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Nonequilibrium molecular dynamics of vapor–liquid interface TAKERU YANO, Osaka University, Japan — Evaporation and condensation at a vapor–liquid interface are studied by moderately large-scale nonequilibrium molecular dynamics simulations for a vapor–liquid two phase system composed of about 0.3 million Lennard-Jones molecules. Constant evaporation and condensation are realized by driving two vapor regions on the either side of a planar liquid film, and thereby the simulation is free from artificial controls of molecular motions in the liquid film and in the neighborhood of the interfaces. This enables us to evaluate the mass, momentum, and energy fluxes across the system, which are relevant to the velocity distribution of molecules leaving the interface at the vapor–liquid nonequilibrium states.

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