ME Seminar

Towards fast and accurate exa-scale quantum-mechanical calculations for material modeling using adaptive finite-elements and mixed-precision computing

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ABSTRACT

Kohn-Sham density functional theory (DFT) calculations based on quantum mechanics have been instrumental in providing many crucial insights into materials behavior and occupy a sizable fraction of world's computational resources today. However, the stringent accuracy requirements in DFT needed to compute meaningful material properties, in conjunction with the asymptotic cubic-scaling computational complexity with number of electrons, demand huge computational resources for accurate DFT calculations. Thus, these calculations are routinely limited to material systems with at most few thousands of electrons, employing plane-wave discretization despite all its limitations which has remained the method of choice for many material science applications. In this talk, I will present some recent advances made in the state-of-the-art for accurate DFT calculations -via- the development of DFT-FE, employing adaptive finite-element discretization, in conjunction with mixed-precision strategies for the solution of governing equations alongside with implementation innovations focusing on significantly reducing the data movement costs and increasing arithmetic intensity on hybrid CPU-GPU architectures. The reported advance discussed in this talk has wide ranging implications in tackling critical scientific and technological problems by making use of the predictive capability of DFT calculations for large-scale material systems.

ABOUT THE SPEAKER

Dr. Phani Motamarri is currently an Assistant Professor at the Department of Computational and Data Sciences, IISc-Bangalore. Prior to this, he served as a research- track faculty member at the University of Michigan, Ann Arbor, USA from where he received his PhD in the area of Computational Materials Physics from the Department of Mechanical Engineering. Before his PhD, he obtained his Master's degree from IISc, Bangalore and Bachelor's degree from NITK, Surathkal both from the Department of Mechanical Engineering. His primary research interests include development of mathematical techniques and HPC centric real-space computational algorithms that can leverage the latest heterogeneous parallel computing architectures and future exa-scale machines for quantum-mechanical material modeling and furthermore, harnessing these computational capabilities to address challenging material modeling problems. He is one of the key developers of DFT-FE—an open-source computational framework for massively parallel large-scale density functional theory calculations that was named as a finalist for 2019 ACM Gordon Bell Prize, the prestigious prize in scientific computing.

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