Linking Composition and Circulation on Intermediate Spatio−Temporal Scales LiCoS (861 and 869)

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Abstract

The description of chemical processes in climate simulations is necessary in order to address questions about the interplay between circulation and air composition and thus climate predictability. For instance, stratospheric ozone depletion has been found to be most important cause of the observed poleward shift in the westerly jet during the austral summer[1]. However, the accurate description of the atmospheric chemistry processes is one of the most computationally intensive tasks in Chemistry-Climate simulations, as it typically accounts for $50\% - 95\%$ of the total computational time. This is obviously a bottleneck for the model performance in high resolution simulations, as well as for the quantification of the model uncertainties. Here, we describe mathematical and computational approaches recently implemented into the ECHAM/MESSy atmospheric chemistry (EMAC) simulation system[2,3] with the aim of reducing the required computational cost. We also present the evaluation of the "Business as Usual" air pollution emission scenario. Finally, we present sensitivity simulations with the MPI-ESM model[4] aimed at investigating the role of clouds and convection on limiting climate predictability.

Chemical ODEs and their integration

In the operator splitting framework individual processes are solved separately in a serial way. The evolution of trace gas concentrations (y) due to chemical kinetics in "closed-system" boxes is then described by a system of Ordinary Differential Equations (ODEs):

$$y' = f(t, y) = P(t, y) - D(t, y) \, y$$

where P and D are the production rate and destruction frequency of the y array. The time integration of the chemical ODEs has to cope with the stiffness phenomenon in which the largest step size h_n^* guaranteeing numerical stability is much smaller than the largest step size h_n for which the discretization error is still sufficiently small[5]. Due to numerical stability considerations, only implicit integration methods can be used with satisfactory results. One of the most common methods is the Rosenbrock algorithm that solves the fully implicit scheme

$$y_{n+1} = y_n + h \, f(y_{n+1})$$

using a generalization of the Euler backward method using more stages[6]. In this work the chemical mechanism used comprises 164 species in 426 reactions.

Stiffness and CPU load distribution

During the ODEs integration, stiffness usually appears when the ratio between the real part of the largest and the smallest Jacobian eigenvalues is $>> 1$. As a consequence, a large number of small time steps ($NSTEPS$) are required for the integration especially of the first second. This is related to the perturbation that processes like changes in photolysis frequency and transport exert on che the chemical system. Thus, very fast transients need to be resolved by the integration method. In order to cope with the diversity of perturbations (and induced stiffnesses) an adaptive time stepping method is used[6]. Usually, the time step size (h_{n+1}) is determined with the formula:

$$h_{n+1} = h_n (\epsilon/r_n)^{1/k}$$

where ϵ = tolerance, r_n = error estimate and $k = p + 1$ (p is order of convergence).
The common adaptive time-stepping is however limited within tight bounds to avoid many step rejections. In 3D atmospheric simulation this leads to a very heterogeneous CPU load distribution. This is shown in the figure in which the column integrated number of subtime steps needed for a $\Delta T^{splitting}$ of 15 min with 39 vertical layers.
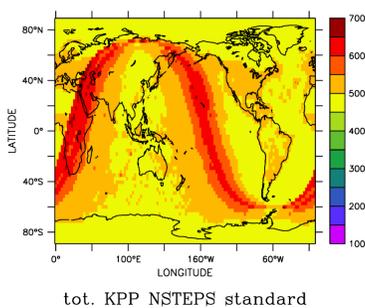
tot. KPP NSTEPS standard

The highest $NSTEPS$ is required for the day-night transition regions in which the time derivative of the photolysis frequencies is very steep. Such a CPU load distribution limits the efficient use of the available computer resources (load imbalance).

Fast chemical integration (WP 1.3-1.4): stiffness reduction

In atmospheric chemical mechanism in which only gas-phase and surface reactions are represented, the stiffness is related to the lifetime (τ) of short-lived species[6]. Their initial concentrations relax very quickly to a steady state that is completely determined by the long-lived species. For such species the concentration can be approximated by the simplest Quasi-Stationary-Steady-Approximation (QSSA) formula

$$P(t, y) - D(t, y) \, y = 0 \implies y = P(t, y)/D(t, y)$$

in order to reduce the stiffness of the ODEs[7]. The error introduced by the QSSA is usually acceptable when τ_i is less than 1s and the QSSA index I, defined as $|(P - L)/(P + L)|$, is less than 10^{-2} [8]. The time QSSA species need to reach the steady stade is called induction period (τ_{ind}) and is estimated to be about 10 times the longest QSSA species lifetime (τ_{QSSA}^{max})[7]. In this work, the QSSA species concentrations are adjusted to their steady state values and the Rosenbrock algorithm is started with an initial time step equal to the induction period.

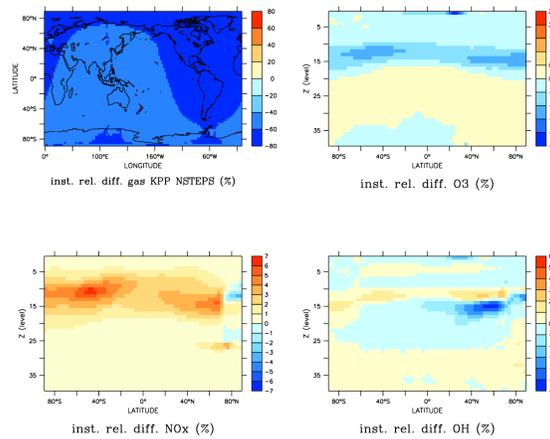## Fast chemical integration (WP 1.3-1.4): time-step control

The more sophisticated step size controller algorithm H211b[9] is used

$$h_{n+1} = (\epsilon/r_n)^{1/(bk)} (\epsilon/r_{n-1})^{1/(bk)} (h_n/h_{n-1})^{-1/b} h_n$$

Differently from the common one, it makes use of the error estimate of the previous time step. This controller is used without bounds.

Fast chemical integration (WP 1.3-1.4): accuracy

A series of tests with different Rosenbrock integrators, τ_{QSSA}^{max} and time stepping parameters have been performed. The optimum for speedup and accuracy has been found with Rosenbrock-Rodas3 in the autonomous mode, $\tau_{QSSA}^{max} = 1s$, and the H211b controller with $b = 1$ and $k = 2$. Zonal mean differences from the reference configuration for O_3, NO_x and OH at the end of a 1-year simulation with EMAC in the quasi CTM mode are shown below.

inst. rel. diff. gas KPP NSTEPS (%)   inst. rel. diff. O3 (%)

inst. rel. diff. NOx (%)   inst. rel. diff. OH (%)

Fast chemical integration (WP 1.3-1.4): speedup

ODEs integration has been sped up by a factor of **4-5**, globally. However, the speedup of the overall model is about **2**. The speedup as a function of the number of CPUs is shown below.
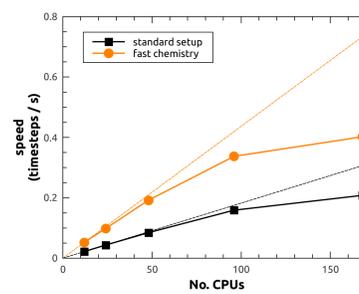
"Business as Usual" scenario (WP 2.1)

Evaluation of the "Business as Usual" emission scenario from EDGAR-CIRCE project has been performed [10].
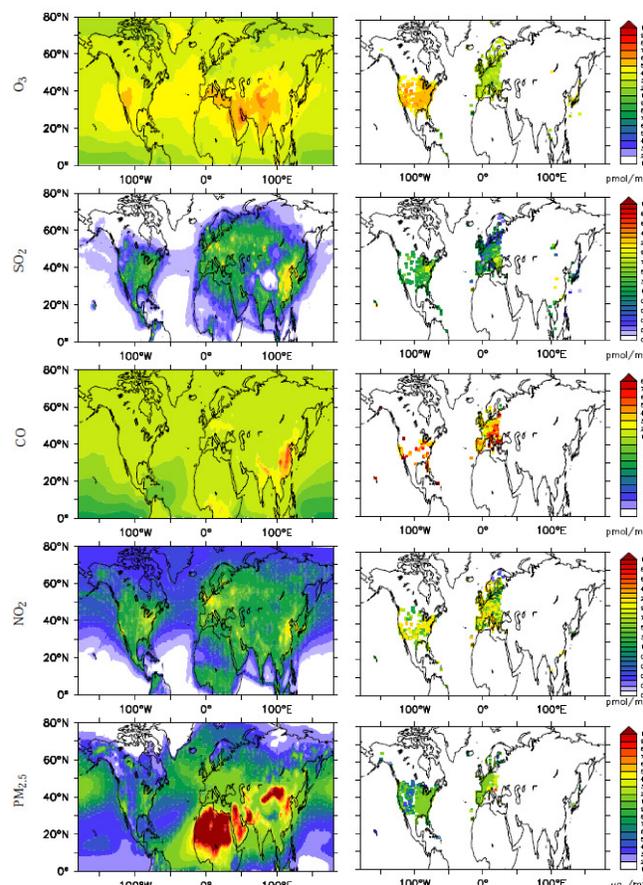
LEFT PANELS: simulated annual mean mixing ratios (in pmol mnol^{-1} and μg m^{-3} for PM2.5) for the year 2005. RIGHT PANELS: annual mean (in pmol mnol^{-1} and μg m^{-3} for PM2.5) from the EPA, EEA and EANET network observations for the year 2005.

Clouds, convection and climate predictability (WP 1.6)

Approach

- How do clouds and biases in cloud representation affect surface temperature anomalies?
- How important are cloud processes for predictability?

Influence of low cloud variability on SST anomalies have not been studied much. There are hints from observations for positive feedback among low-level clouds, large scale circulation and SST's on decadal time scales in NE Pacific. The change in stratocumulus cloud cover is principal factor maintaining decadal SST anomalies in NE Pacific [11].
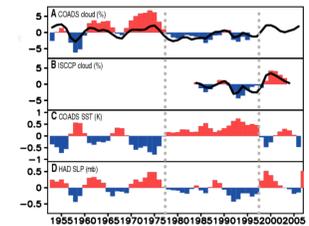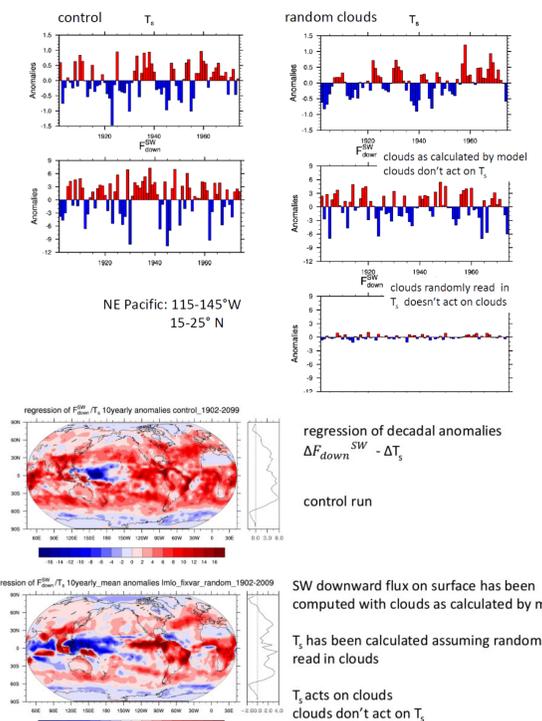

So far two lines of analysis:
- Analysis of existing runs (CMIP5)
- New simulations in which clouds are partially de-coupled from surface temperature anomalies

Decoupling clouds from SST anomalies

In order to decouple cloud and temperature anomalies: prescribe cloud feedbacks

- Special ECHAM6 run with randomly read in (each time radiation is called) cloud parameters: for calculated fluxes Ts doesn't influence clouds
- in a second call to radiation, fluxes are computed with original cloud properties: here clouds don't influence Ts (method adapted from T. Mauritsen)
- First preliminary results with ECHAM6 coupled to a slab ocean

NE Pacific: 115-145°W
15-25° N

regression of decadal anomalies
ΔF_{down}^{SW} - ΔT_s

control run

SW downward flux on surface has been computed with clouds as calculated by model

T_s has been calculated assuming randomly read in clouds

T_s acts on clouds
clouds don't act on T_s

Work in progress.

Recommedations

Next steps

- Speed up the aerosol module GMXe
- Establish relationships between meteorological and air quality indices
- Investigate impact of the "Climate and Air-Quality Policy" emission scenario on air quality and climate predictability
- Repeat simulations for decoupling clouds effect from SST's with the fully coupled MPI-ESM

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