Open and reproducible science: from theory to equations and algorithms

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Scientific theory is commonly formulated using mathematical equations and new theory is often derived from a set of pre-existing equations. Most of us have experienced difficulty in following mathematical derivations in scientific publications and even more so their transfer into numerical algorithms that eventually result in quantitative tests and predictions of data in plots. The Python package Environmental Science using Symbolic Math (ESSM, https://github.com/environmentalscience/essm) offers an open and transparent way to (a) verify derivations in the literature, (b) ensure dimensional consistency of the equations, (c) perform symbolic derivations, and (d) transfer mathematical equations into numerical code, perform computations and generate plots.

Here we present an example workflow using Jupyter notebooks illustrating the capabilities of the package from (a) to (d). For another example, see https://datascience.ch/article-3-2/.