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EDUCATION

- **Ph.D. Mechanical Engineering** May 2007–May 2011
University of California at Berkeley
Thesis: Homogeneous Non-Equilibrium Molecular Dynamics Methods for Calculating the Heat Transport Coefficient of Solids and Mixtures
Mentor: Prof. Panayiotis Papadopoulos
Minors: Mathematics and Physics
Thesis Committee: Prof. Alexander Chorin and Prof. David Steigmann
- **M.S. Civil Engineering** August 2005–May 2007
University of California at Berkeley
Thesis: Cytoskeleton and Soft Glassy Rheology
Mentors: Prof. Sanjay Govindjee and Prof. Mohammad R. K. Mofrad
- **B.S. Civil Engineering** August 2001–May 2005
Indian Institute of Technology at Madras
Thesis: Multiscale Modeling of Mechanical Behavior of Polycrystalline Shape Memory Alloys
Mentor: Prof. Srinivasan M. Sivakumar

PROFESSIONAL APPOINTMENTS

- **Post-Doctoral Scholar – Chemistry** August 2013–Present
University of California at Berkeley and LBNL
Mentors: Prof. David Chandler and Prof. George Oster
- **Post-Doctoral Scholar** July 2011–July 2013
Sandia National Laboratories at Livermore
Host: Dr. Jeremy A. Templeton

HONORS AND AWARDS

- **Poster Prize, 2015**, Berkeley Mini Statistical Mechanical Meeting, 2015, for elucidating a self-assembly force for proteins in lipid bilayers based on its order-disorder phase transition.
- **Editors Choice Award, 2011**, The Journal of Chemical Physics, for developing a non-equilibrium molecular dynamics algorithm for thermal conductivity calculations of mixtures and alloys.
- **Block Grant Award, 2010**, Department of Mechanical Engineering, University of California at Berkeley for distinguished academic record and promise for noteworthy achievement.
- **Prathibha Scholarship, 2001 – 2005**, Government of Andhra Pradesh in India for distinguished academic record at Indian Institute of Technology at Madras.
- **Prathibha Award, 1999**, Government of Andhra Pradesh in India for securing State 7th rank out of 600,000 students in Secondary Board Examination.

PUBLICATIONS

• Journals (In Preparation)

*Equal Contribution

1. *Katira, S., *Mandadapu, K. K., *Vaikuntanathan, S., Smit, B., and Chandler, D., The order-disorder transition in lipid bilayers mediates a force for assembly of transmembrane proteins, *Preprint on Request*.
2. *Katira, S., *Mandadapu, K. K., *Vaikuntanathan, S., Smit, B., and Chandler, D., The order-disorder transition in model lipid bilayers is a hexatic to liquid first-order phase transition, *Preprint on Request*.
3. Kshirsagar, S., Mandadapu, K. K., and Papadopoulos, P., Classical molecular dynamics simulations with a general interatomic potential, *Preprint on request*.
4. Mandadapu, K. K., and Papadopoulos, P., A homogenization method for thermomechanical continua using extensive physical quantities: Frame Invariance, *In preparation*.

• Journals (Submitted)

*Equal Contribution

1. *Mandadapu, K. K., *Nirody, J., Berry, R., and Oster, G., A mechano-chemical model for the bacterial flagellar motor with a new stator mechanism, arXiv:1501:02883. *In review with PNAS* (Preprint on request).

• Journals (Published and Accepted)

1. Mercer, B., Mandadapu, K. K., and Papadopoulos, P., Novel formulations of microscopic boundary-value problems in continuous multiscale finite element methods, *Computer Methods in Applied Mechanics and Engineering* (In press) (2014).
2. Rangamani P., Mandadapu, K. K., and Oster, G., Protein-induced membrane curvature alters local membrane tension, *Biophysical Journal*, 107, 751-762 (2014).
3. Mandadapu, K. K., Jones, R. E., and Zimmerman, J. A., On the microscopic definitions of dislocation density tensor, *Mathematics and Mechanics of Solids* 19, 744-757 (2014).
4. Mandadapu, K. K., Templeton, J. A., and Lee, J. W., Polarization as a field variable from molecular dynamics simulations, *Journal of Chemical Physics*, 139, 054115-1-10 (2013).
5. Lee, J. W., Templeton, J. A., Mandadapu, K. K., and Zimmerman J. A., Investigation of various molecular dynamics models of electrical double layers in nanochannels, *Journal of Chemical Theory and Computation*, 9, 3051-3061 (2013).
6. Rangamani, P., Agrawal, A., Mandadapu, K. K., Oster, G., and Steigmann, D. J., Interaction between surface shape and intra-surface viscous flow on lipid membranes, *Biomechanics and Modeling in Mechanobiology*, 12, 833-845 (2013).
7. Ulz, M., Mandadapu, K. K., Papadopoulos, P., On the estimation of spatial averaging volume for determining stress using atomistic methods, *Modeling and Simulation in Materials Science and Engineering*, 21, 015010 (2013).
8. Jones, R. E., and Mandadapu, K. K., Adaptive Green-Kubo estimates of transport coefficients from molecular dynamics based on robust error analysis, *Journal of Chemical Physics*, 136, 154102 (2012).
9. Mandadapu, K. K., Sengupta, A., and Papadopoulos, P., A homogenization method for thermomechanical continua using extensive physical quantities, *Proceedings of Royal Society A : Mathematical, Physical and Engineering Sciences*, 468, 1696-1715 (2012).

10. Mandadapu, K. K., Jones, R. E., and Papadopoulos, P., A homogeneous non-equilibrium molecular dynamics method for calculating the heat transport coefficient of mixtures and alloys, *Journal of Chemical Physics*, 133, 034122 (2010). (**Editor's Choice Award**)
11. Mandadapu, K. K., Jones, R. E., and Papadopoulos, P., Generalization of the homogeneous non-equilibrium molecular dynamics method for calculating thermal conductivity to multi-body potentials, *Physical Review E*, 80, 047702 (2009).
12. Mandadapu, K. K., Jones, R. E., and Papadopoulos, P., A homogeneous non-equilibrium molecular dynamics method for calculating thermal conductivity with a three-body potential, *Journal of Chemical Physics*, 130, 204106 (2009).
13. Mandadapu, K. K., Govindjee, S., and Mofrad, M. R. K., On the cytoskeleton and soft glassy rheology, *Journal of Biomechanics*, 41, 1467-1478 (2008).
14. Guthikonda, V. S. R., Mandadapu K. K., Sivakumar, S. M., and Srinivasa, A. R., On smeared and micromechanical approaches to modeling martensitic transformations in shape memory alloys, *Nonlinear Analysis: Real World Applications*, 9, 990-1011 (2008).

CONFERENCES AND LECTURES

1. Nontrivial correlation length distinguishes melt from glass in a large-scale atomistic non-equilibrium simulation of a glass transition. *APS March Meeting, San Antonio, TX* (2015). (Joint Work with Hudson, A., and Chandler, D.)
2. Physical principles of organization in biological membranes. *Department of Chemical and Bio-molecular Engineering, University of California, Berkeley* (2015). **Invited Lecture**
3. Physical principles of organization in biological membranes. *Department of Chemical and Biological Engineering, University of Wisconsin Madison* (2015). **Invited Lecture**
4. The orderphobic effect: A fundamental force for self-assembly of proteins in lipid bilayers. *Kuriyan Lab, University of California, Berkeley* (2015). (Joint Work with Katira, S., and Vaikuntanathan, S.) **Invited Lecture**
5. The orderphobic effect: A fundamental force for self-assembly of proteins in lipid bilayers. *Membrane Supergroup Meeting, University of California, Berkeley* (2015). (Joint Work with Katira, S., and Vaikuntanathan, S.)
6. The orderphobic effect: A fundamental force for self-assembly of proteins in lipid bilayers. *Poster at Mini Stat-Mech Meeting, Berkeley* (2015). (Joint Work with Katira, S., and Vaikuntanathan, S.) **(Poster Prize)**.
7. Physical principles of organization in biological membranes. *Benoit Roux Lab, University of Chicago* (2014).
8. Energy transduction in the bacterial flagellar motor. *DARPA DSRC Microsystem-Scale Energy Conversion* (2014). (Joint work with Oster, G.) **Invited Lecture**
9. Effect of protein induced spontaneous curvature on membrane surface tension. *USNCCM MMVMB II, Berkeley* (2014). (Joint Work with Rangamani, P., and Oster, G.)
10. Polarization as a field variable from molecular dynamics simulations: Applications to water at solid interfaces. *Poster at Mini Stat-Mech Meeting, Berkeley* (2014).
11. Polarization as a field variable from molecular dynamics simulations: Applications to electrical double layers, *USNCCM, Raleigh* (2013). (Joint Work with Templeton, J. A., and Lee, J. W.)
12. Theoretical and computational aspects of homogenization in thermo-mechanical continua. *USNCCM, Raleigh* (2013). (Joint work with Mercer, B., and Papadopoulos, P.) **Invited Lecture**

13. Effect of protein induced spontaneous curvature on membrane surface tension. *Sandia National Laboratories* (2013). (Joint Work with Rangamani, P., and Oster, G.) **Invited Lecture**
14. Theoretical and computational aspects of homogenization in thermo-mechanical continua, *Multiscale Modeling Workshop, Sandia National Laboratories* (2013). (Joint work with Mercer, B., and Papadopoulos, P.) **Invited Lecture**
15. Homogeneous non-equilibrium molecular dynamics methods for calculating the heat transport coefficient of solids and mixtures, *Mini Statistical Mechanics Seminar, Department of Chemistry, University of California, Berkeley* (2013). (Joint Work with Jones, R. E., and Papadopoulos, P.) **Invited Lecture**
16. Polarization as a field variable from molecular dynamics simulations, *65th Annual meeting of American Physical Society, Division of Fluid Dynamics* (2012). (Joint work with Templeton, J. A., and Lee, J. W.)
17. Homogeneous non-equilibrium molecular dynamics methods for calculating the heat transport coefficient of solids and mixtures, *International Workshop on Computational Mechanics of Materials IWCMXXII* (2012). (Joint Work with Jones, R. E., and Papadopoulos, P.)
18. Accurate transport coefficients based on robust error analysis of the Green-Kubo method, *ASME Micro/Nanoscale Heat & Mass Transfer International Conference* (2012). (Joint work with Jones, R. E.) *Presentation by Jones, R. E.*
19. Examining permittivity effects in electric double layers using molecular dynamics and atomistic-to-continuum Modeling, *Bulletin of the American Physical Society, 64th Annual Meeting of the APS Division of Fluid Dynamics* (2011). (Joint Work with Templeton, J. A., Lee, J. W., Jones, R. E., and Zimmerman, J.) *Presentation by Templeton, J. A.*
20. Homogeneous non-equilibrium molecular dynamics methods for calculating the heat transport coefficient of solids and mixtures, *Sandia National Laboratories* (2010). (Joint work with Jones, R. E., and Papadopoulos, P.) **Invited Lecture**
21. Equilibrium and non-equilibrium molecular dynamics methods for thermal conductivity calculations, *Majumdar Lab, University of California at Berkeley* (2010). (Joint work with Jones, R. E., and Papadopoulos, P.) **Invited Lecture**
22. Thermal conductivity calculations using homogeneous non-equilibrium molecular dynamics (HNEMD) method, *Indian Institute of Technology at Kanpur* (2008). (Joint work with Jones, R. E., and Papadopoulos, P.) **Invited Lecture**
23. Cytoskeleton and soft glassy rheology, *Summer Bioengineering Conference* (2007). (Joint work with Govindjee, S., and Mofrad, M. R. K.)

PROFESSIONAL SERVICE

- Mini-Symposium chair for *Membranes: Biological and Synthetic at APS March Meeting*, San Antonio, March 2-6, 2015.
- Conference co-organizer for *Multiscale Methods and Validation in Medicine and Biology II: Biomechanics and Mechanobiology (MMVMB II)*, Berkeley, February 13-14, 2014.
- Mini-Symposium co-organizer in *United States National Congress on Computational Mechanics US-NCCM*, Raleigh, July 22-25, 2013.
- Mini-Symposium co-organizer in *International Workshop on Computational Mechanics of Materials IWCMXXII*, Baltimore, September 24-26, 2012.
- Reviewer for
 1. *Proceedings of Royal Society London Series A*

2. *eLife*
3. *Journal of Molecular Biology*
4. *Mathematics and Mechanics of Solids*
5. *IEEE Transactions on Biomedical Engineering*
6. *International Journal of Heat and Mass Transfer*
7. *Journal of Applied Physics*
8. *Journal of Chemical Physics*
9. *Biomechanics and Modeling in Mechanobiology*
10. *Journal of Biomechanics*
11. *Langmuir*

- Advising graduate students towards their Ph.D.
 1. Shrikant Kshirsagar (UC Berkeley)
Topic: Thermal conductivity calculations of rough nanowires
 2. Brian Mercer (UC Berkeley)
Topic: Multiscale modeling of thermo-mechanical continua
 3. Shachi Katira (UC Berkeley)
Topic: Modeling of biological membranes

TEACHING EXPERIENCE

- Teaching Assistant for Statistical Mechanics of Elasticity, Fall 2010.
- Notes for a short course on Modeling and Simulation of Multiscale Continuum Systems, International Center for Mechanical Sciences, Udine, Italy, June 28-July 2, 2010.
- Reader for Introduction to Continuum Mechanics, University of California at Berkeley, Fall 2008.
- Reader for Advanced Computer Programming, University of California at Berkeley, Spring 2008.
- Teaching Assistant for Introduction to Computer Programming, University of California at Berkeley, Fall 2007, Spring 2009, and Fall 2009.
- Statistical Mechanics to Continuum Mechanics, a full semester course notes in preparation.