Geoscientific

Model Development

Discussions

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Interactive comment on "GPU accelerated atmospheric chemical kinetics in the ECHAM/MESSy (EMAC) Earth system model (version 2.52)" *by* Michail Alvanos and Theodoros Christoudias

Anonymous Referee #1

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The manuscript presents a description and accuracy and performance evaluation of a software that enables the established Earth System Model EMAC to offload its most demanding calculations onto GPUs. Such a development is very welcome and highly needed in order to address the challenges of atmospheric chemistry modelling under changing climate. The manuscript is well written and structured. However, results for non-homogeneous ODE system are not presented and the evaluation of model accuracy should be expanded both in terms of key atmospheric species and of time integration length.

Major comments

1) At page 6 it is written that RCONST, the array of the rate constants, is calculated only once at the beginning of the integration. This is correct for the setup the authors have chosen. However, the default MECCA chemical mechanism in EMAC 2.52 is translated by KPP in a ODE system with varying (rate) coefficients which has to be integrated as a non-homogeneous system. This means that the RCONST array has to be re-calculated at each substeps. How does this additional memory allocation affect accuracy and performance ? The test should be done with the unchanged gas.eqn file of MECCA without replacement of the reactions for MIM1.

2) To Figure 3. The largest deviations from zero seem to be for soluble species whose aqueous-phase chemistry is very important and solved with KPP1 by the submodel SCAV. The ODE system for aqueous-phase chemistry is notoriously much stiffer than the one for the gas-phase. This hints to a potential amplification of errors. One could check the accuracy of a simulation without scavenging.

3) For climatic simulations it is important to ensure no drift in the results. A 10-year simulation is desirable when one thinks about chemistry-climate feedbacks in the stratosphere and methane lifetime in the troposphere.

4) The manuscript would profit from showing the distribution of the differences at simulations' end. For instance, the relative differences for the zonal mean ozone and surface OH are worth showing. Given their importance for aerosols differences for surface NH_3 and SO_2 are desirable.

Minor comments

1) A reference to the actual KPP version used (likely v 2.2.3-rs) published in Sander et al.(2011) (http://www.geosci-model-dev.net/4/373) and slightly modified from KPP-2.1 by Sandu and Sander (2006) (http://www.atmos-chem-phys.net/6/187/2006/) is better. The main difference to KPP1 is the generated code in Fortran 90 and not anymore in

FORTRAN.

2) What is meant by statistical reduction of results at page 6? Why is it needed?

3) Page 13, line 1. How can it be "climatic" if the climate is understood to be at least a ~30 yr average state of the atmosphere?

4) To Figure 3. Could you show the differences for OH, N2O5, HNO3, HCOOH and H2O2? Could you also explain the meaning of the bar widths and shaded areas?

5) Which chemical species shows the maximum error of 0.54% ?

6) The chemical solver of MECCA in EMAC has a default relative tolerance (rtol) of 1E-2 and a absolute tolerance (atol) of 1E1 although for key short-lived radicals the atol = 1 is used. This implies a maximum 1% error.

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