The python packages CompartmentalSystems, LAPM and bgc-md

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1 People and Contributions

The presented Software is the fruit of genuine teamwork. To be able to compete in the catagories of group leaders, postdocs and Ph.D. students we give a simplified summary.

Name	Position	Contributions
Verónika Ceballos-Núñez	Ph.D. student	database population report generation abstract vegetation model
Holger Metzler	Ph.D. student	algorithm implementation, testing, database population report generation
Markus Müller	postdoc, developer	technical lead, algorithm implementation, testing, report generation, webfrontend, refactoring, infrastructure
Carlos Sierra	postdoc, group-leader	abstract ecosystem model formulations, database population, outside collaboration, organization, funding

2 Introduction

The presented software framework consists of three open source python packages:
that serve to represent, classify and analyse compartmental systems of ordinary differential equations (see Definition 1 in Appendix A)with special emphasis on the computation of age and transit time densities of the content.

2.1 CompartmentalSystems package

https://github.com/MPIBGC-TEE/CompartmentalSystems
The package allows the computation of ages and transit times for nonlinear, nonautonomous well mixed compartmental systems. A brief summary if found under the link above. A more detailed discription of the concepts and their application is given in Metzler et al. (2018). A preprint is attached ./PNAS.pdf. An example jupyther notebook that shows how to use the package can be found here: http://compartmentalsystems.readthedocs.io/en/latest/_downloads/nonl_gcm_3p.html

2.2 LAPM package

https://github.com/MPIBGC-TEE/LAPM

2.3 The biogeochemical model data base

https://github.com/MPIBGC-TEE/bgc-md
Short summaries are found under the link above or on our group website https://www.bgc-jena.mpg.de/TEE/software/bgc-md/. The package provides

1. Collections of yaml files each encoding a published carbon cycling model
2. The code to produce (at the moment still static) html for user specified queries.

A Compartmental systems

For the purpose of understanding the applications of the software it suffices to interpret all state variables as contents of reservoirs. In the following we treat here reservoir, pool, and compartmental systems as synonymous, and use relevant definitions from Jacquez and Simon (1993, and references therein). The interpretation easiest to imagine is content measured in units of mass stored in a reservoir defined by its spatial boundaries. However, reservoirs as well as contents can be much more abstract.

Definition 1 (Compartmental system) *Let $F_{i,j}$ be the flux from pool j to pool i, for all $i, j \neq i \in \{1 \ldots n\}$, $F_{i,0} = I_i$ define the influx to pool i and $F_{0,i} = O_i$ the outflux from pool i.*
If $F_{i,j}(\vec{C}, t) \geq 0$, for all $i, j \in \{0 \ldots n\}$ and

$$C_j = 0 \implies F_{i,j}(\vec{C}, t) = 0 \tag{1}$$

we call the ODE system:

$$\dot{C}_i = \sum_{i=0.i\neq j} (-F_{j,i}(\vec{C},t) + F_{i,j}(\vec{C},t)) \quad \forall i \tag{2}$$

compartmental.

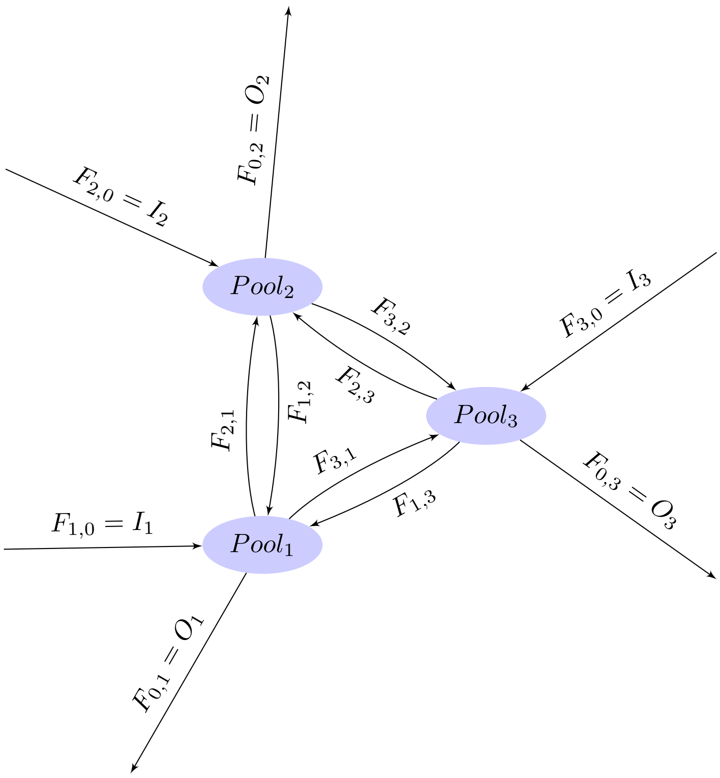

Figure 1: A compartmental model with three pools and all possible connections between the pools and the environment. Note that the flux between pool$_k$ and pool$_l$ is considered a property of the *pipeline*, meaning the flux from pool$_k$ into the pipeline is the same as the flux out of the pipeline into pool$_k$. This ensures mass balance for all fluxes and pools and also for the model as a whole, and makes this the prototype or normal form of mass balanced models with internal connections. Every model that can be drawn in this form is mass balanced. Examples are not limited to networks of pipelines and reservoirs of fluids. Instead of a fluid the total amount of a chemical element in different chemical substances (represented by the pools) can be described by it.

Remarks:
The conditions guarantee mass balance, non-negative fluxes, and ensure that there cannot be any flux out of an empty pool. For non-negative initial values $\vec{C}_0 \in \mathbb{R}^{+^n}$ the pool contents stay non-negative for $t \geq t_0$.

References

Jacquez, J. A. and Simon, C. P. (1993). Qualitative theory of compartmental systems. *Siam Review*, 35(1):43–79.

Metzler, H., Müller, M., and Sierra, C. A. (2018). Transit-time and age distributions for nonlinear time-dependent compartmental systems. *Proceedings of the National Academy of Sciences*, page 201705296.