DCMIP2016, Part 2: Moist Baroclinic Wave

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Abstract. This paper discusses a new idealized test for atmospheric dynamical cores.

1   Introduction

The baroclinic instability test of Ullrich et al. (2014) considers a reference state in geostrophic and hydrostatic balance that satisfies the conditions for baroclinic instability. Although a perfect model should be able to maintain this state indefinitely, small truncation errors associated with numerical inaccuracies and grid structure will trigger the development of the wave modes associated with baroclinic development. To control the development of the baroclinic wave, a small perturbation (but one which is large compared with machine truncation) is added to the flow so as to trigger the development of a wave over a period of approximately 10 days. A moist variant of the dry dynamical test of Ullrich et al. (2014) is considered here so as to understand the impact of moisture feedbacks on the development of the wave.

This test case is similar in character to the test of Jablonowski and Williamson (2006), but has a number of key differences: (1) this test is an analytical solution of the equations of motion in height (z) coordinates, (2) the bottom topography is zero

throughout the domain, (3) the new test case does not have a distinct stratosphere (the presence of a stratosphere is largely irrelevant for understanding baroclinic development), and (4) the velocity field goes to zero at the model surface.

Table 1. List of constants used for the Moist Baroclinic Wave test case

Constant	Value	Description
z_{top}	44000 m	Recommended height position of the model top
p_{top}	≈ 2.26 hPa	Recommended pressure at the model top
X	1	Reduced-size planet scaling factor, see below
a	a_{ref}/X	Scaled radius of the Earth
Ω	$\Omega_{\text{ref}}X$	Scaled angular speed of the Earth
p_s	1000 hPa	Surface pressure (constant)
p_0	1000 hPa	Reference pressure (constant)
u_0	35 m s^{-1}	Maximum amplitude of the zonal wind
b	2	Half-width parameter
K	3	Power used for temperature field
T_E	310 K	Horizontal-mean temperature at the surface
T_P	240 K	Temperature at the polar surface
u_p	1 m s^{-1}	Maximum amplitude of the zonal wind perturbation
z_p	15000 m	Maximum height of the zonal wind perturbation
λ_p	$\pi/9$	Longitude of the zonal wind perturbation centerpoint (20° E)
φ_p	$2\pi/9$	Latitude of the zonal wind perturbation centerpoint (40° N)
R_p	$a/10$	Radius of the zonal wind perturbation
Γ	0.005 K m^{-1}	Temperature lapse rate
ΔT	4.8×10^5 K	Empirical temperature difference
φ_w	$2\pi/9$	Specific humidity latitudinal width parameter (40°)
p_w	340 hPa	Specific humidity vertical pressure width parameter
q_0	0.018 kg/kg	Maximum specific humidity amplitude
q_t	1.0×10^{-12} kg/kg	Specific humidity above artificial tropopause
p_t	10000 hPa	Pressure at artificial tropopause

1.1 Reference State

This section describes the analytical form of the reference state for the baroclinic wave. The test case is initialized with a constant surface pressure and with a surface geopotential equal to zero. The meridional wind in the reference state is zero.

In the reference state, the virtual temperature is given by

$$T_v(\varphi,z) = \frac{1}{\tau_1(z) - \tau_2(z) I_T(\varphi)}, \tag{1}$$

2

where $I_T(\varphi)$ is defined as

$$I_T(\varphi) = (\cos\varphi)^K - \frac{K}{K+2}(\cos\varphi)^{K+2}, \tag{2}$$

and $\tau_1(z)$ and $\tau_2(z)$ are defined as follows:

$$\tau_1(z) = \frac{1}{T_0}\exp\left(\frac{\Gamma z}{T_0}\right) + \left(\frac{T_0 - T_P}{T_0 T_P}\right)\left[1 - 2\left(\frac{zg}{bR_d T_0}\right)^2\right]\exp\left[-\left(\frac{zg}{bR_d T_0}\right)^2\right] \tag{3}$$

$$\tau_2(z) = \frac{(K+2)}{2}\left(\frac{T_E - T_P}{T_E T_P}\right)\left[1 - 2\left(\frac{zg}{bR_d T_0}\right)^2\right]\exp\left[-\left(\frac{zg}{bR_d T_0}\right)^2\right], \tag{4}$$

with $T_0 = \frac{1}{2}(T_E + T_P)$. To maintain hydrostatic balance, the pressure is given by:

$$p(\varphi, z) = p_0 \exp\left[-\frac{g}{R_d}(\tau_{\text{int},1}(z) - \tau_{\text{int},2}(z)I_T(\varphi))\right] \tag{5}$$

with $\tau_{\text{int},1}(z)$ and $\tau_{\text{int},2}(z)$ given by

$$\tau_{\text{int},1}(z) = \frac{1}{\Gamma}\left[\exp\left(\frac{\Gamma z}{T_0}\right) - 1\right] + z\left(\frac{T_0 - T_P}{T_0 T_P}\right)\exp\left[-\left(\frac{zg}{bR_d T_0}\right)^2\right] \tag{6}$$

$$\tau_{\text{int},2}(z) = \frac{(K+2)}{2}\left(\frac{T_E - T_P}{T_E T_P}\right)z\exp\left[-\left(\frac{zg}{bR_d T_0}\right)^2\right]. \tag{7}$$

If density is a prognostic variable, it can be obtained from p, T_v and the ideal gas law (**??**). Finally, the zonal velocity is

$$u_{\text{ref}}(\varphi, z) = -\Omega_{\text{ref}}a_{\text{ref}}\cos(\varphi) + \sqrt{(\Omega_{\text{ref}}a_{\text{ref}}\cos(\varphi))^2 + a_{\text{ref}}\cos(\varphi)U(z,\varphi)}, \tag{8}$$

where

$$U(z,\varphi) = \frac{gK}{a_{\text{ref}}}\tau_{\text{int}_2}(z)\left[(\cos\varphi)^{K-1} - (\cos\varphi)^{K+1}\right]T_v(\varphi, z). \tag{9}$$

1.2 Perturbations

To trigger the development of the baroclinic wave, a perturbation is applied to the zonal velocity field that takes the form of a simple exponential bell with a vertical taper:

$$u'(\lambda, \varphi, z) = \begin{cases} u_p Z_p(z)\exp\left[-\left(\frac{R(\lambda, \varphi; \lambda_p, \varphi_p)}{R_p}\right)^2\right], & \text{if } R(\lambda, \varphi; \lambda_p, \varphi_p) < R_p, \\ 0, & \text{otherwise,} \end{cases} \tag{10}$$

where

$$Z_p(z) = \begin{cases} 1 - 3\left(\frac{z}{z_p}\right)^2 + 2\left(\frac{z}{z_p}\right)^3, & \text{if } z \le z_p, \\ 0, & \text{otherwise.} \end{cases} \tag{11}$$

Consequently, the perturbed velocity field takes the form

$$u(\lambda, \varphi, z) = u_{\text{ref}}(\varphi, z) + u'(\lambda, \varphi, z). \tag{12}$$

1.3 Moist initial conditions

We define the vertical η coordinate as

$$\eta(\lambda, \varphi, z) = p(\lambda, \varphi, z)/p_s. \tag{13}$$

Since the surface pressure of the moist air p_s is constant with $p_s = p_0 = 1000$ hPa the vertical coordinate η is represented by $\eta = p/p_0$. Specific humidity is specified in terms of η as

$$q(\lambda, \varphi, \eta) = \begin{cases} q_0 \exp\left[-\left(\dfrac{\varphi}{\varphi_w}\right)^4\right] \exp\left[-\left(\dfrac{(\eta-1)p_0}{p_w}\right)^2\right], & \text{if } \eta > p_t/p_s, \\ q_t, & \text{otherwise.} \end{cases} \tag{14}$$

The functional form of q and its parameters were inspired by observations. This moisture fields leads to maximum relative humidities around 85% in the lower levels of the midlatitudes.

Note that the moist temperature is colder than the temperature one would obtain with $q = 0$. However, note that in the moist case the virtual temperature and moist pressure determine the strength of the pressure gradient term in the momentum equations. Since these are identical to the temperature and pressure in the dry case, the forcing by the pressure gradient term is the same in both the dry and moist variant of the baroclinic wave. The moist variant of the baroclinic wave without the temperature forcing from large-scale condensation should lead to almost identical results when compared to the dry version. Very small variations are expected since the moisture gets independently transported as a passive tracer in this case and some models utilize the moist variant of the physical constant c_p. If possible, the dry c_p should be used. Comparing the evolution of the dry baroclinic wave to its moist variant (without large-scale condensation) can serve as a first sensibility check.

1.4 Terminator 'toy'-chemistry

The terminator 'toy'-chemistry is presented in Lauritzen et al. (2015) and mimics photolysis-driven processes near the solar terminator. Two passive[1] tracers, Cl and Cl_2, that are chemically reactive are transported. The sources and sinks are given by a simple, but non-linear, 'toy' chemistry. As a result, strong gradients in the spatial distribution of the species develop near the edge of the terminator. Despite the large spatial variations in Cl and Cl_2 the weighted sum $Cl_y = Cl + 2Cl_2$ should always be preserved in any flow field (if the initial condition for Cl_y is constant). An overview of the 'toy' terminator chemistry is given in Appendix A. The terminator test demonstrates how well the advection/transport scheme and/or physics-dynamics coupling preserves linear correlations.
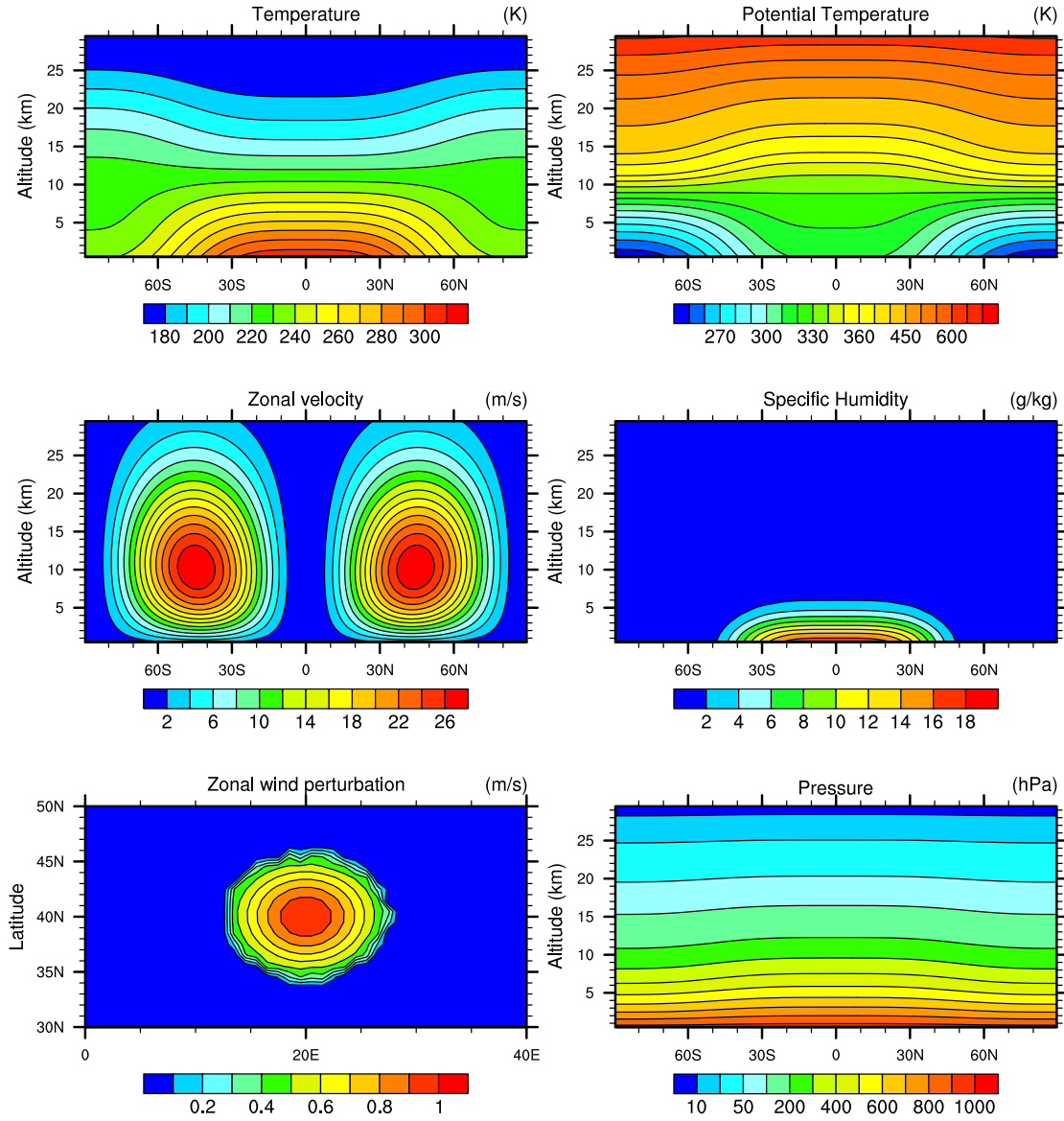
The initial conditions for Cl and Cl_2 (in terms of **dry** mixing ratios q_{Cl} and q_{Cl2}, respectively) are the steady-state solutions to the terminator chemistry with no flow Lauritzen et al. (2015) (see Figure 2):

$$q_{Cl}(\lambda, \theta, z, t=0) = D - r, \tag{15}$$

$$q_{Cl2}(\lambda, \theta, z, t=0) = \frac{1}{2}\left(q_{Cly} - D + r\right), \tag{16}$$
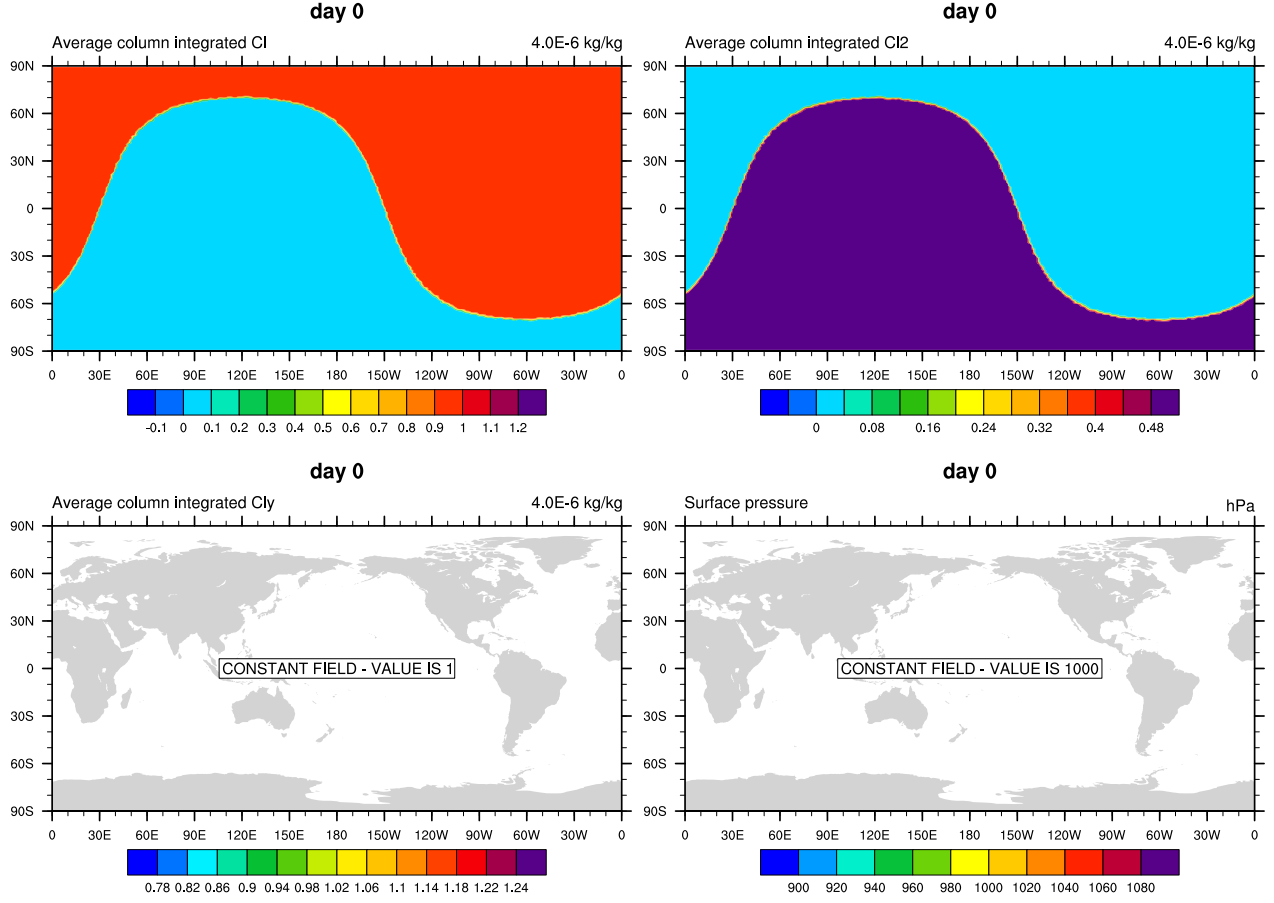
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[1] i.e. tracers do not feed back on the flow

Figure 1. Initial state for the moist baroclinic wave test.

where $q_{Cly} = 4.0 \times 10^{-6}$kg/kg,

$$r = \frac{k_1}{4k_2}, \tag{17}$$

$$D = \sqrt{r^2 + 2rq_{Cly}}, \tag{18}$$

5

HOMME

Figure 2. Contour lines of $< q_{Cl} > /(4.0 \times 10^{-6})$, (upper left), $< q_{Cl2} > /(4.0 \times 10^{-6})$ (upper right), $< q_{Cly} >$ (lower left) and surface pressure (lower right) at day 0 (initial conditions).

and reaction coefficients k_1 and k_2 are given in appendix A (equations (A8) and (A9)). Please note that the mixing ratios are dry, i.e. the ratio between the density of the species and the density of dry air.

The forcing terms are computed analytically (assuming no flow) over a (physics/chemistry) time-step Δt:

$$F_{Cl}^n = -L_{\Delta t} \frac{(q_{Cl}^n - D + r)(q_{Cl}^n + D + r)}{1 + e^{-4k_2 D \Delta t} + \Delta t L_{\Delta t}(q_{Cl}^n + r)}. \tag{19}$$

5 where q_{Cl}^n is the value of q_{Cl} at the beginning of the n'th time step and

$$L_{\Delta t} = \begin{cases} \frac{1 - e^{-4k_2 D \Delta t}}{D \Delta t} & \text{if } D > 0 \\ 4k_2 & \text{if } D = 0. \end{cases} \tag{20}$$

6

and by conservation,

$$F_{Cl_2}^n = -\frac{1}{2} F_{Cl}^n. \tag{21}$$

In implementation, $L_{\Delta t}$ needs some care. As $4 k_2 D \Delta t$ approaches machine precision, it is useful to simply use the formula for $D = 0$ rather than the expression for $D > 0$. The chemistry/physics updated mixing ratios are given by

$$q_{Cl}^n + \Delta t \, F_{Cl}^n, \tag{22}$$

$$q_{Cl2}^n + \Delta t \, F_{Cl2}^n. \tag{23}$$

In terms of Fortran code the analytical forcing is given by:

```
! dt is size of physics time step
cly = cl + 2.0*cl2

r = k1 / (4.0*k2)
d = sqrt( r*r + 2.0*r*cly )
e = exp( -4.0*k2*d*dt )

if( abs(d*k2*dt) .gt. 1e-16 )
   el = (1.0-e) / (d*dt)
else
   el = 4.0*k2
endif

f_cl  = -el * (cl-d+r) * (cl+d+r) / (1.0 + e + dt*el*(cl+r))
f_cl2 = -f_cl / 2.0
```

The reaction rates are defined by

```
! k1 and k2 are reaction rates
k1_lat_center =  20.0 ! degrees
k1_lon_center = 300.0 ! degrees
k1 = max(0.d0,sin(lat)*sin(k1_lat_center)
          + cos(lat)*cos(k1_lat_center)*cos(lon-k1_lon_center))
k2 = 1.0
```

The initial condition is defined by

```
cly = 4.0e-6
```

```
      r = k1 / (4.0*k2)
      d = sqrt( r*r + 2.0*cly*r )

5     cl = d-r
      cl2 = cly / 2.0 - (d-r) / 2.0
```

Fortran subroutines that, given (λ, θ) will return the tendencies for q_{Cl} (mixing ratio) and q_{Cl2} (mixing ratio), are provided as supplemental material in Lauritzen et al. (2015). Similarly for the forcing terms.

The 'toy' terminator chemistry test here uses the baroclinic wave initialization (described in section **??**) based on the moist
10 setup and the flow will transport the two species that interact non-linearly with each other through the toy chemistry. A physics time-step of 30 minutes and 15 minutes, respectively, is used. Note that if the user has the baroclinic wave setup the only additional work is to initialize two tracers and implement the chemistry. Example solutions are shown for HOMME (High-Order Method Modeling Environment) Dennis et al. (2012) spectral elements and HOMME-CSLAM Lauritzen et al. (2016). The latter model is based on CSLAM Lauritzen et al. (2010) transport of tracers consistently coupled with spectral element
15 dynamics.

1.4.1 Diagnostics

If the initial conditions for q_{Cl} and $2q_{Cl2}$ add up to a constant (as is the case in this setup) then no matter how the individual species evolve the weighted sum $q_{Cly} = q_{Cl} + 2q_{Cl2}$ should be constant in space and time. Hence the analytical solution for q_{Cly} is known. The terminator chemistry preserves the linear relationship between q_{Cl} and q_{Cl2} so the only causes for this
20 relationship to break are:

- the transport operator (usually the limiter/filter) does not exactly preserve linear relations, and/or,

- physics-dynamics coupling breaks the relationship (see, e.g., Figure 3).

The following diagnostics are used in this test case:

- Average column integrated mixing ratio (two-dimensional variable):

25
$$< q > = \frac{\int_{z=0}^{z_{top}} q\, dz}{\int_{z=0}^{z_{top}} dz}. \tag{24}$$

where $q = q_{Cl}, q_{Cl2}$. The global integrals should be computed consistently with the numerical method (preferably 'inline' in the source code on the native grid and not using interpolated data).

– $\ell_2(t)$, $\ell_\infty(t)$ and relative mass change $\Delta M(t)$ error norms for Cl_y:

$$\ell_2(t) = \frac{\sqrt{\int_{z=0}^{z_{top}} (<q_{Cly}> -4.0 \times 10^{-6})^2 \, dz}}{\sqrt{\int_{z=0}^{z_{top}} (4.0 \times 10^{-6})^2 \, dz}}, \qquad (25)$$

$$\ell_\infty(t) = \frac{\max_{\text{all } \lambda,\theta} |<q_{Cly}> -4.0 \times 10^{-6}|}{4.0 \times 10^{-6}}, \qquad (26)$$

$$\Delta M(t) = \frac{\int_{z=0}^{z_{top}} q_{Cly} dz - M_0}{M_0} \qquad (27)$$

respectively, where

$$<q_{Cly}> = <q_{Cl} + 2q_{Cl2}> . \qquad (28)$$

and M_0 is the initial mass of Cl_y

$$M_0 = \int_{z=0}^{z_{top}} 4.0 \times 10^{-6} dz. \qquad (29)$$

Note that if the physics-dynamics coupling procedure breaks Cl_y conservation it can be very subtle but shows in the $\Delta M(t)$ diagnostic (see, e.g., Figure 3).

1.5 Grid spacings, simulation time, output and diagnostics

Reference simulations (dry and moist) are performed at $1°$ resolution with 30 vertical levels for 15 days. Plots should be produced for the moist simulation and the anomaly between moist and dry simulations at day 9, 12 and 15.

– Plots of minimum surface pressure over the duration of the simulation for both dry and moist configurations.

– A variable resolution simulation should be performed that (a) studies the effect of the baroclinic wave transitioning from coarse resolution to fine resolution and (b) studies the effect of enhanced resolution near the front.

– Terminator chemistry (use physics time-step of 30 minutes and 15 minutes):

– Please plot contour lines for $<q_{Cl}>/(4.0 \times 10^{-6})$ at day 9. Contour interval must be 0.1 with zero contour. Please offset the zero contour $-1.0\text{E}-12$ to avoid contouring round-off undershoots. Contour levels used in Figure 4 are
`(-0.1,-1.0E-12,0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.8,0.9,1.0,1.2)`

– Please plot contour lines for $<q_{Cl2}>/(4.0 \times 10^{-6})$ at day 9. Contour interval must be 0.04 with round-off offset zero contour. Contour levels used in Figure 4 are
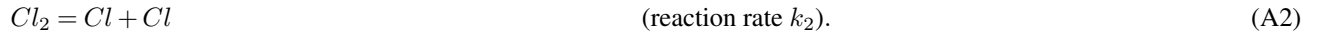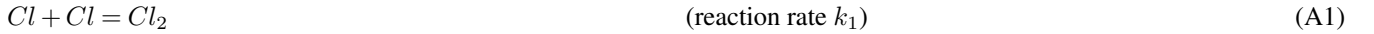`(-0.04,-1.0E-12,0.04,0.08,0.12,0.16,0.20,0.24,0.28,`
`0.32,0.36,0.40,0.44,0.48)`

25   – Please plot contour lines for $< q_{Cly} > /(4.0 \times 10^{-6})$ at day 9. Contour interval must be 0.04 (or 0.02 or 0.01 depending on your data) excluding the 1.0 contour but symmetric about 1.0. Contour levels used in Figure 4 are

$(0.78, 0.82, 0.86, 0.90, 0.94, 0.98, 1.02, 1.06, 1.1, 1.14, 1.18, 1.22, 1.24, 1.08, 1.12, 1.16, 1.20)$

     – Please plot global error norms $\ell_2(t)$, $\ell_\infty(t)$ and relative mass change $\Delta M(t)$ for q_{Cly} as a function of time from day 0 to 30 preferably with 3 hourly time spacing. Use vertical axis adjusted to your data. See example on Figure

5   3.

2   Conclusions

TEXT

Appendix A: 'Toy' Chemistry

The toy chemistry module represents a simple photolysis-driven chemical reaction that incorporates combination and the

10   dissociation of a chemical species:

$$Cl + Cl = Cl_2 \qquad\qquad \text{(reaction rate } k_1\text{)} \qquad\qquad \text{(A1)}$$
$$Cl_2 = Cl + Cl \qquad\qquad \text{(reaction rate } k_2\text{)}. \qquad\qquad \text{(A2)}$$

Observe that the total number of molecules of the chemical species are conserved in this reaction,

$$Cl_T = Cl + 2Cl_2. \qquad\qquad \text{(A3)}$$

15   Representing the mixing ratios of these species as q_{Cl} and q_{Cl2}, we can define the total mixing ratio of Chlorine atoms as

$$q_{Cly} = q_{Cl} + 2q_{Cl2}. \qquad\qquad \text{(A4)}$$

The differential equations describing the evolution of Cl and Cl_2 under this reaction take the form

$$\frac{Dq_{Cl}}{Dt} = 2k_1 q_{Cl2} - 2k_2 q_{Cl}^2, \qquad\qquad \text{(A5)}$$
$$\frac{Dq_{Cl2}}{Dt} = -k_1 q_{Cl2} + k_2 q_{Cl}^2, \qquad\qquad \text{(A6)}$$

20   where D/Dt denotes the Lagrangian derivative. Observe that the total mixing ratio of Chlorine atoms then satisfies

$$\frac{Dq_{Cly}}{Dt} = \frac{Dq_{Cl}}{Dt} + 2\frac{Dq_{Cl2}}{Dt} = 0, \qquad\qquad \text{(A7)}$$

and so the total mixing ratio of Chlorine is held constant.

The two reaction rate coefficient k_1 and k_2, representing the the photolytic dissociation and recombination of Chlorine gas are defined as

$$k_1(\lambda, \theta) = \max\left[0, \sin\theta\sin\theta_c + \cos\theta\cos\theta_c, \cos(\lambda - \lambda_c)\right] \tag{A8}$$

$$k_2(\lambda, \theta) = 1, \tag{A9}$$

where $(\lambda_c, \theta_c) = (20°N, 300°E)$ denote the sub-solar point on the Earth's surface.

5 *Author contributions.* TEXT

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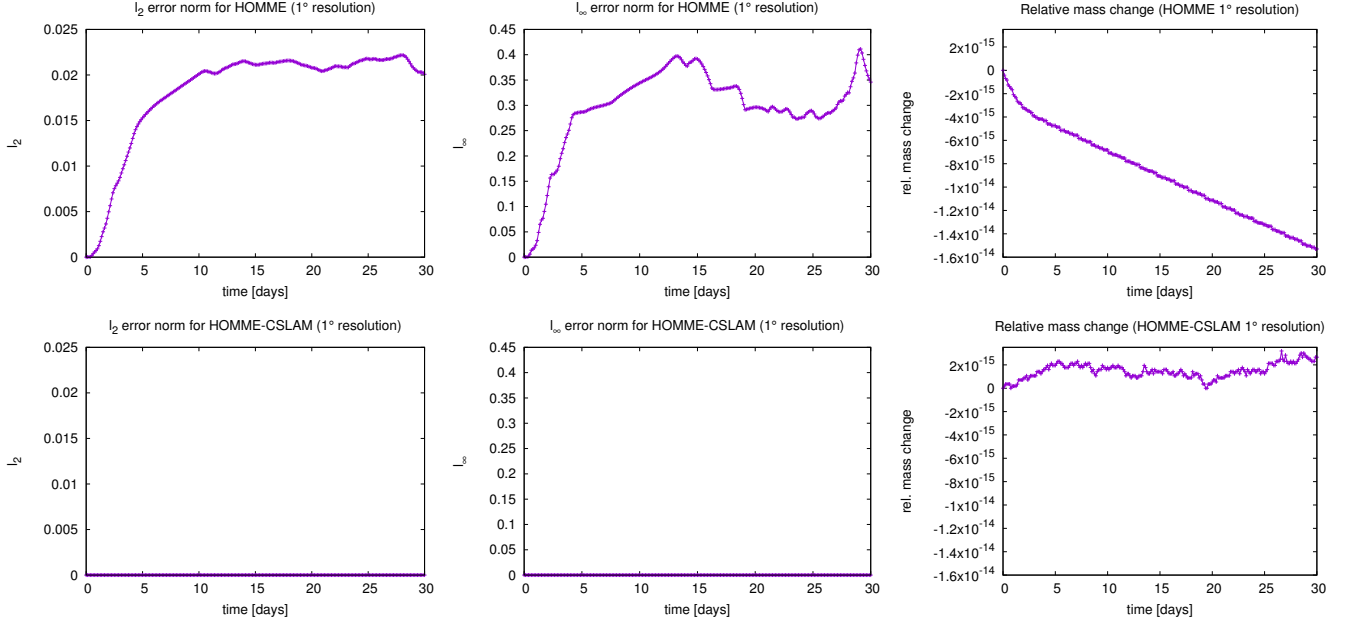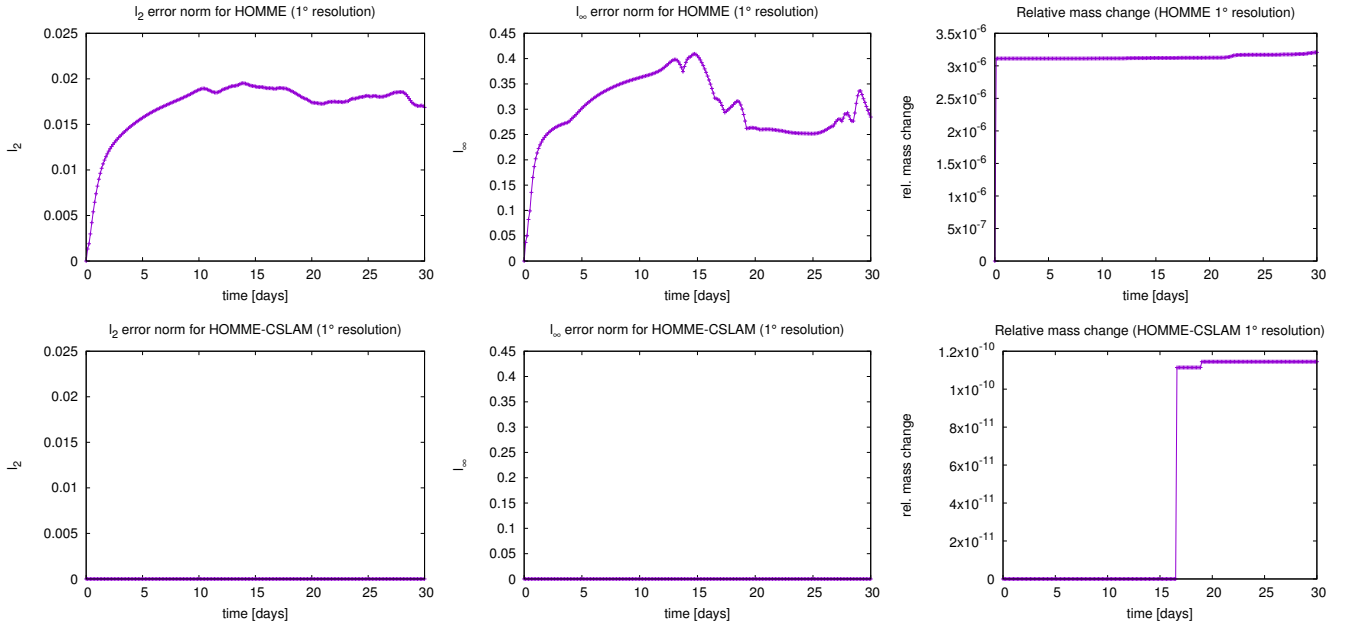
Figure 3. Global error norms $\ell_2(t)$ (column 1), $\ell_\infty(t)$ (column 2) and relative mass change $\Delta M(t)$ (column 3) for q_{Cly} for HOMME (row 1 and 3) and HOMME-CSLAM (row 2 and 4) with physics/chemistry time-step of 15 minutes (row 1 and 2) and 30 minutes (row 3 and 4), respectively. The non-conservation of Cl_y mass ($\Delta M(t)$) for physics time-step of 30 minutes is due to physics-dynamics coupling in which the tendencies are altered if they result in negative mixing ratios. For HOMME-CSLAM this happens at one point around day 16 and 18, respectively, whereas it happens frequently (in time and space) for HOMME.

HOMME

day 9

Average column integrated Cl   4.0E-6 kg/kg

day 9

Average column integrated Cl2   4.0E-6 kg/kg

-0.1 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1 1.1 1.2

0   0.08   0.16   0.24   0.32   0.4   0.48

day 9

Average column integrated Cly   4.0E-6 kg/kg

day 9

Surface pressure   hPa

0.78 0.82 0.86 0.9 0.94 0.98 1.02 1.06 1.1 1.14 1.18 1.22 1.24

968 972 976 980 984 988 992 996 1000 1004 1008 1012

HOMME-CSLAM

day 9

Average column integrated Cl   4.0E-6 kg/kg

day 9

Average column integrated Cl2   4.0E-6 kg/kg

-0.1 0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1 1.2

0   0.08   0.16   0.24   0.32   0.4   0.48

day 9

Average column integrated Cly   4.0E-6 kg/kg

day 9

Surface pressure implied by CSLAM   hPa

CONSTANT FIELD - VALUE IS 1

14