

Application of high-performance computing for bubble simulations in sonochemistry

Content

The objective of sonochemistry is to increase the yield of chemical processes in a fluid with ultrasound excitation. It is based on a special case of cavitation called acoustic cavitation. Because of the ultrasound excitation, several bubbles and bubble-clouds can be formed in a liquid. During the radial oscillation of the bubbles, their compression can be so large that the internal temperature can reach several thousands of Kelvins inducing chemical reactions. The importance of sonochemistry is in its potential applications, e.g., nano-metal particle production, organic synthesis, or water purification.

Understanding the behaviour of a single bubble in an acoustic field is an important topic of sonochemistry, with many open questions. The presentation focuses on the break-up mechanism of a bubble into several smaller bubbles. To directly observe the behaviour of a single bubble, a computational approach is used (CFD). This requires a multiphase model (gas and liquid). Another difficulty is the differences in spatial scales: the size of a bubble in sonochemistry is usually a few micrometres, while the wavelength of the used ultrasound is a few millimetres. An appropriate spatial resolution of the problem requires a highly resolved adaptive mesh with millions of cells. Furthermore, the problem must be solved in time with an appropriately small step size to correctly simulate the propagation of acoustic waves around the bubble. **Due to the high spatial and temporal resolution, the solution must be parallelized, and supercomputers must be used to reduce the runtime of the simulations.**

To simulate a single bubble, the open-source program package called *ALPACA* is used, which is capable of simulating compressible multiphase flows in 2D or 3D. A multiresolution algorithm is employed to automatically adapt the numerical mesh during the solution process; thus, it is suitable for bubble simulations. Moreover, *ALPACA* is designed to be run on supercomputers. During the research, the *SUPERMUC-NG* supercomputer in Germany is used in collaboration with the *Nanoshock* research group from the *Technical University of Munich*. In this presentation, **we demonstrate the basics of a bubble simulation and analyse the strong scaling of such simulations for up to 300 CPU cores.** Based on the scaling analysis, an appropriate configuration can be found for efficient simulations with which several different parameters (e.g., bubble radius, acoustic excitation frequency) can be tested. Finally, the results of the bubble simulations are discussed.

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Contribution Type: Lecture

Submitted by NAGY, Dániel on Monday 13 June 2022