# SYSTEM SIZE DEPENDENCE OF THE DIFFUSION COEFFICIENTS IN MD SIMULATIONS: A SIMPLE PRACTICAL CORRECTION FORMULA

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A practical correction formula relating the self-diffusion coefficient of dense liquids from molecular dynamics simulations with periodic boundary conditions to the self-diffusion coefficient in the thermodynamic limit is discussed. This formula has a very simple form $D = D_0(1 - \gamma N^{-1/3})$, where $D_0$ is the self-diffusion coefficient in the thermodynamic limit and $N$ is the number of particles in the simulation. The numerical factor $\gamma$ depends on the geometry of the simulation cell. Remarkably, $\gamma \simeq 1.0$ for the most popular cubic geometry. The success of this formula is supported by results from MD simulations, including very recent simulations with a "magic" simulation geometry.