Daniel C. Elton

EDUCATION

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

Bachelor of Science, Physics
Rensselaer Polytechnic Institute, Troy, NY — Aug. 2009
GPA 3.87

PROFESSIONAL EXPERIENCE

National Institutes of Health, Bethesda, MD

Staff Scientist — Jan 2019 - present

Contractor supervised by Dr. Ronald M. Summers at the NIH Clinical Center, Department of Radiology and Imaging Sciences.

- Developed a fully automated deep learning based system for bone mineral density measurement in CT scans which utilizes an iterative instance algorithm to segment and label the entire spine.
- Developed and validated a patch-based 3D U-Net for segmentation of plaque in the aorta and pelvic arteries. The segmentations yield plaque severity scores which correlate well with manual measurements ($r^2 = 0.94$).
- Supervised and mentored a post-baccalaureate fellow (Hima Tallam, Fall 2020) and a summer intern (Sai Sriram, 2019).
- Developed a 3D U-Net for pancreas segmentation using an active learning approach which achieves state-of-the art performance on non-contrast CT. Ran the model on $\approx 22,000$ cases to correlate pancreas features with diabetes diagnosis.
- Constructed a large dataset of $\approx$ 20,000 MRI scans and annotations which is being used for machine learning endeavours in the lab. Worked on registration of different MRI series.
- Made numerous improvements to NIH C++ codes for automated bone mineral density measurement, fat measurement, and fracture detection. Did comparison of the accuracy of automated measurement and AI segmentation tools on contrast vs non-contrast CT.
- Trained multiclass 3D U-Net models for vertebral segmentation and liver region segmentation which are being used for projects in the lab.
- Helped develop and test the use of the CycleGAN and UNIT image translation models for CT data augmentation for deep learning.
- Performed GPU server installation, maintenance, and backups.

University of MD, College Park, MD

Postdoctoral Researcher — March 2017 – Dec 2019

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

- Demonstrated for the first time how machine learning models can predict the properties of propellants & explosives with high accuracy.
- Developed a natural language processing pipeline to extract chemical names, properties, and applications from large corpora of text extracted from PDFs and patent applications.
- Supervised a masters student (Dhruv Turakhia) and an undergraduate student (Nischal Reddy Chandra) who contributed to the NLP project.
- Explained the utility of machine learning methods to program managers and chemists in DoD research labs by participating in numerous talks and discussions. Wrote a four page white paper grant proposal on applying machine learning to energetic materials processing optimization.
- 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.
- 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.

Stony Brook University, Stony Brook, NY

Graduate Research Assistant — June 2012 – December 2016

Ph.D. adviser: Prof. Marivi Fernández-Serra. Thesis: *Understanding the Dielectric Properties of Water*.

- Wrote a Fortran code (*PIMD-F90*) for simulation of nuclear quantum effects in liquid water 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.

Graduate Teaching Assistant — September 2010 - May 2012

- Taught "Physics for the Life Sciences II" lab component and tutored students in help room.

Los Alamos National Laboratory, Los Alamos, NM

Science Undergraduate Laboratory Internship — June – August 2010

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

COMPUTER SKILLS

- My primary programming language is Python. I have extensive experience with Matlab and Fortran and some recent experience with C++.
- Python libraries: pytorch, keras, scikit-learn, pandas, numpy, and matplotlib.
- git, LaTeX, MS Excel, MS Access, 3D Slicer, GNU/Linux, slurm

PEER REVIEWED JOURNAL ARTICLES

C. S. Greene, D. S. Himmelstein, **D. C. Elton**, A. J. Titus, A. Gitter, B. C. Christensen, J. J. Levy, et al. "Opportunities and obstacles for deep learning in biology and medicine: Version 2.0", 2020. (in prep)

D. C. Elton. "Applying Deutsch's concept of good explanations to artificial intelligence and neuroscience - an initial exploration", 2020. (under review)

P. J. Pickhardt, P. M. Graffy, A. A. Perez, M. G. Lubner, **D. C. Elton**, R. M. Summers. "Opportunistic Screening at Abdominal CT using Automated Biomarkers: Adding Value Beyond the Clinical Indication". To appear in *Radiographics*, 2021.

P. J. Pickhardt, G. Blake, P. M. Graffy, V. Sandfort, **D. C. Elton**, A. A. Perez, R. M. Summers. "Liver Steatosis Categorization on Contrast-Enhanced CT Using a Fully-Automated Deep Learning Volumetric Segmentation Tool: Evaluation in 1,204 Healthy Adults Using Unenhanced CT as Reference Standard", *American Journal of Roentgenology*, 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", *Abdominal Radiology*, 2020.
• I did all of the deep learning and data analysis work for this paper.

R. M. Summers, **D. C. Elton**, S. Lee, Y. Zhu, J. Liu, M. Bagheri, V. Sanfort, P. C. Grayson, 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 on Noncontrast and Contrast-enhanced Scans", *Academic Radiology*, 2020.
• I did all of the deep learning and most of the data analysis work for this paper.

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", *International Journal of Molecular Sciences*, **21** (14), 5041, 2020.

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, 2019.

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, 2018.

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, 2017.

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

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, 2014.

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, 2009.

PEER REVIEWED CONFERENCE PAPERS

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

D. C. Elton. "Common pitfalls when explaining AI and why mechanistic explanation is a hard problem". *to appear in Proceedings of the 6th International Congress on Information and Communication Technology*, 2021.

Y. Peng, S. Lee, **D. C. Elton**, T. Shen, Y. Tang, Q. Chen, S. Wang, Y. Zhu, R. M. Summers, Z. Lu "Automatic recognition of lymph nodes from clinical text". *to appear in Proceedings of the 3rd Workshop on Clinical Natural Language Processing (ClinicalNLP)*, 2020.

S. Y. Shin, S. Lee, **D. C. Elton**, J. Gulley, R. M. Summers. "Deep Small Bowel Segmentation with Cylindrical Topological Constraints", *Medical Image Computing and Computer Assisted Intervention (MICCAI) 2020*, edited by Anne L. Martel et al., Springer International Publishing, **12264**, 207–15.

Y. Zhu, Y. Tang, Y. Tang, **D. C. Elton**, S. Lee, P. J. Pickhardt, R. M. Summers. "Cross-Domain Medical Image Translation by Shared Latent Gaussian Mixture Model", *Medical Image Computing and Computer Assisted Intervention (MICCAI) 2020*, edited by Anne L. Martel et al., Springer International Publishing, **12262**, 379–389, 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 Knowledge Discovery of Energetic Materials", *Proceedings of the 28th European Signal Processing Conference (EUSIPCO)*, 2020.

D. C. Elton."Self-explaining AI as an alternative to interpretable AI", *Proceedings of the 13th Annual Conference on Artificial General Intelligence*, pg. 95, 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", *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: Computer-Aided Diagnosis, 113140O*, 2020.

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*, 2019.

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*, 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*, 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, 2018.

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, 2009.

PEER REVIEWED BOOK CHAPTERS

D. C. Elton and P. D. Spencer. "Four examples of pathological water science and what they have in common". To appear in *Water in Biomechanical Related Systems*, A. Gadomski, editor. Springer. (2021)

HONORS

Kelly Government Solutions Distinguished Achievement Award, 2020
Foresight Institute Foresight Fellow in Artificial Intelligence, 2020
Talent, MindFire Mission-1, 2018
Peter B. Kahn travel prize, Stony Brook University Physics Department, 2014
Rensselaer Founder's Award of Excellence, 2009
Sigma Pi Sigma, 2008
Rensselaer Medal/Scholarship, 2006
Willits Foundation Scholarship, 2006
RIT Computing Award/Scholarship, 2006
National Merit Scholarship Finalist, 2006

TALKS

"Applying Deutsch's concept of good explanations to artificial intelligence and neuroscience - an initial exploration", Biologically Inspired Cognitive Architectures (BICA) conference, Online. 10 November 2020.

"Why self-explanation and applicability domain analysis are key to building more robust and trustworthy AI systems", INFORMS 2020 Conference, Online. 13 November 2020.

"Pitfalls with explainability techniques and self-explaining AI as a possible remedy", Foresight Institute Salon on "Key issues in near-term AI Safety research", Online. 7 July 2020.

"Self-explaining AI as an alternative to interpretable AI", Artificial General Intelligence Conference, Online. 24 June 2020.

"AI for medical imaging", TAFFD's International Conference on Future Africa, Online. 22 April 2020.

"Accurately identifying vertebral levels in large datasets", SPIE: Medical Imaging Conference, Houston, Texas. 17 February 2020.

"Societal, Policy, and Regulatory Implications of AI for Healthcare and Medicine", Envision Conference, Princeton University, Princeton, New Jersey. 23 November 2019.

"Introduction to machine learning topics : optimization techniques and convolutional neural networks", Deep Learning RIT (Research Interaction Team), UMD Mathematics Department, College Park, MD. 21 September 2018.

"Machine learning and AI for navy energetics", Talk to SEAP interns from Indian Head Naval Surface Warfare Center, College Park, MD. 2 August 2018.

"Machine learning for design and discovery of new energetic materials", Broad Institute Seminar, Cambridge, Massachusetts. 7 June 2018.

"Machine learning for design and discovery of new energetic materials", Gordon Research Seminar - Advances in Modeling, Experimental Developments and Synthesis of Energetic Materials, Newry, Maine. 3 July 2018.

"Machine learning of energetic molecule performance", Army Research Laboratory, Aberdeen, MD. 20 April 2018.

"Pitfalls of machine learning", Artificial Intelligence Information Meetup, Silver Spring, MD. 21 February 2018.

"Pitfalls and biases in machine learning", Bellevue Machine Learning & Artificial Intelligence Meetup, Bellevue, WA. 10 February 2018.

"Machine learning pitfalls", Tech Valley Machine Learning Meetup, Troy, NY. 28 December 2017. 28 December 2017.

"Interpretable machine learning for molecular design and discovery", Tech Valley Machine Learning Meetup, Troy, NY. 20 November 2017.

"Scikit-learn & Keras applied to digit recognition", Tech Valley Machine Learning Meetup, Troy, NY. 12 February 2016.

"Accurate path integral molecular dynamics simulation of ab-initio water at near-zero added cost". American Physical Society March Meeting, Baltimore, MD. 3 March 2016.

"Propagating optical phonon-like modes in liquid water", Institute for Advanced Computational Science, Stony Brook University. 3 February 2016.

"Propagating optical phonon-like modes in liquid water", Young Researcher Symposium, Brookhaven National Lab. 27 November 2015.

"Exploring the nonlocal dielectric susceptibility of liquid water in the terahertz regime - propagating modes, Debye relaxation, and overscreening", American Physical Society March Meeting, San Antonio, Texas. 2 March 2015.

"Water - a relaxor ferroelectric?", Gordon Research Seminar - Water & Aqueous Solutions, Holderness, NH. 26 July 2014.

"Water - a relaxor ferroelectric?", Graduate Student Friday Afternoon Seminar, Stony Brook University, Stony Brook, NY.

"Polar nanoregions in water - a study of the dielectric properties of TIP4P/2005, TIP4P2005f and TTM3F", American Physical Society March Meeting, Denver, Colorado. 5 March 2014.