# *NUCLEAR ENERGY RESEARCH INITIATIVE*

## Deployment of a Suite of High-Performance Computational Tools for Multi-scale Multi-physics Simulation of Generation IV Reactors

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**Project Description**

The overall purpose of this collaboration is to deploy advanced simulation capabilities for next generation reactor systems utilizing newly available, high-performance computing facilities. The goals are 1) to develop and deploy high-performance computing tools for coupled thermal-hydraulic, neutronic, and materials multi-scale simulations of the sodium fast reactor (SFR) and 2) apply the new computational methodology to study reactor fuel and core transient response under beyond-design and accident conditions.

The work will encompass a broad spectrum of issues that are critical for developing next-generation reactors. Deliverables will include multi-physics, multi-scale computational modeling capabilities to investigate the impact of long-term thermal and mechanical loads and high-burnup fuel on reactor safety and accident mitigation strategies. The consortium will address three major groups of problems: 1) development of new simulation capabilities for state-of-the-art computer codes (FronTier, PHASTA, and NPHASE) coupled with MD-type analysis, 2) development of advanced numerical solvers for massive parallel computing, and 3) deployment of a multiple-code computational platform for the Blue Gene supercomputer simulations of SFR fuel performance during accidents.

Researchers will use the simulation codes to study fuel performance, including molecular-scale fission product release from ceramic fuel material, local core degradation, and fission product/fuel particle transport and release in the reactor core. Since no single computer code or technology level can be expected to cover such a broad range of design and operation issues during the reactor's lifetime, it is anticipated that the proposed suite of tools will dramatically improve the accuracy and efficiency of reactor simulations. This, in turn, will significantly reduce conservative design and safety margins that are inherently associated with current reactor engineering methods.