

ASSESSMENT OF THE ADAPTATIVE QUICKEST SCHEME FOR EULER EQUATIONS WITH APPLICATION TO INCOMPRESSIBLE FLOWS

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Abstract. *We present an assessment of the adaptative QUICKEST upwind scheme of Kaibara et al. (Proceedings of 18th International Congress of Mechanical Engineering, Ouro Preto, MG - COBEM 2005), for the numerical solution of the 1D Euler equations with application to 2D Navier-Stokes equations. The numerical experiments for the shock tube problem with two different initial data and incompressible flows with free surfaces show that this high order bounded upwind scheme is a good technique for convectively dominated problems.*

Keywords: *Convective terms, finite difference, high order upwind, TVD limiter, NVD*

1. INTRODUCTION

The discretization of the convective terms is not straightforward and requires additional attention, particularly the non-linear ones appearing in high Reynolds Navier-Stokes equations. The desirable properties of an advection scheme are generally the following (see [Verma and Eswaran (1997)]): a) boundedness, i.e., a such scheme must be able to eliminate spurious oscillation; b) minimal diffusion, i.e., it does not spread the solution by introducing too much artificial (numerical) diffusion; c) accuracy, i.e., the scheme does not produce too great a degradation of accuracy; d) non-compression, i.e., it does not tend to "square off" a smooth profile; and e) algorithmic simplicity. These five properties can easily be reached for linear problems with smoothly varying variables. However, in turbulent flows (or compressible flows with shocks/discontinuities), for instance, the appearance of severe gradients makes the approximation of the non-linear convective terms a very difficult job.

Although classical upwinding (e.g. first order upwind/hybrid) is bounded, it is highly diffusive. On the other hand, traditional high order upwind schemes (e.g. Central, QUICK, Lax-Wendroff, etc) are less diffusive, but they are susceptible to numerical instabilities.

Over the past years, a great deal of research has been done in developing and applying innovative high order upwind convection schemes for approximating the non-linear convective terms. Among these, the technique based on the combination of TVD (Total Variation Diminishing) [Harten (1984)] and NVF (Normalized Variable Formulation) [Leonard (1988)] has been the most widely used. In particular, the well recognized Superbee [Roe (1985)] and Van-Leer [van Leer (1974)] schemes, and, more recently, the adaptative QUICKEST (Quadratic Upstream Interpolation for Convective Kinematics with Estimated Streaming Terms) scheme by [Kaibara et al. (2005)] (see also [Ferreira et al. (2007)]) have been proposed to deal with unsteady problems.

The objective of this study is to present the results of the development and implementation of the bounded high order upwind adaptative QUICKEST scheme for solving 1D Euler equations with application to 2D incompressible Navier-Stokes equations at high Reynolds numbers.

2. TVD Advection Schemes

The same approach that it will be shown below can be followed for derivation of any high order TVD upwind scheme. The advection schemes used in this paper are based on the numerical solution of the 1D linear advection equation

$$\phi_t + a\phi_x = 0, \quad a > 0, \tag{1}$$

with a given initial value $\phi(x,0) = \phi_0(x)$. In order to present the main ingredient of our study, lets us consider the following finite difference discretized form of equation (1)

$$\phi_i^{n+1} = \phi_i^n - \theta(\phi_{i+1/2} - \phi_{i-1/2}), \tag{2}$$

where $\theta = a\frac{\Delta t}{\Delta x}$ is the Courant number; Δt and Δx are, respectively, the time step and the cell size; $\phi_{i+1/2}$ and $\phi_{i-1/2}$ are interface fluxes. In the case of Lax-Wendroff scheme, the flux $\phi_{i+1/2}$ is calculated as

$$\phi_{i+1/2} = \phi_i^n + \frac{1}{2}(1-\theta)(\phi_{i+1}^n - \phi_i^n). \tag{3}$$

TVD schemes are usually based on the Lax-Wendroff scheme (3). And this basic scheme can be modified by introducing a flux limiter ψ

$$\phi_{i+1/2} = \phi_i^n + \frac{1}{2}\psi_i(1-\theta)(\phi_{i+1}^n - \phi_i^n), \tag{4}$$

so that when $\psi_i = 1$ equation (4) reduces to the Lax-Wendroff scheme, and when $\psi_i = 0$ it reduces to the first order upwind scheme. More generally, $\psi_i = \psi(r_{i+1/2})$, where $r_{i+1/2} = (\phi_i^n - \phi_{i-1}^n)/(\phi_{i+1}^n - \phi_i^n)$ is the ratio of two consecutive gradients. Equations (2) and (4) can be combined and rearranged into the Harten's formulation (a combination of a first order scheme and an antidiffusive flux) (see [Harten (1984)])

$$\phi_i^{n+1} = \phi_i^n - \theta\Big[1 - \frac{1}{2}(1-\theta)\psi_{i-1} + \frac{1}{2}(1-\theta)\frac{\psi_i}{r_{i+1/2}}\Big](\phi_i^n - \phi_{i-1}^n). \tag{5}$$

Provided that $\theta < 1$, the following conditions on ψ, proposed in [Jeng and Payne (1995)], imply that the scheme is TVD

$$0 \leq \psi_i \leq 2/(1-\theta), \qquad 0 \leq \frac{\psi_i}{r_{i+1/2}} \leq 2/\theta. \tag{6}$$

The dependence on θ can be avoided by accepting the following subset of the preceding TVD constraints, proposed by Sweby in [Sweby (1984)],

$$0 \leq \psi_i \leq 2, \qquad 0 \leq \frac{\psi_i}{r_{i+1/2}} \leq 2. \tag{7}$$

The choice of $\psi = \psi(r)$ dictates the order of the scheme and its boundedness properties. For example, second order accuracy (but not TVD) can be attained by the choice of a convex linear combination of Lax-Wendroff and Warming-Beam ,$\psi(r) = r$, schemes (see [Warming and Beam (1976)]), that is

$$\psi(r) = (1-\alpha)1 + \alpha r, \qquad 0 \leq \alpha \leq 1. \tag{8}$$

So, the interface fluxes in Equation (2) can be approximated by many different ways, by selecting different flux limiter $\psi(r)$ as described above, leading to different high order TVD upwind schemes. In this work, we selected the well known Superbee and Van-Leer schemes, and the modern adaptative QUICKEST scheme. The flux limiters for these schemes are as follows:

- **Superbee**:

$$\psi(r) = max\{0, min\{2r, 1\}, mim\{r, 2\}\} \tag{9}$$

- **Van-Leer**:

$$\psi(r) = \frac{r + |r|}{1 + |r|} \tag{10}$$

- **Adaptative QUICKEST**:

$$\psi(r) = max\left\{0, min\left[2r(1-\theta), \frac{2}{3} - |\theta| + \frac{\theta^2}{3} + \left(\frac{1-\theta^2}{3}\right)r, 2(1-\theta)\right]\right\} \tag{11}$$

Within the Sweby TVD region, the plot of the flux limiter for the adaptative QUICKEST scheme, for several values of θ, is presented in Fig. 1. It is interesting to note that when the parameter θ tends to 0, the flux limiter passes through the point (1,1) in the TVD region, which is the necessary and sufficient condition for second order accuracy [Harten (1984)].

3. NUMERICAL RESULTS

In this section, we examine the performance of the Lax-Wendroff, Van-Leer, Superbee and adaptative QUICKEST schemes for solving 1D test problems. The adaptative QUICKEST scheme is then applied to solving 2D fluid flow problems. For 1D tests, we have chosen two Riemann problems from [Sod (1978)] and [Shu and Osher (1988)] (see also [Toro (1997)]). For the 2D case, the collapse of a liquid column and a turbulent jet impinging onto a rigid surface were selected. The computer code employed in this study to solve the Navier-Stokes equations is a modified version of the Freeflow simulation system developed by Castelo et al. [Castelo et al. (2000)] (see also [Ferreira et al. (2007)]).

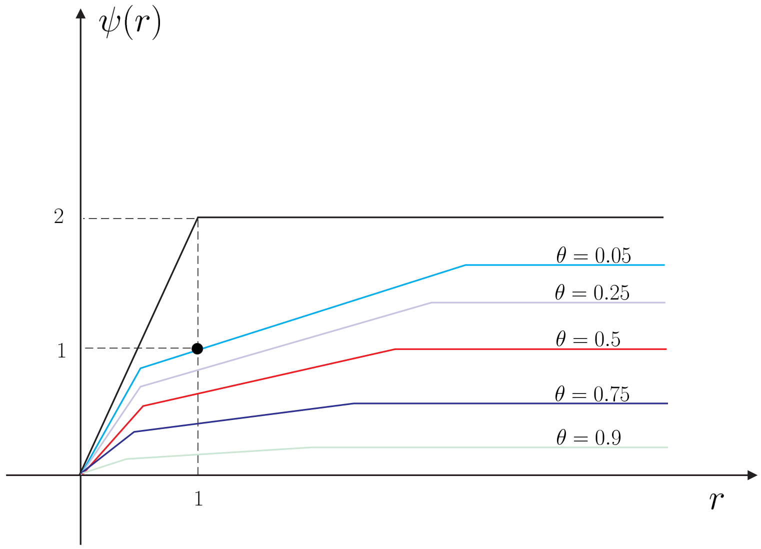

Figure 1. Flux limiter of the adaptative QUICKEST scheme in the Sweby TVD region for several values of θ.

3.1 1D Riemann problems

The first test case is the well known Riemann-Sod's 1D shock tube problem [Sod (1978)]. This problem is used in the experimental investigation of several physical phenomena, such as chemical reaction kinetics, shock structure, and aerothermodynamics of supersonic/hypersonic vehicles. The governing equations are the 1D Euler equations

$$\mathbf{u}_t + \mathbf{f}(\mathbf{u})_{\mathbf{x}} = 0, \tag{12}$$

with $\mathbf{u} = (\rho, \rho v, E)^T$, $\mathbf{f}(\mathbf{u}) = (\rho v, \rho v^2 + p, v(E+p))^T$ and initial conditions $(\rho, v, p)^T = (1, 0, 1)^T$ for $x < 0.5$ and $(\rho, v, p)^T = (0.125, 0, 0.1)^T$ for $x \geq 0.5$. The variables ρ, v, p and E are the density, velocity, pressure, and the total energy per unit volume respectively, with $p = (\gamma - 1)[E - \rho v^2/2]$. Due to the unavailability of an exact solution to this problem, a numerical solution using a fine mesh is considered as the most accurate solution (the Exact one). Displayed in Figs. 2 and 3 are the exact solution and the numerical results for density produced by the Lax-Wendroff, Superbee, Van-Leer, and adaptative QUICKEST schemes on a uniform mesh of 60 computational cells over $0 \leq x \leq 1$ and at time 0.2 seconds. For this case, one can see that, on average, the differences among the results produced by Superbee, Van-Leer and adaptative QUICKEST schemes are, practically, not visible. On the other hand, as it is well recognized, the Lax-Wendroff schemes presented poor results.

In order to show that the adaptative QUICKEST scheme is more appropriated for solving more difficult problem, we present next the simulation of the Shu-Osher problem [Shu and Osher (1988)]. The initial condition is $(\rho, v, p)^T = (3.86, 2.63, 10.33)^T$ if $x < 0.8$ and $(\rho, v, p)^T = (1 + 0.2 sin 5x, 0, 1)^T$ if $x \geq 0.8$, which represents a shock front propagating into a sinusoidal density distribution. Figures 4 and 5 depict the numerical results for density obtained with Lax-Wendroff, Superbee, Van-Leer and adaptative QUICKEST schemes, on the 200 computational cells and at time $t = 1.5$s. It can be seen from these pictures that the adaptative QUICKEST produces, in fact, the most accurate solution, that is very close to the analytical solution. The Van-Leer and Superbee schemes offer poor results. The numerical results by Lax-Wendroff scheme is not acceptable, because it presents spurious oscilations and the peack clipping problem.

3.2 2D Collapse of a liquid column

The collapse of a column of water onto a horizontal wall is a popular test case to validate numerical schemes for calculating transient free surface flows. The experimental results are available in [Martin and Moyce (1952)]. The geometry used is a rectangular column (a=0.050 m wide and $2a$=0.100 m high) in hydrostatic equilibrium and confined between walls. At the beginning, a dam is instantaneously removed and the fluid is subject to vertical gravity and is free to flow out along a rigid horizontal wall. In order to compare with the experimental data given in [Martin and Moyce (1952)], the free-slip boundary condition was used to correctly model this flow at walls. The Reynolds number based on the characteristic length $L = 2a$ and the characteristic velocity $U = \sqrt{L|\mathbf{g}|}$ was $Re \approx LU/\nu = 99 \times 10^3$ ($|\mathbf{g}| = 9.81$ ms^{-2}). Four meshes were used in this problem, namely: 150×75 ($\delta_x = \delta_y = 0.002$ m) computational cells; 300×150 ($\delta_x = \delta_y = 0.001$ m) computational cells; 600×300 ($\delta_x = \delta_y = 0.0005$ m) computational cells; and 750×375 ($\delta_x = \delta_y = 0.0004$ m) computational cells. Figures 6 and 7 show, respectively, the comparison of the numerical results and experimental data for the position of the fluid front ($Xmax$) versus time and the height of residual fluid column ($Ymax$) versus time. Good

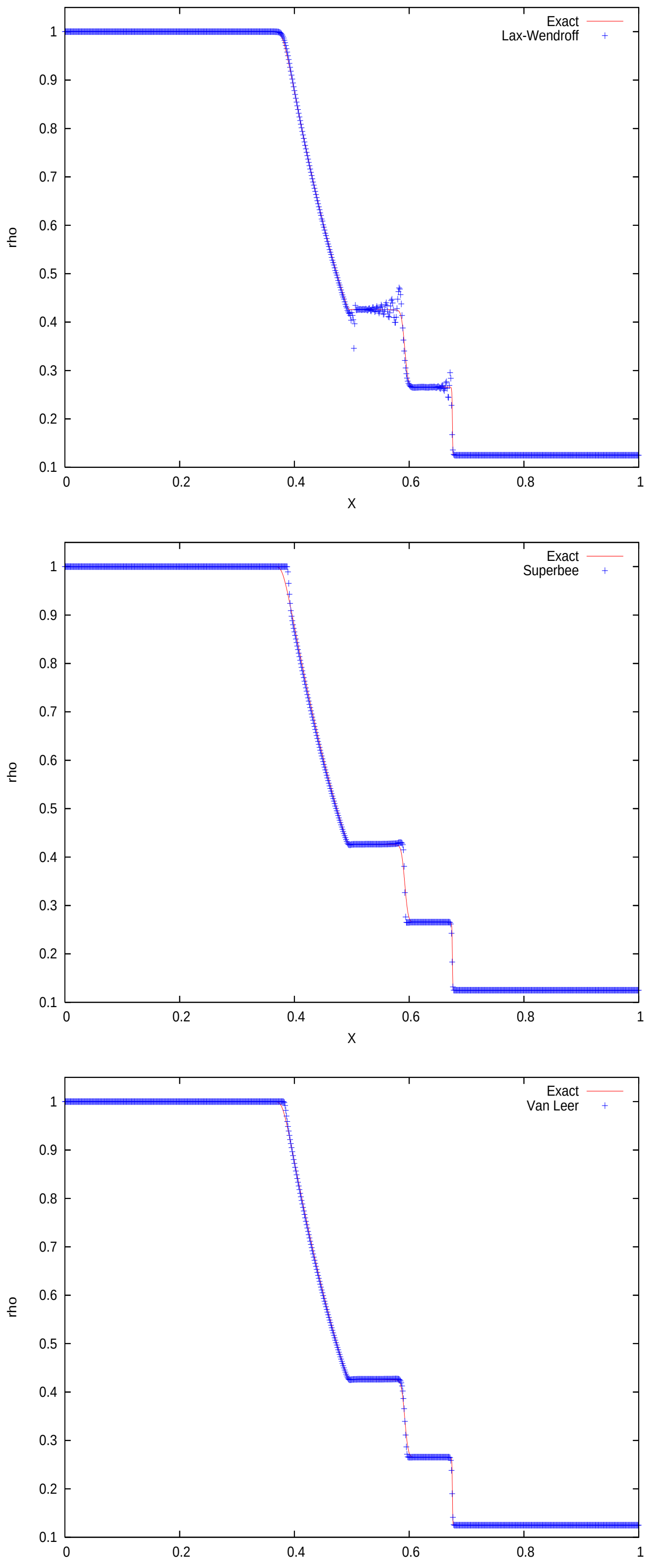

Figure 2. Results for density (ρ) of the Sod shock tube problem, at time $t = 0.2$s and with 60 cells, using Lax-Wendroff, Superbee and Van-Leer schemes.

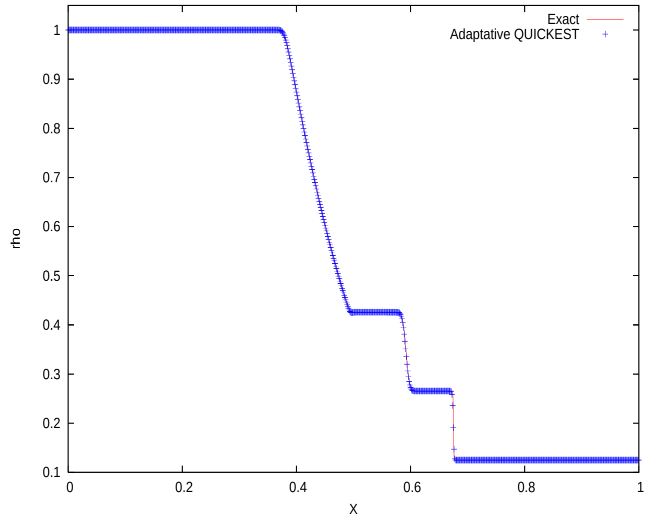

Figure 3. Results for density (ρ) of the Sod shock tube problem, at time $t = 0.2$s and with 60 cells, using adaptative QUICKEST scheme.

agreement between numerical and experimental results is observed from these figures.

3.3 2D Turbulent impinging jet flow

A jet impinging normally onto a flat rigid surface is a good example of a free surface flow, but it is difficult to simulate this problem because the free surface boundary conditions must be specified on an arbitrarily moving boundary. This free surface flow in turbulent regime is also chosen as a representative test case because there is (see [Watson (1964)]) an approximated analytical solution for the total thickness of the fluid layer flowing on the surface. In summary, for a given volumetric flux Q through the inlet section of diameter $L = 2a$, the analytical solution is

$$\begin{cases} h(x) = \dfrac{81(7A)^{\frac{1}{4}}k}{800}\left(\dfrac{\nu}{Q}\right)^{\frac{1}{4}}(x+l), & \text{if} \quad x \geq x_0 \\ h(x) = a + \left(1 - \frac{A}{k}\right)\delta, & \text{if} \quad x < x_0, \end{cases} \tag{13}$$

where

$$\delta(x) = \left(\frac{81}{320(9A-2)}\right)^{\frac{4}{5}} 7^{\frac{1}{5}} k \left(\frac{a\nu}{Q}\right)^{\frac{1}{5}} x^{\frac{4}{5}},$$

$$x_0 = \frac{320(9A-2)}{81 \times 7^{\frac{1}{4}} A^{\frac{5}{4}}} a Re^{\frac{1}{4}},$$

$$l = \frac{160(1-2A)}{9 \times 7^{\frac{1}{4}} A^{\frac{5}{4}}} a Re^{\frac{1}{4}}, \quad A = 0.239, \quad k = 0.260.$$

We simulated this free surface flow, in turbulent regime, using the Freeflow code equipped with the standard $\kappa - \varepsilon$ model on three different meshes, namely: the coarse mesh (200×50 computational cells, $\delta x = \delta y = 0.001$ m); the medium mesh (400×100 computational cells, $\delta x = \delta y = 0.0005$ m); and the fine mesh (800×200 computational cells, $\delta x = \delta y = 0.00025$ m). The Reynolds number involved was 5.0×10^4, which was based on the maximum velocity $U_{max} = 1.0$ m/s and diameter of the inlet $L = 0.01$ m (or $Q = \nu Re = 0.01$ m^2/s). On these three meshes, a comparison is made between the free surface height (the total thickness of the layer), obtained from our numerical solutions and from the analytical viscous solution of Watson. This is displayed in Fig. 8. One can see from this figure that the numerical results on these meshes are similar, showing, in some regions, a small difference when compared to Watson's solution.

4. ACKNOWLEDGEMENTS

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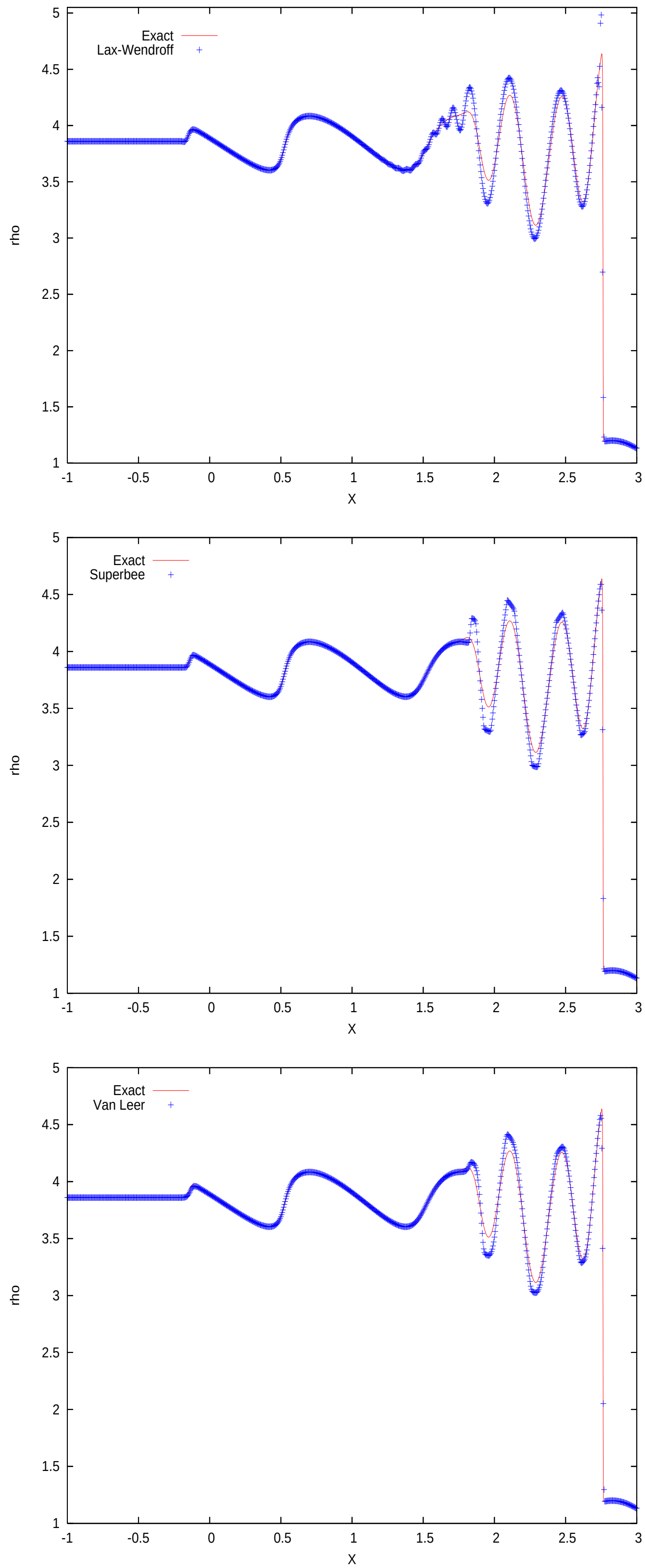

Figure 4. Results for density (ρ) of the Shu-Osher shock tube problem, at time $t = 1.5$s and with 200 cells, using Lax-Wendroff, Superbee and Van-Leer and schemes.

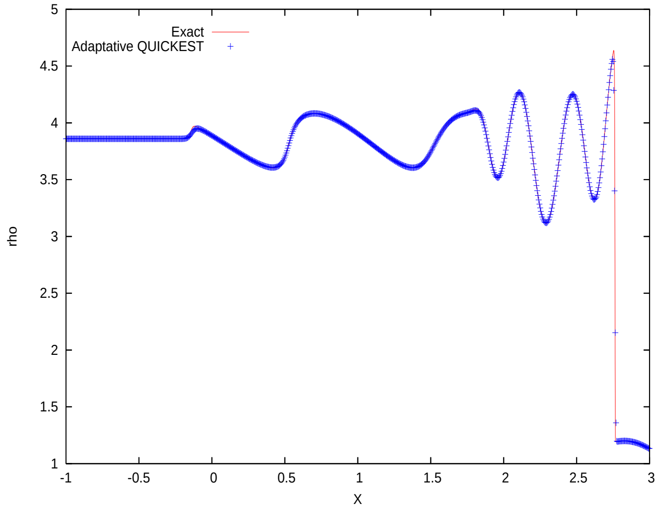

Figure 5. Results for density (ρ) of the Shu-Osher shock tube problem, at time $t = 1.5$s and with 200 cells, using adaptative QUICKEST scheme.

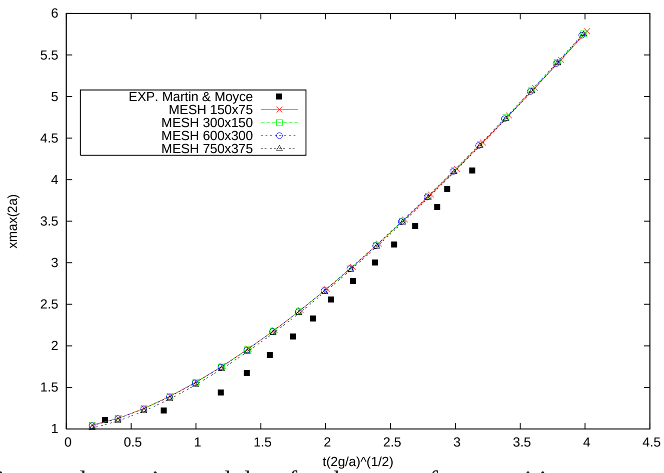

Figure 6. Computations and experimental data for the surge front position versus nondimensional time.

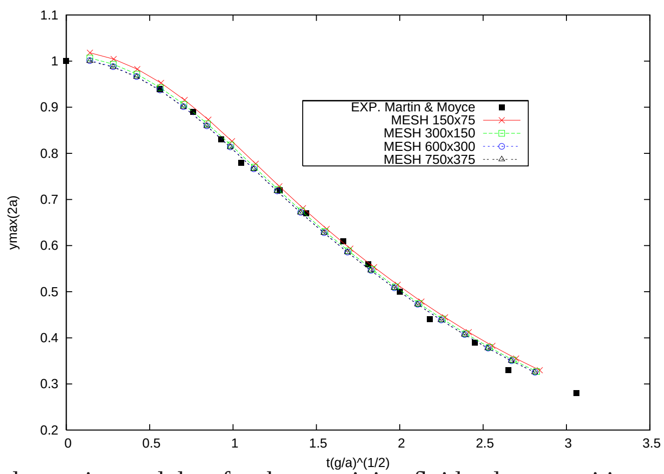

Figure 7. Computations and experimental data for the remaining fluid column position versus nondimensional time.

5. REFERENCES

Castelo, A.F., Tomé, M.F., Cesar, M.L., Cuminato, J.A., Mckee. S., 2000, "Freeflow: An Intregated Simulation System for Three-dimensional Free Surface Flows, Journal of Computing and Visualization in Science, Vol. 2, pp. 199-210.

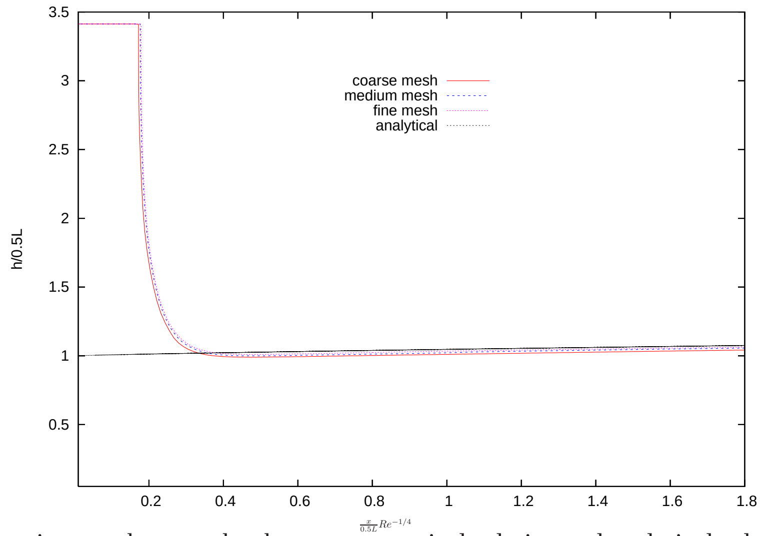

Figure 8. Comparison on three meshes between numerical solution and analytical solution of Watson.

Ferreira, V.G., Oishi, C.M., Kurokawa, F.A., Kaibara, M.K., Cuminato, J.A., Castelo, A., Mangiavacchi, N., Tomé, M.F., McKee, S., 2007 “A combination of implicit and adaptative upwind tools for the numerical solution of incompressible free surface flows”, Communications in Numerical Methods in Engineering, (In press).

Gaskell, P.H., Lau, A.K., 1988, “Curvature-compensated convective transport: SMART, a new boundedness-preserving transport algorithm”, International Journal for Numerical Methods in Fluids, Vol. 8, pp. 617-641.

Harten, A., 1984, “On a class of high resolution total-variation-stable finite-difference schemes”, SIAM Journal of Numerical Analysis, Vol. 1, pp. 1-23.

Jeng, Y.N., Payne, U.J., 1995, “An Adaptive TVD Limiter”, Journal of Computational Physics, Vol, 118, pp. 229-241.

Lax, P.D., Wendroff, B., 1960, “Systems of conservations laws ”, Communications in Pure and Applied Mathematics, Vol. 13, pp. 217.

Kaibara, M.K., Ferreira, V.G., Navarro, H.A., Cuminato, J.A., Castelo, A. Tomé, M.F., 2005, "Upwind Schemes for Convection Dominated Problems", Proceedings of the 18th International Congress of Mechanical Engineering, Ouro Preto-MG, Brazil.

Leonard, B.P., 1988, “Simple high-accuracy resolution program for convective modeling of discontinuities”, International Journal for Numerical Methods in Fluids, Vol. 8, pp. 1291-1318.

Martin, J.C., Moyce, W.J., 1952, “An experimental study of the collapse of liquid columns on a rigid horizontal plate ”, Philosophical Transactions of the Royal Society of London, Series A Mathematical, Physical and Engineering Sciences, Vol. 244, pp. 312-324, 1952.

Roe, P.L., 1985, “Some Contributions to the Modelling of Discontinuous Flows”, Lectures Notes in Applied Mathematics, Summer Seminar on Large Scale Computing in Fluid Mechanics, SIAM, Philadelphia, Vol. 12, pp. 163.

Shu, C.-W., Osher, S., 1988, “Efficient implementation of essentially non-oscillatory shock-capturing schemes”, Journal of Computational Physics, Vol. 77 pp. 439-471.

Sod, G., 1978, “A survey of several finite difference methods for systems of nonlinear hyperbolic conservation laws”, Journal of Computational Physics, Vol. 27 pp. 1.

Sweby, P.K., 1984, “High resolution schemes using flux limiters for hyperbolic conservation laws”, SIAM Journal of Numerical Analysis, Vol. 21, pp. 995-1011.

Toro, E., 1997, “Riemann Solves and Numerical Methods for Fluid Dynamics, Springer-Verlag, Berlin, Heidelberg”.

van Leer, B., 1974, “ Towards the Ultimate Conservative Difference Scheme II: Monotonicity and Conservation Combined in a Second Order Scheme, Journal of Computational Physics, Vol. 14, pp. 361-370.

Verma, A.K. and Eswaran, V., 1997, “A Bounded Convection Scheme for the Overlapping Control Volume Approach, International Journal for Numerical Methods in Fluids, Vol. 25, pp. 1137-1161.

Warming, R.F., Beam, R.M., 1976, “Upwind Second Oerder Difference Schemes and Applications in Aerodynamics, AIAA Journal, Vol. 14, pp. 1241.

Watson, E.J., 1964, “The Radial Spread of a Liquid Jet Over a Horizontal Plane, Journal of Fluid Mechanics, Vol. 20, pp. 481-499.

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