

## VIKRAM GAVINI

Department of Mechanical Engineering  
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University of Michigan  
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### EDUCATION

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- **Doctor of Philosophy (Ph.D)** June 2004 - May 2007  
California Institute of Technology  
Mechanical Engineering
- **Master of Science (M.S.)** Sept 2003 - June 2004  
California Institute of Technology  
Applied Mechanics
- **Bachelor of Technology (B.Tech.)** July 1999 - May 2003  
Indian Institute of Technology, Madras  
Mechanical Engineering

### PROFESSIONAL APPOINTMENTS

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- **Associate Professor** September 2013 - Present  
Department of Mechanical Engineering  
University of Michigan
- **Associate Professor** September 2015 - Present  
Department of Materials Science and Engineering  
University of Michigan
- **Visiting Associate** January 2015 - June 2015  
Department of Mechanical and Civil Engineering  
California Institute of Technology
- **Visiting Scientist** 2012/2013/2014  
Max Planck Institute for Mathematics in Sciences, Leipzig, Germany
- **Visiting Scientist** 2012/2013  
Institute for Mechanics  
University of Stuttgart, Germany
- **Assistant Professor** September 2007 - August 2013  
Department of Mechanical Engineering  
University of Michigan

## HONORS AND AWARDS

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- *Finalist, 2019 Gordon Bell prize* (final decision to be made at SC19), awarded by the Association of Computing Machinery (ACM).
- *Gallagher Young Investigator Award, 2015*, awarded by the United States Association for Computational Mechanics (USACM).
- *Humboldt Research Fellowship (Experienced Researcher), 2012-2014*, awarded by the Alexander von Humboldt foundation, Germany.
- *Young Investigator Award, 2103*, Air Force office of Scientific Research.
- *NSF CAREER Award, 2011*, National Science Foundation.
- *Robert J. Melosh Medal, 2007*, awarded by a consortium including Duke University, ETH Zürich, Elsevier and International Association for Computational Mechanics.
- *Allan Acosta endowed Fellowship, 2003*, California Institute of Technology.
- *Institute Silver Medal, 2003*, Indian Institute of Technology.

## SCIENTIFIC PUBLICATIONS AND TALKS

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- **Books/Book Chapters**

1. Radhakrishnan, B. G., Gavini, V., Electronic structure calculations at macroscopic scales using orbital-free DFT, In Wang, Y.A., Wesolowski, T. (Ed.) Recent Advances in Orbital-free DFT, *World Scientific*, Singapore (2013). (*Invited Book Chapter*)

- **Journal Publications**

1. Das, S., Motamarri, P., Gavini, V., Turcksin, B., Li, Y.W., Leback, B., Fast, scalable & accurate finite-element based first-principles calculations using mixed precision computing: 40 PFLOPS simulation of a metallic dislocation system, The International Conference for High Performance Computing Networking, Storage, and Analysis, to appear (2019) (*ACM Gordon Bell Prize*)<sup>1</sup>.
2. Kanungo, B., Zimmerman, P., Gavini, V., Exact exchange-correlation potentials from ground-state electron densities, *revision submitted to Nature Communications* (2019).
3. Motamarri, P., Das, S. Rudraraju, S. Davydov, D., Gavini, V., DFT-FE: A massively parallel adaptive finite-element code for large-scale density functional theory calculations, *revision submitted to Comput. Phys. Commun.* (2019). arXiv: <https://arxiv.org/abs/1903.10959>
4. Ghosh, K., He, M., Gavini, V., Galli, G., All-electron density functional calculations for electron and nuclear spin interactions in molecules and solids, *Phys. Rev. Mater.*, 3 043801 (2019).

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<sup>1</sup>Selected as finalist; final decision will be made at SC19

5. Kanungo, B., Gavini, V., Real-time time-dependent density functional theory using higher order finite element methods, *submitted to Phys. Rev. B* (2019). arXiv: <https://arxiv.org/abs/1810.13130>.
6. Aagesen, L.K., Adams, J.F., Allison, J.E., Andrews, B., Araullo-Peters, V., Berman, T., Chen, Z., Daly, S., Das, S., Dewitt, S., Ganesan, S., Garikipati, K., Gavini, V., Githens, A., Hedstrom, M., Huang, Z., Jagadish, H.V., Jones, J.W., Luce, J., Marquis, E.A., Misra, A., Montiel, D., Motamarri, P., Murphy, A.D., Natrajan, A.R., Panwar, S., Puchala, B., Qi, L., Rudraraju, S., Sagiya, K., Soloman, E.L.S, Sundararaghavan, V., Tarcea, G., Teichert, G.H., Thomas, J.C., Thorton, K., Van der Ven, A., Wang, Z., Weymouth, T., Yang, C., PRISMS: An integrated, open-source framework for accelerating predictive structural materials science, *JOM - J. Min. Met. Mat. S.* 70, 2298-2314 (2018).
7. Motamarri, P., Gavini, V., Configurational forces in electronic structure calculations using Kohn-Sham density functional theory, *Phys. Rev. B* 97, 165132 (2018).
8. Das, S., Gavini, V., Electronic structure study of screw dislocation core energetics in Aluminum and core energetics informed forces in a dislocation aggregate, *J. Mech. Phys. Solids* 104, 115-143 (2017).
9. Kanungo, B., Gavini, V., Large-scale all-electron density functional theory calculations using an enriched finite element basis, *Phys. Rev. B* 95, 035112 (2017).
10. Motamarri, P., Bhattacharya, K., Ortiz, M., Gavini, V., Spectrum-splitting approach for Fermi-operator expansion in all-electron Kohn-Sham DFT calculations, *Phys. Rev. B* 95, 035111 (2017).
11. Radhakrishnan, B., Gavini, V., Orbital-free DFT study of the energetics of vacancy clustering and prismatic dislocation loop nucleation in aluminum, *Philosophical Magazine* 96, 2468-2487 (2016).
12. Motamarri, P., Blesgen, T., Gavini, V., Tucker-tensor algorithm for large-scale Kohn-Sham density functional theory calculations, *Physical Review B* 93, 125104 (2016).
13. Das, S., Iyer, M., Gavini, V., Real-space formulation of orbital-free density functional theory using finite-element discretization: The case for Al, Mg, and Al-Mg intermetallics, *Physical Review B* 92, 014104 (2015).
14. Radhakrishnan, B., Iyer, M., Gavini, V., Electronic structure study of edge dislocation in aluminum and the role of volumetric deformations on its energetics, *Journal of the Mechanics and Physics of Solids* 76, 260-275 (2015).
15. Motamarri, P., Gavini, V., A subquadratic-scaling subspace projection technique for Kohn-Sham DFT calculations using spectral finite-element discretization, *Physical Review B* 90, 115127 (2014).
16. Iyer, M., Pollock, T.M., Gavini, V., Energetics and nucleation of point defects in aluminum under extreme tensile hydrostatic stresses *Physical Review B* 89, 014108 (2014).
17. Balachandran, J., Reddy, P., Dunietz, B., Gavini, V., End-group influence on frontier molecular reorganization and thermoelectric properties of molecular junctions, *Journal of Physical Chemistry Letters* 4, 3825-3833 (2013).
18. Motamarri, P., Nowak, M.R., Leiter, K., Knap, J., Gavini, V., Higher-order adaptive finite-element methods for Kohn-Sham density functional theory, *Journal of Computational Physics* 253, 308-343 (2013).
19. Pisutha-Arnond, N., Chan, V. W. L., Iyer, M., Gavini, V., Thornton, K., Modeling classical density functional theory and phase-field crystal method using rational function to describe two-body direct correlation function, *Physical Review E* 87, 013313 (2013).

20. Tan, A., Balachandran, J., Dunietz, B., Gavini, V., Reddy, P., Length dependence of frontier orbital alignment in aromatic molecular junctions, *Applied Physics Letters* 101, 243107 (2012) .
21. Balachandran, J., Reddy, P., Dunietz, B., Gavini, V., End-group induced charge transfer in molecular junctions: Effect on electronic structure and thermopower, *Journal of Physical Chemistry Letters* 3, 1962-1967 (2012).
22. Motamarri, P., Iyer, M., Knap, J., Gavini, V., Higher-order adaptive finite-element methods for orbital-free density functional theory, *Journal of Computational Physics* 231, 6596-6621 (2012).
23. Blesgen, T., Gavini, V., Khoromskaia, V., Approximation of the electron density of aluminum clusters in tensor-product format, *Journal of Computational Physics* 231, 2551-2564 (2012) .
24. Tan, A., Balachandran, J., Sadat, S., Gavini, V., Dunietz, B., Jang, S.-Y., Reddy, P., Effect of length and contact chemistry on the electronic structure and thermoelectric properties of molecular junctions, *Journal of American Chemical Society Communications* 133, 8838-8841 (2011).
25. Gavini, V., Liu, L., An analysis of the field theoretic approach to the quasi-continuum method, *Journal of the Mechanics and Physics of Solids* 59, 1536-1551 (2011) .
26. Iyer, M., Gavini, V., A field theoretical approach to the quasi-continuum method, *Journal of the Mechanics and Physics of Solids* 59, 1506-1535 (2011).
27. Radhakrishnan, B.G., Gavini, V., Effect of cell size on the energetics of vacancies in aluminum studied via orbital-free density functional theory, *Physical Review B* 82, 094117 (2010) .
28. Suryanarayana, P., Gavini, V., Blesgen, T., Ortiz, M., Bhattacharya, K., Non periodic finite element formulation of Kohn Sham Density functional theory, *Journal of the Mechanics and Physics of Solids* 58, 256-280 (2010).
29. Gavini, V., Role of the defect-core in energetics of vacancies, *Proceedings of the Royal Society of London, Series A* 465, 3239-3266 (2009).
30. Gavini, V., Role of macroscopic deformation in energetics of vacancies in aluminum, *Physical Review Letters* 101, 205503 (2008). (**Cover Article**)
31. Gavini, V., Bhattacharya, K., Ortiz, M., Vacancy clustering and prismatic dislocation loop formation in aluminum, *Physical Review B* 76, 180101(R) (2007).
32. Gavini, V., Bhattacharya, K., Ortiz, M., Quasi-continuum orbital-free density-functional theory: A route to multi-million atom non-periodic DFT calculation, *Journal of the Mechanics and Physics of Solids* 55, 697-718 (2007).
33. Gavini, V., Knap, J., Bhattacharya, K., Ortiz, M., Non-periodic finite-element formulation of orbital-free density-functional theory, *Journal of the Mechanics and Physics of Solids* 55, 669-696 (2007).
34. Vikram, G., Babu, N.R., Modelling and analysis of abrasive water jet cut surface topography, *International Journal of Machine Tools and Manufacturing* 42, 1345-1354 (2002).

- **Invited Talks in Seminar, Conferences and Workshops**

*Department Seminar*, Brown University, 2019.

*Applied Mathematics Colloquim*, Penn State University, 2019.

*IMA workshop on Multiscale Strategies*, University of Minnesota, 2018.

*Colloquium on Micromechanics of Defects in Crystalline Solids and Metals*, Sevilla (Spain), 2018.

*Scientific Computing Seminar*, University of Warwick, Coventry (United Kingdom), 2018.

*Nonlinear Mechanics Seminar*, University of Bath, Bath (United Kingdom), 2018.

*Invited talk*, 2017 Materials Research Society Meeting, Boston, 2017.

*Keynote talk*, 14th U.S. National Congress on Computational Mechanics, Montreal, 2017.

*Dislocations 2016*, Purdue University, 2016.

*2016 Annual TMS meeting*, Nashville, 2016.

*Mathematical Aspects of Materials Science*, Society of Industrial and Applied Mathematics meeting, Philadelphia, 2016.

*2nd Schoental meeting on dislocation based plasticity*, Schoental (Germany), 2016.

*26th Biennial Numerical Analysis Conference*, University of Starthclyde, Glasgow (Scotland, UK), 2015.

*Department Seminar*, Materials Science and Engineering Seminar, University of Michigan, 2015.

*52nd Society of Natural Philosophy Meeting*, Universidade Federal do Rio de Janeiro, Rio de Janeiro (Brazil), 2014.

*Workshop on multi-scale modeling and computation of nano-optics*, Michigan State University, Lansing, 2014.

*IUTAM Symposium on Innovative numerical approaches for materials and structures in multi-field and multi-scale problems*, Schnellenberg (Germany), 2014.

*Oberseminar*, Max-Planck Institute for Mathematics in Sciences, Leipzig (Germany), 2014.

*IUTAM Symposium on Microstructure of Defect in Solids*, Sevilla (Spain), 2014.

*Frontiers Seminar*, Qatar Energy & Environment Research Institute, Doha (Qatar), 2014.

*Applied and Interdisciplinary Mathematics seminar*, University of Michigan, 2014.

*NSF Symposium on Defect Mechanics*, University of California San Diego, San Diego, 2014.

*Seminar*, Institute of Mechanics, Technische Universität Dortmund, Dortmund (Germany), 2013.

*Workshop on Mathematics and Mechanics in the search for new materials*, Banff (Canada), 2013.

*Seminar*, Max-Planck Institute for Solid State Research, Stuttgart (Germany), 2013.

*Department Seminar*, Mechanical & Aerospace Engineering, University of Minnesota, Minneapolis, 2013.

*Invited presentation*, Symposium on Concurrent Multi-scale Modeling, American Physical Meeting, Baltimore, 2013.

*SimTech Colloquium*, Universität Stuttgart, Stuttgart (Germany), 2012.

*Analysis Seminar*, Technische Universität München, München (Germany), 2012.

*CECAM Workshop on Orbital-free DFT*, Paris (France), 2012.

*Department Seminar*, Materials Department, University of California Santa Barbara, Santa Barbara, 2012.

*Workshop on Materials Defects*, Institute for Pure and Applied Mathematics, University of California Los Angeles, Los Angeles, California, 2012.

*Materials Genome: Simulations, Synthesis, Characterization and Manufacturing*, USC-DOE Materials Genome Conference, Los Angeles, California, 2012.

*Workshop on Averaging Methods for Multiscale Phenomena in Engineering Materials*, Carnegie Mellon University, Pittsburgh, Pennsylvania, 2012.

*Materials and Mechanical Engineering Seminar*, University of California Santa Barbara, Santa Barbara, California, 2012.

*Center for Multiscale Modeling of Engineering Materials (CM2EM) Seminar*, Carnegie Mellon University, Pittsburgh, Pennsylvania, 2011.

*Mechanical Engineering Seminar*, University of Houston, Houston, 2011.

*IEA Fusion Modeling Workshop*, Lawrence Livermore National Laboratories, Livermore, 2011.

*Density Functional Theory: Fundamentals and Applications in Condensed Matter Physics*, BIRS workshop, Banff, 2011.

*Recent Advances in Orbital-free DFT*, Pacificchem Meeting, Honolulu, 2010.

*Drucker Medal Symposium*, ASME International Mechanical Engineering Congress and Exposition, Vancouver, 2010.

*Mathematical Aspects of Materials Science*, Society of Industrial and Applied Mathematics meeting, Philadelphia, 2010.

*Institute of Applied Mechanics Seminar*, University of Stuttgart, Stuttgart (Germany), 2010.

*NSF Dislocation Dynamics Symposium*, University of California, San Diego, 2010.

*Numerics Seminar*, Max-Planck Institute for Mathematics in Sciences, Leipzig (Germany), 2009.

*Nanotechnology Seminar*, Purdue University, 2009.

*Applied Mechanics Colloquium*, Harvard University, 2008.

*Army Research Labs Seminar*, ARL, Aberdeen Proving Grounds, 2008.

*NSF Dislocation Dynamics Symposium*, University of California, San Diego, 2008.

*Density Functional Theory Meeting*, Princeton University, 2007.

*Applied and Interdisciplinary Mathematics seminar*, University of Michigan, 2007.

*Mechanical Engineering Seminar*, University of Michigan, 2007.

*Mechanical Engineering Seminar*, University of Illinois, Urbana Champaign, 2007.

*Mechanical Engineering Seminar*, Johns Hopkins University, 2007.

## PROFESSIONAL ACTIVITIES

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- *Leading* the development of open-source codes for large-scale real-space electronic structure calculations. Released the beta version of DFT-FE: A massively parallel real-space DFT code using finite-elements, in September 2018 (<https://github.com/dftfeDevelopers/dftfe>). The code, to date, has  $\sim 160$  unique clones.
- *Reviewer* for articles in the following journals: Science, Proceedings of the National Academy of Sciences, Nano Letters, Journal of the American Chemical Society, Journal of Mechanics and Physics of Solids, Physical Review (Letters, B, E, Applied), Journal of Computational Physics, Journal of Physics: Condensed Matter, SIAM Multi-scale Modeling of Materials, Acta Materialia, Nonlinearity, International Journal of Solids and Structures, International Journal of Fracture, Extreme Mechanics Letters.
- *Lead Organizer*, USACM Thematic Workshop on “Recent Advances in Computational Methods for Nanoscale Phenomena”, with Prof. Dennis Kochmann (Caltech), Prof. Greg Wagner (Northwestern University) and Dr. Jonathan Zimmerman (Sandia National Laboratory), in Ann Arbor August 28-31, 2016.
- *Chair*, USACM Technical Trust area on Nanotechnology and Lower Scale Phenomena, 2015-present.
- *Guest Editor* for Journal of Materials Research, special issue on “Advanced Atomistic Algorithms in Materials Science” (2017) (along with Dr. Enrique Matrinez, Dr. Danny Perez and Prof. Steven Kenny).
- *Guest Editor* for The International Journal for Multi-scale Computational Engineering, special issue on “Multi-scale Computation and Modeling of Defects in Materials” (2012).
- *Organizer*, symposium on “Modeling at the Intersection of First Principles Methods, Mechanics and Mathematics”, with Prof. P. Suryanarayana (G. Tech.) and Prof. Amartya Banerjee (UCLA), in 15th U.S. National Congress on Computational Mechanics, Austin, July 28-August 1, 2019.
- *Organizer*, symposium on “Data-driven Modeling in Multi-scale Materials Physics”, with Prof. Krishna Garikipati (U. Mich), Dr. Jaroslaw Knap (Army Research Laboratory), Dr. Reese Jones (Sandia National Laboratory) in SIAM Mathematical Aspects of Materials Science, Portland, July 9-13, 2018.
- *Organizer*, symposium on “Modeling at the Intersection of First Principles Methods, Mechanics and Mathematics”, with Prof. P. Suryanarayana (G. Tech.), in 14th U.S. National Congress on Computational Mechanics, Montreal, Canada, July 17-20, 2017.
- *Organizer*, symposium on “Recent Progress in Multi-scale Modeling at the Intersection of Ab-initio Methods, Mechanics and Mathematics”, with Prof. P. Suryanarayana (G. Tech.) and Dr. Amartya Banerjee (LLNL), in 13th U.S. National Congress on Computational Mechanics, San Diego, CA, July 26-30, 2015.
- *Organizer*, symposium on “Ab-Initio Methods in the Mechanics of Materials and Structures”, with Prof. P. Suryanarayana (G. Tech.), in 2014 U.S. National Congress of Theoretical and Applied Mechanics, Lansing, MI, June 15-20, 2014.

- *Organizer*, symposium on “Advances in the study of defects through Atomistic/Continuum coupling methods”, with Professor P. Suryanarayana (G. Tech.), in 2012 Society of Engineering Sciences annual technical meeting, Atlanta, GA, Oct. 10-12, 2012.
- *Organizer*, symposium on “Recent Advances in the Quasicontinuum Method and other Atomistic/Continuum coupling Techniques, and Studies of Microstructural Defects in Materials”, with Dr. J. Marian, Prof. C.-S. Chen, Prof. E. Tadmor, Prof. R. Miller, Prof. Y. Kulkarni, Prof. K. Dayal, in the 11th U.S. National Congress on Computational Mechanics, Minnesota, MN, July 25-29, 2011.
- *Organizer*, symposium on “Multi-scale modeling of defects in materials”, with Prof. K. Dayal (CMU) and Prof. Y. Kulkarni (U. Houston), in the 10th U.S. National Congress on Computational Mechanics, Columbus, OH, July 16-19, 2009.
- *Organizer*, symposium on “Multi-scale computation and modeling of defects in materials”, with Prof. K. Dayal (CMU) and Prof. C. Maloney (CMU), in the 2009 ASCE-ASME-SES conference on mechanics and materials, Blacksburg, VA, June 24-27, 2009.
- *Organizer*, symposium on “Multi-scale models and techniques for defects in solids”, with Prof. K. Dayal (CMU), in the 2008 SIAM conference on mathematical aspects of materials science, Philadelphia, PA, May 11-14, 2008.
- *Organizer*, symposium on “Multi-scale modeling and defects in solids”, with Prof. K. Dayal (CMU), in the 45th Annual technical meeting of the Society of Engineering Sciences, Urbana, IL, Oct. 12-15, 2008.
- *Organizer*, symposium on “Defects in materials: Theory and applications”, with Prof. K. Dayal (CMU), in the 2008 ASME International Mechanical Engineering Congress & Exposition, Boston, MA, Oct. 31-Nov 6, 2008.
- *Panelist*, NSF Panel review 2008, 2010, 2011, 2012, 2014, 2016 (Division of Engineering).
- *Panelist*, XSEDE Research Allocation Committee, June 2012–Sept 2014.
- *Technical program committee*, 45th Annual technical meeting of the Society of Engineering Sciences, Urbana, IL, Oct. 12-15, 2008.
- *Reviewer* of proposals for the following federal agencies: NSF Division of Materials Research, NSF Division of Mathematical Sciences, Department of Energy (BES), Army Research Office, Air Force Office of Scientific Research.
- *Coordinator* at University of Michigan for Midwest Mechanics Seminar Series, 2008-2013.
- *Steering Committee* for Michigan Institute of Computational Discovery and Engineering, 2013-2016.
- *Management Committee* for Michigan Institute of Computational Discovery and Engineering, 2016-present.
- *Advisory Board* for Advanced Research Computing at University of Michigan, 2014, 2017-present.
- *CoE Mathematics Curriculum Review Committee* for reviewing the mathematics curriculum for CoE undergraduate students, 2018-2019.
- *ME Information Technology Committee*: Member 2009-2015; Chair 2015-present.
- *ME Faculty Search Committee*, 2015-2017.