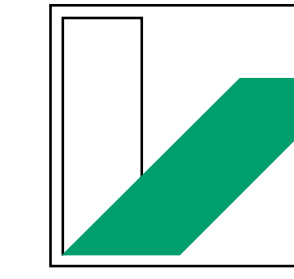


Neural functionals in statistical mechanics

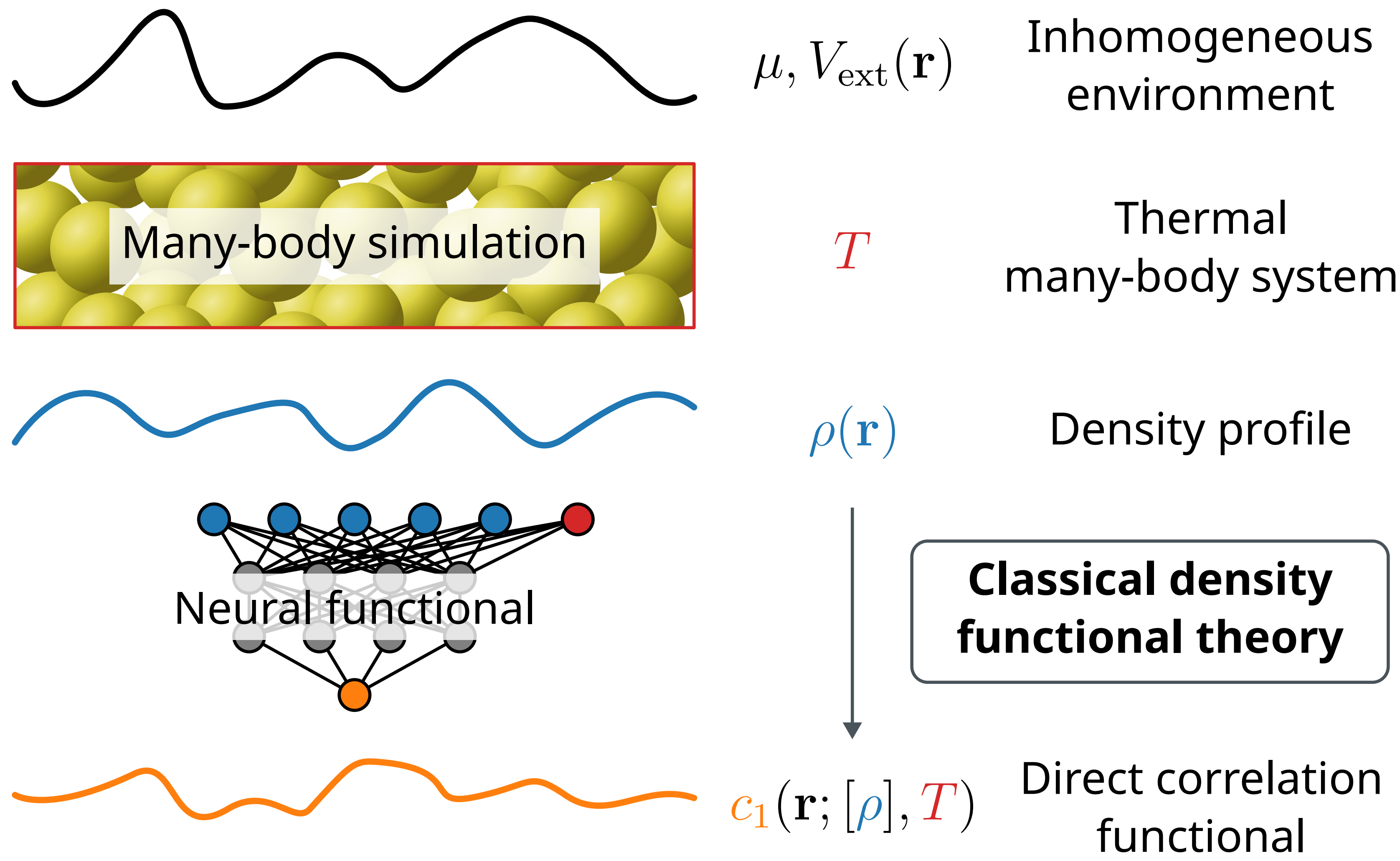
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Theory and workflow



Methods

Calculation of density profiles

$$\rho(\mathbf{r}) = \exp(-\beta(V_{\text{ext}}(\mathbf{r}) - \mu) + c_1(\mathbf{r}; [\rho], T))$$

self-consistent iteration

Neural functional calculus

Pair correlations

$$c_2(\mathbf{r}, \mathbf{r}'; [\rho], T) = \frac{\delta}{\delta \rho(\mathbf{r}')} c_1(\mathbf{r}; [\rho], T)$$

autodiff

Free energy

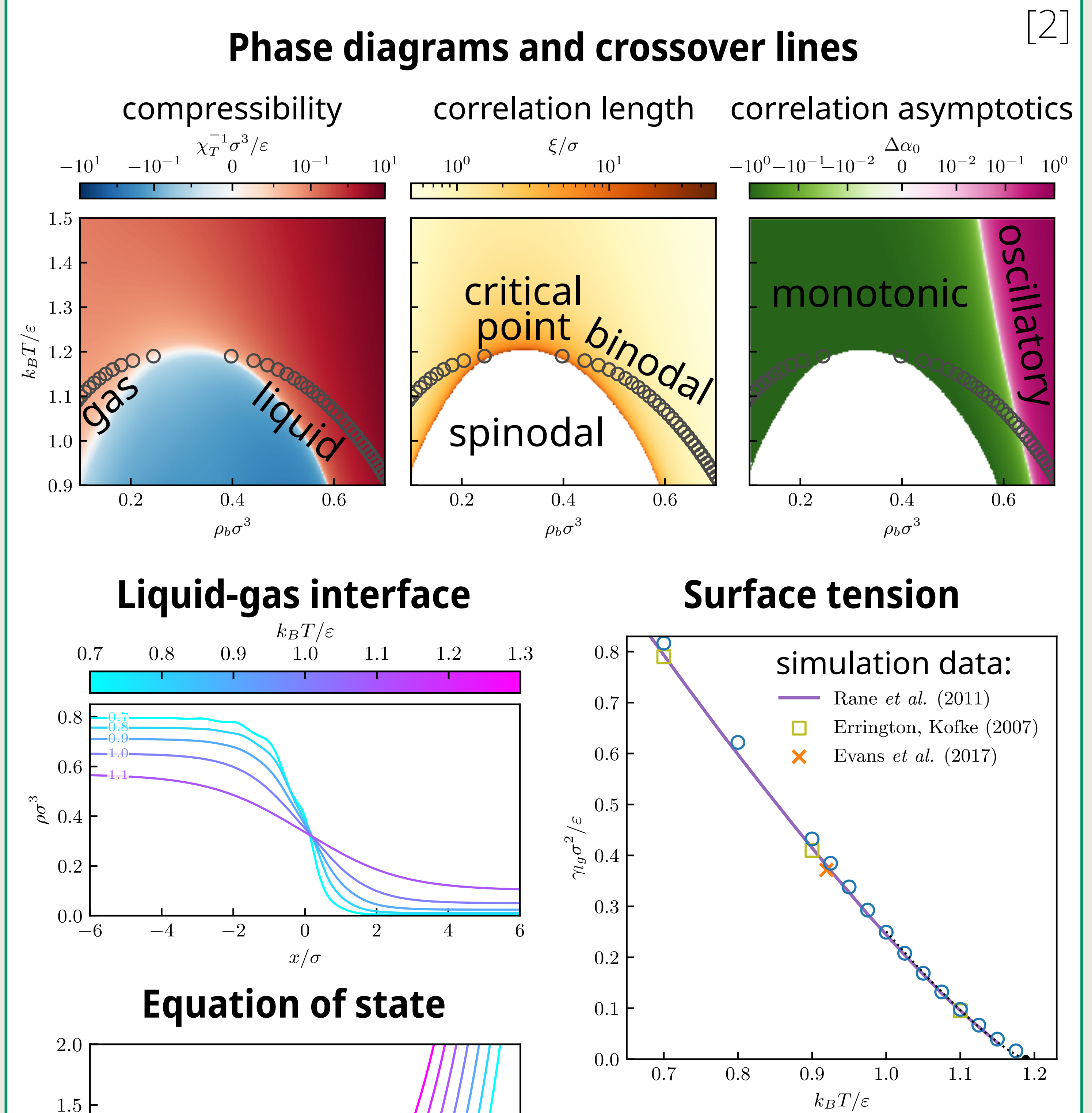
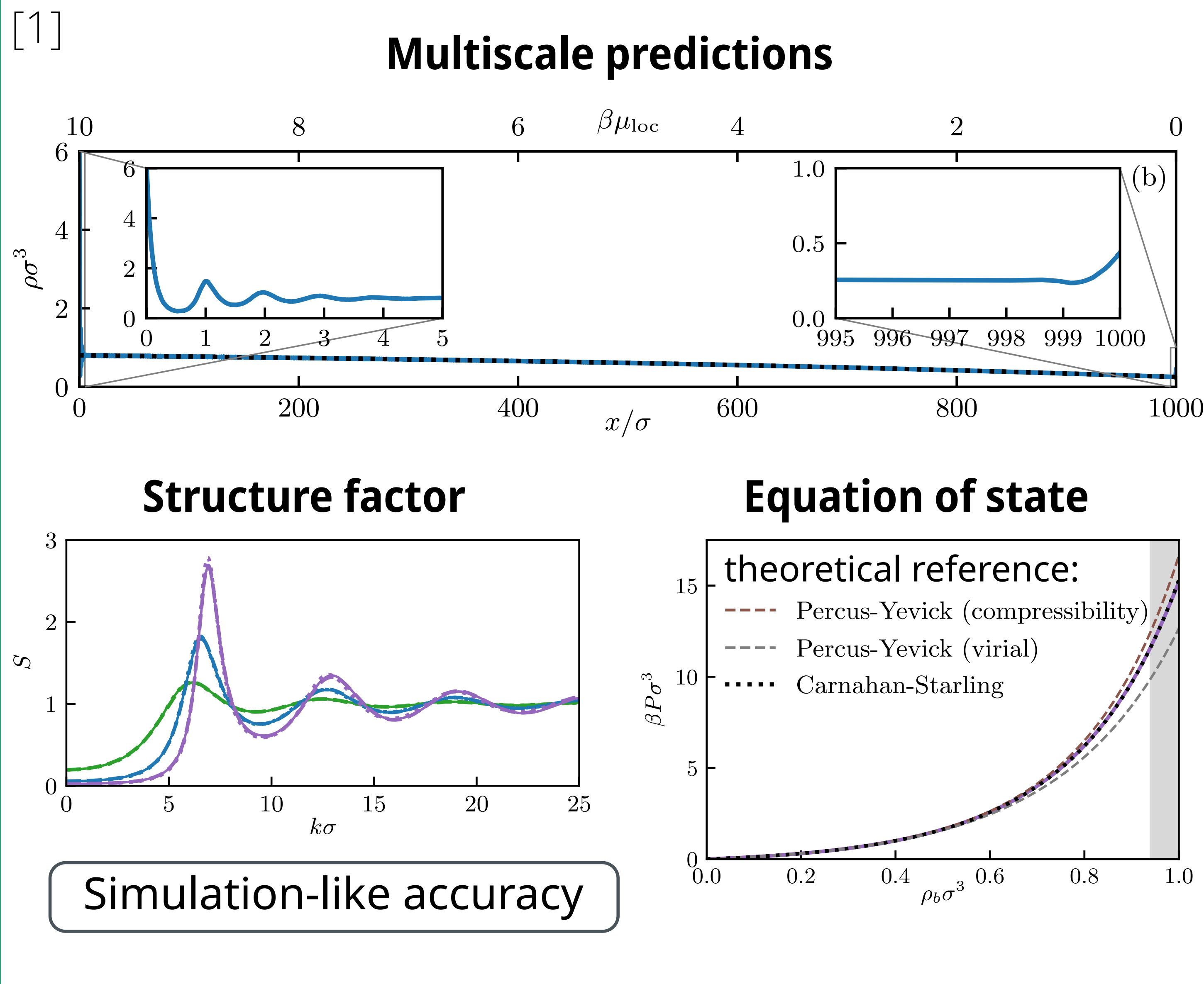
$$F_{\text{exc}}([\rho], T) = -k_B T \int \mathcal{D}[\rho] c_1(\mathbf{r}; [\rho], T)$$

functional line integral

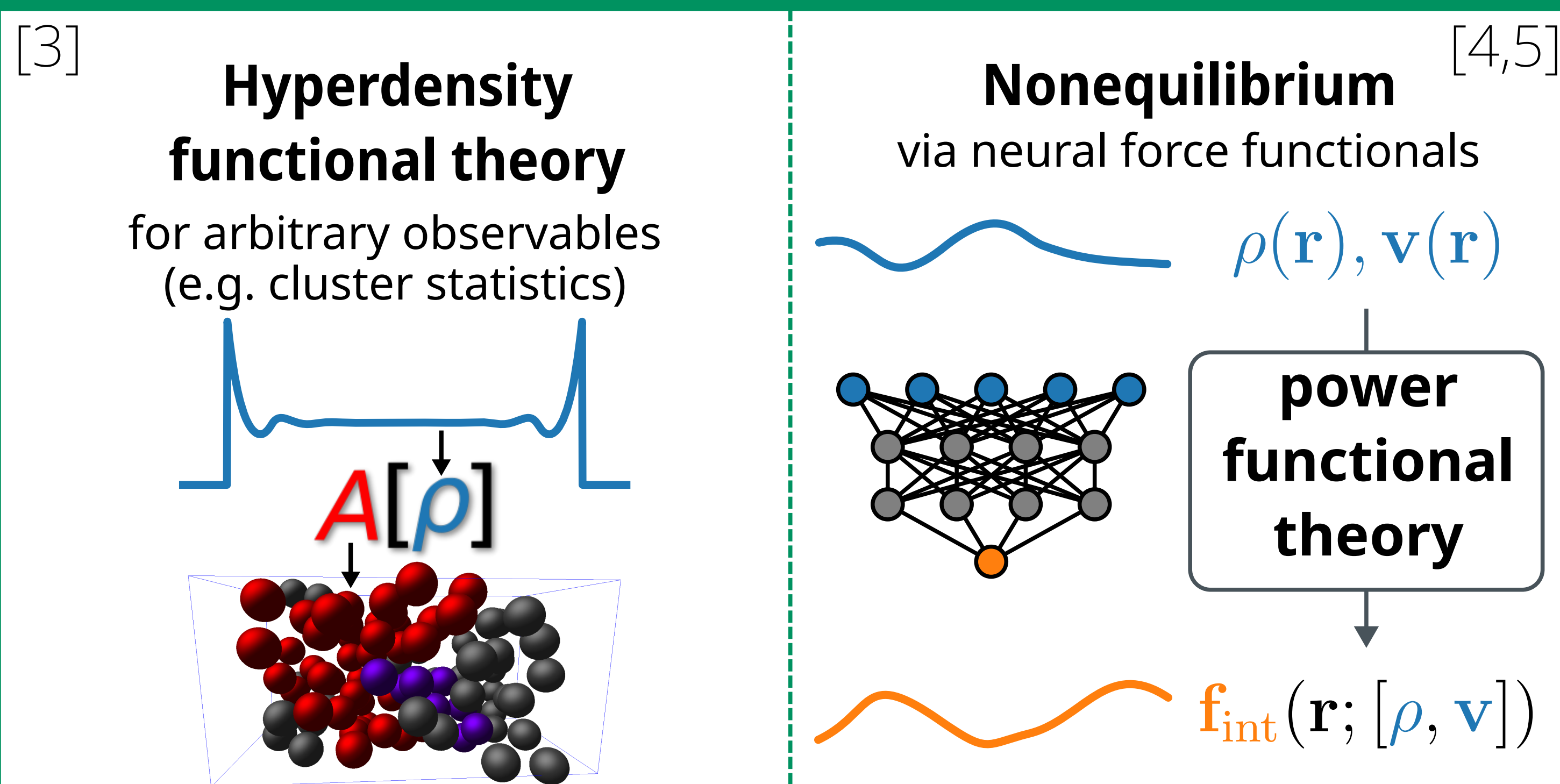
Hard spheres

Results

Lennard-Jones



Extensions



For purely supercritical training:
Discovery of phase coexistence via extrapolation

[1] F. Sammüller, S. Hermann, D. de las Heras, M. Schmidt, Proc. Natl. Acad. Sci. **120**, e2312484120 (2024).

[2] F. Sammüller, M. Schmidt, R. Evans, Phys. Rev. X **15**, 011013 (2025).

[3] F. Sammüller, S. Robitschko, S. Hermann, M. Schmidt, Phys. Rev. Lett. **133**, 098201 (2024).

[4] D. de las Heras, T. Zimmermann, F. Sammüller, S. Hermann, M. Schmidt, J. Phys.: Condens. Matter **35**, 271501 (2023).

[5] T. Zimmermann, F. Sammüller, S. Hermann, M. Schmidt, D. de las Heras, Mach. Learn.: Sci. Technol. **5**, 035062 (2024).

[6] F. Sammüller, S. Hermann, M. Schmidt, J. Phys.: Condens. Matter **36**, 243002 (2024).

Code and data [1,2]



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Tutorial [6]



github.com/sfalmo/NeuralDFT-Tutorial