Implementing Harmonically Mapped Averaging Methods on Popular Molecular Simulation Platforms

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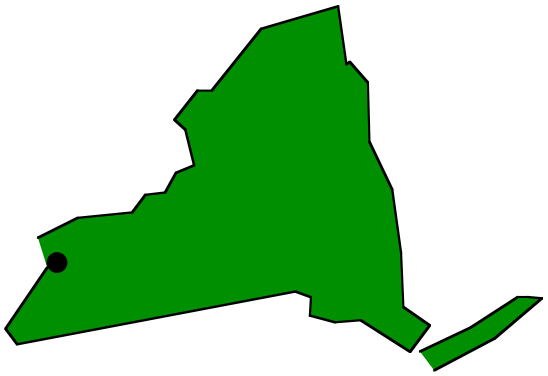

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Ensemble Averages

- Core of statistical mechanics
- Relate averages over molecule coordinates to thermophysical properties
- Example: Pressure tensor (pairwise-additive potential)

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

Mapped Averaging

- We invented a new general framework relate properties to ensemble averages
- Writes averages rigorously as deviation from an approximate starting point
- For crystals, a good starting point is a harmonic lattice
- Example: internal energy

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

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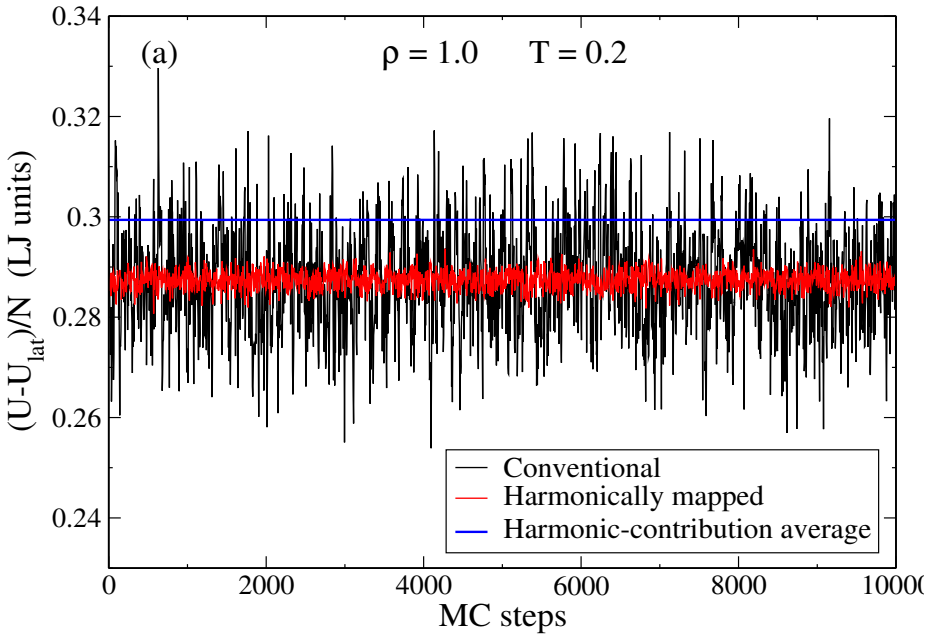
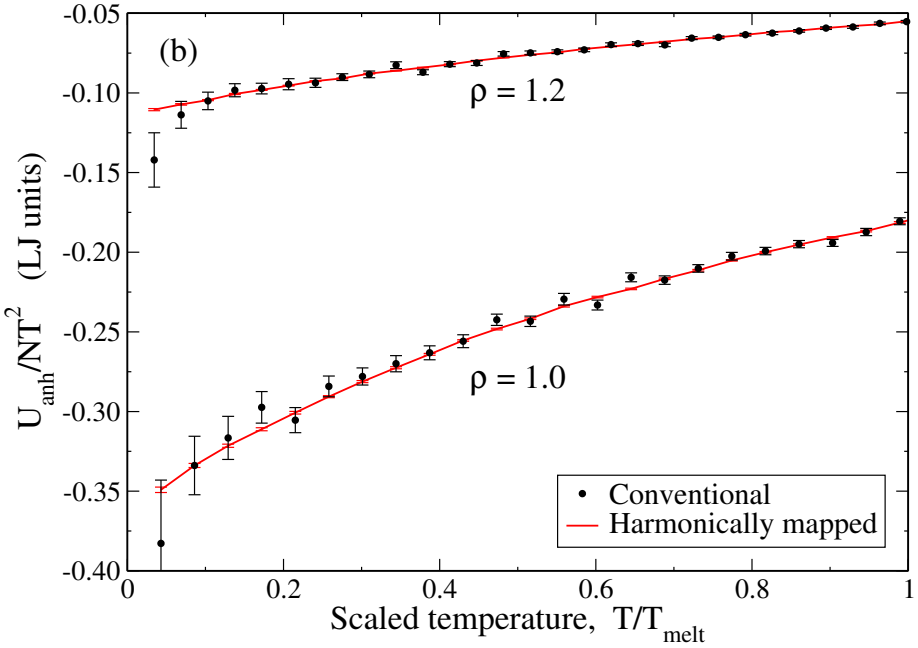
Mapped Averaging – Performance

- The result is a vast improvement in precision





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SSE Project

- Our goal in this project is to implement harmonically mapped averaging on popular molecular simulation codes
  - LAMMPS
  - HOOMD-Blue
  - Cassandra
  - VASP
- We also aim to develop, test, and implement new HMA formulas for other properties
- Supporting activities, broader impact efforts

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