HPC Access to Advance Understanding of Fission Gas Behavior in Nuclear Fuel

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Program: NSUF-2 Access Only to provide HPC resources to DOE ASCR-NE Pilot SciDAC project

ABSTRACT:

This proposal is requesting access to 10 Million cpu hours of high performance computing (HPC) resources each of 2 years, at the INL through the NSUF to support a high visibility pilot project demonstrating the ability of the DOE Office of Nuclear Energy to work with the Office of Science as part of the Scientific Discovery through Advanced Computing (SciDAC) program. The objective of this project is to develop high-performance simulation tools to predict fission gas bubble evolution in nuclear fuel, and to demonstrate a SciDAC partnership project between the DOE Office of Advanced Scientific Computing Research (ASCR) and DOE NE. Deployment of these tools will require the utilization of high performance computing resources, in addition to the development of a leadership-class computational code capable of spanning the multiple length and time scales needed to address the complex physical and computational challenges associated with accurately modeling nuclear fuel. More specifically, the research activities will focus on two research thrusts:

- **Thrust 1: Large-scale atomistic simulations to understand fission gas behavior.** Molecular dynamics (MD) and accelerated MD (AMD) simulations of Xe diffusion and gas bubble re-solution, supplemented by selected ab-initio calculations to validate specific gas-defect cluster diffusion mechanisms;
- **Thrust 2: Continuum model development to treat fission gas bubbles.** Development of a hybrid and spatially dependent continuum model, which we will call Xolotl-fission to model fission gas bubble evolution in nuclear fuel.

The outcome of this project will be improved insight into the atomistic processes of Xe diffusion and clustering, along with gas re-solution by energetic fission fragments; and the development of a leadership class fission gas simulator, Xolotl-fission, for modeling the spatially dependent bubble population evolution within nuclear fuel. Ultimately this will lead to the development of physically-motivated, computationally benchmarked and experimentally validated engineering-scale models of fission gas release to be used in fuel performance codes like BISON.