fabulous-paths

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`fabulous-paths` connects OpenPathSampling, a package for path sampling simulations, to FABULOUS, a machine learning approach to identify important collective variables in transitions.

This package is just the glue between those two projects. Most of the documentation can be found in the individual packages. The documentation includes details on how to use this code as a library and specifics of the OpenPathSampling CLI plugin.

To install `fabulous-paths` just ???. You can verify that the installation worked by running the command `openpathsampling fabulous --help`.

Details on how to use OpenPathSampling to perform path sampling simulations can be found in the OpenPathSampling documentation. Details on how to use FABULOUS to extract important CVs from path sampling data can be found in the documentation for FABULOUS.

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USAGE

This package adds a subcommand `fabulous` to the OpenPathSampling CLI.

API

`fabulous-paths` provides a few functions that can be used in Python to facilitate the conversion of OpenPathSampling data to the input formats required by FABULOUS. This is the documentation for that (very simple) API.

2.1 `fabulous_paths`