Erratum: Energy and pressure of shearing fluids at different state points [Phys. Rev. E 64, 021201 (2001)]

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In the above-mentioned paper, we reported the strain rate dependence of energy and pressure for a system of shearing Lennard-Jones atoms at three distinct state points. We have since discovered an error with the input parameters for the Lennard-Jones potential that implies the calculations were not conducted at the strain rates and state points given in the original paper. This led to systematically higher values in the actual temperature, density, and strain rates compared to those quoted by 18.5%, 4%, and 10.3%, respectively. We also note that the energy reported in the paper was the potential energy per particle (the kinetic energy is kept fixed by the thermostat).

In this Erratum we repeat all the simulations at the intended state points and strain rates. The results of our simulations are presented in Figs. 1, 2, and 3, along with the average absolute deviations (AADs). Clearly, we observe the same trends as previously reported, i.e., the $\dot{\gamma}^{3/2}$ behavior of pressure and energy is only observed at the Lennard-Jones triple point. The midpoint and high-point data are more accurately described by a $\dot{\gamma}^2$ dependence.

Since the temperatures and densities in the original paper were actually different from those reported (18.5% higher in temperature and 4% higher in density), there is one important consequence of this, namely, that the $\dot{\gamma}^{3/2}$ dependence occurs *in the vicinity* of the triple point, not exactly at the triple point. It implies that the exponent of the strain rate dependence varies from ~2 to ~1.5 as the triple point is approached. We are conducting further simulations to confirm this.

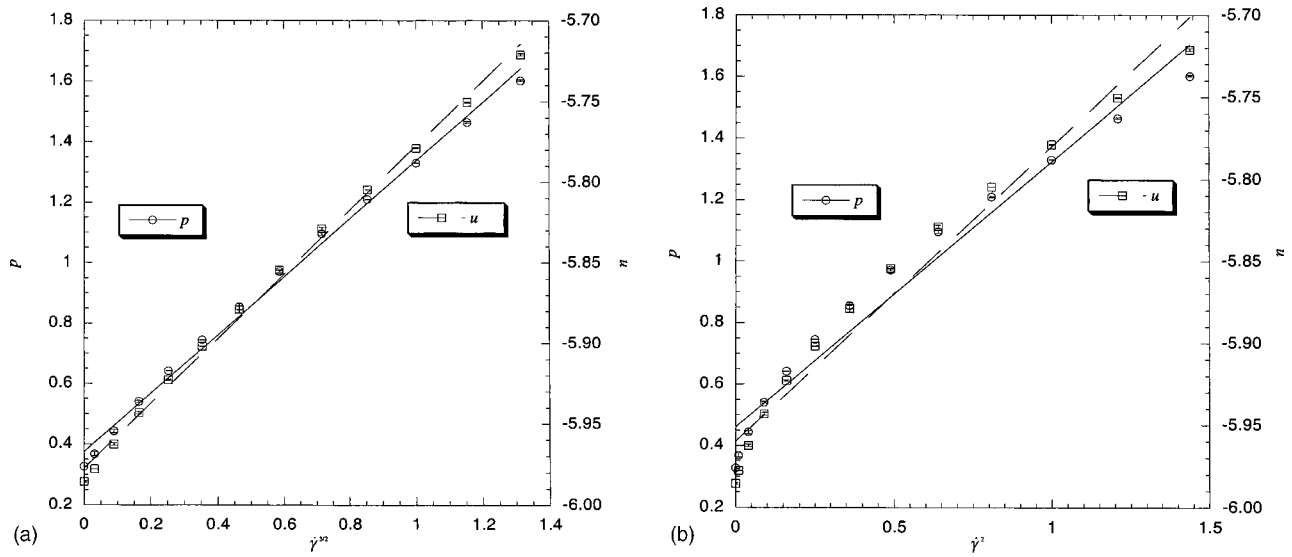

FIG. 1. Reduced pressure and potential energy per particle as functions of (a) $\dot{\gamma}^{3/2}$ and (b) $\dot{\gamma}^2$ at the Lennard-Jones triple point. AADs are 2.62% and 0.45% for the pressure and energy of (a), respectively, and 6.58% and 1.28%, respectively, for (b).

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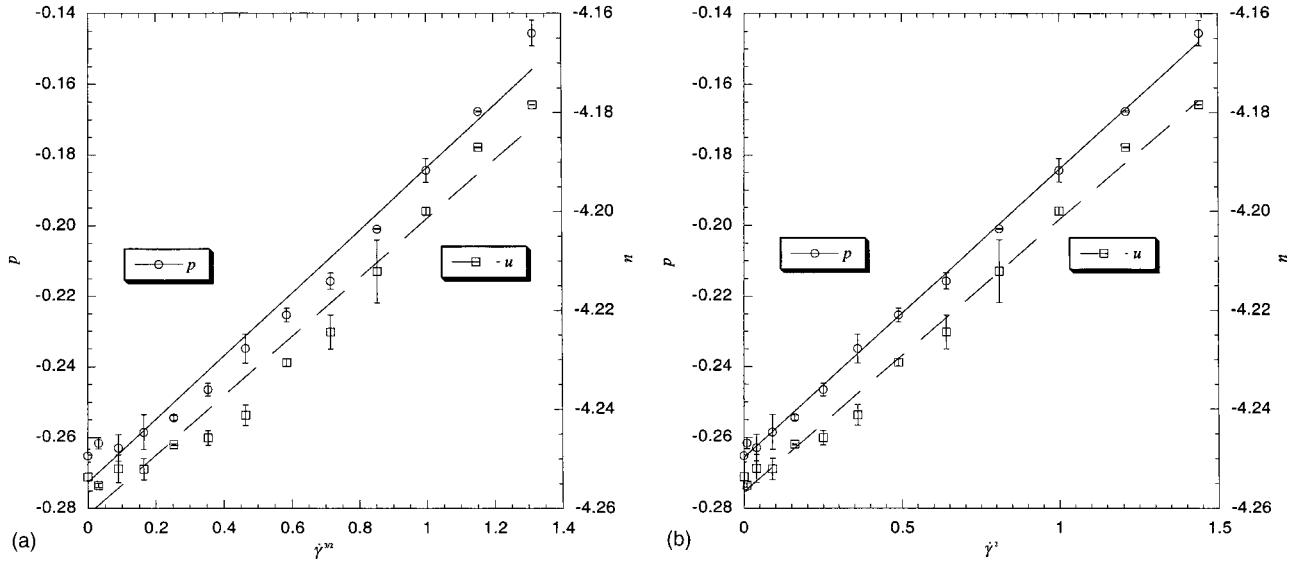

FIG. 2. Reduced pressure and potential energy per particle as functions of (a) $\dot{\gamma}^{3/2}$ and (b) $\dot{\gamma}^2$ at the midpoint. AADs are 0.46% and 0.41% for the pressure and energy of (a), respectively, and 0.13% and 0.19%, respectively, for (b).

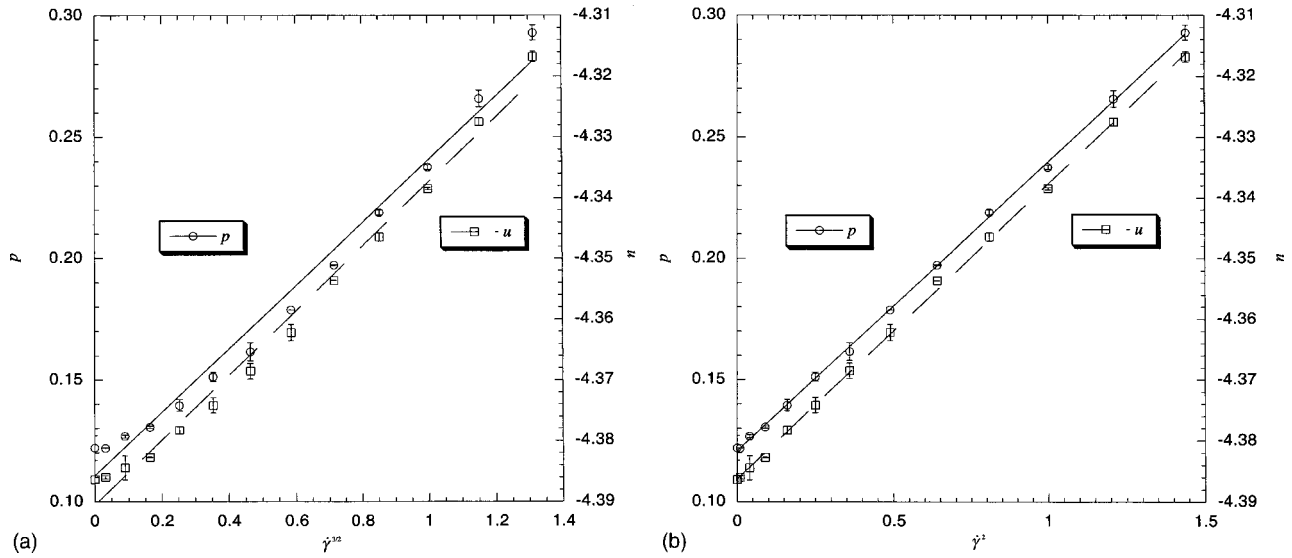

FIG. 3. Reduced pressure and potential energy per particle as functions of (a) $\dot{\gamma}^{3/2}$ and (b) $\dot{\gamma}^2$ at the high point. AADs are 0.61% and 0.21% for the pressure and energy of (a), respectively, and 0.09% and 0.04%, respectively, for (b).