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Toward the development of an efficient and scalable computational fluid dynamics solver for mesoscale phase separation problems

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The separation of a dispersed mixture of immiscible fluids is a common problem that arises in many fields of engineering. Such mixtures can take the form of emulsions of one liquid in another, mists or sprays of liquid droplets in a gas continuum, or foams of gas bubbles separated by thin liquid films. Numerous physical phenomena play a part in the behaviour of groups of droplets or bubbles including gravitational settling, steric interactions, film drainage effects, and coalescence or break-up. These phenomena typically operate over a very widerange of length and time scales, making numerical solution with unified solvers extremely challenging. Existing methods for such problems have focused on either resolving the macro scales, typically using Euler-Euler or CFD-DEM coupling algorithms which require empirical closures, or resolving only the micro scales, using direct numerical simulation in small regions around individual particles.

In this talk an alternative approach for such problems, the dynamic multi-marker method, is discussed. The new algorithm draws from fully-resolved VOF techniques developed for the micro scale and extends them efficiently to the mesoscale, permitting systems with hundreds or thousands of dispersed particles to be modelled. Such models are capable of acting as virtual prototypes and numerical experimentation platforms, and can be used to develop a better understanding of the dynamic structures that form in dispersed phase flow problems. They are also potentially useful in generating and refining closures required for macro scale methods. An implementation of the dynamic multi-marker method as a multiphase solver in the OpenFOAM® computational mechanics framework will be presented, together with some discussion of the interesting challenges and difficulties that were encountered in the process of optimising it for modern highly-parallel HPC architectures.

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