Adriana Ladera

My motivation to obtain a Ph.D. is two-fold: (i) to take a step towards an interdisciplinary career centered around my deep interests in numerical methods and algorithms, high-performance computing, modeling, and simulation, and (ii) —inspired by my work with faculty at Penn State, the University of South Florida (USF), and MIT— to become a professor or industry scientist who can instill in younger individuals, especially those of underrepresented communities, a long-lasting passion for STEM and its career paths.

My first exposure to computational studies was a material science REU at Penn State University that I attended the summer after my first year. I worked with Dr. Long-Qing Chen to create phase-field simulations of potassium sodium niobate (KNN) thin films. The piezoelectric properties of KNN could provide a more environmentally friendly alternative to lead zirconate titanate piezoelectrics. My work contributed to co-authorship in three publications and was presented at the AAAFM Conference at UCLA. Intrigued by the idea that experiments could be feasibly simulated with code and mathematical models, I sought to replicate this experience back at my home institution. Back at USF, I joined the Computational Nanoscience Group with Dr. Inna Ponomareva. My ongoing work is a self-directed project that employs unsupervised k-means clustering to reveal hidden dynamics of the barium zirconate titanate (BZT) relaxor ferroelectric. Preliminary results of clustering applied to simulations of barium titanate (BTO), the parent compound of BZT, demonstrate very good agreement between clusters and simulations.

My greatest and proudest accomplishment was being selected to participate in the 2021 MIT Summer Research Program. I worked with Dr. Heather Kulik to explore transition metal complex (TMC) molecules with computational methods and artificial neural networks (ANNs). TMCs have an elaborate electronic structure, which often results in electronic structure methods (i.e. density functional theory) computing their properties with large error. However, TMCs could be used to benchmark the development of new electronic structure methods. We aimed for TMCs whose evaluation of energy properties produced large disagreement among a selection of 23 different density functionals. I created a workflow that used the density functionals to calculate 23 total atomization energies (TAE) per TMC for over one thousand TMCs. For each functional, I also trained a separate ANN on the set of TAEs produced by that functional. From the ANNs' predictions, I discovered that TMCs with large absolute TAE values tend to have larger functional disagreement. I continued my research through a Fall MSRP Expansion Program invite and am also co-authoring an in-preparation manuscript based on this work.

Although personal and familial issues affected my academic performance in the latter half of 2020, research and the strong network of supportive people around me kept me motivated throughout my journey. I am grateful to have encouragement from people at MIT, USF, and Penn State who helped shape my path as a scientist, and I hope that I can one day do the same for students who are just as curious as I am about the inner mechanisms of science and the universe. Additionally, being a TA, Peer Leader, and the Vice President of Women in Computer Science and Engineering allowed me to see the importance of my role in making a positive impact on others through mentorship and leadership. As a scientist who is also a queer Filipina woman, I want to continue cultivating a welcoming and diverse environment for underrepresented groups in STEM, especially for my intersecting communities: women, people of color, and LGBTQ+ individuals. I will devote my extracurricular time to collaborating with organizations that can target cycles of systemic problems and promote an interest in STEM for underrepresented communities.

Across the research groups I worked with, I was a computer science major who was initially unfamiliar with their fields of study, but it was my determination to learn and the strong support from my mentors that ensured my success in these projects. I collaborated with people of different expertise, adapted to new learning environments, gained scientific communication skills, and co-authored publications. My interdisciplinary training also spanned various areas of computational science and simulation and led my curiosity to the computational frameworks behind these studies, where I grew an affinity for numerical and algorithmic aspects of scientific computing. Through an independent study, I taught myself topics such as finite elements, boundary-value problems, and potential flow based on the MIT OCW "Computational Science and Engineering" course by Professor Gilbert Strang. Recently, I also wrote an NSF Graduate Research Fellowship proposal on efficient high-performance and numerical computing for turbulence simulations, and I hope to work in related areas of scientific computing in graduate school.

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Because of the research offered, the MIT Computational Science and Engineering Ph.D. program strongly aligns with my goals. Professor Wim van Rees and Professor Ahmed F. Ghoniem have made significant contributions in numerical simulations of fluid flow problems and high-performance computing for turbulence, while Professor Rodolfo Ruben Rosales and Professor Alan Edelman made great advancements in fluid mechanics, numerical algorithms, and Julia computing, respectively. I know that with any of these professors I will thrive under their apprenticeship. Additionally, MIT's commitment to diversity reinforces my desire to carry out my plans to help make STEM a more inclusive place. I am very confident that pursuing a doctoral degree in Computational Science and Engineering at MIT will provide me with strong foundations to pursue a career as a professor or industry scientist, where I can hone my research skills and encourage alliances between students, faculty, and industry while working to make STEM more diverse and inclusive.