



Richard Thigpen
B.S. Graduate
Fisk University
Major:
Computer Science & Mathematics

Faculty Advisor:
Dr. Stephen Egarievwe

Program:
Research Alliance for Minorities

Research Area:

This work will implement a simple and generic interface between the Basic Linear Algebra Subroutine (BLAS) library and codes written in C++, in particular the \square -MAG toolset for computational magnetism in particular. BLAS is a highly optimized implementation of the dense linear-algebra on which many algorithms of computational materials science rely. To achieve maximum sustained performance on modern high performance computing architectures, it is therefore essential that implementations make rigorous use of the BLAS library. The C++ interface developed here will facilitate such implementations in the future and is thus expected to have a high impact on the development of computational materials science codes.

Research Mentor:

Thomas Schulthess, Ph.D.
Computer Science and Engineering
Oak Ridge National Laboratory