Scalable High-Performance Algorithms for Phonon Calculations in Complex Materials

Juntang Wang

February 11

Proposal Study Planner

1 Executive Summary

This proposal targets the development of scalable, high-performance algorithms for phonon calculations in complex materials, addressing the significant computational challenges these calculations present. By leveraging advancements in numerical analysis, matrix theory, and high-performance computing, this research aims to bridge the gap between the current computational capabilities and the demands of phonon calculations, significantly reducing computation times while maintaining or improving accuracy. The expertise of Prof. Xiaobai Sun in these areas will be a guiding force in the project, aiming to achieve a suite of algorithms that could transform computational materials science.

2 Survey of Background Literature

2.1 Overview

The study of phonons is critical for understanding the thermal and electronic properties of materials. However, the computational intensity required for phonon calculations in complex materials necessitates advancements in computational methodologies to optimize large matrix operations and exploit parallel computing architectures effectively.

2.2 Background

Phonons, as quantized modes of vibrations in a crystalline lattice, play a pivotal role in determining materials' properties. This proposal is inspired by the foundational work of Togo and Tanaka [1], aiming to advance computational methodologies to address the challenges inherent in phonon calculations. This initiative is further supported by the potential for technological advancements outlined by Maldovan [2].

2.3 Relevance/Impact

The development of scalable, high-performance algorithms for phonon calculations has the potential to significantly impact computational materials science. The efficiency of scalable phonon calculation approaches demonstrated by Zhang et al. [3] and the novel pathway for phononic property analysis offered by machine learning techniques explored by Chen et al. [4] underscore the transformative potential of this research.

3 Proposed Methodology

3.1 Algorithm Development

Design and implement scalable, accurate algorithms for dynamical matrix computations, leveraging advancements in numerical analysis and matrix theory. This objective draws on the insights provided by Nomura et al. [5] regarding phonon engineering through tailored nanostructures.

3.2 Parallel Processing Techniques

Optimize parallel processing techniques, including CUDA and MPI, to enable scalable execution across various hardware platforms, from personal computing devices to supercomputers.

3.3 High-Performance Computing (HPC) Optimization

Implement optimizations specific to HPC environments to ensure efficient utilization of computational resources. This includes leveraging GPU acceleration for phonon computations, as demonstrated by Wei et al. (2020), who identified performance bottlenecks in ShengBTE, a software package used for phonon computation, and proposed various optimizations that significantly improved performance. Such strategies will be crucial for developing our scalable high-performance algorithms, ensuring they can handle the intensive large matrix computations required for accurate phonon calculations in complex materials. [6]

3.4 Benchmarking and Validation

Conduct comprehensive benchmarking against existing methods across different material systems to assess speed, scalability, and accuracy, validating the new framework's improvements.

3.5 Integration with Material Science Applications

Collaborate with material scientists to integrate the algorithms into computational material science software, enhancing phonon calculation capabilities for the research community.

4 Research Plan

Outline short-term and long-term objectives, including the development of algorithm prototypes and their integration into existing software. The plan includes timelines for each stage and dissemination of results through publications and presentations.

5 Resources

Detail the high-performance computing facilities, collaboration with material scientists, and human resources required for the project, emphasizing the multidisciplinary nature of the research team.

References

[1] A. Togo, & I. Tanaka, (2015). First principles phonon calculations in materials science. *Scripta Materialia*, 108, 1-5. `https://doi.org/10.1016/J.SCRIPTAMAT.2015.07.021`

[2] M. Maldovan, (2013). Sound and heat revolutions in phononics. *Nature*, 503, 209-217. `https://doi.org/10.1038/nature12608`

[3] J. Zhang, Y.Q. Cheng, W. Lu, E. Briggs, A. Ramirez-Cuesta, & J. Bernholc, (2019). Large-Scale Phonon Calculations Using the Real-Space Multigrid Method. *Journal of Chemical Theory and Computation*. `https://doi.org/10.1021/acs.jctc.9b00802`

[4] Z. Chen, N. Andrejevic, T. Smidt, Z. Ding, Q. Xu, Y. Chi, Q.T. Nguyen, A. Alatas, J. Kong, & M. Li, (2020). Direct Prediction of Phonon Density of States With Euclidean Neural Networks. *Advanced Science*, 8. `https://doi.org/10.1002/advs.202004214`

[5] M. Nomura, J. Shiomi, T. Shiga, & R. Anufriev, (2018). Thermal phonon engineering by tailored nanostructures. *Japanese Journal of Applied Physics*, 57. `https://doi.org/10.7567/JJAP.57.080101`

[6] Yiming Wei, Xin You, Hailong Yang, Zhongzhi Luan, & Depei Qian. (2020). Towards GPU Acceleration of Phonon Computation with ShengBTE. In *Proceedings of the International Conference on High Performance Computing in Asia-Pacific Region*. `https://doi.org/10.1145/3368474.3368487`