

Skills

- Machine learning, physics, scientific writing and presentation
- My primary programming language is Python. I have extensive experience with Matlab and Fortran and some recent experience with C++.
- Python libraries I am proficient with include pytorch, keras, scikit-learn, pandas, numpy, and matplotlib.
- git, L^AT_EX, 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 supervised by 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 the L1 vertebra with 95% identification accuracy, and developed a system for full spine segmentation using iterative instance segmentation.
- Helped develop and test the use of the CycleGAN and UNIT (Liu, et al. 2017) image translation models for CT data augmentation for deep learning.
- Developed a patch-based 3D U-Net for segmentation of plaque in the aorta which performed better than models previously developed in the lab.
- Constructed a large database of 21,761 MRI scans and annotations for future machine learning endeavours.
- 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 GPU 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 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.
- Worked with Zois Boukouvalas comparing the utility of PCA, ICA, and IVA for dimensionality reduction.
- 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

- 2020 P. J. Pickhardt, **D. C. Elton**, P. M. Graffy, S. J. Lee, J. Liu, V. Sandfort, R. M. Summers. "Fully-automated CT Imaging Biomarkers of Bone, Muscle, and Fat: Correcting for the Effect of Intravenous Contrast" (in prep)

- 2020 R. M. Summers, **D. C. Elton**, Y. Zhu, J. Liu, M. Bagheri, N. N. Mehta, P. A. Pinto, W. M. Linehan, A. A. Perez, P. M. Graffy, S. O'Connor, P. J. Pickhardt. "Atherosclerotic Plaque Burden on Abdominal CT: Automated Assessment with Deep Learning". (in prep)
- 2020 **D. C. Elton**, P. D. Spencer, J. D. Riches, E. D. Williams. "Exclusion zone phenomena in water - a critical review of experimental findings and theories". (under review) (arXiv:1909.06822)
- 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 α -RDX", *MRS Advances*, **4**, 2191
- 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

- 2020 **D. C. Elton**, Y. Zhu, Y. Tang, R. M. Summers. "Improving the transferability of 3D segmentation models using cycle consistent adversarial networks". (in prep)
- 2020 S. Y. Shin, S. Lee, **D. C. Elton**, J. Gulley, R. M. Summers. "Deep Small Bowel Segmentation with Cylindrical Topological Constraints" (under review)
- 2020 Y. Zhu, Y. Tang, Y. Tang, **D. C. Elton**, S. Lee, P. J. Pickhardt, R. M. Summers. "Cross-Domain Image Translation by Shared Latent Gaussian Mixture Model". (under review)
- 2020 Z. Boukouvalas, M. Puerto, **D. C. Elton**, P. W. Chung, M. D. Fuge. "Independent Vector Analysis for Molecular Data Fusion: Application to Property Prediction and Molecular Knowledge Discovery", (under review)
- 2020 **D. C. Elton**. "Self-explaining AI as an alternative to interpretable AI", forthcoming in *Proceedings of the 13th Annual Conference on Artificial General Intelligence (AGI-2020)* (arXiv:2002.05149)
- 2020 Y. Zhu, **D. C. Elton**, S. Lee, P. J. Pickhardt, R. M. Summers. "Image Translation by Latent Union of Subspaces for Cross-Domain Plaque Detection", forthcoming in *Proceedings of the International Conference on Medical Imaging with Deep Learning (MIDL)*
- 2020 **D. C. Elton**, V. Sandfort, P. J. Pickhardt, R. M. Summers. "Accurately identifying vertebral levels in large datasets", *Proceedings of SPIE: Medical Imaging 2020: Computer-Aided Diagnosis, 113140O* (arxiv:2001.10503)
- 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", *Proceedings of the 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", *Proceedings of the 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

Honors

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| 2020 | Kelly Government Solutions Distinguished Achievement Award | |
| 2020 | AI Fellowship, Foresight Institute | 2006 Rensselaer Medal/Scholarship |
| 2018 | Talent, MindFire Mission-1 | 2006 Willits Foundation Scholarship |
| 2014 | Peter B. Kahn travel prize | 2006 RIT Computing Award/Scholarship |
| 2009 | Rensselaer Founder's Award | 2006 National Merit Scholarship Finalist |
| 2008 | Sigma Pi Sigma | 2004 Eagle Scout Award |

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*.
- 2019- Co-organiser, DC Transhumanists Meetup
- 2016-2017 Founder & Organizer, Tech Valley Machine Learning, Data Science, & AI Meetup
- 2015-2016 Writer & Public Relations Director, *Stony Brook Frontiers* magazine
- 2013-2015 Senator & Social Concerns Committee member, Stony Brook Graduate Student Organization

Talks

- 04-22-20 TAFFD's International Conference on Future Africa, *Online*
Invited talk: "AI for Medical Imaging"
- 02-17-20 SPIE: Medical Imaging Conference, *Houston, Texas*
Invited talk: "Accurately identifying vertebral levels in large datasets"
- 11-23-19 Envision Conference, *Princeton University, Princeton, New Jersey*
Invited workshop 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 Talk to 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

- 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