BUG REPORT

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Synopsis: In CMAQ, the horizontal diffusion process is only partially complete when sub-cycling is triggered. This would happen when the characteristic time for diffusion is shorter than the process synchronization time step.

Description: Inside of the DO loop labeled 344, where sub time steps are taken, the CONC array is not updated between the steps. When NSTEPS, the number of sub time steps determined based on the eddy time scale, is larger than 1, CGRID will be updated using the same CONC array loaded from the CGRID before the 344 loops.

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C Loop over species, layers, nsteps

      DO 366 S = 1, N_SPC_DIFF
         D2C = DIFF_MAP( S )

         DO 355 L = 1, NLAYS

C Load working array (CGRID is coupled, CONC is mixing ratio)

            DO R = 1, MY_NROWS
               DO C = 1, MY_NCOLS
                  CONC( C,R ) = CGRID( C,R,L,D2C ) / RHOJ( C,R,L )
                  END DO
               END DO

            DO 344 N = 1, NSTEPS

#ifdef parallel
!*begin change by snl
C Fill 4 boundaries of working array CONC: south, north, west, east

               do c = 1, ncols
                  conc( c,0 ) = bound_south( c,l,s )
                  conc( c,nrows+1 ) = bound_north( c,l,s )
               end do

               do r = 1, nrows
                  conc( 0,r ) = bound_west( r,l,s )
                  conc( ncols+1,r ) = bound_east( r,l,s )
               end do
!*end change by snl
#else
C South boundary

               R = 1
               DO C = 1, MY_NCOLS
                  CONC( C,R-1 ) = CONC( C,R )
                  END DO

C North boundary
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                R = MY_NROWS
                DO C = 1, MY_NCOLS
                   CONC( C,R+1 ) = CONC( C,R )
                   END DO

C West boundary

                C = 1
                DO R = 1, MY_NROWS
                   CONC( C-1,R ) = CONC( C,R )
                   END DO

C East boundary

                C = MY_NCOLS
                DO R = 1, MY_NROWS
                   CONC( C+1,R ) = CONC( C,R )
                   END DO

                CALL SUBST_COMM ( CONC, DSPL_N1_E1_S1_W1, DRCN_N_E_S_W,
COMMSTR )
                CALL SUBST_COMM ( RK11, DSPL_N0_E1_S0_W0, DRCN_E )
                CALL SUBST_COMM ( RK22, DSPL_N1_E0_S0_W0, DRCN_N )
#endif

C Update CGRID

                DO R = 1, MY_NROWS
                   DO C = 1, MY_NCOLS

                      CGRID( C,R,L,D2C ) = RHOJ( C,R,L ) * CONC( C,R )
     &                                     + DTDX1S
     &                                     * ( RK11( C+1,R,L )
     &                                     * ( CONC( C+1,R ) - CONC( C,R )
)
     &                                     - RK11( C,R,L )
     &                                       * ( CONC( C,R )   - CONC( C-
1,R ) ) )
     &                                     + DTDX2S
     &                                     * ( RK22( C,R+1,L )
     &                                       * ( CONC( C,R+1 ) - CONC( C,R
) )
     &                                       - RK22( C,R,L )
     &                                       * ( CONC( C,R )   - CONC(
C,R-1 ) ) )

                      END DO
                   END DO

344             CONTINUE

355          CONTINUE
366       CONTINUE

       RETURN
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1001  FORMAT( 5X, 'Negative concentrations reset to', 1PE11.3 )
1003  FORMAT( 1X, 4I7, 9X, 1PE11.3)
1005  FORMAT( / 5X, 'H-eddy DT & integration steps: ', 1PE15.7, I8 )

      END
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Remedy:

The loading of CONC from CGRID should be re-located inside of the 344 loop in the very beginning of the loop.