Ellen A. Mulvihill, Ph.D.

211 E Ohio St. Apt 2511, Chicago, IL 60611
emulvi@umich.edu, (630) 991-6336
ellenmulvihill.com

Education

University of Michigan - Ann Arbor, MI — December 2020
Ph.D. in Chemistry and Scientific Computing
Relevant Coursework: Quantum Mechanics, Statistical Mechanics, Chemical Dynamics, Spectroscopy, Computational Physics, Methods and Practices of Scientific Computing, Computer Programming for Scientists and Engineers

University of Chicago - Chicago, IL — Class of 2015
B.A. in Chemistry and minor in Physics with General Honors, Dean's List

Fellowships and Awards

Rackham Predoctoral Fellowship — March 2020
University of Michigan, Rackham Graduate School

One-Term Dissertation Fellowship — June 2019
University of Michigan, Department of Chemistry

PPG Summer Research Fellowship — May 2019
University of Michigan, Department of Chemistry

Florence Fenwick Outstanding Graduate Student Award — May 2018
University of Michigan, Department of Chemistry

Research Experience

University of Michigan, Department of Chemistry — January 2021 - Present
Postdoctoral Researcher, Geva Group
- Exploring quantum computing and quantum dynamics research for open systems
- Continuing graduate research on generalized quantum master equation (GQME) extensions and applications
- Communicating with group members to transfer the GQME project effectively for further application

University of Michigan, Department of Chemistry — August 2015 - Present
PhD Candidate, Geva Group
- Derived memory kernel terms of the GQME to simulate energy and charge transfer
- Computed the kernel terms in various limits of the quantum master equation and compared to literature
- Compared a new modified approach to the GQME developed in the group to previously used approaches
- Explored various input methods for the GQME to compute system dynamics, including approximate and exact methods
- Computed dynamics for the spin-boson model and photovoltaic and photosynthetic systems with the GQME

University of Chicago, Department of Geophysical Sciences — June 2014 - June 2015
Undergraduate Research Assistant with Dr. Reika Yokochi
- Designed catalytic methane decomposition experiment from published scientific papers
- Built experimental apparatus including electrical wiring and Swagelok and national pipe thread connections
- Collaborated with PI to develop improvements to the catalyst from scanning electron microscope results

Sherwin-Williams, Protective and Marine Research and Development Division — June 2013 - September 2013
Research Intern
- Created and tested paint samples for durability in high temperature, high pressure, and corrosive situations
- Collaborated with a team to develop strategies to improve the paint and consider applications of innovations
- Presented a final report on my findings throughout the internship to my team and several division executives
- Received offer from Sherwin-Williams to intern again the following summer

Teaching Experience

University of Michigan, Department of Chemistry — May 2016 - Present
Future Faculty Graduate Student Instructor; Chem 230/260H - FA16, WN17, FA17, WN18, FA18, WN19
- Contributed to the Compute-to-Learn (C2L) course for five semesters, an honors studio where students learn Mathematica and create Wolfram demonstrations (http://umich.edu/~pchem/compute-to-learn.html)
- Ran the Fall 2017 semester as the lead GSI, which had all-time high of 23 students complete the course
- Assisted students in creating Wolfram Mathematica demonstrations based on physical chemistry concepts

- Analyzed student performance through surveys and interviews for the purpose of understanding the impact of course design and develop improvements
- Contributed to C2L's overall enrollment of 55% women, especially high for a programming-based course

University of Michigan, Department of Chemistry August 2015 - May 2017
Graduate Student Instructor; Courses: Chem 130 - FA15, WN16; Chem 453 - FA16, FA17; Chem 260 - WN17
- Designed weekly quizzes and worksheets for general chemistry discussion sections (100 level)
- Lead discussion sections for physical chemistry course (260) and biophysical chemistry course (453)
- Held weekly office hours to assist students with questions outside of discussion

Paradigm Shift August 2012 - June 2015
Mentor
- Organized lesson plans to instruct classes of 6th-8th graders on science
- Mentored between four to twenty students once a week at a local middle school

Leadership Experience

ACS Graduate Student Symposium Planning Committee (GSSPC) October 2018 - April 2020
Speaker Liaison, Committee Member
- Applied for and was chosen to become the Graduate Student Symposium Planning Committee (GSSPC) for the Spring 2020 American Chemical Society (ACS) National Meeting
- Organized a symposium involving speakers in a variety of disciplines and programming for attendees in various stages of their careers
- Offered undergraduate travel awards for underrepresented minorities
- Invited nine leaders in the field of smart materials to speak at our symposium and managed communication with them leading up to the event, including the process of shifting to a virtual symposium
- Applied for and received a National Science Foundation grant of $15,000 for the symposium
- First-ever University of Michigan GSSPC

Women in High Performance Computing at U-M October 2018 - Present
Member
- Member of one of the first WHPC chapters in the WHPC Pilot Programme in the United States

Chemistry Mentorship Program September 2018 - September 2019
Mentor
- Mentored a first-year student regarding graduate research and experience during first mentorship program

Chemistry Graduate Student Council September 2016 - May 2019
Executive Committee Member, Treasurer (September 2016-2018)
- Developed and implemented ideas to improve the role of CGSC as a liaison between graduate students and the Chemistry Department
- Organized events to facilitate interactions between graduate students, faculty, and staff
- Managed CGSC budget to ensure effective use of funds and developed a budget plan that resulted in the tripling of CGSC funds while increasing the number of and average attendance at CGSC events

Senior Class Gift Committee September 2014 - June 2015
Committee Member
- Collaborated with committee in developing strategies to increase class participation and donations
- Ran a successful campaign with $104,700 raised for UChicago student funds and scholarships

Delta Gamma, Eta Zeta Chapter, University of Chicago October 2011 - June 2015
President (January 2014-2015)
- Communicated with Executive Offices on a weekly basis with chapter updates
- Lead chapter board meetings each week to develop a calendar of events and oversee Vice President activities
- Organized and managed a chapter of 126 women
- Presented in front of the chapter weekly regarding upcoming events and requirements
- Oversaw the annual philanthropy event which raised a chapter all-time high $25,000 for Service for Sight

Publications

E. Mulvihill, E. Geva, "Exploration of Various Approaches to the Memory Kernel of the Generalized Quantum Master Equation," Manuscript in preparation.

E. Mulvihill, K. Lenn, X. Gao, A. Schubert, B. D. Dunietz, E. Geva, "On Simulating Energy Transfer Dynamics in the Fenna-Matthews-Olson Complex via the Generalized Quantum Master Equation," Submitted.

Y. Liu, X. Gao, Y. Lai, E. Mulvihill, E. Geva, "Electronic Dynamics through Conical Intersections via Quasiclassical Mapping Hamiltonian Methods," *J. Chem. Theory Comput*. 2020, 16, 7, 4479–4488.

E. Mulvihill, X. Gao, Y. Liu, A. Schubert, B. D. Dunietz, E. Geva, "Combining the mapping hamiltonian linearized semiclassical approach with the generalized quantum master equation to simulate electronically non adiabatic molecular dynamics," *J. Chem. Phys.*, **2019** *151*, 074103

E. Mulvihill, A. Schubert, X. Sun, B. D. Dunietz, E. Geva, "A modified approach for simulating electronically nonadiabatic dynamics via the generalized quantum master equation," *J. Chem. Phys.*, **2019** *150*, 034101

M. Jafari, A. R. Welden, K. L. Williams, B. Winograd, E. Mulvihill, H. P. Hendrickson, M. Lenard, A. Gottfried, and E. Geva, "Compute-to-Learn: Authentic Learning via Development of Interactive Computer Demonstrations within a Peer-Led Studio Environment," *J. Chem. Educ.*, **2017** *94* (12) 1896-1903

Presentations

2020 Karle Symposium at the University of Michigan July 2020
Poster Session - ***Won Best Physical Chemistry Poster***
"Generalized Quantum Master Equation: a reduced dynamics approach for electronically nonadiabatic dynamics," E. Mulvihill, X. Gao, Y. Liu, A. Schubert, X. Sun, Barry D. Dunietz, E. Geva. July 31st, 2020.

2020 Virtual Conference in Theoretical Chemistry July 2020
Poster Session and Lightning Talk - ***Won Outstanding Lightning Talk Graduate Student Award***
"Simulating Electronically Nonadiabatic Dynamics via the Generalized Quantum Master Equation," E. Mulvihill, X. Gao, Y. Liu, A. Schubert, X. Sun, Barry D. Dunietz, E. Geva. July 29th, 2020.

2019 Penn Conference in Theoretical Chemistry August 2019
Poster Session
"Simulating Electronically Nonadiabatic Dynamics via a Modified Approach to the Generalized Quantum Master Equation." E. Mulvihill, X. Gao, Y. Liu, A. Schubert, X. Sun, B. D. Dunietz, E. Geva. August 14th, 2019.

2019 Karle Symposium at the University of Michigan August 2019
Poster Session
"Simulating Electronically Nonadiabatic Dynamics via a Modified Generalized Quantum Master Equation," E. Mulvihill, X. Gao, Y. Liu, A. Schubert, X. Sun, Barry D. Dunietz, E. Geva. August 2nd, 2019.

2019 Midwest Theoretical Chemistry Conference June 2019
Oral Presentation
"Generalized Quantum Master Equation-based Approaches to Electronically Nonadiabatic Dynamics: Mapping Hamiltonian + LSC," E. Mulvihill, X. Gao, Y. Liu, A. Schubert, X. Sun, B. D. Dunietz, E. Geva. June 8th, 2019.

Quantum Science and Technology Workshop at University of Michigan, Ann Arbor, MI April 2019
Poster Session
"A Modified Generalized Quantum Master Equation for Simulating Electronically Nonadiabatic Dynamics," E. Mulvihill, A. Schubert, X. Gao, Y. Liu, X. Sun, Y. Lai, B. D. Dunietz, E. Geva. April 12th, 2019.

Invited Research Presentation at Lafayette College, Easton, PA November 2018
Oral Presentation
"A Modified Generalized Quantum Master Equation for Simulating Electronically Nonadiabatic Dynamics," E. Mulvihill, Y. Lai, A. Schubert, X. Sun, B. D. Dunietz, E. Geva. November 1st, 2018.

2018 Midwest Theoretical Chemistry Conference June 2018
Oral Presentation
"A Modified Generalized Quantum Master Equation for Simulating Electronically Nonadiabatic Dynamics," E. Mulvihill, Y. Lai, A. Schubert, X. Sun, B. D. Dunietz, E. Geva. June 22nd, 2018.

ACS National Meeting, New Orleans, LA March 2018
Physical Chemistry Poster Session - ***Won Outstanding Student Poster Award***
"A Modified Generalized Quantum Master Equation for Simulating Electronically Nonadiabatic Dynamics," E. Mulvihill, A. Schubert, X. Sun, Y. Lai, B. D. Dunietz, E. Geva. March 21st, 2018.

Chemistry Education Poster Session
"Compute-to-Learn: Authentic learning via development of interactive computer demonstrations within a peer-led studio environment," M. Jafari, A. R. Welden, K. L. Williams, B. Winograd, E. Mulvihill, H. P. Hendrickson, M. Lenard, A. Gottfried, and E. Geva. March 18th, 2018.

2017 Midwest Theoretical Chemistry Conference June 2017
Poster Session
"Post-Marcus Electronic Transition Dynamics via the Generalized Quantum Master Equation," E. Mulvihill, A. Schubert, X. Sun, B. D. Dunietz, E. Geva. June 1st, 2017.

2017 MICDE Annual Symposium April 2017
Poster Session
"Post-Marcus Electronic Transition Dynamics via the Generalized Quantum Master Equation," E. Mulvihill, A. Schubert, X. Sun, B. D. Dunietz, E. Geva. April 18th, 2017.

ACS National Meeting, San Francisco, CA April 2017
Physical Chemistry Poster Session
"Post-Marcus Electronic Transition Dynamics via the Generalized Quantum Master Equation," E. Mulvihill, A.Schubert, X. Sun, B. D. Dunietz, E. Geva. April 5th, 2017.

Related Professional Experiences

Graduate Poster Judging for 2019 Karle Symposium August 2019
Judged four graduate student posters based on content, presentation, and ability to answer audience questions

Undergraduate Poster Judging for Chem 125 general chemistry lab April 2019
Judged seven undergraduate posters based on content and conversation on the topic of perovskite solar cells

Compute-to-Learn Workshop - Lafayette College, Easton, PA November 2018
Workshop co-facilitator; Led faculty members in various fields through a Mathematica tutorial and assisted in developing the Compute-to-Learn course for their own courses

Chemistry Department External Review October 2017
One of ten graduate students chosen to represent the department in the external review committee meeting

Skills

Developed programs in C++, Python, and Mathematica
Experience programming in Fortran, Bash, Matlab, and HTML
Experience with Git and GitHub