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Accelerating a multiscale continuum-particle fluid dynamics model with on-the-fly machine learning

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Abstract: In fluid dynamics, understanding the complex flows in nanoscale geometries is crucial for a number of engineering applications, from efficient electronic cooling systems and desalination membranes, to precise drug delivery systems and reliable gas pumps which require no moving parts. However, modelling these flows poses a problem: we require an atomistic resolution to capture the non-equilibrium/non-continuum behaviour which dominates fluid flows at this scale, but the state-of-the-art computational techniques to do so are highly computationally expensive. Here we present the application and verification of a hybrid continuum-particle multiscale technique to transient fluid flows in high-aspect-ratio nanoscale channels. To do this, we couple a macroscopic continuum model (derived from mass and momentum continuity) with an array of particle simulations, exploiting the scale separation between the macro and micro models in both time and space. Further, we suggest a general enhancement to hybrid methods by modelling a growing database of particle simulations with a Gaussian process, and using Bayesian inference to predict the output of new configurations; this removes a common flaw whereby many similar particle simulations are performed and information is discarded after one use. We validate our hybrid method results against experimental data and full particle simulations, and estimate our computational savings to be up to several orders of magnitude.

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