

# Reproducible Carbon Cycle Models

## Biogeochemical Model Database `bgc_md2`



Markus Müller, Holger Metzler, Verónica Ceballos Núñez, Kostiantyn Viatkin, Thomas Lotze, Jon Wells, Yu Zhou, Cuijuan Liao, Aneesh Chandel, Feng Tao, Yuanyuan Huang, Alison Bennett, Chenyu Bian, Lifeng Jiang, Song Wang, Chengcheng Gang, Carlos Sierra, Yiqi Luo

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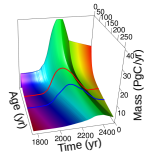
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leaf wood



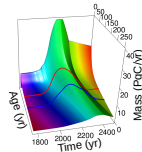
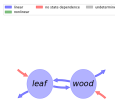
leaf wood lit som cwd



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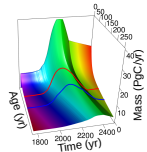


- Find and **reduce** sources of **uncertainty** in carbon predictions

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- ... ???

Biogeochemical Model Database bgc\_md2



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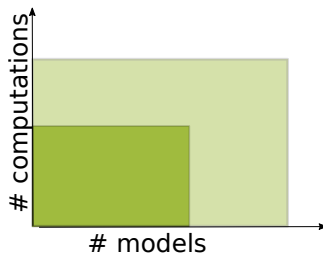
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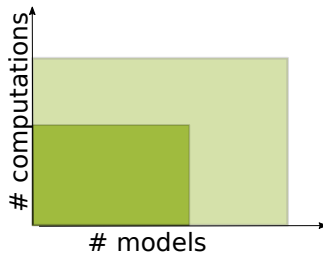
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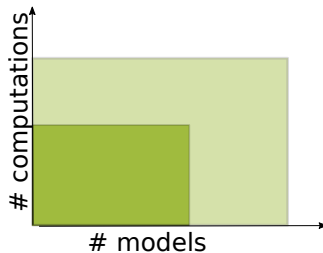
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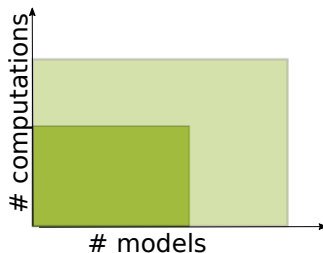
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- Ways of **organizing** both collections
  - ▶ building blocks for models



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- ▶ building blocks for models
- ▶ functions of building blocks

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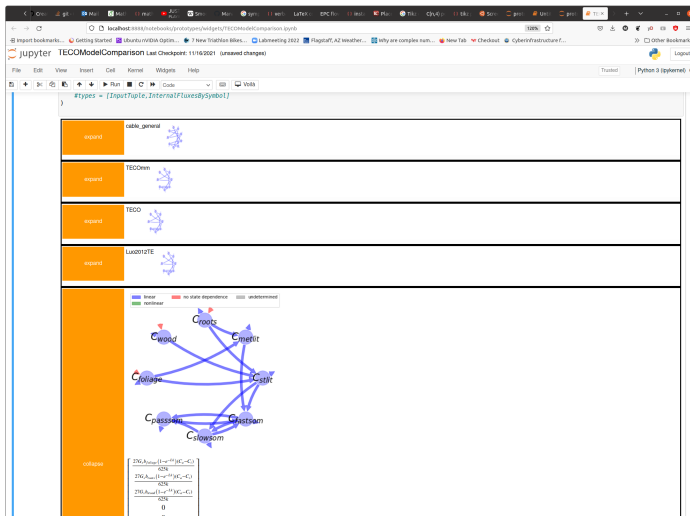
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## Example widget for query result



## Analysis with symbolic tools (sympy) ...

The screenshot displays a Jupyter Notebook environment with the following content:

- Code Cell:** Imports `inspectModel` and defines a function `inputtuple, compartmentalMatrix, compartmentalMatrix, infFluxesBySymbol, inputtuple, internalFluxesBySymbol, smoothReservoirModel, outFluxesBySymbol, compartmentalMatrix, infFluxesBySymbol, inputtuple, internalFluxesBySymbol, smoothReservoirModel, outFluxesBySymbol`.
- Output [3]:** A network diagram showing carbon pools ( $C_{wood}$ ,  $C_{root}$ ,  $C_{leaf}$ ,  $C_{DPM}$ ,  $C_{RPM}$ ,  $C_{HUM}$ ,  $C_{BIO}$ ) and their interactions with arrows indicating fluxes.
- Code Cell:** Executes `mvs.get_CompartmentalMatrix()`.
- Output [28]:** A large matrix representing the compartmental matrix, showing various fluxes and their dependencies on state variables like  $\xi(t)$ .
- Code Cell:** Executes `mvs.get_BibInfo()` and displays a list of attributes including `get_CompartmentalMatrix`, `get_InfFluxesBySymbol`, `get_InputTuple`, `get_InternalFluxesBySymbol`, `get_OutFluxesBySymbol`, `get_SmoothReservoirModel`, and `get_StateVariableTuple`.
- Code Cell:** Executes `get_StateVariableTuple` and displays the output.

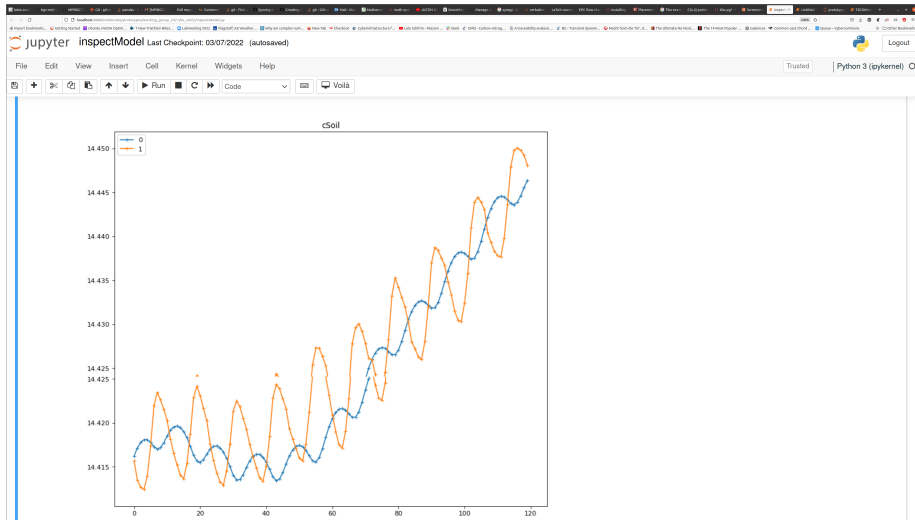
# Reproducible Carbon Cycle Models

## Biogeochemical Model Database `bgc_md2`



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...or numerically



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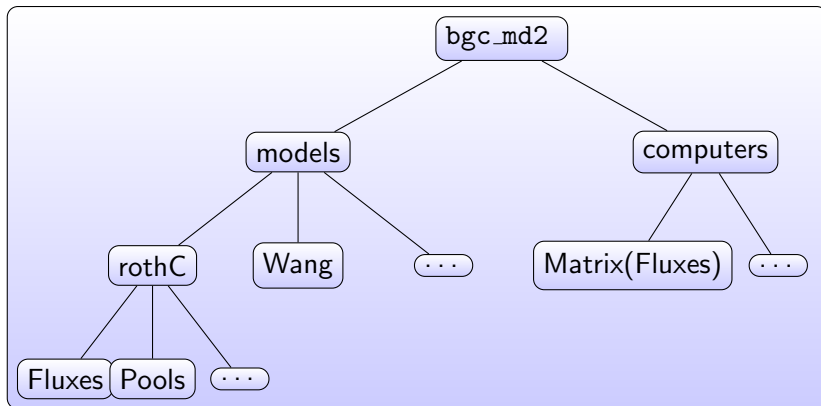


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## Database records are python modules

```
1 from sympy import Symbol, Function
2 from CerebralBiologyModels.OHMS import OHMS
3 from bgc_md2.helper import module_computers
4 from bgc_md2.models.BBInfo import BBInfo
5 from bgc_md2.resolver.mwars import (
6     InfluxesBySymbol,
7     OutFluxesBySymbol,
8     InternalFluxesBySymbol,
9     TimesSymbol,
10     StateVariableTable,
11 )
12 import bgc_md2.resolver.computers as bgc_c
13
14 # Make a small dictionary for the variables we will use
15 syn_dict = {
16     'r_leaf_2_w': 'Internal flux rate from leaf to wood',
17     'r_w_2_l': 'Internal flux rate from wood to leaf',
18     'C_soil_fast': '',
19     'C_soil_slow': '',
20     'C_soil_passive': '',
21     'C_leaf': '',
22     'C_root': '',
23     'C_wood': '',
24     'C_leaf_litter': '',
25     'C_root_litter': '',
26     'C_wood_litter': '',
27     'r_C_leaf_2_C_leaf_litter': '',
28     'r_C_root_2_C_root_litter': '',
29     'r_C_wood_2_C_wood_litter': '',
30     'r_C_leaf_litter_rh': '',
31     'r_C_root_litter_rh': '',
32     'r_C_wood_litter_rh': '',
33     'r_C_soil_fast_rh': '',
34     'r_C_soil_slow_rh': '',
35     'r_C_soil_passive_rh': '',
36     'r_C_leaf_litter_2_C_soil_fast': '',
37     'r_C_leaf_litter_2_C_soil_slow': '',
38     'r_C_leaf_litter_2_C_soil_passive': '',
39     'r_C_wood_litter_2_C_soil_fast': '',
40     'r_C_wood_litter_2_C_soil_slow': '',
41     'r_C_wood_litter_2_C_soil_passive': '',
42     'r_C_root_litter_2_C_soil_fast': '',
43     'r_C_root_litter_2_C_soil_slow': '',
44     'r_C_root_litter_2_C_soil_passive': '',
45     'tair': 'Air temperature',
46     'tsoil': 'Soil temperature',
47     'tveg': 'Vegetation temperature',
48     'tveg': 'Vegetation temperature',
49     'tveg': 'Vegetation temperature',
50     'beta_leaf': '',
51     'beta_wood': '',
52 }
53
54 for k in syn_dict.keys():
55     codekv = syn_dict[k].format(k)
56     exec(code)
57
58 # some we will also use some symbols for functions (which appear with an argument)
59 func_dict = {
60     'tair': 'A scalar function of temperature and moisture and thereby ultimately of time',
61     'tsoil': '',
62     'tveg': ''
63 }
64
65 for k in func_dict.keys():
66     codekv = Function(k).format(k)
67     exec(code)
68
69 t=timesymbol('t')
70 beta_root = 1-i- (beta_leaf+beta_wood)
71 mw = OHMS()
72
73 StateVariableTable(
74     C_leaf,
75     C_wood,
76     C_soil_fast,
77     C_soil_slow,
78     C_soil_passive,
79 )
80
81 InfluxesBySymbol(
82     C_leaf: NPP(t) * beta_leaf,
83     C_root: NPP(t) * beta_root,
84     C_wood: NPP(t) * beta_wood
85 )
86
87 OutFluxesBySymbol(
88     C_leaf_litter: r_C_leaf_litter_rh * C_leaf_litter * t,
89     C_wood_litter: r_C_wood_litter_rh * C_wood_litter * t,
90     C_root_litter: r_C_root_litter_rh * C_root_litter * t,
91     C_soil_fast: r_C_soil_fast_rh * C_soil_fast * t,
92     C_soil_slow: r_C_soil_slow_rh * C_soil_slow * t,
93     C_soil_passive: r_C_soil_passive_rh * C_soil_passive * t,
94 )
95
96 InternalFluxesBySymbol(
97     (C_leaf, C_leaf_litter): r_C_leaf_2_C_leaf_litter * C_leaf,
98     (C_wood, C_wood_litter): r_C_wood_2_C_wood_litter * C_wood,
99     (C_root, C_root_litter): r_C_root_2_C_root_litter * C_root,
100     (C_leaf_litter, C_soil_fast): r_C_leaf_litter_2_C_soil_fast * C_leaf_litter * t,
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106     (C_root_litter, C_soil_fast): r_C_root_litter_2_C_soil_fast * C_root_litter * t,
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108     (C_root_litter, C_soil_passive): r_C_root_litter_2_C_soil_passive * C_root_litter * t,
109     (C_soil_fast, C_soil_slow): r_C_soil_fast_2_C_soil_slow * C_soil_fast * t,
110     (C_soil_slow, C_soil_passive): r_C_soil_slow_2_C_soil_passive * C_soil_slow * t,
111     (C_soil_passive, C_soil_fast): r_C_soil_passive_2_C_soil_fast * C_soil_passive * t,
112 )
113
114 BBInfo(
115     new='t',
116     longname='',
117     version='',
118     entryAuthor='Kostiantyn Viatkin',
119     entryAuthorId='',
120     entryCreatedDate='',
121     doi='',
122 )
```

## Internal Structure of bgc\_md2



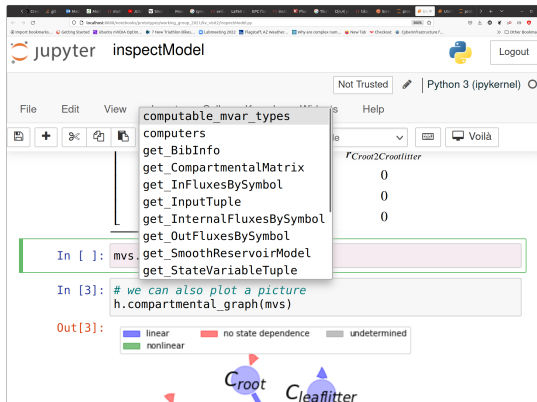
The `bgc_md` library provides 1:

- 1 Datatypes defining **building blocks** of models e.g. CompartmentalMatrix, InternalFluxesBySymbol, ...
- 2 Functions operating on those properties (forming the edges of the graph where the Datatypes are nodes)
- 3 A user interface based on graph algorithms to
  - 1 compute the set of computable properties (e.g. the comparable criteria for a set of models, database queries )
  - 2 actually compute the desired properties by recursively connecting several function applications.
  - 3 show what is missing to compute a desired property.





## Userinterface using computability graphs

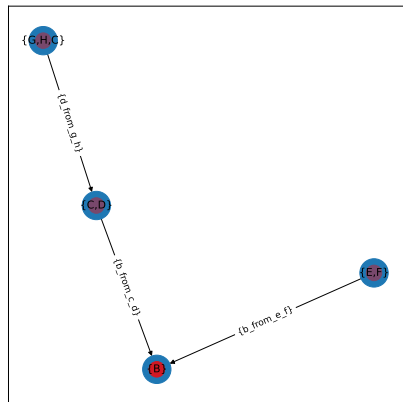


Suggested methods automatically created by ComputabilityGraphs



## Finding what's missing in the model description

given a set of  
functions:  
 $a(i)$ ,  $b(c,d)$ ,  $b(e,f)$ ,  
 $c(b)$ ,  $d(b)$ ,  $d(g,h)$ ,  
 $e(b)$ ,  $f(b)$  and the  
target variable **B** e.g.  
CompartmentalMatrix,  
The algorithm  
computes all possible  
combinations and  
paths from which **B**  
can be computed.

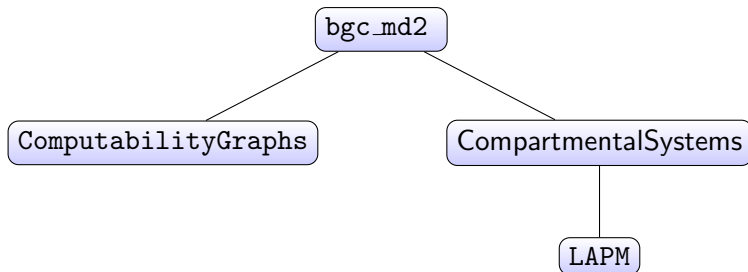




## The `bgc_md` library provides II:

- 1 30+ vegetation, soil or ecosystem models for carbon and nitrogen cycling as reusable python modules using the building blocks in a flexible way.
- 2 An interface to *many algorithms* in `CompartmentalSystems` to compute diagnostic variables for *many models* in `bgc_md2`.

## Relation to other Python Packages



## Example computation via CompartmentalSystems

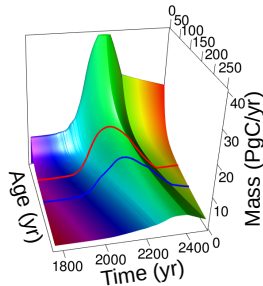


Figure: age distribution of a pool as function of time



Metzler, H., Müller, M., and Sierra, C. (2018).

Transit-time and age distributions for nonlinear time-dependent compartmental systems.

*Proceedings of the National Academy of Sciences*, 115:201705296.

## Links

- The README of the package on github (with installation instructions): [https://github.com/MPIBGC-TEE/bgc\\_md2](https://github.com/MPIBGC-TEE/bgc_md2)
- [https://mybinder.org/v2/gh/MPIBGC-TEE/bgc\\_md2/binder](https://mybinder.org/v2/gh/MPIBGC-TEE/bgc_md2/binder) binder for testing some tutorials (jupyter notebooks) for the creation of new models or a model comparison No installation necessary.