Implementation of a positive definite mass-flux scheme for tracers in the NCEP GFS PBL and cumulus convection schemes

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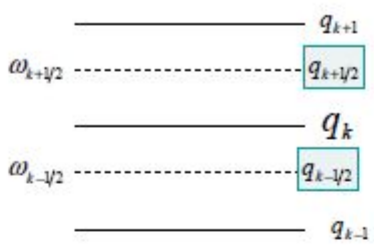
Convection parameterization meeting, August 13, 2021

Outline

- Brief introduction of positive definite TVD (Total Variation Diminishing) advection scheme
- Test of the TVD scheme
- Development of a method removing the negative tracer values
- Summary

Vertical Advection of Tracers: Current GFS Scheme



$$\frac{\partial q}{\partial t} = -\omega \frac{\partial q}{\partial p} = -\left(\frac{\partial \omega q}{\partial p} - q \frac{\partial \omega}{\partial p} \right)$$

Flux form conserves mass

$$A_k = \frac{1}{\Delta p_k}\left(\omega_{k-\frac{1}{2}} q_{k-\frac{1}{2}} - \omega_{k+\frac{1}{2}} q_{k+\frac{1}{2}} \right) - \frac{1}{\Delta p_k} q_k \left(\omega_{k-\frac{1}{2}} - \omega_{k+\frac{1}{2}} \right)$$

$$\Delta p_k = p_{k-\frac{1}{2}} - p_{k+\frac{1}{2}}$$

Currently GFS uses central differencing in space and leap-frog in time.

$$q_{k-\frac{1}{2}} = \frac{1}{2}(q_{k-1} + q_k)$$

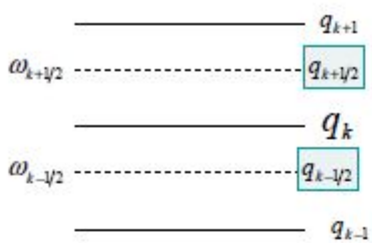
$$A_k = \frac{1}{2\Delta p_k}\left(\omega_{k-\frac{1}{2}}(q_{k-1} - q_k) + \omega_{k+\frac{1}{2}}(q_k - q_{k+1}) \right)$$

The scheme is not positively definite for tracers and may produce negative tracers.

$$q_k^{n+1} = q_k^{n-1} - 2\Delta t \cdot A_k^n$$

From Fanglin Yang et al (2009)

Vertical Advection of Tracers: Upwind Scheme



$$\frac{\partial q}{\partial t} = -\omega \frac{\partial q}{\partial p} = -\left(\frac{\partial \omega q}{\partial p} - q \frac{\partial \omega}{\partial p} \right)$$

Flux form conserves mass

$$A_k = \frac{1}{\Delta p_k}\left(\omega_{k-\frac{1}{2}} q_{k-\frac{1}{2}} - \omega_{k+\frac{1}{2}} q_{k+\frac{1}{2}} \right) - \frac{1}{\Delta p_k} q_k \left(\omega_{k-\frac{1}{2}} - \omega_{k+\frac{1}{2}} \right)$$

For computational stability, upwind-in-space scheme must use forward-in-time integration.

$$q_{k-\frac{1}{2}} = \begin{cases} q_{k-1} & \text{if } \omega_{k-1/2} < 0 \\ q_k & \text{if } \omega_{k-1/2} \geq 0 \end{cases}$$

$$q_k^{n+1} = q_k^n - \Delta t \cdot A_k^n$$

From Fanglin Yang et al (2009)

Positive definite TVD (Total Variation Diminishing) flux-limiter scheme

Vertical Advection of Tracers: Flux-Limited Scheme

$$\text{if } \omega_{k-1/2} < 0 \qquad q_{k-1/2} = q_{k-1} + \Phi_{k-1}^{-}\left(q_{k-1/2}^{H} - q_{k-1}\right)$$

Thuburn (1993)

$$q_{k-1/2}^{H} = \frac{1}{2}\left(q_k + q_{k-1}\right)$$

$$\Phi_{k-1}^{-} = \frac{r_{k-1}^{-} + \left|r_{k-1}^{-}\right|}{1 + \left|r_{k-1}^{-}\right|}$$

Van Leer (1974) Limiter, anti-diffusive term

$$r_{k-1}^{-} = \frac{q_{k-2} - q_{k-1}}{q_{k-1} - q_k} = \frac{\Delta q_{k-2}}{\Delta q_{k-1}}$$

Special boundary conditions

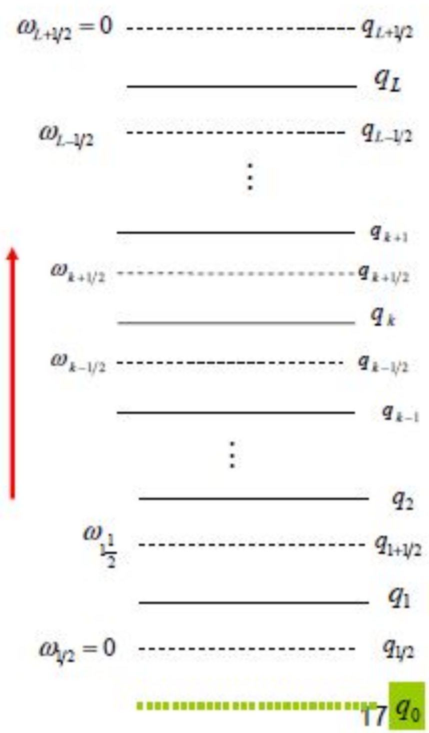
for $k = 1$ $\quad \omega_{1/2} q_{1/2} = 0 \quad$ since $\quad \omega_{1/2} = 0$

for $k = 2$

$$q_{3/2} = q_1 + \Phi_1^{-}\left(q_{3/2}^{H} - q_1\right)$$

$$\Phi_1^{-} = \frac{r_1^{-} + \left|r_1^{-}\right|}{1 + \left|r_1^{-}\right|} \qquad r_1^{-} = \frac{q_0 - q_1}{q_1 - q_2} = \frac{\Delta q_0}{\Delta q_1}$$

$$q_0 = \begin{cases} \max\left(0, 2q_1 - q_2\right) & \text{if } q_1 \geq 0 \\ \min\left(0, 2q_1 - q_2\right) & \text{if } q_1 < 0 \end{cases}$$



From Fanglin Yang et al (2009)

Vertical Advection of Tracers: Flux-Limited Scheme

if $\omega_{k-1/2} \geq 0$

$$q_{k-1/2} = q_k + \Phi_k^+ \left(q_{k-1/2}^H - q_k\right)$$

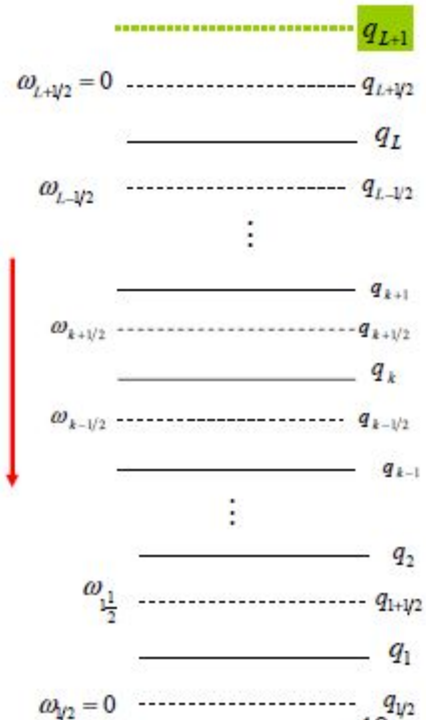
Thuburn (1993)

$$q_{k-1/2}^H = \frac{1}{2}\left(q_k + q_{k-1}\right)$$

$$\Phi_k^+ = \frac{r_k^+ + \left|r_k^+\right|}{1 + \left|r_k^+\right|}$$

Van Leer (1974) Limiter, anti-diffusive term

$$r_k^+ = \frac{q_k - q_{k+1}}{q_{k-1} - q_k} = \frac{\Delta q_k}{\Delta q_{k-1}}$$



Special boundary condition for $k = L$

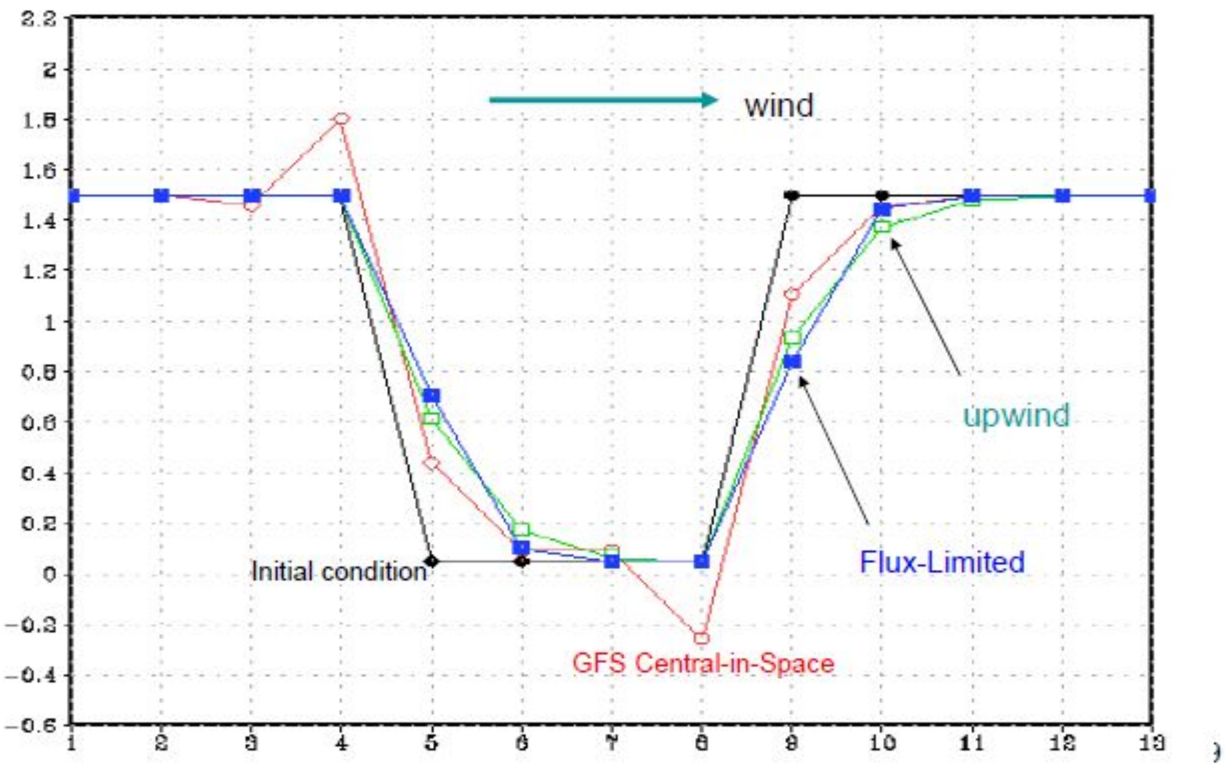
$$q_{L-1/2} = q_L + \Phi_L^+ \left(q_{L-1/2}^H - q_L\right)$$

$$\Phi_L^+ = \frac{r_L^+ + \left|r_L^+\right|}{1 + \left|r_L^+\right|} \qquad r_L^+ = \frac{q_L - q_{L+1}}{q_{L-1} - q_L} = \frac{\Delta q_L}{\Delta q_{L-1}}$$

$$q_{L+1} = \begin{cases} \max\left(0, 2q_L - q_{L-1}\right) & \text{if} \quad q_L \geq 0 \\ \min\left(0, 2q_L - q_{L-1}\right) & \text{if} \quad q_L < 0 \end{cases}$$

From Fanglin Yang et al (2009)

Vertical Advection of Tracers: Idealized Case Study



From Fanglin Yang et al (2009)

Mass-flux scheme

$$\frac{\partial \bar{\phi}}{\partial t} = -\frac{\partial \overline{w'\phi'}}{\partial z} + F_{\phi}$$

$$\overline{w'\phi'} = -K_{\varphi}\frac{\partial \bar{\phi}}{\partial z} + M_u(\phi_u - \bar{\phi})|_{up} - M_d(\phi_d - \bar{\phi})|_{dn}$$

Assuming F_{Φ}=0,

$$\frac{\partial \bar{\phi}}{\partial t} = \underbrace{\frac{\partial}{\partial z}\left(K_{\phi}\frac{\partial \bar{\phi}}{\partial z}\right)}_{(1)} + \underbrace{\frac{\partial}{\partial z}\left((M_u - M_d)\bar{\phi}\right)}_{(2)} + \underbrace{\frac{\partial}{\partial z}(-M_u\phi_u + M_d\phi_d)}_{(3)}$$

- Subtract the double counting change rates of the variable at updraft and downdraft boundaries.

- Check conservation after implementing numerical discretization as:

$$\int_{bot}^{top}\frac{\partial \bar{\phi}}{\partial t}dz = \int_{bot}^{top}\frac{\partial\left(-\overline{w'\phi'}\right)}{\partial z}dz = \left(-\overline{w'\phi'}\right)_{top} - \left(-\overline{w'\phi'}\right)_{bot}$$

Central differencing scheme: ~10^{-17} for TKE
TVD scheme: 10^{-5}~10^{-2} for TKE

GFS-CCPP medium-range forecast experiments

- Resolution: C768L127 (about 13km)
- 6-day warm start forecasts at 00Z cycle every 5 days were conducted for the winter period of Dec. 02, 2019 – Feb. 29, 2020 using initial conditions from the GFSv16 retrospective (v16retro3e) runs.

ccab07: control (updated physics in PBL & SAS: GFS P7c)
ccab42: experiments with the TVD scheme

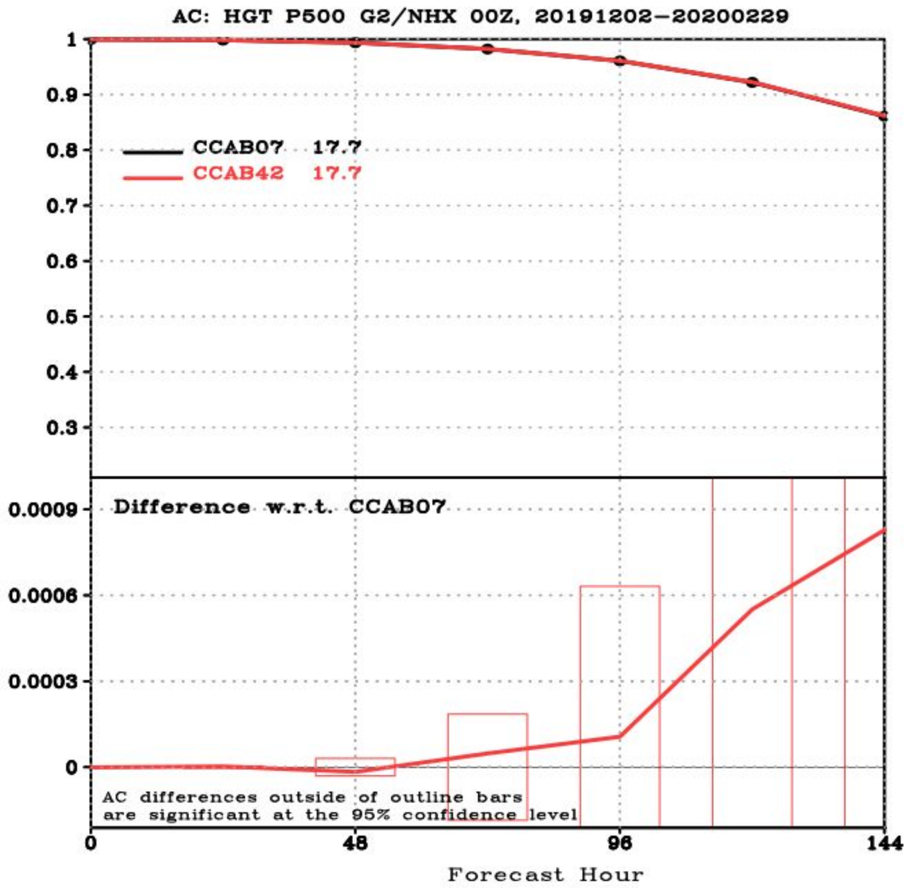
http://www.emc.ncep.noaa.gov/gmb/jhan/vsdbw/ccab42w

Central			TVD	
max TKE	min TKE		max TKE	min TKE
37.01081	-2.91881		37.74255	-0.8153
63.64521	-2.188344		63.97289	-0.59283
84.49205	-2.677069		88.21877	-0.88441
147.0343	-2.362137		128.9055	-1.27692
166.4528	-2.26057		157.634	-0.67856
102.2713	-3.043875		98.10609	-1.97941
45.92924	-2.220357		47.97842	-0.87563
44.87528	-2.64257		45.23304	-0.88497
50.37382	-2.325083		60.52139	-0.98047
62.76791	-2.019215		73.22465	-0.4367
168.5564	-2.355599		61.29884	-0.75169
60.22577	-3.040793		71.64494	-0.7452
42.57714	-2.992054		41.48038	-3.09797
51.07372	-1.874743		40.58673	-0.72027
47.18581	-2.359504		33.16606	-0.52156
41.46842	-3.216556		56.3333	-0.66239
52.59673	-3.246931		42.22956	-0.80629
46.27276	-2.272117		51.83812	-0.5497

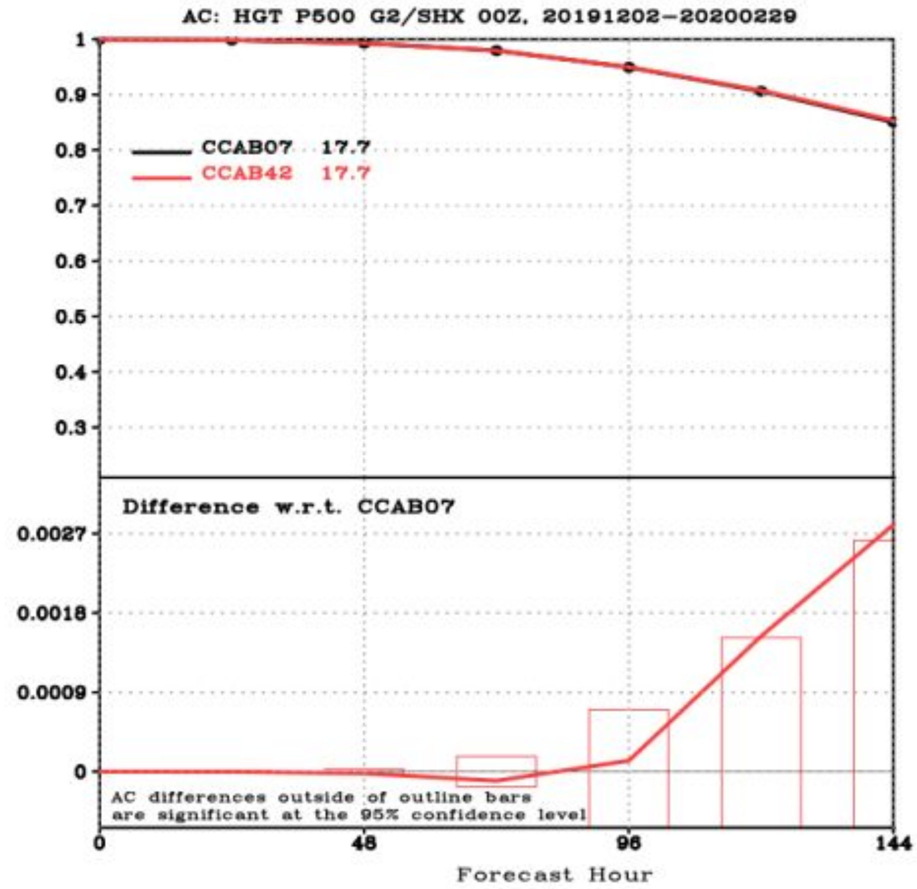
Divergence of parcel flux [term (3) in slide 8] and vertically unequal grid sizes might have caused the negative TKE in the TVD scheme

500 mb height anomaly correlation

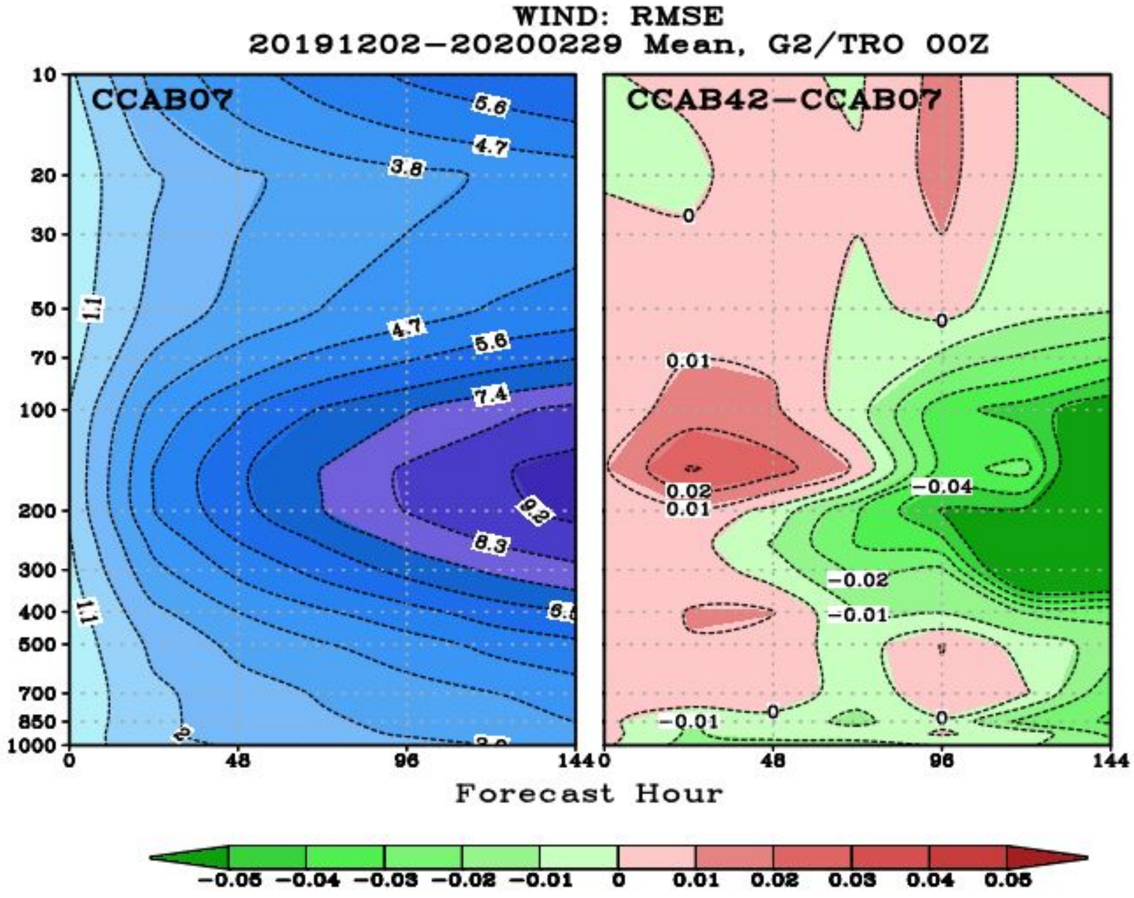
NH



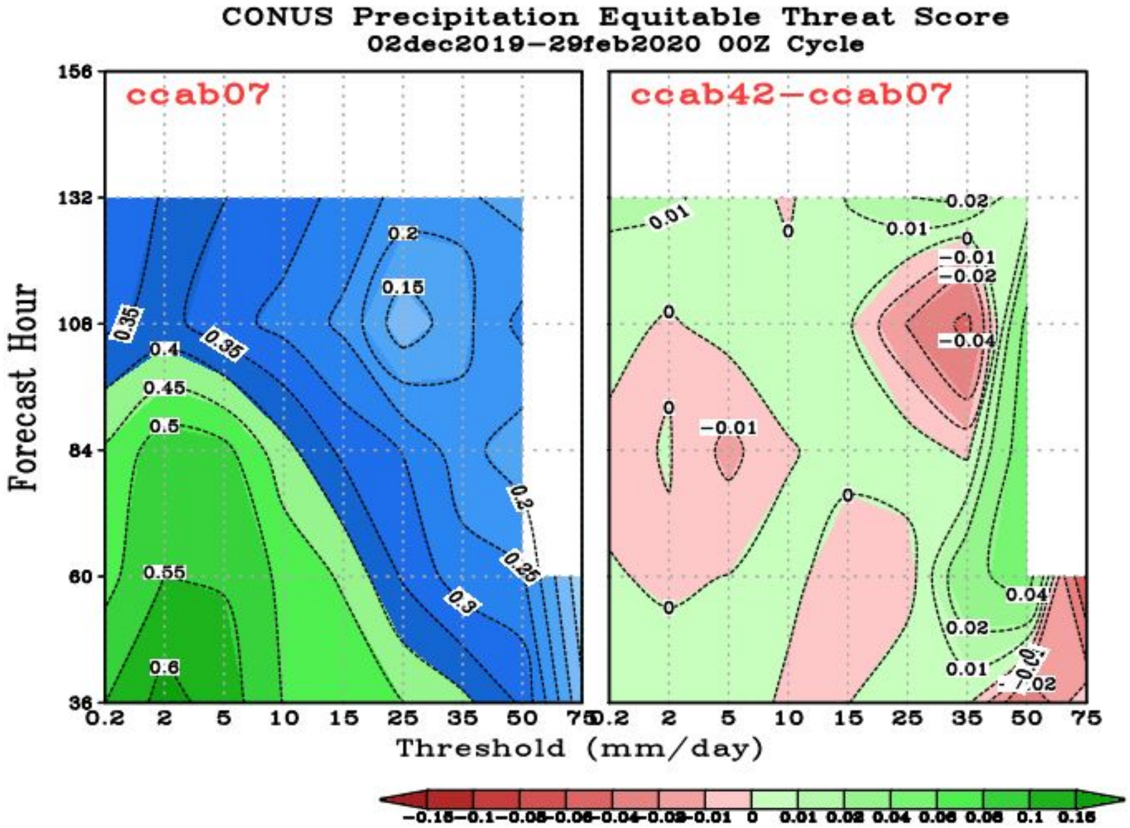
SH



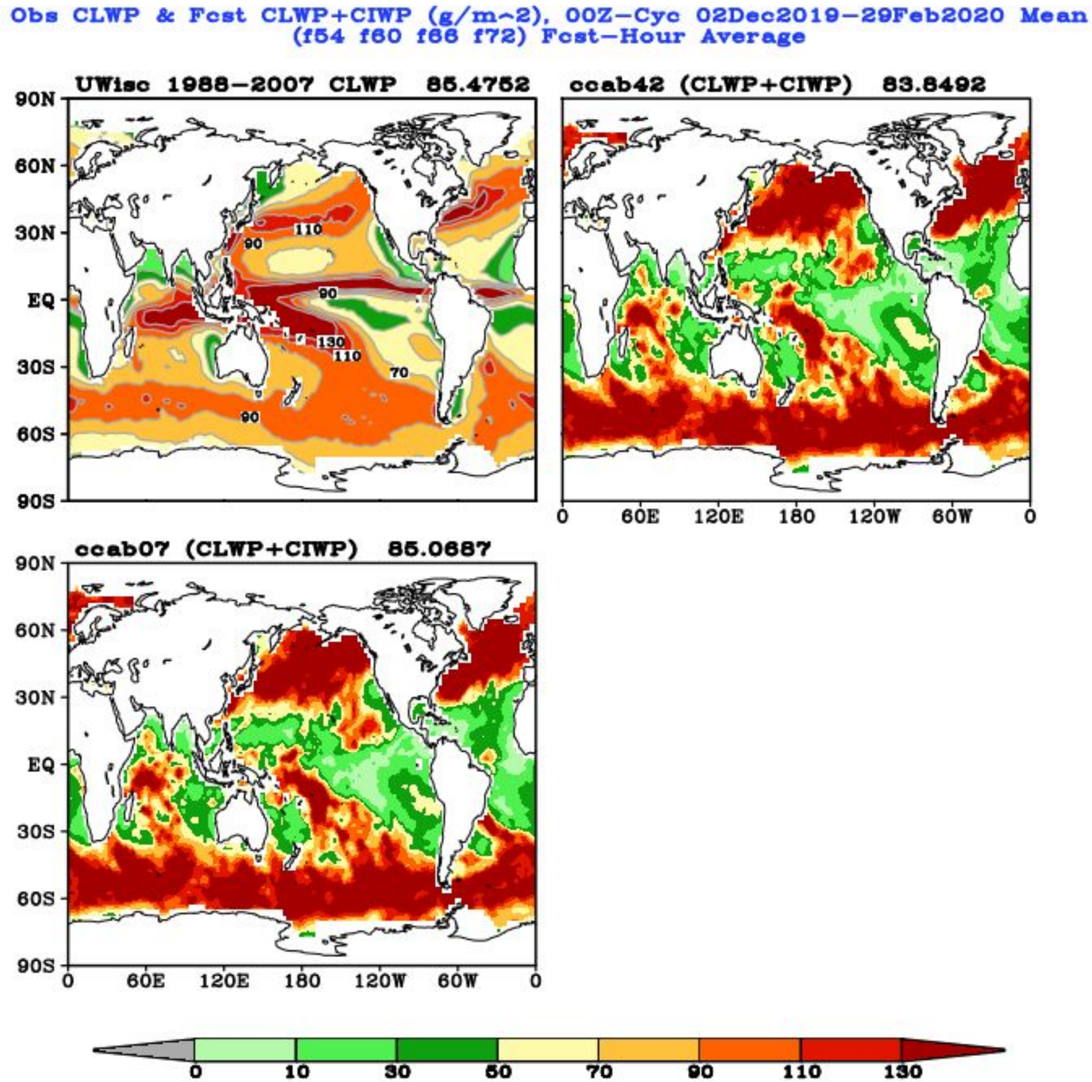
Wind RMSE over Tropics



CONUS Precip ETS



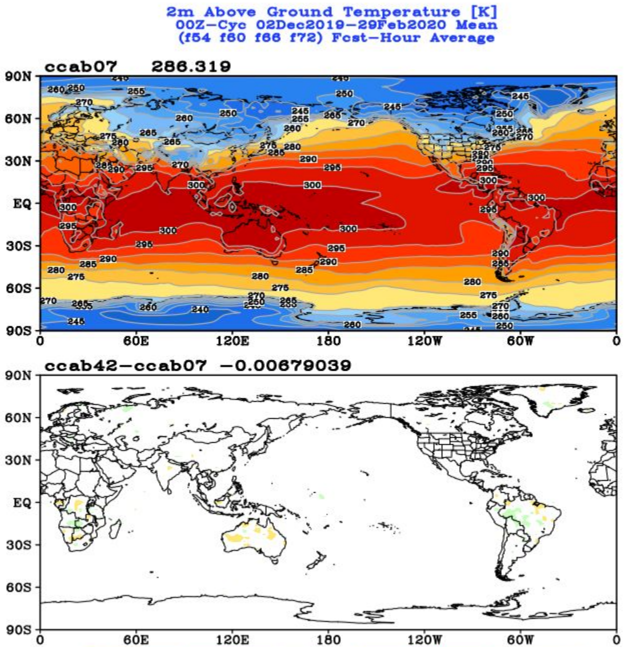
Column liquid and ice water path



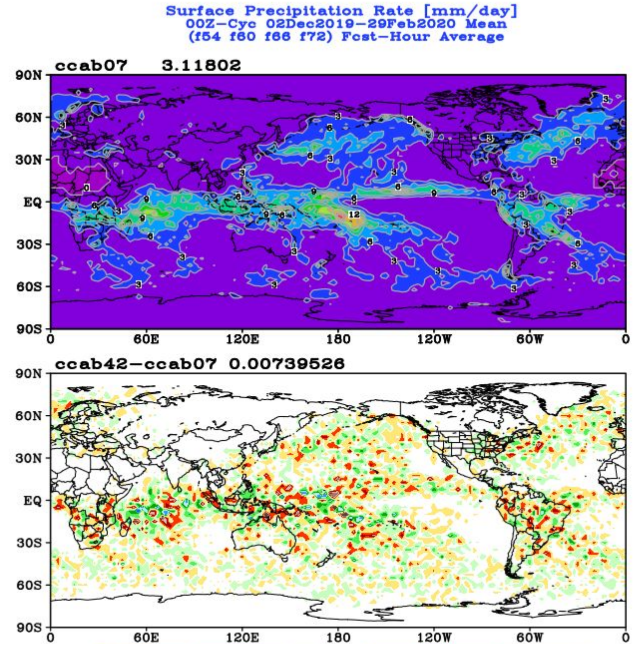
EXP

CTL

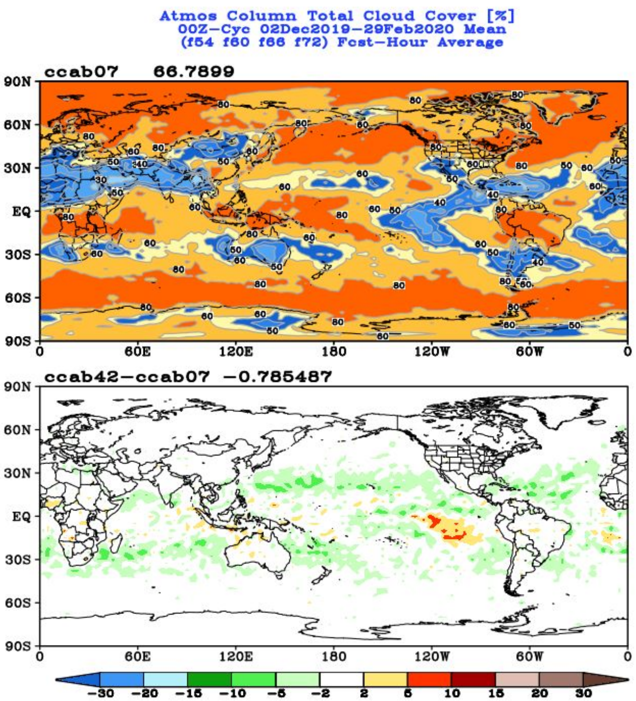
2mT



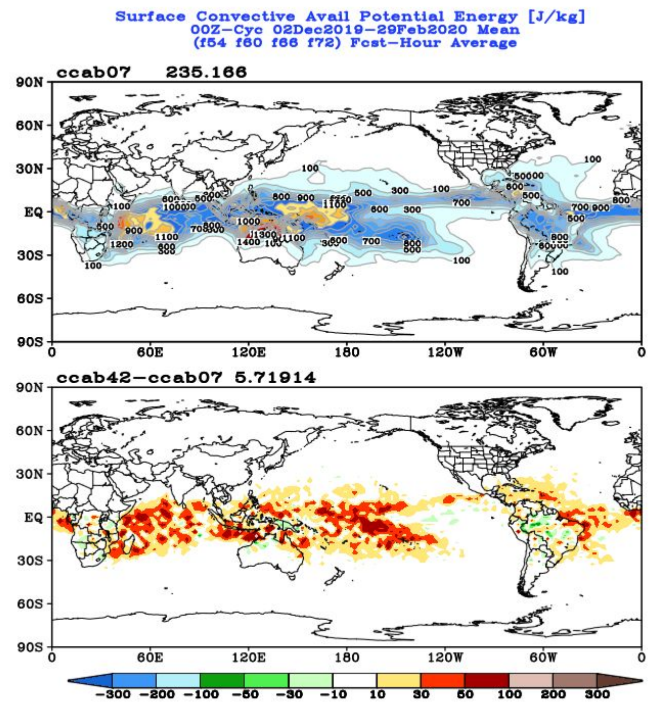
Total precip



Total cloud cover

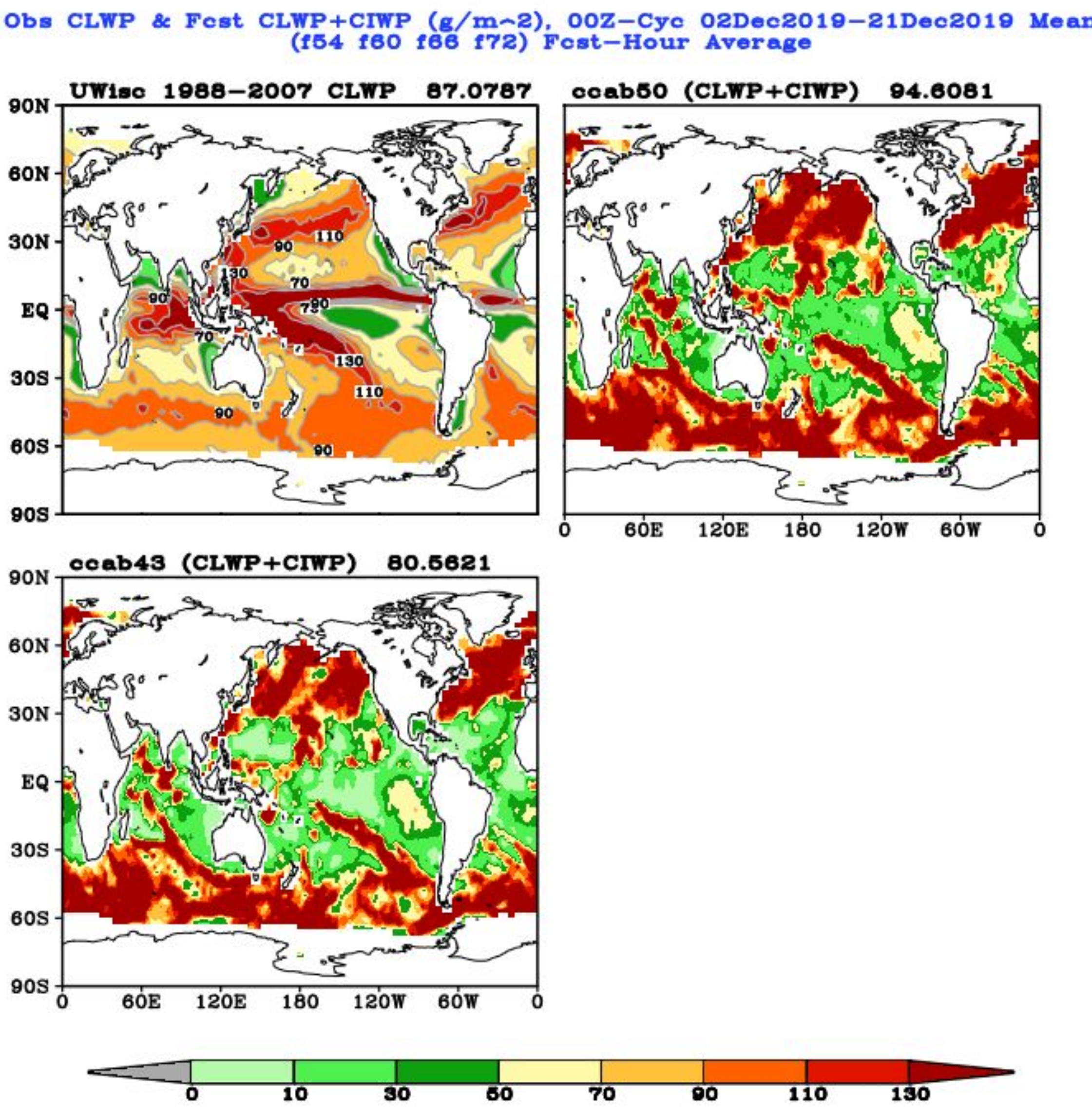


CAPE



Simply zeroing out the negative tracers (TKE, moisture, hydrometeors, and aerosol) can cause a conservation problem and would keep to increase them with time (http://www.emc.ncep.noaa.gov/gmb/jhan/vsdbw/ccab50x)

Column liquid and ice water path

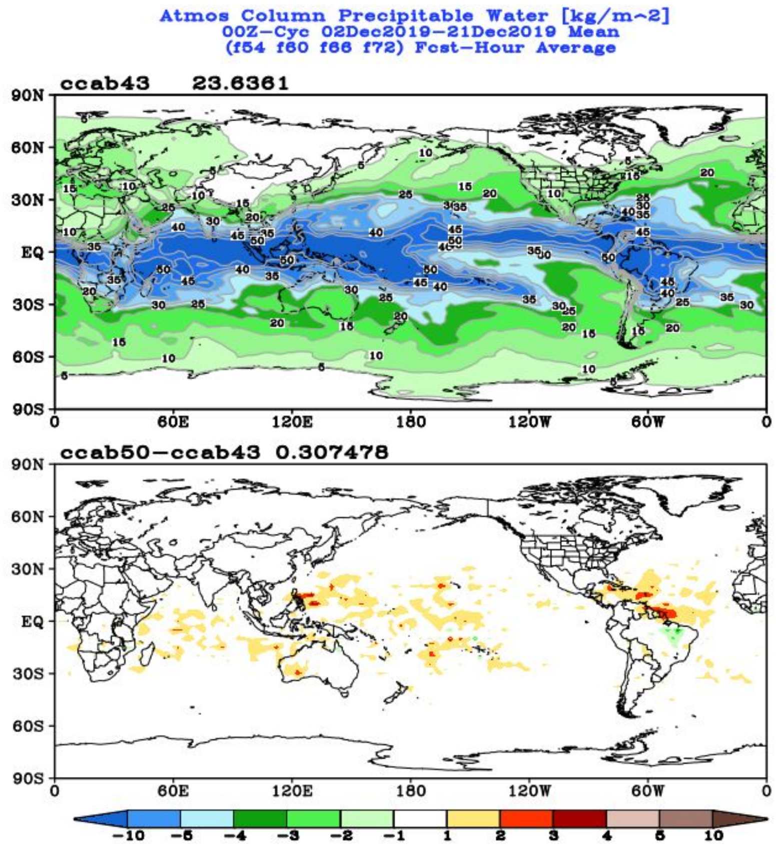


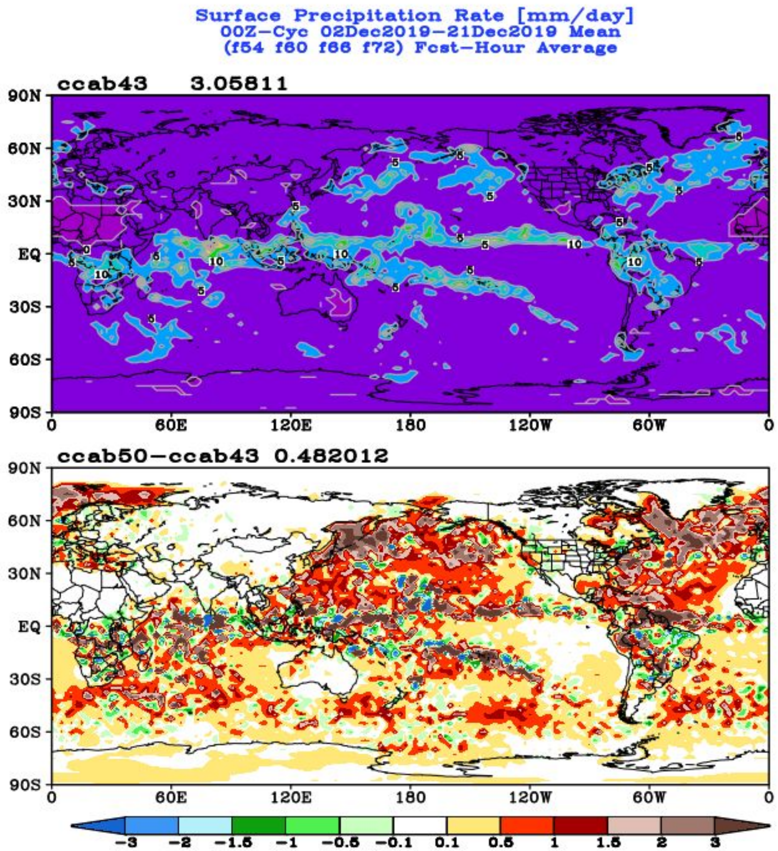
EXP: zeroing out negative values

CTL

Column precipitable water

Total precipitation





Implementation of positive definite upwind scheme for aerosol transport in SAS convection (samfaerosols.F) by Georg Grell

qaero: aerosol concentration

1) qaero=max(qaero, 10^{-22}) initially => conservation issue
2) If qaero < 0 after mass-flux transport,
   wet_dep=wet_dep-qaero*dp (borrow it from wet deposition)
   (=>wet_dep=wet_dep+qaero*dp)
   and set qaero=10^{-22}
   - cannot apply to TKE, moisture, and hydrometeors
   - if wet_dep < -qaero*dp, wet deposition becomes negative

Development of a method removing the negative tracer values

- Borrow positive tracers from other layers within PBL or cumulus clouds after mass-flux transport

$$Ratio = \frac{\sum_{bot}^{top} q_{neg}}{\sum_{bot}^{top} q_{pos}}$$

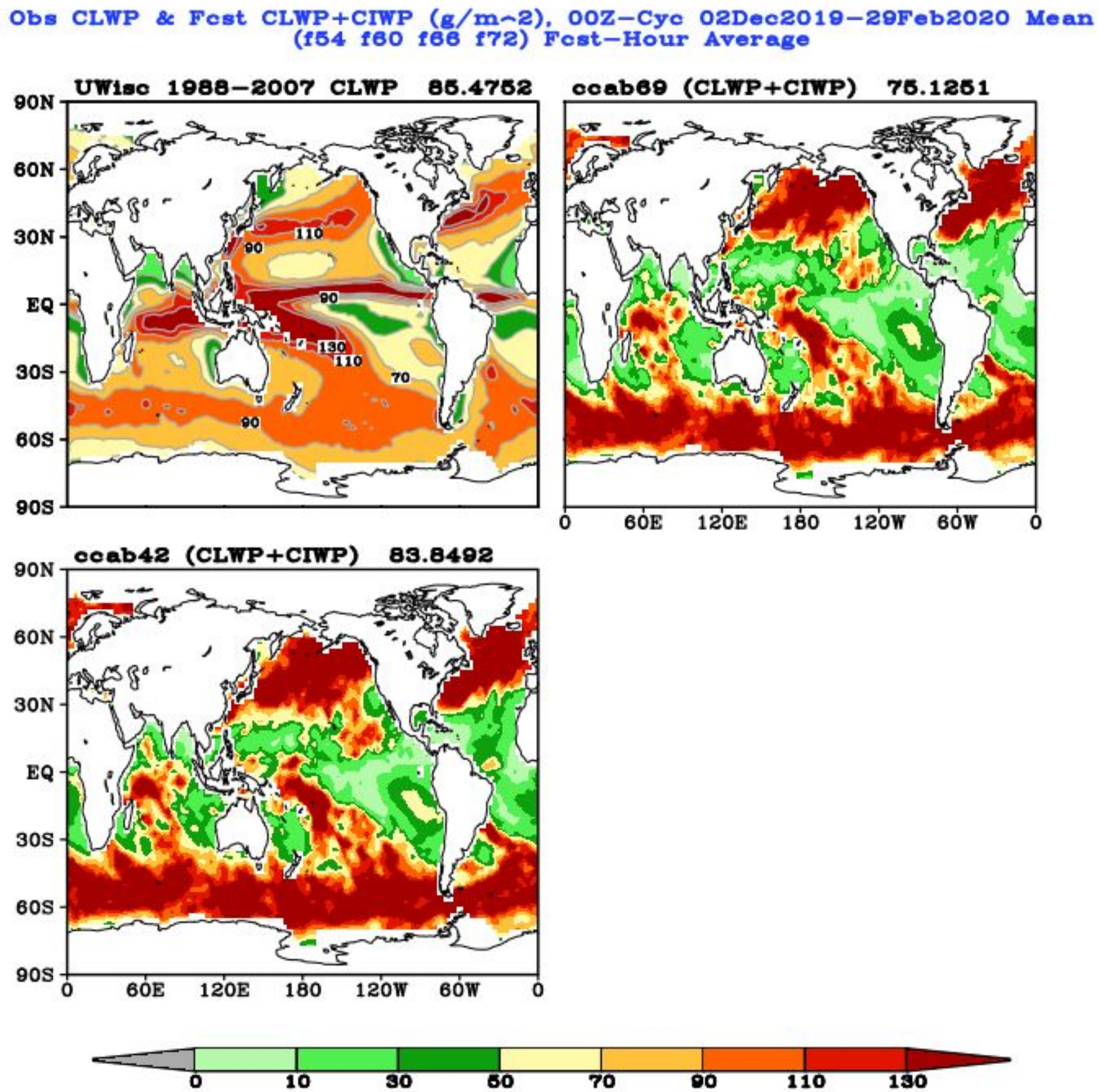
Ratio < 0

```
do k=kbot, ktop
    if (q(k) < 0), q(k)=0
    if (q(k) > 0), q(k)=(1+Ratio) * q(k)
enddo
```

Results: http://www.emc.ncep.noaa.gov/gmb/jhan/vsdbw/ccab69

Borrowing positive values	
max TKE	min TKE
37.0415	-9.02E-17
64.40881	-6.59E-17
89.12389	-1.11E-16
151.9699	-2.08E-16
162.2496	-1.94E-16
105.492	-6.07E-17
46.84769	-1.98E-16
47.31166	-1.39E-16
58.40775	-1.13E-16
59.53362	-2.39E-16
49.4918	-1.80E-16
68.02324	-1.27E-16
46.55048	-1.07E-16
40.5466	-1.13E-16
68.66727	-2.19E-16
65.04642	-1.56E-16
52.83929	-1.04E-16
52.49757	-2.12E-16

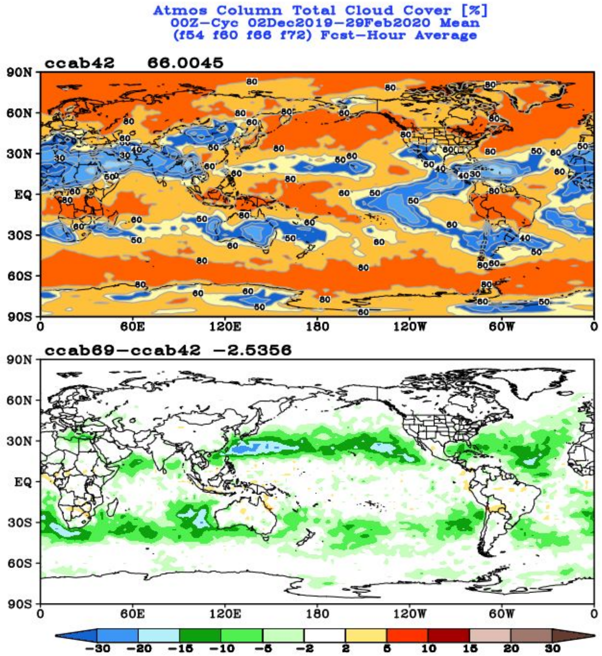
Column liquid and ice water path



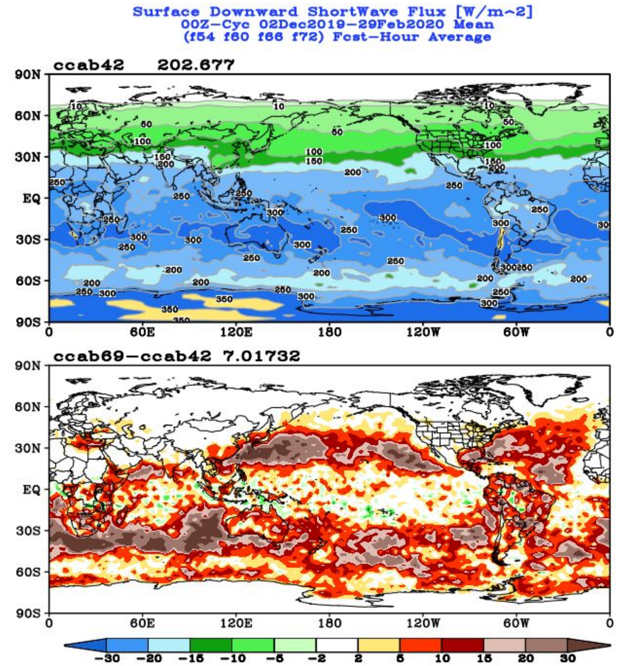
EXP

CTL

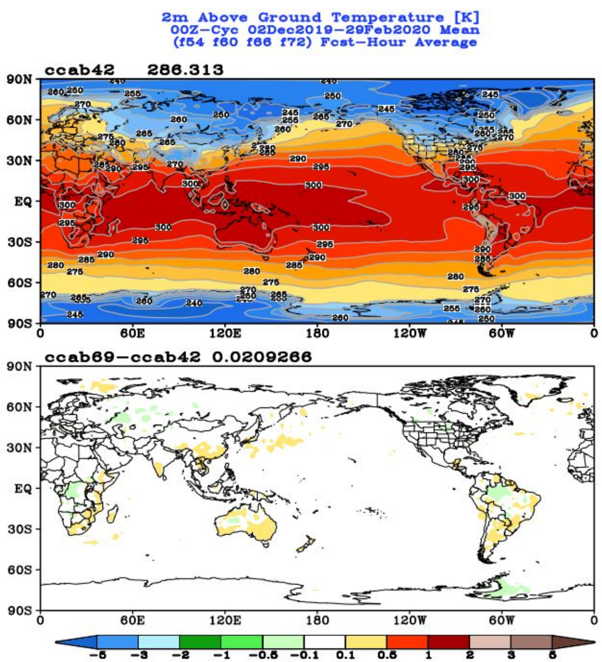
Total cloud cover



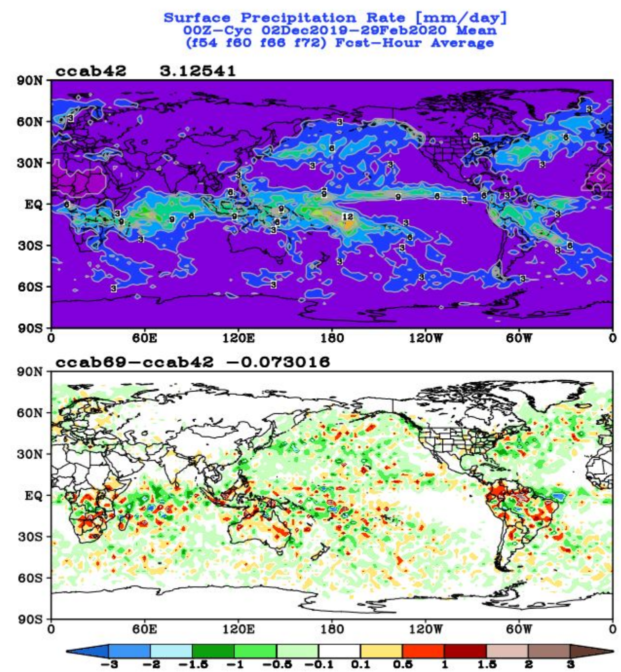
Dn SW



2mT



Total precip



Development of a method removing the negative tracer values

- For the negative liquid water, not to reduce the low clouds, we first borrow water from vapor as done in the Zhao-Carr MP scheme and then borrow it from other layers if the negative liquid water still exists.

```
do k=kbot, ktop
    if (cw(k) < 0) then
       tem = q(k) + cw(k)
       if (tem>=0) then
           q(k) = tem
           T(k) = T(k) – L/cp * cw(k)
           cw(k) = 0
       elseif (q(k) > 0) then
           cw(k) = tem
           T(k) = T(k) + L/cp * q(k)
           q(k) = 0
       endif
    endif
enddo
```

Development of a method removing the negative tracer values

- Significant negative moistures (q) mostly at the model 1st layers (occasionally at the model 2nd and 3rd layers) are found, caused by the downward surface latent heat flux in dry regions during nighttime. This can occur in any PBL scheme as well as in TKE-EDMF and MYNN-EDMF PBL schemes.

$$\frac{\partial \overline{q}}{\partial t} = -\frac{\partial \overline{w'q'}}{\partial z}$$

At the model first layer,

$$\frac{\overline{q}^{\,n+1} - \overline{q}^{\,n}}{\Delta t} = \frac{\left(-\overline{w'q'}\right)_1 - \left(-\overline{w'q'}\right)_s}{\Delta z}$$

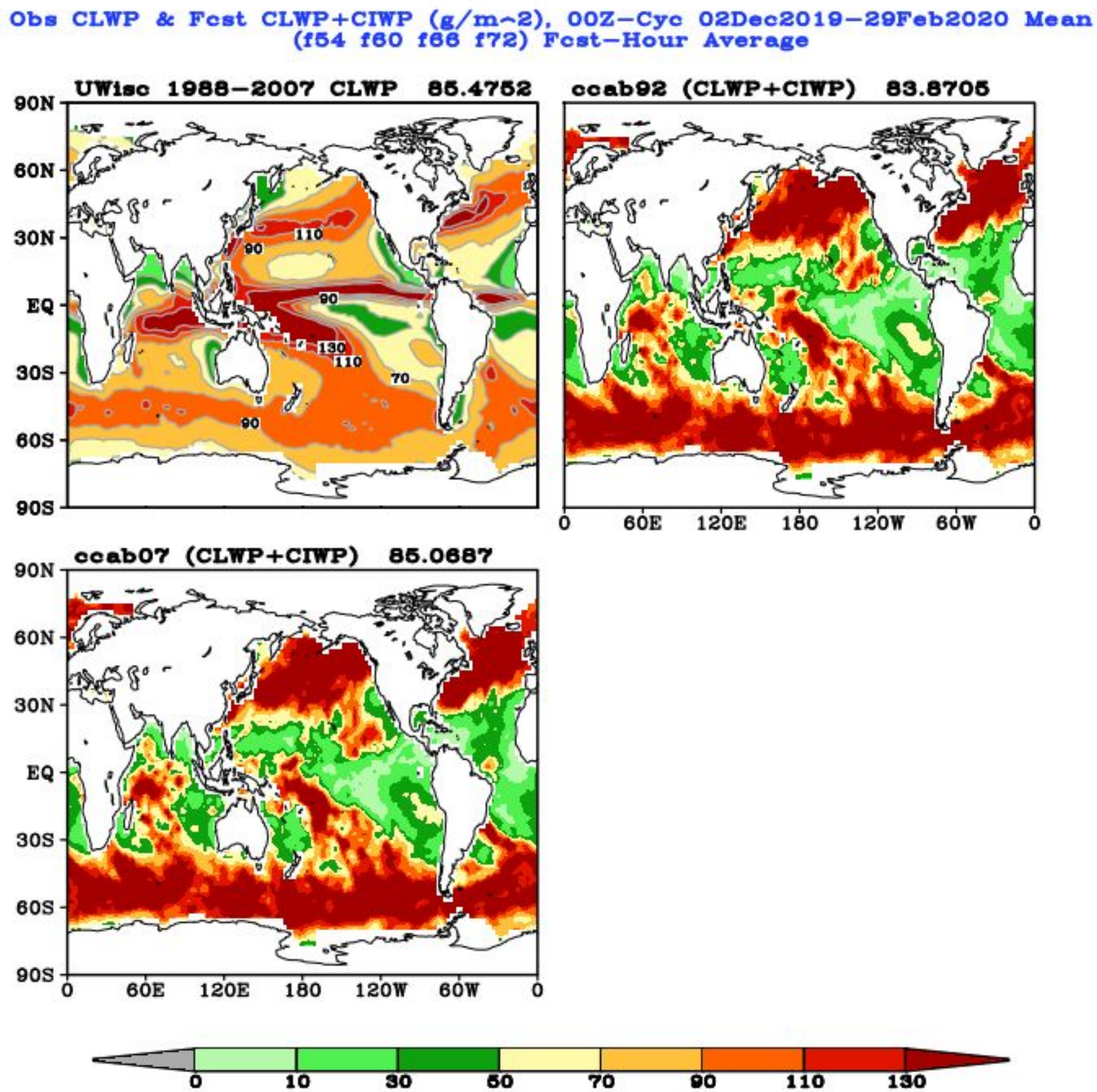
In dry regions during nighttime, both q^n (q at the current time step) and the downward surface latent heat flux [$(-w'q')_s$] are very small. If [$(-w'q')_s$ is relatively large compared to q^n , q^{n+1} (q at the next time step) can be negative.

Development of a method removing the negative tracer values

- Another possibility for negative tracers is that when the mass-flux transport and eddy diffusion are simultaneously computed as in the current TKE-EDMF PBL scheme, the eddy diffusion can leak out the negative tracers out of the mass-flux transport layers before borrowing positive tracers within the mass-flux transport layers.
- In a final TKE-EDMF-TVD version, therefore, the negative tracers produced by the mass-flux scheme are first removed by borrowing the positive tracers within the mass-flux transport layers, and then additional negative tracers leaked out of the mass-flux transport layers due to eddy diffusion or by downward surface fluxes during nighttime (which are usually quite small) are removed by borrowing the positive tracers from the entire column layers.
- For aerosols with wet deposition in the cumulus convection schemes, the potential tiny negative values due to a numerical artifact are further removed by borrowing them from the wet deposition.

Final results: http://www.emc.ncep.noaa.gov/gmb/jhan/vsdbw/ccab92a

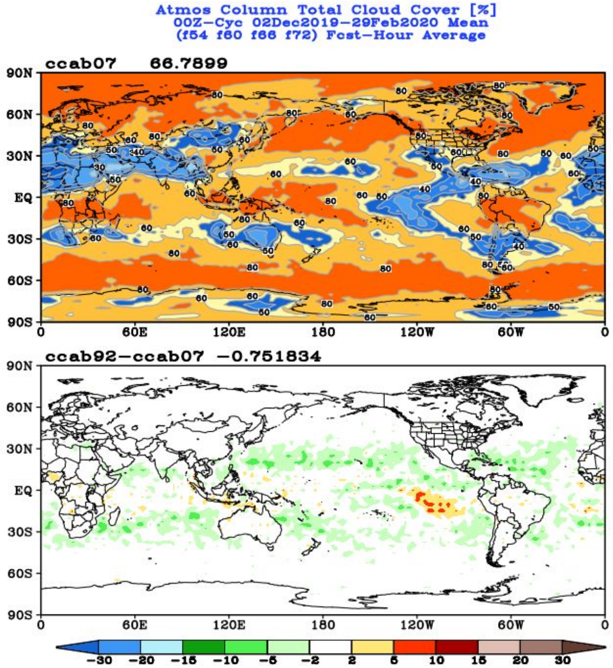
Column liquid and ice water path



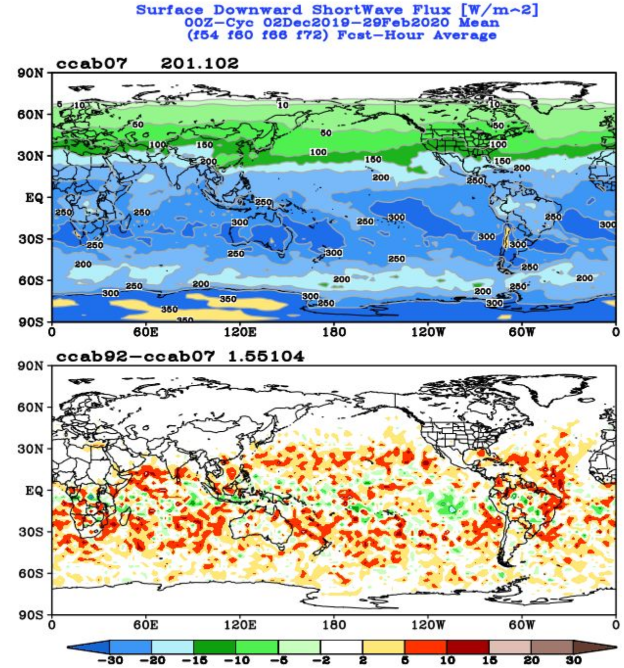
EXP

CTL

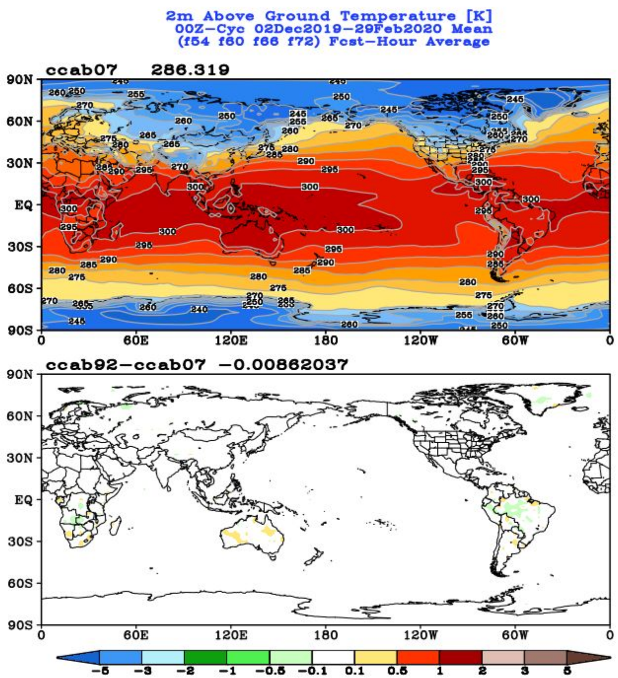
Total cloud cover



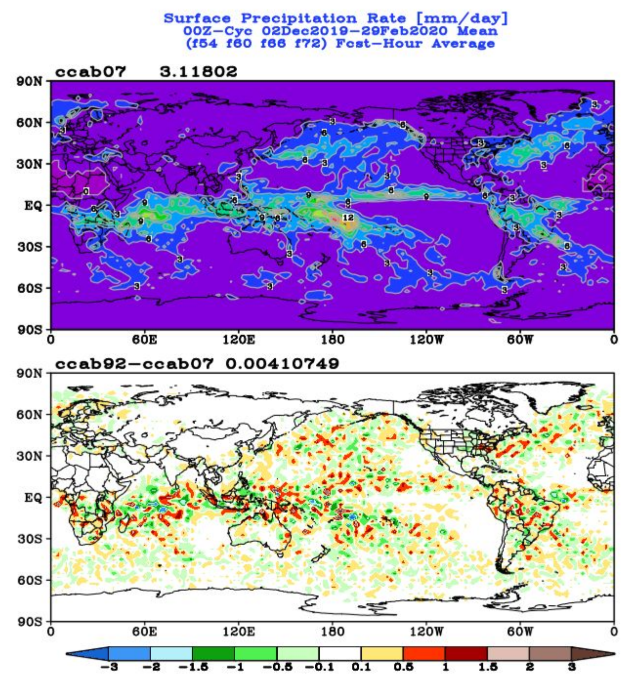
Dn SW



2mT

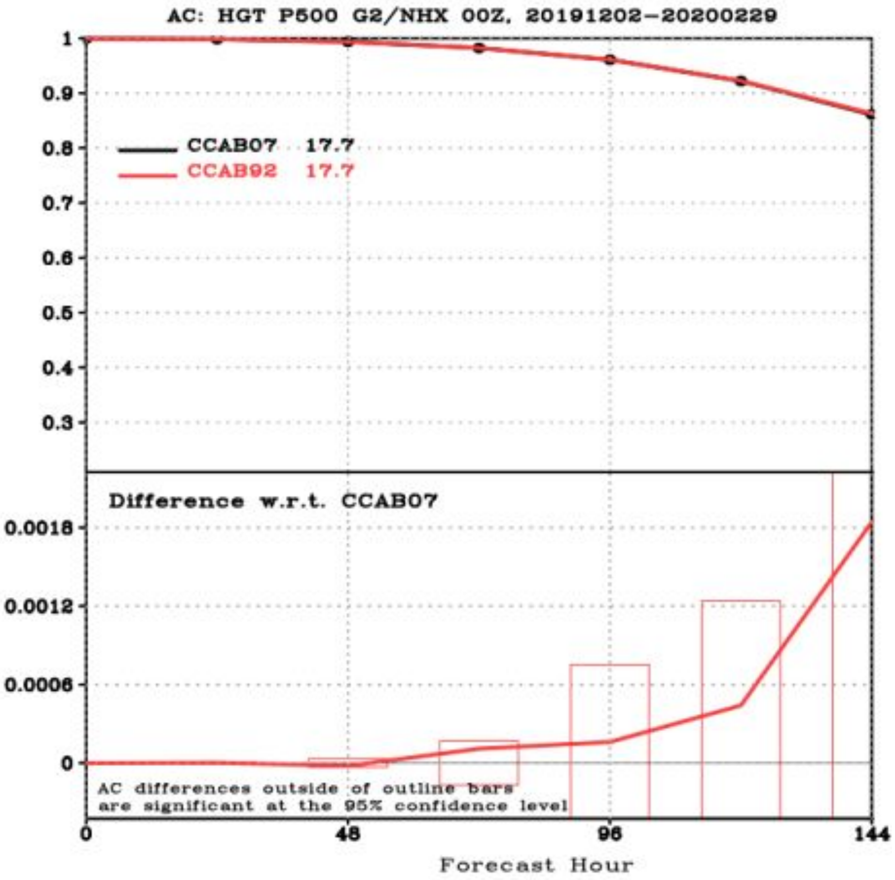


Total precip

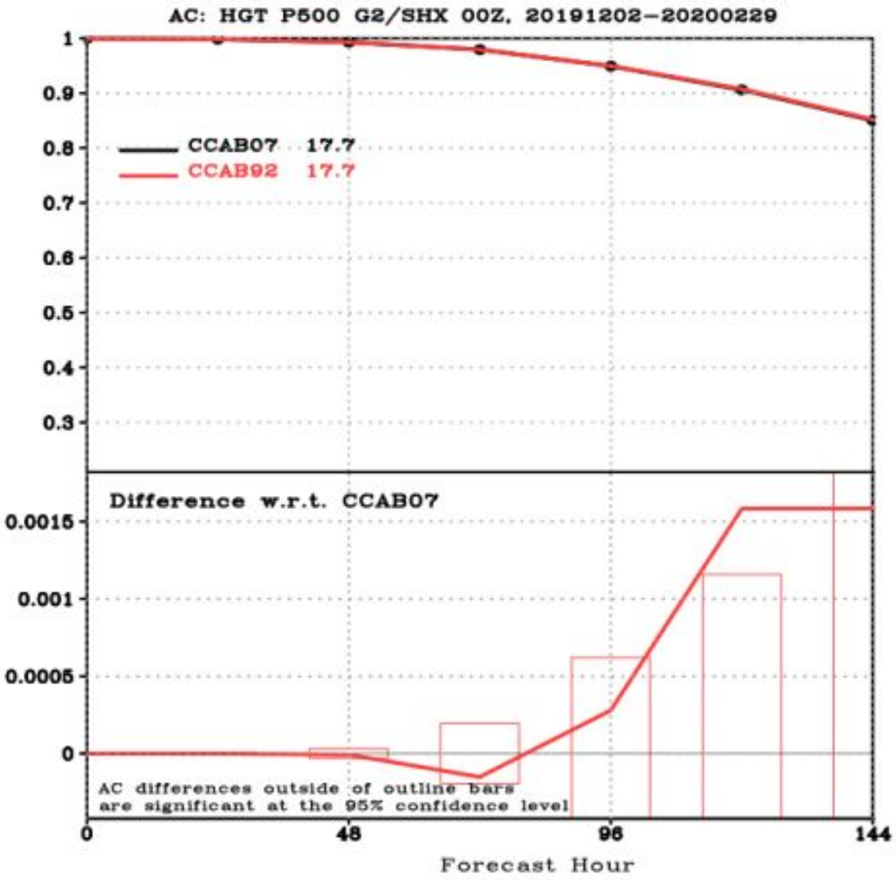


500 mb height anomaly correlation

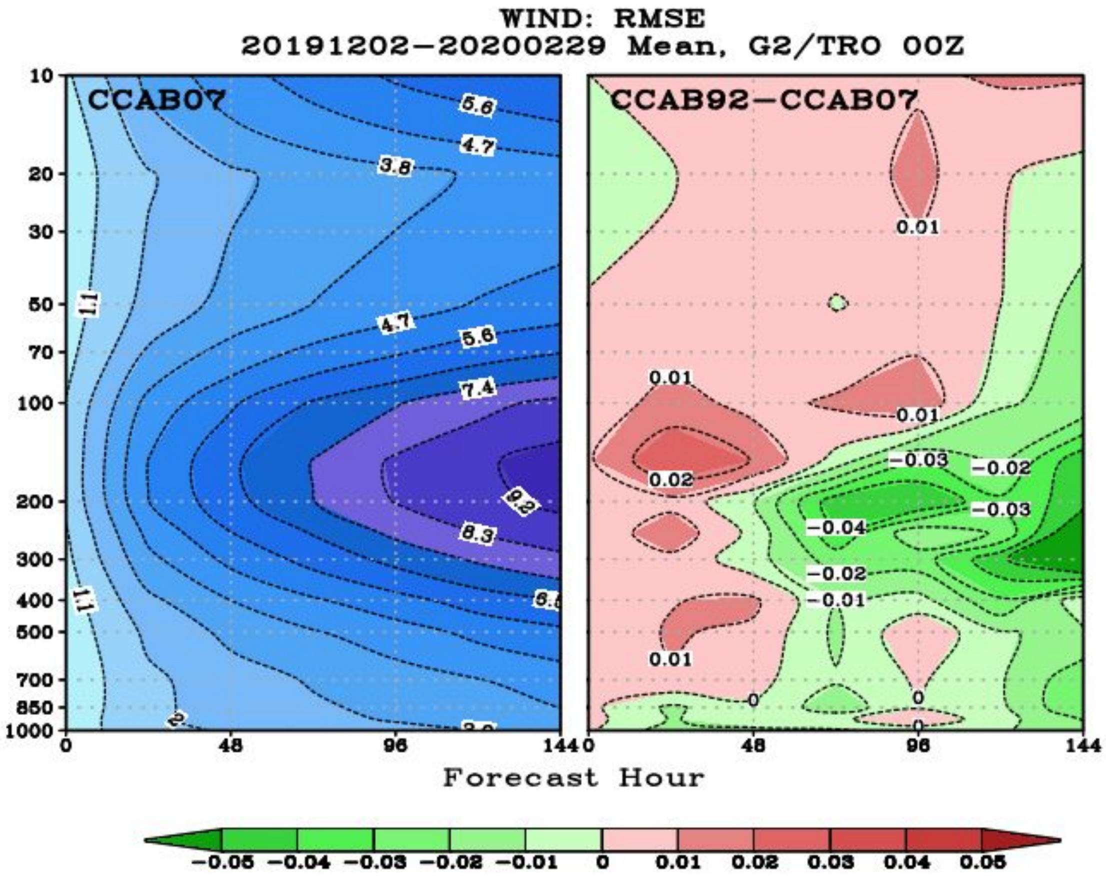
NH



SH



Wind RMSE over Tropics



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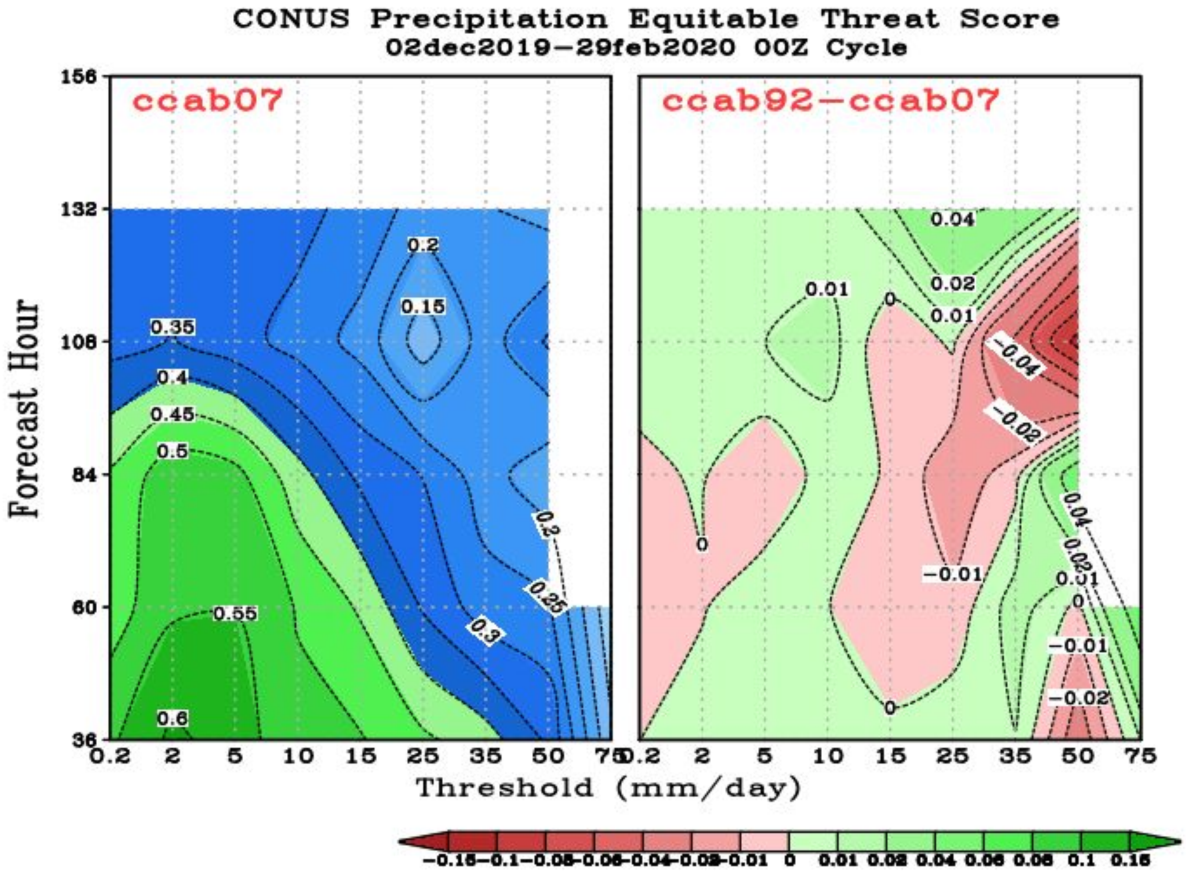

Summary

- A positive definite TVD scheme has been applied for the mass-flux transport of tracers including TKE, moisture & hydrometeors in the NCEP GFS PBL and cumulus convection schemes.
- The TVD mass-flux scheme largely reduces the negative tracer values and shows the medium-range forecast skills and surface fields comparable to the control using a central differencing scheme.
- It appears that small negative values are unavoidable even with the positive definite TVD mass-flux scheme, probably due to divergence of parcel flux and vertically unequal grid sizes.
- Simply zeroing out the negative tracers is not recommended because it can cause a conservation problem and would keep to increase the total tracer amount with time.

Summary (cont.)

- A method removing the negative tracer values has been developed by borrowing positive tracers from other layers within PBL or cumulus clouds after mass-flux transport. Although its impact on the medium-range forecast skills is small, it tends to reduce the low clouds because some of liquid waters in low clouds are subtracted to compensate the negative ones.
- For the negative liquid water, not to reduce the low clouds, we first borrow water from vapor as done in the Zhao-Carr MP scheme and then borrow it from other layers if the negative liquid water still exists. With this method, the low cloud fields are similar to the control while the negative water is removed.

Summary (cont.)

- Significant negative moistures mostly at the model 1st layers (occasionally at the model 2nd and 3rd layers) are caused by the downward surface latent heat flux in dry regions during nighttime.
- When the mass-flux transport and eddy diffusion are simultaneously computed as in the current TKE-EDMF PBL scheme, the eddy diffusion can leak out the negative tracers out of the mass-flux transport layers.
- In the final version of the TKE-EDMF-TVD PBL scheme, the negative tracers produced by the mass-flux scheme are first removed by borrowing the positive tracers within the mass-flux transport layers, and then additional negative tracers leaked out of the mass-flux transport layers due to eddy diffusion or by downward surface fluxes during nighttime are removed by borrowing the positive tracers from the entire column layers.
- For aerosols with wet deposition in the cumulus convection schemes, the potential tiny negative values due to a numerical artifact are further removed by borrowing them from the wet deposition.