Multiphase flow numerics: Perspectives from exascale simulation

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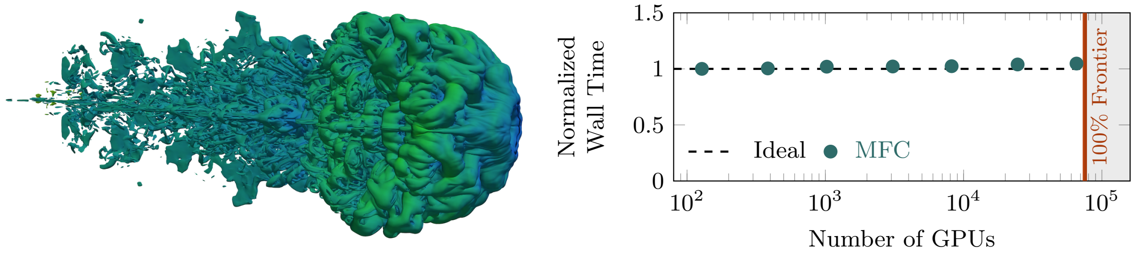
Multi-phase and multi-component flows arise broadly, from cavitation around high speed underwater vehicles to biomedical treatments for kidney stones. The combination of scales in these problems, and others like them, lead to simulations with large grid sizes and small time steps. Still, understanding multiphase flow phenomenologies and the quantities of interest that buttress them are required to develop sub-grid models for them, such as those of Euler–Euler and Euler–Lagrange types. This work presents the use of CFD software at exascale to conduct full-resolution simulation for computational modeling.



(a) Shock–droplet breakup (b) Weak Scaling

Figure 1: (a) Representative MFC simulation and (b) its weak scaling on OLCF Frontier.

We show that exascale supercomputers, like OLCF Frontier, can enable unprecedented resolution and simulation of compressible multi-phase problems. These simulations are conducted via the Multi-component Flow Code (MFC) [1]. MFC is open source (mflowcode.github.io) and GPU-accelerated. The MFC solver uses high-order accurate numerics and marshals different multi-component diffuse interface (4–6 equation models) and sub-grid models for particles, bubbles, and droplets. Figure 1a shows the vorticity around an atomizing droplet via an impinging shock-wave, conducted with MFC.

Efficient use of exascale systems requires performant numerics on NVIDIA- and AMD-GPU-based supercomputers. We accomplish this via high-order WENO reconstructions and HLL-type approximate Riemann solvers. Flux computations are dimensionally-split and array reshaping enables performant nested loop computation in the most expensive kernels: reconstructions and Riemann solves. These methods are offloaded to GPU devices via OpenACC, achieving about a 300-times speedup in the most expensive kernels over single CPU cores. Figure 1b shows that our combination of numerics and GPU acceleration has weak scale nearly ideally (within 95%) to all of Frontier, the first exascale GPU supercomputer (66K GPUs).

References

[1] A. Radhakrishnan, H. Le Berre, B. Wilfong, J. -S. Spratt, M. Rodriguez, T. Colonius, S. H. Bryngelson, *Method for portable, scalable, and performant GPU-accelerated simulation of multiphase compressible flow*, arXiv:2305.09163.

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