Zhen Li Updated: July 20, 2023

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Zhen Li's Profiles on Google Scholar, Researchgate

Summary

Assistant Professor of Mechanical Engineering at Clemson University. Research interest is on multiscale modeling of complex fluids, soft matter and biophysics, using both **bottom-up** (coarse-grained molecular modeling) and **top-down** (from continuum descriptions to fluctuating hydrodynamics) approaches, along with high performance computing. Specific research topics include **mathematical theory** of coarse-graining and model reduction, **physics-informed machine-learning methods** applied to **data-driven** modeling of soft matter and biochemical systems, **memory effects** in complex fluids and **non-local approaches**, and concurrent coupling of heterogeneous solvers for **scale-bridging**.

Professional Experience

Clemson University – Department of Mechanical Engineering — Clemson, SC, USA
Assistant Professor (Tenure-Track) — *Aug. 2019 – present*

Brown University – Division of Applied Mathematics — Providence, RI, USA
Research Associate Professor (Research-Track) — *Jan. 2019 – Jul. 2019*

National Polytechnic Institute of Toulouse – Laboratory of Chemical Engineering — Toulouse, France
Visiting Professor (Fellowship) — *Dec. 2018 – Dec. 2018*

Brown University – Division of Applied Mathematics — Providence, RI, USA
Research Assistant Professor (Research-Track) — *Jan. 2016 – Dec. 2018*

Brown University – Division of Applied Mathematics — Providence, RI, USA
Postdoctoral Research Associate — *Jan. 2013 – Dec. 2015*

University of California, Merced – School of Engineering — Merced, CA, USA
Postdoctoral Research Associate — *Feb. 2012 – Dec. 2012*

Academic Degrees

Shanghai University — Shanghai, China
Ph.D. in Fluid Mechanics — *April 2012*

Shanghai University — Shanghai, China
M.Eng. in Fluid Mechanics — *October 2008*

Wuhan University — Wuhan, China
B.Eng. in Engineering Mechanics — *June 2005*

Publications/Creative Works (* represents the co-first author, † represents the corresponding author)

Year 2023:

65. E. Kiyani, M. Kooshkbaghi, K. Shukla, R. Koneru, **Z. Li**, L. Bravo, A. Ghoshal, G. Karniadakis and M. Karttunen. Characterization of partial wetting by CMAS droplets using multiphase many-body dissipative particle dynamics and data-driven discovery based on PINNs. Journal of Fluid Mechanics, 2023 (under review). arXiv:2307.09142

64. P. Kunwar, A. Poudel, U. Aryal, R. Xie, Z. J. Geffert, H. Wittmann, T. H. Chiang, M. M. Maye, **Z. Li** and P. Soman. Meniscus-enabled Projection Stereolithography (MAPS). Advanced Materials, 2023 (under review). bioRxiv: 2023.06.12.544584

63. S. Sheikh, A. Mohammadi, L. Lonetti, **Z. Li**† and M. Abbas. Anomalous diffusion of soft particles near a fluctuating lipid bilayer. The Journal of Chemical Physics, 2023 (under review).

62. X. Cai, **Z. Li** and X. Bian. Arbitrary slip length for fluid-solid interface of arbitrary geometry in smoothed particle dynamics. Journal of Computational Physics, 2023 (under review). arXiv.2303.06327

61. **Z. Li**†, G. Hu, Z. Wang and G.E. Karniadakis. Preface: machine-learning approaches for computational mechanics. Applied Mathematics and Mechanics, 2023, 44(7): 1035-1038. (Guest Editor of the Special Issue) DOI: 10.1007/s10483-023-2999-7

60. M. Lu, A. Mohammadi, Z. Meng, X. Meng, G. Li and **Z. Li**†. Deep neural operator for learning transient response of interpenetrating-phase composites subject to dynamic loading. Computational Mechanics, 2023, 72: 563-576. DOI: 10.1007/s00466-023-02343-6

59. K.C. Chan, **Z. Li** and W. Wenzel. A Mori-Zwanzig dissipative particle dynamics approach for anisotropic coarse grained molecular dynamics. Journal of Chemical Theory and Computation, 2023, 19(3): 910-923. DOI: 10.1021/acs.jctc.2c00960

Year 2022:

58. R. Koneru, **Z. Li**†, L. Bravo, M. Murugan, A. Ghoshal, G. Karniadakis and A. Flatau. Quantifying the dynamic spreading of a molten sand droplet using multiphase mesoscopic simulations. Physical Review Fluids, 2022, 7: 103602. DOI: 10.1103/PhysRevFluids.7.103602

57. Y. Xia, Q. Rao, A. Hamed, J. Kane, V. Semeykina, I. Zharov, M. Deo and **Z. Li**. Flow reduction in pore networks of packed silica nanoparticles: Insights from mesoscopic fluid models. Langmuir, 2022, 38(26): 8135-8152. DOI: 10.1021/acs.langmuir.2c01038

56. M. Deng, F. Tushar, L. Bravo, A. Ghoshal, G. Karniadakis and **Z. Li**†. Theory and simulation of electrokinetic fluctuations in electrolyte solutions at the mesoscale. Journal of Fluid Mechanics, 2022, 942: A29. DOI: 10.1017/jfm.2022.377

55. K. Zhang, J. Li, W, Fang, C. Lin, J. Zhao, **Z. Li**, Y. Liu, S. Chen, C. Lv and X.-Q. Feng. An energy-conservative many-body dissipative particle dynamics model for thermocapillary drop motion. Physics of Fluids, 2022, 34: 052011. DOI: 10.1063/5.0088238

54. H. Li, Y. Deng, **Z. Li**, A. Gallastegi, C. Mantzoros, G. Frydman and G. Karniadakis. Multiphysics and multiscale modeling of microthrombosis in COVID-19. PLOS Computational Biology, 2022, 18(3): e1009892. DOI: 10.1371/journal.pcbi.1009892

53. S. Ma, S. Wang, X. Qi, K. Han, X. Jin, **Z. Li**†, G. Hu and X. Li. Multiscale computational framework for predicting viscoelasticity of red blood cells in aging and mechanical fatigue. Computer Methods in Applied Mechanics and Engineering, 2022, 391: 114535. DOI: 10.1016/j.cma.2021.114535

52. H. Li, Y. Deng, K. Sampani, S. Cai, **Z. Li**, J.K. Sun and G. Karniadakis. Computational investigation of blood cell transport in retinal microaneurysms. PLOS Computational Biology, 2022, 18(1): e1009728. DOI: 10.1371/journal.pcbi.1009728

Year 2021 and before:

51. C. Lin, M. Maxey, **Z. Li** and G. Karniadakis. A seamless multiscale operator neural network for inferring bubble dynamics. Journal of Fluid Mechanics, 2021, 929: A18. DOI: 10.1017/jfm.2021.866

50. Q. Rao, Y. Xia, J. Li, M. Deo and **Z. Li**†. Flow reduction of hydrocarbon liquid in silica nanochannel: Insight from many-body dissipative particle dynamics simulations. Journal of Molecular Liquids, 2021, 344: 117673. DOI: 10.1016/j.molliq.2021.117673

49. A. Blumers, M. Yin, H. Nakajima, Y. Hasegawa, **Z. Li** and G. Karniadakis. Multiscale parareal algorithm for long-time mesoscopic simulations of microvascular blood flow in zebrafish. *Computational Mechanics*, 2021, 68: 1131-1152. DOI: 10.1007/s00466-021-02062-w

48. C. Lin, **Z. Li**, L. Lu, S. Cai, M. Maxey and G. Karniadakis. Operator learning for predicting multiscale bubble growth dynamics. *The Journal of Chemical Physics*, 2021, 154: 104118. DOI: 10.1063/5.0041203

47. A. Yazdani, Y. Deng, H. Li, E. Javadi, **Z. Li**†, S. Jamali, C. Lin, J. Humphrey, C. Mantzoros and G. Karniadakis. Integrating blood cell mechanics, platelet adhesive dynamics and coagulation cascade for modeling thrombus formation in normal and diabetic blood. *Journal of the Royal Society Interface*, 2021, 18: 20200834. DOI: 10.1098/rsif.2020.0834

46. Q. Rao, Y. Xia, J. Li, J. McConnell, J. Sutherland and **Z. Li**†. A modified many-body dissipative particle dynamics model for mesoscopic fluid simulation: methodology, calibration, and application for hydrocarbon and water. *Molecular Simulation*, 2021 (in press). DOI: 10.1080/08927022.2021.1876233

45. L. Zhao, **Z. Li**†, Z. Wang, B. Caswell, J. Ouyang and G. Karniadakis. Active- and transfer-learning applied to microscale-macroscale coupling to simulate viscoelastic flows. *Journal of Computational Physics*, 2021, 427: 110069. DOI: 10.1016/j.jcp.2020.110069

44. X. Meng, **Z. Li**⋆, D. Zhang and G. Karniadakis. PPINN: Parareal Physics-Informed Neural Network for time-dependent PDEs. *Computer Methods in Applied Mechanics and Engineering*, 2020, 370: 113250. DOI: 10.1016/j.cma.2020.113250

43. Y. Xia, A. Blumers, **Z. Li**†, L. Luo, Y.H. Tang, K.Joshua, H. Huang, M. Andrew, M. Deo and J. Goral. A GPU-accelerated package for simulation of flow in nanoporous source rocks with many-body dissipative particle dynamics. *Computer Physics Communications*, 2020, 247: 106874. DOI: 10.1016/j.cpc.2019.106874
    - This work won the **Best Research Poster Award** of SC19 (The International Conference for High Performance Computing, Networking, Storage, and Analysis, November, 2019).

42. Y. Wang, **Z. Li**[†], J. Ouyang and G. Karniadakis. Controlled release of entrapped nanoparticles from thermoresponsive hydrogels with tunable network characteristics. *Soft Matter*, 2020, 16: 4756-4766. [Selected as the **Back Cover of Soft Matter**] DOI: 10.1039/D0SM00207K

41. L. Lu, **Z. Li**[⋆], H. Li, X. Li, P. Vekilov and G. Karniadakis. Quantitative prediction of erythrocyte sickling for the development of advanced sickle cell therapies. *Science Advances*, 2019, 5(8): eaax3905. DOI: 10.1126/sciadv.aax3905

40. S. Wang, **Z. Li** and W. Pan. Implicit-solvent coarse-grained modeling for polymer solutions via Mori-Zwanzig formalism. *Soft Matter*, 2019, 15: 7567-7582. [Selected as the **Back Cover of Soft Matter**] DOI: 10.1039/C9SM01211G

39. A. Hemeda, S. Pal, A. Mishra, M. Torabi, M. Ahmadlouydarab, **Z. Li**, J. Palko and Y. Ma. Effect of wetting and dewetting on the dynamics of atomic force microscopy measurements. *Langmuir*, 2019, 35(41): 13301-13310. DOI: 10.1021/acs.langmuir.9b02575

38. K. Zhang, **Z. Li**[†] and S. Chen. Analytical prediction of electrowetting-induced jumping motion for droplets on hydrophobic substrates, *Physics of Fluids*, 2019, 31(8): 081703. DOI: 10.1063/1.5109164

37. A.L. Blumers, **Z. Li**[†] and G.E. Karniadakis. Supervised parallel-in-time algorithm for long-time Lagrangian simulations of stochastic dynamics: Application to hydrodynamics. *Journal of Computational Physics*, 2019, 393: 214-228. DOI: 10.1016/j.jcp.2019.05.016

36. Y. Wang, **Z. Li**[⋆,†], J. Xu, C. Yang and G.E. Karniadakis. Concurrent coupling of atomistic simulation and mesoscopic hydrodynamics for flows over soft multi-functional surfaces, *Soft Matter*, 2019, 15: 1747-1757. [Selected as the **Back Cover of Soft Matter**] DOI: 10.1039/C8SM02170H

35. Z. Mao, **Z. Li**[†] and G.E. Karniadakis. Nonlocal flocking dynamics: Learning the fractional order of PDEs from particle simulations, *Communication on Applied Mathematics and Computation*, 2019, 1(4): 597-619 (**Invited Paper** for Special Issue) DOI: 10.1007/s42967-019-00031-y

34. K. Zhang, **Z. Li**[⋆,†], M. Maxey, S. Chen and G.E. Karniadakis. Self-cleaning of hydrophobic rough surfaces by coalescence-induced wetting transition, *Langmuir*, 2019, 35(6): 2431-2442. [Selected as the **Cover of Langmuir**] DOI: 10.1021/acs.langmuir.8b03664

33. B. Drawert, B. Jacob, **Z. Li**, T.-M. Yi and L. Petzold. A hybrid smoothed dissipative particle dynamics spatial stochastic simulation algorithm for advection-diffusion-reaction problems. *Journal of Computational Physics*, 2019, 378: 1-17. DOI: 10.1016/j.jcp.2018.10.043

32. B. Drawert, B. Jacob, **Z. Li**, T.-M. Yi and L. Petzold. Validation data for a hybrid smoothed dissipative particle dynamics (S-DPD) spatial stochastic simulation algorithm (sSSA) method. *Data in Brief*, 2019, 22: 11-15. DOI: 10.1016/j.dib.2018.11.103

31. L. Zhao, **Z. Li**[⋆,†], J. Ouyang, B. Caswell and G.E. Karniadakis. Active learning of constitutive relation from mesoscopic simulations for continuum modeling of non-Newtonian fluids. *Journal of Computational Physics*, 2018, 363: 116-127. DOI: 10.1016/j.jcp.2018.02.039

30. **Z. Li**[†], X. Bian, Y.-H. Tang and G.E. Karniadakis. A dissipative particle dynamics method for arbitrarily complex geometries. *Journal of Computational Physics*, 2018, 355: 534-547. DOI: 10.1016/j.jcp.2017.11.014

29. K. Kim, M.H. Han, C. Kim, **Z. Li**, G.E. Karniadakis and E.K. Lee. Nature of intrinsic uncertainties in equilibrium molecular dynamics estimation of shear viscosity for simple and complex fluids. *The Journal of Chemical Physics*, 2018, 149: 044510. DOI: 10.1063/1.5035119

28. **Z. Li**[†], G. Hu and G.E. Karniadakis. Preface: theory, methods, and applications of mesoscopic modeling. *Applied Mathematics and Mechanics*, 2018, 39(1): 1-2. DOI: 10.1007/s10483-018-2260-6 (**Organizer** of Special Issue)

27. X. Bian, **Z. Li** and N.A. Adams. A note on hydrodynamics from dissipative particle dynamics. *Applied Mathematics and Mechanics*, 2018, 39(1): 63-82. DOI: 10.1007/s10483-018-2257-9 (**Invited Paper** for Special Issue)

26. Y. Yoshimoto, **Z. Li**, I. Kinefuchi and G.E. Karniadakis. Construction of non-Markovian coarse-grained models employing the Mori-Zwanzig formalism and iterative Boltzmann inversion. *The Journal of Chemical Physics*, 2017, 147: 244110. DOI: 10.1063/1.5009041 (Selected as **Editor's Pick** featured article)

25. A.L. Blumers, Y.-H. Tang, **Z. Li**[†], X. Li and G.E. Karniadakis. GPU-accelerated red blood cells simulations with transport dissipative particle dynamics. *Computer Physics Communications*, 2017, 217: 171-179. DOI: 10.1016/j.cpc.2017.03.016 (Released open source code – **USERMESO2.0**)

24. **Z. Li**, C. Lan, L. Jia and Y. Ma. Ground effects on separated laminar flows past an inclined flat plate. *Theoretical and Computational Fluid Dynamics*, 2017, 31(2): 127-136. DOI: 10.1007/s00162-016-0410-0

23. **Z. Li**, H.S. Lee, E. Darve and G.E. Karniadakis. Computing the non-Markovian coarse-grained interactions derived from the Mori–Zwanzig formalism in molecular systems: Application to polymer melts. *The Journal of Chemical Physics*, 2017, 146(1): 014104. DOI: 10.1063/1.4973347

22. H. Lei, X. Yang, **Z. Li** and G.E. Karniadakis. Systematic parameter inference in stochastic mesoscopic modeling. *Journal of Computational Physics*, 2017, 330: 571–593. DOI: 10.1016/j.jcp.2016.10.029

21. M. Deng, **Z. Li**[†], O. Borodin and G.E. Karniadakis. cDPD: A new dissipative particle dynamics method for modeling electrokinetic phenomena at the mesoscale. *The Journal of Chemical Physics*, 2016, 145(14): 144109. DOI: 10.1063/1.4964628

20. **Z. Li**, X. Bian, X. Yang and G.E. Karniadakis. A comparative study of coarse-graining methods for polymeric fluids: Mori-Zwanzig vs. iterative Boltzmann inversion vs. stochastic parametric optimization. *The Journal of Chemical Physics*, 2016, 145(4): 044102. DOI: 10.1063/1.4959121

19. Y.-H. Tang, **Z. Li**, X. Li, M. Deng and G.E. Karniadakis. Non-equilibrium dynamics of vesicles and micelles by self-assembly of block copolymers with double thermoresponsivity. *Macromolecules*, 2016, 49(7): 2895–2903. DOI: 10.1021/acs.macromol.6b00365

18. **Z. Li**, X. Bian, X. Li and G.E. Karniadakis. Incorporation of memory effects in coarse-grained modeling via the Mori-Zwanzig formalism. *The Journal of Chemical Physics* (**Invited Paper** for Special Topic: Coarse Graining of Macromolecules, Biopolymers, and Membranes), 2015, 143(24): 243128. DOI: 10.1063/1.4935490

17. X. Bian, **Z. Li**, M. Deng and G.E. Karniadakis. Fluctuating hydrodynamics in periodic domains and heterogeneous adjacent multidomains: Thermal equilibrium. *Physical Review E*, 2015, 92(5): 053302. DOI: 10.1103/PhysRevE.92.053302

16. C. Lan, S. Pal, **Z. Li** and Y. Ma. Numerical simulations of digital microfluidic manipulation of single microparticles. *Langmuir*, 2015, 31 (35): 9636–9645. DOI: 10.1021/acs.langmuir.5b02011

15. **Z. Li**, A. Yazdani, A. Tartakovsky and G.E. Karniadakis. Transport dissipative particle dynamics model for mesoscopic advection-diffusion-reaction problems. *The Journal of Chemical Physics*, 2015, 143: 014101. DOI: 10.1063/1.4923254

14. X. Bian, **Z. Li** and G.E. Karniadakis. Multi-resolution flow simulations by smoothed particle hydrodynamics via domain decomposition. *Journal of Computational Physics*, 2015, 297: 132–155. DOI: 10.1016/j.jcp.2015.04.044

13. **Z. Li**, Y.-H. Tang , X. Li and G.E. Karniadakis. Mesoscale modeling of phase transition dynamics of thermoresponsive polymers. *Chemical Communications*, 2015, 51: 11038-11040. DOI: 10.1039/C5CC01684C

12. Y.-H. Tang, S. Kudo, X. Bian, **Z. Li** and G.E. Karniadakis. Multiscale Universal Interface: A concurrent framework for coupling heterogeneous solvers. *Journal of Computational Physics*, 2015, 297: 13–31. DOI: 10.1016/j.jcp.2015.05.004 (Released open source C++ library – **Multiscale Universal Interface (MUI)**)

11. S. Pal, C. Lan, **Z. Li**, E.D. Hirleman and Y. Ma. Symmetry boundary condition in dissipative particle dynamics. *Journal of Computational Physics*, 2015, 292: 287–299. DOI: 10.1016/j.jcp.2015.03.025

10. **Z. Li**, X. Bian, B. Caswell and G.E. Karniadakis. Construction of dissipative particle dynamics models for complex fluids via the Mori-Zwanzig formulation. *Soft Matter*, 2014,10: 8659–8672. DOI: 10.1039/C4SM01387E

9. **Z. Li**, Y.-H. Tang, H. Lei, B. Caswell and G.E. Karniadakis. Energy-conserving dissipative particle dynamics with temperature-dependent properties. *Journal of Computational Physics*, 2014, 265: 113–127. DOI: 10.1016/j.jcp.2014.02.003

8. **Z. Li**, G. Hu, Z. Wang, Y. Ma and Z. Zhou. Three dimensional flow structures in a moving droplet on substrate: a dissipative particle dynamics study. *Physics of Fluids*, 2013, 25: 072103. DOI: 10.1063/1.4812366

7. C. Lan, L. Jia, **Z. Li** and Y. Ma. Wall effect on separated flow around an inclined flat plate at high incidence. *Proceedings of the ASME 2013 International Mechanical Engineering Congress and Exposition*. 2013, 7A: T08A022. DOI: 10.1115/IMECE2013-65261

6. **Z. Li**, Z. Zhou and G. Hu. Dissipative particle dynamics simulation of droplet oscillations in AC electrowetting. *Journal of Adhesion Science and Technology*. 2012, 26: 1883–1895. DOI: 10.1163/156856111X600217 (**Invited Paper** for Special Issue: Electrowetting)

5. **Z. Li**, C. Lan and Y. Ma. Effects on dust emission from an inclined flat solar panel. *Proceedings of the ASME 2012 International Mechanical Engineering Congress and Exposition*. 2012, 6: 619–624. DOI: 10.1115/IMECE2012-89463

4. C. Lan, **Z. Li** and Y. Ma. Numerical study of sand deposition and control by flat solar panels. *Proceedings of the ASME 2012 International Mechanical Engineering Congress and Exposition*. 2012, 6: 643–649. DOI: 10.1115/IMECE2012-89648

3. **Z. Li**, G. Hu, J. Zhou and Z. Zhou. Effects of elasticity of substrate on dewetting process of evaporable ultra-thin liquid film. *Chinese Journal of Theoretical and Applied Mechanics*. 2011, 43(4): 699–706. (in Chinese) DOI: 10.6052/0459-1879-2011-4-lxxb2010-459

2. **Z. Li**, G. Hu and Z. Zhou. A numerical method to impose slip boundary conditions in dissipative particle dynamics. *Journal of Shanghai University*. 2009, 15(6): 628–633. (in Chinese) DOI: 10.3969/j.issn.1007-2861.2009.06.014

1. **Z. Li**, G. Hu and Z. Zhou. Floquet instability of a large density ratio liquid-gas coaxial jet with periodic fluctuation. *Applied Mathematics and Mechanics*. 2008, 29(8): 975–984. DOI: 10.1007/s10483-008-0801-y

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Book/Chapters

4. **Z. Li**, W. Pan and A.M. Tartakovsky. Particle-based methods for mesoscopic transport processes. In book: Handbook of Materials Modeling – Volume 2 Applications: Current and Emerging Materials, Editor: W. Andreoni and S. Yip. Publisher: Springer, Cham, 2020. DOI: 10.1007/978-3-319-50257-1_64-1

3. **Z. Li**, X. Bian, X. Li, M. Deng, Y.-H. Tang, B. Caswell and G.E. Karniadakis. Dissipative Particle Dynamics: Foundation, Implementation and Applications. In book: Particles in Flows, Editor: T. Bodnár, G.P. Galdi and Š. Nečasová. Publisher: Birkhäuser, 2017. DOI: 10.1007/978-3-319-60282-0_5

2. X. Li, **Z. Li**, X. Bian, M. Deng, C. Kim, Y.-H. Tang, A. Yazdani and G.E. Karniadakis. Dissipative Particle Dynamics, Overview. In book: Encyclopedia of Nanotechnology, Editor: B.Bhushan, Publisher: Springer, 2016. DOI: 10.1007/978-94-007-6178-0_100954-1

1. **Z. Li**, G. Hu and Z. Zhou. Dissipative Particle Dynamics for Complex Fluid. In book: Mechanics and Engineering – A 21st Century Engineering Technology and Mechanical Cutting-edge Research, SJTU Press, 2009, 385–397. (in Chinese)

Conference Activities in Recent Years

14. **Z. Li**, Invited Minisymposium Talk: Parareal Physics-Informed Neural Network for Solving Time-Dependent PDEs. The 16th U.S. National Congress on Computational Mechanics, Jul. 2021 (online).

13. **Z. Li**, Invited Workshop Talk: Non-Markovian coarse-grained models of polymeric fluids derived via the Mori-Zwanzig formalism. 2020 CECAM Workshop "Multiscale Simulations of Soft Matter: New Method Developments and Mathematical Foundations", Oct. 2020 (online), Mainz, Germany.

12. **Z. Li**, Active- and transfer-learning applied to microscale-macroscale coupling in modeling of viscoelastic flows. The 91st Annual Meeting of The Society of Rheology, Oct. 2019, Raleigh, NC, USA.

11. **Z. Li**, Invited Minisymposium Talk: Dissipative particle dynamics methods for mesoscopic problems. The 13th World Congress on Computational Mechanics (WCCM-XIII), Jul. 2018, New York City, USA.

10. **Z. Li**, Invited Minisymposium Talk: Active learning of constitutive relations from mesoscopic dynamics for macroscopic modeling of soft matter. 2018 SIAM Conference on Mathematical Aspects of Materials Science (MS18), July 2018, Portland, OR, USA.

9. **Z. Li**, Talk: Computing memory effects in coarse-grained modeling derived from the Mori-Zwanzig formalism: Application to polymer melts, 2017 MRS Spring Meeting, Apr. 2017, Phoenix, AZ, USA.

8. **Z. Li**, Talk: Non-Markovian coarse-grained models derived from the Mori-Zwanzig formalism, 2017 Mach Conference, Apr. 2017, Annapolis, MD, USA.

7. **Z. Li**, Talk: Arbitrary-shaped walls with controllable surface roughness in dissipative particle dynamics simulations, 2017 SIAM Conference on Computational Science and Engineering (CSE), Feb. 2017, Atlanta, GA, USA.

6. **Z. Li**, **Keynote** Minisymposium Talk: Construction of coarse-grained models for polymeric fluids via the Mori-Zwanzig formalism. The 12th World Congress on Computational Mechanics (WCCM-XII), Jul. 2016, Seoul, Korea.

5. **Z. Li**, Invited Minisymposium Talk: Bottom-up construction of non-Markovian coarse-grained model for polymeric fluids. VII European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS), Jun. 2016, Grete, Greece.

4. **Z. Li**, Invited Minisymposium Talk: Practices of coarse-graining based on the Mori-Zwanzig formalism. 2016 SIAM Conference on Mathematical Aspects of Materials Science (MS16), May 2016, Philadelphia, PA, USA.

3. **Z. Li**, Talk: Non-Markovian coarge-grained modeling of polymeric fluids based on the Mori-Zwanzig formalism, 2016 APS March Meeting, Mar. 2016, Baltimore, MD, USA.
2. **Z. Li**, Talk: Modeling of advection-diffusion-reaction processes using transport dissipative particle dynamics, The 68th Annual Meeting of the APS Division of Fluid Dynamics, Nov. 2015, Boston, MA, USA.
1. **Z. Li**, Invited Minisymposium Talk: Mesoscopic modeling of temperature-dependent properties in non-isothermal fluid systems, 2015 SIAM Conference on Computational Science and Engineering (CSE), Mar. 2015, Salt Lake City, UT, USA.

Released Open Source Codes:

• Multiscale Universal Interface (MUI) library for multiscale simulations: MUI is a C++ header-only library that integrates MPI MPMD support and an asynchronous communication protocol to handle inter-solver information exchange and to couple multiple heterogeneous solvers to perform multi-physics and multiscale simulations.

• USER-MESO package in Large-scale Atomic/Molecular Massively Parallel Simulator (**LAMMPS**): The USER-MESO package appends new capabilities to LAMMPS for DPD simulations (beyond the classical DPD model). It includes the many-body DPD (mDPD) model for multiphase problems, the energy-conserving DPD (eDPD) model for non-isothermal dynamics, and the transport DPD (tDPD) for mesoscopic problems involving advection-diffusion-reaction processes.

• USERMESO-2.0 for GPU-accelerated particle-based simulations: USERMESO-2.0 is a GPU-accelerated extension to LAMMPS that migrates most computation workload onto GPUs and achieves more than twenty times speedup on a single GPU over 16 CPU cores. For a typical system containing 1,000,000 particles, USERMESO-2.0 allows running 1,000,000 time steps overnight with a single GPU. For parallel computations, USERMESO-2.0 has linear speedup up to 1024 GPUs.

Research Projects:

6. DOE/EFRC (Co-Lead of Thrust II: AI Models): Artificially Intelligent Manufacturing Paradigm for Composites (AIM for Composites), $10.35M in total, $3.5M to Clemson University (2022-2026).
5. NSF project (Co-PI): CDS&E: HAM3R: Heterogeneous Automated Management of Multiscale Methods and Resources, $500K to Clemson University (2022-2025).
4. NSF project (PI): Collaborative Research: SciMem: Enabling High Performance Multi-Scale Simulation on Big Memory Platforms, $140K to Clemson University (2021-2024).
3. NASA/EPSCoR project (PI): Impacts of Gravity and Surfactants on Drainage Flow and Rheology of Wet Foams, $88K to Clemson University (2021-2022).
2. MURI/ARO project (Subaward PI): Fractional PDEs for Conservation Laws and Beyond; Theory, Numerics and Applications - Extension, $75K to Clemson University (2020-2021).
1. DOE/PNNL ASCR project (Co-PI at Brown, 2018-2019): PhILMS: Collaboratory on Mathematics and Physics-Informed Learning Machines for Multiscale and Multiphysics Problems, $10M in total, $1.2M to Brown University (2018-2022).

Student Supervision:

7. Ansel L. Blumers: (PhD student at Brown, now at MathWorks), fall 2015 to 2019. Topic: Parallel-in-time algorithms for large-scale simulations of stochastic dynamics.
6. Lifei Zhao: (visiting PhD student at Brown), fall 2016 to 2018. Topic: Active-learning methods applied to multiscale simulation of complex fluids.
5. Kaixuan Zhang: (visiting PhD student at Brown), 2017-2018. Topic: Stochastic simulations of mesoscale multiphase flows and wetting phenomena.
4. Yuying Wang: (visiting PhD student at Brown), 2017-2018. Topic: Concurrent coupling of heterogeneous solvers for multiscale biological processes.
3. Theodora Myrto Perdikari: (visiting B.S. student at Brown, now is PhD student at Brown), 2016 summer intern. Topic: Particle-based methods for simulations of amphiphilic molecules.
2. Yu-Hang Tang: (PhD student at Brown, now at NVIDIA), 2013-2017. Topic: Multiscale methods and applications to functional materials and soft matter.
1. Mingge Deng: (PhD student at Brown, now at Google), 2013-2016. Topic: Lagrangian approach for mesoscopic electrokinetics with electrostatic fluctuations.

Professional Services

Reviewer of [1] Journal of Computational Physics (2017 Outstanding Reviewer) • [2] Physics of Fluids • [3] Physical Review Letter • [4] Physical Review E • [5] Physical Review Fluids • [6] RSC Advances • [7] The Journal of Chemical Physics • [8] Langmuir • [9] Soft Matter • [10] International Journal of Thermal Sciences • [11] International Journal of Heat and Mass Transfer • [12] IEEE Transactions on Nanotechnology • [13] Molecular Simulation • [14] Applied Mathematics and Mechanics • [15] Colloids and Surfaces A • [16] Computational Materials Science • [17] Fluid Dynamics Research • [18] Journal of Hydrodynamics • [19] Computer Methods in Applied Mechanics and Engineering • [20] Fluid Phase Equilibria • [21] Computer & Fluids • [22] SIAM Journal on Scientific Computing.

Topic Editor in the Editorial Board of *Fluids.*

Established the weekly CFSM Seminar Series (cecas.clemson.edu/zhenli/cfsm/) to promote interdisciplinary communication and improve research collaborations between researchers especially young scientists whose interests and research connect, and foster a well-connected research community in the field of complex fluids and soft matter.

Reviewer of Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), DOE, and NSF.

Established DPDForun (www.dpdforum.org) to enhance the academic communications and collaborations in the DPD community and to share useful materials through its Virtual Resource Center.

Organized 2015 International Workshop of Dissipative Particle Dynamics held in Shanghai, China during September 21-23, 2015. Website: www.cfm.brown.edu/dpd-workshop.

Organized the minisymposium "MS-917 Mesoscopic Methods for Complex Fluids and Soft Matter" in the VII European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS Congress 2016) held in Crete, Greece during June 5-10, 2016. Website: www.eccomas2016.org.

Chaired the minisymposium "MS110C Particle-based Methods for the Simulation of Complex Fluids" in the 12th World Congress on Computational Mechanics (WCCM XII) held in Seoul, Korea during July 24-29, 2016. Website: wccm2016.org.

Lead Guest Editor of Applied Mathematics and Mechanics, Special Issue on: Theory, Methods and Applications of Mesoscopic Modeling. Website: Applied Mathematics and Mechanics: Special Issue.

Organized the minisymposium "MS-917 Numerical Methods for Mesoscale Modeling of Complex Fluids and Soft Matter" in 2018 SIAM Annual Meeting (SIAM-AN18) held in Portland, Oregon, USA during July 9-13, 2018. Website: www.siam.org.

Organized the minisymposium "Multiscale Modeling and Mechanics of Soft Matter and Hierarchical Materials" in the 57th SES Annual Technical Meeting held virtually during September 28-30, 2020. Website: ccaps.umn.edu/SES.

Organized the minisymposium "Multiscale methods and Data-driven Models" in 2021 SIAM Conference on Computational Science and Engineering (SIAM-CSE21) held virtually during March 1-5, 2021. Website: SIAM-CSE21.

Teaching Experiences:

- Teach: **ME 3080: Fluid Mechanics** (undergraduate course, Fall 2019, Spring & Fall 2020, Spring & Fall 2021, Spring 2022)
  Department of Mechanical Engineering, Clemson University

  ME 4230/6230: Introduction to Aerodynamics (undergraduate & graduate course, Spring 2022)
  Department of Mechanical Engineering, Clemson University

  ME 3900/4900 Creative Inquiry + Undergraduate Research (undergraduate level, Fall 2021, Spring 2022)
  Department of Mechanical Engineering, Clemson University

  APMA 1660: Statistical Inference II (undergraduate course, Spring 2019)
  Division of Applied Mathematics, Brown University
- Teaching Credential: **Teaching Certificate I**
  Harriet W. Sheridan Center for Teaching and Learning, Brown University
- Lectures in Graduate Courses: **ME 8930: Introduction to Atomistic Modeling** (Fall 2019)
  Department of Mechanical Engineering, Clemson University

  APMA 2580: Multiscale Computational Fluid Dynamics (Fall 2016)
  Division of Applied Mathematics, Brown University

  APMA 2811T: Dissipative Particle Dynamics (Spring 2016)
  Division of Applied Mathematics, Brown University