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Reformulation of the Muffin-Tin Problem in Electronic Structure Calculations within the FEAST Framework

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Abstract
This thesis describes an accurate and scalable computational method designed to perform nanoelectronic structure calculations. Built around the FEAST framework, this method directly addresses the nonlinear eigenvalue problem. The new approach allows us to bypass traditional approximation techniques typically used for first-principle calculations. As a result, this method is able to take advantage of standard muffin-tin type domain decomposition techniques without being hindered by their perceived limitations. In addition to increased accuracy, this method also

has the potential to take advantage of parallel processing for increased scalability.

The Introduction presents the motivation behind the proposed method and gives an overview of what will be presented for this thesis. Chapter 1 explains how electronic structure calculations are currently performed, including an overview of Density Functional Theory and the advantages and disadvantages of various numerical techniques. Chapter 2 describes, in detail, the method proposed for this thesis, including mathematical justification, a matrix-level example, and a description of implementing the FEAST algorithm. Chapter 3 presents and discusses results from numerical experiments for Hydrogen and various Hydrogen molecules, Methane, Ethane, and Benzene. Chapter 4 concludes with a summary of the presented work and its impact in the field.

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