

DMRG++ Code Refactoring: Implementing a JSON Format for the Input File

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A Numerical Method

The Density Matrix Renormalization Group (DMRG) is a numerical variational method used to study quantum many-body physics. This method is used to diagonalize the density matrix in order to truncate the system. Using only the dominant eigenvalues of this matrix, instead of the system matrix, reduce the calculations and the needed computational power.

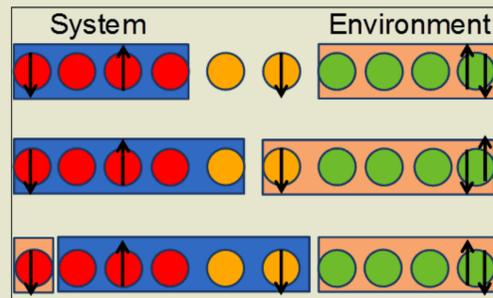


Fig. 1: Combination process of blocks to form new geometries

Figure 1 shows how the system and environment blocks combine to form the final geometry.

DMRG is used to study the behavior of materials with special characteristics like new high temperature superconductors. As shown in figure 2, superconductivity can be achieved at liquid nitrogen temperature.

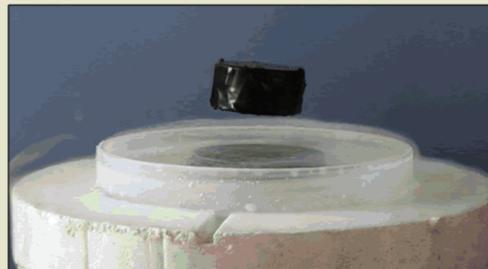


Fig. 2: Magnet floating on top of a nitrogen cooled superconductor .

Figure 3 shows how the Hubbard model is used to characterize the electrons spin fluctuations that cause the superconducting state in the cuprates.

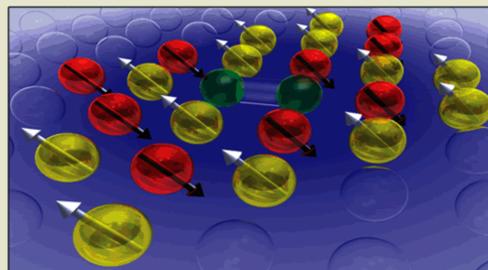


FIG. 3: Electron spin model of cuprate superconductor.

Research Objectives

Modify the DMRG++ code to read a JSON input file

Test all the changes to ensure proper functioning

Convert the old input files, that were in plain text format, to JSON format using a PERL script

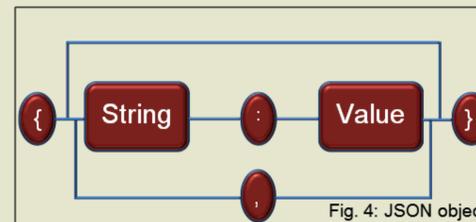
Tools and Methods

The DMRG++ is Oak Ridge National Laboratory's (ORNL) implementation of the DMRG in the C++ programming language.



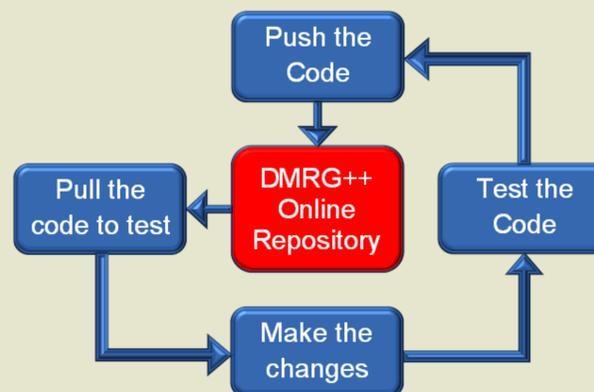
An input file describing the model parameters is needed to start the code. This file is written in plain text format.

Using the Java-Script Object Notation (JSON) we wrote one new input file for testing. Figure four shows an example of the JSON object. The new structured format makes the file more readable and easier to find errors.

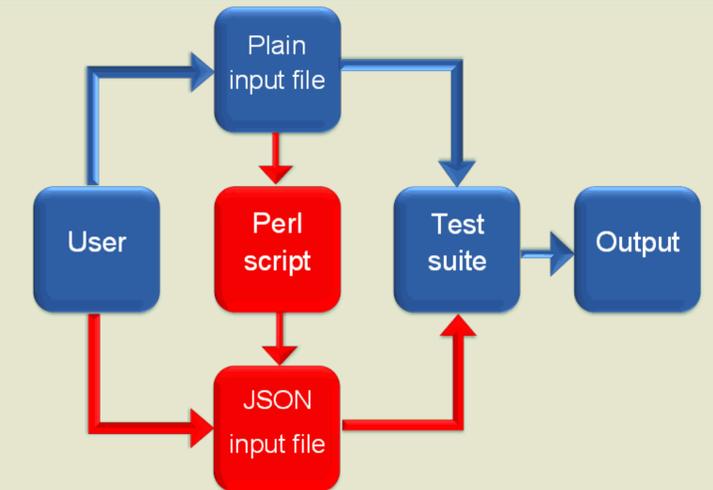


The old input files were changed to the new format using a script written in the Practical extraction and reporting language (Perl).

Git-Hub was used to keep track of the changes to the code that we made through the process. It also serves as interchange channel for feedback.



Results and Conclusions



A Perl script transforms plain format DMRG++ input files into a JSON format.

Changes to the code make it capable of accepting the new input format.

The code is available to physicists, and other interested scientists and researchers, through a free GitHub repository.

For a limited time, the code will accept the old and the new data formats to help smooth the transition.

Future Work

Implement a JSON format to the output file

Create a Graphical User Interface

Implement parallelization with MPI libraries

References

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