Response to Reviewers of the manuscript, **"Development of a grid-independent GEOS-chem chemical transport model as an atmospheric chemistry module for Earth System Models"** by M.S. Long et al.

Jan. 9, 2015

We thank the two reviewers and the Executive Editor for their thoughtful comments and recommendations for improving the manuscript. To the extent possible, we have addressed the reviewers' concerns. Each comment (in italics) followed by our corresponding response to that comment is listed below. Unless otherwise noted, line numbers refer to those in the original, PDF version of the discussion manuscript published online.

Reviewer 1 – C2459

http://acmg.seas.harvard.edu/geos/geos_benchmark.html

It would be useful to outline details of QA procedures involved in ensuring that the "state-of-science" and other developments mentioned are safe and fit for purpose in terms of scientific and technical performance. For example:

p.7507, lines 19-29: The document refers to quick and efficient implementation of new developments. It would be useful to outline what quality assurance methods are employed to prevent new developments being taken up before they are proved beneficial and/or safe. (e.g. any automated testing? "Benchmarking" may mean different things to different people, so it would be helpful if this were briefly clarified in terms of how scientifically valid model evolution is ensured as well as technical performance.)

We now specify in the introduction that "benchmarking" refers to rigorous QA. Further QA details are given at the end of Section 2.1 and we have expanded on those in revision.

p.7508, lines 13-15: This seems to suggest new developments are immediately adopted without any QA. Presumably the impression is incorrect in which case it would be useful to discuss such procedures.

We now clarify that QA is applied to any new developments. Again, further QA details are given at the end of Section 2.1.
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It would be interesting, if possible, to comment in more detail, in the context of the abstract and the main document on the expected scalability and performance beyond the range of processors actually tested.

The following text has been included in the manuscript starting on p. 7515, L21:

“The results further suggest that the chemistry module would remain efficient for simulations beyond the range of values tested”

Individual Issues:

p.7510, line 18: Use of the term "leverage" seems rather flowery. Words with more obviously understandable meaning such as "use", "adopt" or "employ" would aid clarity.

The sentence now reads, ” much of the FORTRAN-77 code base was updated to Fortran-90”.

p.7511, line 7: It seems unclear unclear what "hooks" are in this context. Are these additional interface or wrapper routines or some sort of trigger mechanism?

The text has been revised. The text at p. 7511, L7 now reads,
“The GEOS-Chem code includes specific conditional-compilation flags to accommodate the ESMF interface and permit coupling with external data streams. These flags do not interfere with GEOS-Chem’s scientific operation and are used exclusively in grid, I/O, and utility operations. There are three flags invoked as C-preprocessor statements: *ESMF_*, *EXTERNAL_GRID*, and *EXTERNAL_FORCING*.”

p.7511, line 10: Re the sentence: "They can remain invisible to the scientific programmer." To what end? i.e. When would that be desirable and how is it achieved?

This statement has been removed from the text.

p.7512, lines 3-8: It would help the document flow to establish this as a standard working practice earlier in the document. (See earlier specific comments about QA.)

We have added mention of QA in the introduction.

p.7512, line 21: Missing word? Existing wording seems to imply that initialization is performed at the beginning of each time step. That seems unlikely. Should this say "at the beginning of the first time step" or at the "start of the run" or something similar?

The words “time step” have been replaced with “simulation”.

p.7514, line 22: Use of the term: "Scalability simulations" for clarity of meaning. Earth system simulations have been run using different resource configurations in order to establish scalability, so the term "scalability tests" or "scalability analysis" would seem more appropriate. i.e. scalability itself is not being simulated.

The line has been revised. It now reads, “Simulations used to test strong scalability of the coupled system were run…”

p.7515, line 8: Suggest the use of "Wall-clock time", "elapsed time" or two separate words "wall time" rather than "walltime".

Instances of “walltime” were replaced with “wall time”.

p.7515, line 19: Suggest rewording to avoid the suggestion that scaling efficiency has truly been demonstrated for ANY number of cores.

The words, “all numbers of cores”, have been replaced with “the range of cores tested.”

p.7515, line 22: The word "other" is in quotes. The reason for this is unclear. Would it help to provide general examples of the scalability, performance and code structure characteristics of the important elements of these "other" components as compared with the chemistry module?

The word “other” has been removed from the text.

Reviewer 2 – C2525

Specific comments:

1. The authors claim that the new GEOS-Chem code can serve as an atmospheric chemistry module for Earth System Models (plural). In practice, this will be limited to those ESMs that make use of the ESMF interface. The authors should indicate which ESMs besides GEOS-5 actually use ESMF, and if there are concrete plans for integrating GEOS-Chem in other ESMs.

The inclusion of data sockets as described in the text (p. 7510, L24) places all of the data structures required to couple the system within any ESM in a few modules. This is intended to simplify coupling in any configuration. Further the use of the C-preprocessor flags "EXTERNAL_GRID" and "EXTERNAL_FORCING" automatically configure GEOS-Chem for sending and receiving data necessary for coupling. While this was not specified in the text, it was our intention from the outset to make the code as general as possible to facilitate generic coupling.

The following text has been included after p. 7512, L2:
"The redesign of GEOS-Chem's data structures was meant to simplify coupling of GEOS-Chem with any ESM regardless of its ESMF compatibility. In the absence of an ESMF interface, users would be required to engineer a specific interface for their ESM, However, GEOS-Chem's data sockets and conditional-compilation flags facilitate this task by having all input and output data structures and associated methods conveniently located in a few specific modules."

2. The splitting in a transport operator and a local or chemical operator, indicated in Equations (2) and (3) in Section 2, is inconsistent with the actual implementation, described in Section 3. According to Section 2, wet deposition is described by the chemical operator in GEOS-Chem. According to Section 3, however, cloud processing and in-cloud scavenging of chemical tracers are described as part of GEOS-5 native moist physics. Please make sure that the theoretical description given in Section 2 is consistent with the actual implementation, and adapt the equations accordingly.

The reviewer makes a good point that needs clarification. Convective scavenging fits into Eq. (2) vs. Eq. (3) since it cannot be decoupled from transport. This is now addressed in the text at p. 7509, L13:

"Wet deposition involving sub-grid convection cannot be decoupled from transport and is treated as part of convection in the transport operator".

3. According to Section 2, the transport operator describes advection, convection, and boundary layer mixing. I assume that sedimentation of large particles is also described by the transport operator. Please mention this in the text, or clarify why it is not.

The following text has been added at p. 7509, L13:

"Gravitational settling of particles is treated as part of the chemical operator."

4. Please add a statement on the mass-conserving character of the semi-lagrangian advection scheme used in GEOS-5, and explain why and for which tracers this is important.

This does not seem relevant to our work.

5. The HEMCO emission module is presented as a general tool to describe emissions in CTMs and ESMs. Please indicate how widespread its use is. Is it used in other models besides GEOS-Chem?

We deleted as indeed unnecessary "HEMCO was designed by Keller et al. (2014) as a flexible general tool for facilitating the implementation and update of emission inventories in CTMs and ESMs"

6. Page 7515, line 19: The scaling efficiency using 192 cores is close to 0.7. On a scale from 0 to 1, I wouldn't call that "close to unity".

The phrase "close to unity" has been removed from the text.

7. Page 7517, line 2: Quantitative comparison of the GEOS-5/GEOS-Chem and CTM systems does not necessarily require using the same meteorological data in both. Quantitative comparison of the climatological behavior of both systems could also be of interest, e.g. to study to role of climate biases in the GEOS-5 ESM.

The word "quantitative" has been removed, and the sentence now reads, "A more thorough evaluation of GEOS-Chem's chemistry within the GEOS-5 system would require the use of the same meteorological data as the offline CTM…"

8. Last sentence of the summary: "Although the inclusion of detailed atmospheric chemistry in an ESM is a major computational expense, it becomes relatively more efficient as the number of cores increases due to its consistent scalability." Since the chemical tracers are transported within the GEOS-5 general circulation model, the inclusion of GEOS-Chem will affect the scaling efficiency of the dynamics. The reduced scalability of the dynamics could therefore also be related to the addition of chemical tracers, in which case the concluding sentence would not hold. Please clarify this issue.

The last sentence in the summary has been revised. It now reads,
"Although the inclusion of detailed atmospheric chemistry in an ESM is a major computational expense, chemistry operations become relatively more efficient as the number of cores increases due to its consistent scalability."
As well, the sentence, "This result also likely reflects the additional burden associated with the greater number of tracers.", was added to the text.

Technical corrections:

1. In the title, please change "GEOS-chem" to "GEOS-Chem".

The title has been corrected.

2. On page 7511, line 13, please add a space between "ESMF_" and "macro".

A space has been added.

Editor's Comment – C2771

In my role as Executive editor of GMD, I would like to bring to your attention our Editorial:
http://www.geoscientific-model-development.net/gmd_journal_white_paper.pdf
http://www.geosci-model-dev.net/6/1233/2013/gmd-6-1233-2013.html

This highlights some requirements of papers published in GMD, which is also available on the GMD website in the 'Manuscript Types' section:
http://www.geoscientific-model-development.net/submission/manuscript_types.html

In particular, please note that for your paper, the following requirements have not been met in the Discussions paper – please correct this in your revised submission to GMD.

"– The paper must be accompanied by the code, or means of accessing the code, for the purpose of peer-review. If the code is normally distributed in a way which could compromise the anonymity of the referees, then the code must be made available to the editor. The referee/editor is not required to review the code in any way, but they may do so if they so wish. "

"– All papers must include a section at the end of the paper entitled "Code availability". In this section, instructions for obtaining the code (e.g. from a supplement, or from a website) should be included; alternatively, contact information should be given where the code can be obtained on request, or the reasons why the code is not available should be clearly stated. "

The following section and text has been added at the end of the manuscript prior to Acknowledgements:

"**Code Availability.** GEOS-Chem source code is freely available to the public. Source code may be downloaded by following instructions found at http://wiki.seas.harverd.edu/geos-chem."

"– All papers must include a model name and version number (or other unique identifier) in the title. "

The title has been amended to include the model version.