

Phani Motamarri

*Assistant Professor, Department of Computational and Data Sciences,
Indian Institute of Science, Bangalore, India (from Dec 2019)*

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Research Interests

- Mathematical techniques and real-space computational algorithms for large-scale ab-initio calculations using density functional theory (DFT).
- Ab-initio modeling of defect properties in structural and functional materials, thereby informing higher-scale models for accurate prediction of macroscopic material properties.
- Computational solid mechanics, Finite-element methods.
- Numerical analysis, Scientific computing, Open-source DFT-FE code development.

Education

- 2009 – 2014 **Doctor of Philosophy (Ph.D) – Computational Materials Physics**, *Department of Mechanical Engineering*, University of Michigan Ann Arbor, USA
“Large-scale real-space Kohn-Sham density functional theory calculations using adaptive finite-element discretization” **Advisor:** Prof. Vikram Gavini
- 2005 – 2007 **Master of Engineering (M.E) – Computational Solid Mechanics**, *Department of Mechanical Engineering*, Indian Institute of Science Bangalore (IISc), India
“An energy-momentum conserving algorithm for nonlinear elastodynamics within the framework of hybrid finite-elements”. **Advisor:** Prof. C. S. Jog
- 2001 – 2005 **Bachelor of Engineering (B.E)**, *Department of Mechanical Engineering*, National Institute of Technology Karnataka, Surathkal, India

Professional Appointments

- from Dec 2019 **Assistant Professor**, *Department of Computational and Data Sciences (CDS)*, Indian Institute of Science, Bangalore, India
- since April 2015 **Assistant Research Scientist (Research Faculty)**, *Department of Mechanical Engineering*, University of Michigan Ann Arbor, USA
- since April 2015 **Affiliate Faculty**, *Michigan Institute for Computational Discovery and Engineering*, University of Michigan Ann Arbor, USA
- October 2014 – March 2015 **Postdoctoral Research Fellow**, *Computational Materials Physics Group*, Department of Mechanical Engineering, University of Michigan Ann Arbor, USA
Post-doc Advisor: Prof. Vikram Gavini
- 2007 – 2009 **Researcher**, *India Science Lab*, General Motors R&D Center, Bangalore, India

Honors & Awards

- 2020 **INCITE Award**, *US Department of Energy (DOE) Leadership Computing award to solve grand scientific challenges (role: Co-Principal Investigator)*
- 2019 **Finalist – ACM Gordon Bell Prize Competition**, *SC’19 to be held in Nov 2019, Colorado, USA*, (One of the lead authors of the Gordon Bell Prize nomination)
🔗 (hyperlink)
- 2016 **Finalist - Alston S. Householder fellowship**, *Computational and Applied Math Group, Oak Ridge National Laboratory, USA*
- 2014 **Robert J Melosh Medal**, *International Association of Computational Mechanics (IACM) and Duke University, North Carolina, USA*, 🔗 (hyperlink)

- 2013 **Rackham Predoctoral Fellowship**, Awarded to few selected doctoral students across various disciplines who have achieved PhD candidacy, University of Michigan, Ann Arbor, USA, [🔗](#) (hyperlink)
- 2009 **Dwight F. Benton fellowship**, Awarded to first year PhD students based on the academic accomplishments prior to joining the PhD program at University of Michigan.
- 2004 **Indian Academy of Sciences Research Fellowship**, Awarded to few selected undergraduate students across India to conduct summer research at some of the finest research labs in India.

Peer-reviewed Journal and Conference Publications

- Phani Motamarri, Sambit Das, Shiva Rudraraju, Krishnendu Ghosh, Denis Davydov, Vikram Gavini: DFT-FE — A massively parallel adaptive finite-element code for large-scale density functional theory calculations, *Computer Physics Communications*, 246 (2020) 106853. [🔗](#) (journal)
- Sambit Das, Phani Motamarri, Vikram Gavini, Bruno Turcksin, Ying Wai Li, Brent Leback: Fast, scalable and accurate finite-element based ab-initio calculations using mixed precision computing: 46 PFLOPS simulation of a metallic dislocation system. *Proceedings of SC19, The International Conference for High Performance Computing, Networking, Storage, and Analysis (2019)*.
- Aagesen et al. PRISMS – An Integrated, Open Source Framework for Accelerating Predictive Structural Materials Science, *Journal of Mechanics–J. Min. Met. Mat. S.*, (2018) p1-17 [🔗](#) (journal)
- Phani Motamarri, Vikram Gavini: Configurational force approach for atomic relaxations in electronic-structure calculations using Kohn-Sham density functional theory. *Physical Review B*, 97 (2018) 165132 [🔗](#) (journal)
- Phani Motamarri, Kaushik Bhattacharya, Michael Ortiz, Vikram Gavini: Spectrum splitting approach for Fermi-operator expansion in all-electron Kohn-Sham DFT calculations, *Physical Review B*, 95 (2017) 035111. [🔗](#) (journal)
- Phani Motamarri, Thomas Blesgen, Vikram Gavini: Tucker-tensor algorithm for large scale Kohn-Sham density functional theory calculations, *Physical Review B*, 93 (2016) 125104. [🔗](#) (journal)
- Phani Motamarri, Vikram Gavini: Subquadratic-scaling subspace projection method for large-scale Kohn-Sham density functional theory calculations using spectral finite-element discretization, *Physical Review B*, 90 (2014) 115127. [🔗](#) (journal)
- Phani Motamarri, Mike Nowak, Kenneth Leiter, Jaroslaw Knap, Vikram Gavini: Higher-order adaptive finite-element methods for Kohn-Sham density functional theory, *Journal of Computational Physics*, 253 (2013) (308-343). [🔗](#) (journal)
- Phani Motamarri, Mrinal Iyer, Jaroslaw Knap, Vikram Gavini: Higher-order adaptive finite-element methods for orbital-free density functional theory, *Journal of Computational Physics*, 231 (2012) 6596-6621. [🔗](#) (journal)
- Phani Motamarri, Anand Ramani, Anshul Kaushik: Structural topology synthesis with dynamics and nonlinearities using equivalent linear systems, *Structural and Multidisciplinary Optimization*, 45 (2012) 545-558. [🔗](#) (journal)
- Phani Motamarri, Srinivasan Suryanarayan: Unified analytical solution for dynamic elastic buckling of beams for various boundary conditions and loading rates, *International Journal of Mechanical Sciences*, 56 (2012) 60-69. [🔗](#) (journal)
- C. S. Jog, Phani Motamarri: An energy momentum conserving algorithm for nonlinear transient analysis within the framework of hybrid elements, *Journal of Mechanics of Materials and Structures*, 4 (2009) 157-186. [🔗](#) (journal)
- M. Phani Sudheer, Ravi S. Nanjundiah and A. S. Vasudevamurthy: Revisiting the slow manifold of the Lorenz-Krishnamurthy Quintet, *Discrete and Continuous Dynamical Systems-Series B*, 6 (2006) 1403-1416. [🔗](#) (journal)

In preparation:

- *Sambit Das, Phani Motamarri, Vikram Gavini*: GPU accelerated real-space Kohn-Sham density functional theory calculations using adaptive finite-element discretization. (in preparation for *SIAM Journal of Scientific Computing*).
- *Ian Lin, Phani Motamarri, Vikram Gavini*: Linear-scaling Tucker tensor approach for large-scale Kohn-Sham density functional theory calculations. (in preparation for *PNAS*).
- *Phani Motamarri, Vikram Gavini*: Energetics and nucleation of point defects in magnesium under extreme tensile hydrostatic stresses. (to be submitted to *J. Mech. Phys. Solids*)
- *Phani Motamarri, Linda Zotti, Juan Carlos Cuevas, Vikram Gavini*: Large-scale electronic structure calculations in double-stranded DNA molecule for bio-molecular applications.
- *Phani Motamarri, Sambit Das, Vikram Gavini*: Core-energetics of dislocations in aluminum and magnesium using Kohn-Sham density functional theory with bulk boundary conditions.

Professional Activities

- Reviewer for articles in Journal of Computational Physics, Journal of Scientific Computing, Computer Modeling in Engineering and Sciences, Structural and Multidisciplinary Optimization

Invited Talks

- *Mechanical Engineering Department Seminar*, University of California, San Diego, USA, 2019.
- *Computational and Data Sciences Department Seminar*, Indian Institute of Science (IISc), Bangalore, India, 2019.
- *Engineering Mechanics Unit Seminar*, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bangalore, India, 2019.
- *Computational Materials Science Group Seminar*, Shell Technology Centre, Bangalore, India, 2019.
- *Toyota Research Institute Conference on Accelerated Materials Discovery*, San Francisco, USA, 2018.
- *SIAM Conference on Computational Science and Engineering*, Atlanta, USA 2017.
- *Mechanical Engineering Seminar*, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia. 2016.
- *Computational Mathematics, Science and Engineering Seminar*, Michigan State University, East Lansing, USA, 2016.
- *Alston S. Householder Fellowship Seminar*, Oak Ridge National Laboratory, USA, 2016.
- *Invited talk*, Simulators Meeting, Carnegie Mellon University, Pittsburgh, USA, 2016.
- *Invited talk*, The 8th International Congress on Industrial and Applied Mathematics, Beijing, China, 2015.
- *Army High Performance Computing Research Center Seminar*, Stanford University, Stanford, USA, 2014.
- *Robert J Melosh Symposium*, Duke University, Raleigh, USA, 2014. (Student finalist presentation for Melosh competition)
- *Invited talk*, IBM Semiconductor Research and Development Center (SRDC), Bangalore, India, 2014..
- *Invited talk*, SIAM Conference on Mathematical Aspects of Material Science, Philadelphia, USA, 2013.
- *Invited talk*, General Motors India Science Lab, Bangalore, India, 2007.