Geoscientific Model Development Discussions

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Comment on gmd-2022-76

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Community comment on "Downscaling atmospheric chemistry simulations with physically consistent deep learning" by Andrew Geiss et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2022-76-CC1, 2022

The authors in this work develop a neural network (NN) approach for super-resolution, allowing atmospheric chemistry simulations to be run at coarser grid resolutions for computational efficiency. The convolutional NN super resolution is in better agreement with fine resolution output than other interpolation methods. Particularly interesting is the incorporation of scientific fundamentals in the NN, by using a layer in the NN that enforces physical consistency. Specifically, a conservation layer in the NN ensures that the mixing ratio of chemical species in super-resolved regions agrees with the mixing ratio of the corresponding coarse grid cells.

Physically consistent machine learning (ML) tools in the field of atmospheric chemistry modeling are quite new, and this study seems to me to make a novel and potentially valuable contribution in a relatively underexplored area. That being said, I'd like to bring to the authors' attention some prior related work that develops physically consistent machine learning tools for use in atmospheric chemistry modeling. This manuscript shares goals and has some conceptual overlap with recent work published and under review in GMD:

Sturm, P. O. and Wexler, A. S.: A mass- and energy-conserving framework for using machine learning to speed computations: a photochemistry example, Geosci. Model Dev., 13, 4435–4442, https://doi.org/10.5194/gmd-13-4435-2020, 2020.

Sturm, P. O. and Wexler, A. S.: Conservation laws in a neural network architecture: Enforcing the atom balance of a Julia-based photochemical model (v0.2.0), Geosci. Model Dev. Discuss. [preprint], https://doi.org/10.5194/gmd-2021-402, in review, 2021.

The neural network used in this work has some similarities to the physics-constrained NN architecture developed in Sturm and Wexler (2021) in that a layer at the end of a neural network enforces conservation laws. The approach in Sturm and Wexler (2021) has some similarities to the Beucler et al. (2021) approach already cited in line 86, but with a specific focus for conserving mass in atmospheric chemistry. This work is distinct in its application (super-resolution in a spatial domain) and for that reason strictly conserves mixing ratio in space.

The work in this manuscript additionally develops a way of re-dimensionalizing quantities before enforcing the conservation of mixing ratios. This allows the CNN to operate on

normally distributed data, which has shown to improve convergence while training neural networks. The re-dimensionalized data is then passed to a layer that enforces hard constraints (conservation of mixing ratio of chemical species). This is an interesting method that allows for normalization while still enforcing conservation in a dimensionalized space; this approach could also be used to improve upon the physics-constrained NN developed in Sturm and Wexler (2021) in future studies.

If the authors think these recent papers are relevant, a short discussion of them might fit after the sentence on lines 81-83 "Several studies have addressed this problem by adding terms to the neural network's loss function that nudge it towards better agreement", or perhaps after the motivation for NN tools that contain "internal representations of known physical properties of the underlying system" in line 86. Sturm and Wexler (2020) contributed the first framework towards strict conservation laws in ML surrogate models of atmospheric chemistry. The physics-constrained NN in Sturm and Wexler (2021), despite not being a convolutional NN, is a type of NN architecture that contains an internal representation of the system (atom flux continuity/ a stoichiometric balance) which is applied to strictly conserve atoms in a neural network surrogate model of atmospheric chemistry.