Project ID: jh180026-NAJ

Project Title

High Performance Computational (HPC) Studies on Beyond the Standard Model of Particle Physics Using Atoms and Molecules

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Abstract:
The focus of our project for FY 2018 was the computation of the electric dipole moment of xenon, which is an important ingredient for probing new physics beyond the Standard Model of particle interactions. To this end we used the relativistic coupled cluster theory, which is currently one of the leading quantum many body theories and has been successfully applied to wide range of physical systems. This theory is both compute and memory intensive. We performed our computations using Tsubame 3.0 at the Tokyo Institute of Technology. Our relativistic coupled cluster theory codes were parallelized using MPI and the large memory available in this was used across multiple nodes. A new version of the code utilizing a hybrid approach based on OpenMP and MPI has been developed and applied to argon atom.

The results for the electric dipole moment of xenon of two different formulations of the relativistic coupled cluster theory using Tsubame 3.0 were found to be in good agreement. Higher order relativistic and many-body effects were included in these calculations. This updated work has been submitted for publication to Physical Review Letters and presented in an international workshop. These results in combination with future experiments of the electric dipole moment of xenon will provide insights into new physics beyond the Standard Model. We have also carried out preliminary studies on the polarizabilities of certain closed shell atoms. We performed simple tests of our relativistic coupled cluster molecular codes on TSUBAME 3.0

1. Basic Information

(1) Collaborating JHPCN Centers

Tokyo Institute of Technology

(2) Research Areas

✓ Very large-scale numerical computation
☐ Very large-scale data processing
☐ Very large capacity network technology

☐ Very large-scale information systems

(3) Roles of Project Members

Das: Dirac-Fock Codes and Management
Sahoo: Relativistic Coupled Cluster Code
Abe: Relativistic Molecular Code
Sakurai: Xe EDM Computation using RCC
Shitara: Computation of Polarizabilities
Watanabe: OpenMP and MPI of RCC code
Dyall: Advice on Dirac-Fock Codes
Harrison: Advice on Basis Sets and HPC

2. Purpose and Significance of the Research

The purpose of the present research project is to use high performance computing(HPC) techniques to probe new physics beyond the Standard Model (BSM) of elementary particles. For our proposed research, the BSM physics that we have explored is the nuclear electric dipole moment (EDM) which can arise due to the violations of symmetries of space and time reversal due to exotic forces between subatomic particles. In particular, we have computed the size of the nuclear EDM by performing HPC studies on xenon atom and combining them with data from experiments that are in progress in laboratories in Japan, USA and Europe. The results that we have obtained for the xenon nuclear EDM would provide important insights into BSM physics and also deepen our understanding of why there is more matter in the universe than antimatter.

3. Significance as a JHPCN Joint Research Project

The high performance computations of the nuclear EDMs to test BSM physics have been carried out in the framework of relativistic quantum mechanics. To this end, we have solved the many electron Dirac equation for different xenon atom in three steps: (i) Solution of the Dirac-Hartree-Fock (DHF equation) in the mean field approximation (ii) Solution of the relativistic coupled cluster (RCC) amplitude equations using the results of the previous step. It would be appropriate to mention here that the RCC theory is currently the most advanced theoretical method describing atoms and molecules (iii) Evaluation of the nuclear EDM using the input from Steps 1 and 2. The input from the DHF code for xenon atom was used for solving the RCC amplitude equations, which are nonlinear equations of the type **A(t)t = B**, where **A** is a matrix of size **N X N** and **N** is of the order of a few million, **t** is a vector of size **N** and it represents the RCC amplitudes and B is a known vector of size **N**. It is necessary to solve these equations iteratively since the matrix **A** is a function **t.** The solution of the RCC amplitude equations clearly requires large scale HPC resources which are available in TSUBAME. We used the Jacobi iterative method to solve these equations as it is robust and amenable to parallelization. Using MPI, we have parallelized those parts of our RCC codes for atoms where these equations are solved and the vector **B** evaluated.

The calculation of the RCC amplitudes for xenon mentioned above are both compute and memory intensive, and require state of the art high performance computing resources. include higher order relativistic effects using 12 nodes (96 cores) and also higher order many body effects using 12 node (120 cores). These amplitudes are necessary to compute nuclear EDMs. The result for xenon nuclear EDM in combination with those of EDM experiments would be an important step towards understanding BSM physics.

4. Outline of the Research Achievements up to FY2017

Not Applicable

5. Details of FY2018 Research Achievements

We have made significant progress in our theoretical studies on the nuclear EDM of the xenon atom due to violations of parity and time-reversal symmetries. There are currently three EDM experiments underway on xenon EDM. The results of EDM calculations for this atom in combination with those of the experiments can probe BSM physics. Our calculations were carried out using two different versions of the relativistic coupled cluster theory and they include higher order relativistic effects using 12 nodes (96 cores) and also higher order many body effects using 12 nodes (120 cores).. The codes for both cases were run on TSUBAME 3.0 using MPI. The two results were close, and they can in the future be combined with those of the EDM experiments in the to test BSM physics. This work has been submitted for publication to Physical Review Letters. Prof Watanabe has been able successful in parallelizing the RCC code for argon atom by combining features of OpenMP and MPI.

Computations were carried out to determine the polarizabilities of certain closed shell atoms.

We have performed DHF and RCC computations for helium-like xenon, which were used as inputs for quantum simulations that were performed on a different computer.

6. Progress of FY2018 and Future Prospects

We were successful in installing our relativistic coupled cluster codes for atoms in TSUBAME 3.0 and parallelizing them using MPI. Prof Watanabe has been successful in parallelizing the RCC code for argon atom by combining certain features of OpenMP and MPI. Using the former code we performed theoretical studies of the EDM of atomic xenon, which we had set as one of our principal objectives for our objective. In addition, we have also carried out calculations of polarizabilities for various closed shell atoms.

We made progress in making our relativistic molecular codes

UTCHEM and DIRAC compatible with TSUBAME 3.0.

7. List of Publications and Presentations

(1) Journal Papers

"Relativistic many body theory of the electric dipole moment of ^{129}Xe and its implications for probing new physics beyond the Standard Model (Submitted to Physical Review Letters)"

A. Sakurai, B. K. Sahoo, K. Asahi and B. P. Das

(2) Conference Papers

"Relativistic Theory of the electric dipole moment of xenon atoms to probe new physics beyond the Standard Model" (International Workshop on Fundamental Physics Using Atoms, Okinawa 2019)

A. Sakurai, B. K. Sahoo, K. Asahi and B. P. Das

(3) Oral Presentations

(4) Others