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New formulas for exploring the age structure of non-linear dynamical systems

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Mathematical models about how mass moves in natural systems are used in various scientific fields such as to understand the global carbon and water cycles, or predicting the spread of contaminants or tracers in water bodies, soils, or organisms. These models, technically known as compartmental systems, are common in medical sciences, biology, and geosciences. Scientists from the Max Planck Institute for Biogeochemistry in Jena made a big step forward in this field by developing formulas and algorithms that help to describe the evolution of the age of particles in such systems when these are out of equilibrium. Their findings, just published in the scientific journal Proceedings of the National Academy of Sciences (PNAS), extend the existing theory that so far was only available for systems resting in equilibrium. The new formulas and algorithms will allow much faster computations. In addition, they will also improve the investigation and understanding of non-linear dynamical systems, which describe many physical and biological processes in nature.

As matter enters a natural system, there is a constant replacement of the particles or atoms that are present in there. For example, a tree that fixes carbon from the atmosphere puts some of this carbon in its leaves, stems, and roots, but at the same time carbon is removed from these compartments by the respiratory activity of the tree. “It is common for scientists to think about how much time carbon atoms spend in each of these compartments. In our general approach, we are interested in learning about the time it takes for atoms or particles to stay in the compartments and the time they need to travel across a system,” says Holger Metzler, first author of the study and PhD student at the Max Planck Institute for Biogeochemistry (MPI-BGC). “In many cases we know, based on measurements, that there is a mix of ages in compartmental systems, but until now we did not have formulas to calculate the proportion of atoms in different ages and how this age structure changes over time as the system evolves,” Carlos Sierra, leader of the Theoretical Ecosystem Ecology group, further explains.

The new mathematical theory developed by the scientists at MPI-BGC in Jena focuses on describing the age structure of mass in a compartmental system. The new set of formulas allows scientists to compute the complete age structure of each individual compartment as well as of the entire system, and to observe how the system evolves over time. The researchers also developed a computer program to perform these complex computations.

“These new formulas and algorithms are highly versatile and can be used for a number of different scientific questions. We implemented them in open source software, which is publicly available to other scientists to corroborate our findings and use them in other scientific studies” illustrates Markus Müller who took an active role in the development of the software. For example, the formulas can be used to calculate how long it would take to remove all the carbon dioxide from the atmosphere that is emitted by humans through combustion of fossil fuels. Furthermore, they can be applied to determine how much time it takes for a drug to be assimilated by an organism that is actively moving such as an athlete; or the time period needed to naturally degrade a contaminant dumped into a lake experiencing a drought. Many different questions of scientific or societal interest can now be tackled with the new mathematical and computational theory.

Original publication:

Metzler H., Müller M., Sierra C. (2018) Transit-time and age distributions for nonlinear time-dependent compartmental systems. *Proceedings of the National Academy of Sciences* doi:10.1073/pnas.1705296115

See also:

Metzler, H., & Sierra, C. A. (2018). Linear Autonomous Compartmental Models as Continuous-Time Markov Chains: Transit-Time and Age Distributions. *Mathematical Geosciences*, *50*(1), 1–34. doi:10.1007/s11004-017-9690-1

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Coal-burning power plant Staudinger, Germany; an example for industrial fossil fuel emissions released to the atmosphere. (© Dr. Klaus-Uwe Gerhardt /pixelio.de)