

Kelin Xia

Assistant Professor

Nanyang Technological University,
SPMS-DMS-05-18, 21 Nanyang Link,
Singapore 637371

Phone: +65 65137464
Email: xiakelin@ntu.edu.sg
Homepage: <http://www.ntu.edu.sg/home/xiakelin/>

Educational and Professional Qualifications

- **Ph.D. Graduate University of Chinese Academy of Sciences, China**
Ph.D in Applied Mathematics Jun. 2007 – Jan. 2013
– Advisor: Meng Zhan and Guo-Wei Wei
- **Michigan State University**
Visiting scholar Dec. 2009 – Jan. 2013
– Advisor: Guo-Wei Wei
- **Michigan State University**
Visiting Assistant Professor Jan. 2013 – May 2016
– Mentor: Guo-Wei Wei
- **Nanyang Technological University**
Assistant Professor Jun. 2016 – Present

Research Interests

- **Mathematical Modeling of Biomolecular Systems**
Geometric and topological modeling of biomolecules;
Variational multiscale modeling of biomolecules;
Flexible-Rigidity Index
- **Topological Data Analysis**
Persistent homology analysis for big data in biomolecules
- **Scientific Computing**
Matched interface and boundary (MIB) method for multidomain interface problem;
Adaptive mesh based MIB method;
MIB Galerkin method

Grants and Awards

Research Funding

- Nanyang Technological University, SUG-M4081842.110
- Co-PI (PI: Guo-Wei Wei), National Science Foundation, DMS-1160352, \$319,477, “FRG: Collaborative research: Variational multiscale approaches to biomolecular structure, dynamics and transport” 09/15/2012-08/31/2015. Personal annual allocation: 2 mo. salary.
- Co-PI (PI: Guo-Wei Wei), NIH/NIGMS, 3R01GM090208-04S1, \$103,339 “Geometric flow approach to implicit solvation modeling” 07/29/2014-06/30/2015. Personal annual allocation: 1 mo. salary.

- Investigator (PI: Guo-Wei Wei), NIH/NIGMS, R01GM090208, \$1,239,500, "Geometric flow approach to implicit solvation modeling" 07/29/2009-07/28/2014. Personal annual allocation: 6 mo. salary.

Awards

- Traveling award: IMA Annual Program Year Workshop Topological Structures in Computational Biology, December 9-13, 2013
- Traveling award: Mathematical Challenges in Biomolecular/Biomedical Imaging and Visualization, Mathematical Biosciences Institute, Ohio State University, February 18-22, 2013
- Traveling award: Modeling and Computation of Biomolecular Structure and Dynamics, Mathematical Biosciences Institute, Ohio State University, April 25-29, 2011
- Traveling award: Fluid Motion Driven by Immersed Structures, University of Toronto, August 9-13, 2010

Publications

Under Review Articles

1. Yin Cao, Bao Wang, **Kelin Xia** and Guo-Wei Wei, "Finite volume formulation of the MIB method for elliptic interface problems", *Journal of Computational Physics*, submitted, 2015

Published Articles and Articles Accepted for Publication

28. Duc D Nguyen, **Kelin Xia** and Guo-Wei Wei, "Generalized flexibility-rigidity index", *Journal of Computational Chemistry*, 144, 234106, 2016
27. Kristopher Opron, **Kelin Xia**, Zachary F. Burton and Guo-Wei Wei, "Flexibility-Rigidity index for protein-nucleic acid flexibility and fluctuation analysis", *Journal of Computational Chemistry*, 37, 1283-1295, 2016
26. Zixuan Cang, Lin Mu, Kedi Wu, Kristopher Opron, **Kelin Xia** and Guo-Wei Wei, "A topological approach to protein classification", *Molecular Based Mathematical Biology*, 3, 140-162, 2015
25. **Kelin Xia**, Kristopher Opron and Guo-Wei Wei, "Multiscale Gaussian network model (mGNM) and multiscale anisotropic network model (mANM)", *Journal of Chemical Physics*, 143, 204106, 2015
24. **Kelin Xia**, Zhixiong Zhao and Guo-Wei Wei, "Multiresolution persistent homology for excessively large biomolecular datasets", *Journal of Chemical Physics*, 143, 134103, 2015
23. **Kelin Xia** and Guo-Wei Wei, "Multiresolution topological simplification", *Journal of Computational Biology*, 22(9), 1-5, 2015
22. **Kelin Xia** and Guo-Wei Wei, "Multidimensional persistence in biomolecular data", *Journal of Computational Chemistry*, 36, 1502-1520, 2015
21. **Kelin Xia** and Guo-Wei Wei, "Persistent homology for cryo-EM data analysis", *International Journal for Numerical Methods in Biomedical Engineering*, 31(8), e02719, 2015
20. Jinkyong Park, **Kelin Xia** and Guo-Wei Wei, "Atomic scale design and three dimensional simulations of nanofluidic systems", *Microfluidics and Nanofluidics*, 19(3), 665-692, 2015

19. Kristopher Opron, **Kelin Xia** and Guo-Wei Wei, "Communication: Capturing protein multiscale thermal fluctuations", *Journal of Chemical Physics*, 142, 211101, 2015
18. Bao Wang, **Kelin Xia** and Guo-Wei Wei, "Second order method for solving 3D elasticity equations with complex interfaces", *Journal of Computational Physics*, 294, 405-438, 2015
17. **Kelin Xia**, Xin Feng, Yiyong Tong and Guo-Wei Wei, "Persistent homology for the quantitative prediction of fullerene stability", *Journal of Computational Chemistry*, 36, 408-422, 2015
16. Bao Wang, **Kelin Xia** and Guo-Wei Wei, "Matched interface and boundary method for elasticity interface problems", *Journal of Computational and Applied Mathematics*, 285, 203-225, 2015
15. **Kelin Xia** and Guo-Wei Wei, "A Galerkin formulation of the MIB method for three dimensional elliptic interface problems", *Computers and Mathematics with Applications*, 68, 719-745, 2014
14. **Kelin Xia** and Guo-Wei Wei, "Persistent homology analysis of protein structure, flexibility and folding", *International Journal for Numerical Methods in Biomedical Engineering*, 30, 814-844, 2014
13. Kristopher Opron, **Kelin Xia** and Guo-Wei Wei, "Fast and anisotropic flexibility-rigidity index for protein flexibility and fluctuation analysis", *Journal of Chemical Physics*, 140, 234105, 2014
12. **Kelin Xia**, Meng Zhan and Guo-Wei Wei, "MIB Galerkin method for elliptic interface problems", *Journal of Computational and Applied Mathematics*, 272, 195-220, 2014
11. **Kelin Xia** and Guo-Wei Wei, "Molecular nonlinear dynamics and protein thermal uncertainty quantification", *Chaos*, 24, 013103, 2014
10. **Kelin Xia** and Guo-Wei Wei, "Stochastic model for protein flexibility analysis", *Physical Review E*, 88, 062709, 2013
9. **Kelin Xia**, Kristopher Opron and Guo-Wei Wei, "Multiscale multiphysics and multidomain models—Flexibility and rigidity", *Journal of Chemical Physics*, 139, 194109, 2013.
8. **Kelin Xia**, Xin Feng, Zhan Chen, Yiyong Tong and Guo-Wei Wei, "Multiscale geometric modeling of macromolecules I: Cartesian representation", *Journal of Computational Physics*, 257, 912-936, 2014
7. Xin Feng, **Kelin Xia**, Zhan Chen, Yiyong Tong and Guo-Wei Wei, "Multiscale geometric modeling of macromolecules II: Lagrangian representation", *Journal of Computational Chemistry*, 34, 2100-2120, 2013
6. Xin Feng, **Kelin Xia**, Yiyong Tong and Guo-Wei Wei, "Geometric modeling of subcellular structures, organelles, and multiprotein complexes", *International Journal for Numerical Methods in Biomedical Engineering*, 28(12), 1198-1223, 2012
5. Guo-Wei Wei, Qiong Zheng, Zhan Chen and **Kelin Xia**, "Variational multiscale models for charge transport", *SIAM Review*, 54(4), 699-754, 2012
4. **Kelin Xia**, Meng Zhan, Decheng Wan and Guo-Wei Wei, "Adaptively deformed mesh based interface method for elliptic equations with discontinuous coefficients", *Journal of Computational Physics*, 231(4), 1440-1461, 2012
3. **Kelin Xia**, Meng Zhan and Guo-Wei Wei, "MIB method for elliptic equations with multi-material interfaces", *Journal of Computational Physics*, 230(12), 4588-4615, 2011
2. Ming Yi, **Kelin Xia** and Meng Zhan, "Theoretical study for regulatory property of scaffold protein on MAPK cascade: a qualitative modeling", *Biophysical Chemistry*, 147(3), 130-139, 2010
1. Qi Zhao, Ming Yi, **Kelin Xia** and Meng Zhan, "Information propagation from IP₃ to target protein: a combined model for encoding and decoding of Ca²⁺ signal", *Physica A*, 388, 4105-4114, 2009

Conferences and Presentations

- (upcoming) Invited speaker: Department of Mathematics, National University of Singapore, August 31, 2016
- (upcoming) Invited speaker: Bioinformatics Institute, A*STAR, August 23, 2016
- (upcoming) Invited speaker: School of Biological Science, Nanyang Technological University, August 15, 2016
- Organizer: Mini-symposium "Molecular Biosciences and Biophysics: Topological and Geometric methods" at SIAM Conference on Life Sciences, Boston, Massachusetts, July 13, 2016 (Co-organizer: Prof. Natasha Jonoska)
- Invited speaker: Department of Mathematics and Statistics, University of North Carolina Charlotte, April 25, 2016
- Invited speaker: School of Mathematical Science, Monash University, April 21, 2016
- Invited speaker: School of Physical and Mathematical Science, Nanyang Technological University, March 8, 2016
- Invited speaker: Department of Mathematics, The university of Tennessee at Chattanooga, February 30, 2016
- Invited speaker: Department of Mathematical Science, Georgia Southern University, February 22, 2006
- Invited speaker: Department of Mathematics, North Carolina State University, January 21, 2016
- Invited speaker: MBI emphasis workshop Geometric and Topological Modeling of Biomolecules, Mathematical Biosciences Institute, Ohio State University, September 28-October 2, 2015
- Invited speaker: IMA hot topic workshop Mathematics of Biological Charge Transport: Molecular and Beyond, Institute for Mathematics and its Applications, Twin Cities, 2015
- Invited speaker: Geometric and Topological Modeling of Biomolecules, Mathematical Biosciences Institute, Ohio State University, September 28-October 02, 2015
- Organizer: Workshop on persistent homology for biosciences, East Lansing, October 18, 2014 (With Prof. Guo-Wei Wei and Prof. Yiyong Tong)
- Organizer: Mini-symposium "Molecular Biosciences: Topological modeling of biomolecules" at SIAM Conference on Life Sciences, Charlotte, North Carolina, August 4-7, 2014 (Co-organizer: Prof. Yuanan Diao)
- Invited speaker: Mini-symposium "Modeling and computation of problems in mathematical biology" at The 38th annual meeting of the SIAM Southeastern Atlantic Section, Florida Institute of Technology in Melbourne, Florida, March 28-30, 2014
- Poster: IMA Annual Program Year Workshop Topological Structures in Computational Biology, December 9-13, 2013
- Poster: 2013 Great Lakes SIAM Conference: Computational Mathematics: Modeling, Algorithms and Applications, Central Michigan University, April 20, 2013
- Invited speaker: Mathematical Challenges in Biomolecular/Biomedical Imaging and Visualization, Mathematical Biosciences Institute, Ohio State University, February 18-22, 2013

- Invited speaker: 12th International Symposium on Mathematical and Computational Biology, Tempe, Arizona, November 7-10, 2012
- Speaker: SMB Annual Meeting and Conference, Knoxville, Tennessee, July 25-28, 2012
- Participation: 2nd Midwest Conference on Mathematical Methods for Images and Surfaces, East Lansing, August 27-28, 2011
- Participation: Modeling and Computation of Biomolecular Structure and Dynamics, Mathematical Biosciences Institute, Ohio State University, April 25-29, 2011
- Poster: Fluid Motion Driven by Immersed Structures, University of Toronto, August 9-13, 2010
- Participation: Workshop on Nano-Bio Mathematics and Mechanics, Michigan State University, August 5, 2010
- Participation: Modeling and Numerical PDEs in Mathematical Biology and Applications, Oakland University, April 16, 2011
- Participation: Frontiers in Mathematical Biology: NSF-NIH PIs Meeting 2010, University of Maryland, College Park, April 26-27, 2010
- Participation: SIAM Great Lakes Conference: Modeling and numerical PDEs in Mathematical Biology, University of Michigan at Dearborn, April 17, 2010

Teaching

- **Instructor**
MH9200, 2016
MTH 132 (Section 016 and Section 020), 2015;
MTH 132 (Section 014 and Section 033), 2014;
MTH 132 (Section 016 and Section 024), 2013
- **Series of lectures**
MTH 995 (Modeling and Computation of human sensory systems), 2013
- **Mentor for undergraduates (with Prof. Guo-Wei Wei)**
Archie Brown III, Summer Research Opportunities Program at MSU, 2012;
Rinaldi Romulus, Summer Research Opportunities Program at MSU, 2013;
Zhuozhuo Tu, International Exchange Program at Department of Mathematics in MSU, 2013;
Fengze Cao, International Exchange Program at Department of Mathematics in MSU, 2014

Journal Reviewer

- Applied Mathematics and Computation
- Chemical Physics Letters
- Computer Methods in Applied Mechanics and Engineering
- European Journal of Applied Mathematics
- International Journal for Numerical Methods in Biomedical Engineering
- International Journal of Biomathematics

- Journal of Applied Mathematics
- Journal of Computational and Applied Mathematics
- Journal of Chemical Physics
- Journal of Theoretical and Computational Chemistry
- Mathematics of Computation
- Molecular Based Mathematical Biology
- Nonlinearity
- Statistical Applications in Genetics and Molecular Biology
- Symmetry