Integrating HOOMD-blue with SSAGES for Advanced Sampling

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Introduction

The SSAGES (Software Suite for Advanced General Ensemble Simulations) project **[1]**...

- provides methods for advanced sampling and free energy calculations
- works with multiple simulation engines, including GROMACS, LAMMPS, OpenMD, and Qbox (as of v0.8.2)
- generalizes to a wide variety of atomistic, coarse grained, classical, and quantum simulations

This work adds support to SSAGES for the open-source GPU-accelerated simulation engine, HOOMD-blue **[2,3]**.

Implementation

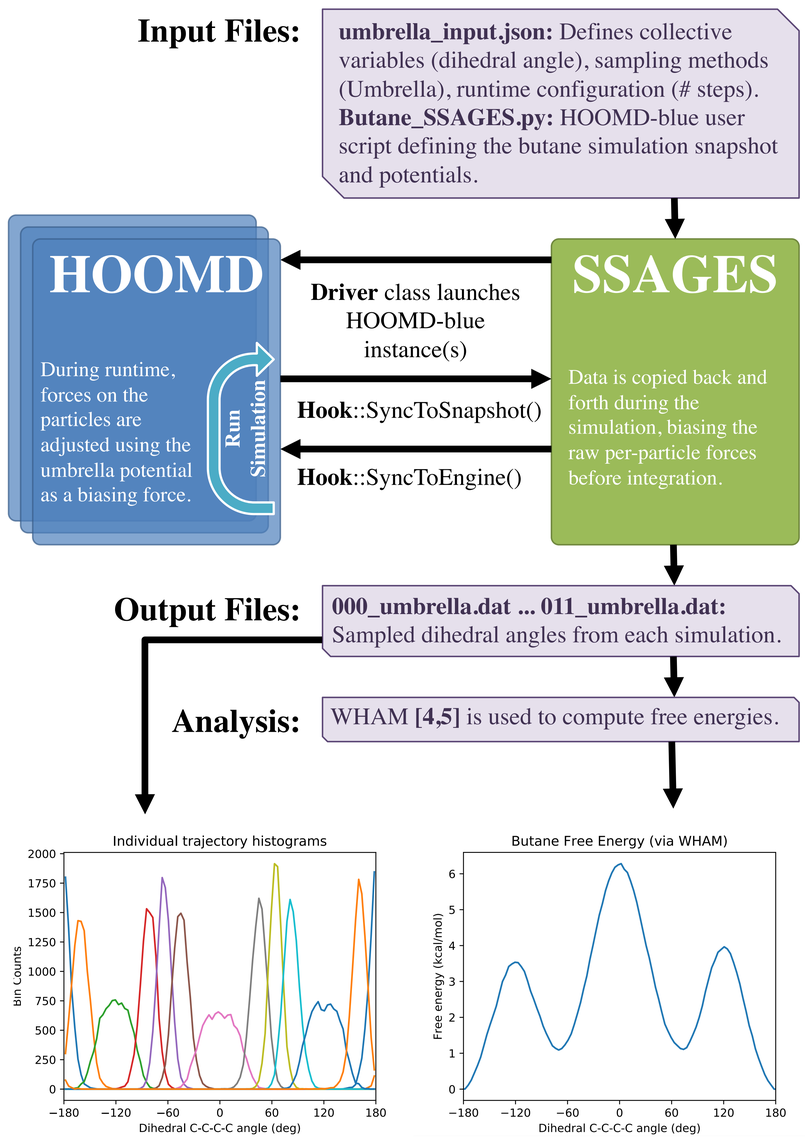
SSAGES computes collective variables (CVs) derived from snapshots of particle-level data, captured from HOOMD-blue at runtime. SSAGES integrates with HOOMD-blue through C++ classes and callbacks, and can read or overwrite snapshot data to bias the system toward certain configurations and measure results.

SSAGES simulations can be run in parallel, via separate instances of the MD/MC engine. The system communications are managed via SSAGES over MPI, allowing systems to share information such as what portions of a free energy landscape are already sampled (as in metadynamics).

SSAGES integrates with HOOMD-blue through a *driver* and a *hook*. The driver launches each instance of the the simulation engine and provides it with a partitioned MPI communicator. The hook is injected into the simulation engine and triggers actions in SSAGES when the simulation starts/stops and during the integration step, after forces are computed.

Example: Determining the Free Energy of Butane via Umbrella Sampling

The example below demonstrates the use of SSAGES with HOOMD-blue for sampling the free energy of a butane molecule. The four carbon atoms rotate into different conformations (*anti*, *gauche*, and *eclipsed*). The free energy of this rotation can be computed to know the energy cost of any dihedral angle between -180 and 180 degrees. Umbrella Sampling is used with the Weighted Histogram Analysis Method (WHAM) to determine the free energy **[4,5]**.



Use Cases & Future Work

Advanced sampling methods are complicated to write, and difficult to parallelize effectively. Scaling such codes to large compute environments such as Titan provides a significant challenge with substantial development work required. Using SSAGES reduces the duplication of such efforts between researchers and across different advanced sampling methods, offering a major benefit to many simulation workflows.

The SSAGES framework provides an excellent starting point for building simulations that employ advanced sampling. By integrating SSAGES and HOOMD-blue, HOOMD users gain access to a growing set of advanced sampling methods implemented in SSAGES, including metadynamics, forward flux sampling, finite temperature string, and adaptive biasing force algorithms.

Future work could add features to SSAGES that improve its utility within the soft matter community:

- Support for anisotropic particles (orientations, torques)
- GPU acceleration for computing collective variables from the GPU's device memory, instead of host-device copying
- Additional collective variables useful for soft matter order parameters

Get the Software

HOOMD-blue: http://glotzerlab.engin.umich.edu/hoomd-blue/
SSAGES: http://miccomcodes.org/

HOOMD-blue v2.4.0+ will support SSAGES integration.

References and Acknowledgements

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