Application of high-order numerical methods for modeling multicomponent and multiphase flows

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1 Introduction

At EDF R&D and IMSIA, the field of aeroacoustics has been the pioneering one in developing and using high order methods for numerical simulations. For carrying out such computations, a numerical tool called *Code_Safari* has been developed. The governing equations and the computational methods are extensively presented in Daude *et al.* [1]. The compressible Navier-Stokes equations are solved using high order centered finite difference schemes on cartesian curvilinear grids. In order to be able to compute complex configurations, an overset capability is implemented.

But other application fields need high resolution methods. This is the case of multi-component and two-phase flows when the transient evolution of interfaces have to be computed.

2 Computational Methods

For computing multi-component and two-phase flows, it is necessary to introduce some upwind treatment at interfaces. Since *Code_Safari* was developed with a grid structure adapted to a finite difference scheme, a WENO type finite difference scheme developed by Nonomura [8] has been implemented. This scheme is a Weighted Compact Nonlinear Scheme (WCNS) and the flux derivative is approximated by :

$$\left.\frac{\partial f(u)}{\partial x}\right|_{t,x_i} = \frac{1}{\Delta x}\sum_{k=0}^{r-1}\beta_k(f_{i+k+\frac{1}{2}} - f_{i-k-\frac{1}{2}}) + o(\Delta x^{2r}),$$

It is called the midpoint-to-node (**MD**) differencing scheme. MD difference gives a more robust scheme than HOFD. However, it still failed in solving stiff shock tube problems, so another differencing approach, proposed by Nonomura [7], was implemented.

In this scheme, the flux derivative approximation uses not only the flux at the interfaces, but also the flux at the nodes. The $2r^{th}$ approximation is :

$$\left.\frac{\partial f(u)}{\partial x}\right|_{t,x_i} = \frac{1}{\Delta x}\sum_{k=0}^{r-1}\gamma_k(f_{i+\frac{k+1}{2}} - f_{i-\frac{k+1}{2}}) + o(\Delta x^{2r}),$$

It is called the midpoint-and-node-to-node differencing scheme (**MND**).

At interfaces, fluxes are computed through WENO interpolation and HLLC Riemann solvers. In order to obtain very sharp interfaces, THINC method [10, 5] is also used.

3 Multi-component and two-phase flow models

For modeling multi-component flows, the 4-eq equation system is applied with the appropriate treatment at interfaces for avoiding pressure oscillations [6, 9]. For modeling two-phase flow, two systems of equations are used : the 4-eq HEM/HRM system [2] and the 6-eq one velocity two pressure system [4, 3].

4 Numerical results

Numerical results concerning a simple shock tube test case to check the capabilities of the high order methods applied to the 6-eq one velocity two pressure model are presented here. The initial conditions are :

$$(p, \alpha_2, \rho_1, \rho_2, u, v) = \begin{cases} (1.1\times 10^5, 0.1, 10, 1, 50, 0) & x < 0 \\ (1.0\times 10^5, 0.9, 10, 1, 50, 0) & x \geq 0 \end{cases}$$

The equation of state is the stiffened gas law, with the following parameters : $(\gamma_1, P_{\infty 1}) = (1.4, 0)$ on the left, and $(\gamma_2, P_{\infty 2}) = (1.1, 0)$ on the right. The test case was made on a 400-cell mesh, with a CFL number equal to 0.5.

As an example of the results obtained, we compare WENO5-MND4 results and CLAWPACK results (Conservation Laws Package, a package that solves hyperbolic PDEs with low-order methods) and WENO-THINC-BVD [10] reconstruction scheme results. We used a 5^{th}-order WENO interpolation and a 4^{th}-order flux derivative.

Figure 1 shows the void fraction result. It confirms that the THINC approach is able to give very sharp discontinuties. The zoom given in the same figure makes it more evident.

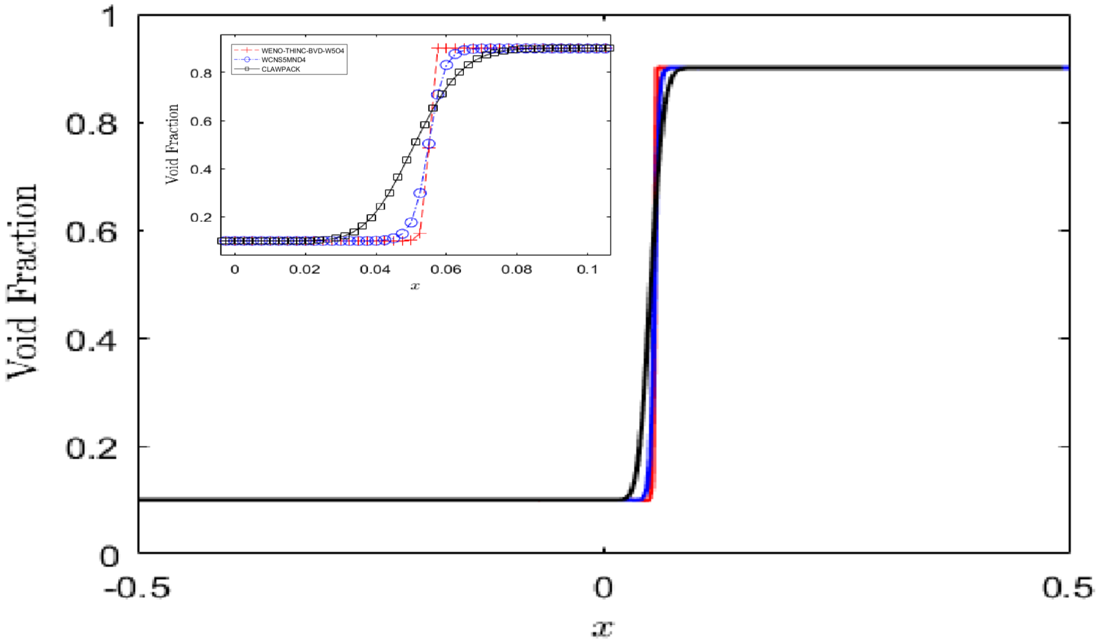

FIGURE 1 – Two-phase shock tube with the 6-equation model. Void fraction. Comparison between WCNS, WENO-THINC-BVD and CLAWPACK at $t = 1.0 \times 10^{-3}$ s.

5 Conclusion

A software dedicated to the development of high-order finite difference methods (Centered, WCNS, WENO, THINC, ...) for solving multi-component and multi-phase flows is being developed and tested. The aim of this project is to be able to apply such approaches to simplified problem of industrial interest : transient vaporization, explosions, ... in order to understand the role of local mecanisms in global non-equilibrium phenomena.

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