# Code Refactoring and Test Suite Development for the Density Matrix Renormalization Group Algorithm

**Eduardo Ponce Mojica**
**Polytechnic University of Puerto Rico**
**http://sites.google.com/a/g.ornl.gov/eponce/**

**Research Alliance in Math and Science**

**Mentor: Dr. Gonzalo Alvarez-Campot**
**Oak Ridge National Laboratory**
**Computer Science and Mathematics Division**

## Strongly Correlated Electron Systems

Strong electronic interactions appear in many materials of technological interest, such as manganites, high-temperature superconductors, and multiferroics. Condensed matter physics studies phenomena related to strongly correlated electron systems. Several methods have been developed to model the relevant interactions of a given compound and the relevant degrees of freedom. Tight-binding lattice models (Hubbard, t-J, and spin ½ Heisenberg) aid in determining the materials characteristics. These models exhibit exponential complexity due to their Hilbert space and require a great deal of computational power. In solid-state physics, density matrix renormalization group (DMRG) is a numerical variational method used to describe quantum many-body systems. Physicists from the Nanomaterials Theory Institute at Oak Ridge National Laboratory are producing a free and open source generic implementation of the DMRG technique using the C++ Standard Template Library (DMRG++), to model strongly correlated interacting electrons in one-dimensional chains and n-leg ladders. DMRG++ needs a framework that enables incremental changes with the ability to detect if it the code is in a valid state.

## Research Objectives

- Develop test suite for DMRG++ code using Perl language
- Create a scalable and flexible framework enabling implementation for other similar codes
- Compute oracles of DMRG++ tests for results validity
- Construct libraries to parallelize sparse linear algebra present in DMRG++ code

Figure 1. Development tools used: Perl, DMRG++, MPI, and github.

## Test Suite Framework

The density matrix renormalization group is an algorithm which uses states and sites to represent electronic interactions. DMRG++ requires a number of inputs and configurations prior to execution. Test's speed is essential for physicists studying the interactions in materials. In addition, features and changes made to the code require some sort of validation tool.

Figure 2. DMRG++ algorithm decomposes the system followed by a sweep to compute ground state characteristics

Test suite development for DMRG++ consists of a framework that runs tests automatically with simple configurations. The framework uses a hierarchy of directories and files to configure, compile, and execute the algorithm. Each test has associated files containing inputs for each type of model and geometry used. A common library allows to add or remove analyses for the tests with minimal modifications. A hash table is maintained to avoid the compilation phase if same configurations are inputted. The results are extracted from the raw output data and compared with pre-determined oracles to validate.

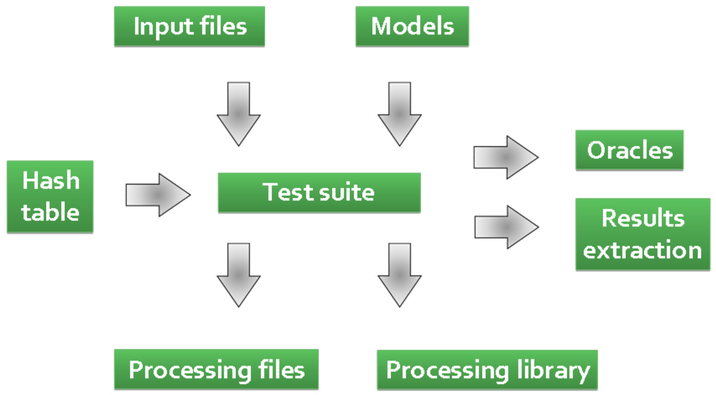


Figure 3. Information flow diagram of DMRG++ test suite framework.

## Results

(A) (B)

Figure 4. (A) Perl routine used in the execution of DMRG++. (B) Output representation after running a single test.

The main purpose of DMRG++ is to compute ground state energies in strongly correlated systems, average spin coefficients, and densities of states (charges per site). The test suite framework simplifies single or multiple test runs by running with a single command as input. All the results are saved in files associated to each test which are then compared to oracles, determining the validity of the code state. The framework allows the addition or removal of analyses without hindering results and provides exception handling capabilities.

## Future Research

The general methodology used in the test suite can be adapted to similar codes, Dynamic Cluster Approximation, by undergoing minor programming changes. Additional processing methods can be incorporated to the processing library. Still to be developed is the implementation code parallelization using message passing interface libraries. This feature will help reduce bottlenecks due to sparse linear algebra parts of the code, thus improving the DMRG++ performance allowing to study materials more in depth.

## References

White, S. R. (1992) *Density Matrix Formulation for Quantum Renormalization Groups*. Physical Review Letters, Vol. 69, No 19, pp. 2863-2866.
Alvarez, G. (2009) *The Density Matrix Renormalization Group for Strongly Correlated Electron Systems: A Generic Implementation*. Computer Physics Communications, Vol. 180, No 9, pp. 1572-1578.

U.S. DEPARTMENT OF ENERGY
Office of Science

The Research Alliance in Math and Science program is sponsored by the Office of Advanced Scientific Computing Research, U.S. Department of Energy. The work was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under Contract No. De-AC05- 00OR22725.
This work has been authored by a contractor of the U.S. Government, accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.
I would like to thank Dr. Gonzalo Alvarez for the opportunity to work on this project, Rashida E. Askia for her continued support, and Debbie McCoy, who made provisions for this research experience along with exceptional professional support.

POLYTECHNIC UNIVERSITY
UT-BATTELLE
Management Contractor for DOE's Oak Ridge National Laboratory