NPLinker Community Meeting

2024-09-10

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Agenda

16:00	Short Introduction
16:05	Announcements and upcoming events
16:10	NPLinker development
16:25	Monthly plan
16:30	Q&A
17:00	.

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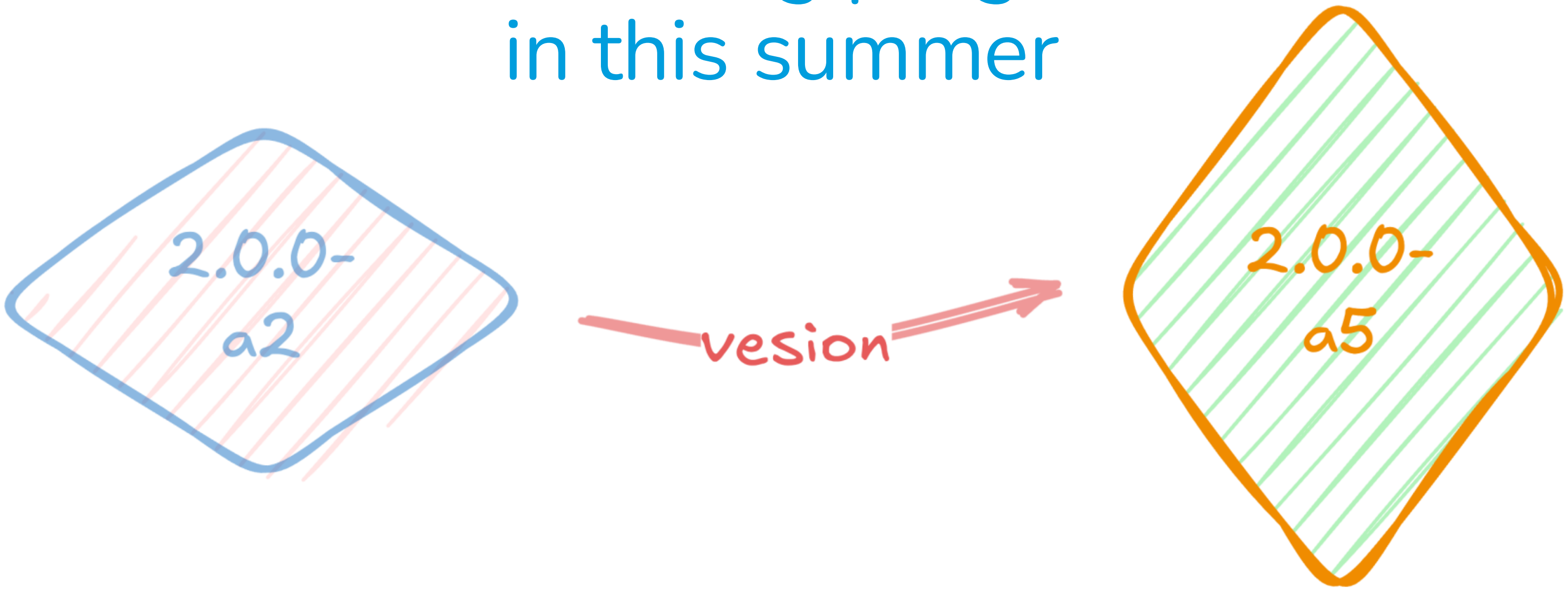
Announcements and upcoming events?

NPLinker Development

New features & changes

Contributors: Cunliang Geng, Giulia Crocioni, Arjan Draisma

Refactoring progress in this summer



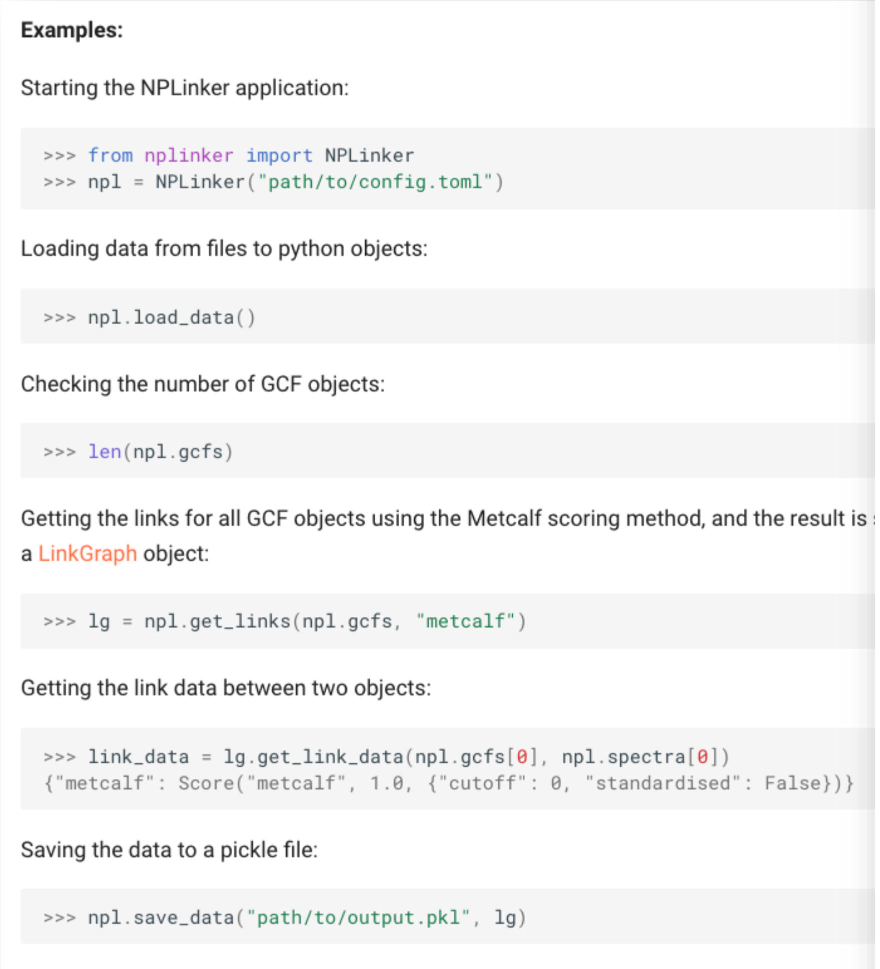
Added

- The check of available disk space when downloading data. You will get a warning if having <50GB
- Warning with details when it fails to download some antiSMASH data
- OpenSSF scorecard for code quality and security openssf scorecard 6

Improved

- The detection of tabular file delimiter
- docstrings: added code examples, link to specific function/class, and more explanations

Improved docstrings -> doc



Examples:

Starting the NPLinker application:

```
>>> from nplinker import NPLinker
>>> npl = NPLinker("path/to/config.toml")
```

Loading data from files to python objects:

```
>>> npl.load_data()
```

Checking the number of GCF objects:

```
>>> len(npl.gcfs)
```

Getting the links for all GCF objects using the Metcalf scoring method, and the result is a LinkGraph object:

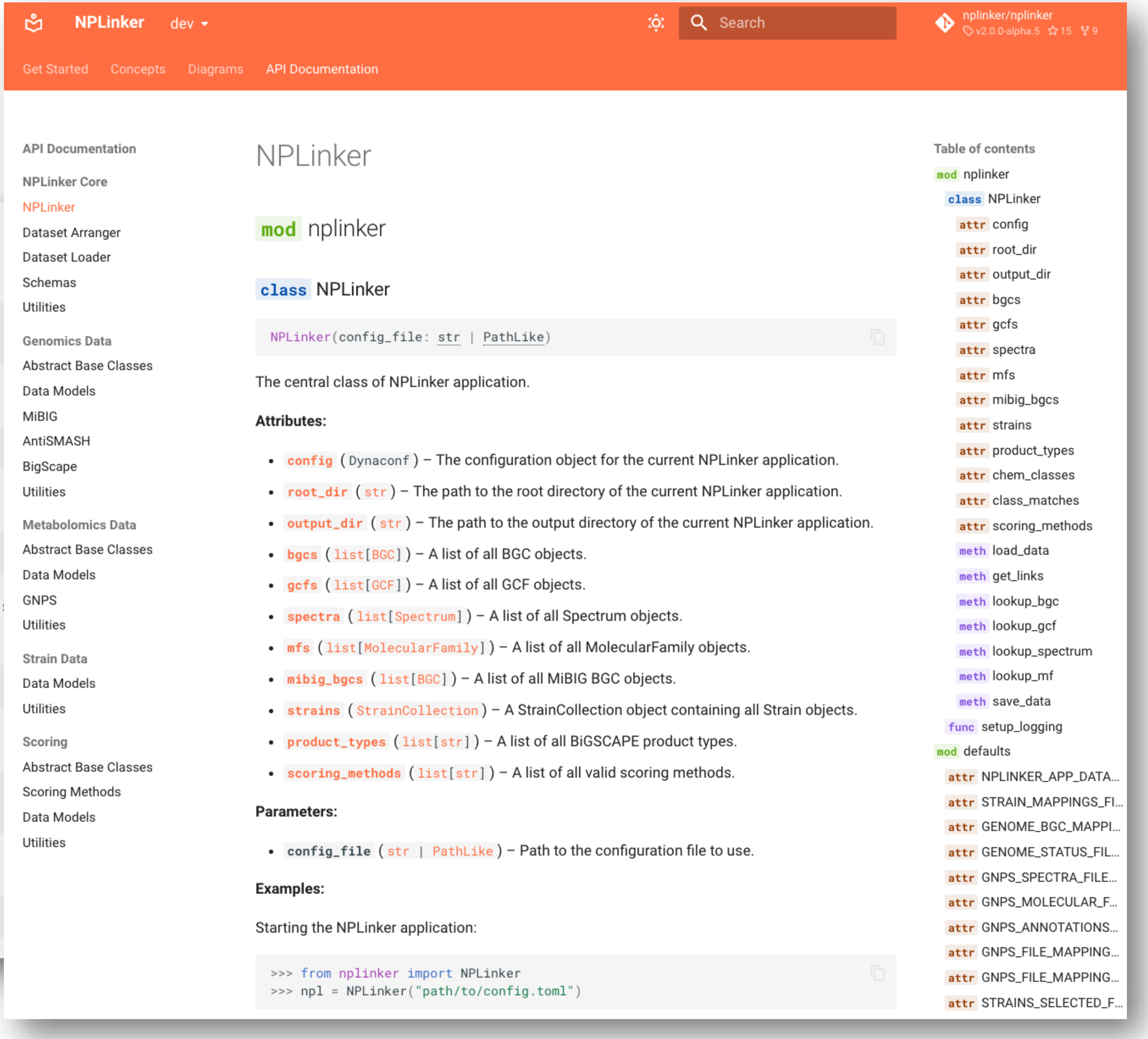
```
>>> lg = npl.get_links(npl.gcfs, "metcalf")
```

Getting the link data between two objects:

```
>>> link_data = lg.get_link_data(npl.gcfs[0], npl.spectra[0])
{"metcalf": Score("metcalf", 1.0, {"cutoff": 0, "standardised": False})}
```

Saving the data to a pickle file:

```
>>> npl.save_data("path/to/output.pkl", lg)
```



NPLinker

mod nplinker

class NPLinker

```
NPLinker(config_file: str | PathLike)
```

The central class of NPLinker application.

Attributes:

- `config` (`Dynaconf`) – The configuration object for the current NPLinker application.
- `root_dir` (`str`) – The path to the root directory of the current NPLinker application.
- `output_dir` (`str`) – The path to the output directory of the current NPLinker application.
- `bgcs` (`list[BGC]`) – A list of all BGC objects.
- `gcfs` (`list[GCF]`) – A list of all GCF objects.
- `spectra` (`list[Spectrum]`) – A list of all Spectrum objects.
- `mfs` (`list[MolecularFamily]`) – A list of all MolecularFamily objects.
- `mibig_bgcs` (`list[BGC]`) – A list of all MiBIG BGC objects.
- `strains` (`StrainCollection`) – A StrainCollection object containing all Strain objects.
- `product_types` (`list[str]`) – A list of all BiGSCAPE product types.
- `scoring_methods` (`list[str]`) – A list of all valid scoring methods.

Parameters:

- `config_file` (`str | PathLike`) – Path to the configuration file to use.

Examples:

Starting the NPLinker application:

```
>>> from nplinker import NPLinker
>>> npl = NPLinker("path/to/config.toml")
```

[PR 266]

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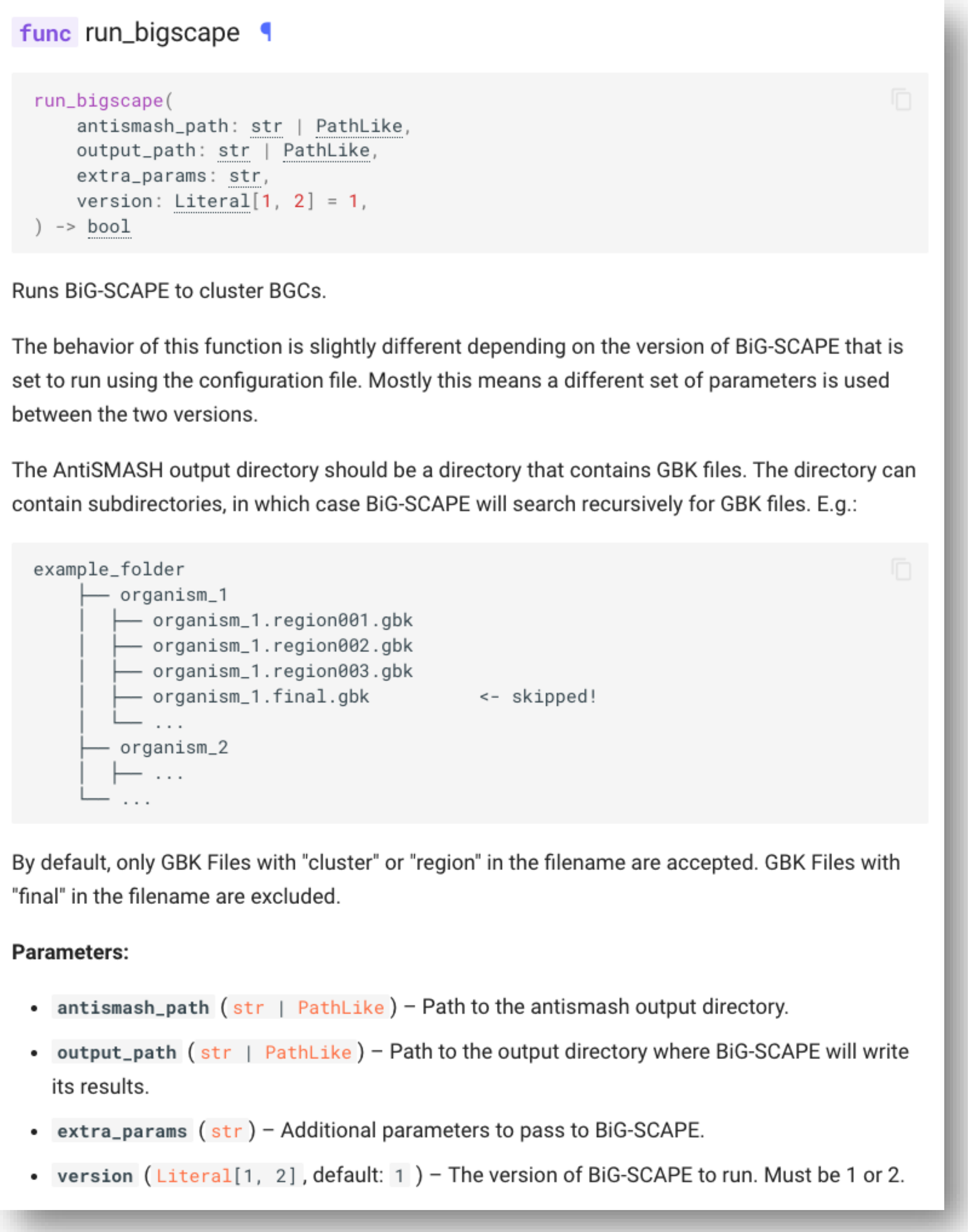
Integrated BigScape V2

Now you can run BigScape V1 and V2 in NPLinker

[PR 251 by Arjan]



func run_bigscape ¶

```
run_bigscape(
    antismash_path: str | PathLike,
    output_path: str | PathLike,
    extra_params: str,
    version: Literal[1, 2] = 1,
) -> bool
```

Runs BiG-SCAPE to cluster BGCs.

The behavior of this function is slightly different depending on the version of BiG-SCAPE that is set to run using the configuration file. Mostly this means a different set of parameters is used between the two versions.

The AntiSMASH output directory should be a directory that contains GBK files. The directory can contain subdirectories, in which case BiG-SCAPE will search recursively for GBK files. E.g.:

```
example_folder
    ├── organism_1
    │  ├── organism_1.region001.gbk
    │  ├── organism_1.region002.gbk
    │  ├── organism_1.region003.gbk
    │  ├── organism_1.final.gbk          <- skipped!
    │  └── ...
    ├── organism_2
    │  ├── ...
    └── ...
```

By default, only GBK Files with "cluster" or "region" in the filename are accepted. GBK Files with "final" in the filename are excluded.

Parameters:

- `antismash_path` (`str | PathLike`) – Path to the antismash output directory.
- `output_path` (`str | PathLike`) – Path to the output directory where BiG-SCAPE will write its results.
- `extra_params` (`str`) – Additional parameters to pass to BiG-SCAPE.
- `version` (`Literal[1, 2]`, default: `1`) – The version of BiG-SCAPE to run. Must be 1 or 2.

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NPLinker Webapp Development

Contributors: Giulia Crocioni, Cunliang Geng

Demo

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Monthly plan

What will happen before next meeting

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Need your tests and feedback on the refactored NPLinker

Questions? Ideas? Feedback?