How we can make DSMC more computationally scalable, while preserving its accuracy

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In this talk, I will describe our latest developments of DSMC-continuum multiscale methods. The goal of multiscaling involves using DSMC in parts of the solution, but achieving an overall faster computation than DSMC would alone, with minimal losses in predictive accuracy. The target market of these multiscale methods has been either in comparing with experimental results, and for industrial design of low-pressure, low-speed microsystems, where in both cases DSMC is too prohibitive to provide any meaningful solution.

Many important publications have sparked this research field of multiscaling using DSMC, including at its infancy, the use of domain decomposition (DD) [1]. In DD, the method resolves regions of thermodynamic non-equilibrium (such as near wall regions, or regions of shockwaves in bulk [2]) using DSMC, while coupling the flow physics with a computationally cheaper Navier-Stokes continuum solver in the far-field.

Our vision for the next-generation multiscale methods has been to make larger computational savings that DD simply does not always offer, such as in microscale gas flows. In this talk I will describe some of these developments in depth. Broadly speaking, I will talk about three areas of development. (1) In *concurrent multiscaling*, like in DD, the DSMC runs concurrently as the continuum solver, exchanging information as the simulation evolves. I will show our heterogeneous methodologies [3,4] that have led to agreement of thermal transpiration flows in Knudsen pump experiments [5]. (2) In *sequential multiscaling*, the DSMC is first run on simple, small representative cases of the full problem, with data tabulated, or relationships developed manually and numerically incorporated to correct traditional and fast computational fluid dynamics (CFD) solvers. I will show the high scalability of these type of simulations on quasi-3D lubrication flow problems. (3) Finally, in *smart concurrent/sequential methods*, we have recently adopted physics-informed learning approaches in concurrent multiscale methods to automate the development of the underlying physical relationships from the DSMC training of surrogate models, which could be then used in a sequential simulation. This framework provides us with smooth flow fields, a probability criterion to stop the DSMC once the models are found and calibrated, as well as the ability to quantify the uncertainty of the final macroscopic flow fields.

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