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Numerical modelling of compressible flows using pressure-correction algorithms.

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ABSTRACT. Two pressure-correction Finite Volume algorithms are evaluated on compressible flows with shock wave patterns. Both algorithms are compared with a classical hyperbolic scheme based on the approximate solution of a Riemann problem on each cell interface. Schemes are briefly described. Test cases involve standard Riemann problems with or without shocks, in both homogeneous and inhomogeneous cases. The L^1 norm of the error is presented in each case. As expected, it is shown that conservative schemes enable to compute meaningful compressible solutions, whenever rarefaction waves, contact discontinuities and even shock waves occur. Rates of convergence are very similar to those observed for upwinding schemes.

KEYWORDS: Compressible flow, pressure-correction algorithm, Godunov scheme, Finite Volume conservative scheme, positivity, total enthalpy conservation

1. Introduction

The main objective of this work is to check whether pressure-correction algorithms enable to retrieve meaningful solutions of compressible Euler equations, even when unsteady shock waves occur. Actually, in order to compute Euler equations with shock waves, hyperbolic schemes are usually considered and have already proved to provide very good approximate solutions on any mesh size ([GOD 96]): the huge amount of literature is of course not recalled here. On the contrary, few papers address the suitability of pressure-correction algorithms for such a purpose. Here, two pressure-correction algorithms are presented (see [ARC 07] for details, in particular space discretizations) and compared on test-cases for which an exact solution is available. The L^1 -norm of the error is displayed, which enables to compare with the literature ([GAL 02-1]). Eventually, these algorithms and an approximate Godunov scheme are used to compute a test-case with a strong local and constant heat source term, for which no exact solution exists. The effect of the mesh refinement is studied.

The system to solve is recalled below. We note: $c^2 = \partial_\rho P|_s$ and $\beta = \partial_s P|_\rho$ where P , ρ and s stand for pressure, density and entropy. With standard notations for the momentum $q = \rho u$, the velocity u , the total enthalpy $H = E + P/\rho$ and the total energy $E = \epsilon(P, \rho) + u^2/2$, we consider the 1D Euler equations with a perfect gas EOS ($P = (\gamma - 1)\rho\epsilon(P, \rho) = \rho r T$) and a heat source term Φ independant of time:

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) & = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2) + \partial_x P & = 0 \\ \partial_t(\rho H) + \partial_x(\rho u H) & = \partial_t P + \Phi \end{cases} \quad [1]$$

2. NLK algorithm: a pressure-correction algorithm with sub-iterations

This pressure-correction algorithm sequentially solves the equations of momentum, mass and enthalpy, with sub-iterations to ensure conservativity in time. The algorithm also conserves the total enthalpy along a streamline, in a steady flow when no dissipation/source term is present. At each time step, a global iterative process couples the velocity and the enthalpy-pressure steps: one iterates for $m = 1$ to $m = ntg > 0$ (a given integer) over the steps **[[1.]]** and **[[2.]]** defined below, starting from $Q_{m=1}^{n+1} = q^n$ (for $n = 0$, u^0 , P^0 and H^0 are given, we take $q^0 = \rho^0 u^0$ and ρ^0 from the EOS).

[[1.]] velocity step: a predicted velocity u_m^* is computed from:

$$\rho^n \frac{u_m^* - u^n}{\Delta t} - u_m^* \partial_x Q_m^{n+1} + \partial_x(q^n u_m^*) = -\partial_x P^n \quad [2]$$

[[2.]] enthalpy-pressure step: a sub-iterative process couples enthalpy and pressure: one iterates for $k = 1$ to $k = nthm > 0$ (a given integer) over the steps **[[2.1.]]** to **[[2.3.]]** defined below, starting from $(u, H, P, q)_{m,k=1}^{n+1} = (u_m^*, H^n, P^n, \rho^n u_m^*)$:

[[2.1.]] enthalpy step: $H_{m,k+1}^{n+1}$ (total enthalpy) and an updated density $\rho_{m,k+1/2}^{n+1}$ are computed from:

$$\begin{aligned} \rho^n \frac{H_{m,k+1}^{n+1} - H^n}{\Delta t} - H_{m,k+1}^{n+1} \partial_x q_{m,k}^{n+1} + \partial_x(q_{m,k}^{n+1} H_{m,k+1}^{n+1}) &= \frac{P_{m,k}^{n+1} - P^n}{\Delta t} + \Phi \\ \rho_{m,k+1/2}^{n+1} &= \frac{\gamma P_{m,k}^{n+1}}{(\gamma - 1)(H_{m,k+1}^{n+1} - \frac{1}{2}u_{m,k}^{n+1} u_{m,k}^{n+1})} \end{aligned} \quad [3]$$

[[2.2.]] stopping test and updates: detailed below

[[2.3.]] pressure step: an updated pressure $P_{m,k+1}^{n+1}$ is computed and is used to update the mass flux $q_{m,k+1}^{n+1}$, the velocity $u_{m,k+1}^{n+1}$ and the density $\rho_{m,k+1}^{n+1}$:

$$\frac{P_{m,k+1}^{n+1} - P_{m,k}^{n+1}}{(c^2)^n \Delta t} - \partial_x \Delta t \partial_x (P_{m,k+1}^{n+1} - P_{m,k}^{n+1}) = -\frac{\rho_{m,k+1/2}^{n+1} - \rho^n}{\Delta t} - \partial_x q_{m,k}^{n+1} \quad [4]$$

$$\begin{cases} \frac{u_{m,k+1}^{n+1} - u_{m,k}^{n+1}}{\Delta t} = -\frac{\partial_x (P_{m,k+1}^{n+1} - P_{m,k}^{n+1})}{\rho_{m,k+1/2}^{n+1}} \\ \frac{q_{m,k+1}^{n+1} - q_{m,k}^{n+1}}{\Delta t} = -\partial_x (P_{m,k+1}^{n+1} - P_{m,k}^{n+1}) \end{cases} \quad [5]$$

$$\rho_{m,k+1}^{n+1} = \frac{\gamma P_{m,k+1}^{n+1}}{(\gamma - 1)(H_{m,k+1}^{n+1} - \frac{1}{2}u_{m,k+1}^{n+1} u_{m,k+1}^{n+1})} \quad [6]$$

The pressure correction equation [4] is derived from the discrete mass equation:

$\frac{\rho_{m,k+1}^{n+1} - \rho^n}{\Delta t} + \partial_x q_{m,k+1}^{n+1} = 0$. To do so, the mass flux $q_{m,k+1}^{n+1}$ is replaced by its expression according to [5]: $q_{m,k}^{n+1} - \Delta t \partial_x (P_{m,k+1}^{n+1} - P_{m,k}^{n+1})$. Moreover, the density variation is split into two parts: $\rho_{m,k+1}^{n+1} - \rho_{m,k+1/2}^{n+1}$ and $\rho_{m,k+1/2}^{n+1} - \rho^n$; the first part vanishes when the iterative process converges and it is modelled as: $(P_{m,k+1}^{n+1} - P_{m,k}^{n+1})/(c^2)^n$.

The stopping test and subsequent updates are detailed hereafter. The iterations are not necessarily executed up to $k = nthm$ and $m = ntg$. **To end a given m -cycle**, a convergence test ($C1$) is carried out at the end of the enthalpy step, at each k -iteration (except at the first one): the current m -cycle is interrupted (and the last pressure step of the cycle is skipped) if ($C1$) is true, that is if $k = nthm$ or if the discrete mass equation (rhs of [4]) is satisfied. **To end a given time step**, a convergence test ($C2$) is carried out at the end of each m -cycle: the current time step is interrupted if ($C2$) is true, that is if $m = ntg$ or if the discrete divergence of the mass flux Q_l^{n+1} did not vary between the last two cycles $l = m - 1$ and $l = m$. With these stopping tests:

- **at the end of the last m -cycle**¹, we update the variables for the next time-step:

$$(u, P, q)^{n+1} = (u, P, q)_{m_{max}, k_{max}}^{n+1}, H^{n+1} = H_{m_{max}, k_{max}+1}^{n+1}, \rho^{n+1} = \rho_{m_{max}, k_{max}+1/2}^{n+1} \quad [7]$$

- **at the end of all other m -cycles**², only Q is updated for the next m -cycle:

$$Q_{m+1}^{n+1} = q_{m, k_{max}}^{n+1} \quad [8]$$

The discretization in space relies on a cell-centred Finite Volume technique. A first order upwind discretization³ is used for the terms of the form $\partial_x(q\phi)$ with ϕ standing for u or H . All other gradients are centred.

Conservativity in time⁴ needs $\rho^n \frac{u_{m_{max}}^* - u^n}{\Delta t} - u_{m_{max}}^* \partial_x Q_{m_{max}}^{n+1} = \frac{\rho^{n+1} u^{n+1} - \rho^n u^n}{\Delta t}$ and $\rho^n \frac{H_{m_{max}, k_{max}+1}^{n+1} - H^n}{\Delta t} - H_{m_{max}, k_{max}+1}^{n+1} \partial_x q_{m_{max}, k_{max}}^{n+1} = \frac{\rho^{n+1} H^{n+1} - \rho^n H^n}{\Delta t}$. These relations hold if the enthalpy-pressure and the global iterative cycles are converged. Indeed, convergence yields:

- $u_{m_{max}}^* = u^{n+1}$ and $H_{m_{max}, k_{max}+1}^{n+1} = H^{n+1}$
- $\rho_{m_{max}, k_{max}+1/2}^{n+1} = \rho^{n+1}$ so that: $\frac{\rho^{n+1} - \rho^n}{\Delta t} + \partial_x q_{m_{max}, k_{max}}^{n+1} = 0$
- $\partial_x q_{m_{max}, k_{max}}^{n+1} = \partial_x q_{m_{max}-1, k_{max}}^{n+1}$, so that, with: $Q_{m_{max}}^{n+1} = q_{m_{max}-1, k_{max}}^{n+1}$, we have: $\frac{\rho^{n+1} - \rho^n}{\Delta t} + \partial_x Q_{m_{max}}^{n+1} = 0$

1. ($C1$) and ($C2$) are true, $m = m_{max} \leq ntg$ and $k = k_{max} \leq nthm$

2. ($C1$) is true, ($C2$) is false, $m < ntg$ and $k = k_{max} \leq nthm$

3. On a regular mesh with cells numbered i and interfaces $i + \frac{1}{2}$, we have:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} q \phi dx = q_{i+\frac{1}{2}} (\alpha_{i+\frac{1}{2}} \phi_i + (1 - \alpha_{i+\frac{1}{2}}) \phi_{i+1}) - q_{i-\frac{1}{2}} (\alpha_{i-\frac{1}{2}} \phi_{i-1} + (1 - \alpha_{i-\frac{1}{2}}) \phi_i) \text{ with}$$

$\alpha_{k+\frac{1}{2}} = 1$ for $q_{k+\frac{1}{2}} > 0$ and $\alpha_{k+\frac{1}{2}} = 0$ otherwise.

4. Conservativity in space is ensured by construction with the Finite Volume scheme used.

3. SLK algorithm: a conservative pressure-correction algorithm

This pressure-correction algorithm sequentially solves the equations of mass, momentum and energy without sub-iteration [MAT 03]. By construction, this scheme is conservative in space *and time*. Provided a condition on the time step value, the scheme ensures the discrete positivity of the density and of scalar variables when no source term is present. The algorithm also preserves the total enthalpy along a streamline, in a steady flow when no dissipation/source term is present. At each time step the sequential procedure is the following:

[[1.]] compute the density ρ^{n+1} and the mass flux q_{ac}^{n+1} from:

$$\frac{\rho^{n+1} - \rho^n}{\Delta t} + \partial_x (q^n - \Delta t \beta^n \partial_x s^n) - \partial_x (\Delta t (c^2)^n \partial_x \rho^{n+1}) = 0 \quad [9]$$

$$q_{ac}^{n+1} = q^n - \Delta t ((c^2)^n \partial_x \rho^{n+1} + \beta^n \partial_x s^n) \quad [10]$$

[[2.]] sequentially compute the velocity u^{n+1} and the total energy E^{n+1} from:

$$\rho^n \frac{u^{n+1} - u^n}{\Delta t} - u^{n+1} \partial_x q_{ac}^{n+1} + \partial_x (q_{ac}^{n+1} u^{n+1}) = -\partial_x P^n \quad [11]$$

$$\rho^n \frac{E^{n+1} - E^n}{\Delta t} - E^{n+1} \partial_x q_{ac}^{n+1} + \partial_x \left(q_{ac}^{n+1} \left(E^{n+1} + \frac{P^n}{\rho^{n+1}} \right) \right) = \Phi \quad [12]$$

[[3.]] update the pressure from: $P^{n+1} = (\gamma - 1) \rho^{n+1} (E^{n+1} - \frac{1}{2} u^{n+1} u^{n+1})$

As for NLK, the discretization in space relies on a cell-centred Finite Volume technique. A first order upwind discretization is used for terms of the form $\partial_x(q\phi)$, with ϕ standing for u or $E + P/\rho$. All other gradients are centred.

Conservativity in space is ensured by construction (Finite Volume scheme). Conservativity in time is ensured if $\rho^n \frac{u^{n+1} - u^n}{\Delta t} - u^{n+1} \partial_x q_{ac}^{n+1} = \frac{\rho^{n+1} u^{n+1} - \rho^n u^n}{\Delta t}$ (and a similar relation for E instead of u). This relation is ensured by the discrete form of the mass equation (from [9] and [10]): $-\partial_x q_{ac}^{n+1} = \frac{\rho^{n+1} - \rho^n}{\Delta t}$.

4. VFRoe-ncv: a conservative approximate Godunov scheme

To provide a reference solution for the present computations with a heat source term, many Godunov type schemes may be selected (see [GOD 59] [GOD 96]). Here, the VFRoe-ncv scheme has been adopted: a detailed description can be found in [BUF 00] and comparisons with various Riemann solvers in [GAL 02-1] and [GAL 02-2].

5. Numerical results

We present analytical test-cases and one test-case with a constant heat source term. Convergence studies are carried out keeping $\Delta t/\Delta x$ constant for all meshes.

First, the L^1 -norm of the error obtained with the pressure-correction schemes is studied on the basis of test-cases for which an exact solution is available: double rarefaction wave, contact discontinuity, double shock wave, Sod shock tube and a test-case including a heat source term⁵. Indeed, the four first ones enable to study the elementary wave configurations which are encountered, in a combined or complex way, in industrial studies, and in particular in nuclear thermalhydraulic scenarii. The last test-case is important for industrial problems with a strong heat source term, such as, for instance, some safety studies on large electrical power transformers. The analytical solution of the test case including a heat source term is available in [ARC 07].

Both pressure-correction algorithms converge towards the correct solutions, even when shocks are involved. Moreover, the classical convergence rates expected for so-called "first-order" schemes are retrieved (see figure 1 for SLK, figure 2 for NLK and [GAL 02-1] for the same test-cases computed with VFRoe-ncv). If NLK is operated with too little sub-iterations (conservativity in time can not be ensured), convergence properties may be lost: see figure 3 for the double shock wave and the Sod shock tube test-cases. This is well known for non-conservative schemes applied to systems of conservation laws (for instance [HOU 94], [GAL 02-2]). For these simulations, the coarser and finer meshes contain respectively 80 and 10 240 regular cells.

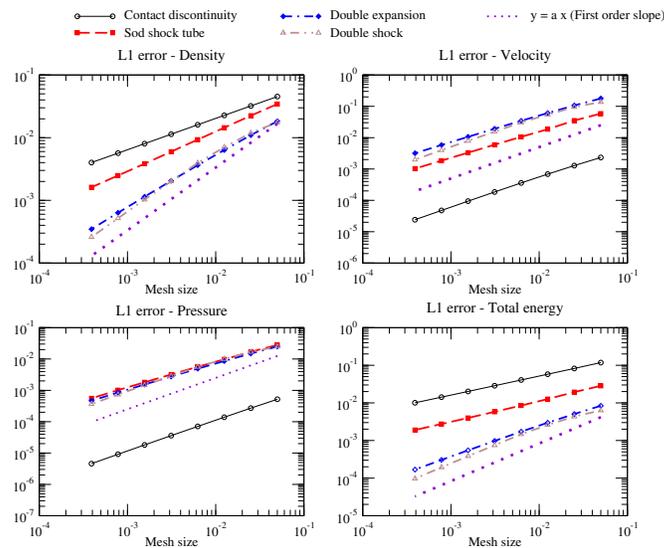


Figure 1. SLK - L^1 -errors for the test-cases without heat source term.

Moreover, a 1D test-case with a constant heat source term has been considered (see [DOU 03] for the industrial context): it is defined by the initial conditions $\rho = 1$,

⁵ Only the results obtained without heat source term are reported here; see [SMO 83] for the analytical solutions.

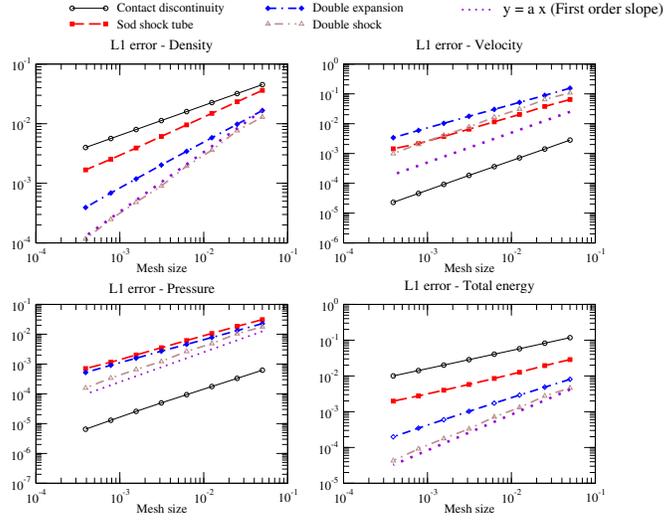


Figure 2. NLK with $ntg = 20$ and $nthm = 20$ - L^1 -errors for the test-cases without heat source term.

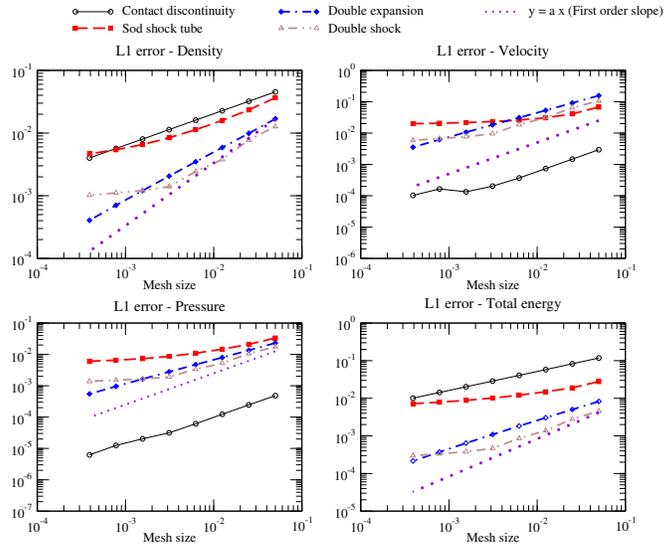


Figure 3. NLK with $ntg = 1$ and $nthm = 2$ - L^1 -errors for the test-cases without heat source term.

$u = 0$, and $P = 10^5$. The constant heat source term Φ is zero everywhere except in the centre of the domain ($\Phi = 10^{10}$ in a zone extending over a length of 0.1). It is observed that when the mesh is refined, the solutions obtained with SLK and NLK converge towards the VFroen-cv reference solution⁶. If NLK is operated with an insufficiently large number of sub-iterations to ensure conservativity, the solution does not converge as the mesh is refined (figure 4). For these simulations, the coarser and finer meshes contain respectively 80 and 6 480 regular cells.

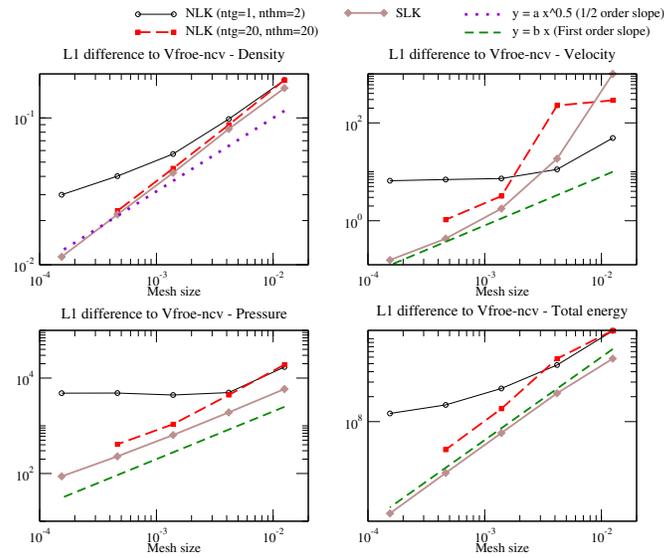


Figure 4. L^1 -difference between NLK and VFroen-cv (curves NLK) and between SLK and VFroen-cv (curves SLK) for the test-case with a constant heat source term; the results with NLK were obtained with two sets of parameters: ($ntg = 1$; $nthm = 2$) and ($ntg = 20$; $nthm = 20$). The dashed lines represent the slopes of 0.5 and 1.

6. Conclusion

The ability to solve compressible flows with pressure correction algorithms has been investigated. Two algorithms have been studied: one of them ensures conservativity using a sub-iterative process, while the second one is conservative by construction. For the former, it has been demonstrated numerically that if the maximum number of sub-iterations was not large enough, the right shock solutions could not be captured. On the other hand, as long as conservativity is ensured, it has been numerically verified that both pressure-correction algorithms can solve compressible flows and capture the right shock solutions.

⁶ VFroen-cv reference solution has been obtained on a mesh containing 174 960 regular cells.

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