J-value diagnostic update: netCDF output

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J-value diagnostic (ND22, bpch)

- J-values for most species are archived in PHOTO_JX (in fast_jx_mod.F) which handles the photolysis for a column
- Some special reactions are archived in PHOTRATE_ADJ (also in fast_jx_mod.F), after some adjustments are made to certain J-values
  - NOTE: For tropchem, the unadjusted O3P J-values for (ND22 slot #5) and POH (ND22 slot #6) are archived. This is probably historical.
- The mapping from FAST-JX species to GEOS-Chem species indices is messy and hardwired
- Because the J-value diagnostics are attached in fast_jx_mod.F, all levels are available in the diagnostics.

J-value diagnostic (ND22, bpch)

- J-values are “noontime” values, averaged between 11AM and 1PM local solar time
  - Diagnostic array LTJV(I,J) is used to determine if it is near local noon in grid box (I,J). If not, the J-values at (I,J) are ignored.
  - Counter array CTJV(I,J) keeps track of the number of times each grid box (I,J) was at local noon.
  - To get the average noontime J-value over a day, week, month, etc, the diagnostic array is divided by CTJV. Only those boxes near local noon are included.

```
IF ( ND22 > 0 ) THEN

    ! Save J-values for 2PM diagnostic boxes
    IF ( LTJV(ILON,ILAT) > 0 ) THEN

       DO L = 1, LD22

          ! AD22 IDs 5, 6, and 15 (J-values for O3 and O2)
          ! are handled in routine PHOTRATE_ADJ
          ! Hardcode ZPJ indices based on valued from FJX_j2j.dat
          ! for now (mps, 3/15/16)
          AD22(ILON,ILAT,L, 1) = AD22(ILON,ILAT,L, 1) +  ! JNO2
&                                ZPJ(L,11,ILON,ILAT)
          AD22(ILON,ILAT,L, 2) = AD22(ILON,ILAT,L, 2) +  ! JHNO3
&                                ZPJ(L,16,ILON,ILAT)
          AD22(ILON,ILAT,L, 3) = AD22(ILON,ILAT,L, 3) +  ! JH2O2
&                                ZPJ(L, 9,ILON,ILAT)
          AD22(ILON,ILAT,L, 4) = AD22(ILON,ILAT,L, 4) +  ! JCH2O
&                                ZPJ(L, 7,ILON,ILAT)  +
&                                ZPJ(L, 8,ILON,ILAT)
          AD22(ILON,ILAT,L, 7) = AD22(ILON,ILAT,L, 7) +  ! JGLYX
&                                ZPJ(L,72,ILON,ILAT)  +
&                                ZPJ(L,73,ILON,ILAT)  +
&                                ZPJ(L,74,ILON,ILAT)
          AD22(ILON,ILAT,L, 8) = AD22(ILON,ILAT,L, 8) +  ! JMGLY
&                                ZPJ(L,71,ILON,ILAT)
          AD22(ILON,ILAT,L, 9) = AD22(ILON,ILAT,L, 9) +  ! JBrO
&                                ZPJ(L,28,ILON,ILAT)
          AD22(ILON,ILAT,L,10) = AD22(ILON,ILAT,L,10) +  ! JHOBr
&                                ZPJ(L,32,ILON,ILAT)
```

ND22 bpch J-value diagnostic code in routine **PHOTO_JX**.

The mapping is hardwired to the ordering of the J-value reactions in the **FJX_j2j.dat** input file.

Routine **PHOTRATE_ADJ** has similar hardwiring of values.

NetCDF J-value diagnostics

- The netCDF diagnostics in both GC “Classic” and GCHP cannot handle local-time averaging. Therefore, we have created three different diagnostics:
  - `JVal_?PHO?:` Instantaneous J-values
    - `?PHO?` = wildcard for all photolyzing species
  - `JNoonDailyAvg_?PHO?:` Daily average of noontime J-values. Averaging is done outside of HISTORY. Arrays are zeroed each new day.
  - `JNoonMonthlyAvg_?PHO?:` Monthly average of noontime J-values. Averaging is done outside of HISTORY. Arrays are zeroed each new month.

NetCDF J-value diagnostics

- IMPORTANT: To avoid double-averaging, The **JNoonDailyAvg** and **JNoonMonthlyAvg** diagnostics must be placed within an instantaneous collection.
- Also: The netCDF diagnostics are attached in flexchem_mod.F90, after the call to PHOTRATE_ADJ. This allows that the J-value diagnostics to be attached to only one place in the code (instead of two, as for the bpch diagnostics).
  - CAVEAT: the netCDF J-value diagnostics are attached in a part of the code that only executes if we are in the chemistry grid. Therefore, grid boxes that are outside of the chemistry grid will appear as zeroes. Not sure if this is important but we can discuss later.

```
          ! Loop over the FAST-JX photolysis species
          DO N = 1, JVN_

             ! Copy photolysis rate from FAST_JX into KPP's PHOTOL array
             PHOTOL(N) = ZPJ(L,N,I,J)

#if defined( NC_DIAG )

             ! GC photolysis species index
             P = GC_Photo_Id(N)

             ! If this FAST_JX photolysis species maps to a valid
             ! GEOS-Chem photolysis species (for this simulation)...
             IF ( P > 0 ) THEN

                ! Archive the instantaneous photolysis rate
                ! (summing over all reaction branches)
                IF ( Archive_Jval ) THEN
                   State_Diag%JVal(I,J,L,P) = PHOTOL(N)
                ENDIF


                ! If it is local noon ...
                IF ( IsLocNoon ) THEN

                   ! Compute the noontime sum of the photolysis rate
                   ! over all branches for this GEOS-Chem species
                   ! (for the daily average diagnostic)
                   IF ( Archive_JNoonDailyAvg ) THEN
                      JvSumDay(I,J,L,P) = JvSumDay(I,J,L,P) + PHOTOL(N)
                   ENDIF

                   ! Compute the noontime sum of the photolysis rate
                   ! over all branches for this GEOS-Chem species
                   ! (for the monthly average diagnostic)
                   IF ( Archive_JNoonMonthlyAvg .and. IsLocNoon ) THEN
                      JvSumMon(I,J,L,P) = JvSumMon(I,J,L,P) + PHOTOL(N)
                   ENDIF
                ENDIF
             ENDIF
#endif
          ENDDO
```

Code in **flexchem_mod.F90** showing where the netCDF J-value diagnostics are attached.

Some code and comments are omitted for clarity.

ZPJ(L,N,I,J) represent the J-values for a given species at a given grid box. These are stored in **PHOTOL(N)** for KPP.

IsLocNoon is a logical that is set (in the code above, not shown) if it is near local noon at grid box (I,J,L)

GC_Photo_ID is an array that maps each FAST-JX photolysis species ID **(N)** to a GEOS-Chem species ID **(P)**. More than one FAST-JX species may map to the same GEOS-Chem species ID. This represents multiple branches of a photolysis reaction for a given GEOS-Chem species. This allows us to reduce the complex mapping to just a summation over index **P**.

JvSumDay and **JvSumNoon** are local arrays for computing the **JvNoonDailyAvg** and **JvNoonMonthlyAvg** diagnostics. These are zeroed each new day and each new month, respectively.

```
#if defined( NC_DIAG )
          !-----------------------------------------------------------------
          ! HISTORY (aka netCDF diagnostics)
          !
          ! Take the average of J-values only where it is noon
          !-----------------------------------------------------------------
          IF ( IsLocNoon ) THEN

             ! For the daily-average diagnostic
             IF ( Archive_JNoonDailyAvg ) THEN
                DO P = 1, State_Chm%nPhotol+2
                   State_Diag%JNoonDailyAvg(I,J,L,P) = ( JvSumDay(I,J,L,P)    &
                                                       /   JvCountDay(I,J,L)   )
                ENDDO
             ENDIF

             ! For the monthly-average diagnostic
             IF ( Archive_JNoonMonthlyAvg ) THEN
                DO P = 1, State_Chm%nPhotol+2
                   State_Diag%JNoonMonthlyAvg(I,J,L,P) = ( JvSumMon(I,J,L,P)  &
                                                     /   JvCountMon(I,J,L) )
                ENDDO
             ENDIF
          ENDIF
#endif
```

Code in **flexchem_mod.F90** showing where the netCDF J-value diagnostics are attached.

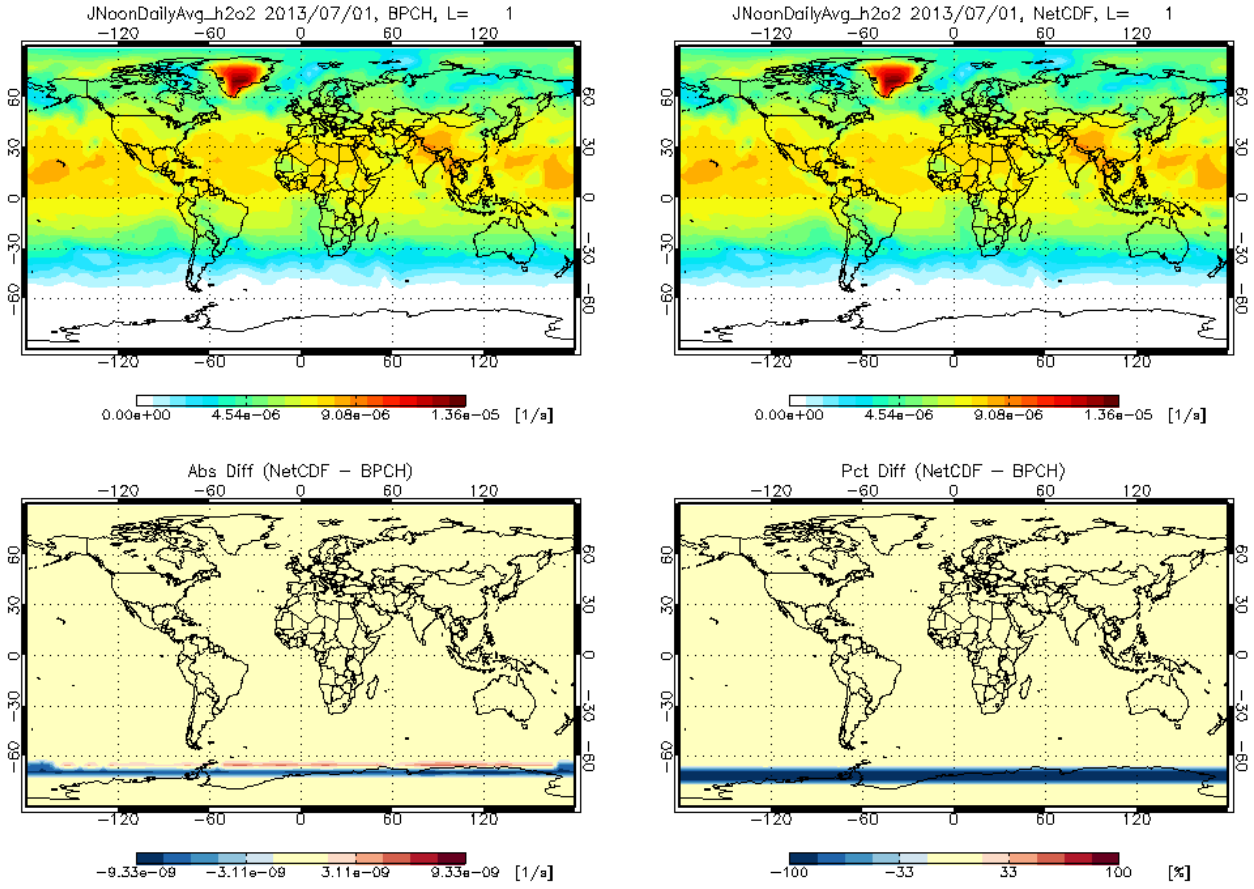
Immediately below the code on the prior slide we have the block of code where we compute the running daily or monthly average of noontime J-values.

For the daily average, we divide the **JvSumDay** array by the **JvCountDay** array. **JvCountDay** is a counter (similar to CTJV) that keeps track of the number of times it was near local noon at each grid box. Then we store into the **State_Diag%JNoonDailyAvg** array.

For the monthly average, it is the same process: we divide **JSumMonth** by **JvCountMonth** and store the result in **State_Diag%JNoonMonthlyAvg**.

Again, the **JNoonDailyAvg** and **JNoonMonthlyAvg** diagnostics must be placed into an instantaneous collection, because we have done the averaging here.

Comparisons: Bpch vs. NetCDF

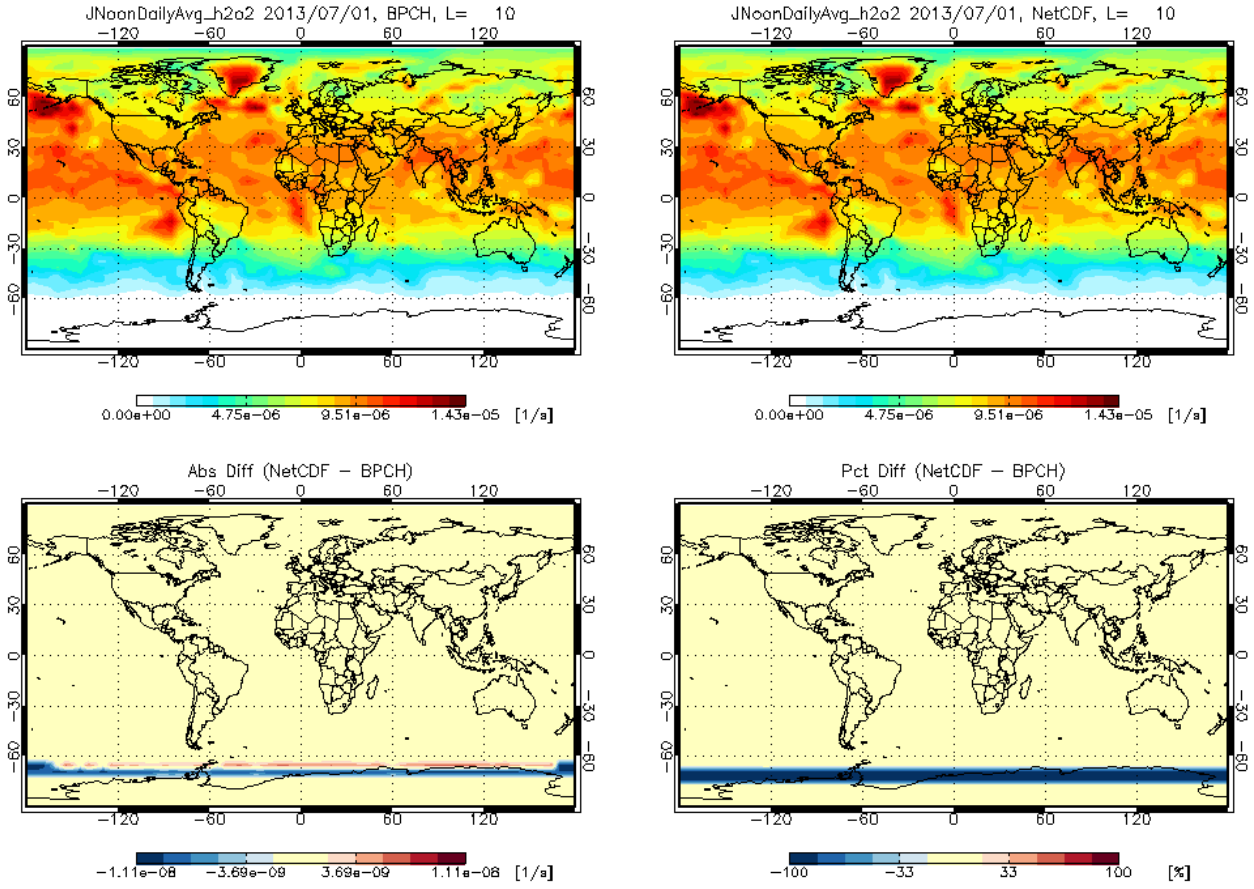


Simulation: geosfp_4x5_tropchem
Diagnostic: JNoonDailyAvg
Species: H2O2
Model Level: 1 (surface)

4-panel plot ordering:

Bpch output	netCDF output
Absolute diff	% diff

Comparisons: Bpch vs. NetCDF

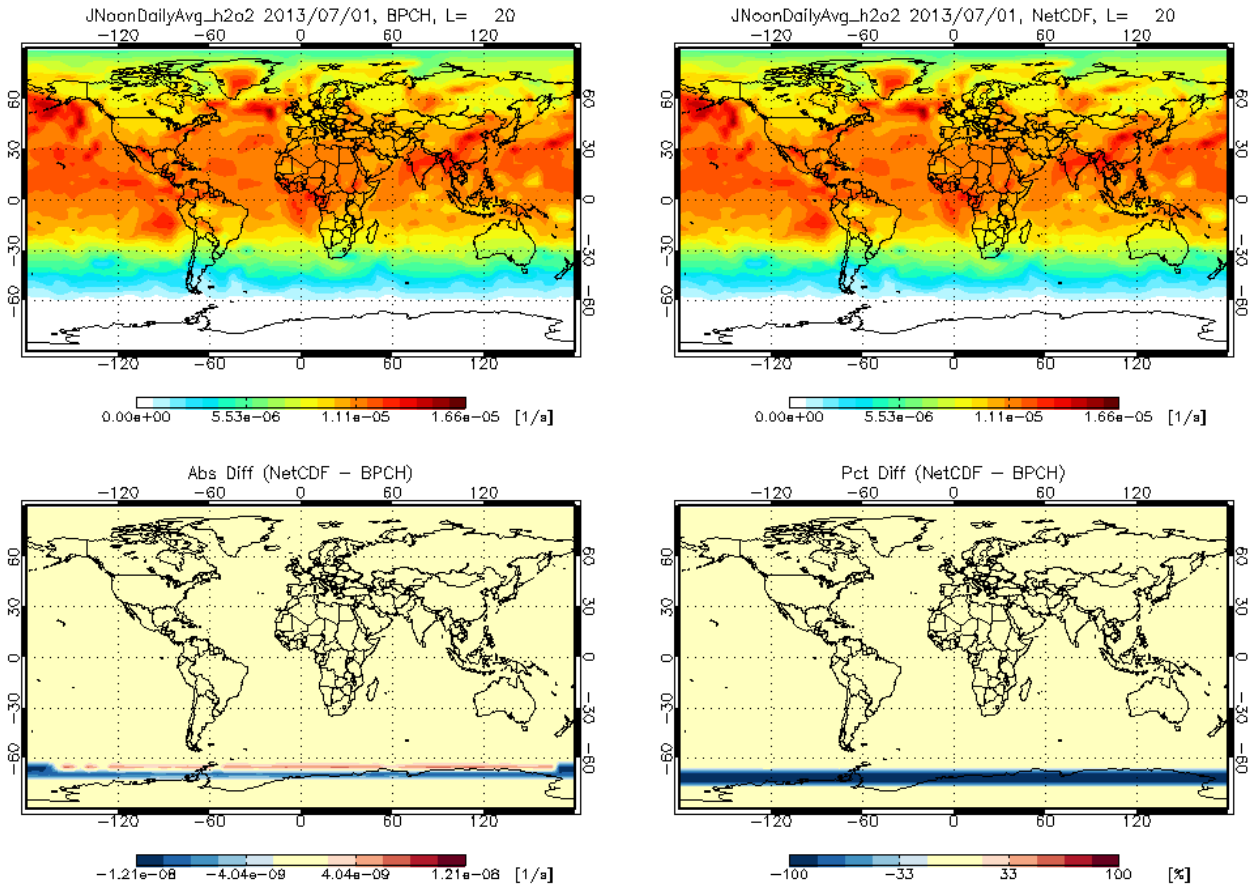


Simulation: geosfp_4x5_tropchem
Diagnostic: JNoonDailyAvg
Species: H2O2
Model Level: 10 (~ 870 hPa)

4-panel plot ordering:

Bpch output	netCDF output
Absolute diff	% diff

Comparisons: Bpch vs. NetCDF

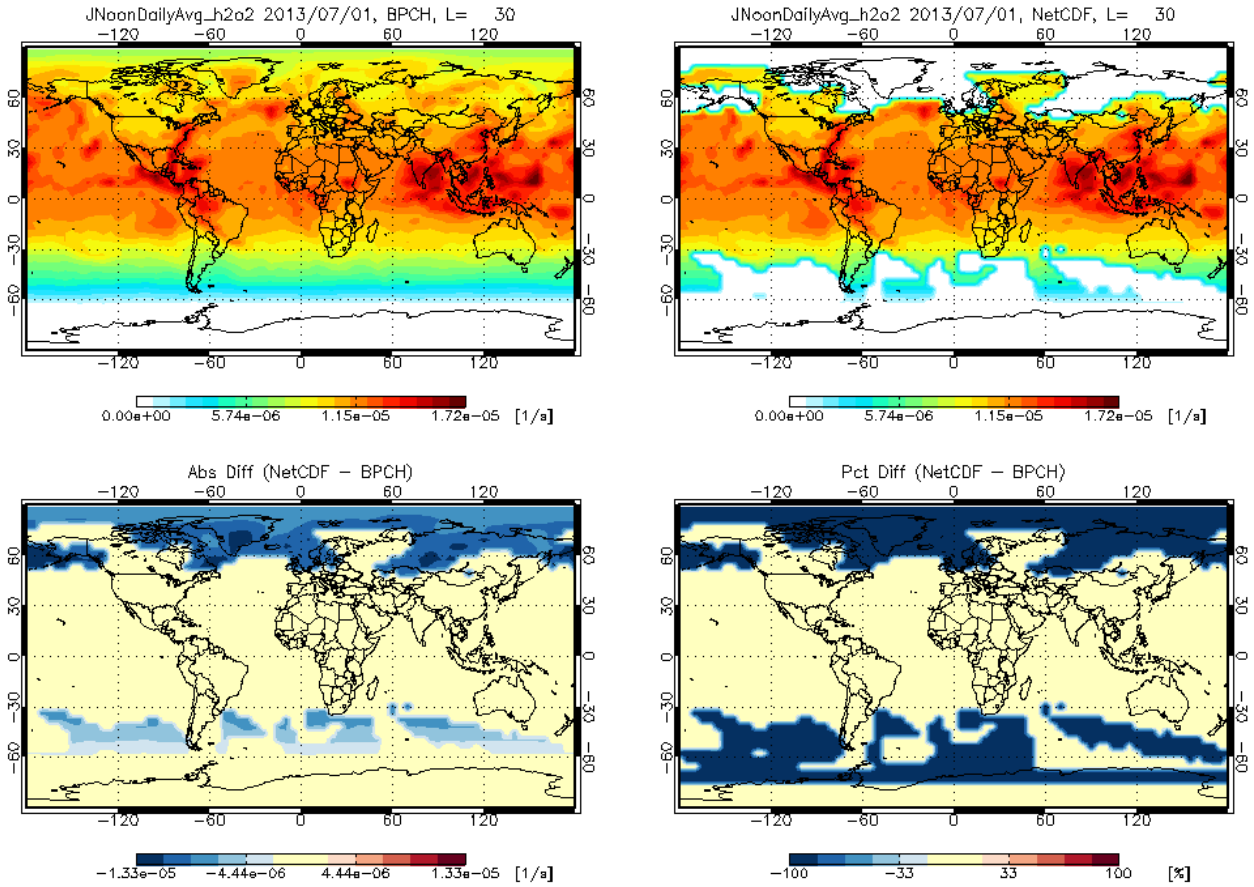


Simulation: geosfp_4x5_tropchem
Diagnostic: JNoonDailyAvg
Species: H2O2
Model Level: 20 (~ 625 hPa)

4-panel plot ordering:

Bpch output	netCDF output
Absolute diff	% diff

Comparisons: Bpch vs. NetCDF



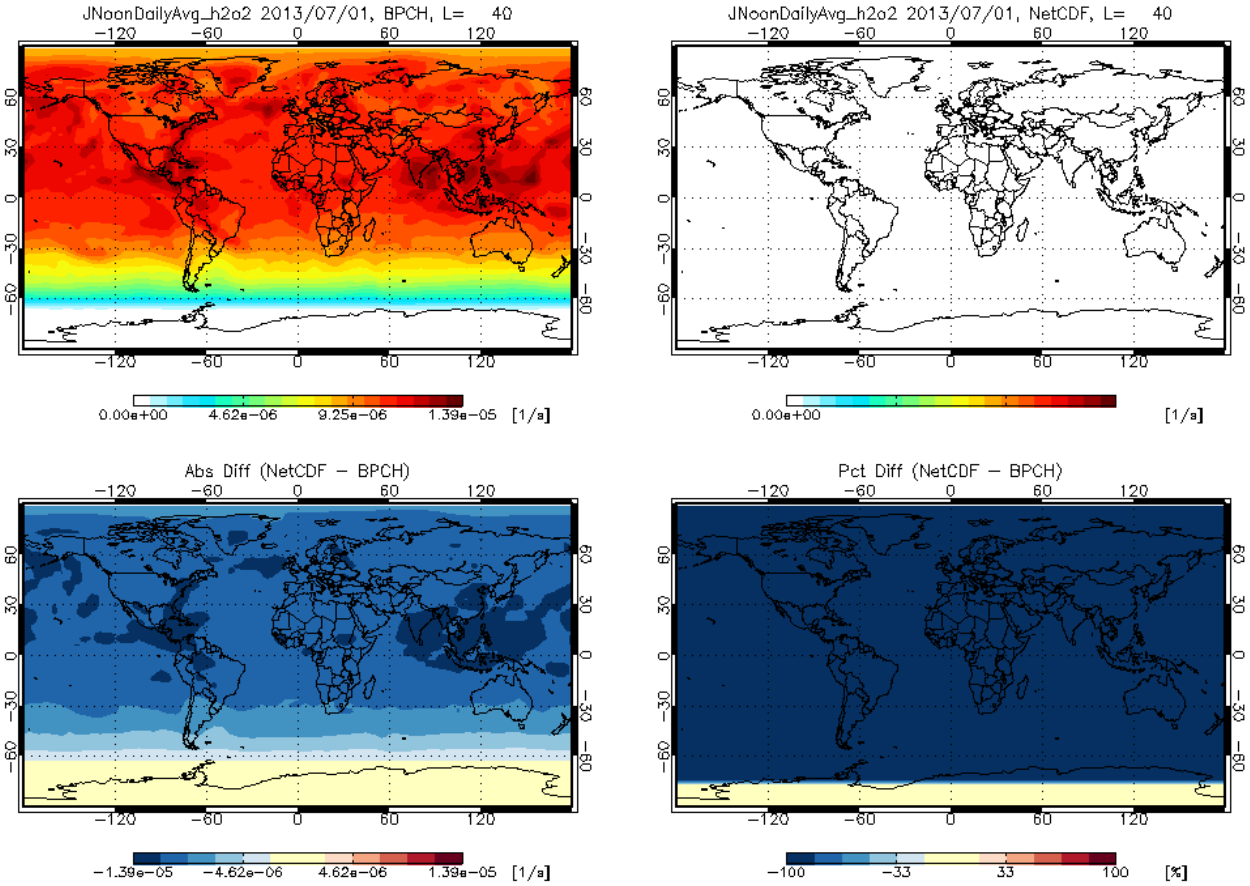
Simulation: geosfp_4x5_tropchem
Diagnostic: JNoonDailyAvg
Species: H2O2
Model Level: 30 (~ 225 hPa)

4-panel plot ordering:

Bpch output	netCDF output
Absolute diff	% diff

NOTE: Boxes that are in the stratosphere show up as white in the netCDF output. This is due to us attaching the netCDF diagnostics at a point in the code where it only executes if grid box (I,J,L) is within the chemistry grid.

Comparisons: Bpch vs. NetCDF



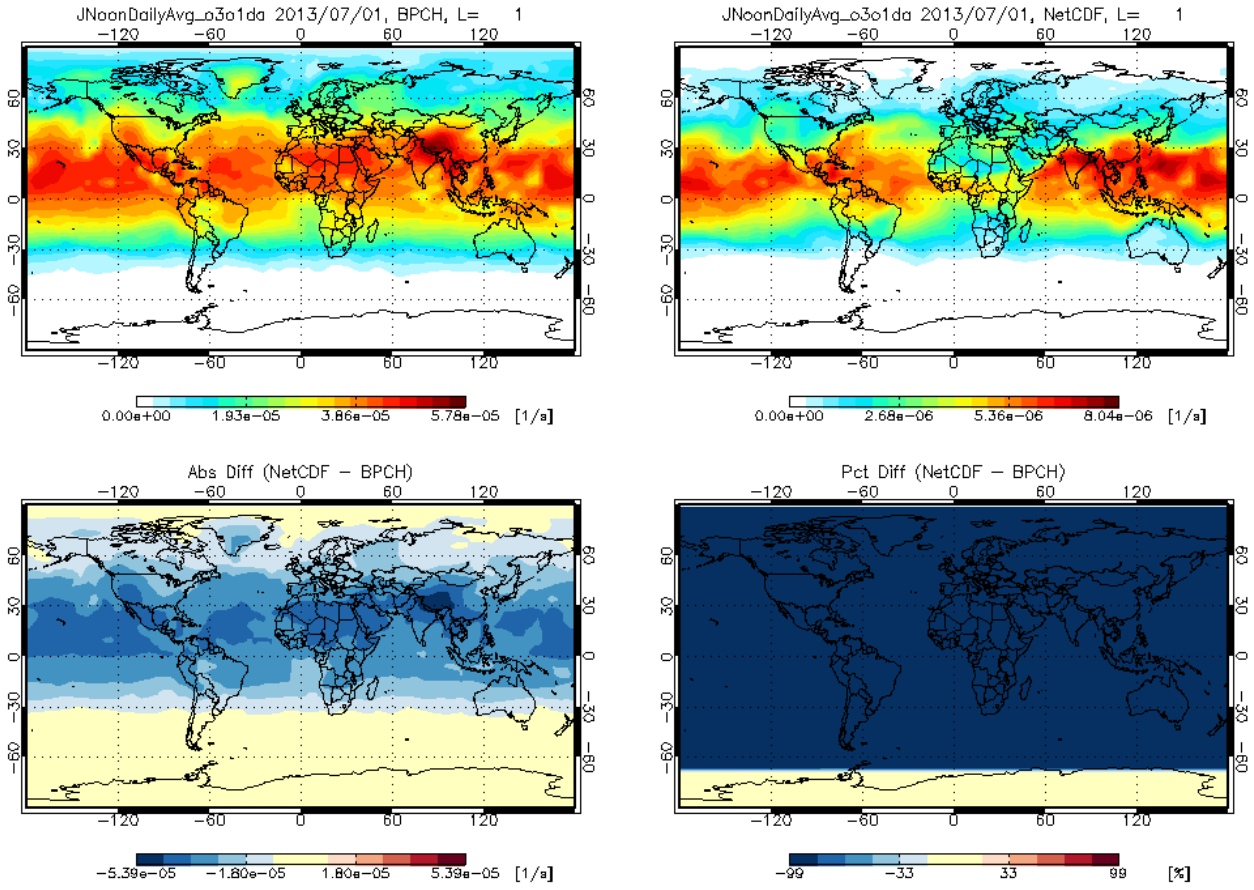
Simulation: geosfp_4x5_tropchem
Diagnostic: JNoonDailyAvg
Species: H2O2
Model Level: 40 (~ 25 hPa)

4-panel plot ordering:

Bpch output	netCDF output
Absolute diff	% diff

NOTE: At this level, all boxes (I,J,L) are in the stratosphere.

Comparisons: Bpch vs. NetCDF



Simulation: geosfp_4x5_tropchem
Diagnostic: JNoonDailyAvg
Species: O3P
Model Level: 1 (surface)

4-panel plot ordering:

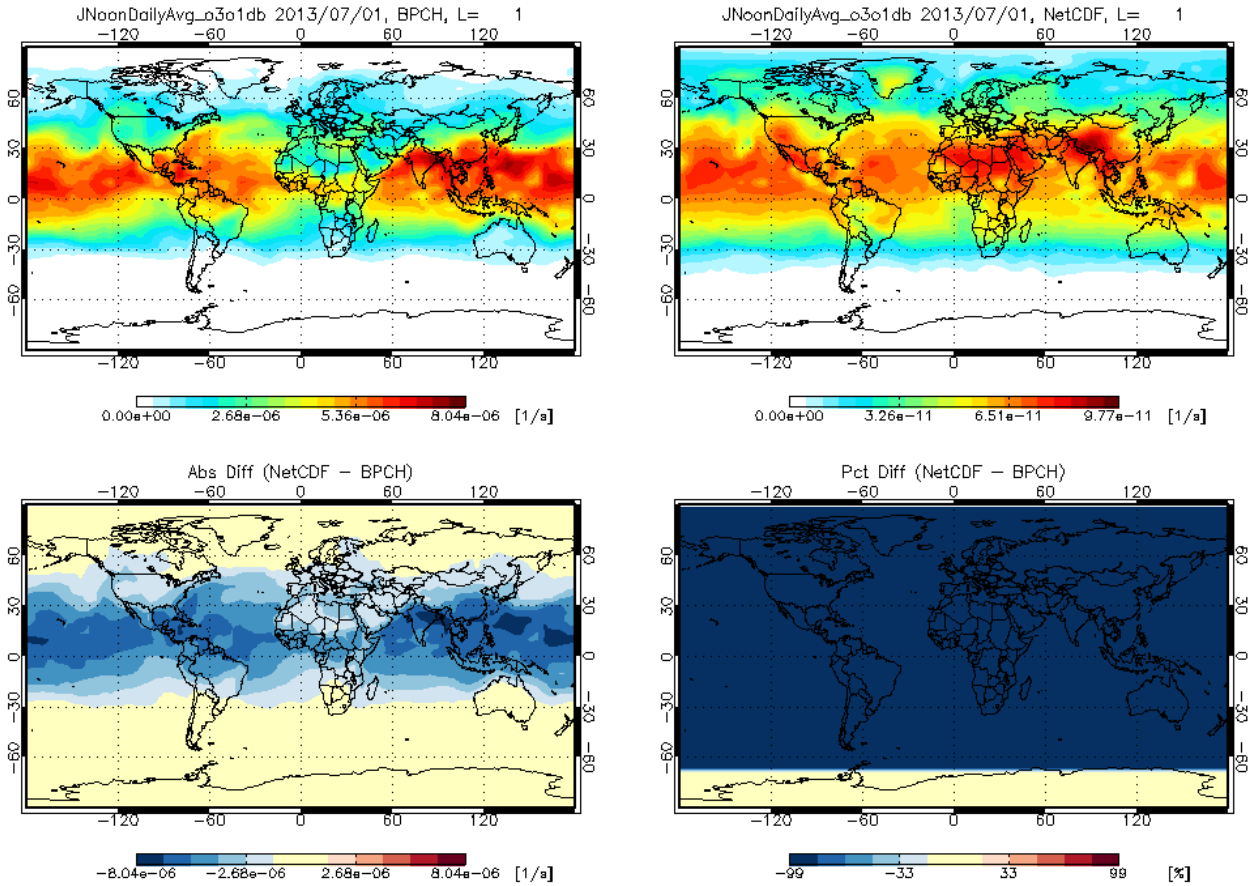
Bpch output	netCDF output
Absolute diff	% diff

This is O3P (which corresponds to ND22 slot #5 for the tropchem simulation).

The bpch diagnostic archives the unadjusted rate (i.e. diagnostic is attached in PHOTRATE_ADJ before adjustment)

On the other hand, the netCDF diagnostic archives the adjusted rate, by virture of where the netCDF diagnostics are attached in flexchem_mod.F90.

Comparisons: Bpch vs. NetCDF



Simulation: geosfp_4x5_tropchem
Diagnostic: JNoonDailyAvg
Species: POH
Model Level: 1 (surface)

4-panel plot ordering:

Bpch output	netCDF output
Absolute diff	% diff

This is POH (which corresponds to ND22 slot #6 for the tropchem simulation).

The bpch diagnostic archives the unadjusted rate (i.e. diagnostic is attached in PHOTRATE_ADJ before adjustment)

On the other hand, the netCDF diagnostic archives the adjusted rate, by virture of where the netCDF diagnostics are attached in flexchem_mod.F90.

Conclusions

- We have successfully added netCDF diagnostics for J-values
  - But we had to make some machinations
  - “Noontime” J-values are only valid for 1-day and 1-month averaging periods

- NetCDF diagnostics are attached in flexchem_mod.F90
  - But only if the grid box is within the chemistry grid
  - If desired, we could move the block where netCDF J-value diagnostics are archived further up in the loop (before the test for ITS_IN_THE_CHEMGRID)

- Some issues still exist for the tropchem simulation
  - O3P, POH J-values are adjusted rates, but bpch are unadjusted
  - How should we deal with this? Does it really matter?