Testing "Soft" Fundamental Measure Theory for not-so-hard-sphere fluids ERIC KREBS, PATRICK KREITZBERG, DAVID ROUNDY, Oregon State University — A standard approach for modelling in-homogeneous distributions of the hard-sphere fluid is the Fundamental Measure Theory (FMT) formulation of classical density functional theory. Due to the paucity of truly hard spheres in the real world, it seems advisable to consider interactions that are not quite so "hard," a challenge tackled by the "Soft" FMT (SFMT) introduced by Schmidt [1]. We apply SFMT to a simple potential describing slightly penetrable spheres, that is, spheres at moderate temperatures—such that the spheres are thermally able to penetrate by a short distance. We compare the predicted equation of state with the result of Monte Carlo simulations, and also compare the free energy and density distribution near a hard wall with simulation.

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

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Date submitted: 19 Nov 2012   Electronic form version 1.4