

CONTACT  
INFORMATION

Assistant Professor  
Department of Mathematics  
University of Kentucky  
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RESEARCH  
INTERESTS

**Machine learning:** Multiscale manifold regularization, convolution neural network (CNN), graph convolution neural network (GNN), multitask learning, transfer learning, autoencoder, generative adversarial network (GAN), reinforcement learning  
**Data analysis:** low-dimensional mathematical representations, knowledge based driven data analysis  
**Mathematical models for bioscience:** Differential geometry representations, multiscale weighted colored algebraic graphs, topological learning  
**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

RESEARCH GRANT NSF CDSE&E-MSS-2053284 (awarded) (\$150,000.00), 09/01/2021 – 08/31/2024  
AWARDS

- 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
- 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
- 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) (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

**NSF-Mathematical Biology** (pending) (\$215,397.00), 09/01/2021 – 08/31/2024

- Role: PI
- Topic: Differential geometry and graph theory approaches for biomolecular data
- Aim: The goal of this study is to develop new spectral graph theory and differential geometry based approaches for biomolecular data analysis

#### PATENTS

System and Methods for Machine Learning for Drug Design and Discovery

(Publication Number: US2019/0304568 A1)

Authors: Guo-Wei Wei, Duc Nguyen, and Zixuan Cang

#### HIGHLIGHTS

**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 1<sup>st</sup> in 6 of a total of 26 contests
- In D3R Grand Challenge 2 (2016-2017), my submission were ranked 1<sup>st</sup> for the binding affinity ranking of Set 1 in Stage 2

#### Teaching

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

#### Software packages development

- **FRI**: Online server for the flexibility analysis of biomolecules based on flexibility and rigidity index
- **RI-Score**: Online server for geometric graph theory or rigidity index (RI) based scoring function for protein ligand binding affinity prediction
- **DG-GL**: Online server for differential geometry based geometric data analysis (DG-GDA) of molecular datasets
- **AGL-Score**: Online server for algebraic graph theory based protein-ligand binding scoring, ranking, docking and screening.

#### 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

APPOINTMENTS	<b>Assistant Professor (Tenure Track)</b> Department of Mathematics, University of Kentucky	Aug. 2020 – Present
	<b>Assistant Professor (Fixed Term)</b> Department of Mathematics, Michigan State University	Jan. 2019 – Jul. 2020
	<b>Research Associate</b> Department of Mathematics, Michigan State University Mentor: Guowei Wei	Aug. 2015 – Dec. 2018
	<b>Graduate Research Assistantship</b> Department of Mathematics, The University of Alabama	Aug. 2013 – Aug. 2015
	<b>Graduate Teaching Assistantship</b> Department of Mathematics, The University of Alabama	Jan. 2011 – May 2013
	<b>Lecturer</b> Department of Mathematics and Computer Science, University of Science, Vietnam	Aug. 2009 – Aug. 2010

## MENTOR

**Graduate Students**

- David Storey (Sept. 2018 – Jul. 2020)
- Christopher Matthew Grow (Sept. 2018 – Jul. 2020)
- Rui Wang (Female, Aug. 2018 – Jul. 2020)
- Timothy Andrew Szocinski (May 2018 – Jul. 2020)

**Undergraduate Students**

- 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)

TEACHING  
EXPERIENCE

**University of Kentucky**, Lexington, KY

Instructor

- (MA 421G) Mathematics Introduction to Deep Learning Spring 2021
- (MA 777) Mathematical Seminar Spring 2021
- (MA 138) Calculus II with Life Science Fall 2020

**Michigan State University**, East Lansing, MI

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

Training

- Attained conditional pass for GTA training on teaching methods Fall 2013
- Attended GTA Workshop Fall 2011

Other experience

- Member of the test development committee for Alabama Statewide High School Mathematics Contest Fall 2011, Spring & Fall 2012
- Proctored Alabama Statewide High School Mathematics Contest Spring 2011, 2012

**University of Sciences**, Ho Chi Minh City, Vietnam

Teaching Assistant

- Real Analysis I Fall 2009

HONORS AND  
AWARDS

- SCMLLS Travel Support Fund 2019  
*(For presenting a poster at Scientific Computing meets Machine Learning and Life Sciences conference at Texas Tech University)*
- NSF-CBMS Travel Support Fund 2019  
*(For giving a talk at NSF-CBM conference at University of Alabama)*
- Field Institute Travel Support Fund 2018  
*(For giving a talk at Workshop on the Mathematics of Drug Design/Discovery in Field Institute at University of Toronto)*
- MBI Travel Support Fund 2013, 2016  
*(For attending conferences in Mathematical Biosciences Institute at Ohio State University)*

	College of Arts & Sciences Outstanding Dissertation Award, University of Alabama	2016 <i>(Awarded to a Doctoral Candidate who has the best dissertation in College of Arts &amp; Sciences division)</i>
	Outstanding Research Award, University of Alabama	2015 <i>(Awarded to a Doctoral Candidate who has the best research performance in Department of Mathematics)</i>
	IMA Travel Support Fund	2015 <i>(For attending conferences in Institute for Mathematics and its Applications at University of Minnesota)</i>
	Best Poster Prize, SIAM-SEAS	2015 <i>(Awarded to the graduate student who has the best poster in SIAM-SEAS 2015 conference)</i>
	AMS Travel Support Fund	2015 <i>(For attending 2015 Joint Math Meetings)</i>
	Ainsworth Fellowship, University of Alabama	2014 – 2015 <i>(Awarded to the top three students in the Mathematics Department, University of Alabama with outstanding research performance)</i>
	Travel Support Fund, University of Alabama	2013, 2014 <i>(For attending meetings and conferences )</i>
	NSF funded Graduate Research Assistantship (DMS-1016579)	2013 – 2015
	Henry Miller Fellowship, University of Alabama	2011 – 2013 <i>(Awarded to students in the Mathematics Department, University of Alabama with excellent performance on qualifying exam and teaching)</i>
	Travel Award for Dissertation Research Enhancement, PUF	2010 <i>(Awarded to top ranking students in PUF-Master Program)</i>
	Honors Program Scholarship, University of Sciences, Vietnam	2005 – 2009 <i>(Awarded to students with exceptional performance on national entrance exams)</i>
SERVICES	<b>Assistant Editors</b> , Computational and Mathematical Biophysics	2015 – Present
	<b>Guest Editor</b> , Special Issue: Mathematical Molecular Bioscience and Biophysics	2019
	<b>Lead Guest Editor</b> , Special Issue: Computational and Mathematical Drug Design and Discovery	2018
REFeree/ REVIEWER EXPERIENCES	Scientific Report, Bioinformatics, Journal of Computer-Aided Molecular Design, International Journal for Numerical Methods in Biomedical, Communications in Information & Systems, Journal of Computation Chemistry, Bioinformatics and Biology Insights, 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	
ACADEMIC INVITED VISIT	<b>Mathematical Biosciences Institute</b> Ohio State University, Columbus, OH	Aug. 2015 – Dec. 2015
	<b>Laboratoire Analyse, Géométrie et Applications</b> Universite Paris 13, Paris, France	May 2010 – Aug. 2010

REFEREED  
JOURNAL  
PUBLICATIONS

- [23] **Duc 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*, doi: 10.1039/D0SC04641H, (2020)
- [22] Jiahui Chen, Kaifu Gao, Rui Wang, **Duc Nguyen**, and Guo-Wei Wei, Review of COVID-19 antibody therapies, *Annual Review of Biophysics*, **50(1)**, (2020)
- [21] Kaifu Gao, **Duc Nguyen**, Meihua Tu, and Guowei Wei, Generative network complex for the automated generation of druglike molecules, *Journal of Chemical Information and Modeling*, doi: 10.1021/acs.jcim.0c00599 (2020)
- [20] 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*, doi: 10.1021/acs.jpcelett.0c01579 (2020)
- [19] Rui Wang, **Duc Duy Nguyen**, and Guo-Wei Wei, Persistent spectral graph, *International journal for numerical methods in biomedical engineering*, doi: 10.1002/cnm.3376 (2020)
- [18] Kaifu Gao, **Duc D. Nguyen**, Vishnu Sresht, Alan M. Mathiowetz, Meihua Tu and Guo-Wei Wei, Are 2D fingerprints still valuable for drug discovery?, *Physical Chemistry Chemical Physics*, doi: 110.1039/D0CP00305K (2020)
- [17] Jian Jiang, Rui Wang, Menglun Wang, Kaifu Gao, **Duc D. Nguyen**, and Guo-Wei Wei, Boosting tree-assisted multitask deep learning for small scientific datasets, *Journal of Chemical Information and Modeling*, doi: 10.1021/acs.jcim.9b01184 (2020)
- [16] **Duc D. Nguyen**, Zixuan Cang, and Guo-Wei Wei, A review of mathematical representations of biomolecular data, *Physical Chemistry Chemical Physics*, doi: 10.1039/C9CP06554G (2020)
- [15] **Duc D. Nguyen**, Kaifu Gao, Menglun Wang, and Guo-Wei Wei, MathDL: Mathematical deep learning for D3R Grand Challenge 4, *Journal of Computer Aided Molecular Design*, doi:10.1007/s10822-019-00237-5 (2019)
- [14] Christopher Grow, Kaifu Gao, **Duc D. Nguyen**, and Guo-Wei Wei, Generative network complex (GNC) for drug discovery, *Communications in Information and Systems*, **19(3)**, 241–277 (2019)
- [13] **Duc D. 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*, (2019)
- [12] **Duc D. 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 D 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 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 D 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 D 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 D Nguyen**, Kelin Xia and Guo-Wei Wei, Generalized flexibility-rigidity index, *Journal of Chemical Physics*, **144**, 234106 (2016)
- [5] **Duc D. Nguyen** and S. 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] Y. Zhang, **D.D. Nguyen**, K. Du, J. Xu, and S. 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 D. Nguyen** and S. 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 D. Nguyen** and S. 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 D. Nguyen** and S. Zhao, High order FDTD methods for transverse magnetic modes with dispersive interfaces, *Applied Mathematics and Computation*, **226**, 699–707, (2014)

CONFERENCE  
PUBLICATIONS

- [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)

SUBMITTED

- [1] Ekaterina Rapinchuk, **Duc Nguyen**, and Guo-Wei Wei, Multiscale Laplacian Learning, (2021)
- [2] Timothy Szocinski, **Duc Nguyen**, and Guo-Wei Wei, AweGNN: Auto-parametrized weighted element-specific graph neural networks, (2021)
- [3] Dong Chen, Kaifu Gao, **Duc Nguyen**, Xin Chen, Yi Jiang, Guowei Wei, and Feng Pan, Algebraic Graph-assisted Bidirectional Transformers for Molecular Prediction, (2021)

CONFERENCES

- Unviersity of Georgia Applied Mathematics Seminar, Mar. 10, 2021
- Georgia Southern University General Mathematics Sciences Colloquium, Feb. 26, 2021
- TSIMF Conference on Computational and Mathematical Bioinformatics and Biophysics, Dec. 19–23, 2020, Virtual Format (invited talk)

- Commonwealth Computational Summit 2020 , Oct. 12–16, 2020, Virtual Format (invited lightning talk)
- Fall Eastern Sectional Meeting , Oct. 03–04, 2020, Virtual Format (invited talk)
- SIAM Conference on Mathematics of Data Science 2020 , May 04–June 30, 2020, Virtual Format (invited talk)
- Scientific Computing meets Machine Learning and Life Sciences, Oct. 07–09, 2019, Texas Tech University, Lubbock, TX (contributed poster)
- D3R 2019 Workshop, Aug. 22–23, 2019, Hotel La Jolla, La Jolla, CA (participant)
- NSF-CBMS Conference: Mathematical Molecular Bioscience and Biophysics, May 13–17, 2019, University of Alabama (invited talk)
- Workshop on the Mathematics of Drug Design/Discovery, Jun. 4–7, 2018, The Fields Institute, University of Toronto, Canada (invited talk)
- D3R Workshop, Feb. 22–23, 2018, Scripps Institution of Oceanography, UC San Diego, CA (participant)
- The 3rd Annual Meeting of SIAM Central States Section, Sep. 30–Oct. 1, 2017, Colorado State University, Fort Collins, CO (invited talk)
- Workshop 1: Topological, Geometric, and Statistical Techniques in Biological Data Analysis, Sep. 12–16, 2016, Mathematical Biosciences Institute, Ohio State University, OH (contributed poster)
- SIAM Conference on the Life Sciences (LS16), Jul. 11–14, 2016 The Westin Boston Waterfront, Boston, Massachusetts (invited speaker)
- Workshop 4: Mathematical Challenges in Drug and Protein Design, Dec. 7–11, 2015, Mathematical Biosciences Institute, Ohio State University , OH (contributed poster)
- Workshop 3: Modeling and Computation of Transmembrane Transport, Nov. 16–20, 2015, Mathematical Biosciences Institute, Ohio State University , OH (participant)
- Workshop 2: Multiple Faces of Biomolecular Electrostatics, Oct. 12–16, 2015, Mathematical Biosciences Institute, Ohio State University , OH (participant)
- Workshop 1: Geometric and Topological Modeling of Biomolecule, Sep. 28–Oct. 2, 2015, Mathematical Biosciences Institute, Ohio State University , OH (participant)
- Mathematics of Biological Charge Transport: Molecular and Beyond, Jul. 20–24, 2015, IMA, University of Minnesota, Minneapolis, MN (contributed poster)
- SIAM Southeastern Atlantic Section Conference (SIAM-SEAS 2015), Mar. 20–22, 2015, University of Alabama at Birmingham, Birmingham, AL (contributed poster)
- Graduate Recruiting Expo 2015, Feb. 27, 2015, University of Alabama, Tuscaloosa, AL (contributed talk)
- 2015 Joint Mathematics Meetings, Jan. 10–13, 2015, San Antonio, TX (contributed talk)
- 3MT - Three Minute Thesis Competition: Semi-Final Competition: Department Winners compete, Nov. 05, 2014, University of Alabama, Tuscaloosa, AL (contributed talk)
- Joint Applied Mathematics Meeting, University of Alabama at Birmingham, Birmingham, Nov. 8, 2014 (contributed talk)



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

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

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

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

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

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

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

- 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