

FEASST: Free Energy and Advanced Sampling Simulation Toolkit

Harold W. Hatch, Nathan A. Mahynski, and Vincent K. Shen

National Institute of Standards and Technology,
Gaithersburg, MD 20899

harold.hatch@nist.gov

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1. Summary

The Free Energy and Advanced Sampling Simulation Toolkit (FEASST) is a free, open-source, modular program to conduct molecular and particle-based simulations with Metropolis, Wang-Landau and Transition-Matrix Monte Carlo methods [1–7]. FEASST is implemented in C++ and may be imported as a module within Python 2 or 3.¹

This document describes the initial public release version 1.0 with the following features:

1. Simulation techniques
 - Wang-Landau Monte Carlo
 - Transition-matrix Monte Carlo
 - Metropolis Monte Carlo
2. Thermodynamic ensembles
 - Grand canonical ensemble
 - Isothermal isobaric ensemble
 - Canonical ensemble
3. Advanced Monte Carlo algorithms
 - Parallel configuration swaps

¹Certain commercial firms and trade names are identified in this document in order to specify the installation and usage procedures adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that related products are necessarily the best available for the purpose.

- Floppy box
4. Intermolecular interactions
- Charged interactions with the Ewald summation
 - Lennard-Jones with different exponential parameters, long range corrections, Yukawa, force shifted and/or Gaussians
 - Hard spheres, soft spheres and square wells
5. Modern software
- Interface with C++ or as a Python module
 - Open Multi-Processing (OpenMP) parallelization
 - Check points to save and restart simulations
 - Robust unit testing

Many more features are planned for release in future versions of FEASST including expanded ensembles in temperature and alchemical transformations, configurational bias, geometric cluster algorithm, aggregation volume bias, confinement, patchy particle potentials and Mayer-sampling Monte Carlo.

2. Software Specifications

NIST Operating Unit	Material Measurement Laboratory, Chemical Sciences Division, Chemical Informatics Group
Category	Classical molecular and particle-based simulation
Targeted Users	Researchers, educators, and students
Operating Systems	Cross platform CMake 2.8 build. Automated build testing on Linux and macOS
Programming Language	C++11 with optional Python 2.7 or 3.6
Inputs/Outputs	FEASST interfaces with C++ or Python. It may require many parameters and/or configurations typically required by complex molecular simulation code, and FEASST may output structural and thermodynamic properties (instantaneous and statistic ensemble averages).
Documentation	https://doi.org/10.18434/M3S095
Accessibility	N/A, small-scale research tool
Disclaimer	https://www.nist.gov/director/licensing

3. Methods for Validation

The software was validated by reproducing published results, as documented in the website listed above. An extensive suite of unittests for both C++ and Python provides coverage for the majority of lines of code. In addition to unittests, potential memory leaks are detected using Valgrind as part of a nightly automated build. Source code style follows recommendations from Google C++ Style Guide, cplint, and pylint.

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About the authors: *H.W.H., N.A.M. and V.K.S. are chemical engineers at NIST. The National Institute of Standards and Technology is an agency of the U.S. Department of Commerce.*