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- <u>Research</u>
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- Teaching and course development
- <u>Book</u>

Research:

Summary: My work draws inspiration from various disciplines of sciences and has made an impact in fluid dynamics, chemistry, material sciences, and soft condensed matter physics. I have contributed to the resolution of some long standing scientific problems such as the Burgers turbulence problem (which was the original motivation of Burgers for proposing the well-known Burgers equation), the Cauchy-Born rule for crystalline solids (which indeed dates back to Cauchy, and provides a microscopic foundation for the elasticity theory), and the moving contact line problem (which is still largely open). A common theme is to try bringing clarity to scientific issues through mathematics. A second theme is multi-scale and/or multiphysics problems. I have also worked on building the mathematical framework and finding effective numerical algorithms for modeling rare events which is a very difficult class of problems involving multiple time scales (string method, minimum action methods, transition path theory, etc). I have also worked on multiscale analysis and algorithms for stochastic simulation algorithms, homogenization problems, problems with multiple time scales, complex fluids, etc. My book provides a broad introduction to this subject. A third theme is to develop and analyze algorithms in general. In computational fluid mechanics, I was involved in analyzing and developing vorticity-based methods, the project method and the gauge method. In density functional theory (DFT), my collaborators and I have developed the selected inversion algorithm, which is so far the most efficient algorithm for DFT.

Here are some examples of the work I have been involved with (*click on the* ``+'' *sign to read more*):

Burgers turbulence

We have analyzed the statistical properties of solutions to the Burgers equation with random initial data and random forcing. This series of work provided answers to some of the questions that Burgers proposed back in the early 20th century, and resolved some of controversies concerning the asymptotics of the probability distribution functions for the random forced Burgers equation.

• W. E and E. Vanden-Eijnden. Asymptotic theory for the probability density functions

- in Burgers turbulence. Phys. Rev. Lett., vol. 83, no. 13, pp. 2572-2575, 1999.
- W. E, K. Khanin, A. Mazel and Ya. Sinai. <u>Probability distribution functions for the</u> random forced Burgers equation. *Phys. Rev. Lett.*, vol. 78, no. 10, pp. 1904-1907, 1997.
- M. Avellaneda and W. E. <u>Statistical properties of shocks in Burgers turbulence</u>. *Comm. Math. Phys.*, vol. 172, no. 1, pp. 13-38, 1995.
- M. Avellaneda, R. Ryan and W. E. <u>PDFs for velocity and velocity gradients in Burgers'</u> <u>turbulence</u>. *Phys. Fluids*, vol. 7, no. 12, pp. 3067-3071, 1995.

From quantum and molecular mechanics to macroscopic theories of solids (Cauchy-Born rule and related topics)

The objective here is to understand solids at the level of quantum mechanics or molecular mechanics. As a by-product, we give a rigorous derivation of the macroscopic continuum models of solids. A key ingredient in this analysis is to understand the various levels of stability conditions (quantum, classical but at the atomic level and classical but at the macro level).

- W. E and J. Lu, "<u>The Kohn-Sham equation for deformed crystals</u>," *Memoire of the American Math Socieety*, 2012.
- W. E and J. Lu, "<u>The electronic structure of smoothly deformed crystals: Wannier functions and the Cauchy-Born rule</u>," *Arch. Ration. Mech. Anal.*, vol. 199, pp. 407-433, 2011.
- W. E and J. Lu, "<u>The electronic structure of smoothly deformed crystals: Cauchy-Born</u> <u>rule for the nonlinear tight-binding model</u>," *Comm. Pure Appl. Math.*, vol. 63, pp. 1432-1468, 2010.
- W. E, J. Lu and X. Yang, "Effective Maxwell equations from time-dependent density functional theory," *Acta Math. Sinica*, vol. 27, pp. 339-368, 2011.
- W. E, J. Lu and X. Yang, "Asymptotic analysis of the quantum dynamics: The Bloch-Wigner transform and Bloch dynamics," *Acta. Appl. Math. Sinica.*, (25 July 2011), pp. 1-12.
- W. E and D. Li, "<u>On the crystallization of 2D hexagonal lattices</u>," *Comm. Math. Phys.*, vol. 286, no. 3, pp. 1099-1140, 2009.
- W. E and P.B. Ming, <u>"Cauchy-Born Rule and the Stability of Crystalline Solids:</u> <u>Dynamic Problems</u>," *Acta. Math. Appl. Sin. Engl. Ser.*, vol. 23, no. 4, pp. 529-550, 2007.
- W. E and P.B. Ming, "<u>Cauchy-Born Rule and the Stability of Crystalline Solids: Static</u> <u>Problems</u>," *Arch. Rat. Mech. Anal.*, vol. 183, no. 2, pp. 241-297, 2007.

Stochastic PDEs

We have developed a new way of studying stochastic PDEs, by viewing the stationary solutions as functionals of the stochastic forcing. This has led to a very elegant description of the stationary solutions of the stochastic Burgers equation and the stochastic passive scalar equation as well as the ergodicity of the stochastic Navier-Stokes equation.

• W. E and D. Liu. <u>Gibbsian dynamics and invariant measures for stochastic dissipative</u>

- PDEs. J. Stat. Phys., vol. 108, no. 5-6, pp. 1125-1156, 2002.
- W. E. "<u>Stochastic PDES in turbulence theory</u>," Proc. 1st Intl. Congress Chinese Math. (Beijing, 1998), pp. 27-46. <u>AMS/IP Stud. Adv. Math</u>, vol. 20, Amer. Math. Soc., Providence, RI, 2001.
- W. E and J.C. Mattingly. <u>Ergodicity for the Navier-Stokes equation with degenerate</u> <u>random forcing: Finite-dimensional approximation</u>. *Comm. Pure Appl. Math.*, vol. 54, no. 11, pp. 1386-1402, 2001.
- W. E, J.C. Mattingly and Ya. Sinai. <u>Gibbsian dynamics and ergodicity for the</u> <u>stochastically forced Navier-Stokes equation</u>. *Comm. Math. Phys.*, vol. 224, no. 1, pp. 83-106, 2001.
- W. E and J.C. Mattingly. <u>Ergodicity for the Navier-Stokes equation with degenerate</u> <u>random forcing: Finite-dimensional approximation</u>. *Comm. Pure Appl. Math.*, vol. 54, no. 11, pp. 1386-1402, 2001.
- W. E, J.C. Mattingly and Ya. Sinai. <u>Gibbsian dynamics and ergodicity for the</u> <u>stochastically forced Navier-Stokes equation</u>. *Comm. Math. Phys.*, vol. 224, no. 1, pp. 83-106, 2001.
- W. E and E. Vanden-Eijnden. <u>Generalized flows, intrinsic stochasticity and turbulent</u> <u>transport</u>. *Proc. Natl. Acad. Sci.*, vol. 97, no. 15, pp. 8200-8205, 2000.

■ Modeling rare events

My work on modeling rare events (joint with Weiqing Ren and Eric Vanden-Eijnden) has centered around developing the string method, which is now quite popular in cmputational chemistry and begins to get popularity in material science, as well as the transition path theory, which is a general theoretical framework for analyzing transition events in complex systems.

- W. E and X. Zhou, <u>The gentlest ascent dynamics</u>.*Nonlinearity*, vol. 24, no. 6, pp. 1831, 2011.
- W. E and E. Vanden-Eijnden, <u>The transition path theory and path-finding algorithms</u> for the study of rare events. *Ann. Rev. Phys. Chem.*, vol. 61, pp. 391-420, 2010.
- X. Cheng, L. Lin, W. E, A-C. Shi, and P. Zhang, <u>Nucleation of Ordered Phases in</u> <u>Block Copolymers</u>. *Phys. Rev. Lett.*, vol. 104, pp. 148301-148301-4, 2010.
- X. Wan, X. Zhou, and W. E, <u>Study of noise-induced transitions in the Kuramoto-</u> <u>Sivashinsky equation via the minimum action method</u>. *Nonlinearity*, vol. 23, no. 3, pp. 475-494, 2010.
- X. Zhou and W. E, <u>Study of noise-induced transitions in the Lorenz system using the minimum action method</u>. *Comm. Math. Sci.*, vol. 8, pp. 341-355, 2010.
- W. E, W. Ren, E. Vanden-Eijnden. <u>Simplified and improved string method for</u> <u>computing the minimum energy paths in barrier-crossing events</u>. *J. Chem. Phys.*, vol. 126, no. 16, 164103, 2007.
- W. E and E. Vanden-Eijnden. <u>Towards a theory of transition paths</u>. J. Stat. Phys., vol. 123, No. 3, 503-523, 2006.
- W. Ren, E. Vanden-Eijnden, P. Maragakis and W. E. <u>Transition pathways in complex</u> <u>systems: Application of the finite temperature string method to the alanine dipeptide</u>. *J. Chem. Phys.*, vol. 123, 134109, 2005.
- W. E, W. Ren and E. Vanden-Eijnden. Finite temperature string method for the study

of rare events. J. Phys. Chem. B, 109, 6688-6693, 2005.

• W. E, W. Ren and E. Vanden-Eijnden. <u>String method for the study of rare events</u>. *Phys. Rev. B*, vol. 66, no. 5, 052301, 2002.

■ Multiscale methods

We have developed the framework of the heterogeneous multiscale method (HMM). HMM has led to very promising applications to stochastic simulation algorithms, ODEs with multiple time scales, and many other areas. It also provides a very nice framework for analyzing multiscale methods.

- A. Abdulle, W. E, B. Engquist and E. Vanden-Eijnden, <u>The heterogenous multiscale</u> <u>methods</u>. *Acta. Numerica*, pp. 1-87, 2012.
- W. E, B. Engquist, X. Li, W. Ren and E. Vanden-Eijnden. <u>Heterogeneous multiscale</u> <u>methods: A review</u>. *Comm. Comput. Phys.*, vol. 2, no. 3, pp. 367-450, 2007.
- W. E, P.B. Ming and P.-W. Zhang. <u>Analysis of the heterogeneous multiscale method</u> <u>for elliptic homogenization problems</u>. *J. Amer. Math. Soc.*, vol. 18, no. 1, pp. 121-156, 2005.
- W. E, D. Liu and E. Vanden-Eijnden. <u>Analysis of multiscale methods for stochastic</u> <u>differential equations</u>. *Comm. Pure Appl. Math.*, vol. 58, No. 11, 1544-1585, 2005.
- W. E. <u>Analysis of the heterogeneous multiscale method for ordinary differential</u> equations. *Comm. Math. Sci.*, vol. 1, no. 3, pp. 423-436, 2003.
- W. E and B. Engquist. <u>The heterogeneous multiscale methods</u>. *Comm. Math. Sci.*, vol. 1, no. 1, pp. 87-132, 2003.
- W. E and B. Engquist. <u>Multiscale modeling and computation</u>. *Notices Amer. Math. Soc.*, vol. 50, no. 9, pp. 1062-1070, 2003.
- W. E, D. Liu and E. Vanden-Eijnden. <u>Nested stochastic simulation algorithms for</u> <u>chemical kinetic systems with multiple time scales</u>. *J. Comput. Phys.*, vol. 221, no. 1, pp. 158-180, 2007.
- W. E, D. Liu and E. Vanden-Eijnden. <u>Nested stochastic simulation algorithm for</u> <u>chemical kinetic systems with disparate rates</u>. J. Chem. Phys., vo. 123, 194107, 2005.

Soft condensed matter physics

We have developed the first general nonlinear model for smectic A liquid crystals and used it to study the interesting filamentary structures arising in isotropic-smectic phase transition. We have also developed models for the dynamics of membranes and polymer phase separations that are consistent with thermodynamics. In addition, we have developed models for general inhomogeneous liquid crystal polymer systems using the one-particle probability distribution function as the order parameter.

- D. Hu, P. Zhang and W. E. <u>Continuum theory of a moving membrane</u>. *Phys. Rev. E*, vol. 75, no. 4, 041605, 2007.
- Q. Wang, W. E, C. Liu, P.-W. Zhang. <u>Kinetic theory for flows of nonhomogeneous</u> <u>rodlike liquid crystalline polymers with a nonlocal intermolecular potential</u>. *Phys. Rev. E*, vol. 65, no. 5, 051504, 2002.
- W. E and P. Zhang. <u>A molecular kinetic theory of inhomogeneous liquid crystal flow</u>

- and the small Deborah number limit. *Methods Appl Anal.*, vol 13, no. 2, pp. 181-198, 2006.
- D. Zhou, P. Zhang and W. E. <u>Modified models of polymer phase separation</u>. *Phys. Rev. E*, vol. 73, 061801, 2006.
- C.B. Muratov and W. E. <u>Theory of phase separation kinetics in polymer-liquid crystal</u> <u>systems</u>. *J. Chem. Phys.*, vol. 116, no. 11, pp. 4723-4734, 2002.
- W. E and P. Palffy-Muhoray. <u>Dynamics of filaments during the isotropic-smectic A</u> <u>phase transition</u>. *J. Nonlin. Sci.*, vol. 9, no. 4, pp. 417-437, 1999.
- W. E. Nonlinear continuum theory of smectic-A liquid crystals. Arch. Rat. Mech. Anal., vol. 137, no. 2, pp. 159-175, 1997.
- W. E and P. Palffy-Muhoray. <u>Phase separation in incompressible systems</u>. *Phys. Rev. E*, vol. 55, no. 4, pp. R3844-R3846 , 1997.
- F. Otto and W. E. <u>Thermodynamically driven incompressible fluid mixtures</u>. J. Chem. *Phys.*, vol. 107, no. 23, pp. 10177-10184, 1997.

Generational fluid dynamics

Jian-Guo Liu and I addressed long time controversies in vorticity boundary conditions and the numerical boundary layers for the projection method.

A posteriori error estimates

In my master degree thesis completed in 1985 under the supervision of Prof. Huang Hongci, I established some of the earliest results on a posteriori error estimates for finite element methods. I introduced the Clement interpolation technique, and proved upper and lower bounds for local error estimators.

- W. E, M. Mu and H.C. Huang. <u>A posteriori error estimates in finite element methods</u>. *Chinese Quart. J. Math.*, (Chinese) vol. 3, no. 1, pp. 97-107, 1988.
- H.C. Huang and W. E. <u>A posteriori error estimates for finite element methods for one-dimensional boundary value problems</u>. *Chinese Quart. J. Math.*, (Chinese) vol. 2, no. 1, pp. 43-47, 1987.

Weak KAM theory

Under the influence of Jurgen Moser, I independently (of Fathi) developed the weak KAM theory. This was one of the first application of PDE methods to the study of dynamical systems. The most interesting aspect is to study the implication of weak solutions of the Hamilton-Jacobi equation to Hamiltonian systems. This gives an alternative (and much simplified) viewpoint for the Aubry-Mather theory.

• W. E. <u>Aubry-Mather theory and periodic solutions of the forced Burgers equation</u>. *Comm. Pure Appl. Math.*, vol. 52, no. 7, pp. 811-828, 1999.

I Numerical algorithms for Kohn-Sham density functional theory

• L. Lin, C. Yang, J. Lu, L. Ying and W. E, "<u>A fast parallel algorithm for selected</u> inversion of structured sparse matrix with application to 2D electronic structure calculations," *SIAM J. Sci. Computing*, vol. 33, 1329-1351, 2011.

- W. E, T. Li and J. Lu, "Localized basis of eigen-subspaces," *Proc. Natl. Acad. Sci.* USA, vol. 109, pp. 1273-1278, 2010.
- L. Lin, C. Yang, J. C. Meza, L. Ying and W. E, "SelInv An algorithms for selected inversion of a sparse symmetric matrix," *ACM Transactions on Mathematical Software*, vol. 37, no. 4, pp. 40:1-40:19, 2011.
- L. Lin, C. Yang, J. Lu, L. Ying and W. E, "A fast parallel algorithm for selected inversion of structured sparse matrices with application to 2D electronic structure calculation," *Lawrence Berkeley National Laboratory*. LBNL Paper LBNL-2677E. Retrieved from: <u>http://escholarship.org/uc/item/46q6w084</u>, 2010.
- L. Lin, J. Lu, L. Ying and W. E, "<u>Pole-based approximation of the Fermi-Dirac</u> <u>function</u>," *Chin. Ann. Math.*, vol. 30B, pp. 729-742, 2009.
- L. Lin, J. Lu, L. Ying, R. Car and W. E, "<u>Fast algorithm for extracting the diagonal of the inverse matrix with application to the electronic structure analysis of metallic systems,</u>" *Comm. Math. Sci.*, vol. 7, pp. 755-777, 2009.
- L. Lin, J. Lu, R. Car and W. E, "<u>Multipole representation of the Fermi operator with</u> application to electronic structure analysis of metallic systems," *Phys. Rev. B*, vol. 79, no. 11, pp. 115133-115113-10, 2009.
- W. Gao and W. E, "<u>Orbital minimization with localization</u>," *Discrete and Continuous Dynamical Systems*, vol. 23, no. 1-2, pp. 249-264, 2009.

Other topics I have made contributions to include: Onsager's conjecture on the energy conservation for weak solutions of the 3D Euler's equation, homogenization and two-scale convergence, singularity formation in solutions of Prandtl's equation, Ginzburg-Landau vortices, micromagnetics and the Landau-Lifshitz equation, stochastic resonance, etc.

- <u>String Method Webpage</u>
- <u>HMM webpage</u>

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Analysis and algorithms for multiscale problems

■ Mathematical theory of solids at the atomic and macroscopic scales

The main objective is to develop a rigorous mathematical theory for solids. This requires understanding models of solids at the electronic, atomistic and continuum level, as well as the relation between these models. Problems of interest include: (1). The crystallization problem: Why solids take the form of crystal lattice at zero temperature? (2). The Cauchy-Born rule, which serves as a connection between atomistic and continuum models of solids.

- W. E and D. Li. <u>On the crystallization of 2d hexagonal lattice</u>. *Comm. Math. Phys.*, submitted.
- W. E and J.F. Lu. <u>The continuum limit and QM-continuum approximation of quantum</u> <u>mechanical models of solids</u>. *Comm. Math. Sci.*, vol. 5, no. 3, pp. 679-696, 2007.
- W. E and J.F. Lu. <u>The elastic continuum limit of the tight binding model</u>. *Chinese Ann. Math. Ser. B*, vol. 28, no. 6, pp. 665-676, 2007.

- W. E and P.B. Ming. <u>Cauchy-Born rule and the stability of crystalline solids: Dynamic problems</u>. *Acta Math. Appl. Sin. Engl. Ser.*, vol. 23, no. 4, pp. 529-550, 2007.
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Electronic structure, density functional theory

The main objective is to understand the mathematical foundation of electronic structure analysis, to develop and analysis efficient algorithms.

• W. E and J.F. Lu. <u>The continuum limit and QM-continuum approximation of quantum</u> <u>mechanical models of solids</u>. *Comm. Math. Sci.*, vol. 5, no. 3, pp. 679-696, 2007.

General issues in multiscale modeling

- S. Chen, W. E, Y. Liu and C.-W. Shu. <u>A discontinuous Galerkin implementation of a domain decomposition method for kinetic-hydrodynamic coupling multiscale problems in gas dynamics and device simulations</u>. *J. Comput. Phys.*, vol. 225, no. 2, pp. 1314-1330, 2007.
- W. E, B. Engquist, X. Li, W. Ren and E. Vanden-Eijnden. <u>Heterogeneous multiscale</u> <u>methods: A review</u>. *Comm. Comput. Phys.*, vol. 2, no. 3, pp. 367-450, 2007.
- W. E and J.F. Lu. <u>Seamless multiscale modeling via dynamics on fiber bundles</u>. *Comm. Math. Sci.*, vol. 5, no. 3, pp. 649-663, 2007.
- X. Yue and W. E. <u>The local micro-scale problem in the multiscale modelling of</u> <u>strongly heterogeneous media: Effect of boundary conditions and cell size</u>. *J. Comput. Phys.*, vol. 222, no. 2, pp. 556-572, 2007.
- S. Chen, W. E and C.-W. Shu. <u>The heterogeneous multiscale method based on the discontinuous galerkin method for hyperbolic and parabolic problems</u>. *Multiscale Model. Simul.*, vol. 3, no. 4, pp. 871-894, 2005.
- W. E and B. Engquist. <u>The heterogeneous multi-scale method for homogenization</u> <u>problems</u>. Multiscale Methods in Sci. and Eng., pp. 89-110. *Lect. Notes in Comput. Sci. Eng.*, vol. 44, Springer, Berlin, 2005.
- W. E and P.B. Ming. Analysis of the local quasicontinuum method. <u>Frontiers and</u> <u>Prospects of Contemp. Appl. Math.</u>, pp. 18-32. *Contemporary Appl. Math.*, vol. 6, Higher Education Press, Beijing, 2005.
- W. E, P.B. Ming and P.-W. Zhang. <u>Analysis of the heterogeneous multiscale method</u> for elliptic homogenization problems. *J. Amer. Math. Soc.*, vol. 18, no. 1, pp. 121-156, 2005.
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- W. E and B. Engquist. The heterogeneous multiscale method. *Second Intl. Congress of Chinese Mathematicians. Proc. of ICCM2001*, Taipei, pp. 57-74, New Studies in Advanced Mathematics, vol. 4, Intl. Press, 2004.
- W. E, X. Li, E. Vanden-Eijnden. Some recent progress in multiscale modeling.

- Multiscale Modelling and Simulation, pp. 3-22. Lect. Notes Comput. Sci. Eng., vol. 39, Springer, Berlin, 2004.
- W. E and X.-T. Li. <u>Analysis of the heterogeneous multiscale method for gas dynamics</u>. *Methods Appl. Anal.*, vol. 11, no. 4, pp. 557-572, 2004.
- W. E and P.B. Ming. <u>Analysis of multiscale methods</u>. J. Comput. Math., vol. 22, no. 2, pp. 210-219, 2004.
- W. E nd X. Yue. <u>Heterogeneous multiscale method for locally self-similar problems</u>. *Comm. Math. Sci.*, vol. 2, no. 1, pp. 137-144, 2004.
- W. E. <u>Analysis of the heterogeneous multiscale method for ordinary differential</u> equations. *Comm. Math. Sci.*, vol. 1, no. 3, pp. 423-436, 2003.
- A. Abdulle and W. E. <u>Finite difference heterogeneous multi-scale method for</u> <u>homogenization problems</u>. J. Comput. Phys., vol. 191, no. 1 pp. 18-39, 2003.
- L.-T. Cheng and W. E. The heterogeneous multi-scale method for interface dynamics. <u>Recent advances in scientific computing and partial differential equations</u> (Hong Kong, 2002), pp. 43-53, *Contemp. Math.*, vol. 330, Amer. Math. Soc., Providence, RI, 2003.
- W. E and B. Engquist. <u>The heterogeneous multiscale methods</u>. *Comm. Math. Sci.*, vol. 1, no. 1, pp. 87-132, 2003.
- W. E and B. Engquist. <u>Multiscale modeling and computation</u>. *Notices Amer. Math. Soc.*, vol. 50, no. 9, pp. 1062-1070, 2003.
- W. E, B. Engquist and Z. Huang. <u>Heterogeneous multiscale method: A general</u> <u>methodology for multiscale modeling</u>. *Phys. Rev. B*, vol. 67, no. 9, 092101, 2003.

■ Problems with multiple time scales

- T. Li, A. Abdulle and W. E. <u>Effectiveness of implicit methods for stiff stochastic</u> <u>differential equations</u>. *Comm. Comput. Phys.*, vol. 3, no. 2, pp. 295-307, 2008.
- W. E, D. Liu and E. Vanden-Eijnden. <u>Nested stochastic simulation algorithms for</u> <u>chemical kinetic systems with multiple time scales</u>. *J. Comput. Phys.*, vol. 221, no. 1, pp. 158-180, 2007.
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- W. E, D. Liu and E. Vanden-Eijnden. <u>Analysis of multiscale methods for stochastic</u> <u>differential equations</u>. *Comm. Pure Appl. Math.*, vol. 58, No. 11, 1544-1585, 2005.
- W. E and X.-T. Li. <u>Analysis of the heterogeneous multiscale method for gas dynamics</u>. *Methods Appl. Anal.*, vol. 11, no. 4, pp. 557-572, 2004.

Stochastic chemical kinetic systems

- W. E, D. Liu and E. Vanden-Eijnden. <u>Nested stochastic simulation algorithms for</u> <u>chemical kinetic systems with multiple time scales</u>. *J. Comput. Phys.*, vol. 221, no. 1, pp. 158-180, 2007.
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■ Multiscale modeling of solids

- W. Guo, T. P. Schulze and W. E. Simulation of impurity diffusion in a strained nanowire using off-lattice KMC. *Comm. Comput. Phys.*, vol. 2, no. 1, pp. 164-176, 2007.
- X. Li and W. E. <u>Variational boundary conditions for molecular dynamics simulations</u> of crystalline solids at finite temperature: Treatment of the thermal bath. *Phys. Rev. B*, vol 76, no. 10, 104107, 2007.
- J.Z. Yang and W. E. <u>Generalized Cauchy-Born rules for elastic deformation of sheets</u>, <u>plates</u>, <u>and rods</u>: <u>Derivation of continuum models from atomistic models</u>. *Phys. Rev. B*, vol. 74, no 18, 184110, 2006.
- Y. Xiang, H. Wei, P.B. Ming and W. E. <u>A generalized Peierls?Nabarro model for</u> <u>curved dislocations and core structures of dislocation loops in Al and Cu</u>. *Acta Materialia*, in press, available online 14 January 2008.
- W. E, J.-F. Lu, J.Z. Yang. <u>Uniform accuracy of the quasicontinuum method</u>. *Phys. Rev. B*, vol. 74, 214115, 2006.
- X.-T. Li and W. E. Variational boundary conditions for molecular dynamics simulation of solids at low temperature. *Comm. Comput. Phys.*, vol. 1, No. 1, 135-175, 2006.
- N. Choly, G. Lu, W. E and E. Kaxiras. <u>Multiscale simulations in simple metals: A</u> <u>density-functional based methodology</u>. *Phys. Rev. B*, vol. 71, 094101, 2005.
- X.-T. Li and W. E. <u>Multiscale modeling of the dynamics of solids at finite temperature</u>. *J. Mech. Phys. Solids*, vol. 53, 1650-1685, 2005.
- W. E and X.-T. Li. <u>Multiscale modeling of crystalline solids</u>. *Handbook of Materials Modeling*, Part A, edited by S. Yip., pp. 1491-1506, Springer Netherlands, 2005.
- Y. Xiang and W. E. <u>Misfit elastic energy and a continuum model for epitaxial growth</u> with elasticity on vicinal surfaces. *Phys. Rev. B*, vol. 69, no. 3, 035409, 2004.
- Y. Xiang, D.J. Srolovitz, L.-T. Cheng and W. E. <u>Level set simulations of dislocation-particle bypass mechanisms</u>. *Acta Materialia*, vol. 52, no. 7, pp. 1745-1760, 2004.
- Y. Xiang, L.-T. Cheng, D.J. Srolovitz and W. E. <u>A level set method for dislocation</u> <u>dynamics</u>. *Acta Materialia*, vol. 51, no. 18, pp. 5499-5518, 2003.
- T. Schulze, P. Smereka and W. E. <u>Coupling kinetic Monte-Carlo and continuum</u> <u>models with application to epitaxial growth</u>. *J. Comput. Phys.*, vol 189, no. 1, pp. 197-211, 2003.
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- W. E and Z. Huang. <u>A dynamic atomistic-continuum method for the simulation of crystalline materials</u>. *J. Comput. Phys.*, vol. 182, no. 1, pp. 234-261, 2002.
- W. E and Z. Huang. <u>Matching conditions in atomistic-continuum modeling of</u> <u>materials</u>. *Phys. Rev. Lett.*, vol. 87, no. 13, 135501, 2001.
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- <u>HMM papers</u>
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 - Analysis and modeling of stochastic problems
 - Other topics
 - Selected Review Papers