The $\chi$–Schemes: A New Consistent High-Resolution Formulation Based on the Normalized Variable Methodology

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Abstract

This paper deals with the formulation and testing of a new class of consistent High-Resolution (HR) schemes, denoted as the $\chi$-schemes. These schemes, combine consistency, accuracy and boundedness across systems of equations and are suitable for use in the simulation of multi-phase and multi-component flows. The consistency feature refers to the capability of these schemes to implicitly satisfy the additional algebraic constraint representing a global conservation relation governing certain sets of equations (e.g., species mass fraction, volume fraction, etc.). Four $\chi$–schemes are implemented within an unstructured grid finite-volume framework, tested by solving four multi-component pure-advection test problems, and shown to be consistent.

Keywords: Advection schemes, High Resolution, Consistent, Multi-Component, Multiphase.
A new Consistent High Resolution Formulation

**Nomenclature**

- \( c \): mass fraction of a specie.
- \( F \): neighbouring control volume nodes.
- \( f() \): functional relationship.
- \( g \): geometric factor.
- \( P \): node at control volume centre.
- \( r \): position vector.
- \( S \): surface area of control volume face or source term.
- \( u, v \): velocity components in the x- and y- directions.
- \( v \): velocity vector.

**Greek Symbols**

- \( \alpha \): refers to species or volume fractions.
- \( \Delta \): measure of inconsistency.
- \( \Gamma \): diffusion.
- \( \chi \): consistency factor.
- \( \phi \): general dependent variable.
- \( \rho \): density.

**Superscripts**

- \( \tilde{} \): refers to normalized variable.
- \( HO \): refers to High Order value.
- \( HR \): refers to High Resolution value.
Subscripts

C  central grid node.
D  downstream grid node.
E  east neighbouring node
EE east neighbouring node of the east node with respect to the P node
f  refers to control volume faces.
F  refers to neighbours of P grid node.
N  North neighbouring node
nb refers to neighbouring faces
NB refers to neighbouring nodes.
P  main grid node
S  south neighbouring node
U  upstream grid node.
W  west neighbouring node
WW west neighbouring node of the west node with respect to the P node
\( \alpha \) refers to species.
Introduction

Interest in the simulation of multi-fluid and multi-component systems has sharply increased over the last decade, partly due to the maturity of computational Fluid Dynamics (CFD) as a numerical technique and also because of the exponential increase in microprocessor power and the associated decrease in unit cost. Multiprocessor systems with large memory, set up at a fraction of the cost of the super-computers of a decade ago, have pushed the limits on the size and complexity of the problems that can be tackled [1,2]. On the numerical side, many of the developments in the simulation of single fluid flows [3-5] can readily be used in the simulation of multi-fluid and/or multi-component systems. For optimal performance however, some of these techniques need to be modified [6]. High Resolution (HR) schemes [7-10] represent one of the areas where adjustment is required for optimal performance in the simulation of such systems. High Resolution schemes are generally derived by enforcing a Boundedness criterion, such as the Convection Boundedness Criterion (CBC) [11] or the Total Variation Diminishing (TVD) [12,13], on a base High-Order (HO) scheme. This procedure transforms the linear but unbounded high-order scheme into a bounded but non-linear high-resolution scheme. The non-linearity results from the dependence of the Boundedness criterion on the local solution field.

When dealing with multi-component or multi-fluid system of equations, the transport conservation equations (species mass fraction and volume fraction equations) describing the behaviour of the system are implicitly coupled by an algebraic equation representing a global conservation relation; the algebraic relation represents the conservation of mass for multi-component systems and the conservation of volume for multi-fluid systems. If this algebraic relation is properly accounted for in the
discretization process the solution of the individual equations can be guaranteed to satisfy
global conservation across the whole computational domain, i.e. at control volume centres
and all control volume faces, in which case the discretization scheme is said to be **consistent**. When using the first order upwind scheme or indeed any high order
advection scheme this property, consistency, is inherently satisfied. Taking a multi-
component species system as an example: the global mass conservation translates into the
following relationship (the sum of all mass fractions, \( C_\alpha \), for the different species is 1):

\[
\sum_{\alpha=\text{all species}} C_\alpha = 1 \quad (1)
\]

When considering the discretization of the advection term using the first order
upwind scheme, the mass fraction at face ‘f’ of the control volume ‘P’ can be written as:

\[
C_{(\alpha),f} = \begin{cases} 
C_{(\alpha),P} & U_f \geq 0 \\
C_{(\alpha),F} & U_f < 0 
\end{cases} \quad (2)
\]

where \( U_f = v_f \cdot s_f \) is the velocity flux through face f. Summing the mass fractions over
all the species equations over face f, it is found that the conservation relation is satisfied:

\[
\sum_{\alpha=\text{species}} C_{(\alpha),f} = \begin{cases} 
\sum_{\alpha=\text{species}} C_{(\alpha),P} = 1 \quad \text{for } U_f \geq 0 \\
\sum_{\alpha=\text{species}} C_{(\alpha),F} = 1 \quad \text{for } U_f < 0 
\end{cases} \quad (3)
\]

Similarly when using the central difference scheme for the discretization of the advection
term, the mass fraction for any species at face f is given by:

\[
C_{(\alpha),f} = \frac{1}{2} C_{(\alpha),P} + \frac{1}{2} C_{(\alpha),F} \quad (4)
\]

Summing over all species at that face one gets:

\[
\sum_{\alpha=\text{species}} C_{(\alpha),f} = \sum_{\alpha=\text{species}} \left( \frac{1}{2} C_{(\alpha),P} + \frac{1}{2} C_{(\alpha),F} \right) = 1 \quad (5)
\]

where P and F denote the nodes straddling the face f (see figure 1(a)). Equation (5)
clearly obeys the global mass fractions conservation relation.
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Indeed as long as the advection coefficients of the mass fraction equations are constant (i.e. only geometry dependent) and sum to 1, for all species then any conservation relation enforced over the mass fraction equations at the centre of a control volume will be enforced for the interpolated face values of that control volume.

In general, for third and second high order scheme, the interpolated face value can be written in the form:

\[
C_{(a),f} = f(C_{(a),WW}, C_{(a),W}, C_{(a),P}, C_{(a),E}, C_{(a),EE})
\]

\[
= g_{WW} C_{(a),WW} + g_{W} C_{(a),W} + g_{P} C_{(a),P} + g_{E} C_{(a),E} + g_{EE} C_{(a),EE}
\]

(6)

Note that the discretization factor \(g\) is a pure geometric factor that is scheme dependent but not species dependent, and that for a finite volume discretization we have \(\sum g_N = 1\).

For higher order schemes the stencil becomes larger, but the relation remains linear. Thus at any interface, the conservation property is satisfied as long as values at the control volume centre satisfy the conservation property, which in turn yields new control volume values that again satisfy the conservation property. These schemes are said to be *consistent* i.e. they satisfy the *consistency* property.

Because high order schemes generates over/under shots and oscillatory behaviour in the presence of steep gradients [14], their use is not practical in the simulation of multi-fluid and multi-component systems: under/overshoots would yield either negative mass or volume fractions, or mass or volume fractions larger than one. High Resolution (HR) schemes are designed so as not to generate unphysical over/undershoots, but on the other hand suffer from inconsistency, paradoxically, a side effect of the current methods of enforcing the monotonicity criterion.

In this paper a new class of **consistent** High Resolution schemes is presented. This class of schemes, denoted by \(\chi\)–scheme (\(\chi\) is the Greek equivalent of c), combines consistency, accuracy and boundedness across systems of equations. The new consistent formulation
A new Consistent High Resolution Formulation is based on a modified form of the Normalized Variable Formulation (NVF) of Leonard [15], hence providing a simple and elegant framework for its development. In what follows, the construction of HR schemes using the NVF is briefly reviewed and shown to be non-consistent. Then, the $\chi-$schemes formulation is detailed, and four HR schemes (the SMART scheme of Gaskel and Lau [7], the MUSCL scheme of van Leer [16] based on Fromm’s scheme [17], the Osher scheme [18], and the Gamma scheme of Jasak et al. [19]) are reformulated as $\chi-$schemes, gaining consistency in the process. Finally the four schemes in their original and consistent form are tested in four pure advection problems.

The Normalized Variable Formulation

In the NVF of Leonard [15], the local variables are transformed into normalized variables defined by:

$$\tilde{\phi} = \frac{\phi - \phi_U}{\phi_D - \phi_U}$$  \hspace{1cm} (7)

Where $\phi_D$ is the downwind value, $\phi_C$ is the upstream value and $\phi_U$ is the far upstream value (Fig. 1(b)), note that with this normalization $\tilde{\phi}_D = 1$ and $\tilde{\phi}_U = 0$. The use of the normalized variable simplifies the definition of the functional relationships of HR schemes and is helpful in defining the conditions that the functional relationships should satisfy in order to have the property of boundedness and stability.

For example, the functional relationship for the “Quadratic Upstream Interpolation for Convection Kinematic” (QUICK) [11] scheme for steady flow is given by:

$$\phi_t = f(\phi_U, \phi_C, \phi_D) = \frac{1}{2}(\phi_C + \phi_D) - \frac{1}{8}(\phi_D - 2\phi_C + \phi_U) = \frac{3}{8}\phi_D + \frac{3}{4}\phi_C - \frac{1}{8}\phi_U$$  \hspace{1cm} (8)

Using Equation (7) and normalizing the variable in Equation (9), we get:
A number of schemes written using the NVF are given in Table 1. Note that the functional relationships for these schemes are all linear functions of $\tilde{\phi}_c$.

The functional relationship of any scheme can be plotted on a Normalized Variable Diagram (NVD), i.e., by plotting $\tilde{\phi}_j$ vs. $\tilde{\phi}_c$. Figure 2(a) shows the normalized variable diagram (NVD) for the schemes of Table 1. The NVD is an effective tool for assessing the accuracy and relative diffusivity of schemes. For example, Leonard [12] has shown that any scheme that has a functional relationship passing through point 'Q' in Fig. 2(a) is at least second order accurate, and if the slope at point 'Q' is equal to 0.75, then the scheme is third order accurate. Also schemes that have an NVD plot near the first order upwind NVD plot tend to be highly diffusive, while schemes whose NVD plot is near the first order downwind NVD plot (the line $\tilde{\phi}_j = 1$) tend to be highly compressive.

The Convective Boundedness Criterion (CBC)

The Convection Boundedness Criterion (CBC) for implicit steady state flow calculation was first explicitly formulated by Gaskell and Lau [7], based on the NVD introduced earlier by Leonard [11] and other implicit criteria implicit in reference [11]. The CBC states that for a scheme to have the boundedness property its functional relationship should be continuous, should be bounded from below by $\tilde{\phi}_j = \tilde{\phi}_c$ and from above by unity, should pass through the points (0,0) and (1,1) in the monotonic range ($0 < \tilde{\phi}_c < 1$), and for $1 < \tilde{\phi}_c$ or $\tilde{\phi}_c < 0$ the functional relationship $f(\tilde{\phi}_j)$ should be equal to $\tilde{\phi}_c$.

The above conditions illustrated in Fig. 2(b), can be formulated as:

$$\tilde{\phi}_j = f(\tilde{\phi}_c) = \frac{3}{8} + \frac{3}{4} \tilde{\phi}_c$$ (9)
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\[
\tilde{\phi}_r = \begin{cases} 
    f(\tilde{\phi}_C) & \text{continuous} \\
    f(\tilde{\phi}_C) = 1 & \tilde{\phi}_C = 1 \\
    f(\tilde{\phi}_C) < 0 & \tilde{\phi}_C < 1 \\
    f(\tilde{\phi}_C) = 0 & \tilde{\phi}_C = 0 \\
    f(\tilde{\phi}_C) = \tilde{\phi}_C & \tilde{\phi}_C < 0 \text{ or } \tilde{\phi}_C > 1 
\end{cases}
\]  

(10)

**NV Formulation of High-Resolution Schemes**

High Resolution schemes are derived by enforcing a boundedness criterion on HO schemes [7,20]. Starting with a base High-Order (HO) scheme, the CBC criterion is enforced by modifying the high order profile to fit within the advection boundedness region. Examples of HR schemes are shown in Fig. 3 for a number of base HO schemes.

For these HR schemes [15,21,22] the advection coefficients are non-linear as they are not based on geometric quantities, rather in order to enforce the (CBC), they become variable-dependent. In multi-fluid or multi-component systems, this implies that the various variables of the implicitly coupled equations will have unequal face coefficients. Thus the algebraic relation initially satisfied at the control volume centres by the cell values and/or cell averages is no more satisfied at the control volume faces, leading to an inconsistent solution at the control volume centres, again this is purely due to the inconsistent interpolation functions used by the different mass or volume fractions.

**The \( \chi \)-Schemes**

The new consistent formulation of non-linear HR schemes is based on the observation that the upwind scheme and all HO schemes are consistent. Thus, if the HR scheme at a control volume face is forced to share across the system of equations the same linear combination of high-order schemes then it will be consistent. In the \( \chi \) formulation, the value at a control volume face using a HR scheme is written as:
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\[ \tilde{\phi}_f^{HR} = \tilde{\phi}_c + \chi(\tilde{\phi}_f^{HO} - \tilde{\phi}_c) \quad (11) \]

It is clear that with this formulation, forcing all the related equations to share the same value of \( \chi \) at any control volume face can ensure consistency. What is equally important is to enforce the boundedness of the different schemes through the proper choice of the single \( \chi \) value at any face. Moreover, the above equation can be equally written in terms of the un-normalized variables i.e.

\[ \phi_f^{HR} = \phi_c + \chi(\phi_f^{HO} - \phi_c) \quad (12) \]

The dual formulation is very useful since a \( (\chi, \tilde{\phi}_c) \) diagram can be developed based on Eq. (11) while Eq. (12) could be used for implementation.

\( \chi \)-Scheme Formulation

The derivation of the different \( \chi \)-HR schemes starts by re-writing equation (11) in the following form:

\[ \chi = \frac{\tilde{\phi}_f^{HR} - \tilde{\phi}_c}{(\tilde{\phi}_f^{HO} - \tilde{\phi}_c)} \quad (13) \]

With this definition, the \( \chi \) forms of the OSHER, MUSCL, SMART, and GAMMA schemes will be as follows.

The \( \chi \)-OSHER Scheme

In the NVF the OSHER scheme is written as

\[ \tilde{\phi}_f = \begin{cases} 
\frac{3}{2} \tilde{\phi}_c & 0 < \tilde{\phi}_c < \frac{2}{3} \\
1 & \frac{2}{3} < \tilde{\phi}_c < 1 \\
\tilde{\phi}_c & \text{elsewhere}
\end{cases} \quad (14) \]

with the HO base scheme (the SOU scheme [23]) taking the form
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\[ \tilde{\phi}_f = \frac{3}{2} \tilde{\phi}_C \]  

(15)

The basic \( \chi \) formulation for the OSHER scheme is thus written as

\[ \chi = \frac{\tilde{\phi}_f^{HR} - \tilde{\phi}_C}{\frac{3}{2} \tilde{\phi}_C - \tilde{\phi}_C} = \frac{\tilde{\phi}_f - \tilde{\phi}_C}{\frac{1}{2} \tilde{\phi}_C} = 2\left(\frac{\tilde{\phi}_f^{HR} - \tilde{\phi}_C}{\tilde{\phi}_C}\right) \]  

(16)

This translates into the following relationships for \( \chi \)-OSHER:

\[
\begin{array}{c|c}
\chi & \\
\hline
1 & 0 < \tilde{\phi}_C < \frac{2}{3} \\
\frac{2(1 - \tilde{\phi}_C)}{\tilde{\phi}_C} & \frac{2}{3} < \tilde{\phi}_C < 1 \\
0 & \text{elsewhere}
\end{array}
\]  

(17)

The \( \chi \)-MUSCL Scheme

For the case of the MUSCL scheme, the base HO scheme is the Fromm scheme [14], which itself is formed from the arithmetic mean of the second order upwind (Eq. 15) and second order central differencing schemes (Eq. 26). The base HO scheme is written as

\[ \tilde{\phi}_f = \frac{1}{4} + \tilde{\phi}_C \]  

(18)

The expression for the base \( \chi \) emerges as

\[ \chi = \frac{\tilde{\phi}_f^{HR} - \tilde{\phi}_C}{\frac{1}{4} + \tilde{\phi}_C - \tilde{\phi}_C} = 4\left(\frac{\tilde{\phi}_f^{HR} - \tilde{\phi}_C}{\frac{1}{4} + \tilde{\phi}_C - \tilde{\phi}_C}\right) \]  

(19)

The NVF form of the MUSCL scheme is given by
The \( \tilde{\phi}_j \) formulation for the MUSCL scheme becomes

\[
\tilde{\phi}_j = \begin{cases} 
2\tilde{\phi}_c & 0 < \tilde{\phi}_c < \frac{1}{4} \\
\frac{1}{4} + \tilde{\phi}_c & \frac{1}{4} < \tilde{\phi}_c < \frac{3}{4} \\
1 & \frac{3}{4} < \tilde{\phi}_c < 1 \\
\tilde{\phi}_c & \text{elsewhere}
\end{cases}
\] (20)

The \( \chi \) formulation for the MUSCL scheme becomes

\[
\chi = \begin{cases} 
4\tilde{\phi}_c & 0 < \tilde{\phi}_c < \frac{1}{4} \\
1 & \frac{1}{4} < \tilde{\phi}_c < \frac{3}{4} \\
4(1 - \tilde{\phi}_c) & \frac{3}{4} < \tilde{\phi}_c < 1 \\
0 & \text{elsewhere}
\end{cases}
\] (21)

The \( \chi \)-SMART Scheme

The base scheme for SMART is the QUICK scheme of Leonard [11] and is given by:

\[
\tilde{\phi}_j = \frac{3}{8} + \frac{3}{4}\phi_c
\] (22)

Thus, the base \( \chi \)-SMART formulation is

\[
\chi = \frac{\tilde{\phi}_{j}^{HR} - \tilde{\phi}_c}{\left(\frac{3}{8} + \frac{3}{4}\phi_c - \tilde{\phi}_c\right)} = \frac{8(\tilde{\phi}_{j}^{HR} - \tilde{\phi}_c)}{\left(3-2\tilde{\phi}_c\right)}
\] (23)

Moreover, the NVF form of the SMART scheme is written as

\[
\tilde{\phi}_j = \begin{cases} 
3\tilde{\phi}_c & 0 < \tilde{\phi}_c < \frac{1}{6} \\
\frac{3}{8} + \frac{3}{4}\tilde{\phi}_c & \frac{1}{6} < \tilde{\phi}_c < \frac{5}{6} \\
1 & \frac{5}{6} < \tilde{\phi}_c < 1 \\
\tilde{\phi}_c & \text{elsewhere}
\end{cases}
\] (24)

The equivalent \( \chi \) formulation is
The \( \chi \)-GAMMA Scheme

The base scheme for GAMMA [19] is the second-order central difference scheme, which can be written as

\[
\tilde{\phi}_j = \frac{1}{2} + \frac{\tilde{\phi}_c}{2}
\]

(26)

Therefore the base \( \chi \)-GAMMA formulation is

\[
\chi = \frac{\tilde{\phi}_j^{HR} - \tilde{\phi}_c}{\left(\frac{1}{2} + \frac{1}{2} \tilde{\phi}_c - \tilde{\phi}_c\right)} = \frac{2(\tilde{\phi}_j^{HR} - \tilde{\phi}_c)}{(1 - \tilde{\phi}_c)}
\]

(27)

The GAMMA scheme in the NVF is written as

\[
\tilde{\phi}_j = \begin{cases} 
3\tilde{\phi}_c & 0 < \tilde{\phi}_c < \frac{1}{5} \\
\frac{1}{2} + \frac{1}{2} \tilde{\phi}_c & \frac{1}{5} < \tilde{\phi}_c < 1 \\
\tilde{\phi}_c & \text{elsewhere}
\end{cases}
\]

(28)

The equivalent \( \chi \) formulation is found to be

\[
\chi = \begin{cases} 
\frac{4\tilde{\phi}_c}{(1 - \tilde{\phi}_c)} & 0 < \tilde{\phi}_c < \frac{1}{5} \\
1 & \frac{1}{5} < \tilde{\phi}_c < 1 \\
0 & \text{elsewhere}
\end{cases}
\]

(29)
Similar to the NVD, the \( (\chi, \tilde{\phi}_C) \) relationships of the above schemes can be visualized on a \( \chi \)-NVD diagram as depicted in Fig. 3. Moreover, after computing the \( \chi \_f \) value along a control volume face, the interpolated \( \phi_f \) value is computed from Eq. (12).

**NVF for unstructured grids and gradient interpolation**

In the above formulation, the functional relationships of HR schemes were defined as functions of \( \tilde{\phi}_C \), the normalized upwind nodal value, Eq. (7). To compute \( \tilde{\phi}_C \), \( \phi_U \) is needed. In unstructured grids the node \( \phi_U \) is not naturally defined. However, following Jasak et al. [19], a virtual value can be reconstructed from the cell gradient given by

\[
\nabla \phi_C \cdot \mathbf{r}_{UD} = \phi_D - \phi_U
\]

(30)

By choosing the U node such that the C grid point is at the centre of the segment (UD), one can write

\[
\phi_U = \phi_D - \nabla \phi_C \cdot \mathbf{r}_{UD} = \phi_D - 2\nabla \phi_C \cdot \mathbf{r}_{CD}
\]

(31)

With this simple re-formulation, all NVF-based schemes can be used with unstructured grids.

In addition to \( \phi_U \), face gradients are needed for the diffusive fluxes in the solution process and are usually obtained by a weighted interpolation from the neighbouring cell gradients. This simple interpolation procedure leads to an extended stencil as shown in Fig. 4(a). A better method is to force the face gradient along the PF direction (F being the neighbour of P), Fig. 4(b), to be directly computed from the cell nodes in a manner similar to the Rhie-Chow interpolation [24] for pressure gradients. This was found to improve the accuracy and stability of HR schemes defined as functions of face gradients such as the SMART, GAMMA, and OSHER schemes. Thus the equation used in computing the gradient along a control volume face is:
\[
(\nabla \phi)_j = (\nabla \phi)_j + \left( \frac{\phi_F - \phi_P}{r_{PF}} \right) e_{PF} - (\nabla \phi)_j \cdot e_{PF} \]

(32)

where \((\nabla \phi)_j\) is the simple weighted gradient interpolated from the two adjacent cell values.

**Enforcing Consistency**

As mentioned earlier, any scheme formulated as a linear combination of HO schemes across the related equations would have the consistency property. As such, the only remaining condition in the \(\chi\) formulation for the resultant schemes to be consistent is to force all equations to share the same \(\chi\). It is obvious that forcing all related equations to share the same \(\chi\) can yield oscillations unless the value chosen is the minimum of all computed \(\chi\) values. Thus in this case the shared \(\chi\) value is computed as:

\[
\chi_{\text{shared}} = \text{MIN}(\chi_k) \quad k = 1..\text{Number of Related Equations}
\]

(33)

Two different but equally relevant routes can be pursued:

- In the first the \(\chi\) values are specified on faces i.e. they are face-based quantities shared across components and/or fluids
- In the second approach the \(\chi\) values are defined on cell centres. In this case in addition to being shared across components and fluids, the \(\chi\)'s are shared by the “upwinded” faces of the relevant cells.

In this work the face-based method is adopted, as it leads to a less diffusive schemes. From Eq. (12) it is obvious that the \(\phi_f^{\text{HR}}\) is the sum of the upwind value and an anti-diffusive part given by \(\chi(\phi_f^{\text{HO}} - \phi_C)\). Thus, the higher \(\chi\) is, the less diffusive the scheme will be. Since the minimum value of \(\chi\) is used at a control volume face, the resultant \(\chi\)-schemes will be a little more diffusive than their original NVF counterparts since lower
anti-diffusive correction will be added to the upwind value. This is the penalty paid in order to restore consistency. The effect of this newly suggested treatment on the quality of the solution is assessed by comparing profiles obtained using both the NVF and $\chi$ formulations and is shown to be tolerable.

**Results and Discussion**

The performance of the various $\chi$–schemes is assessed by presenting solutions to four pure advection problems. In these problems, two different types of profiles (step and sinusoidal, Figs. 5(a) and 5(b), respectively) and two different types of flow fields (oblique and rotational, Figs. 5(c) and 5(d), respectively) are used. Computations are performed using either three or four scalar variables, which may represent the mass or volume fractions of a multiphase/multi-component system. The computational domains along with the grid networks used are depicted in Figs. 5(e) and 5(f). Results generated are displayed in terms of maps showing the locations where inconsistency exists. In addition, profiles obtained employing both the NVF and $\chi$-NVF formulations are presented.

To measure the inconsistency two parameters are adopted in this work, the first defines the maximum inconsistency that occurs in any cell, this is denoted by:

$$\Delta_{I,cell} = \left(1 - \sum_{k=cell}^{\phi_k}\right) \quad k = \text{number of related scalars}$$

with the maximum value computed as

$$\Delta_{I,\text{max}} = \text{abs}\left(1 - \sum_{k=cell}^{\phi_k}\right) \quad k = \text{number of related scalars}$$

(34)

(35)
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The inconsistency, $\Delta t$, can be thought of as a measure of the over/undershoot across the system of equations (i.e. the global mass fraction or volume fraction conservation equation).

We also define the Global Consistency Measure (GCM) as

$$
GCM = \sum_{\text{cells}} \left( \frac{\text{vol}_{\text{cell}} \cdot \left( 1 - \sum_{k} \phi_{k}^{~} \right)}{\text{total \_ volume}} \right)
$$

$$
= \sum_{\text{cells}} \left( \frac{\text{vol}_{\text{cell}} \cdot \Delta_{t,\text{cell}}}{\text{total \_ volume}} \right)
$$

(36)

GCM for the different test problems is shown in table 2.

**Problem 1: Advection of Step Profiles in an oblique flow field**

In this test, three non-reactive scalars ($\phi_{1}$, $\phi_{2}$ and $\phi_{3}$) are convected in an oblique flow field, Fig. 5(e). The sum of these scalars at inlet is 1 and the initialized values of the scalars also sum to 1. The inlet profiles, shown in Figure 5(a), involve two double step profiles for $\phi_{1}$ and $\phi_{2}$, with the $\phi_{3}$ profile computed so that the sum of all three equals 1.

Mathematically this is represented as

$$
\begin{align*}
\phi_{1} &= \begin{cases} 
0.50 & 0 < x(y) < 0.4 \\
0 & \text{otherwise}
\end{cases} \\
\phi_{2} &= \begin{cases} 
0.25 & 0.2 < x(y) < 0.6 \\
0 & \text{otherwise}
\end{cases} \\
\phi_{3} &= 1 - (\phi_{1} + \phi_{2})
\end{align*}
$$

(37)

The physical domain and grid network used are presented in Figs. 5(c) and 5(e), respectively. The governing conservation equation for the kth scalar is given by:

$$
\nabla \cdot (\rho \nabla \phi_{k}) = 0
$$

(38)

The velocity field is oblique at 45° and its magnitude is 1. In order to assess the effect of using a shared $\chi$ on the accuracy of the schemes, the profiles of the convected scalars
obtained using the NV-SMART and $\chi$-SMART formulations are displayed in Fig. 6 along a diagonal that slices the domain from point $(1,0)$ to $(0,1)$. As expected, a sharper profile is obtained with the NVF formulation. However, the difference in accuracy between the two formulations is relatively small, and is accomplished in the case of the NV formulation at the expense of a substantial inconsistency (see Fig. 7).

Fig. 7 shows a plot of the discretized computational domain with cells having $\Delta > 0.0001$ clearly outlined. The numbers of cells not satisfying this requirement along with the maximum inconsistency are indicated directly below each figure. It is clear from the maps depicted in Fig. 7 that results obtained using the $\chi$ formulation do satisfy to a large extent the consistency criterion. The few cells with $\Delta$ larger than $10^{-4}$ are suspected to be caused by numerical round-offs in the computation of the gradients used in the HR schemes. The average number of cells for the four schemes where inconsistency occurs is 0.5 for the $\chi$-formulation as compared to 1180 for the NV-formulation. Moreover, the maximum average inconsistency is $9 \times 10^{-3}\%$ ($\pm 0$) for the $\chi$-schemes, whereas it is about 6% for the NVF schemes. The inconsistency obtained with the NVF schemes is detrimental when simulating multiphase/multi-component flow problems, as it destroys global conservation and causes divergence. This is even more so in the case when high-density ratios exist among the different components. An explicit ad-hoc treatment is usually adopted to enforce consistency at the expense of a lower convergence rate and additional algorithmic instability [6].

**Problem 2: Advection of Sinusoidal Profiles in an oblique flow field**

For this test, four scalar variables, $\phi_1$, $\phi_2$, $\phi_3$ and $\phi_4$, are used for which the inlet profiles are graphically shown in Fig. 5(b). Mathematically the profiles are given by:
\[
\left\{
\begin{array}{ll}
\phi_1 = & 0.5 \cos \left( \frac{\pi}{0.3} x \right) \quad \text{for } 0 < x < 0.3 \\
\phi_2 = & 0 \quad \text{otherwise}
\end{array}
\right.
\] 
\[
\left\{
\begin{array}{ll}
\phi_2 = & 0.25 \sin \left( \frac{\pi(x - 0.2)}{0.2} \right) \quad \text{for } 0.2 < x < 0.4 \\
\phi_3 = & 0 \quad \text{otherwise}
\end{array}
\right.
\] 
\[
\left\{
\begin{array}{ll}
\phi_3 = & 0.125 \sin \left( \frac{\pi(x - 0.1)}{0.4} \right) \quad \text{for } 0.1 < x < 0.5 \\
\phi_4 = & 0 \quad \text{otherwise}
\end{array}
\right.
\] 
\[
\phi_4 = 1 - \left( \phi_1 + \phi_2 + \phi_3 \right) \quad \text{for all } x
\] 

The physical domain, velocity field, grid network used, and governing equation for each scalar variable are the same as those of problem 1. Profiles generated using the \( \chi \)-SMART and NVF-SMART schemes are displayed in Fig. 8. Similar to profiles presented in Fig. 6, the \( \chi \)-SMART profiles are slightly more diffusive for the reasons stated earlier. Because of the constantly changing profiles, the NVF schemes show more inconsistency in comparison with the previous problem, as there is more opportunity for them to fall out of sync. This is clearly shown in Fig. 9, where the number of cells at which the schemes are inconsistent is higher than that in test 1. The \( \chi \) schemes on the other hand preserve consistency except at few cells, where numerical round-off errors are again suspected to be the cause. The average number of cells for the four schemes where inconsistency occurs is 1.5 for the \( \chi \)-formulation and 1646 for the NV-formulation. Moreover, the maximum average inconsistency is 2.275x10^{-2}\% (\approx 0) for the \( \chi \)-schemes whereas it is about 5.22\% for the NVF schemes. The value of the maximum inconsistency is slightly lower than that in test 1 due to the gradual variation in the profiles. In both tests 1 and 2 cells showing consistency with the NVF schemes are cells where the profiles of the respected scalars are not changing. At these locations, the CBC is automatically satisfied and is not explicitly enforced. In other words, in these areas the HR schemes behave basically as HO schemes. It is also worth noting that when only two scalars are varying the standard NVF formulation yields consistent results. This serendipitous behaviour is
due to the fact that for this special case $\tilde{\phi}_c$ is the same for both profiles. In terms of the $\chi$-formulation this means that the $\chi$ values for both profiles are equal. This explains the regions where consistency is satisfied for the NVF-schemes.

**Problem 3: Advection of square profiles in a rotational field**

The same inlet step profiles (Fig. 5(a)) of problem 1 are convected here in the presence of a rotational flow field. The velocity field is a Smith-Hutton [25] type rotational field from the inlet plane ($0<x<1$, $y=0$) to the outlet plane ($1<x<2$, $y=0$), for which the analytical solution is given by:

$$
\mathbf{v} = \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 2y(1-x^2) \\ -2x(1-y^2) \end{bmatrix}
$$

As detailed in [26], the use of the above equation to compute the convective fluxes yields a non-conservative velocity field. The reason for this behaviour is that equation (40) represents a point wise analytical solution, while a face-averaged (integrated) solution is needed for the discretized computational domain. Therefore, in order to satisfy continuity over each cell in the computational domain equation (38) is integrated over the cell faces to yield the following divergence-free velocity field [26]:

$$
\mathbf{v} = \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} \frac{1}{x_{n_2} - x_{n_1}} \left[ m(x_{n_2}^2 - x_{n_1}^2) + 2n(x_{n_2} - x_{n_1}) \right] - \frac{1}{2} m(x_{n_2}^4 - x_{n_1}^4) - \frac{2}{3} n(x_{n_2}^3 - x_{n_1}^3) \\ \frac{1}{x_{n_2} - x_{n_1}} \left[ -x_{n_2}^2 - x_{n_1}^2 \right] + n^2(x_{n_2}^2 - x_{n_1}^2) + \frac{1}{2} m^2(x_{n_2}^4 - x_{n_1}^4) - \frac{4}{3} mn(x_{n_2}^3 - x_{n_1}^3) \end{bmatrix}
$$

(41)

Where $m$ and $n$ define the slope and intercept of the equation passing through nodes $n_1$ and $n_2$, i.e. the cell face. Equation (41) could also be obtained as the difference of stream function values across the control volume face. In fact, streamfunction computation of face-average velocity components is ideal for a two-dimensional unstructured mesh.
Results for the problem displayed in Fig. 10 reveal once more that the NVF formulation produces inconsistent predictions in the simulation of multiphase/multi-component flow systems. As shown (Fig. 10), imbalance reaches a value as high as 10% with NVF-MUSCL. The $\chi$-schemes results, on the other hand, are nearly inconsistency free except over two control volumes in $\chi$-MUSCL and $\chi$-SMART where the maximum imbalance is 0.025%.

**Problem 4: Advection of sinusoidal profiles in a rotational field**

In this last test case, the sinusoidal profiles displayed in Fig. 5(b) are used for the same physical domain and rotational flow field of problem 3. The inconsistency maps presented in Fig. 11, show the same trend of results obtained earlier. The entire domain is flagged when using the NVF schemes (due to the continuously changing profiles) except the central circular region where the profiles of the various variables are not changing ($\phi_1 = \phi_2 = \phi_3 = 0$ and $\phi_4 = 1$). By contrast, the $\chi$-schemes results are consistent across the system of equations except at few locations with the maximum imbalance being less than 0.03463% as compared to a maximum value of 21.79% obtained with the NVF-OSHER scheme.

**Closing Remarks**

A new consistent reformulation of NVF-based High Resolution schemes was presented. The resultant $\chi$-schemes were shown to be inherently consistent across system of equations preserving global conservation, and as such suitable for use in the simulation of multi-phase and multi-component flows. Tests indicated that if the consistency property during the discretization process is not given adequate attention, unphysical results would be obtained over large areas of the computational domain. Consistency as defined in this
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work could be thought of as a boundedness criterion applied across a special system of equations where an implicit global conservation relation should be satisfied. The suppressed over/undershoots in this case are those values, whether positive or negative, that do not satisfy the conservation relation. A minor deficiency of this method is the slight increase in the numerical diffusion. A similar deficiency exits when enforcing boundedness at locations where physical extrema occur, resulting in a loss of the extrema in pure advection fields. Such behaviour has been minimized in some previous work of the authors [21], and similar techniques could be developed for the $\chi$-formulation.

**Acknowledgments**

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References

1. Shanley A. “CFD Comes of Age in the CPI industry, Chemical Engineering”, vol. 103, Issue 12, 1996


### Table 1: Functional Relationships for the different linear schemes.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Functional Relationship</th>
<th>Functional Relationship (NVF)</th>
</tr>
</thead>
<tbody>
<tr>
<td>First order upwinding</td>
<td>( \phi_f = \phi_C )</td>
<td>( \tilde{\phi}_f = \tilde{\phi}_C )</td>
</tr>
<tr>
<td>Second order upwinding</td>
<td>( \phi_f = \frac{3\phi_C - \phi_U}{2} )</td>
<td>( \tilde{\phi}_f = \frac{3}{2}\tilde{\phi}_C )</td>
</tr>
<tr>
<td>Second order central</td>
<td>( \phi_f = \frac{\phi_D + \phi_C}{2} )</td>
<td>( \tilde{\phi}_f = \frac{1 + \tilde{\phi}_C}{2} )</td>
</tr>
<tr>
<td>Fromm’s method</td>
<td>( \phi_f = \phi_C + \frac{\phi_D - \phi_U}{4} )</td>
<td>( \tilde{\phi}_f = \frac{1 + \tilde{\phi}_C}{4} )</td>
</tr>
<tr>
<td>QUICK</td>
<td>( \phi_f = \frac{\phi_C + \phi_D}{2} - \frac{\phi_D - 2\phi_C + \phi_U}{8} )</td>
<td>( \tilde{\phi}_f = \frac{3}{8} + \frac{3}{4}\tilde{\phi}_C )</td>
</tr>
</tbody>
</table>
Table 2: Consistency Index for the various test problems.

<table>
<thead>
<tr>
<th></th>
<th>MUSCL</th>
<th>Osher</th>
<th>GAMMA</th>
<th>SMART</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\chi$</td>
<td></td>
<td>$\chi$</td>
<td></td>
</tr>
<tr>
<td>Test 1</td>
<td>0.89x10$^6$</td>
<td>3.7x10$^6$</td>
<td>1.85x10$^6$</td>
<td>1.32x10$^6$</td>
</tr>
<tr>
<td></td>
<td>6.2x10$^{-3}$</td>
<td>4.4x10$^{-3}$</td>
<td>4.8x10$^{-3}$</td>
<td>4.6x10$^{-3}$</td>
</tr>
<tr>
<td>Test 2</td>
<td>0.76x10$^6$</td>
<td>2.5x10$^6$</td>
<td>0.69x10$^6$</td>
<td>1.96x10$^6$</td>
</tr>
<tr>
<td></td>
<td>6.1x10$^{-3}$</td>
<td>6.1x10$^{-3}$</td>
<td>6.2x10$^{-3}$</td>
<td>6.5x10$^{-3}$</td>
</tr>
<tr>
<td>Test 3</td>
<td>0.57x10$^6$</td>
<td>1.7x10$^6$</td>
<td>0.76x10$^6$</td>
<td>0.88x10$^6$</td>
</tr>
<tr>
<td></td>
<td>7.0x10$^{-3}$</td>
<td>11.0x10$^{-3}$</td>
<td>6.7x10$^{-3}$</td>
<td>7.7x10$^{-3}$</td>
</tr>
<tr>
<td>Test 4</td>
<td>3.80x10$^6$</td>
<td>5.5x10$^6$</td>
<td>1.8x10$^{-6}$</td>
<td>2.4x10$^{-6}$</td>
</tr>
<tr>
<td></td>
<td>10.5x10$^{-3}$</td>
<td>15.2x10$^{-3}$</td>
<td>8.7x10$^{-3}$</td>
<td>13.7x10$^{-3}$</td>
</tr>
</tbody>
</table>
**Figure Captions**

Figure 1: (a) unstructured grid and advection node notation; (b) virtual Upwind node

Figure 2: (a) NVD representation of High Order schemes; (b) Advection Boundedness Criteria.

Figure 3: High-Resolution schemes in the NV and $\chi$–NV Diagrams.

Figure 4: (a) extended stencil for face gradient, and (b) compact stencil for face gradient.

Figure 5: (a) Square profiles for 3 species; (b) sinusoidal profiles for 4 species; (c) physical domain and flow field for tests 1 and 2; (d) physical domain and flow field for tests 3 and 4; (e) grid used for tests 1 and 2; (f) grid used for tests 3 and 4.

Figure 6: Comparison of square profiles obtained using NVF-SMART and $\chi$-SMART schemes.

Figure 7: Inconsistency maps for square profiles in an oblique flow field (sum of 3 species > 1.0001 or < 0.9999).

Figure 8: Comparison of sinusoidal profiles obtained using NVF-SMART and $\chi$-SMART schemes.

Figure 9: Inconsistency maps for sinusoidal profiles in an oblique flow field (sum of 4 species > 1.0001 or < 0.9999).

Figure 10: Inconsistency maps for square profiles in a rotational flow field (sum of 3 species > 1.0001 or < 0.9999).

Figure 11: Inconsistency maps for sinusoidal profiles in a rotational flow field (sum of 4 species > 1.0001 or < 0.9999).
Figure 1
Figure 2

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Figure 3
Figure 5
Figure 6
χ−MUSCL, # cells = 0; $\Delta_{\text{max}} = 0.000077$

χ−OSHER, # cells = 2; $\Delta_{\text{max}} = 0.00024$

χ−GAMMA, # cells = 0; $\Delta_{\text{max}} = 0.00008$

χ−SMART, # cells = 1; $\Delta_{\text{max}} = 0.000156$

NVF-MUSCL, # cells = 1239; $\Delta_{\text{max}} = 0.0525$

NVF-OSHER, # cells = 1322; $\Delta_{\text{max}} = 0.0531$

NVF-GAMMA, # cells = 1165; $\Delta_{\text{max}} = 0.0674$

NVF-SMART, # cells = 1089; $\Delta_{\text{max}} = 0.0595$

Figure 7
Figure 8
Darwish and Moukalled

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χ−MUSCL, # cells = 1; Δ_{max} = 0.000109

NVF-MUSCL, # cells = 1612; Δ_{max} = 0.0580

χ−OSHER, # cells = 0; Δ_{max} = 0.000044

NVF-OSHER, # cells = 1633; Δ_{max} = 0.0479

χ−GAMMA, # cells = 0; Δ_{max} = 0.000044

NVF-GAMMA, # cells = 1658; Δ_{max} = 0.0593

χ−SMART, # cells = 2; Δ_{max} = 0.000358

NVF-SMART, # cells = 1620; Δ_{max} = 0.0653

Figure 9
Figure 10

\(\chi - \text{MUSCL}, \# \text{cells} = 0; \Delta_{\text{max}} = 0.00009\)

\(\chi - \text{OSHER}, \# \text{cells} = 0; \Delta_{\text{max}} = 0.00003\)

\(\chi - \text{GAMMA}, \# \text{cells} = 0; \Delta_{\text{max}} = 0.00001\)

\(\chi - \text{SMART}, \# \text{cells} = 1; \Delta_{\text{max}} = 0.00024\)

\(\text{NVF-MUSCL}, \# \text{cells} = 1273; \Delta_{\text{max}} = 0.0782\)

\(\text{NVF-OSHER}, \# \text{cells} = 1589; \Delta_{\text{max}} = 0.4269\)

\(\text{NVF-GAMMA}, \# \text{cells} = 1144; \Delta_{\text{max}} = 0.0706\)

\(\text{NVF-SMART}, \# \text{cells} = 1386; \Delta_{\text{max}} = 0.0854\)
χ-MUSCL, # cells 4; \( \Delta_{\text{max}} = 0.000375 \)

NVF-MUSCL, # cells = 1528; \( \Delta_{\text{max}} = 0.1102 \)

χ-OSHER, # cells = 1; \( \Delta_{\text{max}} = 0.000113 \)

NVF-OSHER, # cells = 1564; \( \Delta_{\text{max}} = 0.4069 \)

χ-GAMMA, # cells = 0; \( \Delta_{\text{max}} = 0.000043 \)

NVF-GAMMA, # cells = 1550; \( \Delta_{\text{max}} = 0.0681 \)

χ-SMART, # cells = 6; \( \Delta_{\text{max}} = 0.000305 \)

NVF-SMART, # cells = 1556; \( \Delta_{\text{max}} = 0.0928 \)