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## **Exascale Simulation of Thermal-Hydraulics Phenomena in Advanced Reactors and Validation Using High Resolution Experimental Data**

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### **ABSTRACT:**

Two Minority Serving Institutions, the City College of New York (CCNY) and University of New Mexico (UNM), with a strong record in nuclear reactor thermal-hydraulics research and minority student education, will work together with collaborators at Argonne National Laboratory (ANL) and Purdue University to expand their expertise and capabilities in nuclear reactor simulation work and train minority students in numerical simulations of Gen IV reactors. They will use an advanced thermal-hydraulics code, Nek5000 or its GPU-oriented version, NekRS, which is a spectral element open source CFD solver developed by the Department of Energy and designed to simulate low Mach number flows of compressible fluids such as a gaseous coolant in a High Temperature Gas Reactor (HTGR), and low Prandtl number molten metal flows in a Sodium Fast Reactor (SFR). Unlike commercial CFD codes such as FLUENT, Nek5000/RS is especially suitable for performing Multiphysics simulations within the MOOSE framework.

Both CCNY and UNM will recruit and train graduate students from underrepresented minority groups in the use of Nek5000/RS and STAR-CCM+ CFD codes to simulate thermal hydraulics phenomena in a HTGR and SFR. The students will perform exascale simulations and validate their models using existing experimental data available from CCNY and Purdue University. All the members of the IRP team will then compare the simulation results between Nek5000/RS and STAR-CCM+, and identify the limitations and areas in need of improving the simulation performance of the two codes. Although Nek5000/RS is not expected to be used on a routine basis or as part of an Evaluation Model for licensing by NRC, it would be highly useful for verifying the accuracy of commercial CFD codes such as STAR-CCM+ and FLUENT, and licensing codes to be used by NRC.

After the completion of this project, the students will be able to join DOE's National Laboratories, Nuclear Regulatory Commission (NRC) and industry developing HTGRs and SFRs such as Framatome and GE-Hitachi, respectively. This proposed project could thus contribute directly to the training of future engineers with expertise in the use of Nek5000/RS and CFD codes for large scale simulations of Gen IV reactors.

CCNY and UNM will work with ANL to guide and train the students in the use and development of Nek5000/RS for simulations of two benchmark problems: CCNY's experiments on helium-air mixing in HTGR cavities and Purdue University's experiments on thermal stratification of a liquid metal in a pool-type SFR. UNM will conduct CFD simulations of the same benchmark experiments using a commercial CFD code, STAR-CCM+, used widely by the industry. The results of Nek5000/RS and commercial CFD code simulations will be compared to not only help achieve a better understanding of the physics underlying the helium-air gas mixing in HTGR cavities and thermal stratification phenomena in a Sodium



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Fast Reactor, but also in identifying the limitations and improvements needed in Nek5000/RS and the CFD codes commonly used in the development and licensing of HTGRs and SFRs in the future.

ANL will help train the CCNY and UNM students in the use of High-Performance Computing paradigms and platforms and provide support for the simulation model development, computational performance and optimization for each problem. ANL will also enable and facilitate large-scale, computationally intensive simulations which will run on the latest, leadership-class supercomputers (ThetaGPU, Polaris and Aurora) at the Argonne Leadership Computing Facility (ALCF). For validation of the Nek5000/RS and STAR-CCM+ simulations, the experimental data from the current NEUP R&D projects underway at CCNY and Purdue will be used, so all the experimental data will be made available at practically no cost to this IRP project.

Graduate students to be supported and trained at CCNY and UNM would be recruited from underrepresented minority groups. They would study nuclear engineering subjects at the graduate level and receive training in the use of Nek5000/RS and STAR-CCM+, and High-Performance Computing for the simulation of advanced reactors and model validation methodologies. UNM students would study in a graduate level CFD course taught at CCNY, and CCNY students would study advanced nuclear engineering courses offered by UNM. This mutual course offering would help both CCNY and UNM students gain basic knowledge of exascale simulation using advanced codes, as well as knowledge of nuclear engineering subjects including reactor thermal-hydraulics.

During the summer, these students will visit the partner institutions and interact with the faculty, students and research staff, so they could broaden their learning experiences and improve their research skills. They will also experience research internships at ANL or other National Laboratories such as Sandia, LANL, and INL. Before graduating, they will pass on their knowledge of large-scale computing using Nek5000/RS and STAR-CCM+ to other students conducting nuclear engineering research at their own institutions. After completion of their graduate programs, the students will be highly skilled in modeling of advanced reactors and able to enter and contribute to the nuclear engineering workforce at DOE's National Laboratories, NRC and industry.