Preserving Positivity when Advecting Interacting Biological Scalar Fields

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Overview

Over the last couple of years, Alan Wallcraft has introduced several biological models into the trcupd.f code in HYCOM. However, problems with positivity can arise due to the nature of the nonlinear interactions, for example zooplankton consume phytoplankton, etc. In particular, although the MPDATA approach, for example, preserves sign in the advection/diffusion of the scalar fields, it is not guaranteed that sign is preserved if the nonlinear interactions are computed using a separate method under the framework of operator splitting.

Fortunately, Smolarkiewicz and Margolin (1998) have devised a scheme that preserves the sign in the presence of “source” terms. An abbreviated version of their Eq. (19) is

\[ \frac{\partial \psi}{\partial t} + \text{div} (v \, \psi) = R, \]

where \( \psi \) is any biological entity, e.g. N, Z, P or D, \( v(x,t) \) is the fluid velocity, and \( R(x,t) \) is an appropriate source function. For biological modeling, it would represent the nonlinear interactions among the distinct constituents (R is a function of NZPD). However for present purposes the precise form is irrelevant.

The aim of this note is to incorporate the Smolarkiewicz - Margolin formulation of the inclusion of R into HYCOM.

Implementation

The basic ideas are contained in the following statements. As originally formulated, A is the complete MPDATA advection-diffusion operation, although it can represent any alternative advection scheme that preserves positivity. The expressions \( \Psi(n) \) and \( R(n) \) refer to the values at time indexed by n, while dt is the discretized timestep. An asterisk refers to an intermediate updated value through the operation A or evaluation of the source term R.

1) \( \Psi^* = A[\Psi(n) + dt \, R(n)] \)

2) \( R^* = R(\Psi^*) \)

3) \( \Psi(n+1) = A[\Psi(n) + dt/2 \, R(n)] + dt/2 \, R^* \)

4) \( R(n+1) = R(\Psi(n+1)) \)
To carry out these operations, Willemsen initially introduced an array “sterm” to represent the source term R with the same dimensions as “tracer” (ψ), together with storage arrays sterm0 and tracer0. Later Wallcraft showed that there is no need for sterm0.

We start with line 466 of tsadvec, do ktr = 1, ntracr. The specific line number referred to the version of src being used at the time, but it has been verified that after revisions since then this line number is still correct.

c STERM ADDED FOR BIO line 466 in tsadvc.f
   do ktr= 1,ntracr
      call xctilr(tracer( 1-nbdy,1-nbdy,1,1,ktr),1,2*kk, 6,6, halo_ps)
      call xctilr(sterm( 1-nbdy,1-nbdy,1,1,ktr),1,2*kk, 6,6, halo_ps)
   enddo

c store values at time n
   do ktr= 1,ntracr
      trold(i,j,ktr)=tracer(i,j,k,n,ktr)
      if (trcflg(ktr).eq.2) then
         tracer(i,j,k,n,ktr)=tracer(i,j,k,n,ktr)+pdtemp
      endif
   enddo

c construct the quantity to be advected (operator A in 1))

c ADDED FOR BIO line 551
   tracer0(i,j,k,n,ktr)=tracer(i,j,k,n,ktr)
      & +0.25*delt1*sterm(i,j,k,m,ktr)
   tracer( i,j,k,n,ktr)=tracer(i,j,k,n,ktr)
      & +0.5*delt1*sterm(i,j,k,m,ktr)

c END ADDED

   enddo

c advect it with the understanding that tracer is both input and output from c advem -this is unchanged from previous location, but note there are 2 calls

call advem(2,tracer..,....)
call advem(2,tracer0..,....)

c to implement step 2, the R operation refers to a call to trcupd which has sterm c in common block just like tracer – the modifications to trcupd will be seen c below then construct new quantity to be advected ( step 3)

c ADDED FOR BIO line 858
   call trcupd(n,n)
   tracer(:,:,:,n,:)=tracer0(:,:,:,n,:)+
      & +0.5*delt1*sterm(:,:,:,n,:)
c step 4, since trcupd is now a calculation using tracer(n+1), update the sources outside of last ijk loop.

call trcupd(n,n)

Note that while the calls to advem invoke MPDATA in the current version of HYCOM, the method should be robust to changes in the advection method since the treatment of the source term is a standard predictor-corrector method.

**Modifications to trcupd**

Roughly speaking the dynamics was initially evaluated using, with m and n the leapfrogging steps,

\[
\begin{align*}
\text{bm} &= \text{tracer}(m) \\
\text{bn} &= \text{tracer}(n) \\
\text{tracer}(n) &= \text{bn} + S(m) \cdot \text{dt} \quad \text{! where the S(m) are the explicit nonlinear interactions evaluated with tracer(m)’s.}
\end{align*}
\]

A different version appropriate for use within the present scheme involves

1) Removing the bm fields;
2) computing S(n) rather than S(m) and these become the sterm outputs;
3) do not compute any update to tracer here, it’s done in tsadvec as above.

In detail,

c NEW VERSION line 683 in trcupd.f
! tracer(i,j,k,n,ibio) = bn_n + delt1/86400.0 * bu_n
! tracer(i,j,k,n,ibio+1) = bn_p + delt1/86400.0 * bu_p
! tracer(i,j,k,n,ibio+2) = bn_z + delt1/86400.0 * bu_z
! tracer(i,j,k,n,ibio+3) = bn_d + delt1/86400.0 * bu_d

sterm(i,j,k,n,ibio) = 1.0/86400.0 *bu_n
sterm(i,j,k,n,ibio+1) = 1.0/86400.0 *bu_p
sterm(i,j,k,n,ibio+2) = 1.0/86400.0 *bu_z
sterm(i,j,k,n,ibio+3) = 1.0/86400.0 *bu_d

endo
endo !i
endo !l
endo !j
return
end subroutine trcupd_904

Note the 1.0 rather than delt1 because the delt1 are introduced in the calls.
Reference