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NUMERICS FOR DIVERSE EXASCALE PLATFORMS WITH APPLICATION TO MULTI-PHASE AND SPECIES FLOW

Spencer Bryngelson[1], Benjamin Wilfong[1] and Anand Radhakrishnan[1]*

[1]Georgia Institute of Technology

ABSTRACT

Exascale computing devices came online in 2024 and are diversifying. These span GPU-focused machines (AMD MI250X for OLCF Frontier and Intel Max for ALCF Aurora) to superchip-based devices (AMD MI300A for LLNL El Capitan and NV GraceHopper for JSC JUPITER). The numerical method often has the primary computational cost in multiphase flow simulation, so appropriate methods and implementations are required to use these machines efficiently. The numerical method's performance is often stunted by the low arithmetic intensity it presents to the GPU device. Beholden to this constraint, crafting new methods or implementations is required for efficient device use. This work presents optimizations and algorithmic strategies for maximizing the device's computational capability. We focus on maintaining the robustness the computational multiphase flow community expects, including treatment shock and interface discontinuities and positivity of advected fields. All methods are implemented in MFC [Bryngelson et al. Comp. Phys. Comm (2021)]. Results are presented for methods of finite difference and ENO flavors. Device-focused optimization, both on GPU and superchip devices, will be presented. We show that high-order accurate WENO methods can achieve near-peak compute utilization. We navigate concerns like large on-device memory footprints, which can constrain simulated problem size. Application results are shown for canonical multiphase flows, including shock-bubble and shock-droplet interaction problems.