Executive Summary

Scientific Merit: This project will use high performance computing for assessment of predictive uncertainty in groundwater reactive transport modeling. Due to the high computational cost of reactive transport modeling and the proposed method of uncertainty analysis, the project objectives can only be obtained by using advanced computing capabilities.

This project will develop a parallel code for simulating movement of groundwater contaminants through geological media for environmental protection and restoration. This code will resolve the great challenge in reactive transport modeling that simulating geochemical reactions of contaminants is computationally demanding. The parallel computing will be based on a physically-based parallelization mechanism that reaction equations can be simulated simultaneously at each node of a computational grid. This feature enables petascale simulation and analysis for a grid of millions nodes, which is not uncommon in groundwater modeling. Developing and benchmarking the proposed parallel code is impossible without high performance computing capabilities.

The developed code will be used to assess predictive uncertainty caused by parametric uncertainty and model uncertainty. The model uncertainty arises when multiple models are all acceptable given available knowledge and data. While the model uncertainty is prevalent in groundwater reactive transport modeling, it has been ignored in most, if not all, modeling practice by using a singe model. This introduces biased modeling results and/or underestimation of predictive uncertainty, leading to improper decisions for environmental management. This project will jointly assess the parametric and model uncertainty using a Bayesian model averaging (BMA) method. The parallel code enables a Monte Carlo implementation of BMA, and the results will provide a reference to evaluate previous approximations of the BMA method, a unique chance only possible with high performance computing capabilities.

Collaboration with ORNL Scientist: This project is to tackle the uranium reactive transport problem occurred since the Cold War Era at many sites national-wide managed by the Department of Energy (DOE). The study site is the Oak Ridge Field Research Center (ORFRC), and this project will leverage previous and on-going research at the site. A supporting letter from Dr. Phil Jardine, an ORNL Distinguished Research Staff Scientist, is attached.

In addition to computing staff at ORNL, we will collaborate with Dr. Zhang at the ORNL Environmental Science Division, who is currently supported by the ORFRC project and a key modeler simulating uranium reactive transport at the site. Dr. Zhang will assist the parallel code development and uncertainty assessment, when the faculty-student team works in Oak Ridge during summer. Her commitment letter is attached to this proposal.

Faculty-Student Approach and Qualification: The research team consists of the Principle Investigator (PI), an Assistant Professor in the Department of Scientific Computing of the Florida State University (FSU), and a graduate student. This team will perform the research at ORNL in summer. The PI has substantial experience of parallel computing, uncertainty analysis, and numerical modeling at DOE sites. The proposed research is built on his previous experience and will expand his research area in reactive transport modeling. The graduate student (female) is pursuing her Ph.D. degree with the PI, and well qualified for performing the proposed research.

Institution Alignment: The FSU Department of Scientific Computing will support the graduate student for 9 months during Spring and Fall semesters, and provide support to the PI for traveling to Oak Ridge. A total of 16 processors will be allocated at FSU High Performance Computer (HPC) to facilitate code development at FSU.