Author response to referee technical corrections on
Conservation laws in a neural network architecture: Enforcing the atom balance of a Julia-based photochemical model (v0.2.0)
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29 March 2022

We would like to thank the referees and the editor for their time. Below are point-by-point responses to technical corrections required for acceptance of the final manuscript. Points from referee reports are in *italic*, our responses are in **bold**, and updates to the manuscript are shown in blue.

Report #1
Submitted on 25 Mar 2022
Anonymous referee #2
For final publication, the manuscript should be accepted subject to technical corrections.

The authors have addressed my previous comments/questions, however, I am still puzzled with the answer to the following:
Line 115: ... several key differences:
1. Our entire output vector represents a coupled system where all elements are subject to the constraints. This differs from the approach in Beucler et al. (2021). which constrains a chosen subset of the output and allows some output to be unconstrained.

My point was: The approach in Beucler et al allows to constrain any subset of the output, and the subset can also be the whole output. If you restrict to only allowing to constrain all the output, I would say it is just a particular or restricted case, right? If that is the case, then why is the difference a key difference in positive sense?
Response: Our approach is not a subcase of the Beucler et al. (2021) approach, as our formulation using the A matrix does not require relating inputs to the outputs, but rather balances tendencies in the output vector. This core difference can be found by comparing Eqns. 1 and 2 and corresponding discussion in this manuscript to Eq. 1 in the cited Beucler et al. (2021) publication. This difference is also visually illustrated by comparing Figure 1 in this manuscript to Figure 2 in the Beucler et al. (2021) publication, where inputs are fed to the constraints layers. Due to this fundamental difference, we do not want to make the argument that this is a particular or restricted case. We do note, however, that our approach as developed here operates on all output and is therefore more restrictive than the Beucler et al. (2021) approach (though our approach could conceivably be generalized to only enforce a flux continuity constraint on a portion of the output, such a generalization is outside of the scope of our example). Thanks for pointing out that this point could be made clearer; we have refined this point to now read:

1. Our entire output vector represents a coupled system where all elements are subject to the constraints. This formulation is more restrictive than the approach in Beucler et al. (2021), which constrains a chosen subset of the output and allows some output to be unconstrained.

Report #2
Submitted on 28 Mar 2022
Anonymous referee #1
For final publication, the manuscript should be accepted subject to technical corrections.

The paper is in good shape. I only have a few technical corrections

l 60: "these models" should read "air quality and climate models"
Response: Done! Note that this is line 48 now – the previous manuscript had a discrepancy where the count was skipped for 12 lines (somewhere in between 30 and 45).

eq. 3 brackets are in subscript
Response: We have checked to make sure that the parentheses in equation 3 are not in the subscript.

Figure captions: reference to intermediate model is missing in Figure 2, 3, B1, B2.
Response: Thank you for catching this. All four captions are now updated to begin with:
Scatter plots of target values to predicted values, for the naïve NN (orange, top row), the intermediate NN (purple, middle row) and the physics-constrained NN (green, bottom row)…

l 555: contrast, not contract
Response: We have replaced this word in section 3.5 accordingly.

l 644: I would call this a cloud microphysical model rather than an aerosol microphysical model
Response: We have updated this sentence, which now reads:
Recent work has been published on machine learning surrogate models for cloud microphysics with resolved size bins (Gettelman et al., 2021) and aerosol microphysics using a modal approach (Harder et al., 2021).