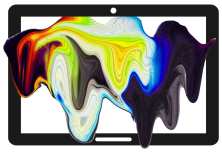

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Massively Parallel Hybrid Molecular-Continuum Simulations

Micro- and nanofluid flow simulations require considering some effects at the molecular scale. Molecular-continuum coupled flow simulations can perform computationally intensive molecular dynamics (MD) simulations in localized regions of a geometry under consideration, and employ classical, computationally cheaper computational fluid dynamics (CFD) solvers for the remaining larger computational domain. This approach reduces computational efforts tremendously while still considering molecular effects in the flow solution. In this poster, we present our methods used in the context of hybrid MD-CFD simulations, such as massively parallel software concepts, parallel-in-time algorithms or multi-MD instance sampling, and their impact on computational time, precision and energy efficiency in comparison to full-MD simulations.

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2,3

Keywords

molecular dynamics, cfd, hpc, multiscale

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