Duc D. Nguyen — *Curriculum Vitae*

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Contact Information

Assistant Professor
Department of Mathematics
University of Kentucky
Lexington, KY 40506 USA

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Appointments

Assistant Professor (Tenure Track) Aug. 2020 – Present
Department of Mathematics, University of Kentucky

Assistant Professor (Fixed Term) Jan. 2019 – Jul. 2020
Department of Mathematics, Michigan State University

Research Associate Aug. 2015 – Dec. 2018
Department of Mathematics, Michigan State University
Mentor: Guowei Wei

Graduate Research Assistantship Aug. 2013 – Aug. 2015
Department of Mathematics, The University of Alabama

Graduate Teaching Assistantship Jan. 2011 – May 2013
Department of Mathematics, The University of Alabama

Lecturer Aug. 2009 – Aug. 2010
Department of Mathematics and Computer Science, University of Science, Vietnam

Education

The University of Alabama, Tuscaloosa, AL

Ph.D., Mathematics Jan. 2011 – Aug. 2015

- Thesis Topic: *High order FDTD methods for electromagnetic systems in dispersive inhomogeneous media*
- Adviser: Shan Zhao

Université d'Orléans, Orléans, France

M.S., Applied Mathematics Aug. 2009 – Aug. 2010

- Thesis Topic: *Preservation of the Discrete Geostrophic Equilibrium in Shallow Water Flows*
- Adviser: Emmanuel Audusse

University of Science, Ho Chi Minh City, Vietnam

B.S., Mathematics and Computer Science Aug. 2005 – May 2009

- Thesis Topic: *Multiple positive fixed points of nonlinear operators on ordered Banach spaces*
- Adviser: Duc M. Duong

Research Interests

Machine learning: Physics-informed machine learning, geometric deep learning, topology deep learning, multiscale manifold regularization, convolution neural network (CNN), graph convolution neural network (GNN), multitask learning, transfer learning, autoencoder, generative adversarial network (GAN), reinforcement learning, large language modeling (LLM)
Mathematical models for bioscience: Differential geometry representations, multiscale weighted colored algebraic graphs, topological learning
Data analysis: low-dimensional mathematical representations, knowledge based driven data analysis
Quantitative systems pharmacology: Develop mechanistic system biology model, investigate potential therapeutic drug targets

Scientific computing: Computational electrodynamics, electrostatic solvation and binding analysis, computational fluid dynamics

FUNDING

Provost's IMPACT Initiative (awarded) ($50,000.00), 06/01/2023 – 05/31/2024
- Role: one of the Multiple PIs (PIs: Katherine Thompson, Zeya Wang, Jiawei Zhang, and Yuanyuan Su)
- Topic: University of Kentucky Hub for Artificial Intelligence and Machine Learning
- Aim: This project proposes an AI/ML symposium for researchers and undergraduate workshops. It aims to form an ongoing AI/ML research workgroup that can address complex scientific problems in various areas.

NSF DMS-2245903 (awarded) ($599,995.00), 08/01/2023 – 07/31/2026
- Role: PI (Co-PI: Chang-Guo Zhan)
- Topic: DMS/NIGMS 1: Data-driven Ricci curvatures and spectral graph for machine learning and adaptive virtual screening
- Aim: This project proposes a data-driven Ricci curvature and associated spectral graph information for the virtual screening. Furthermore, this project will develop the adaptive training data selection integrated with deep learning algorithms to rank the drug candidates

NSF DMS-2151802 (awarded) ($306,750.00), 09/01/2022 – 08/31/2025
- Role: PI (Co-PI: Sally R. Ellingson)
- Topic: Robust and reliable mathematical models for biomolecular data via differential geometry and graph theory
- Aim: The goal of this study is to develop new spectral graph theory and differential geometry based approaches for biomolecular data analysis

NSF DMS-2053284 (awarded) ($150,000.00), 09/01/2021 – 08/31/2024
- Role: PI
- Topic: Collaborative Research: Integrating Algebraic Topology, Graph Theory, and Multiscale Analysis for Learning Complex and Diverse Datasets
- Aim: This project will develop novel topology and graph theory-based approaches to revolutionize the current practice in data analysis and to deal with the challenge of structurally complex data and diverse data

Michigan Economic Development Corp (awarded) ($75,000.00), 02/01/2020 – 01/31/2021
- Role: Co-PI (PI: Guo-Wei Wei)
- Topic: MAID2: Mathematical Artificial Intelligence for Drug Discovery
- Aim: The goal of this study is to develop a commercializable MAID2 software package

Pfizer (awarded) ($221,128.00), 10/01/2018 – 09/31/2020
- Role: Co-PI (PI: Guo-Wei Wei)
- Topic: Topology and manifold based machine learning for de novo hit identification
- Aim: The goal of this study is to develop a mathematical models for drug virtual screening

Bristol Myers Squibb (awarded) ($119,000.00), 01/05/2019 – 12/31/2019
- Role: PI
- Topic: Quantitative systems pharmacological modeling of drug impact to heart failure - Patient study
- Aim: The goal of this study is to develop mathematical models for drug pharmacodynamics and efficacy

Bristol Myers Squibb (awarded) ($112,000.00) 02/27/2018-12/26/2019
- Role: Co-PI (PI: Guo-Wei Wei)

- Topic: Quantitative systems pharmacological modeling of drug impact to heart failure— Modeling and simulation of sodium and potassium based water regulation.
- Aim: The goal of this study is to develop mathematical models for drug pharmacodynamics and efficacy

Bristol Myers Squibb (awarded) ($150,000.00) 12/20/2017-12/19/2018
- Role: Co-PI (PI: Guo-Wei Wei)
- Topic: Quantitative systems pharmacological modeling of drug impact to heart failure.
- Aim: The goal of this study is to develop mathematical models for drug pharmacodynamics and efficacy

Scientific competition

D3R Grand Challenges, a world-wide competition in drug design

- In D3R Grand Challenge 4 (2018-2019), I was the top performer with the most top three submissions
- In D3R Grand Challenge 3 (2017-2018), my submissions were ranked 1st in 6 of a total of 26 contests
- In D3R Grand Challenge 2 (2016-2017), my submission were ranked 1st for the binding affinity ranking of Set 1 in Stage 2

Patents

Systems and Methods for Drug Design and Discovery Comprising Applications of Machine Learning with Differential Geometric Modeling
(US Patent App.: 17/043,551 (2021))
Authors: Guo-Wei Wei, Duc Nguyen, and Zixuan Cang

System and Methods for Machine Learning for Drug Design and Discovery
(US Patent App.: 16/372,239 (2019))
Authors: Guo-Wei Wei, Duc Nguyen, and Zixuan Cang

Software

- **GGL-Score**: A free and open-source software program for calculating protein-ligand binding scores using an extended atom-type graph-based model.
- **EISA-Score**: A free and Open source software program based on element interactive surface curvatures to predict protein-ligand binding affinity.
- **AGL-Score**: Online server for algebraic graph theory based protein-ligand binding scoring, ranking, docking and screening.
- **DG-GL**: Online server for differential geometry based geometric data analysis (DG-GDA) of molecular datasets.
- **RI-Score**: Online server for geometric graph theory or rigidity index (RI) based scoring function for protein-ligand binding affinity prediction.
- **FRI**: Online server for the flexibility analysis of biomolecules based on flexibility and rigidity index.

Journal Publications

[30] Md Masud Rana and **Duc Duy Nguyen**, Geometric Graph Learning to Predict Changes in Binding Free Energy and Protein Thermodynamic Stability upon Mutation , *The Journal of Physical Chemistry Letters*, **14**, 10870–10879 (2023).

[29] Md Masud Rana and **Duc Duy Nguyen**, Geometric Graph Learning with Extended Atom–Types for Protein–Ligand Binding Affinity Prediction, *Computers in Biology and Medicine*, **164**, 107250 (2023)

[28] Edison Mucllari, Vasily Zadorozhnyy, Qiang Ye, and **Duc Duy Nguyen**, Novel Molecular Representations using Neumann-Cayley Orthogonal Gated Recurrent Unit, *Journal of Chemical Information and Modeling*, **63(9)**, 2656–2666 (2023)

[27] Ekaterina Merkurjev, **Duc Duy Nguyen**, and Guo-Wei Wei, Multiscale Laplacian Learning, *Applied Intelligence*, **147** (2022)

[26] Md Masud Rana and **Duc Duy Nguyen**, EISA-Score: Element Interactive Surface Area Score for Protein–Ligand Binding Affinity Prediction, *Journal of Chemical Information and Modeling*, **62(18)**, 4329–4341 (2022)

[25] Timothy Szocinskia, **Duc Duy Nguyen**, and Guo-Wei Wei, AweGNN: Auto-parametrized weighted element-specific graph neural networks for molecules *Computers in Biology and Medicine*, **134**, 104460 (2021)

[24] Dong Chen, Kaifu Gao, **Duc Duy Nguyen**, Xin Chen, Yi Jiang, Guo-Wei Wei, and Feng Pan, Algebraic graph-assisted bidirectional transformers for molecular property prediction, *Nature Communications*, **12(1)**, 3521 (2021)

[23] Jiahui Chen, Kaifu Gao, Rui Wang, **Duc Duy Nguyen**, and Guo-Wei Wei, Review of COVID-19 antibody therapies, *Annual Review of Biophysics*, **50**, 1–30 (2021)

[22] **Duc Duy Nguyen**, Kaifu Gao, Jiahui Chen, Rui Wang, and Guo-Wei Wei, Unveiling the molecular mechanism of SARS-CoV-2 main protease inhibition from 137 crystal structures using algebraic topology and deep learning, *Chemical Science*, **11(44)**, 12036–12046 (2020)

[21] Kaifu Gao, **Duc Duy Nguyen**, Jiahui Chen, Rui Wang, and Guo-Wei Wei, Repositioning of 8565 Existing Drugs for COVID-19, *The Journal of Physical Chemistry Letters*, **11(13)**, 5373–5382 (2020)

[20] Kaifu Gao, **Duc Duy Nguyen**, Meihua Tu, and Guowei Wei, Generative network complex for the automated generation of druglike molecules, *Journal of Chemical Information and Modeling*, **11(60)**, 5682–5698 (2020)

[19] Rui Wang, **Duc Duy Nguyen**, and Guo-Wei Wei, Persistent spectral graph, *International journal for numerical methods in biomedical engineering*, **36(9)**, e3376 (2020)

[18] Kaifu Gao, **Duc Duy Nguyen**, Vishnu Sresht, Alan M. Mathiowetz, Meihua Tu and Guo-Wei Wei, Are 2D fingerprints still valuable for drug discovery?, *Physical Chemistry Chemical Physics*, **22(16)**, 8373–8390 (2020)

[17] Jian Jiang, Rui Wang, Menglun Wang, Kaifu Gao, **Duc Duy Nguyen**, and Guo-Wei Wei, Boosting tree-assisted multitask deep learning for small scientific datasets, *Journal of Chemical Information and Modeling*, **60(3)**, 1235–1244 (2020)

[16] **Duc Duy Nguyen**, Zixuan Cang, and Guo-Wei Wei, A review of mathematical representations of biomolecular data, *Physical Chemistry Chemical Physics*, **22(8)**, 4343–4367 (2020)

[15] **Duc Duy Nguyen**, Kaifu Gao, Menglun Wang, and Guo-Wei Wei, MathDL: Mathematical deep learning for D3R Grand Challenge 4, *Journal of Computer Aided Molecular Design*, **34**, 131–147 (2020)

[14] Christopher Grow, Kaifu Gao, **Duc Duy Nguyen**, and Guo-Wei Wei, Generative network complex (GNC) for drug discovery, *Communications in Information and Systems*, **19(3)**, 241–277 (2019)

[13] **Duc Duy Nguyen** and Guo-Wei Wei, AGL-Score: Algebraic Graph Learning Score for Protein-Ligand Binding Scoring, Ranking, Docking, and Screening, *Journal of Chemical Information and Modeling*, **59(7)**, 3291–3304 (2019)

[12] **Duc Duy Nguyen** and Guo-Wei Wei, DG-GL: Differential geometry based geometric learning of molecular datasets, *International Journal for Numerical Methods in Biomedical Engineering*, **35(3)**, e3179 (2019)

[11] **Duc Duy Nguyen**, Zixuan Cang, Kedi Wu, Menglun Wang, Yin Cao and Guo-Wei Wei, Mathematical deep learning for pose and binding affinity prediction and ranking in D3R Grand Challenges, *Journal of Computer-Aided Molecular Design*, **33**, 71–82 (2018)

[10] **Duc Duy Nguyen**, Tian Xiao, Menglun Wang and Guo-Wei Wei, Rigidity strengthening: A mechanism for protein-ligand binding, *Journal of Chemical Information and Modeling*, **57**, 1715–1721 (2017)

[9] Bao Wang, Zhixiong Zhao, **Duc Duy Nguyen** and Guo-Wei Wei, Feature functional theory - binding predictor (FFT-BP) for the blind prediction of binding free energy, *Theoretical Chemistry Account*, **136**, 55 (2017)

[8] **Duc Duy Nguyen**, Bao Wang and Guo-Wei Wei, Accurate, robust and reliable calculations of Poisson-Boltzmann binding energies, *Journal of Computational Chemistry*, **38**, 941–948 (2017)

[7] **Duc Duy Nguyen** and Guo-Wei Wei, The impact of surface area, volume, curvature and Lennard-Jones potential to solvation modeling, *Journal of Computational Chemistry*, **38**, 24-–36 (2017)

[6] **Duc Duy Nguyen**, Kelin Xia and Guo-Wei Wei, Generalized flexibility-rigidity index, *Journal of Chemical Physics*, **144**, 234106 (2016)

[5] **Duc Duy Nguyen** and Shan Zhao, A second order dispersive FDTD algorithm for transverse electric Maxwell's equations with complex interface, *Computers and Mathematics with Applications*, **71**, 1010–1035 (2016)

[4] Ya Zhang, **Duc Duy Nguyen**, Kewi Du, Jin Xu, and Shan Zhao, Time-domain numerical solutions of Maxwell interface problems with discontinuous electromagnetic waves, *Advances in Applied Mathematics and Mechanics*, **8**, 353–385 (2016)

[3] **Duc Duy Nguyen** and Shan Zhao, A new high order dispersive FDTD method for Drude material with complex interfaces, *Journal of Computational and Applied Mathematics*, **285**, 1–14 (2015)

[2] **Duc Duy Nguyen** and Shan Zhao, Time-domain matched interface and boundary (MIB) modeling of Debye dispersive media with curved interfaces, *Journal of Computational Physics*, **278**, 298–325, (2014)

[1] **Duc Duy Nguyen** and Shan Zhao, High order FDTD methods for transverse magnetic modes with dispersive interfaces, *Applied Mathematics and Computation*, **226**, 699–707, (2014)

Refereed Proceedings

[1] E. Audusse, R. Klein, **D. D. Nguyen**, S. Vater, Preservation of the Discrete Geostrophic Equilibrium in Shallow Water Flows, *Finite Volumes for Complex Applications VI Problems & Perspectives Springer Proceedings in Mathematics*, **04**, pp. 59–67, (2011)

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Preprints

[1] Vasily Zadorozhnyy, Edison Mucllari, Cole Pospisil, **Duc Duy Nguyen**, and Qiang Ye, Orthogonal Gated Recurrent Unit with Neumann-Cayley Transformation, submitted to *Journal Neural Computation*, arXiv:2208.06496 (2023). 16 pages.

Honors and Awards

College of Arts & Sciences Outstanding Dissertation Award, University of Alabama 2016
(Awarded to a Doctoral Candidate who has the best dissertation in College of Arts & Sciences division)

Outstanding Research Award, University of Alabama 2015
(Awarded to a Doctoral Candidate who has the best research performance in Department of Mathematics)

Best Poster Prize, SIAM-SEAS 2015
(Awarded to the graduate student who has the best poster in SIAM-SEAS 2015 conference)

Ainsworth Fellowship, University of Alabama 2014 – 2015
(Awarded to the top three students in the Mathematics Department, University of Alabama with outstanding research performance)

NSF funded Graduate Reasearch Assistantship (DMS-1016579) 2013 – 2015

Henry Miller Fellowship, University of Alabama 2011 – 2013
(Awarded to students in the Mathematics Department, University of Alabama with excellent performance on qualifying exam and teaching)

Travel Award for Dissertation Research Enhancement, PUF 2010
(Awarded to top ranking students in PUF-Master Program)

Honors Program Scholarship, University of Sciences, Vietnam 2005 – 2009
(Awarded to students with exceptional performance on national entrance exams)

Invited conference talks

2023 SIAM-NNP, New Jersey Institute of Technology, Oct. 20-22, 2023.

The 2023 SIAM Great Lakes Meeting, Michigan State University , Oct. 14, 2023.

Spring Central Sectional Meeting, University of Cincinnati , Apr. 15-16, 2023.

Spring Southeastern Sectional Meeting, Georgia Institute of Technology, Mar. 18-19, 2023.

Minisymposium on Molecular Biosciences: Advances in molecular property and structure predictions, SIAM Conference on the Life Sciences, Jul. 11-14, 2022, Virtual Format.

Topology-based Learning, Biomolecular Topology and Related Topics, Institute for Mathematical Sciences, Singapore, Jul. 11–15, 2022, Virtual Format.

Joint Mathematics Meetings, Seattle, WA, Apr. 8, 2022, Virtual Format.

The Fourth TSIMF Conference on Computational and Mathematical Bioinformatics and Biophysics, Dec. 12–15, 2021, Virtual Format.

TSIMF Conference on Computational and Mathematical Bioinformatics and Biophysics, Dec. 19–23, 2020, Virtual Format.

Commonwealth Computational Summit 2020 , Oct. 12–16, 2020, Virtual Format.

Fall Eastern Sectional Meeting , Oct. 03–04, 2020, Virtual Format.

SIAM Conference on Mathematics of Data Science 2020 , May 04–June 30, 2020, Virtual Format.

NSF-CBMS Conference: Mathematical Molecular Bioscience and Biophysics, May 13–17, 2019, University of Alabama.

Workshop on the Mathematics of Drug Design/Discovery, Jun. 4–7, 2018, The Fields Institute, University of Toronto, Canada.

The 3rd Annual Meeting of SIAM Central States Section, Sep. 30–Oct. 1, 2017, Colorado State University, Fort Collins, CO.

SIAM Conference on the Life Sciences (LS16), Jul. 11–14, 2016 The Westin Boston Waterfront, Boston, Massachusetts.

Contributed conference talks

Graduate Recruiting Expo 2015, Feb. 27, 2015, University of Alabama, Tuscaloosa, AL.

2015 Joint Mathematics Meetings, Jan. 10–13, 2015, San Antonio, TX.

3MT - Three Minute Thesis Competition: Semi-Final Competition: Department Winners compete, Nov. 05, 2014, University of Alabama, Tuscaloosa, AL.

Joint Applied Mathematics Meeting, University of Alabama at Birmingham, Birmingham, Nov. 8, 2014.

Seminar talks

University of Cincinnati Applied Mathematics Seminar, Nov. 18, 2022

University of Georgia Applied Mathematics Seminar, Mar. 10, 2021

Georgia Southern University General Mathematics Sciences Colloquium, Feb. 26, 2021

Contributed Conference Posters

Scientific Computing meets Machine Learning and Life Sciences, Oct. 07–09, 2019, Texas Tech University, Lubbock, TX.

Workshop 1: Topological, Geometric, and Statistical Techniques in Biological Data Analysis, Sep. 12-16, 2016, Mathematical Biosciences Institute, Ohio State University, OH.

Workshop 4: Mathematical Challenges in Drug and Protein Design, Dec. 7–11, 2015, Mathematical Biosciences Institute, Ohio State University , OH.

Mathematics of Biological Charge Transport: Molecular and Beyond, Jul. 20–24, 2015, IMA, University of Minnesota, Minneapolis, MN.

SIAM Southeastern Atlantic Section Conference (SIAM-SEAS 2015), Mar. 20–22, 2015, University of Alabama at Birmingham, Birmingham, AL.

South Central Conference on Advanced Numerical Methods and Applications, Apr. 5–7, 2013, University of Arkansas at Little Rock.

Mathematical Challenges in Biomolecular/Biomedical Imaging and Visualization, Feb. 18–22, 2013, MBI, Ohio State University.

Other Conferences attended

NSF-NIH Joint Workshop on Emerging AI in Biology, Jun. 8–9, 2023, Virtual event.

D3R 2019 Workshop, Aug. 22–23, 2019, Hotel La Jolla, La Jolla, CA.

D3R Workshop, Feb. 22–23, 2018, Scripps Institution of Oceanography, UC San Diego, CA.

Workshop 3: Modeling and Computation of Transmembrane Transport, Nov. 16–20, 2015, Mathematical Biosciences Institute, Ohio State University, OH.

Workshop 2: Multiple Faces of Biomolecular Electrostatics, Oct. 12–16, 2015, Mathematical Biosciences Institute, Ohio State University , OH.

Workshop 1: Geometric and Topological Modeling of Biomolecule, Sep. 28–Oct. 2, 2015, Mathematical Biosciences Institute, Ohio State University , OH.

25th Annual University of Alabama System Applied Mathematics Meeting, Nov. 3, 2012, University of Alabama in Huntsville.

Ninth Mississippi State – UAB conference on Differential Equations & Computational Simulations, Oct. 4–6, 2012, Mississippi State University.

36th Annual SIAM Southeastern Atlantic Section Conference (SEAS 2012), Mar. 24–25, 2012, University of Alabama in Huntsville.

Joint Applied Mathematics Meeting, University of Alabama at Birmingham, Birmingham, Nov. 5, 2011.

2nd Midwest Conference on Mathematical Methods for Images and Surfaces, Michigan State University, East Lansing, Aug. 27–28, 2011.

Academic Invited Visit

Mathematical Biosciences Institute Aug. 2015 – Dec. 2015
Ohio State University, Columbus, OH

Laboratoire Analyse, Géométrie et Applications May 2010 – Aug. 2010
Universite Paris 13, Paris, France

Teaching

University of Kentucky, Lexington, KY

Instructor

- (MA 213) Calculus III (116 Students) Fall 2023
- (CS/MA 321) Introduction to Numerical Analysis Fall 2023
- (CS/EGR/MA 537) Numerical Analysis Spring 2022 & 2023
- (MA/BIO 337) Mathematical Modeling in the Life Sciences Spring 2022 & 2023
- (MA 721) Topics in Numerical Analysis: Deep Learning Fall 2022
- (MA 138) Calculus II with Life Science Fall 2020, Fall 2021
- (MA 421G) Mathematics Introduction to Deep Learning Spring 2021
- (MA 777) Mathematical Seminar Spring 2021

Michigan State University, East Lansing, MI

Course development

- Developed machine learning course for Actuarial Science Program and Capstone course at Michigan State University

Instructor

- (MTH 496 (Capstone Course)) Machine learning Spring 2018, Spring 2019, Fall 2019
- (MTH 132) Calculus I Fall 2018
- (MTH 490) Predictive Analysis Spring 2018
- (MTH 309) Linear Algebra Spring 2016, Fall 2016, Spring 2017

The University of Alabama, Tuscaloosa, AL

Grader

- (MATH 126) Calculus II — Fall 2011, Spring 2012

Tutor

- Mathematics Technology Learning Center — Spring & Fall 2011, 2012
- Math tutor in Paty Hall — Fall 2011

University of Sciences, Ho Chi Minh City, Vietnam

Teaching Assistant

- Real Analysis I — Fall 2009

Advising and Mentoring

Postdocs

- Masud Rana (UK, July. 2021 – Present)

Graduate Students

- Farjana Tasnim Mukta (Female, UK, Aug. 2021 – Present)
- David Storey (MSU, Sept. 2018 – Jul. 2020)
- Christopher Matthew Grow (MSU, Sept. 2018 – Jul. 2020)
- Rui Wang (Female, MSU, Aug. 2018 – Jul. 2020)
- Timothy Andrew Szocinski (MSU, May 2018 – Jul. 2020)

Undergraduate Students

- Joyce Yang (Female, UK, Aug 2023 – Present)
- Asmita Karki (Female, UK, Aug 2023 – Present)
- Avery Meyer (Female, UK, May 2022 – May 2023)
- Benjamin Philpot (UK, May 2022 – Aug 2022)
- Cecilia Mikat (Female, Professorial Assistantship (PA) Program, MSU Aug. 2018 – May 2019)
- Jason Charles Kenny (Professorial Assistantship (PA) Program, MSU Aug. 2018 – May 2019)
- Kyle Thomas Cole (Professorial Assistantship (PA) Program, MSU Aug. 2018 – May 2020)
- Jianbin Chen (MSU, Aug. 2018 – May 2020)
- Jonathon Fleck (Professorial Assistantship (PA) Program, MSU Aug. 2016 – May 2020)
- Nick Smentowski (Professorial Assistantship (PA) Program, MSU Aug. 2016 – May 2018)
- Tian Xiao (With Prof. Guowei Wei, Summer Research Opportunities Program at MSU, 2016)

Professional Service

Review Editor, Frontiers in Drug Discovery - In silico Methods and Artificial Intelligence for Drug Discovery 2023 – Present

Editorial Board, Artificial Intelligence Chemistry 2023 – Present

Editorial Board, PeerJ Physical Chemistry 2021 – Present

Review Editor, Computational Physiology and Medicine 2022 – Present

Assistant Editor, Computational and Mathematical Biophysics 2015 – Present

Program Committee, PASC23 Conference 2022 – 2023

Lead Guest & Guest Editors

- FoDS Special Issue: Recent Advances in Topological Deep Learning 2023
- AI Chemistry Special Issue: AI for Drug Discovery 2023
- PeerJ Special Issue: AI-driven chemistry for drug design 2021
- CMB Special Issue: Drug design and discovery for COVID-19 2021
- CMB Special Issue: Mathematical Molecular Bioscience and Biophysics 2019
- CMB Special Issue: Computational and Mathematical Drug Design and Discovery 2018

Journal Reviewer

- Scientific Report
- Journal of Computer-Aided Molecular Design
- International Journal of Numerical Methods in Biomedical
- Artificial Intelligence Chemistry
- Communications in Information & Systems
- Journal of Computation Chemistry
- Bioinformatics and Biology Insights
- PLOS Computational Biology
- Foundations of Data Science
- Inverse Problems and Imaging
- Computational and Mathematical Biophysics
- ACS Synthetic Biology
- Journal of Medicinal Chemistry
- Biophysical Journal
- APL Machine Learning
- Bioinformatics
- Journal of Computational Physics
- Briefings in Bioinformatics
- Journal of Chemical Information and Modeling
- Mathematical Biosciences and Engineering
- Journal of the Royal Society Interface
- ACS Omega
- Computers in Biology and Medicine
- PeerJ Computer Science
- Computers and Mathematics with Applications
- Current Research in Structural Biology
- Cogent Engineering
- iScience
- Proceedings of the Royal Society A

Book Reviewer, Review of new book proposal, publisher: Wiley-VCH 2022

Grant Reviewer, NSF (06/21/2021 – 06/23/2021), NSF (12/12/2022 – 12/14/2022), NSF (06/21/2023 – 06/23/2023)

Conference Organizer

- Organizer (with David Murrugarra), Minisymposium on Molecular Biosciences: Advances in molecular property and structure predictions, SIAM Conference on the Life Sciences July 11-14, 2022

Local service

Department

- Member, Numerical Analysis Prelim committee 2022-2023
- Member, Postdoc Recruiting Committee 2021-2022

Dissertation Committees

- Farjana Tasnim Mukta, PhD in Mathematics Co-chair, In Progress
- Edison Mucllari, PhD in Mathematics In Progress
- Charles Hutchinson, Ms. in Mathematics 2023
- Cole Pospisil, PhD in Mathematics 2023
- Susanna Lange, PhD in Mathematics 2022

Computer Skills

- Programming languages: FORTRAN, C/C++, PYTHON, BASH, PERL, PHP, HTML/CSS
- Mathematical and statistical softwares: Matlab, Mathematica, Maple, R
- Database management system: MySQL