Positivity preserving mixed derivative diffusion

Luke Western

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This document explains the approach and rationale for the positivity-preserving mixed derivative diffusion scheme used in MALTA.

One of the difficulties of 2D modelling of diffusion in Cartesian coordinates is handling of the mixed-derivative diffusion terms. Central difference Eulerian schemes preserve a positive mole fraction field when diffusion is in the horizontal or vertical directions, i.e., that forced by the diagonal components of the diffusion tensor D_{yy} and D_{zz} in the budget equation,

$$\nabla \cdot (\mathbf{D} \cdot \nabla \bar{q}). \tag{1}$$

Central differencing when working with the mixed derivative term, e.g.,

$$D_{yz} \frac{\partial^2 q}{\partial y \partial z} \tag{2}$$

generally gives negative values (a symmetric positive in one diagonal and equally negative in the other diagonal). Instead another method has to be found.

In MALTA, we choose to use the approach proposed by du Toit et al. [1] who use a positivity preserving advection scheme to make an advective-like diffusion field. This is an approximate scheme but seems to be the most physically accurate 2D scheme available, considering computational expense.

The rationale of the du Toit et al. scheme is as follows. For a single mixed-derivate diffusion term, we can write,

$$D_{yz} \frac{\partial^2 q}{\partial y \partial z} = D_{yz} \frac{\partial}{\partial y} (v \cdot q) \text{ where } v = \frac{1}{q} \frac{\partial}{\partial z}. \tag{3}$$

Using Picard linearisation we assume that if dt is small then

$$\frac{1}{q^n} \frac{\partial q^n}{\partial z} \approx \frac{1}{q^{n+1}} \frac{\partial q^{n+1}}{\partial z}, \tag{4}$$

which means that we can use v^n (from the previous timestep) to approximate v^{n+1} (the current time step). This means that in

$$D_{yz} \frac{\partial}{\partial y} vq = D_{yz} v \frac{\partial}{\partial y} q \tag{5}$$

as the v is effectively constant.

We can calculate v using central differencing and define a new parameter

$$v_{\text{diff}} = D_{yz} v, \tag{6}$$

which is interpolated on to a suitable grid structure for a positivity-preserving advection scheme. Following this we end up with

$$D_{yz} \frac{\partial^2 q}{\partial y \partial z} = v_{\text{diff}} \frac{\partial q}{\partial y}, \tag{7}$$

which takes the form of standard advection. This can be similarly applies in the other off-diagonal,

$$D_{zy} \frac{\partial^2 q}{\partial z \partial y} = w_{\text{diff}} \frac{\partial q}{\partial z}, \tag{8}$$

and thus the mixed-derivative diffusion is solved using a suitable advection scheme.

References

[1] du Toit, E., O'Brien, M., & Vann, R. (2018). Positivity-preserving scheme for two-dimensional advection–diffusion equations including mixed derivatives. Computer Physics Communications, 228, 61–68. https://doi.org/10.1016/j.cpc.2018.03.004