Zhen Li Updated: November 15, 2018

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Zhen Li's Profiles on Google Scholar, Researchgate

Summary

Assistant Professor of Applied Mathematics (Research) at Brown University. Research interest is on multiscale modeling of soft matter, complex fluids 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 for **coarse-graining** and model reduction, **machine-learning** applied to **data-driven** multiscale 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**.

Employment History

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

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*

Shanghai University – Shanghai Institute of Applied Mathematics & Mechanics — Shanghai, China
Research Assistant — *Sep. 2005 – Dec. 2011*

Education

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

Shanghai University — Shanghai, China
M.S. in Fluid Mechanics — *August 2008*

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

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

Under review:

1. 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*, 2018 (under review) arXiv: 1810.13041

2. K. Zhang, **Z. Li**⋆,†, M. Maxey, S. Chen and G.E. Karniadakis. Self-cleaning of hydrophobic rough surfaces by coalescence-induced wetting transition, *Langmuir*, 2018 (under review) arXiv: 1810.13073

3. 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*, 2018 (**Invited Paper** for Special Issue, under review) arXiv: 1810.11596

4. L. Lu, **Z. Li**⋆, H. Li, X. Li, P.G. Vekilov and G.E. Karniadakis. Quantitative prediction of erythrocyte sickling for anti-polymerization activities. *Proc. Natl. Acad. Sci. U.S.A*, 2018 (under review)

5. 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*, 2018 (under review)

Year 2018:

6. 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*, 2018 (in press) DOI: 10.1016/j.jcp.2018.10.043

7. 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

8. **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
9. 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
10. **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)
11. 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)

Year 2017:

12. 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)
13. 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**)
14. **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
15. **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
16. 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

Year 2016:

17. 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
18. **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

Year 2015:

20. **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
21. 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
22. 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
23. **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
24. 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
25. **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
26. 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)**)
27. 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

Year 2014 and before:

28. **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
29. **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
30. **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
31. **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)
32. **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
33. 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
34. **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
35. **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
36. **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

1. **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, 2018. DOI: 10.1007/978-3-319-50257-1_64-1
2. **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
3. 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
4. **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

1. **Z. Li**, Invited Minisymposium Talk: Dissipative particle dynamics methods for mesoscopic problems. The 13th World Congress on Computational Mechanics (WCCM-XIII), July 2018, New York City, USA.
2. **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.
3. **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.
4. **Z. Li**, Talk: Non-Markovian coarse-grained models derived from the Mori-Zwanzig formalism, 2017 Mach Conference, Apr. 2017, Annapolis, MD, USA.
5. **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.
7. **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.

8. **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.
9. **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.
10. **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.
11. **Z. Li**, Poster: A particle-based mesoscopic model for simulating advection-diffusion-reaction processes, 2015 Conference on Foundations of Molecular Modeling and Simulation (FOMMS 2015), Jul. 2015, Mt. Hood, OR, USA.
12. **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.

Invited Seminars in Universities

1. **Z. Li**, Theory of coarse-graining and mesoscopic methods applied to multiscale problems, Department of Mechanical Engineering, University of California, Merced (UCM), Oct. 12, 2018.
2. **Z. Li**, Mathematical and physical foundation of mesoscopic methods and its applications to multiscale problems, School of Energy and Power, Huazhong University of Science and Technology (HUST), China, Sep. 6, 2018.
3. **Z. Li**, Mathematical and physical foundation of coarse-graining and applications to multiscale problems, School of Aeronautics and Astronautics, Zhejiang University (ZJU), China, Aug. 29, 2018.
4. **Z. Li**, Mathematical theory of coarse-graining and mesoscopic methods applied to multiscale problems, Department of Modern Mechanics, University of Science and Technology of China (USTC), Aug. 23, 2018.
5. **Z. Li**, Computation of memory effects in coarse-grained modeling through the Mori-Zwanzig formulation, Department of Mathematical Sciences, Worcester Polytechnic Institute (WPI), Sep. 30, 2016.
6. **Z. Li**, Lagrangian modeling framework for stochastic advection-diffusion-reaction processes in biological systems, Department of Computer Science, University of California, Santa Barbara (UCSB), Jul. 18, 2016.
7. **Z. Li**, Coarse-graining of complex fluids and mesoscopic modeling, Department of Mathematics and Statistics, University of North Carolina at Charlotte (UNCC), Mar. 22, 2016.

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:

1. DOE/PNNL ASCR project (Co-PI at Brown, 2018-present): PhILMS: Collaboratory on Mathematics and Physics-Informed Learning Machines for Multiscale and Multiphysics Problems, $\$1,200,000$ to Brown University (2018-2022).
2. MURI/ARO project (2015 to present): Fractional PDEs for Conservation Laws and Beyond; Theory, Numerics and Applications, $\$7,103,239$ in total (2015-2020).
3. Utah/ARL project (2013 to present): Alliance for the Computationally-guided Design of Energy Efficient Electronic Materials (CDE3M), $\$1,056,063$ to Brown University (2012-2021).
4. DOE/PNNL ASCR project: (2013-2018): Collaboratory on Mathematics for Mesoscopic Modeling of Materials (CM4), $\$1,500,000$ to Brown University (2012-2018).

Grant Proposal Writing:

1. Co-PI, 2018DOE ASCR MMICC Project: Collaboratory on Mathematics and Physics-Informed Learning Machines for Multiscale and Multiphysics Problems (PhILMs), with G. Karniadakis (Director, PNNL), A. Tartakovsky (PNNL), M. Ainsworth (Brown), C. Daskalakis (MIT), E. Darve (Stanford) and P. Atzberger (UCSB)
2. Co-PI, 2017DOE ASCR SciDAC Project: Nanoscale Flow at Chemically Reactive Interfaces, with G. Schenter (PNNL), A. Tartakovsky (PNNL), J. Morris (CUNY) and I. Siepmann (UMn)
3. Co-PI, 2017DoD PETTT Project: MUI - Multiscale Universal Interface for Simulating Materials and Complex Fluids at the Exascale, with G. Karniadakis (Brown)

Student Supervision:

1. Ansel L. Blumers: (PhD student at Brown), fall 2015 to present. Topic: Parallel-in-time algorithms for large-scale simulations of stochastic dynamics.
2. Lifei Zhao: (visiting PhD student at Brown), fall 2016 to present. Topic: Active-learning methods applied to multiscale simulation of complex fluids.
3. 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.
5. 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.
6. Yu-Hang Tang: (PhD student at Brown, now at Lawrence Berkeley National Lab), 2013-2017. Topic: Multiscale methods and applications to functional materials and soft matter.
7. 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.

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

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.

Teaching Experiences:

- To Teach: **APMA 1660: Statistical Inference II** (undergraduate course)
  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: **APMA 2580: Multiscale Computational Fluid Dynamics** (2016)
  Division of Applied Mathematics, Brown University
  APMA 2811T: Dissipative Particle Dynamics (2016)
  Division of Applied Mathematics, Brown University