Interface Tracking Capabilities of the Inter-Gamma Differencing Scheme

H. Jasak and H.G. Weller
Department of Mechanical Engineering
Imperial College of Science, Technology and Medicine
London

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Abstract

The purpose of this paper is to describe a new method of convection discretisation specifically developed for interface tracking problems. The discretisation scheme is based on the NVD-diagram with the special attention to the compressive characteristics required for interface tracking. The limitation on the maximum Courant number has been discussed. Two test cases have been selected to illustrate the behaviour of the scheme in one and two spatial dimensions.

1 Introduction

The interface tracking problem in computational fluid dynamics represents a very interesting area of research. The equation that needs to be solved is the Iconal equation 1:

$$\frac{\partial \psi}{\partial t} + \mathbf{U}.\nabla\psi = S|\nabla\psi| \tag{1}$$

where ψ is the scalar field which describes the interface, $\mathbf{U}$ is the convective velocity and S is the propagation speed of the interface itself.

This equation can be modified in order to recognise the fact that the interface moves with the interface velocity which consists of the convective velocity and the propagation velocity of the interface itself (normal to the interface). The interface velocity $\mathbf{U}_T$ is defined according to 2.

$$\mathbf{U}_T = \mathbf{U} + S\hat{\mathbf{n}} \tag{2}$$

The interface unit normal $\hat{\mathbf{n}}$ can be calculated from the ψ field as:

$$\hat{\mathbf{n}} = \frac{\nabla\psi}{|\nabla\psi|} \tag{3}$$

The equation 1 can now be rewritten as

$$\frac{\partial\psi}{\partial t} + \mathbf{U}_T.\nabla\psi = 0 \tag{4}$$

From the form of the equation 4 it can be said that ψ is a bounded and non-conservative property. Examples for such a property could be the indicator function (taking only values of 0 or 1), void fraction in two-phase flows or regress variable in combustion.

The boundedness of ψ should be also preserved in the discretised form of the equation 4. If the value of ψ exceeds its natural bounds it is usually impossible to continue the calculation.

Problems with the discretisation of the modified form of the Iconal equation 4 could be summarised as follows:

- the discretisation practice should not “diffuse” the resolution of the interface,
- it is essential to preserve boundedness of ψ.

The results obtained by tracking the interface with the discretisation scheme with no numerical diffusion are not satisfactory. Spurious oscillations in the vicinity of the interface violate the bounds on ψ and the solution is unacceptable. The boundedness of ψ is not preserved.

2 Alternative Treatment of Numerical Diffusion Problem

From the discussion in the previous section one could conclude that it is more important to preserve the boundedness of ψ than to insist on very sharp resolution of the interface. This enables us at least to continue the calculation. If a procedure for “reconstruction” of the sharpness of the interface could be devised, both objectives could be satisfied simultaneously.

The basic interface-tracking procedure that could be considered a basis for this analysis is the explicit VOF method [1]. This method is based on donor-acceptor cell arrangement and can get quite complicated in multi-dimensional non-orthogonal meshes. The main disadvantage of this method is that it tries to align the interface with the mesh lines.

The analysis of the VOF method can pinpoint the reason for this alignment: the method can be described as the simple combination of upwind and downwind differencing. This enables it to preserve both boundedness of ψ and sharpness of the interface. On the other hand, upwind and downwind differencing are strongly dependent on the directionality of the grid and will always try to align the solution with it.

One of the possible modifications of the method would be to introduce a scheme which is not based purely on upwind and downwind differencing but can also take into account differences in the "sharpness" of the profile. This might sound completely unnecessary if one thinks about the form of the expected solution of the equation 4 (sharp interface). On the other hand, one has got to have in mind that the interface is not necessarily aligned with the mesh, resulting in a finite gradient over the interface (as a consequence of the discrete nature of the solution on the computational grid).

2.1 Boundedness Criterion - NVD Diagram

The basis for the development of the new differencing scheme is the Normalised Variable diagram.

Leonard [2] and Gaskell and Lau [3] show that the boundedness criterion for convection differencing schemes could be defined in the NVD diagram, showing $\widetilde{\phi}_f$ as a function of $\widetilde{\phi}_C$ as the shaded region in fig. 1, or with the following conditions:

- for $0 < \widetilde{\phi}_C < 1$, $\widetilde{\phi}_C$ is bounded below by the function $\widetilde{\phi}_f = \widetilde{\phi}_C$ and above by unity, and passes through the points (0,0) and (1,1),
- for $\widetilde{\phi}_C < 0$ and $\widetilde{\phi}_C > 1$ $\widetilde{\phi}_f$ is equal to $\widetilde{\phi}_C$.

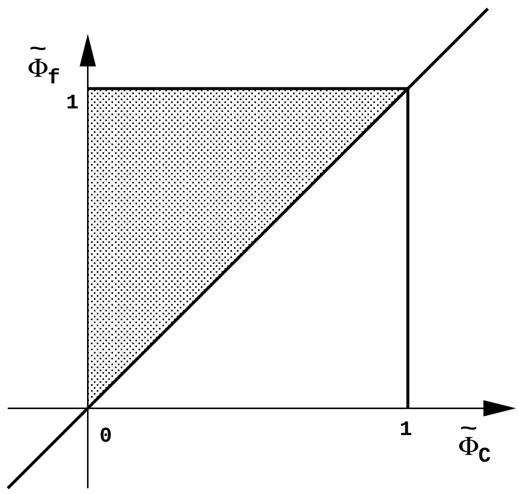

Figure 1: Boundedness criterion in NVD diagram

3 Inter-Gamma Differencing Scheme

From the NVD-diagram (fig.1), it could be seen that the choice of the differencing practice is more or less free for $0 < \widetilde{\phi}_C < 1$. This is where the actual behaviour of the scheme is determined.

The proposed differencing scheme is described by:

- for $\widetilde{\phi}_C < 0$, $\widetilde{\phi}_C > 1 \Rightarrow \widetilde{\phi}_f = \widetilde{\phi}_C$ to obey the NVD-criterion
- for $\frac{1}{2} < \widetilde{\phi}_C < 1 \Rightarrow \widetilde{\phi}_f = 1$ to ensure the compressive behaviour of the scheme.
- for $0 < \widetilde{\phi}_C < \frac{1}{2}$ the change in $\widetilde{\phi}_f$ will be similar the the change proposed in the Gamma differencing scheme. The objective is to create a smooth change from upwind to downwind differencing over this range of $\widetilde{\phi}_C$. In other words, blending factor γ is changing in the following way:
  - $\widetilde{\phi}_C = 0 \Rightarrow \gamma = 0$ (Upwind differencing),
  - $\widetilde{\phi}_C = \frac{1}{2} \Rightarrow \gamma = 2$ (Downwind differencing),

  or in terms of $\widetilde{\phi}_f$:

$$\widetilde{\phi}_f = -2\widetilde{\phi}_C^2 + 3\widetilde{\phi}_C \tag{5}$$

The new differencing scheme is shown in NVD-diagram in fig. 2.

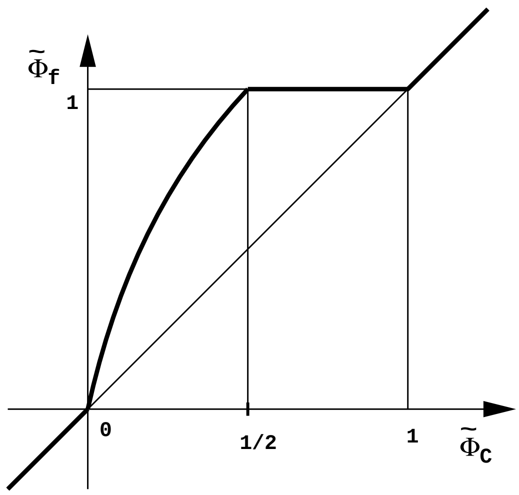

Figure 2: Inter-Gamma in NVD diagram

This scheme is expected to preserve boundedness of ψ and to give a reasonably sharp resolution of the interface. The explanation of the expected behaviour of the scheme can be divided into two parts:

- in order to preserve boundedness, a certain amount of numerical diffusion is introduced. The experience with other differencing schemes shows that this is inevitable. This will naturally smear the resolution of the interface.
- in order to reconstruct the sharp interface, downwind differencing is used.

The special treatment of "smooth" profiles in the differencing scheme is expected to cure the problems of alignment of the solution (interface) with the mesh lines.

At this point it is necessary to explain how and why the use of downwind differencing influences the resolution of the sharp interface.

The use of upwind differencing on the convection term of the equation 4 will effectively introduce another term of the form $\nabla \bullet \Gamma_N \nabla \psi$ - obviously diffusion-like. This term (which is purely numerical) will smear the solution as if there exist an amount of "real" diffusion corresponding to numerical diffusion Γ_N.

On the other hand, downwind differencing will introduce a similar term but in this case the numerical diffusion Γ_N is going to be negative. That means that the problem that is actually being solved effectively includes an antidiffusion term. This results in sharpening of all the gradients in the solution.

One should have in mind that the negative numerical diffusion of downwind differencing will not "cancel out" with the positive numerical diffusion of upwind differencing. As it will be shown later both schemes in conjunction can still produce results that are quite satisfactory.

3.1 Courant Number Limit

When simple upwind or downwind differencing schemes are selected for discretisation of the convection term of 4, the fluxes on the faces of the control volume guarantee the the central coefficient will not be zero. In the case of central differencing on the uniform mesh this coefficient is exactly zero. The requirement on the Courant number for central differencing comes from the condition of the diagonal equalness of the matrix.

In the case of Inter-Gamma differencing scheme the situation is a bit more complicated: the choice between upwind and downwind differencing is not made just by checking the direction of the flux. The choice is actually made based both on the flux direction and the local shape of the solution. This means that the continuity criterion is not enough to guarantee the existence of the central coefficient. It often happens (say in 1D) that one of the faces of the control volume uses upwind and the other uses downwind differencing. The result is that the central coefficient from the convection discretisation comes out to be zero and the sum of the neighbouring coefficients is twice as much as in the case of central differencing.

It is easy to show that this results in the Courant number limit of $Co < \frac{1}{2}$ (compared with $Co < 1$ for central differencing). In multidimensions the situation gets even more severe and it is usually necessary to keep the Courant number to be less than $\frac{1}{3}$. At the same time one should have in mind that the lower Courant number results in a better conditioned matrix, less smearing and better temporal accuracy.

Having in mind the existing Courant number limit, it might be interesting to consider the use of Inter-Gamma differencing scheme in the explicit mode. In this paper the possibility of explicit evaluation has been neglected because of the possible problems with operator splitting on arbitrary unstructured meshes.

4 Test Cases

Two test cases have been selected:

- 1-D transport of the step profile
- transport of a sine-shaped interface 30 degrees skew to the mesh

4.1 1-D Transport of the Step Profile

The test setup is a simple transport the step profile through one-dimensional duct by the prescribed velocity field. The result is shown in fig. 3.

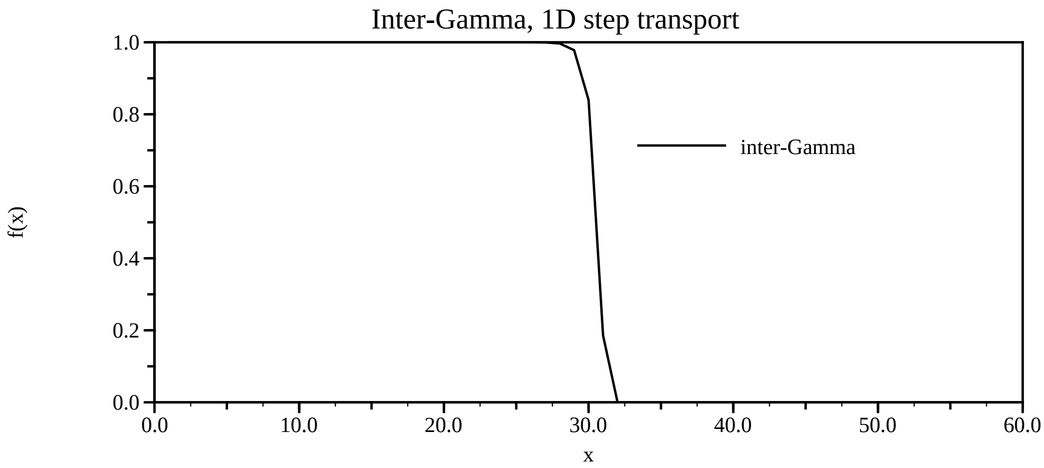

Figure 3: 1-D test step profile transport

From the raw data it can be seen that the resolution of the interface is smeared over only two cells, which is considered acceptable.

4.2 Transport of a Sine-shaped Interface

This test case has been selected to test the behaviour of the scheme in more realistic circumstances: transport of a curved surface through the mesh with the velocity field which is not aligned with the mesh.

The purpose of this test is to see whether the smearing of the profile gets unacceptably large after it has been transported about 30 cell sizes from its initial position. The ideal surface tracking scheme should show no smearing whatsoever, irrespective of how far the interface has been transported.

The setup of the test case is shown in fig. 5 together with the initial field of ψ in fig. 6. The consecutive positions of the interface are shown in figs. 7 to 10.

The smearing of the interface unfortunately still exists but it is not as severe as in the case of some other high resolution schemes. It should be noted that the problem of alignment between the interface and the mesh lines is much less obvious than in the case of the VOF method.

In order to illustrate the problem, a similar test has been performed with a larger Courant number (Co = 0.3). The result is presented in fig 4.

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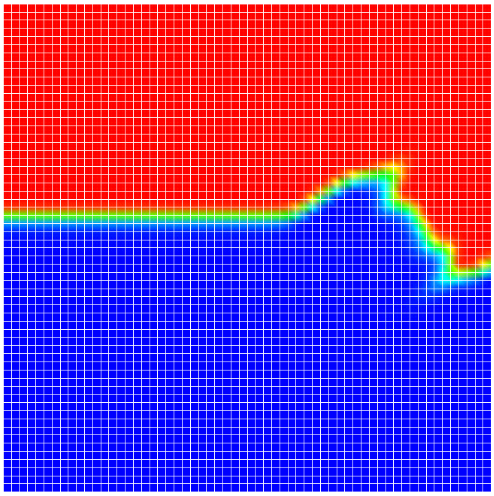

Figure 4: Problem of alignment of interface with grid lines

The problem of interface to grid alignment can now be clearly seen. Unfortunately, the only obvious solution to the problem at this stage is to decrease the Courant number. One should have in mind that this will not eliminate the problem completely, but only postpone it.

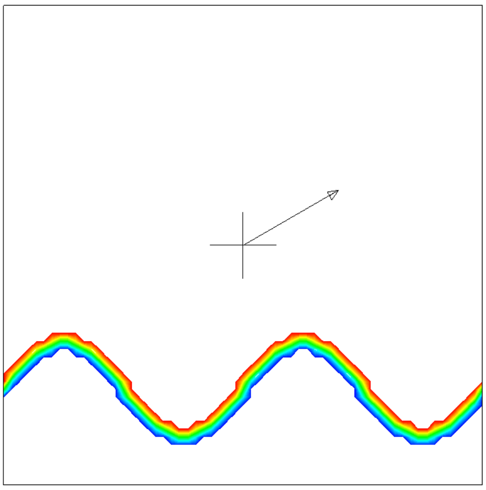

Figure 5: Test case setup

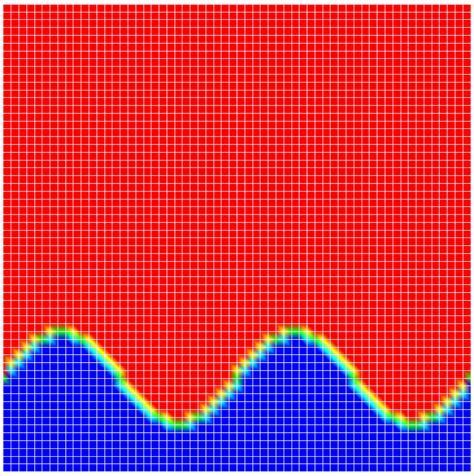

Figure 6: Initial field

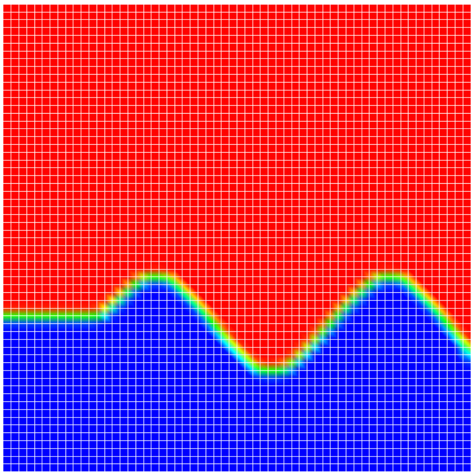

Figure 7: Moving interface i

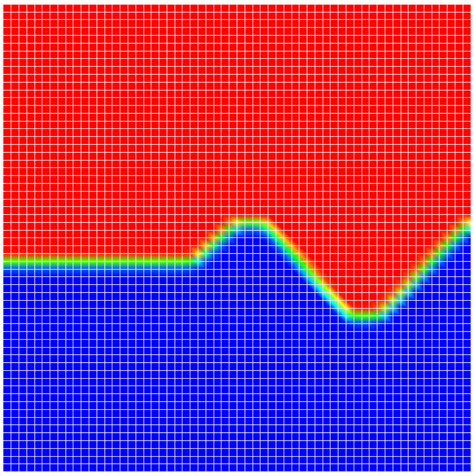

Figure 8: Moving interface ii

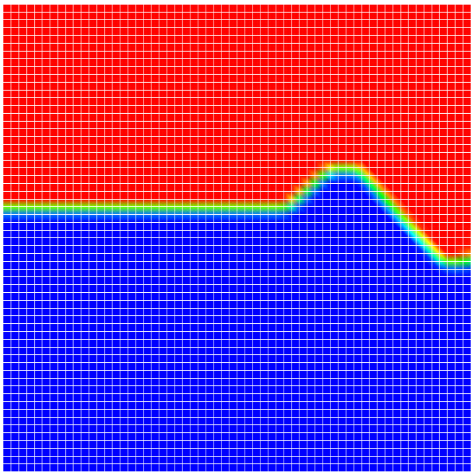

Figure 9: Moving interface iii

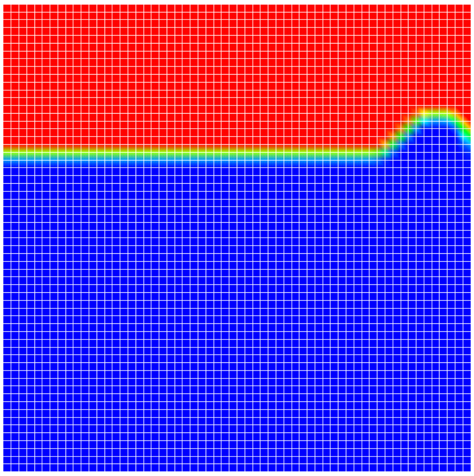

Figure 10: Moving interface iv

5 Conclusion

A simple discretisation practice enabling the tracking of an interface with an Eulerian approach has been presented. The main objective in the development of the new convection differencing scheme proposed in this paper was to keep the boundedness property of the variable ψ and at the same time to try to get as good resolution of step profiles as possible. The new differencing scheme is based on the NVD-approach and it has been made compressive by the use of downwind differencing. It is applicable in multidimensions and on arbitrary unstructured meshes.

The main disadvantage of the proposed differencing scheme is a severe Courant number limit. This is a consequence of the compressive character of the scheme and cannot be overcome easily. Having in mind that the expected use of this differencing scheme is the tracking of the interface (transient problem) the temporal accuracy is usually the one dictating maximum Courant numbers of about 0.2.

The explicit version of the proposed discretisation scheme is yet to be tested.

References

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[3] Gaskell, P.H. and Lau, A.K.C.: "Curvature-compensated convective transport: SMART, a new boundedness-preserving transport algorithm", *Int. J. Num. Meth. Fluids*, 8:617–641, 1988.