing automatic measurements in CT scans. Ran these codes on an HPC cluster for 14,000+ scans.
- Performed data center server installation, maintenance, and backups.

2018-2019 **Assistant Research Scientist**, *University of Maryland, College Park*

Supervised by Prof. Peter W. Chung and Prof. Mark D. Fuge.

- Wrote a detailed review article on deep learning techniques for molecular design and demonstrated how a generative adversarial network can be used to generate sets of potentially useful molecules.
- Demonstrated for the first time how machine learning models can predict the properties of propellants & explosives with high accuracy and low computational cost. (ridge and LASSO regression, kernel ridge regression, random forest models)
- Worked with Zois Boukouvalas comparing the utility of PCA, ICA, and IVA for dimensionality reduction.
- Explained the utility of machine learning methods to program managers and chemists in DoD research labs by participating in numerous talks and discussions.
- Developed a natural language processing pipeline to extract chemical names, properties, and functionalities from large corpora of text extracted from pdfs and patent applications. Supervised a masters student and an undergraduate student who helped with the NLP project.
- Explored how sensitivity analysis of machine learning models and feature ranking techniques can be used to help illuminate possible relationships between molecular structures and properties.

2017-2018 **Postdoctoral Associate**, *University of Maryland, College Park*, Same as above.

Spring 2017 **STEM Tutor**, *Schenectady County Community College*

2012-2016 **Graduate Research Assistant**, *Stony Brook University*

Ph.D. adviser: Prof. Marivi Fernández-Serra

- Wrote a Fortran code (*PIMD-F90*) for quantum molecular dynamics simulation and a Python package (*spectrumfitter*) for fitting dielectric spectra. Parallelized code with MPI and ran large scale molecular dynamics simulations on HPC clusters.
- Planned and executed a detailed simulation study of the dielectric properties of water which led to the discovery of optical phonon-like modes in liquid water.

2010-2012 **Graduate Teaching Assistant**, *Stony Brook University*

2010 **Summer Internship**, *Los Alamos National Laboratory*

- Worked with Dr. Garrett Kenyon on biologically-inspired neural networks for computer vision.

Education

Dec. 2016 **Ph.D. Physics**, *Stony Brook University*, Stony Brook, NY

Aug. 2009 **B.S., Physics**, *Rensselaer Polytechnic Institute* , Troy, NY

Mathematics minor, Magna Cum Laude, GPA 3.87

Peer reviewed journal articles

2019 **D. C. Elton**, Z. Boukouvalas, M. D. Fuge, and P. W. Chung. "Deep learning for molecular design - a review of the state of the art", Molecular Systems Design & Engineering, **4**, 828

2019 G. Kumar, F. G. VanGessel, **D. C. Elton**, and P. W. Chung. "Phonon Lifetimes and Thermal Conductivity of the Molecular Crystal -RDX", *MRS Advances*

2019 **D. C. Elton**, M. Fritz, and M.-V. Fernández-Serra, "Using a monomer potential energy surface to perform approximate path integral molecular dynamics simulation of ab-initio water at near-zero added cost", *Phys. Chem. Chem. Phys.*, **21**, 409

2018 **D. C. Elton**, Z. Boukouvalas, M. S. Butrico, M. D. Fuge, and P. W. Chung, "Applying machine learning techniques to predict the properties of energetic materials", *Scientific Reports* **8**, 9059

2017 **D. C. Elton** "The origin of the Debye relaxation in liquid water and fitting the high frequency excess response", *Phys. Chem. Chem. Phys.*, **19**, 18739

2016 **D. C. Elton** and M.-V. Fernández-Serra, "The hydrogen-bond network of water supports propagating optical phonon-like modes", *Nature Communications*, **7**, 10193

2014 **D. C. Elton** and M.-V. Fernández-Serra, "Polar nanoregions in water - a study of the dielectric properties of TIP4P/2005, TIP4P/2005f and TTM3F", *The Journal of Chemical Physics*, **140**, 124504

2009 J. J. Podesta, M. A. Forman, C. W. Smith, **D. C. Elton**, and Y. Malecot, "Accurate Estimation of Third-Order Moments from Turbulence Measurements", *Nonlin. Proc. Geophys*, **16**, 99

Peer reviewed conference proceedings

2019 **D. C. Elton**, Y. Zhu, Y. Tang, R. M. Summers. "Improving the transferability of 3D segmentation models using cycle consistent adversarial networks". In prep.

2019 **D. C. Elton**, V. Sandfort, P. J. Pickhardt, R. M. Summers. "Accurately identifying vertebral levels in large datasets". Forthcoming in SPIE: Medical Imaging 2020.

2019 **D. C. Elton**, D. Turakhia, N. Reddy, Z. Boukouvalas, R. M. Doherty, M. D. Fuge, and P. W. Chung. "Using natural language processing techniques to extract information on the properties and functionalities of energetic materials from large text corpora" Proceedings of the 22nd International Seminar on New Trends in Research of Energetic Materials. (arxiv:1903.00415)

2018 Z. Boukouvalas, **D. C. Elton**, M. D. Fuge, and P. W. Chung. "Independent Vector Analysis for Data Fusion Prior to Molecular Property Prediction with Machine Learning" 2018 Neural Information Processing Systems (NIPS) workshop on Machine Learning for Molecules and Materials. (arxiv:1822.00628)

2018 B. C. Barnes, **D. C. Elton**, Z. Boukouvalas, D. E. Taylor, W. D. Mattson, M. D. Fuge, and P. W. Chung, "Machine Learning of Energetic Material Properties", 16th International Detonation Symposium, Cambridge MD (arXiv:1807.06156)

2018 F. G. VanGessel, G. Kumar, **D. C. Elton**, and P. W. Chung, "A Phonon Boltzmann Study of Microscale Thermal Transport in α-RDX Cook-Off", 16th International Detonation Symposium, Cambridge MD (arXiv:1808.08295)

2010 M. A. Forman, C. W. Smith, B. J. Vasquez, B. T. MacBride, J. E. Stawarz, J. J. Podesta, **D. C. Elton**, U. Y. Malecot, and Y. Gagne. "Using Third-Order Moments of Fluctuations in V and B to Determine Turbulent Heating Rates in the Solar Wind.", *AIP Conference Proceedings, 12th International Solar Wind Conference*, **1216**, 176

Professional development & service

2015- Peer Review Reviewer

I have reviewed for *Neural Computing and Applications*, *Journal of Physics Communications*, *Scientific Reports*, *Journal of Chemical Physics*, and *Journal of Physical Chemistry Letters*.

2016-2017 Founder & Organizer, Tech Valley Machine Learning, Data Science, & AI Meetup

I hosted 18 meetups on topics in data science and machine learning, three of which were talks I gave myself.

2015-2016 Writer & Public Relations Director, *Stony Brook Frontiers* magazine

2013-2015 Senator & Social Concerns Committee member, Stony Brook Graduate Student Organization

2014-2015 Volunteer, Stony Brook Astronomy Open Nights

2014,2015 Judge, Nassau County Science Competition

2012 Improvisation for Scientists Course, Alda Center for Communicating Science

Honors

2018 Talent, MindFire Mission-1
2014 Peter B. Kahn travel prize
2009 Rensselaer Founder's Award
2008 Sigma Pi Sigma
2006 Rensselaer Medal/Scholarship
2006 Willits Foundation Scholarship
2006 RIT Computing Award/Scholarship
2006 National Merit Scholarship Finalist
2004 Eagle Scout Award

Talks

11-23-19 Envision Conference, *Princeton University, Princeton, New Jersey*
Invited talk: "Societal, Policy, and Regulatory Implications of AI for Healthcare and Medicine "

9-21-18 Deep Learning RIT (Research Interaction Team), *UMD Mathematics Department, College Park, Maryland*
"Introduction to machine learning topics : optimization techniques and convolutional neural networks"

8-2-18 Visit of SEAP interns from Indian Head Naval Surface Warfare Center, *College Park, Maryland*
Invited talk: "Machine Learning and AI for Navy Energetics"

6-7-18 Talk to Gad Getz's group at the Broad Institute, *Cambridge, Massachusetts*
"Machine Learning for Design and Discovery of New Energetic Materials"

6-3-18 Gordon Research Seminar - Advances in Modeling, Experimental Developments and Synthesis of Energetic Materials, *Newry, Maine*
"Machine Learning for Design and Discovery of New Energetic Materials"

4-20-18 Army Research Laboratory, *Aberdeen, Maryland*
Invited talk: "Machine Learning of Energetic Molecule Performance"

2-21-18 Artificial Intelligence Information Meetup, *Silver Spring, Maryland*
"Pitfalls of Machine Learning"

2-10-18 Bellevue Machine Learning & Artificial Intelligence Meetup, *Bellevue, Washington*
"Pitfalls and Biases in Machine Learning"

12-28-17 Tech Valley Machine Learning Meetup, *Troy, New York*
"Machine learning pitfalls"

11-20-17 Tech Valley Machine Learning Meetup, *Troy, New York*
"Interpretable machine learning for molecular design and discovery"

12-12-16 Tech Valley Machine Learning Meetup, *Troy, New York*
"Scikit-learn & Keras applied to digit recognition"

3-16-16 American Physical Society March Meeting, *Baltimore, Maryland*
"Accurate path integral molecular dynamics simulation of *ab-initio* water at near-zero added cost"

2-3-16 Institute for Advanced Computational Science, *Stony Brook University*
Invited talk: "Propagating Optical-Phonon Like Modes in Liquid Water"

11-27-15 Young Researcher Symposium, *Brookhaven National Lab*
"Propagating optical phonon-like modes in liquid water"

3-2-15 American Physical Society March Meeting, *San Antonio, Texas*
"Exploring the nonlocal dielectric susceptibility of liquid water in the terahertz regime - propagating modes, Debye relaxation, and overscreening"

7-26-14 Gordon Research Seminar - Water & Aqueous Solutions, *Holderness School, New Hampshire*
Invited talk: "Water - a Relaxor Ferroelectric?"

4-17-14 Graduate Student Friday Afternoon Seminar, *Stony Brook University*
"Water - a Relaxor Ferroelectric?"

3-5-14 American Physical Society March Meeting, *Denver, Colorado*
"Polar nanoregions in water - a study of the dielectric properties of TIP4P/2005, TIP4P2005f and TTM3F"

Poster presentations

9-17-18 Postdoctoral Research Symposium, *University of Maryland, College Park*
"Machine learning for molecular property prediction and discovery"

8-7-18 Artificial Intelligence for Materials Science (AIMS) Workshop, *NIST, Gaithersburg, Maryland*
"Machine learning for molecular property prediction and discovery"

6-3-18 Gordon Research Seminar - Advances in Modeling, Experimental Developments and Synthesis of Energetic Materials, *Newry, Maine*
"Machine learning for molecular property prediction and discovery"

2-5-18 New Deep Learning Techniques Workshop, *Institute for Pure and Applied Mathematics*
"Interpretable machine learning for molecular property prediction and discovery"

6-29-17 Machine Learning for Materials Research Workshop, *University of Maryland*
"Fitting and Understanding the Dielectric Spectra of Liquid Water"

4-13-16 Institute for Advanced Computational Sciences Research Day, *Stony Brook University*
"The H-bond network of liquid water supports propagating phonons"

3-17-16 American Physical Society March Meeting, *Baltimore, Maryland*
"The hydrogen bond network of water supports propagating optical phonon-like modes"

10-23-15 Chemistry Research Day, *Stony Brook University*
"The H-bond network of liquid water supports propagating phonons"

9-18-15 Institute for Advanced Computational Science Grand Opening, *Stony Brook University*
"The H-bond network of liquid water supports propagating phonons"

7-29-14 Gordon Research Conference - Water & Aqueous Solutions, *Holderness School, NH*
"Water - a Relaxor Ferroelectric?"

3-21-14 5th New York Theoretical and Computational Chemistry Conference, *Stony Brook University*
"Polar nanoregions in water - a study of the dielectric properties of TIP4P/2005, TIP4P/2005f and TTM3F"

1-14-13 4th New York Theoretical & Computational Chemistry Conference, *City University of New York*
"The Dielectric Properties and Dipolar Correlations of Liquid Water Investigated using TIP4P/2005 Rigid and Flexible Models"

11-6-12 8th Gotham-Metro Condensed Matter Meeting, *New York Academy of Sciences*
"The Dielectric Properties and Dipolar Correlations of Liquid Water Investigated using TIP4P/2005 Rigid and Flexible Models"

References

- Dr. Ronald M. Summers, rsummers@cc.nih.gov, 301-402-5486
- Prof. Peter W. Chung, pchung15@umd.edu, 301-405-4543
- Prof. Mark D. Fuge, fuge@umd.edu, 301-405-2558
- Prof. Marivi Fernández-Serra, maria.fernandez-serra@stonybrook.edu, 631-632-8244