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Determination of the shear and bulk viscosity from equilibrium molecular-dynamics simulations[1] FREDERIKE JAEGER, ERICH MULLER, OMAR K. MATAR, Imperial College London — Determining fluid properties accurately is essential for large-scale fluid dynamics simulations where only a few parameters determinethe behaviour of an entire system. Even though many properties are well known, others are more obscure and difficult to determine experimentally. One such property is the bulk viscosity which plays a particularly large role in compressible fluids but is rarelyconsidered in fluid-dynamics simulations. We determine both the shear and bulk viscosity using equilibrium methods within themolecular-dynamics framework using both atomistic and coarse-grained models with a view of assessing both the accuracy of coarse-grained models for transport-property calculations and the necessity of including such properties at various scales and scenarios.

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