ADVANCED PARALLEL COMPUTING METHODLOGIES FOR MULTl-PHYSICS INDUSTRIAL PROBLEMS

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Summary. High performance computing of multi-scale and multiphase flows using two different and novel approaches will be highlighted in this work.

Computational Fluid Dynamics (CFD) is routinely used to model many problems of engineering interests that involve turbulent mixing, multi-phase flows, chemically reactive flows and flows with heat transfer. The governing equations and numerical/physical model formulations are being constantly improved which enables accurate and faster computations of many physical phenomena. However, thermal and fluid flow problems encountered in realistic engineering applications are often multi-scale and multi-physics in nature and hence are computational resource intensive. High performance computations using multiple cores are being routinely used in industry for design and to address product issue that may arise in the field. In this work, two example problems from multi-scale, turbulent reacting flows and multiphase flows applied to heat transfer applications will be used to highlight UTRC’s exploration in the field of high performance parallel computing.

Direct Numerical Simulation of Reacting Flows using Heterogeneous computing:

The first problem is an idealized problem looking at the micro-physics of turbulent mixing and combustion investigated using Direct Numerical Simulations, where all physical length and times scales are fully resolved. It is preferable to use detailed chemical kinetic mechanisms to describe the evolution of species concentration during chemical reactions. However, computing chemical kinetic equations takes nearly 50-90% of the time in reactive CFD codes. In the final manuscript and presentation, we will describe a novel approach in which the chemical kinetics Ordinary Differential Equations (ODEs) were solved using Graphical Processing Units (GPU) while the fluid transport equations (partial differential equations) were solved using Central Processing Units. Results from the performance of this heterogeneous computing approach will be presented.

High Fidelity Simulation of boiling flows:

The particular focus is to develop a simulation technique that is capable of predicting the heat transfer and hydrodynamic characteristics of nucleate boiling and the transition to critical heat flux on surfaces of arbitrary shape and roughness distribution addressing a critical need to design enhanced boiling heat transfer surfaces. The macro-scale of the phase change and
bubble dynamics is addressed through employing fully-resolved Computational Fluid Dynamics (CFD) methods for interface tracking and interphase mass and energy transfer. The microscale of the microlayer, which forms at early stage of bubble nucleation near the wall, is resolved through asymptotic approximation of the thin-film theory which provides a closed-form solution for the distribution of the micro-layer and its influence on the evaporation process. In addition, the sub-grid surface roughness is represented stochastically through probabilistic density functions and its role in bubble nucleation and growth is then represented based on the thermodynamics of nucleation process. This combination of deterministic CFD, local approximation, and stochastic representation allows the simulation of pool boiling on any surface with known roughness and enhancement characteristics. In addition, an extension to high-Reynolds number convective boiling flows is presented where multiphase heat transfer phenomena span scales of many orders of magnitude, from nucleation of bubble embryo (10–7m) all the way to macroscale (1m) geometry felt by the flow. To overcome such multiscale challenges, two different models have been developed to resolve different physics with relevant range of scales. The characteristics of nucleate boiling near the wall are resolved through a previously developed high-fidelity model for pool boiling flows. The information from this model is transmitted through a buffer layer into a large-scale LES-based model to simulate the large-scale two-phase flow away from the wall (e.g. in the core for an in-tube configuration) allowing one to capture the hydrothermal characteristics of convective boiling flow in a practical fashion.