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Geoscientific Model Development Discussions
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Interactive comment on "MP CBM-Z V1.0: design for a new CBM-Z gas-phase chemical mechanism architecture for next generation processors" *by* Hui Wang et al.

Anonymous Referee #2

Received and published: 22 June 2018

This paper describes improvements in vectorisation of the Carbon Bond Mechanism Z. While interesting, significant problems need to be addressed before I can recommend its publication in GMD.

General Comments

1. The manuscript contains numerous grammatical and spelling mistakes, and I will attempt to highlight these in detail in my specific comments below. I would recommend the authors check any resubmission carefully.

2. Throughout the manuscript the authors make reference to "the chemistry transport model", "the CTM", and "the air quality model" without first describing which specific

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CTM or AQ model they are referring to, if any. I believe from the context that the model the authors use is in fact the GNAQPMS model, first mentioned on P2L13. If the authors mean a specific CTM it should be discussed in this context, although in some places (e.g. P3L15) the authors mean CTMs in general. If the authors mean any CTM then the phrase "Chemistry Transport Models" or "CTMs" would be appropriate.

3. The paper itself only covers improvements to the CBM-Z module, which I assume is included in some way into GNAQPMS, although this is not discussed by the authors. The CBM-Z code is provided by the authors on Zenodo, which is great to see, although I find it difficult to understand the improvements made in the code by examining Figures 2 and 3 in the manuscript. While graphical representations of these optimisations are useful, I would like to see how these were implemented in practice by the authors giving specific code examples within the manuscript.

4. The authors only give results from a CBM-Z standalone model, rather than having incorporated these improvements back into their CTM and presenting results from there. If available, I would certainly like to see what this does to model performance, as I feel it would strengthen this work greatly. As it is, they present only two case studies, where emissions are zero and meteorological conditions were constant. I would expect to see simulations of a number of different environments similar to those seen in simulations, i.e. free troposphere, boundary layer, urban, rural etc.

5. CBM-Z output is plotted for 10 model hours, and within this time the relative error introduced by the optimisations is less than 0.05

6. The authors describe running the CBM-Z model using a single point and over a number of grids for testing, which I believe to be a spatial grid from the context. In this case, is there any transport or mixing between grid-points, or any differences in meteorological variables? If not, how was this configured and set-up - is each point solving the same conditions at all times? If so, this will not be representative of real-world usage where there will be a large amount of variation across the domain. For the

single-point model, is it integrated in time? If not, how is it configured? I again question whether it would be better to perform these 3D simulations with a CTM instead of a stand-alone CBM-Z model, as it would then allow for a better understanding of how these improvements impact their model in practice. If this is not possible, the authors should give reasons as to why this is.

My major concerns with the manuscript as presented are:

A. Insufficient conditions used for testing

B. Insufficient analysis of the errors introduced by the optimisations.

Specific Comments and Technical Corrections

P1L11 - computational

P1L12 - model used.

P1L18 - Knights Landing

P1L19 - I question whether the <0.05

P1L29 - Chemistry Transport Models

P2L1 - a CTM

P2L1 - computational

P2L3 - relatively simple processes are adopted in CTMs to minimize

P2L4 - computational

P2L5-6 - I would suggest this: "Therefore, air quality simulation studies can benefit significantly by improving the performance of the CTM used."

P2L16 - what is meant by "improving the frequency of air quality forecasting" in this context?

P2L19-21 - do you have any references for the trend in changes to computing architecture that can be quoted here?

P3L4 - what is "the air quality model" in this context? Do you mean "in several air quality models"?

P3L9 - what do you mean by "architecture" in this context?

P3L14 - tropospheric

P3L15 - in CTMs

P4L1 - delete "The" and just start the sentence "CBM-Z also. . ."

P4L6 - simulations

P4L14 - space after AVX-512

P4L19 - do you mean "implement fine-grained parallelization"?

P4L21 - fine-grained

P4L21 - delete the comma after SIMD

P5L5 - does the solver use a fixed number of iterations, or does it integrate to convergence?

P5L13-14 - does the fact that calculations are performed on all grids but not all grids are copied back introduce a possible inefficiency? Are these grids taking time to solve that could be better spent doing something else?

P5L22-23 - as I have mentioned in the General Comments, how representative are these examples? How exactly were they configured?

P6L17 - as I have mentioned in the General Comments, how robust is the error of range <0.05

P7L4-9 - Please provide more details of these 3D simulations, as I am unclear exactly

how they were set-up.

P8L10 - It's great to see that the code is provided, but I found the structure provided confusing and the README provided lacking. However, this isn't part of this manuscript, but I would urge the authors to improve the documentation provided, include a directory listing with what the files do etc.

P10 - Caption to Table 2: versions

P11 - Table 3: How many times were these tests run? Is it possible to provide an error estimate for these numbers?

P12 - Caption to Figure 2: vectors

P12 - Figures 2: As mentioned in the General Comments, I believe that this manuscript would benefit from seeing how the code is altered with these optimizations.

P12 - Caption to Figure 3: grids

P13 - Figure 4: As mentioned in the General Comments, do these trends continue? How long until they become significant?

P13/P14 - Figures 4 5: Which simulations are these figures from, the single-point case or the 3D simulation? I would suggest more species are analyzed, covering a range of chemical lifetimes.

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