Harmonically Mapped Averaging for Everyone

Ensemble Averages

- Core of statistical mechanics
- Relate molecule coordinate averages to material properties
- Example: Pressure tensor

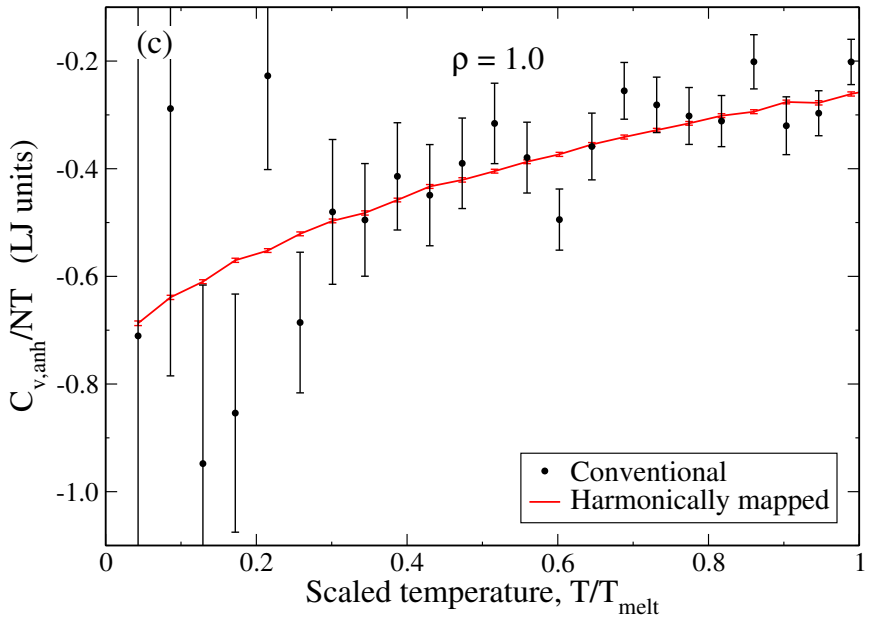
$$\mathbf{P} = \rho kT\,\mathbf{I} + \frac{1}{3V}\left\langle \sum_{i<j} \mathbf{f}_{ij}\mathbf{r}_{ij} \right\rangle$$

Mapped Averages

- Writes averages rigorously as deviation from an approximate starting point
- For crystals, a good starting point is a harmonic lattice
- Example: internal energy

$$U = \frac{3}{2}NkT + \left\langle U_{\text{config}} + \frac{1}{2}\mathbf{F}\cdot\Delta\mathbf{r} \right\rangle$$

Performance: Heat capacity



SSE project: Implement in these codes

LAMMPS ✓

etomica ✓

VASP (b-initio ienna ackage imulation) ✓

HOOMD-blue

Cassandra Monte Carlo SOFTWARE