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# RPPR Final Report
as of 27-Aug-2019

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Proposal Number: 72111MARIP **Agreement Number: W911NF-18-1-0242**
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**Report Date:** 28-Aug-2019 Date Received: 26-Aug-2019
**Final Report** for Period Beginning 02-Jun-2018 and Ending 28-May-2019
**Title:** COMPUTING CLUSTER FOR THE DEVELOPMENT OF FAST AND SCALABLE ALGORITHMS FOR LARGE SCALE REAL-SPACE ELECTRONIC STRUCTURE CALCULATIONS
**Begin Performance Period:** 02-Jun-2018 **End Performance Period:** 28-May-2019
**Report Term:** 0-Other
Submitted By: Vikram Gavini Email: vikramg@umich.edu
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**STEM Degrees:** 2 **STEM Participants:** 5

**Major Goals:** The major goal of this proposal is to acquire a large memory computing cluster to support the development of fast, error-controllable, and scalable algorithms for large-scale real-space electronic structure calculations to understand and accurately predict a wide range of materials properties and phenomena relevant to the Army Research Office and the Department of Defense. The DoD-funded research areas to be supported by the acquisition include the development of fast and scalable algorithms for time dependent density functional theory calculations, and the development of computational methods for fast electronic structure calculations using tensor-structured techniques. The proposed acquisition will also aid the development of computational methods for real-space all-electron electronic structure calculations, as well as the development of a computational framework for large-scale materials simulations with quantum accuracy, which will tackle two significant approximations in electronic structure calculations, i.e., the pseudopotential approximation and approximations in modeling electron-electron correlations.

**Accomplishments:** A computing cluster was acquired in early 2019 to support the various aspects of proposed method development of fast, error-controllable, and scalable algorithms for large-scale real-space electronic structure calculations. The acquired computing cluster comprises of 22 nodes of dual socket Intel Xeon Gold 6154 processors with 36 cores per each node. Each node has a 192 GB of random access memory (RAM) and 480 GB of solid state drive (SSD) and 4 TB of hard disk drive (HDD). The compute nodes are all interconnected with InfiniBand HDR100 networking, capable of 100 Gb/s throughput. The computing cluster will be maintained by advanced research computing technology services at University of Michigan for a period of four years to aid the proposed research work. This includes housing the computing cluster, periodic maintenance of the computing cluster, and any support needed to fix hardware or software issues.

Significant progress has been made in many of the proposed research activities, which are briefly summarized below:

1. Fast, accurate and scalable large-scale real-space DFT calculations: We have further advanced our work on developing fast and scalable algorithms for large-scale DFT calculations. In particular, using a higher-order adaptive finite element basis, in conjunction with the developed algorithms (including mixed precision algorithms) for a fast an accurate solution of the Kohn-Sham eigenvalue problem, we have demonstrated pseudo potential DFT calculations on 100,000 electrons. The developments in the computational framework and algorithms have been released as an open source code DFT-FE. The details of the framework, algorithms and detailed benchmark studies on the accuracy, computational efficiency and scalability will shortly be appearing in Computer Physics

Communications (arXiv:1903.10959). Based on the unprecedented parallel performance of DFT-FE, this work has also been selected as one of the finalists of the ACM Gordon Bell prize (with the final decision to be made at SC19).

2. Large-scale all-electron calculations: Building on our preliminary work on using an enriched finite element (EFE) basis for all-electron calculations, we now have extended the formulation and computational framework to consider both non-periodic and periodic systems. Our benchmark studies are suggesting that we gain almost 10-fold advantage on degrees of freedom by using EFE basis (in comparison to just FE basis), and ~30-60 fold advantage on computational times (due to synergistic improvement in the efficiency of the solver). For systems involving more than 50 atoms, we are significantly outperforming existing state-of-the-art all-electron codes. More comprehensive benchmark studies are ongoing along this direction.

3. Time dependent DFT calculations: We have extended the higher-order adaptive FE framework for ground-state DFT to time dependent DFT. In particular, the adaptive nature of the FE basis plays a significant role in TDDFT calculations, due to which we are observing a 3-5 fold improvement over well developed TDDFT codes such as OCTOPUS. We are currently working on subspace approaches to accelerate the TDDFT calculations, that has the potential to enable long time-scale TDDFT calculations. A manuscript reporting some aspects of this work is currently in review in Physical Review B (arXiv:1810.13130).

4. Inverse DFT: We have a recent breakthrough in a long-standing open problem in computational chemistry. The inverse DFT problem comprises of computing the exchange correlation (XC) potential from a given ground-state density. Besides the importance of inverse DFT in embedding techniques, it can also provide a path towards improving the exchange-correlation description in DFT by deriving the exact XC potentials computed from ab-initio correlated ground-state densities, and subsequently learning the relationship between exact XC potentials and ground-state densities. However, the problem has remained an open numerical challenge for over two decades. We have developed a framework to compute exact XC potentials, to chemical accuracy, from correlated ground-state densities. This involves: (i) a PDE constrained formulation of inverse DFT; (ii) use of a systematically improvable and complete basis, the FE basis, to discretize the problem; (iii) use a cusp-correction to correct for the incorrect asymptotics in the ab initial correlated densities computed from a gaussian basis; (iv) employ asymptotically correct far-field boundary conditions from the exact XC potentials. The findings of this work are under consideration in Nature Communications (nominally accepted, pending requested editorial changes).

**Training Opportunities:** The computing resources provided by the cluster has contributed to the research activities of 4 graduate studies and a research scholar. The computational cluster and the research activities it supports resulted in training opportunities spanning high performance computing, numerical analysis, fast algorithms and condensed matter theory.

**Results Dissemination:** The following publications have resulted from this work (in the past one year), which are either accepted or under consideration. Four other publications are under preparation.

1. Motamarri, P., Das, S., Rudraraju, S., Ghosh, K., Davydov, D., Gavini, V., DFT-FE: A massively parallel adaptive finite-element code for large-scale density functional theory calculations, Comput. Phys. Commun., to appear (2019).

2. Das, S., Motamarri, P., Gavini, V., Turcksin, B., Li, Y.-W., Leback, B., 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). (Gordon Bell Prize)

3. Kanungo, B., Zimmerman, P., Gavini, V., Exact exchange-correlation potentials from ground-state electron densities, Nature Communications, nominally accepted pending editorial revisions (2019).

4. Kanungo, B., Gavini, V., Real-time time-dependent density functional theory using higher order finite element methods, Phys. Rev. B, in review (2019).

**Honors and Awards:** The parallel performance of DFT-FE has been selected as one of the two finalists for the 2019 ACM Gordon Bell Prize.

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**Protocol Activity Status:**

**Technology Transfer:** The computational framework and algorithmic developments in ground-state DFT have been released as an open source code: DFT-FE. The link to the GitHub page of the DFT-FE is: https://github.com/dftfeDevelopers/dftfe. Unique capabilities of DFT-FE include: (i) the treatment of both pseudopotential and all-electron calculations in periodicals semi-periodic and non-periodic systems using density and gradient density based XC functionals; (ii) massive scalability of the code, with scaling demonstrated to 200,000 MPI tasks on Cori super computer.

**PARTICIPANTS:**

**Participant Type:** PD/PI
**Participant:** Vikram Gavini
**Person Months Worked:** 2.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

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**Participant:** Phani Motamarri
**Person Months Worked:** 4.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

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**Participant:** Sambit Das
**Person Months Worked:** 4.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

**Participant Type:** Graduate Student (research assistant)
**Participant:** Bikash Kanungo
**Person Months Worked:** 8.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

**Participant Type:** Graduate Student (research assistant)
**Participant:** Chih-Chuen Lin
**Person Months Worked:** 4.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

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**Participant Type:** Graduate Student (research assistant)
**Participant:** Nelson Rufus
**Person Months Worked:** 6.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Nothing to report in the uploaded pdf (see accomplishments)