

ForceBalance Developer API Guide version 1.3

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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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3 File Index

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4 Namespace Documentation

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4.2 ForceBalance Namespace Reference

4.3 MakeInputFile Namespace Reference

4.4 src Namespace Reference

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- [abinitio.internal](#)

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- [chemistry](#)
- [contact](#)
- [counterpoise](#)
- [custom_io](#)
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5.3 abinitio_internal.py File Reference

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5.4 amberio.py File Reference

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5.5 api.dox File Reference

5.6 binding.py File Reference

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5.7 chemistry.py File Reference

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- [src.hydration](#)

5.18 interaction.py File Reference

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- [src.interaction](#)

5.19 leastsq.py File Reference

Namespaces

- [src.leastsq](#)

5.20 LICENSE.txt File Reference

Functions

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5.20.1 Function Documentation

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