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1 ESBMTK - An Earth-sciences box modeling toolkit

ESBMTK is python library which aims to simplify typical box modeling projects the in Earth-Sciences. I started this project to teach myself python and explore object oriented programming. The code became however functional enough that the focus of this project has shifted to make box modeling more approachable for classroom teaching. So performance and scalability are not great. Specifically, the solver is just a simple forward Euler scheme, so stiff problems are not handled gracefully.

At present, it will calculate masses/concentrations in reservoirs and fluxes including isotope ratios. It provides a variety of classes which allow the creation and manipulation of input signals, and the generation of graphical results. There is however no support for chemical reactions (including equilibrium reactions).

2 News

- Dec. 20th, added a new connection type (`flux_balance`) which allows equilibration fluxes between two reservoirs without the need to specify forward and backwards fluxes explicitly. See the equilibration example in the example directory.
- Dec. 9th, added a basic logging infrastructure. Added `describe()` method to `Model`, `Reservoir` and `Connnection` classes. This will list

details about the fluxes and processes etc. Lot's of code cleanup and refactoring.

- Dec. 7th, When calling an instance without arguments, it now returns the values it was initialized with. In other words, it will print the code which was used to initialize the instance.
- Dec. 5th, added a DataField Class. This allows for the integration of data which is computed after the model finishes into the model summary plots.
- Nov. 26th Species definitions now accept an optional display string. This allows pretty printed output for chemical formulas.
- Nov. 24th New functions to list all connections of a reservoir, and to list all processes associated with a connection. This allows the use of the help system on process names. New interface to specify connections with more complex characteristics (e.g., scale a flux in response to reservoir concentration). This will breaks existing scripts which use these kind of connections. See the Quickstart guide how to change the connection definition.
- Nov. 23rd A model can now save it's state, which can then be used to initialize a subsequent model run. This is particularly useful for models which require a spin up phase to reach equilibrium
- Nov. 18th, started to add unit tests for selected modules. Added unit conversions to external data sets. External data can now be directly associated with a reservoir.
- Nov. 5th, released version 0.2. This version is now unit aware. So rather than having a separate keyword for `unit`, quantities are now specified together with their unit, e.g., `rate = "15 mol/s"`. This breaks the API, and requires that existing scripts are modified. I thus also removed much of the existing documentation until I have time to update it.
- Oct. 27th, added documentation on how to integrate user written process classes, added a class which allows for concentration dependent flux. Updated the documentation, added examples
- Oct. 25th, Initial release on github.

3 Contributing

Don't be shy. Contributing is as easy as finding bugs by using the code, or maybe you want to add a new process code? If you have plenty of time to spare, ESBMTK could use a solver for stiff problems, or a graphical interface ;-) See the todo section for ideas.

4 Installation

ESBMTK relies on the following python versions and libraries

- python > 3.6
- matplotlib
- numpy
- pandas
- typing
- nptyping
- pint

If you work with conda, it is recommended to install the above via conda. If you work with pip, the installer should install these libraries automatically. ESBMTK itself can be installed with pip

- pip install esbmtk

5 Documentation

The documentation is available in org format or in pdf format. See the documentation folder, [specifically the quickstart guide](#).

At present, I also provide the following example cases (as py-files and in jupyter notebook format)

- A trivial carbon cycle model which shows how to set up the model, and read an external csv file to force the model.
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6 Todo

- expand the documentation
- provide more examples
- do more testing

7 License

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