Implementing Harmonically Mapped Averaging Methods on Popular Molecular Simulation Platforms

David A. Kofke and Andrew J. Schultz



Department of Chemical and Biological Engineering University at Buffalo, State University of New York

Ensemble Averages

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

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



UNIVERSITY AT BUFFALO

tate University of New York

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

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



3

Mapped Averaging – Performance

• The result is a vast improvement in precision



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



UNIVERSITY AT BUFFALO

state University of New York

Acknowledgements

- Funding
 - National Science Foundation SSE grant, OAC-1739145
- Personnel
 - Dr. Sabry G. Moustafa
 - Apoorva Purohit
 - Arpit Bansal



UNIVERSITY AT BUFFALO

state University of New York