Jiahui Chen

CONTACT INFORMATION

Department of Mathematics
Michigan State University *E-mail:* chenj159@msu.edu
East Lansing, MI 48824

ACADEMIC PREPARATION

Michigan State University, East Lansing, Michigan
Postdoc, 2019-present (Mentor: Guo-Wei Wei)

Southern Methodist University, Dallas, Texas
PhD, Computational and Applied Mathematics, 2014-2019 (Advisor: Weihua Geng)

Xi'an Jiaotong–Liverpool University, Suzhou, China
BSc Applied Mathematics, May 2014

WORKING EXPERIENCE

Michigan State University, East Lansing, MI
Visiting Assistant Professor **August 2019 - Present**

Michigan State University, East Lansing, MI
Visiting scholar **May - July, 2018**

Pacific Northwest National Laboratory, Richland, WA
PhD internship **May - August, 2016**

RESEARCH INTERESTS

Mathematical Biology/Biophysics; Topological Data Analysis; Differential Geometry; Numerical PDB; Boundary Integral Equations; Boundary Element Method; Treecode and Fast Multipole Method; Machine Learning/Deep Learning; and Parallel/GPU Computing

PUBLICATIONS

(* co-first author)
Published/Accepted

16. **J. Chen***, K. Gao*, R. Wang*, and G.W. Wei, Prediction and mitigation of mutation threats to COVID-19 vaccines and antibody therapies, *Chemical Science*, in publication 2021
15. R. Wang, R. Zhao, E. Ribando-Gros, **J. Chen**, Y. Tong, and G.W. Wei, HERMES: Persistent spectral graph software, *Foundations of Data Science*, in publication (2021)
14. J. Strubbe-Rivera, **J. Chen**, B. A. West, K. N. Parent, G.W. Wei, and J. N. Bazil, Modeling the Effects of Calcium Overload on Mitochondrial Ultrastructural Remodeling, *Applied Sciences*, DOI:10.3390/app11052071 (2021)
13. R. Wang, **J. Chen**, K. Gao, Y. Hozumi, C. Yin, and G.W. Wei, Analysis of SARS-CoV-2 mutations in the United States suggests presence of four substrains and novel variants, *Communications Biology*, in press (2021)
12. **J. Chen**, W. Geng, and D. Reynolds, Cyclically parallelized treecode for fast computations of electrostatic interactions on molecular surfaces, *Computer Physics Communication*, 260, 107742 (2021)
11. **J. Chen**, J. Hu, Y. Xu, R. Krasny, and W. Geng, Computing protein pKas using the TABI Poisson-Boltzmann Solver, *Jounal of Computational Biophysics and Chemistry*, 2042006, (2020)
10. R. Wang, **J. Chen**, Y. Hozumi, C. Yin, G.W. Wei, Decoding asymptomatic COVID-19 infection and transmission, *The Journal of Physical Chemistry Letters*, 11 (23), 10007-10015, (2020)
9. **J. Chen**, R. Wang, M. Wang, and G.W. Wei, Mutations strengthened SARS-CoV-2 infectivity, *Joiunral of molecular biology*, 432 (19), 5212-5226, (2020)

8. R. Zhao, M. Wang, **J. Chen**, Y. Tong, and G.W. Wei, The de Rham-Hodge Analysis, and Modeling of Biomolecules, *Bulletin of Mathematical Biology*, 82 (8), 1-38, (2020)
7. **J. Chen***, K. Gao*, R. Wang, D. Nguyen, and G.W. Wei, Review of COVID-19 antibody therapies, Annual Review of Biophysical, 50, (2020)
6. K. Gao, D. Nguyen, **J. Chen**, R. Wang, and G.W. Wei, Repositioning of 8565 existing drugs for COVID-19, *The Journal of Physical Chemistry Letters*, 11, (13), 5373-5382, (2020)
5. D. Nguyen, K. Gao, **J. Chen**, R. Wang, and G.W. Wei, Unveiling the molecular mechanism of SARS-CoV-2 main protease inhibition from 92 crystal structures, *Chemical Science*, 11, 12046-12046, (2020)
4. **J. Chen**, R. Zhao, Y. Tong, Evolutionary de Rham-Hodge method, *Discrete & continuous Dynamical Systems - B*, doi: 10.3934/dcdsb.2020257 (2020)
3. **J. Chen** and W. Geng, On Preconditioning the Treecode-Accelerated Boundary Integral (TABI) Poisson-Boltzmann Solver, *J. Comput. Phys.*, 373, 750-762 (2018)
2. 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)
1. **J. Chen**, W. Geng, 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)

In revision/Revision submitted

2. R. Wang*, K. Gao*, **J. Chen**, and G.W. Wei, Fast-growing mutations in the United Kingdom, the United States, Singapore, Spain, South Africa, and other COVID-19-devastated countries, *The Journal of Physical Chemistry Letters*, in revision, 2021
1. K. Gao*, R. Wang*, **J. Chen**, L. Cheng, J. Frishcosy, Y. Huzumi, Y. Qiu, T. Schluckbler, and G.W. Wei, Methodology-centered review of molecular modeling, simulation, and prediction of SARS-CoV-2, *Chemical Review*, in revision, 2021

Honors and awards

Dedman College, SMU, Graduate Student Travel Grant Award, $500, 2019

Dedman College, SMU, Graduate School Dissertation Completion Fellowship, $20,000, 2018

Math Dept., Southern Methodist University, Teaching Assistant Award, Cash award, 2018

Papers in preparation

With L. Wilson, W. Geng, R. Krasny, "Improvements to the TABIPB C-Version"

With Q. Sun, D. Chan and W. Geng, "Regularization for Boundary Integral Poisson-Boltzmann Equation and Treecode Acceleration"

With W. Geng, J. Tausch, "Adaptive Cartesian FMM Accelerated Poisson-Boltzmann Solver"

With W. Geng, T. Schlick, G. Bascom, "Multipole Method Accelerated Electrostatics Computation for Mesoscale Chromatin Simulation"

With H-X Zhou, W. Geng, J. Tausch, "Cartesian FMM for Modeling Protein Folding and Binding under All-Atom Crowders"

Conferences and presentations

9. Computational Biology Forum, MSU, January 2021 (presentation)
8. Computational topology/geometry/graph seminar, webinar, December 2020 (presentation)
7. Colorado State University, webinar, November 2020 (presentation)
6. NSF-CBMS Conference: Mathematical Molecular Bioscience and Biophysics, the University of Alabama, Tuscaloosa, Alabama, May 2019 (poster)

5. IMSM workshop, SAMSI, North Carolina State University, July 2018 (presentation)
4. Workshop on the Mathematics of Drug Design/Discovery, the Fields Institute, Toronto, Canada, June 2018 (attendance)
3. Multiple Faces of Biomolecular Electrostatics, MBI, Ohio State University, October 2016 (poster)
2. Mathematics of Biological Charge Transport: Molecules and Beyond, IMA, University of Minnesota, Twin Cities, July 2016 (attendance)
1. 2015 SMU PhD interdisciplinary project of data science and analysis (presentation)

Teaching experience

MTH496, Introduction of Machine Learning — Fall 2020 / Spring 2021
Instructor — Michigan State University

Math 3316, Introduction to High Performance Scientific Computing — Fall 2015
Laboratory TA — Southern Methodist University

Graduate research mentoring (With Professor Guo-Wei Wei at MSU)

- Ms. Rui Wang — 2019-present
- Mr. Yuta Hozumi — 2020-present
- Mr. Xiaoqi Wei — 2020-present

Professional services

Journal reviewer
International Journal for Numerical Methods in Biomedical Engineering, Computational and Mathematical Biophysics, Journal of Chemical Information and Modeling
Proposal reviewer
The French National Research Agency

Software

- Wei-Lab (MSU) servers maintenance
- C-version Treecode (http://github.com/jiahuic/treecode)
- Parallel C-version Treecode (http://github.com/jiahuic/treecode_parallel)
- C-version TABI Poisson-Boltzmann Solver (http://github.com/jiahuic/TABI_solver)

Activates

- Math Outreach, Glencairn Elementary School, East Lansing, January 9. 2020

Professional Membership

- American Mathematical Society (2014-)
- Society for Industrial and Applied Mathematics (2014-)

Computer Skills

- Mathematical and statistical modeling and programming
- Parallel programming: MPI, Open MP, GPU/CUDA
- Programming languages: FORTRAN, C/C++, HTML, Python, Java, Cython
- Mathematical and statistical softwares: Matlab, Mathematica, Excel