Domain-level Reaction Enumerator

Karthik Sarma, Casey Grun, and Erik Winfree.

Overview

This package predicts the set of possible reactions between a set of initial nucleic acid complexes. Complexes are comprised of strands, which are subdivided into "domains"—contiguous regions of nucleotide bases which participate in Watson-Crick hybridization. The enumerator only considers reactions between complexes with complementary domains. At this point, only unpseudoknotted intermediate complexes are considered.

This document describes basic usage of the software, automatic generation of API documentation, and running of unit tests. There's a separate document, `architecture.pdf`, which describes the internal architecture of the software.

This package is written for Python 2.7; Python must be installed and in the user's `path` in order to run the program.

Usage

```
usage: enumerator.py [-h] [--infile INPUT_FILENAME]
                     [--outfile OUTPUT_FILENAME] [-o OUTPUT_FORMAT]
                     [-i INPUT_FORMAT] [-c]
                     [--max-complex-size MAX_COMPLEX_SIZE]
                     [--max-complexes MAX_COMPLEX_COUNT]
                     [--max-reactions MAX_REACTION_COUNT]

optional arguments:
    -h, --help            show this help message and exit
    --infile INPUT_FILENAME
                          Path to the input file
    --outfile OUTPUT_FILENAME
                          Path to the output file
    -o OUTPUT_FORMAT      Desired format for the output file; one of: standard,
                          json
    -i INPUT_FORMAT       Desired format for the input file; one of: sbml, json,
                          legacy, pil, standard, graph
    -c                    Condense reactions into only resting complexes
```

```
--max-complex-size MAX_COMPLEX_SIZE
                      Maximum number of strands allowed in a complex (used
                      to prevent polymerization)
--max-complexes MAX_COMPLEX_COUNT
                      Maximum number of complexes that may be enumerated
                      before the enumerator halts.
--max-reactions MAX_REACTION_COUNT
                      Maximum number of reactions that may be enumerated
                      before the enumerator halts.
```

Building documentation

API Documentation is built from comments in the source using Sphinx; Sphinx must be installed. Then you can run:

```
make docs
```

from within the main directory to build HTML documentation; you can find this documentation at `docs/_build/html/index.html`. Additional output formats are available, and can be generated by moving to the `docs/` subdirectory and using `make`. Type `make` within the `docs/` subdirectory to show a list of available output formats. Once you've generated the documentation, it will be available in the folder `docs/_build/{format}`.

This document, and the architecture documentation, are generated from Markdown with Pandoc in PDF or HTML format; Pandoc must be installed; then you can use `make README.pdf` or `make README.html`, or similarly `make architecture.pdf` or `make architecture.html`.

Running unit tests

Unit tests for the project are written using Nosetests. Nosetests must be installed. Then you can run:

```
make tests
```

from within the main directory to run unit tests.