Notes on high resolution discretization

M. Syamlal, 5-20-2005

These notes update the derivation of discretized scalar transport equation shown in pages 15-21 of the MFIX numerics manual (Syamlal 1998). This update ensures that strict conservation is maintained even with the high resolution technique. The derivation is shown only for one component of the convection term, but the extension to the full 3-D equation as shown in the numerics manual is straightforward. The derivation here also shows the implementation of deferred correction.

Scalar transport

As shown in page 4-5 of the numerics manual the discretization of the convection term gives

$$\int \frac{\partial(\phi\rho u)}{\partial x} dV = \left[(\phi\rho u A)_e - (\phi\rho u A)_w\right] \qquad (1)$$

The face values of uA are known. The choice of the face values of $\phi\rho$ would determine the accuracy and stability of the discretized equations. To maintain strict conservation it is essential that the face value of ρ be set exactly equal to the face value used in the continuity equation. That leaves only the face value of ϕ to be determined. We will apply a high resolution method to determine the face value of ϕ to get

$$\int \frac{\partial(\phi\rho u)}{\partial x} dV = \left[\phi_e^H (\rho u A)_e - \phi_w^H (\rho u A)_w\right] \qquad (2)$$

where terms like $(\rho u A)_e$ come from the discretized continuity equation. The stability of the above discretization scheme is not guaranteed. But tests simulating the convection of square waves of void fraction and species mass fraction show that implicit methods do not result in oscillations. To derive a deferred correction scheme we add and subtract low order terms (superscript L). Only the east term is shown below; west and other terms are similar:

$$\phi_e^H (\rho u A)_e + \phi_e^L (\rho u A)_e + \ldots = \phi_e^L (\rho u A)_e + \ldots \qquad (3)$$

which can be rearranged as

$$\phi_e^L (\rho u A)_e + \ldots = (\phi_e^L - \phi_e^H)(\rho u A)_e + \ldots \qquad (4)$$

Express the low-order face value in terms of node values and subtract out continuity equation multiplied by ϕ_P

$$\left[\xi_e^L \phi_E + \bar{\xi}_e^L \phi_P - \phi_P\right](\rho u A)_e + \ldots = \left[\phi_e^L - \phi_e^H\right](\rho u A)_e + \ldots \quad (5)$$

Then using the identity that $\bar{\xi}_e^L = 1 - \xi_e^L$ we get

$$\left[\xi_e^L (\phi_E - \phi_P)\right](\rho u A)_e + \ldots = \left[\phi_e^L - \phi_e^H\right](\rho u A)_e + \ldots \quad (6)$$

And the deferred correction formula is obtained by evaluating the right hand side term from the previous iteration:

$$\left[\xi_e^L (\phi_E - \phi_P)\right](\rho u A)_e + \ldots = \left[\phi_e^L - \phi_e^H\right]^{n-1} (\rho u A)_e + \ldots \quad (7)$$

The above formula conforms to *Rule 4* of Patankar and avoids the assumption mentioned in last paragraph of page 20 of the numerics manual.

Testing of scalar transport

The species conservation was tested with a bubbling bed simulation. The bed is fluidized with a grid flow composed of gas species 1 and a central jet composed of gas species 2. Since the grid flow is much larger gas species 1 is the major species and 2 is the minor species. There are no chemical reactions. All the equations were discretized using Superbee. From past experience it was known that the error in the minor species mass balance is severe when a high resolution scheme Superbee is used for discretizing the continuity equation.

Table 1 compares the percent error in the overall mass balance in the predictions of the old code with that of the new code at 0.1 s intervals. There is some improvement in the overall mass balance and as expected there is no dramatic change. The CPU time for the old simulation was 238 s and that for the new simulation was 232 s.

Table 1. %Error in overall mass balance

Gas		Solids	
Old	New	Old	New
2.77E-03	3.44E-04	2.74E-04	3.77E-04
1.07E-03	-5.60E-04	1.33E-04	8.72E-05
2.62E-03	4.30E-04	8.95E-05	5.15E-05
2.15E-03	1.06E-04	1.01E-04	3.10E-05
2.28E-03	1.63E-04	8.90E-05	5.49E-05
2.91E-03	1.41E-04	1.05E-04	4.15E-05
2.95E-03	2.24E-04	1.84E-04	6.11E-05
2.32E-03	2.99E-04	1.66E-04	6.28E-05
3.06E-03	3.32E-04	1.96E-04	6.98E-05

Table 2 compares the %error in the overall species mass balances. The %error in the mass balance of the major species decreases by several orders of magnitude. There is even greater improvement in the mass balance of the minor species.

Table 2. %Error in overall mass balance of gas species

Major species		Minor species	
Old	New	Old	New
1.94E-02	3.77E-04	-0.169	2.61E-06
-0.964	-6.15E-04	9.63	-9.59E-06
-1.819	4.74E-04	18.2	-1.71E-06
-1.42	1.16E-04	14.2	9.81E-06
-1.10	1.77E-04	11.0	1.86E-05
-1.49	1.55E-04	14.9	4.24E-06
-0.50	2.45E-04	5.02	1.92E-05
-1.07	3.22E-04	10.7	6.62E-05
-0.725	3.57E-04	7.27	7.96E-05

Another test used to evaluate the new algorithm was the Spouted Bed Combustor tutorial problem. This problem considers four gas phase species, two solids phases with two species each, three energy equations, and chemical reactions. Solids phase-2 is injected into a bed of solids phase-1 through a central jet. All the equations were discretized using Superbee. The CPU time for the old simulation was 868 s and that for the new simulation was 291 s. The results are compared in Table 3. The overall mass balances are similar. The drop in the gas phase mass balance is small and can be reduced by increasing the tolerance. Again there is several orders of magnitude improvement in the gas phase species mass balance. The solids phase-1 species balances have also improved.

There is a surprising drop in the accuracy of the overall balance of solids phase-2 species. This anomaly is quite likely because the amount of solids phase-2 in the system is very small.

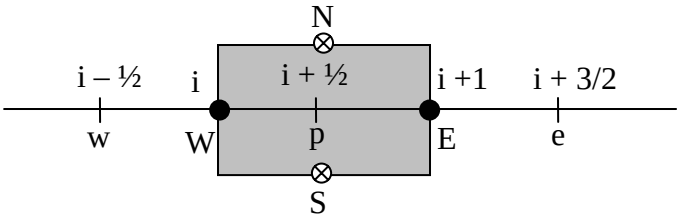
Table 3. %Error in overall mass balance of gas species

	Old	New
Gas	5.85E-04	-1.15E-03
Solids 1	5.84E-08	-1.45E-08
Solids 2	4.45E-06	5.88E-10
Gas sp 1	-2.50E+00	-3.01E-05
Gas sp 2	-8.83E+00	-4.07E-05
Gas sp 3	1.44E+00	-2.14E-05
Gas sp 4	3.86E-01	-1.43E-03
Solids-1 sp 1	-8.51E-02	8.90E-05
Solids-1 sp 2*	3.80E-06	4.20E-07
Solids-2 sp 1	-1.44E-04	-6.23E-02
Solids-2 sp 2	2.27E-04	9.35E-02

* Normalized with the accumulation, since there is no net flow of this species

Momentum equations

As an example we consider the x-momentum equation, which is integrated over the staggered cell. The u-component is stored at locations such as i-1/2, i+1/2 and so on.



$$\int\left[\frac{\partial(\rho u)}{\partial t}+\frac{\partial(u\rho u)}{\partial x}+\frac{\partial(u\rho v)}{\partial y}\right]dV=\left[(\rho u)_p-(\rho u)_p^0\right]\frac{\Delta V}{\Delta t}+\left[(u\rho uA)_E-(u\rho uA)_W\right]+\left[(u\rho vA)_N-(u\rho vA)_S\right] \tag{8}$$

From the above we need to subtract out the continuity equation multiplied by u_p to get

$$\int\left[\frac{\partial(\rho u)}{\partial t}+\frac{\partial(u\rho u)}{\partial x}+\frac{\partial(u\rho v)}{\partial y}\right]dV=\left[u_p-u_p^0\right]\frac{\rho_p^0\Delta V}{\Delta t}+\left[(u_E-u_p)(\rho uA)_E-(u_W-u_p)(\rho uA)_W\right] \tag{9}$$
$$+\left[(u_N-u_p)(\rho vA)_N-(u_S-u_p)(\rho vA)_S\right]$$

So we need the continuity equation in the following form to be satisfied:

$$\left[\rho_p-\rho_p^0\right]\frac{\Delta V_p}{\Delta t}+\left[(\rho uA)_E-(\rho uA)_W\right]+\left[(\rho vA)_N-(\rho vA)_S\right]=R_p\Delta V_p \tag{10}$$

There is no discretized equation like that because continuity equation is integrated over the scalar cell. However we can ensure that such a balance exists by calculating the mass fluxes of the two scalar cells whose intersection gives the x-momentum cell (using i, j subscripts for clarity):

$$\left[\rho_{i,j}-\rho_{i,j}^0\right]\frac{\Delta V_{i,j}}{\Delta t}+\left[(\rho uA)_{i+1/2,j}-(\rho uA)_{i-1/2,j}\right]+\left[(\rho vA)_{i,j+1/2}-(\rho vA)_{i,j-1/2}\right]=R_{i,j}\Delta V_{i,j} \tag{11}$$

$$\left[\rho_{i+1,j}-\rho_{i+1,j}^0\right]\frac{\Delta V_{i+1,j}}{\Delta t}+\left[(\rho uA)_{i+3/2,j}-(\rho uA)_{i+1/2,j}\right]+\left[(\rho vA)_{i+1,j+1/2}-(\rho vA)_{i+1,j-1/2}\right]=R_{i+1,j}\Delta V_{i+1,j} \tag{12}$$

Now adding the two continuity equations, dividing by two, and comparing with equation (10) we get

$$\Delta V_p=0.5\left(\Delta V_{i,j}+\Delta V_{i+1,j}\right)$$
$$\rho_p=\left(\Delta V_{i,j}\rho_{i,j}+\Delta V_{i+1,j}\rho_{i+1,j}\right)/\left(2\Delta V_p\right)$$
$$(\rho uA)_E=0.5\left[(\rho uA)_{i+3/2,j}+(\rho uA)_{i+1/2,j}\right]$$
$$(\rho uA)_W=0.5\left[(\rho uA)_{i+1/2,j}+(\rho uA)_{i-1/2,j}\right]$$

$$(\rho v A)_N = 0.5\left[(\rho v A)_{i+1,j+1/2} + (\rho v A)_{i,j+1/2}\right]$$
$$(\rho v A)_S = 0.5\left[(\rho v A)_{i+1,j-1/2} + (\rho v A)_{i,j-1/2}\right]$$
$$R_p = \left(\Delta V_{i,j} R_{i,j} + \Delta V_{i+1,j} R_{i+1,j}\right)/\left(2\Delta V_p\right)$$

Extension to the k-direction and to other momentum equations is straightforward.

Note that the balance $\Delta V_p = 0.5\left(\Delta V_{i,j} + \Delta V_{i+1,j}\right)$ is guaranteed in cylindrical coordinates only when the radial direction grid is uniform.

Algorithm Changes

1. All the convection terms were changed as per the above formulas.
2. Rearranged the algorithm to do calculations in the following order:
    a. All physical properties, other than reaction rates and densities
    b. Velocity star
    c. Density and reaction rates
    d. Solids volume fractions
    e. Correct solids velocity
    f. Fluid volume fraction
    g. Solids pressure
    h. Face values of densities. (Store rho_g face values used for pressure correction and use it afterward to calculate the fluxes with corrected velocities.)
    i. Fluid pressure correction
    j. Correct fluid pressure
    k. Correct fluid velocity (Do not correct solids velocities.)
    l. Update fluid density (Do not recompute the face densities.)
    m. Face values of mass fluxes
    n. All scalar transport equations
3. Changed density and reaction rate averaging procedure in the u-momentum source routines (source_u_g and source_u_s). This is required only because of the peculiarity of cylindrical coordinates. No changes are required in the other momentum source routines.
4. Included under-relaxation factor for pressure in the term accounting for mild compressibility in the pressure correction equation (i.e., $\left(\frac{\partial \rho_0}{\partial P_g}\right)^* P_g'$).
5. Commented out the adjustment for compressibility in the convection terms (source_pp_g). This may deteriorate the convergence of high speed flows.

Also the velocity calculation routine was changed so as to eliminate the effect – quite likely small – of the order in which the velocity components are calculated; e.g., the updated u-component is not used for solving the v-component until the next iteration.