GREGORY J. WAGNER

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EDUCATION

Ph.D. Mechanical Engineering, *Northwestern University*, Evanston, IL 2001
Thesis title: *A Numerical Investigation of Particulate Channel Flows*

M.S. Mechanical Engineering, *Northwestern University*, Evanston, IL 1999
Thesis title: *A Multi-Scale Approach to Large Eddy Simulation via RKPM*

B.S. Mechanical Engineering, *Boston University*, Boston, MA 1996

PROFESSIONAL EXPERIENCE

Northwestern University Evanston, IL
Associate Professor 1/2015 – Present

- Research interests include multi-scale and multi-physcis simulation methods; computational fluid dynamics; multiphase flows; high-performance computing.

Sandia National Laboratories Livermore, CA
Manager 4/2012 – 12/2014

- Manage the Thermal/Fluid Science and Engineering Department, part of the Transportation Energy Center at Sandia
- Oversee department of around 15 staff, post-docs and contractors with >$3.5M annual budget
- Lead development and application of modeling and simulation capability for fluid and thermal problems in defense, energy and industry applications
- Hire, retain and develop a talented and diverse group of technical staff

Sandia National Laboratories Livermore, CA
Principal Member of Technical Staff 10/2006 – 4/2012
Senior Member of Technical Staff 10/2002 – 9/2006

- Performed extensive research, code development, analysis, and project management, including:
  - Modeling and simulation of incompressible turbulent reacting flows, multiphase and particulate flows, and compressible flows
  - Large-scale molecular dynamics and multi-scale computations of materials
  - Coupled thermo-mechanical-optical analysis for refractive and reflective optics
  - Mesoscale models of materials for hydrogen storage and lithium ion battery modeling applications
- Wrote proposals and obtained funding primarily through Sandia's internal Laboratory Directed Research and Development (LDRD) program and the DOE's Advanced Simulation and Computing program
- Mentored graduate student interns, post-docs and staff

Northwestern University Evanston, IL
Research Assistant Professor 6/2001 – 9/2002

- Introduced Bridging Scale Method for coupling molecular dynamics and finite element method in concurrent multi-scale simulations
- Developed multiple-scale simulation methods for fluid and solid dynamics and multiphase flows
- Performed molecular dynamics and nanoscale simulations for surface science and sensor design applications
- Led research in meshfree computational methods and parallel and high-performance computing
- Mentored undergraduates, graduate students, and post-docs on research projects

Northwestern University Evanston, IL
Graduate Research Assistant 6/1997 – 6/2001

- Developed novel technique for direct simulation of multiphase particulate flows using the eXtended Finite Element Method (XFEM)
- Introduced and tested a method for using the Reproducing Kernel Particle Method (RKPM) in a dynamic subgrid scale Large Eddy Simulation (LES) turbulence model

Moog, Inc. East Aurora, NY
Design Engineering Analyst 5/1996 – 8/1996

- Used commercial finite element codes to perform vibration and stress analysis on device components

FELLOWSHIPS AND AWARDS

- **Zienkiewicz Numerical Methods in Engineering Prize**
  John Wiley and Sons, Ltd., 2004.
- **B.L. Martin Fellowship**
  Northwestern University, 2000-2001
- **National Defense Science and Engineering Graduate Fellowship**
  Department of Defense, 1997-2000
- **Cabell Fellowship**
  Northwestern University, 1996-1997
- **Valedictorian, College of Engineering**
  Boston University, 1996
- **Trustee Scholarship**
  Boston University, 1992-1996

TEACHING

Courses Taught

- ME377 Heat Transfer
- ME424 Advanced Topics in Computational Fluid Dynamics (developed)
- ME495 High Performance Computing for Multiphysics Applications (developed)

PUBLICATIONS

- S. Lin, J. Smith, W.K. Liu, G.J. Wagner. 2017. "An energetically consistent concurrent multiscale method for heterogeneous heat transfer and phase transition applications." *Comput. Methods Appl. Mech. Engrg.*, **315**:100-120.

- S. Tang, Y. Ying, Y. Lian, S. Lin, Y. Yang, G.J. Wagner, W.K. Liu. 2016. "Differential operator multiplication method for fractional differential equations." *Comput. Mech.*, **58**:879-888.
- Y. Lian, Y. Ying, S. Tang, S. Lin, G.J. Wagner, W.K. Liu. 2016. "A Petrov-Galerkin finite element method for the fractional advection-diffusion equation." *Comput. Methods Appl. Mech. Engrg.*, **309**:388-410.
- J. Smith, W. Xiong, W. Yan, S. Lin, P. Cheng, O.L. Kafka, G.J. Wagner, J. Cao, W.K. Liu. 2016. "Linking process, structure, property, and performance for metal-based additive manufacturing: computational approaches with experimental support." *Comp. Mech.*, **57(4)**:583-610.
- M. Markl, G.J. Wagner, A.J. Barker. 2016. "Re: Blood flow analysis of the aortic arch using computational fluid dynamics." *Eur J Cardiothorac Surg*, **49**:1586-1587.
- G.J. Wagner. 2013. "Atomistic-to-Continuum Coupling Methods for Heat Transfer in Solids." in *Multiscale Simulations and Mechanics of Biological Materials*, pp. 3-20. Ed. S. Li and D. Qian. John Wiley & Sons, Ltd.
- J. Deng, G.J. Wagner, R.P. Muller. 2013. "Phase field modeling of solid electrolyte interface formation in lithium ion batteries." *J. Electrochem. Soc.*, **160(3)**:A487-A496.
- B. Jelinek, S. Groh, A. Moitra, M.F. Horstemeyer, J. Houze, S.G. Kim, G.J. Wagner, M.I. Baskes. 2012. "Modified embedded atom method potential for Al, Si, Mg, Cu, and Fe alloys." *Phys Rev. B*, **24**:245102.
- J. Deng, G.J. Wagner, R.P. Muller. 2012. "A phase field model of solid electrolyte interface formation in lithium-ion batteries." *MRS Proceedings*, 1440, DOI:10.1557/op1.2012.1278.
- A.L. Brown, G.J. Wagner, K.E. Metzinger. 2011. "Impact, fire and fluid spread code coupling for complex transportation accident environment simulation." *J. Thermal Sci. and Eng. Appl.*, **4**:021004-1.
- M.P. Klein, B.W. Jacobs, M.D. Ong, S.J. Fares, D.B. Robinson, V. Stavila, G.J. Wagner, I. Arslan. 2011. "Three-dimensional pore evolution of nanoporous metal particles for energy storage." *J. Amer. Chem. Soc.*, **133(24)**:9144-9147.
- A.L. Brown and G.J. Wagner. 2010. "Fluid spread model validation for emerging liquid tank impact predictive methods." *ASME Conf. Proc.* 2010, **925**, DOI:10.1115/IHTC14-23067.
- G.J. Wagner, D. Seif, M.D. Ong. 2010. "Kinetic Monte Carlo simulation of the aging of nanoporous metals." *MRS Online Proceedings Library*, **1263**: 1263-Y04-04.
- G.J. Wagner, X. Zhou, S.J. Plimpton. 2010. "Equation-free accelerated simulations of the morphological relaxation of crystal surfaces." *Int. J. Multiscale. Comp. Eng.*, **8(4)**:423-439.
- J.A. Templeton, R.E. Jones, G.J. Wagner. 2010. "Application of a field-based method to spatially varying thermal transport problems in molecular dynamics." *Mod. Sim. Mat. Sci. Eng.*, **18(8)**:085007.
- R.E. Jones, J.A. Templeton, G.J. Wagner, D. Olmsted, N. Modine. 2010. "Electron-transport enhanced molecular dynamics for metals and semi-metals." *Int. J. Num. Meth. Eng.*, **83(8-9)**:940-967.
- G.J. Wagner, R.E. Jones, J.A. Templeton, M.L. Parks. 2008. "An atomistic-to-continuum coupling method for heat transfer in solids." *Comp. Meth. Appl. Mech. Eng.*, **197**:3351-65.
- M.Q. Chandler, M.F. Horstemeyer, M.I. Baskes, P.M. Gullett, G.J. Wagner, B. Jelinek. 2008. "Hydrogen effects on nanovoid nucleation in FCC single crystals." *Acta Materialia*, **56(1)**:95-104.

- M.Q. Chandler, M.F. Horstemeyer, M.I. Baskes, G.J. Wagner, P.M. Gullett, B. Jelinek. 2008. "Hydrogen effects on nanovoid nucleation at nickel grain boundaries." *Acta Materialia*, **56(3)**:619-631.
- S.G. Srinivasan, M.I. Baskes, G.J. Wagner. 2007. "Atomistic simulations of shock induced microstructural evolution and spallation in single crystal nickel.". *J. Appl. Phys.*, **101(4)**:043504
- S.G. Srinivasan, M.I. Baskes, G.J. Wagner. 2006. "Spallation of single crystal nickel by void nucleation at shock induced grain junctions." *J. Mat. Sci.*, **41(23)**:7838-42.
- H.S. Park, P.A. Klein, G.J. Wagner. 2006. "A surface cauchy-born model for nanoscale materials." *Int. J. Num. Meth. Eng.*, **68(10)**:1072-95.
- G.P. Potirniche, M.F. Horstemeyer, G.J. Wagner, P.M. Gullett. 2006. "A molecular dynamics study of void growth and coalescence in single crystal nickel." *Int. J. Plasticity*, **22**:257-78.
- G.P. Potirniche, M.F. Horstemeyer, B. Jelinek, G.J. Wagner. 2005. "Fatigue damage in nickel and copper single crystals at nanoscale." *Int. J. Fatigue*, **27**:1179-85.
- W.K. Liu, H.S. Park, D. Qian, E.G. Karpov, H. Kadowaki, G.J. Wagner. 2006. "Bridging scale methods for nanomechanics and materials." *Comp. Meth. Appl. Mech. Eng.*, **62**:1250-62.
- E.G. Karpov, G.J. Wagner, W.K. Liu. 2005. "A Green's function approach to deriving non-reflecting boundary conditions in molecular dynamics simulations." *Int. J. Num. Meth. Eng.*, **69(2)**:1250-1262.
- X.Q. Chen, S.L. Zhang, G.J. Wagner, W.Q. Ding, R.S. Ruoff. 2004. "Mechanical resonance of quartz microfibers and boundary condition effects." *J. App. Phys.*, **95**: 4823-4828.
- S. Zhang, G.J. Wagner, S.N. Medyanik, W.K. Liu, Y.H. Yu, Y.W. Chung. 2004. "Experimental and molecular dynamics simulation studies of friction behavior of hydrogenated carbon films." *Surface and Coatings Technology*, **177**: 818-823.
- G.J. Wagner, E.G. Karpov, W.K. Liu. 2003. "Molecular dynamics boundary conditions for regular crystal lattices." *Comp. Meth. Appl. Mech. Eng.*, **193**: 1579-1601.
- G.J. Wagner, W.K. Liu. 2003. "Coupling of atomistic and continuum simulations using a bridging scale decomposition." *J. Comp. Phys.*, **190**: 249-274.
- G.J. Wagner, S. Ghosal, W.K. Liu. 2003. "Particulate flow simulations using lubrication theory solution enrichment." *Int. J. Num. Meth. Eng.*, **56(9)**:1261-1289.
- S.L. Zhang, H.T. Johnson, G.J. Wagner, W.K. Liu, K.J. Hsia. 2003. "Stress generation mechanisms in carbon thin films grown by ion-beam deposition." *Acta Materialia*, **51**:5211-22.
- D. Qian, G.J. Wagner, W.K. Liu. 2003. "A multiscale projection method for the analysis of carbon nanotubes." *Comp. Meth. Appl. Mech. Eng.*, **193**:1603-1632.
- E.G. Karpov, G.J. Wagner, W.K. Liu. 2003. "A Green's function approach to deriving wave-transmitting boundary conditions in molecular dynamics simulations." *Int. J. Num. Meth. Eng.*, **62(9)**:1250-62.
- L.T. Zhang, G.J. Wagner, W.K. Liu. 2003. "Modeling and simulation of fluid structure interaction by meshfree and FEM." *Commun. Numer. Meth. Engng.*, **19**:615-621.
- D.A. Dikin, X. Chen, W. Ding, G. Wagner, R.S. Ruoff. 2003. "Resonance vibration of amorphous SiO_2 nanowires driven by mechanical or electrical field excitation." *J. App. Phys.*, **93(1)**:226-230.
- M.F. Yu, G.J. Wagner, R.S. Ruoff, M.J. Dyer. 2002. "Realization of parametric resonances in a nanowire mechanical system with nanomanipulation inside a scanning electron microscope" *Phys. Rev. B*, **66**: art. no. 073406.

- D. Qian, G.J. Wagner, W.K. Liu, M.F. Yu, R.S. Ruoff. 2002. "Mechanics of carbon nanotubes." *Appl. Mech. Rev*, **55(6)**:495-553.
- L. Zhang, G.J. Wagner, W.K. Liu. 2002. "A parallelized meshfree method with boundary enrichment for large-scale CFD." *J. Comp. Phys*, **176**:483-506.
- W. Han, G.J. Wagner, W.K. Liu. 2002. "Convergence analysis of a hierarchical enrichment of dirichlet boundary conditions in a meshfree method." *Int. J. Num. Meth. Eng*, **53**: 1323-1336.
- G.J. Wagner, N. Moës, W.K. Liu, T. Belytschko. 2001. "The extended finite element method for viscous particulate flows." *Int. J. Num. Meth. Eng.*, **51**: 293-313.
- G.J. Wagner, W.K. Liu. 2000. "Hierarchical enrichment for bridging scales and meshfree boundary conditions." *Int. J. Num. Meth. Eng.*, **50**: 507-524.
- G.J. Wagner and W.K. Liu. 2000. "Turbulence simulation and multiple scale subgrid models." *Comp. Mech.*, **25**: 117-136.
- G.J. Wagner and W.K. Liu. 2000. "Application of essential boundary conditions in mesh-free methods: a corrected collocation method." *Int. J. Num. Meth. Eng.*, **47**: 1367-1379.