

Jin Liu

CONTACT INFORMATION

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EDUCATION

Johns Hopkins University, Baltimore, MD
Ph.D. in Mechanical Engineering, GPA: 3.9/4.0 08/2008
Advisor: Prof. Shiyi Chen

The University of Michigan, Ann Arbor, MI
M.S. in Mechanical Engineering, GPA: 3.8/4.0 12/2003

Univ. of Sci. & Tech. of China, Anhui, China
B.S. in Mechanical Engineering, GPA: 3.7/4.0 06/2001

RESEARCH INTERESTS

- Fluid mechanics, computational fluid dynamics (CFD), turbulent flows, computational biology, drug delivery
- Micro-and nano-fluidics, electrokinetic flows, heat transfer, energy conversion, fuel cells, granular flows, multiscale modeling, electrowetting, bio-fluidics, membrane dynamics
- Spectral method, molecular dynamics, Monte Carlo simulations, lattice Boltzmann method, multigrid method, parallel computing

RESEARCH EXPERIENCE

Postdoctoral Associate 02/2009-present
Department of Bioengineering
University of Pennsylvania, Philadelphia, PA
Prof. Ravi Radhakrishnan, Prof. P. S. Ayyaswamy and Prof. David M Eckmann
Project: Targeted drug delivery: Integrated Multiscale Modeling, supported by NIH

- Developed a numerical protocol to compute the absolute binding free energy between anti-ICAM-1 coated nanocarrier and ICAM-1 expressing endothelial cells.
- Analyzed the effects from a broad range of parameters on the efficiency of nanocarrier drug delivery, closely compared our model predictions to *in vitro* and *in vivo* experiments.
- Developing the procedure to study the membrane and flow mediated nanocarrier drug delivery.

Postdoctoral Research Fellow 09/2008-01/2009
Department of Mechanical Engineering
Johns Hopkins University, Baltimore, MD
Prof. Shiyi Chen

Graduate Student Research Assistant 08/2007-08/2008
Department of Mechanical Engineering,
Johns Hopkins University, Baltimore, MD
Prof. Shiyi Chen
Project: NIRT: Interfacial Forces in Active Nano Devices supported by NSF and Multiscale modeling and simulations of micro- and nano-scale electrokinetic flows, supported by NSF

- Developed a new version of the particle-particle particle-mesh (PPPM) scheme to resolve the long range Coulomb force.
- Implemented a cost efficient multi-grid technique to solve the Poisson equation.
- Extended the above code to study electro-osmosis and electro-wetting problems (contact angle saturation).

Visiting Graduate Student 08/2006-07/2007
Theoretical Division, Fluid Dynamics Group T3,
Los Alamos National Laboratory, Los Alamos NM
Dr. Duan Z Zhang and Prof. Shiyi Chen
Project: Model Simulation of Materials and Particle Interactions

- Incorporated a granular simulation code into CartaBlanca to allow study of granular materials (CartaBlanca is a pure Java, component-based, object oriented simulation tool for non-linear physics maintained in Los Alamos National Lab).
- Performed numerical simulations of mixing of binary particulate systems from molecular to mesoscopic scales.
- Analyzed the numerical results and proposed a possible unified constitutive relation for material mixing at different length and time scales.

Graduate Student Research Assistant 01/2004-07/2006
Department of Mechanical Engineering,
Johns Hopkins University, Baltimore, MD
Prof. Shiyi Chen
Project: Multi-scale simulation of micro/nano flow, supported by NSF

- Developed a new multi-timescale algorithm to allow a hybrid atomistic/continuum scheme to be applied to dynamics on much longer time scales.

- Extended our previous isothermal hybrid scheme to include the energy equation.
- Analyzed heat transfer problems for one and two-dimensional incompressible flows in micro/nano channels.

Graduate Student Research Assistant 10/2001-12/2003

Department of Mechanical Engineering,
The University of Michigan, Ann Arbor, MI

Project: Molecular-Biomolecular Suppression of Turbulence, supported by DARPA/ATO

- Developed a cost-efficient and accurate polymer model, which was implemented in a pseudo-spectral Direct Numerical Simulation (DNS) code using the Eulerian and Lagrangian methods.
- Parallelized the above code using MPI.
- Analyzed the large DNS database produced from the supercomputers in San Diego and Texas.
- Visualized and proposed the mechanism involved in the well-known polymer drag reduction phenomenon.

Research Assistant 09/1999-06/2001

Department of Mechanics and Mechanical Engineering
Univ. of Sci. & Tech. of China, Anhui, China

Prof. Xiyun Lu and Prof. Lixian Zhuang

Project: Large Eddy Simulation of Smoke Movement with Water Spray

- Performed numerical studies of combustion and smoke movement.
- Designed fire extinguishment experiments, collected the experimental data, compared with numerical results and proposed optimal fire extinguishment strategy.

TEACHING EXPERIENCE

Teaching Assistant, Department of Mechanical Engineering, Johns Hopkins University
EN.530.766, Numerical Methods Fall 2007

Teaching Assistant, Department of Mechanical Engineering, Johns Hopkins University
EN.530.621, Fluid Dynamics I Fall 2007

CONFERENCE PRESENTATIONS

Biophysical Society 55th Annual Meeting, 2011, Mar. 5-9, Baltimore, Maryland. Poster session 3327-Pos "Monte Carlo Simulations of Absolute Binding Free Energy of Targeted Nanocarriers to Cell Surfaces".

American Physical Society (APS)-Division of Fluid Dynamics (DFD), 2010, Nov. 21-23, Long Beach, CA. Volume 55, No. 16, MK 4 "Monte Carlo Simulations of Absolute Binding Free Energy of Targeted Nanocarriers to Cell Surfaces".

American Physical Society (APS)-Division of Fluid Dynamics (DFD), 2010, Nov. 21-23, Long Beach, CA. Volume 55, No. 16, MK 8 "Modeling Protein-induced Membrane Deformation using Monte Carlo and Langevin Dynamics Simulations".

Biophysical Society 54th Annual Meeting, 2010, Feb. 20-24, San Francisco, California. Poster session "Simulations of Functionalized Nanocarrier Binding to Cells: Calculations of Absolute Binding Free Energies, Effect of Shear Flow and Glycocalyx and Comparison to Experiments".

ASME Micro/Nanoscale Heat and Mass Transfer International Conference, 2009, Dec.18-21, Shanghai, China. "Molecular simulation of electrokinetic transport in nanofluidics".

American Physical Society (APS)-Division of Fluid Dynamics (DFD), 2008, Nov. 23-25, San Antonio, Texas. Volume 53, No. 15, MN 10 "Molecular simulation of electrokinetic flows".

American Physical Society (APS)-Division of Fluid Dynamics (DFD), 2007, Nov. 18-22, Salt Lake City, Utah. Volume 52, No. 17, JI 12 "Stresses in Binary Particulate Systems".

American Physical Society (APS)-Division of Fluid Dynamics (DFD), 2005, Nov. 20-22, Chicago, IL. Volume 50, No. 9, FC 5 "A hybrid continuum-atomistic simulation of heat transfer in micro flow".

American Physical Society (APS)-Division of Fluid Dynamics (DFD), 2004, Nov. 21-23, Seattle, WA. "A new multiscale time algorithm for Micro/Nano flow".

American Physical Society (APS)-Division of Fluid Dynamics (DFD), 2003, Nov. 23-25, East Rutherford, NJ. Volume 48, No. 10, FC 2 "DNS of Drag Reduction by Dilute Polymer Solutions using a Backward-tracking Lagrangian Particle Method".

DARPA Friction Drag Reduction Program Principal Investigators' Meeting, May 21-22, 2003, San Diego, California.

American Physical Society (APS)-Division of Fluid Dynamics (DFD), 2002, Nov. 24-26, Dallas, TX. Volume 47, No. 10, KK 8 “Direct Numerical Simulation of Polymer Drag Reduction in a Turbulent Channel Flow Using the FENE-P Model”.

DARPA Friction Drag Reduction Program Principal Investigators’ Meeting, November 19-20, 2002, Orlando, Florida.

BOOK CHAPTER

J. Liu, N.J. Agrawal, D.M. Eckmann, P.S. Ayyaswamy and R. Radhakrishnan (2011), chapter “Top-down mesoscale models and free energy calculations of multivalent protein-protein and protein-membrane interactions” for book “Innovations in Biomolecular Modeling and Simulation” edited by Tamar Schlick and published by Royal Society of Chemistry (RSC) (in press).

PUBLICATIONS

J. Liu, N.J. Agrawal, V. Ramanan and R. Radhakrishnan (2011), Migration of curvature inducing proteins in response to mean and Gaussian curvature gradients (under review)

J. Liu, M. Wang, S. Chen and M. Robbins (2011), Uncovering molecular mechanisms of electrowetting and saturation with simulations (under review)

T.N. Swaminathan, **J. Liu**, U. Balakrishnan, P.S. Ayyaswamy, R. Radhakrishnan and D.M. Eckmann, Dynamic factors controlling carrier anchoring on vascular cells, *IUBMB Life* 63 (8): 640-647 (2011)

V. Ramanan, N.J. Agrawal, **J. Liu**, S. Engles, R. Toy and R. Radhakrishnan, Systems biology and physical biology of Clathrin-mediated endocytosis: An integrative experimental and theoretical perspective, *Integr. Biol.* 3 (8): 803-815 (2011)

J. Liu, R. Bradley, D.M. Eckmann, P.S. Ayyaswamy and R. Radhakrishnan, Multiscale modeling of functionalized nanocarriers in targeted drug delivery, *Curr. Nanosci.* 7 (5): 727-735 (2011)

J. Liu, N. Agrawal, A. Calderon, P.S. Ayyaswamy, D.M. Eckmann and R. Radhakrishnan, Multivalent binding of nanocarrier to endothelial cells under shear flow, *Biophys. J.* 101 (2): 319-326 (2011) (**Featured cover story**)

J. Liu, G. Weller, B. Zern, P.S. Ayyaswamy, D.M. Eckmann, V.R. Muzykantov and R. Radhakrishnan, Computational model for nanocarrier binding to endothelium validated using in vivo, in vitro and atomic force microscopy experiments, *Proc. Natl. Acad. Sci. USA.* 107 (38): 16530-16535 (2010)

J. Liu, M. Wang, S. Chen and M. Robbins, Molecular simulations of electroosmotic flows in rough nanochannels, *J. Comput. Phys.* 229 (20): 7834-7847 (2010)

J. Liu, M. Wang, S. Chen and M. Robbins, Molecular simulation of electrokinetic transport in nanofluidics, *Proceedings of ASME Micro/Nanoscale Heat and Mass Transfer International Conference 2009, MNHMT2009*, 1: 233-241 (2010)

J. Liu, S. Chen and D.Z. Zhang, Species interactions in binary particulate systems, *Phys. Rev. E* 77: 066301 (2008)

J. Liu, S. Chen, X. Nie and M. Robbins, A continuum-atomistic multi-timescale algorithm for micro/nano flows, *Commun. Comput. Phys.* 4 (5): 1279-1291 (2008)

J. Liu, S. Chen, X. Nie and M. Robbins, A continuum-atomistic simulation of heat transfer in micro- and nano-flows, *J. Comp. Phys.* 227 (1): 279-291 (2007)

M. Wang, **J. Liu** and S. Chen, Electric potential distribution in nanoscale electroosmosis: from molecules to continuum, *Mol. Simulat.* 33 (15): 1273-1277 (2007)

M. Wang, **J. Liu** and S. Chen, Similarity of electroosmotic flows in nanochannels, *Mol. Simulat.* 33 (3): 239-244 (2007)

J. Liu, X. Lu, G. Liao and W. Fan, Application of large eddy simulation to smoke movement, *J. Fire Safety Science* (in China) 11 (1): 5-14 (2002)

J. Liu, X. Lu, G. Liao and W. Fan, Large eddy simulation of smoke movement with a water spray, *J. Fire Safety Science* (in China) 11 (1): 15-23 (2002)

HONORS AND AWARDS

Graduate Student Research Assistantship, 2004-2008
Johns Hopkins University

NR-Engineering Grad Fellowship 2003
The University of Michigan, Ann Arbor

Graduate Student Research Assistantship 2001-2003
The University of Michigan, Ann Arbor

Climbing Award in Mechanics Univ. of Sci. & Tech. of China	2001
Excellent Student Scholarship Univ. of Sci. & Tech. of China	1997-2000
Excellent New Student Scholarship Univ. of Sci. & Tech. of China	1996