SSAGES (Software Suite for Advanced Generalized Ensemble Simulations) – Development and Applications

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Introduction

SSAGES (Software Suite for Advanced Generalized Ensemble Simulations) is an open-source, engine agnostic, C++11 based advanced sampling package. It is designed to be easy to use, extendable and extremely versatile. It is currently pre-beta, meaning that there are many rough edges, but we are working rapidly to expand its features and fix any bugs.

Highlights

- Engine agnostic framework
- Simple JSON input file syntax
- Easy to add new CVs
- Easy to add new methods
- Much more!

Engines

- Gromacs (5.0.x+)
- LAMMPS (Most recent versions)
- OpenMD (2.4+)
- QBox (1.63+)
- DASH GPU MD Engine

CVs

- Atom group coordinate
- Atom group position
- Atom group separation
- Bend angle
- Torsional angle
- Components of gyration tensor
- Polymer Rouse modes
- Coordination number
- Box volume

Methods

- Metadynamics
- Basis function sampling
- Adaptive biasing force
- Nudged elastic band
- Finite temperature string
- Forward flux sampling
- Swarm of trajectories
- Umbrella sampling

SSAGES can handle interconnected 'walkers' that can each launch their own simulations, with the same, complementary or different CVs, methods and even engines!

SSAGES and GPU-Accelerated Simulations with DASH

About DASH

DASH is a *fast* GPU-Based Molecular Dynamics engine developed by Daniel Reid in the de Pablo Group at the University of Chicago, in collaboration with Julian Helfferich, Marat Andreev, and Mike Webb.

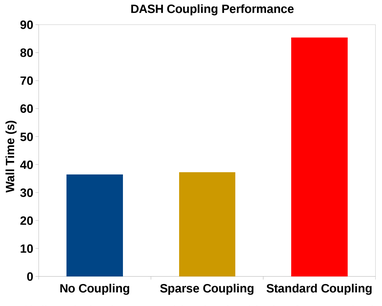
	LAMMPS	GPU code	Speedup
Lennard-Jones fluid	1.8 x 10^6	128 x 10^6	71 X
Atomistic (Organic photovoltaic system)	0.5 x 10^6	18.5 x 10^6	37 X

Units of particle timesteps per seconds.
LAMMPS benchmarked with Intel i7 @ 3.4 GHz
GPU code benchmarked with Geforce 1080 GTX

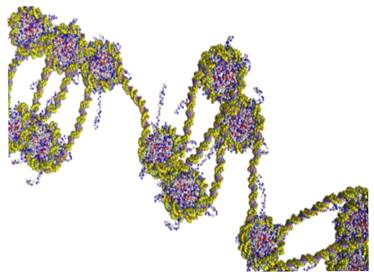
Coupling to SSAGES

CPU-side calculation of CVs and method-specific operations such as biases and histograms, while the molecular dynamics simulation runs on GPUs.

We developed a 'sparse coupling' with SSAGES to minimize PCI-express data transfer bottlenecks and still keep full functionality.

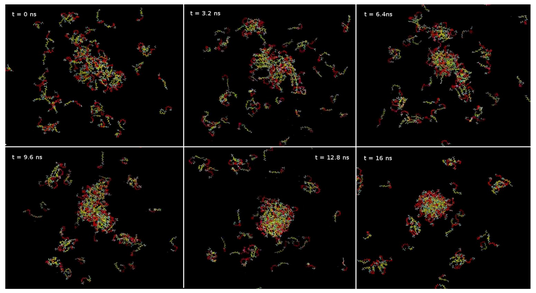


NaCl dissociation in water with adaptive biasing force method
1500 molecules of water. 31Å x 31Å x 31Å



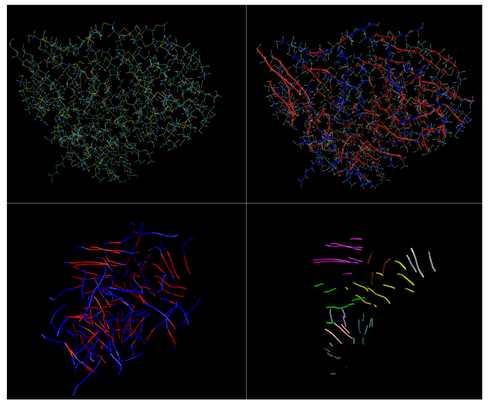
DASH is currently being used to tackle problems intractable with standard MD

Simulations of Self Assembly of Micelles with SSAGES-GROMACS

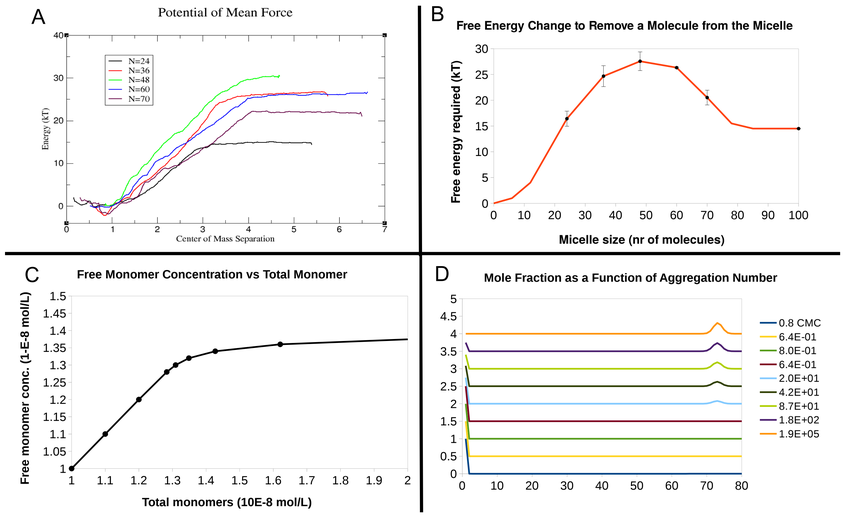


Most amphiphilic systems self-assemble into micellar or fibrillar structures in water with amorphous or semi-crystalline cores, stabilized by hydrophobic or electrostatic interactions. In contrast, Brubaker *et al.* have recently described highly asymmetric, Polyethylene Glycol – *b*–Oligoethylene Sulfide (PEG-*b*-OES) block co-polymers, capable of forming micelles, fibrils and hydrogels with crystalline cores or association domains.

Based on experimental data and theory, PEG-*b*-OES micelles were postulated to be crystalline at their cores - Ethylene sulfide has a strong tendency to crystallize, and differential scanning calorimetry (DSC) results of pure $(OES)_3$ has shown crystallinity. We simulated a box of pure $(OES)_3$, similar to experimental conditions, and reproduced the experimental melting point range. Furthermore, pure $(OES)_3$ spontaneously arranged into hexagonally ordered rods below its melting point. Here, we show that the same ordering is also observed at the center of PEG-*b*-OES micelles. In larger micelles, amorphous regions separate several hexagonally arranged crystal grains.



Calculation of Critical Micelle Concentration via Molecular Dynamics

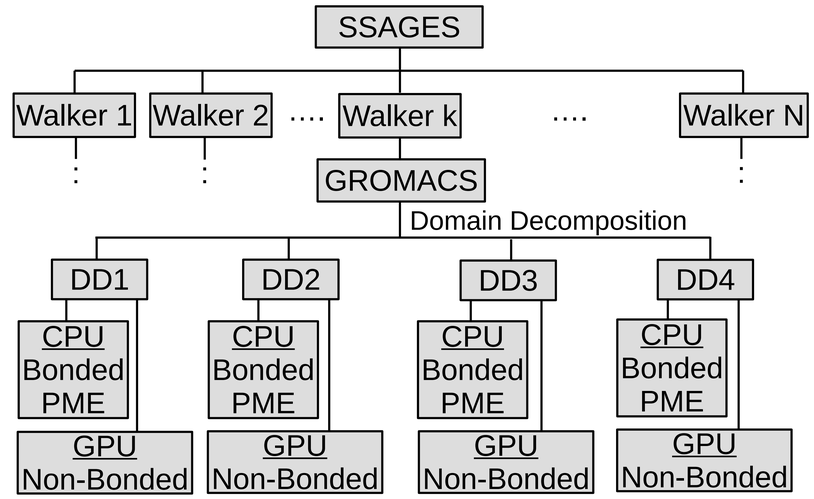


A. Potential of Mean Force of Extracting a Unimer from a Micelle **B.** Free Energy of (A) as a Function of Micelle Size

C. Predicted Behavior Based on $\Delta G_{micelle} = -\frac{RT}{N} ln[micelle] + RT \times ln(CMC)$

D. Behavior at Different Total Concentration of Polymer

SSAGES-GROMACS Simulations on Broadwell-GPU Nodes



1)Each walker collects trajectory information and sends it to SSAGES
2)SSAGES combines all trajectory information and calculates a bias based on a method
3)The bias is communicated to each walker and accelerates sampling

Free Energy Surfaces from *ab-initio* Molecular Dynamics using Qbox and SSAGES

Ab-initio Molecular Dynamics (AIMD) generates a forcefield from first principles quantum-mechanical calculations rather than using a pre-defined, empirical forcefield. Thus, AIMD calculations have the potential to be more accurate, can yield information about electronic states, and can simulate chemical reactions.

Steep computational cost has been limiting adoption of AIMD. However, with SSAGES coupled to Qbox, a C++/MPI scalable parallel implementation of first-principles molecular dynamics, it is now possible to perform advanced sampling using AIMD and significantly accelerate convergence, making it widely applicable. As a proof of concept, we generate the free energy surface of a well-studied system, alanine dipeptide, entirely from AIMD.

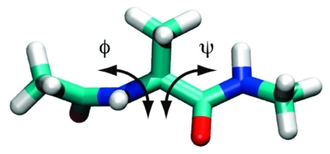
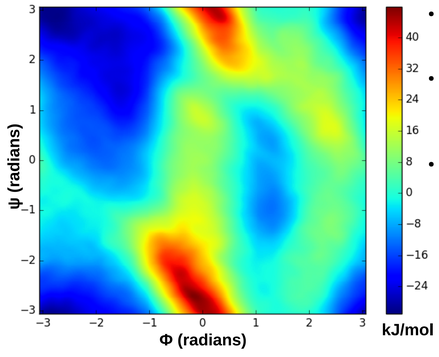


Image Credit: www.cp2k.org

Free Energy as a Function of Dihedral Angles



- SSAGES was used to launch 16 walkers on Qbox instances.
- Each Qbox instance was parallelized onto 28 cores to perform the electronic structure calculations.
- Method used was a fully parallelizable implementation of the Adaptive Biasing Force algorithm.
  → The first implementation that can handle arbitrary number of walkers and domain decomposition schemes
- Wall time: ~ 2 weeks

References

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Acknowledgements

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