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Huge-scale molecular dynamics simulation of gas-liquid two-phase flow

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Summary

Gas-liquid two-phase flow is a system containing gas and liquid phase. While the gas-liquid two-phase flow is important for applications such as power plants and pump cavitations, it is difficult to study gas-liquid multiphase flow theoretically or numerically since it is multi-scale and multi-physics system involving not only flow but also phase transitions. In order to overcome the difficulties, we study the two-phase flow with full particle simulations. In the full-particle simulation, phase boundaries create and annihilate spontaneously, and therefore, multi-physics phenomena are naturally simulated. We developed a parallel molecular dynamics (MD) simulation code which is scalable up to ten thousand processes, and have achieved 4.1 billion particles with 8192 MPI processes. In this talk, we introduce how to achieve huge-scale MD simulations on massively parallel computers and show recent results.