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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 advanced deep learning and high performance computing.

Specific research topics include **mathematical theory** of coarse-graining and model-order 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 and supervised parallel-in-time algorithms for **scale-bridging**.

Professional Experience

Clemson University – Department of Mechanical Engineering Assistant Professor (Tenure-Track)	CLEMSON, SC, USA Aug. 2019 – present
Brown University – Division of Applied Mathematics Research Associate Professor (Research-Track)	PROVIDENCE, RI, USA Jan. 2019 – Jul. 2019
National Polytechnic Institute of Toulouse – Laboratory of Chemical Engineering Visiting Professor (Fellowship)	TOULOUSE, FRANCE Dec. 2018 – Dec. 2018
Brown University – Division of Applied Mathematics Research Assistant Professor (Research-Track)	PROVIDENCE, RI, USA Jan. 2016 – Dec. 2018
Brown University – Division of Applied Mathematics Postdoctoral Research Associate	PROVIDENCE, RI, USA Jan. 2013 – Dec. 2015
University of California, Merced – School of Engineering Postdoctoral Research Associate	MERCED, CA, USA Feb. 2012 – Dec. 2012

Academic Degrees

Shanghai University Ph.D. in Fluid Mechanics	SHANGHAI, CHINA April 2012
Shanghai University M.Eng. in Fluid Mechanics	SHANGHAI, CHINA October 2008
Wuhan University B.Eng. in Engineering Mechanics	WUHAN, CHINA June 2005

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

Year 2024:

69. M. Lu, C. Lin, M. Maxey, G. Karniadakis and **Z. Li**. Bridging scales in multiscale bubble growth dynamics with correlated fluctuations using neural operator learning. *International Journal of Multiphase Flow*, 2024 (under review). [arXiv: 2403.13299](https://arxiv.org/abs/2403.13299)
68. M. Lu, Y. Xia, T. Bhattacharjee, J. Klinger and **Z. Li**. Predicting biomass comminution: Physical experiment, population balance model, and deep learning. *Powder Technology*, 2024 (under review). DOI: [10.2139/ssrn.4684975](https://doi.org/10.2139/ssrn.4684975)
67. 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 Technology*, 2024 (under review). [bioRxiv: 2023.06.12.544584](https://doi.org/10.1002/admt.2023.06.12.544584)
66. Z. Diermyer, Y. Xia, A. Hamed, J. Klinger, V. Thompson, **Z. Li** and J. Li. Mesoscopic flow simulation to understand the percolation through fine-ground electronic waste particle bed. *Powder Technology*, 2024 (under review).
65. P. Kunwar, U. Aryal, A. Poudel, D. Fougner, Z. J. Geffert, R. Xie, **Z. Li** and P. Soman. Droplet bioprinting of acellular and cell-laden structures at high-resolutions. *Biofabrication*, 2024 (accepted). [bioRxiv: 2023.11.18.567660](https://doi.org/10.1063/1.5111111)
64. 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*, 2024, 985: A7. DOI: [10.1017/jfm.2024.270](https://doi.org/10.1017/jfm.2024.270)

Year 2023:

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, 159: 244903. DOI: 10.1063/5.0182499
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, 494: 112509. DOI: 10.1016/j.jcp.2023.112509
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. Hirtleman 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

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

26. Z. Li, Invited Minisymposium Talk: Multiscale Parareal Algorithms for Long-Time Mesoscopic Simulation of Complex Fluids. 2024 SIAM Conference on Parallel Processing for Scientific Computing (SIAM PP24), Mar. 2024.
25. Z. Li, Session Chair: Inferring multiscale bubble growth dynamics by deep neural operator learning. The 76th Annual Meeting of the APS Division of Fluid Dynamics (APS/DFD 2023), Nov. 2023.
24. Z. Li, Minisymposium Organizer: Deep neural operator for learning transient response of composites. 2023 Annual Technical Meeting of the Society of Engineering Science (SES 2023), Oct. 2023.
23. Z. Li, Invited Minisymposium Talk: Deep neural operator for learning transient response of composites subject to dynamic loading. 10th International Congress on Industrial and Applied Mathematics (ICIAM), Aug. 2023.
22. Z. Li, Oral Presentation: Multiphase dissipative particle dynamics modeling of dynamic spreading of a molten sand droplet. 2023 Engineering Mechanics Institute (EMI) Conference, Jun. 2023.

21. **Z. Li, Invited Talk**: Generation of rough surfaces with desired statistic features by training an LSTM neural network. 2023 ARL SMASH Hypersonic Workshop, Apr. 11th, 2023.
20. **Z. Li, Invited Talk**: Deep neural operator for learning transient response of composites subject to mechanical loading. 2023 SIAM-SEAS Conference, Mar. 24th, 2023.
19. **Z. Li, Department Colloquium**: Scale-Bridging in Fluid Systems through Multiscale Modeling and Machine Learning Approaches. Department of Physics and Astronomy, Clemson University, Sep. 29th, 2022.
18. **Z. Li, Department Colloquium**: Memory Effects in Coarse-Grained Modeling of Soft Matter, Department of Mathematics and Statistics, UNC Charlotte, Sep. 16, 2022.
17. **Z. Li, Invited Talk**: Long-Time Mesoscopic Simulation of Microvascular Blood Flow in Zebrafish Enabled by a Multiscale Parallel-in-Time Method, 2022 Platform for Advanced Scientific Computing (PASC) Conference, Jun. 2022.
16. **Z. Li, Invited Talk**: Long-time Mesoscale Fluid Dynamics Simulation Enabled by a Supervised Parallel-in-time Method, 19th U.S. National Congress on Theoretical and Applied Mechanics (USNC/TAM), Jun. 2022.
15. **Z. Li, Invited Minisymposium Talk**: Parallel computing technology and accelerated convergence algorithms. The 21st IACM (International Association for Computational Mechanics) Computational Fluid Conference (CFC), Oct. 2021 (Virtual).
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 (USNCCM16), Jul. 2021 (Virtual).
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 (Virtual), 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, first job 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, joined the PhD program at Brown University), 2016 summer intern. Topic: Particle-based methods for simulations of amphiphilic molecules.
2. [Yu-Hang Tang](#): (PhD student at Brown, first job at Lawrence Berkeley National lab), 2013-2017. Topic: Multiscale methods and applications to functional materials and soft matter.
1. [Mingge Deng](#): (PhD student at Brown, first job 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.[1,500+ participants, 200+ subscribers of the CFSM YouTube Channel]

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

Established DPDForum (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*, and Special Issue on: *Machine-Learning Approaches for Computational Mechanics*.

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.

Organized the minisymposium MS-322 “Multiscale Methods and Mechanics of Soft Matter and Hierarchical Materials” in 19th U.S. National Congress on Theoretical and Applied Mechanics to be held June 19-24, 2022 in Austin, Texas. Website: USNC/TAM 2022.

Organized the minisymposium MS10 “Multiscale Modeling and Mechanics of Soft Matter and Hierarchical Materials” in 2023 Annual Technical Meeting of the Society of Engineering Science (SES 2023) hosted by the University of Minnesota during October 8-11, 2023. Website: SES 2023.

Teaching Experiences:

- Teach: **ME 8190: Computational Methods in Thermal Science** (graduate course, Spring 2024)
Department of Mechanical Engineering, Clemson University
- **ME 8100: Macroscopic Thermodynamics** (graduate course, Spring 2023)
Department of Mechanical Engineering, Clemson University
- **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