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1
2 # =====
3 # 6) Use the HPPM method from CMAQ
4 # CW refers to the paper by Colella and Woodward.
5
6 # 1-D domain covers grid points i = 1 to imax. But 1 and imax are boundary-
7 # condition cells. The main interior computation is for i = 2 to (imax-1).
8
9 # Pre-calculate some constants
10 sixth = 1.0/6.0
11 two3rds = 2.0/3.0
12 oneoverdelx = 1.0 / delx
13
14 # Allocate the vectors
15 dc = numeric(imax)      # nominal difference in concentration across a cell
16 clfirst = numeric(imax) # first guess of conc at left edge of cell i
17 cr = numeric(imax)     # conc at right edge of cell i
18 cl = numeric(imax)     # conc at left edge of cell i
19 c6 = numeric(imax)     # this corresponds to parabola parameter a6 of CW eq.(1.4)
20 FL = numeric(imax)     # pollutant flux into the left side of a grid cell
21 FR = numeric(imax)     # pollutant flux into the right side of a grid cell
22
23
24 # Iterate forward in time
25 for (n in 1:nsteps) {   # for each time step n
26
27
28 # To guarantee that solution is monotonic, check that the left edge of cell i
29 # (which is between cells i and i-1) should not have a concentration lower
30 # or higher than the concentrations in those two neighboring cells
31 # Namely, is clfirst between c[i] and c[i-1]. If not, then fix.
32 for (i in 2:(imax - 1)) { # for each interior grid point i
33   del_cl = conc[i] - conc[i-1] # concentration difference with cell at left
34   del_cr = conc[i+1] - conc[i] # concentration difference with cell at right
35   dc[i] = 0.5*(del_cl + del_cr) # 1st guess of avg conc difference across cell i
36   if ((del_cl*del_cr)>0.0) { # then revise average difference across cell i
37     dc[i] = sign(dc[i]) * min( abs(dc[i]), 2*abs(del_cl), 2*abs(del_cr) )
38   } else {dc[i]=0.0} # for the special case of constant conc across cell
39 } # end of grid-point (i) loop
40
41 # First guess for concentration at left edge of each cell, using revised dc value
42 for (i in 2:(imax - 1)) { # for each interior grid point i
43   clfirst[i] = 0.5*(conc[i]+conc[i-1]) - sixth*(dc[i]-dc[i-1])
44 } # end of grid-point (i) loop
45
46 # find parameters for the piecewise-continuous parabola in cell i
47 for (i in 2:(imax - 1)) { # for each interior grid point i
48
49 # conc at the right edge (cr) of cell i equals concn at left edge of cell i+1
50 cr[i] = clfirst[i+1] # concentration at right edge of cell i
51 cl[i] = clfirst[i] # concentration at left edge of cell i
52
53 # Check whether cell i is an extremum (is a peak or valley in the conc plot)
54 if (( (cr[i]-conc[i]) * (conc[i] - cl[i]) ) > 0.0) { # then not extremum
55
56 # Find the two coefficients of the parabola: dc and c6:
57 dc[i] = cr[i] - cl[i] # updated concn diff. between right and left edges
58 c6[i] = 6*( conc[i] - 0.5*(cl[i]+cr[i]) )
59
60 if ( (dc[i]*c6[i]) > (dc[i]*dc[i]) ) { # then adjust for overshoot at left edge
61   cl[i] = 3.0*conc[i] - 2.0*cr[i]
62 } else if ( (-dc[i]*dc[i]) > (dc[i]*c6[i]) ) { # then adjust for overshoot at right
63   cr[i] = 3.0*conc[i] - 2.0*cl[i]
64 } # end of block of "not extremum" calculations
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66     } else {                               # For an extremum, don't use a parabola.
67         cl[i] = conc[i]                   # Instead, assume concen is constant across the cell,
68         cr[i] = cl[i]                     # Thus, left and right concentrations equal average conc.
69     }                                       # end of grid-point (i) loop
70
71     # second guess of coefficients for the parabola, from CW eq. (1.5)
72     dc[i] = cr[i] - cl[i]
73     c6[i] = 6.0*(conc[i] - 0.5*(cl[i] + cr[i]))
74
75 }                                           # end of grid-point (i) loop
76
77
78 # Initialize to 0 the fluxes into the left and right sides of cell i
79 FL <- rep(0.0, imax)
80 FR <- rep(0.0, imax)
81
82
83 # Next, use parabolic fits within each cell to calculate the fluxes between cells
84
85 # At left side of whole domain (i = 1), assume constant flux. Use FR[1] = FR[2]
86 if (u > 0.0) {                               # if wind enters left boundary of domain
87     y = u*delt                               # distance traversed by wind during delt
88     x = y*oneoverdelx                         # Courant number is fraction of grid cell traversed
89     # Find the flux leaving the right side of left boundary cell
90     FR[1] = y*( cr[2] - 0.5*x*(dc[2] - c6[2]*(1.0 - two3rds*x)) ) # parabolic in x
91 }
92
93 # In interior of whole domain, use parabola eqs. CW (1.12) to find the fluxes
94 for (i in 2:(imax-1)) {                       # for each interior grid point i
95
96     if (u < 0.0) {                             # for wind from right to left
97         y = -u*delt                             # distance traversed by wind during delt
98         x = y*oneoverdelx                         # Courant number is fraction of grid cell traversed
99         FL[i] = y*( cl[i] + 0.5*x*(dc[i] + c6[i]*(1.0 - two3rds*x)) ) # parabolic in x
100    }
101
102    if (u > 0.0) {                               # for wind from left to right
103        y = u*delt                               # distance traversed by wind during delt
104        x = y*oneoverdelx                         # Courant number is fraction of grid cell traversed
105        FR[i] = y*( cr[i] - 0.5*x*(dc[i] - c6[i]*(1.0 - two3rds*x)) ) # parabolic in x
106    }
107
108 }                                           # end of loop over all interior grid cells
109
110 # At right side of whole domain (i = imax), assume const. flux. Use FL[imax] = FL[imax-1]
111 if (u < 0.0) {                               # if wind enters right boundary of domain
112     y = -u*delt                               # distance traversed by wind during delt
113     x = y*oneoverdelx                         # Courant number is fraction of grid cell traversed
114     FL[imax] = y*( cl[imax-1] + 0.5*x*(dc[imax-1] + c6[imax-1]*(1.0 - two3rds*x)) )
115 }
116
117
118 # For a realistic case, you would want to impose the actual fluxes at the boundaries.
119 # But for our simple HW, impose boundry conditions of zero pollutant flux entering the domain.
120 if (u > 0.0) FR[1] = 0.0
121 if (u < 0.0) FL[1] = 0.0
122
123
124 # Update the concentrations in each grid cell. *** This is the forecast equation.***
125
126 for (i in 2:(imax-1)) {                       # for each interior grid point i
127     conc[i] <- conc[i] + oneoverdelx*(FR[i-1] - FR[i] + FL[i+1] - FL[i]) # CW eq. 1.13
128 }                                           # end of loop over all interior grid cells i
129
130 }                                           # end of loop over all time iterations n

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