# Weihua Geng

Contact Information	135 Clements Hall Department of Mathematics Southern Methodist University Dallas, TX 75275	Office Phone: (214) 768-2252 E-mail: wgeng at smu dot edu Website: http://faculty.smu.edu/wgeng	
Research Interests	mathematical biology, finite difference and boundary integral methods for PDEs, algorithms for molecular simulation, algorithms for N-body problems, parallel computing, machine learning		
Academic Preparation	University of Michigan, Ann Arbor, Michigan		
	Postdoc, Applied Mathematics, 2008-2011 (Mentors: Robert Krasny, Daniel Forger)		
	Michigan State University, East Lansing, Michigan		
	<ul><li>Ph.D., Applied Mathematics, 2008 (Advisor: Guowei Wei)</li><li>M.S., Statistics, 2005</li><li>Professional M.S., Industrial Mathematics, 2003</li></ul>		
	Zhejiang University, Hangzhou	ı, Zhejiang, China	
	B.E., Electrical and Computer Engineering, 1999		
Academic Experience	Southern Methodist Universi Associate Professor	ty, Dallas, Texas August, 2019 - presen	
	<ul> <li>Assistant Professor</li> <li>Taught nine undergraduate cou Linear Algebra (Math 3304), Dif puting (Math 3315), PDE and B<sup>A</sup> Mathematics in Machine Learning</li> <li>Taught three graduate courses:</li> <li>6320), Mathematical Biology (Ma</li> <li>Advised/Advising four PhD st Sliheet (2019-2024), Md Abu Tall</li> <li>Mentored four REU students: Ji 2022), Reese Iriye (2022-2024)</li> </ul>	August, 2013 - May, 2019 urses: Calculus I/II/III (Math 1337/1338/3302), Introduction to ferential Equation (Math 3313), Introduction to Scientific Com VPs (Math 4337), Advanced Scientific Computation (Math 4315) g (Math 4377) Finite Element Analysis (Math 6319), Iterative Methods (Math ath 6350) udents: Jiahui Chen (2014-2019), Xin Yang (2019-2024), Elyssa na (2023-) ngzhen Hu (2014-2017), Xin Yang (2017-2019), Yongjia Xu (2019	
	University of Alabama, Tusca Assistant Professor - Taught three undergraduate cour 238), Mathematical Statistics wit - Taught one graduate course: Nu - Mentored an undergraduate stu	ioosa, Alabama August, 2011 - July, 2013 rses: Calculus III (Math 227), Applied Differential Equation (Math h Applications (Math 451) umerical Linear Algebra (Math 510) dent: Tyler Arnold (2012-2013) from Alabama Emerging Scholar	
	<b>University of Michigan</b> , Ann A Postdoctoral Assistant Professor	Arbor, Michigan August, 2008 - May, 201	
	<ul> <li>Taught undergraduate courses:</li> <li>Numerical Methods for Engineers</li> <li>Mentored a REU student: Moi 1</li> </ul>	Calculus I (Math 115), Applied Honors Calculus III (Math 255) (Math 371), Introduction to Numerical Methods (Math 471) Bai (Summer 2010).	
	<b>Michigan State University</b> , E. Research and Teaching Assistant	ast Lansing, Michigan August, 2001 - August, 2008	

	Math Dept., University of Michigan, Spring/Summer Research Fellowship, \$10,000, 2009
	Michigan State University, Graduate School Dissertation Completion Fellowship, \$6,000, 2008
	Math Dept., Michigan State University, Senior Graduate Teaching Award, Honorable Mention, 2006
Grants	NIH R15-xxxxxx, The Art of Feature Generation: A Machine Learning Based Protein Property Pre- diction, Target Program: Model and Analysis of Biological Systems (MABS), to submit: 6/25/2024 PI: W. Geng, 2024-2027
	NSF DMS-2410955, Collaborative Research: Computational Tools for Charge Transport Through Transmembrane Ion Channels, \$259,572 pending, PI: W. Geng, 2024-2027
	NSF DMS-2110922, Collaborative Research: Implicit Solvent Modeling and Fast Algorithm Develop- ment for Simulating Solutes with Atomic Polarizable Multipoles, \$199,216, <u>awarded</u> , PI: W. Geng, 2021-2024
	NSF DMS-2110869, Collaborative Research: Computational Tools for Biomolecular Electrostatics, \$110,000, <u>awarded</u> , PI: W. Geng, 2021-2024
	NSF DMS-1819193, Collaborative Research: Improved Boundary Element Methods for Electrostatics of Interacting Proteins in Solvent, \$155,000, <u>awarded</u> , PI: W. Geng, 2018-2021
	NSF DMS-1836318, CBMS Conference: Mathematical Molecular Bioscience and Biophysics, \$35,000, <u>awarded</u> , PI: S. Zhao, Co-PI: W. Geng, 2018-2019
	NSF DMS-1418957, Collaborative Research: Boundary Integral Simulations for Solvent Effects in Protein Structure and Dynamics, \$114,000, <u>awarded</u> , PI: W. Geng, 2014-2017
	NSF DMS-1318898, Matched alternating direction implicit (ADI) schemes for solving the nonlinear Poisson-Boltzmann equation with complex dielectric interfaces, \$250,000, <u>awarded</u> , PI: S. Zhao, Co-PI: W. Geng, 2013-2016

Math Dept., Southern Methodist University, Betty McKnight Speairs Endowed Teaching Excellence

Honors &

Math Award, 2018

Awards

NSF DMS-0915057, Treecode-Accelerated Implicit Solvent Models for Biomolecular Simulation, \$242,659, <u>awarded</u>, PI: R. Krasny, Co-PI: W. Geng, 2009-2013

PUBLICATIONS

[33] X. Yang, S. Zhao, W. Geng<sup>\*</sup>, A regularized Matched Interface and Boundary Method (MIB) for Solving Polarizable Multipole Poisson-Boltzmann model, in preparation, (2024)

[32] Y. Xu, M.A. Talha, W. Geng<sup>\*</sup>, Temporal and Spacial Studies of Infectious Diseases: Mathematical Models and Numerical Solvers, in preparation, (2024)

[31] E. Sliheet, W. Geng<sup>\*</sup>, A DNN Biophysics Model with Topological and Electrostatic Features, in preparation, (2024)

[30] S. Amihere, Y. Ren, W. Geng, S. Zhao, A New Boundary Condition for the Nonlinear Poisson– Boltzmann Equation in Electrostatic Analysis of Proteins, in preparation, (2024)

[29] J. Chen, Y. Xu, X. Yang, W. Geng<sup>\*</sup>, G-W. Wei, *Poisson-Boltzmann based machine learning* (*PBML*) model for electrostatic analysis, Biophysical Journal, 123, 1-8 (2024)

[28] X. Yang, E. Sliheet, R. Iriye, D. Reynolds, W. Geng<sup>\*</sup> Optimized Parallelization of Boundary Integral Poisson-Boltzmann Solvers, Computer Physics Communications, 299,109125 (2024)

[27] S. Ullaha, X. Yang, B. Jones, S. Zhao, W. Geng<sup>\*</sup>, G-W. Wei, *Bridging Eulerian and Lagrangian Poisson–Boltzmann solvers by ESES*, Journal of Computational Chemistry, (2023)

[26] Z. Chao, W. Geng, Robert Krasny, Integral method for the 1D steady-state Poisson-Nernst-Planck equations, Journal of Computational Electrostatics, 22, 396–1408 (2023)

[25] J. Chen, J. Tausch, W. Geng<sup>\*</sup>, A Cartesian FMM-accelerated Galerkin boundary integral Poisson-Boltzmann solver, Journal of Computational Physics, 478, 111981 (2023)

[24] L. Wilson, W. Geng, R. Krasny, TABI-PB 2.0: An improved version of the treecode-accelerated boundary integral Poisson-Boltzmann solver, Journal of Physical Chemistry B, 126(37), 7104–7113 (2022)

[23] A. Amihere, W. Geng, S. Zhao, *Benchmarking electrostatic free energy of the nonlinear Poisson-Boltzmann model for the Kirkwood sphere*, Communications in Information and Systems, 22(3), 305-315 (2022)

[22] L. Wilson, J. Hu, J. Chen, R. Krasny, W. Geng\*, Computing electrostatic binding energy with the TABI Poisson-Boltzmann solver, Communications in Information and Systems, 22(2), 247-273 (2022)

[21] J. Chen, W. Geng, G-W. Wei, *MLIMC: Machine Learning-Based Implicit-Solvent Monte Carlo*, Chinese Journal of Chemical Physics, 34(6), 683-694 (2021)

[20] A. Lee, W. Geng, S. Zhao, Regularization methods for the Poisson-Boltzmann equation: comparison and accuracy recovery, Journal of Computational Physics, 426, 109958 (2021)

[19] J. Chen, J. Hu, Y. Xu, R. Krasny, W. Geng<sup>\*</sup>, Computing protein pKas using the TABI Poisson-Boltzmann solver, Journal of Computational Biophysics and Chemistry, 2042006 (2021)

[18] J. Chen, **W. Geng\***, and D. R. Reynolds, *Cyclically parallelized treecode for fast computations of electrostatic interactions on molecular surfaces*, Computer Physics Communication, 260, 107742 (2021)

[17] W. Geng<sup>\*</sup> and X. Yang, *Role of combinatorial complexity in genetic networks*, Communications in Information and Systems, 18(4), 209-228, (2018)

[16] J. Chen and W. Geng\*, On preconditioning the treecode-accelerated boundary integral (TABI) Poisson-Boltzmann solver, Journal of Computational Physics, 373, 750-762 (2018)

[15] E. Jurrus, D. Engel, K. Star, K. Monson, J. Brandi, L. E. Felberg, D. H. Brookes, L. Wilson, J. Chen, K. Liles, M. Chun, P. Li, D. W. Gohara, T. Dolinsky, R. Konecny, D. R. Koes, J. E. Nielsen, T. Head-Gordon, W. Geng, R. Krasny, G.-W. Wei, M. J. Holst, J. A. McCammon, and N. A. Baker, *Improvements to the APBS biomolecular solvation software suite*, Protein Science, 27(1), 112-128 (2018).

[14] J. Hu, S. Zhao, and W. Geng\*, Accurate pKa computation using matched interface and bound-

ary (MIB) method based Poisson-Boltzmann solver, Communications in Computational Physics, 23, 520-539 (2018).

[13] W. Geng, S. Zhao, A two-component matched interface and boundary (MIB) regularization for charge singularity in implicit solvation, Journal of Computational Physics, 351, 25-39 (2017) <u>Note:</u> 2020 ICCM Best Paper Award (Distinguished Paper Award).

[12] J. Chen, W. Geng<sup>\*</sup>, Parallel computing of the adaptive N-body treecode algorithm for solving boundary integral Poisson-Boltzmann equation, Lecture Notes in Computer Science, 9576, 1-9, Springer (2016).

[11] W. Geng<sup>\*</sup>, A boundary integral Poisson-Boltzmann solvers package for solvated bimolecular simulations, Computational and Mathematical Biophysics (formerly Molecular Based Mathematical Biology), 3, 43-58 (2015).

[10] D. DeWoskin, W. Geng, A.R. Stinchcombe, and D.B. Forger, *It's not the parts, but how they interact that determines the behavior of circadian rhythms across scales and organisms*, 4, 20130076, Royal Society Interface Focus (2014).

[9] W. Geng and R. Krasny, A treecode-accelerated boundary integral Poisson-Boltzmann solver for continuum electrostatics of solvated biomolecules, Journal of Computational Physics, 247, 62-87 (2013).

[8] W. Geng<sup>\*</sup>, Parallel higher-order boundary integral electrostatics computation on molecular surfaces with curved triangulation, Journal of Computational Physics, 241, 253-265 (2013).

[7] W. Geng<sup>\*</sup> and F. Jacob, A GPU-accelerated direct-sum boundary integral Poisson-Boltzmann solver, Computer Physics Communication, 184, 1490-1496 (2013).

[6] W. Geng and S. Zhao, Fully implicit ADI schemes for solving nonlinear Poisson-Boltzmann equation, Computational and Mathematical Biophysics (formerly Molecular Based Mathematical Biology), 1, 109-123 (2013).

[5] W. Geng and G-W. Wei, Multiscale molecular dynamics using the matched interface and boundary (MIB) method, Journal of Computational Physics, 230, 435-457 (2011).

[4] D. Chen, Z. Chen, C. Chen, W. Geng and G-W. Wei, *MIBPB: A software package for electro-static analysis*, Journal of Computational Chemistry, 32, 756-770 (2011).

[3] W. Geng, S. Yu and G-W. Wei, *Treatment of charge singularities in implicit solvent models*, Journal of Chemical Physics, 127, 114106-114126 (2007).

[2] S. Yu, W. Geng and G-W. Wei, *Treatment of geometric singularities in implicit solvent models*, Journal of Chemical Physics, 126, 244108-244121 (2007).

[1] J. Enders, W. Geng, P. Li, M.W. Frazier, and D.J. Scholl, *The shift-invariant discrete wavelet transform and application to speech waveform analysis*, Journal of Acoustical Society of America, 117, 2122-2133, (2005).

<u>Note</u>: \*: corresponding author

ACADEMIC	Hands-on Summer School: Electronic Structure Theory for Materials and (Bio)molecules, IPAM/UCLA
TRAININGS	Los Angeles, July 21 - August, 2014 (NSF travel fund)

The 2014 NSF-CBMS Conference on Inverse Scattering and Transmission Eigenvalues, UT-Arlington, Arlington, May 27-May 31, 2014 (NSF travel fund)

Hands-on Workshop on Computational Biophysics, The Scripps Research Institute, San Diego, July 12-16, 2010 (NSF/UIUC travel fund)

INDUSTRIAL International MedioNet Association Inc., Shanghai, C	China
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EXPERIENCE Project Manager

September, 2000 - May, 2001

Led the design and implementation of a healthcare website which promotes sharing resources and exchanging information among hundreds of county hospitals.

# SuperSoft International Inc., Zhejiang, China

## Software Engineer

#### August, 1999 - September, 2000

Carried out the specification, design, coding, testing, and documentation of several software projects such as: Localized CitiBank Personal Financing System; TimeCard System (including its internet approach); The Library Management System; BITCO Health Information System.

#### Hangzhou Truth Electronic Inc., Zhejiang, China

#### Intern

#### September, 2000 - May, 2001

Circuit design and software implementation of a computer controlled telephone switching system.

PROFESSIONAL SERVICE

- Liaison, North Texas, SIAM Taxes&LA Section (2024-)
- Adult Mentor/Sponsor, Society for Science (2024-)
- Director of Undergraduate Studies, Math Department, SMU (2021- present)
- Data science graduate program admission committee member, SMU (2023-)
- Faculty search committee member: department of biology, SMU (2019-2020)
- Associate editor, Computational and Mathematical Biophysics (2019-)
- Committee member of SMU Undergraduate Council (2018-2021)
- Lead Guest Editor, Computational and Mathematical Biophysics (formerly Molecular Based Mathematical Biology) (2013-2014)
- Guest Editor, Computational and Mathematical Biophysics (formerly Molecular Based Mathematical Biology) (2012-2013)
- NSF Panelist service on Joint Meeting of Computational Mathematics and Mathematical Biology, Washington DC, April 4-5, 2011
- Referee Services:

Nature Computational Science Journal of Computational Physics Computer Physics Communications Journal of Computational Chemistry Journal of Chemical Theory and Computation SIAM Journal of Computational Science Journal of Chemical Information and Modeling Communications in Computational Physics Journal of Supercomputing

International Journal of Biomedical Image International Journal for Numerical Methods in Biomedical Engineering Journal of Applied Mathematics Journal of Computational and Applied Mathematics Advances in Applied Mathematics and Mechanics Journal of Computational Biophysics and Chemistry Communications in Information and Systems Journal of Computational and Mathematical Biophysics Numerical Algorithms MDPI-Mathematics

- Member of SMU Center for Research Computing Committee (2013-)
- Member of Calculus Book Committee at University of Alabama (2011-2012)
- Member of Linear Algebra Qualify Exam Committee, University of Alabama system (2012-2013)

PROFESSIONAL	• Institute of Electrical and Electronics Engineers (2001-)
MEMBERSHIP	• American Mathematical Society (2003- )
	• Society for Industrial and Applied Mathematics (2008-)
	• Society of Mathematical Biology (2010-)
	• American Chemical Society (2014-)
Computer Skills	• Mathematical and statistical modeling and programming
	• Solid software engineering background on participating and leading software projects
	• Parallel programming: MPI, Open MP, GPU/CUDA
	• Programming languages: FORTRAN, C/C++, Python, VB, HTML, Perl
	• Mathematical and statistical softwares: Matlab, Mathematica, Maple, SAS, Splus/R
	• Database management systems: SQL Server, Oracle, MySQL
	• Bimolecular simulation and dynamics packages: AMBER, CHARMM, APBS, VMD/NAMD
Students	• Current Graduate Students: Md Abu Talha (2023-)
Mentoring	• Graduated PhD Students:
	<ul> <li>Jianui Chen (2014-2019, tenure-track assistant professor at University of Arkansas)</li> <li>Xin Yang (2019-2024, computational scientist at HPC group of UTSW Medical Center)</li> <li>Elyssa Sliheet (2019-2024), TBA</li> </ul>
	• Current REU Students:
	<ul> <li>Graduated REU Students:</li> <li>Jingzhen Hu (2014-2017, PhD at Duke → Ernst Young),</li> <li>Xin Yang (2017-2019, PhD at SMU → computational scientist at HPC group of UTSW Medical Center)</li> <li>Yongjia Xu (2020-2022, Google)</li> <li>Reece Iriye (2022-2024, Verizon)</li> </ul>
Thesis & Dissertation	<ul> <li>Md Abu Talha (Math, 2026, Thesis &amp; Dissertation advisor, tentatively)</li> <li>Xin Yang (Math, 2024, Thesis &amp; Dissertation advisor)</li> <li>Alyssa Sliheet (Math, 2024, Thesis &amp; Dissertation advisor)</li> <li>Sylvia Amihere (Math, University of Alabama, 2024, Thesis &amp; Dissertation committee member)</li> </ul>
	• Ishna Satyarth (CS, 2024, Thesis & Dissertation committee member)
	• Molly Robinson (Math, 2024, Thesis & Dissertation committee member)
	<ul> <li>Tingting Zhao (Chemistry, 2024, Thesis &amp; Dissertation committee member)</li> <li>Morgan Thompson (Biology 2022, Thesis &amp; Dissertation committee member)</li> </ul>
	<ul> <li>Norah Hakami (Math, 2022, Thesis &amp; Dissertation committee member)</li> </ul>
	• Francesco Trozzi (Chemistry, 2022, Thesis & Dissertation committee member)
	• Shihao Wang (Math, 2021, Thesis & Dissertation committee member)
	• Sasan Mohyaddin (Math, 2020, Thesis & Dissertation committee member)
	• Jiahui Chen (Math, 2019, Thesis & Dissertation advisor)

- Yunwen Tao (Chemistry, 2018, Thesis & Dissertation committee member)
  Yang Liu (Math, 2017, Thesis & Dissertation committee member)

Previously Submitted Proposals NSF DMS-2325260, A Structural and Physical Data Driven Deep Learning Model for Protein Properties Prediction, \$235,723, not funded, PI: W. Geng, 2024-2027

SMU-Seed, Collaborative Research: Fast and Accurate Numerical Methods for Protein Simulation and Drug Design, \$194,100, not funded, Lead PI: W. Geng, PIs: Johannes Tausch, Tao Peng, John Wise, 2020-2023

NSF DMS-2012421, Collaborative Research: Mathematical modeling, numerical methods, and machine learning for simulating highly-charged biomolecules, \$243,941, not funded, PI: W. Geng, Co-PI: S. Zhao, 2020-2023

NSF DMS-1951770, Numerical Methods and Machine Learning for Computing Protein Pka Values, \$247,093, not funded, PI: W. Geng, 2020-2023

NSF DMS-1901550, Collaborative research: An integrated computational and experimental study of the gating mechanism and insecticides' effect in sodium channels, \$601,561, not funded, PI: W. Cai, Co-PI: W. Geng, 2019-2024

NSF DMS-1848426, CAREER: Numerical Methods for Interface Problems, \$423,489, not funded, PI: W. Geng, 2019-2024

NSF DMS-1759580, Collaborative research: a combined computational and experimental study of the gating mechanism and insecticides' effect in sodium channels, \$650,107, not funded, PI: W. Cai, Co-PI: W. Geng, 2018-2023

NSF DMS-1753195, CAREER: Fast and accurate algorithms for biomolecular simulations, \$451,107, not funded, PI: W. Geng, 2018-2023

NSF ACI-1739628, Collaborative: SI2-SSE - Treecode-Accelerated Software for Biomolecular Electrostatics, \$194,526, not funded, PI: W. Geng, 2017-2020

NSF DMS-1743914, CBMS Conference: Mathematical Molecular Bioscience and Biophysics, \$35,000, not funded, PI: S. Zhao, Co-PI: W. Geng, 2017-2018

NSF DMS-1720343, Treecode-accelerated Electrostatic Interactions for Biomolecular Applications, \$246,635, not funded, PI: W. Geng, 2017-2020

NSF DMS-1625961, *MRI: Acquisition of a High-Performance Computing Cluster for Computational Mathematics*, \$372,539, <u>not funded</u>, PI: T. Hagstrom, Co-PI(s): B. Lee, W. Geng, S. Xu, D. Reynolds, 2016-2019

Simons Foundation, Simons Investigators in the Mathematical Modeling of Living Systems (MMLS), From Molecular to Sub-Cellular: Numerical Simulation of Electrostatic Interaction for Implicitly Solvated Living Systems, \$500,000, not funded, PI: W. Geng, 2015-2010

NSF DMS-1554839, CAREER: Electrostatic Interactions in Solvated Biomolecules: Modelings, Algorithms and Applications, \$434,791, not funded, PI: W. Geng, 2016-2021

PRESENTATIONS Workshop on Biomolecular Topology: Modeling and Data Analysis, Institute for Mathematical Sciences (IMS), Singapore, June 24-28, 2024 (invited speaker)

Mathematics Seminar at Shanghai Jiaotong University, Shanghai, China, December 19, 2023 (invited speaker)

The 5th TSIMF Conference on Computational and Mathematical Bioinformatics and Biophysics,

Sanya, China, Dec. 11-15, 2021 (invited speaker)

Mathematics Seminar at Zhejiang University, Hangzhou, China, Dec. 8, 2023 (invited speaker)

10th International Congress on Industrial and Applied Mathematics, Waseda University, Tokyo, Japan, Aug. 20-25, 2023 (invited minisymposium speaker)

Protein Electrostatics Conference, Istituto Italiano di Tecnologia, Genoa, Italy, June 26-29, 2023 (invited minisymposium speaker)

Workshop on Scientific Computing, Purdue University, October 8, 2022 (invited speaker)

7th Annual Meeting of SIAM Central States Section, Oklahoma State University, Oct. 1-2, 2022 (invited minisymposium speaker)

SIAM Conference on the Life Sciences and SIAM Annual Meeting, Pittsburgh, July 11-15, 2022 (minisymposium organizer and speaker)

Mathematics Department Colloquium, (Online, University of Idaho), Feb. 10, 2022 (invited speaker)

The Fourth TSIMF Conference on Computational and Mathematical Bioinformatics and Biophysics, (online Tsinghua Sanya International Mathematics Forum), Sanya, China, December 10-14, 2021 (invited speaker)

The 4th Annual Meeting of SIAM Texas-Louisiana Section, Padre Island, November 5-7, 2021 (poster presentation)

Applied and Numerical Analysis Seminar, (Online, University of Florida), December 2, 2021 (invited speaker)

Mathematics in Action (MiA2021), Workshop on Modeling and Analysis in Molecular Biology and Electrophysiology (Online, Duke Kunshan University), June 10-13, 2021 (invited speaker)

Applied Mathematics Seminar, (Online, Texas Tech University), February 10, 2021 (invited speaker)

The 2nd Annual Meeting of SIAM Texas-Louisiana Section, SMU, Dallas November 1-3, 2019 (minisymposium speaker)

Conference on Computational Mathematics and Applications, University of Nevada, Las Vegas October 25 - 27, 2019 (minisymposium speaker)

International Congress on Industrial and Applied Mathematics, Valencia, July 15-19, 2019 (minisymposium speaker)

The Mathematics of Finite Elements and Applications (MAFELAP), Brunel University, London, June 18-21, 2019 (minisymposium speaker)

Finite Element Rodeo, University of Texas, Austin, February 27-28, 2019 (contributed speaker)

The 4th Annual Meeting of SIAM Central States Section, University of Oklahoma, Norman, October 6-7, 2018 (invited speaker)

Mathematics Seminar at Shanghai Jiaotong University, Shanghai, China, December 26, 2018 (invited speaker)

Mathematics Seminar at Zhejiang University, Hangzhou, China, December 19, 2018 (invited speaker)

Computational and Mathematical Approaches for Bioinformatics and Biophysics workshop, Tsinghua Sanya International Mathematics Forum, Sanya, China, December 10-14, 2018 (invited speaker)

SIAM Conference on the Life Sciences, Minneapolis, August 6-9, 2018 (minisymposium speaker)

SIAM Annual Meeting, Portland, July 9-13, 2018 (minisymposium organizer and speaker)

Mathematics in Action (MiA2018): Modeling and Analysis in Molecular Biology and Electrophysiology, Mathematical Center for Inter-discipline Research, Soochow University, China, June 16-18, 2018 (invited speaker)

Modeling, Analysis, Simulations and Applications of Inter-Facial Dynamics and FSI Problems workshop, Tsinghua Sanya International Mathematics Forum, Sanya, China, June 4-8, 2018 (invited speaker)

The 10th International Conference on Computational Physics (ICCP10), Macao, China, January 16-20 (invited symposium speaker)

Mathematics Seminar at Renmin University of China, Beijing, China, January 9, 2017 (invited speaker)

Mathematics Biophysics and Molecular Biosciences workshop, Tsinghua Sanya International Mathematics Forum, Sanya, China, December 19-23, 2016 (invited speaker)

The 20th IMACS World Congress, Xiamen, China, December 10-14, 2016 (invited speaker for the symposium )

SIAM Conference on the Life Sciences & SIAM Annual Meeting, Boston, July 11-15, 2016 (minisymposium organizer and speaker)

UT ICES Seminar-Numerical Analysis Series, Department of Mathematics, UT Austin, Austin, TX, March 11, 2016 (invited speaker)

Research Seminar at Department of Radiation Oncology, UT Southwestern Medical Center, Dallas, TX, February 5, 2016 (invited speaker)

MBI Workshop on "Multiple Faces of Biomolecular Electrostatics", Ohio State University, Columbus, Ohio, October 12-16, 2015 (invited speaker)

MBI Workshop on "Geometric and Topological Modeling of Biomolecules", Ohio State University, Columbus, Ohio, September 28 -October 2, 2015 (poster presenter with travel support)

8th International Congress on Industrial and Applied Mathematics, Beijing, China, August 10-14, 2015 (invited speaker for the symposium on "Free Boundary Problems: Theory, Numerics, and Applications")

The 3rd International Conference on High Performance Computing and Applications, Shanghai, China, July 26-30, 2015 (conference proceedings author and speaker)

Mathematics Seminar at Xian Jiaotong-Liverpool University, Suzhou, China, July 8, 2015 (invited speaker)

Finite Element Rodeo, Southern Methodist University, Dallas, February 27-28, 2015 (contributed speaker)

248th ACS National Meeting & Exposition, San Francisco, August 10-14, 2014 (invited speaker for the minisymposium on "Modeling the Effects of Water and Solvation in Biological Systems: Developments and Applications")

SIAM Conference on the Life Sciences, Charlotte, August 4-7, 2014 (minisymposium organizer and speaker)

Hands-on Summer School: Electronic Structure Theory for Materials and (Bio)molecules, IPAM/UCLA, Los Angeles, July 21 - August 1, 2014 (participant with travel support)

NSF-CBMS Conference on Inverse Scattering and Transmission Eigenvalues, UT Arlington, Arlington, May 27-31, 2014 (participant with travel support)

Scientific Computation Seminar, University of Texas at Dallas, Richardson, March 21, 2014 (invited talk)

Mathematical Biology and Physiology Seminar, Penn State University, University Park, October 24, 2013 (invited talk)

Research Seminar, Pacific Northwest National Laboratory, Richland, July 15-19, 2013 (Visiting

## Scholar)

SIAM Annual Meeting, San Diego, July 8-12, 2013 (two invited minisymposium talks)

SIAM Conference on Computational Science & Engineering, Boston, February 25 - March 1, 2013 (co-author of an invited minisymposium talk)

MBI Workshop on "Mathematical Challenges in Biomolecular/Biomedical Imaging and Visualization", Ohio State University, Columbus, Ohio, February 18-22, 2013 (invited poster)

The Society for Mathematical Biology Annual Meeting and Conference, Knoxville, July 25-28, 2012 (Minisymposium organizer and speaker)

36th Annual SIAM Southeastern Atlantic Section Conference, University of Alabama in Huntsville, Huntsville March 24-25, 2012 (invited minisymposium talk)

Applied Math Seminar, Illinois Institute of Technology, Chicago, March 7, 2012 (invited talk)

Joint Applied Mathematics Meeting, University of Alabama at Birmingham, Birmingham, November 5, 2011 (invited talk)

2nd Midwest Conference on Mathematical Methods for Images and Surfaces, Michigan State University, East Lansing, August 27-28, 2011 (invited poster)

MBI Workshop on "Modeling and Computation of Biomolecular Structure and Dynamics", Ohio State University, Columbus, Ohio, April 25-29, 2011 (invited poster)

SIAM Great Lake Conference, Oakland University, Rochester, April 16, 2011 (contributed poster)

Applied and Interdisciplinary Mathematics Seminar, University of Michigan, Ann Arbor, February 14, 2011 (contributed talk)

Applied Math Seminar, University of Alabama, Tuscaloosa, January 30-31, 2011 (invited talk)

Applied Math Seminar, Colorado State University, Fort Collins, September 1, 2010 (invited talk)

IMA Hot Topics Workshop on "Integral Equations", University of Minnesota, Minneapolis, August 1-5, 2010 (contributed poster)

M Symposium on Biophysics, University of Michigan, Ann Arbor, March 18, 2010 (contributed poster)

SIAM Conference on Parallel Processing for Scientific Computing, Seattle, February 24-26, 2010 (contributed talk)

IMA Workshop on "Molecular Simulations: Algorithms, Analysis, and Applications", University of Minnesota, Minneapolis, May 18-22, 2009 (contributed poster)

International Conference on Engineering and Computational Mathematics, Hong Kong Polytechnic University, Hong Kong, May 27-29, 2009 (contributed talk)

Frontier in Applied and Computational Mathematics, NJIT, Newark, May 19-21, 2008 (contributed talk)

Computer Science Seminar, Purdue University, West Lafayette, February 12, 2008 (invited talk)

Applied Math Seminar, University of Michigan, Ann Arbor, December 14, 2007 (invited talk)

MSU-UM Math Biology Day, Michigan State University, East Lansing, December 1, 2007 (invited talk)

First Annual MSU Student Mathematics Conference, Michigan State University, East Lansing, March 1, 2003 (contributed talk)