U.S. Department of Energy

Project Title

Development of an Efficient Meso-scale Multi-phase Flow Solver in Nuclear Applications

PI: Taehun Lee – City College of City University of New York (CCNY)

Program: NEAMS-2

Collaborators: Sanjoy Banerjee – CCNY

Masahiro Kawaji – CCNY

Kent E. Wardle – Argonne National Laboratory

ABSTRACT

The proposed research aims at formulating a predictive high-order Lattice Boltzmann Equation for multi-phase flows relevant to nuclear energy related applications—namely, saturated and sub-cooled boiling in reactors, and liquid-liquid mixing and extraction for fuel cycle separation. An efficient flow solver will be developed based on the Finite Element based Lattice Boltzmann Method (FE-LBM), accounting for phase-change heat transfer and capable of treating multiple phases over length scales from the submicron to the meter. LBM is a mesoscale approach, which can accommodate coarse-grained, molecular-level information into the macroscopic description of complex interfacial phenomena. This is achieved by introducing a phase field function into a single-phase lattice Boltzmann formulation to distinguish between phases (i.e. liquid-vapor or liquid-liquid), together with a phenomenological free energy functional of the solid-liquid-vapor system whose dissipative minimization constrains the temporal evolution of the phase field. The proposed FE-LBM will provide stability and geometric flexibility while retaining the original LBM's high accuracy and scalability in massively parallel computing platforms.

A thermal LBM will be developed in order to handle adjustable *Prandtl* number, arbitrary specific heat ratio, a wide range of temperature variations, better numerical stability during liquid-vapor phase change, and full thermo-hydrodynamic consistency. Recent advances in multiphase LBM methodology have also demonstrated the potential for extension of LBM beyond two phases. We propose to extend FE-LBM to liquid–liquid–gas multi-phase flows for application to high-fidelity simulations building up from the meso-scale up to the equipment sub-component scale. While several relevant applications exist, the initial applications for demonstration of the efficient methods to be developed as part of this project include numerical investigations of Critical Heat Flux (CHF) phenomena in nuclear reactor fuel bundles, and liquid-liquid mixing and interfacial area generation for liquid-liquid separations. Large Eddy Simulation (LES) based on the dynamic global-coefficient model for multi-phase flows will be carried out. In addition, targeted experiments will be conducted for validation of these advanced multi-phase models.