DFT-FE: Fast, Accurate and Large-scale Ab-initio Calculations for Materials Modeling

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This talk will present our recent advances towards the development of computational methods and numerical algorithms for conducting fast and accurate large-scale DFT calculations using adaptive finite-element discretization, which form the basis for the recently released DFT-FE open-source code (https://github.com/dftfeDevelopers/dftfe). Details of the implementation, including mixed precision algorithms and asynchronous computing, will be presented. The computational efficiency, scalability and performance of DFT-FE will be presented. A few application problems tackled using DFT-FE will be presented.