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Softening the Hard-Sphere Fluid ERIC KREBS, SAMUEL LOOMIS, PATRICK KREITZBERG, DAVID ROUNDY, Oregon State University — The hard-sphere fluid is a widely used reference fluid for theoretical frameworks for real fluids that, while well studied and understood, doesn't match particularly well with real physical fluids. For inhomogeneous hard-sphere fluids, Fundamental Measure Theory (FMT) is a standard classical density functional theory that predicts the hard-sphere free energy. A "soft" FMT (SFMT) was introduced by Schmidt [1] which is based on FMT and allows for penetrable spheres determined by a pair potential. We study a soft fluid with a simple potential describing slightly penetrating spheres at moderate temperatures based on SFMT. We compare the predicted equation of state against Monte-Carlo simulation for a homogeneous soft fluid and for soft spheres near a hard wall.

[1] Schmidt, M. Phys. Rev. E 62(4), 4976 (2000)

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