

ForceBalance Developer API Guide version 1.2

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1 Project Roadmap

ForceBalance is a work in progress and is continually being improved and expanded! Here are some current and future project development ideas.

Some notes on updating the version:

The formalism for the version number goes something like this:

v1.2.1[ab][1-9]

where:

- 1.2.1 stands for major release (may break compatibility), medium-sized release (important features), minor release (improvements)
- a or b, if present, stands for alpha or beta release, with numbers standing for the n-th alpha or beta release

To manually specify a release, create a tag and push it to the remote repository: `git tag -a v1.2.1 -m "version 1.2.1" git push --tags`

The version number should then be automatically generated by "git describe" which is run by `setup.py` at installation. Finally, remember to update the version number in the documentation generation scripts!

1.1 Most Recently Implemented (version 1.3.0):

- Engine class is a unified interface to MD simulation codes.
- Added Gromacs, OpenMM, and TINKER engines.
- Thermo target; simple support for general thermodynamic properties. (Erik)
- Lipid target; lipid bilayer properties. (Keri)
- ForceBalance `--continue` option continues an aborted run and loads as much data as possible from the latest iteration.
- Parameter filtering allows targets to skip over parameters that are known to be irrelevant, for efficiency of finite difference derivatives.
- (Optimizer / Liquid / Lipid) Increase simulation length as we get closer to convergence.
- (Gromacs) Now supports binding energies, interaction energies, multipole moments and vibrational frequencies.
- (OpenMM) Now supports binding energies, interaction energies, and multipole moments.
- ([nifty.py](#)) `exec_()` reads from stdout and stderr asynchronously, allowing us to split the streams and `tail -f` the output at the same time.

1.2 Current Development Goals, for version 1.3.1:

- More comprehensive tutorial to walk users through the initial process of setting up targets and preparing for a successful ForceBalance run

1.3 Longterm Development Ideas

- Visualization of running calculations

2 Namespace Index

2.1 Packages

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