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Interactive comment on "Quasi-Newton Methods for Atmospheric Chemistry Simulations: Implementation in UKCA UM Vn10.8" *by* Emre Esenturk et al.

Anonymous Referee #3

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The manuscript by Esenturk et al. describes application of a new hybrid numerical algorithm for solving the ODEs governing atmospheric chemistry simulations. The is typically a significant computational bottleneck of such simulations, although here the authors focus on chemistry-climate models whereas the issue is even more pronounced for chemical-transport models. Thus, the topic is generally of interest and suitable for GMD. The methods proposed here are not ground-breaking, but contain an incremental idea about replacing some Newton-Raphson steps with those using approximate Jacobians (i.e. quasi-Newton). The results are similarly incremental, resulting in speed ups of the overall model by 2-3%, although tests of box-model simulations show up to $\sim$30% improvement. The authors are diligent about exploring different aspects of this

problem and considering many ways of evaluating their results, which seem to be fairly sound. I just wish... as the authors must... that the paper went further in advancing this field. The modest improvements in performance aren't likely to motivate current researches to make a switch to adapt these methods. But perhaps this is a first step in the right direction, and this type of mixed QN/NR method will have improved performance over time. I've provided detailed comments below, which essentially amount to minor revisions.

1.28: on the –> for the

1.30: can be more specific here? how many fewer grid cells?

1.31: Can be more quantitative here as well?

2.26: I object to the statement that "explicit methods are quick" which isn't necessarily true when solving a stiff system and an explicit method is forced to take times steps that are so small that the total integration cost is larger than implicit methods. But, the authors could modify there statement to be correct by changing the scope to any single internal integration step, which indeed are usually quicker for explicit methods than implicit (but still not always).

3.11: Is 2004 really a "recent year"? Or are there more recent applications to cite here?

6.15: This approach is commonly implemented in numerous models that could be cited, for example any that uses KPP-generated solvers with sparse Jacobian options enabled.

7.25: Please clarify how the increment vector is compared to the converge threshold (a scalar). Presumably some norm of the increment? State which norm and provide some justification for associated threshold value.

I can see the distinction that the authors are making between their method and typical QN, but it's a rather small difference.

12.12: Seems like replacing NR iterations with QN isn't going to always reduce the overall computational cost, as the NR step is less accurate. Does it ever (or could it ever) occur that so many more NR iterations are required that the total cost is increased?

Fig 4: Might also be useful to show the total computational expense, rather than # of iterations, as a function of timestep. Computational expense could be plotted on the right hand side axis.

15: I was a little confused as to why QN2-3 was selected based on Fig 3 and Fig 4. It seems that in terms of overall computational expense (Fig 4), there are several where the net_Avg is about 3.9 NR. I would think then these methods should be evaluated in terms of overall accuracy (Fig 3) in a comprehensive manner, using a metrics such as significant digits of accuracy ,

SDA = -log10(max_k E_k)

where E_k is the root mean square norm of the relative error compared to the CNTRL simulation, and max_k indicates that the species with maximum E_k is considered.

Then the algorithm with the fastest, most accurate, performance selected.

17.25: "did not bit" – typo?

General: The authors might consider the applicability of their work to the field of chemical transport models, which spend a much greater fraction of their wall time on solving chemistry (since transport and dynamics are not solved online).

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