Analysis of chosen numerical methods for the application in high order interior ballistics simulations

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Abstract. Considering constant development of the interior ballistics, along with new gun and ammunition designs, the necessity of in-depth analysis of the shot event is continuously increasing. Numerical simulations of interior ballistics problems are useful for optimising new designs or explaining complex issues, regarding performance instabilities and catastrophic failures. With the rise of the computing power, there is a significant urge to drive the numerical errors towards machine zero. This goal demands using methods of high order of accuracy in both space and time. Current methods allow to achieve an arbitrary order of numerical accuracy, thus allowing to shift the focus towards sophistication of the mathematical model of the studied phenomenon. Therefore, in this work, some numerical schemes, in context of finite volume method, are reviewed and studied using well established test problems. The results of the presented analysis are meant to become the basis for future development of a high order numerical scheme for simulation of interior ballistics problems.

1. Introduction

Interior ballistics is specialized field of science, that deals with the interaction of the gun, projectile and propelling charge, which includes, among other phenomena, the ignition and burning of propellant, and the dynamics of projectile motion in gun during a very short shot event [1]. One of the main goals of interior ballistics of guns is to estimate pressure of gases in combustion chamber and muzzle velocity of projectile and to study factors affecting the ballistic cycle. The gun could be considered as a particular kind of heat engine, exchanging chemical energy, through combustion of propellant, into kinetic energy of projectile and mixture of propellant and combustion gases. Therefore the shot event could be analysed using properly adapted laws of thermodynamics and fluid mechanics [2].

The complexity of the shot phenomenon demands using many simplifications for its mathematical description. Simple lumped-parameter models, like IBHVG2 [3], generalised model of interior ballistics [4] or STANAG 4367 are the main tools used for interior ballistics computations, as they are fast and could be used for, among others, propellant charge optimisation. However, the development of computational methods and constant rise of computing power makes it possible to use more sophisticated mathematical models, thus allowing to study phenomena like pressure waves, propellant grains fracture during shot event or different modes of ignition. The necessity of in-depth analysis of these issues is increasing, as it is useful for explaining performance instabilities in guns or catastrophic failures [5]. This could be achieved by utilising one- or multi-dimensional numerical models. Currently, numerical schemes based on Godunov scheme [6] for solving partial differential equations...
are applied for solving many complex issues, for example fluid dynamics of multiphase flows or astrophysical simulations in multiple dimensions. With the urge to drive numerical errors towards machine zero, there is a need to develop and use numerical schemes of high order of accuracy [7]. Current numerical methods allow to achieve even arbitrary order of numerical accuracy in both space and time, thus making it possible to shift the focus towards sophistication of the mathematical formulation of the studied problem. Therefore, the objective of this work was to study chosen numerical methods, that could be used to develop one-dimensional numerical scheme of high order of accuracy for simulations of interior ballistics problems.

To properly study pressure waves and ignition of propellant the flow in gun cannot be properly modelled as a homogenous mixture of yet unburnt propellant grains and combustion gases. Two-phase flow model has to be used [8], where one phase is the solid phase composed by propellant grains and the second is compressible gas. Although this approach is in constant development, it is broadly used in numerical simulations and in interior ballistics applications [9-16]. The studied numerical schemes for solving two-phase flow systems were then tested and compared using well-established test problems.

2. Mathematical model

The generic mathematical model for one-dimensional two-phase flow has the following form [16]:

\[ \begin{aligned}
\partial_t (\alpha_1 \rho_1 u_1) + \partial_x (\alpha_1 \rho_1 u_1 u_1) &= 0 \\
\partial_t (\alpha_1 \rho_1 u_1) + \partial_x (\alpha_1 \rho_1 u_1^2 + \alpha_1 p_1) - p_1 \partial_x \alpha_1 &= 0 \\
\partial_t (\alpha_1 \rho_1 E_1) + \partial_x (\alpha_1 u_1 (\rho_1 E_1 + p_1)) - p_1 u_1 \partial_x \alpha_1 &= 0 \\
\partial_t (\alpha_1 \rho_2 u_1) + \partial_x (\alpha_1 \rho_2 u_2^2 + \alpha_1 p_2) + p_1 \partial_x \alpha_1 &= 0 \\
\partial_t (\alpha_1 \rho_2 E_2) + \partial_x (\alpha_1 u_2 (\rho_2 E_2 + p_2)) + p_1 u_2 \partial_x \alpha_2 &= 0 \\
\partial_t \alpha_1 + u_1 \partial_x \alpha_1 &= 0
\end{aligned} \]  

(1)

In this work, the flow was considered to be non-viscous and without mass exchange, heat transfer or wall friction, thus the source terms on the right hand side are omitted so the resulting system of equations is homogenous. Here \( \alpha_i \) is the volume fraction, \( \rho_i \), the density, \( u_i \), the velocity, \( E_k = e_k + \frac{1}{2} \rho_k u_k^2 \) is the total specific energy and \( p_i \) the pressure of the phase \( k = 1, 2 \). Variables \( u_i \) and \( p_i \) are interfacial velocity and interfacial pressure respectively. Necessary closure relations [16] are caloric equation of state for phase \( k \):

\[ e_k = e_k(p_k, \rho_k) \]  

(2)

and saturation constraint:

\[ \alpha_1 + \alpha_2 = 1 \]  

(3)

By defining \( u_i \) and \( p_i \) differently, one could obtain distinct models describing two-phase flow, as the chosen definition has significant impact on mathematical properties of the system (1) and the numerical strategy for the discretisation [17]. In this work it was chosen to set these variables as in the original paper of Baer and Nunziato [18], where the two-phase model of flame spreading and deflagration-to-detonation transition in gas-permeable, reactive granular material was proposed. This model is obtained from equation (1) by setting [16]:

\[ u_i = u_1, \quad p_i = p_2 \]  

(4)

where the interfacial velocity \( u_i \) is assumed equal to the velocity of the less compressible phase and the interfacial pressure \( p_i \) is assumed equal to pressure of the most compressible phase [19].

The system of equations (1) could be also written in non-conservative vector form:

\[ \partial_t \mathbf{Q} + \partial_x \mathbf{F} + \mathbf{B} \partial_x \mathbf{Q} = 0 \]  

(5)
where $Q$ is the vector of state variables, $F(Q)$ is the flux vector for the conservative part of the system and $B(Q)$ is the square matrix containing non-conservative part [20]:

$$Q = \begin{bmatrix} \alpha_1 \rho_1 \\ \alpha_1 \rho_1 u_1 \\ \alpha_1 \rho_1 E_1 \\ \alpha_2 \rho_2 \\ \alpha_2 \rho_2 u_2 \\ \alpha_2 \rho_2 E_2 \\ \alpha_1 \end{bmatrix}, \quad F(Q) = \begin{bmatrix} \alpha_1 \rho_1 u_1 \\ \alpha_1 (\rho_1 u_1^2 + p_1) \\ \alpha_1 (\rho_1 E_1 + p_1) \\ \alpha_2 \rho_2 u_2 \\ \alpha_2 (\rho_2 u_2^2 + p_2) \\ \alpha_2 \rho_2 E_2 + p_2 \\ 0 \end{bmatrix}$$

(6)

$$B(Q) = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -p_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -p_1 u_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & p_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & p_1 u_1 & 0 \\ 0 & 0 & 0 & 0 & 0 & u_1 & 0 \end{bmatrix}$$

Rewriting equation (5) in a quasi-linear form gives the following equation:

$$\partial_t Q + A(Q)\partial_x Q = 0$$

(7)

The system matrix $A(Q)$ is defined as:

$$A(Q) = \frac{\partial F(Q)}{\partial Q} + B(Q)$$

(8)

where $\partial F(Q)/\partial Q$ is a Jacobian matrix of the flux vector.

Analysing the eigenstructure of equation (7) it could be seen that the system is non-strictly hyperbolic. Moreover, its important feature is the presence of non-conservative terms:

$$\pm p_i \partial_x \alpha_i , \quad \pm p_i u_i \partial_x \alpha_i$$

(9)

and the transport equation for the volume fraction $\alpha_i$ [16] in addition to equations for conservation of mass, momentum and energy for each phase.

3. Numerical methods

In order to find the solution for a system of hyperbolic partial differential equations like in equation (7), the one-dimensional, Cartesian discretisation of the computational domain was assumed in the framework of the finite volume method, where the vector of state variables is averaged inside every computational cell (finite volume) and the flux vector is defined on the cell interface. In the conservative case, cell-averaged values of the vector $Q$ in the consequent time step could be found using classical Godunov scheme [6]:

$$Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} \left( F_{i+1/2}^n - F_{i-1/2}^n \right)$$

(10)

For non-conservative systems, like in equation (5), classical Rankine-Hugoniot relations for conservation laws are not applicable, therefore it becomes problematic to define the solution of the Riemann problem. To overcome this issue, path-conservative schemes were introduced [21], where the non-conservative product is defined along path $\Psi(s, Q_L, Q_R)$ in the phase-space, connecting left state $Q_L$ and right state $Q_R$, satisfying [19]:

- $\Psi(0, Q_L, Q_R) = Q_L$ and $\Psi(1, Q_L, Q_R) = Q_R$;
- $\Psi(\zeta, Q, Q) = Q$ for any $\zeta \in [0,1]$.  

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It should be noted, that the weak solution of the Riemann problem depends on the choice of path \( \Psi \) [19, 22]. In this work, the straight-line segment path was chosen:

\[
\Psi(s, Q_L, Q_R) = Q_L + (Q_R - Q_L)s, \quad \text{where} \quad s \in [0,1]
\] (11)

This simple path choice is generally accepted for solving Baer-Nunziato equations (see eg. [20, 23-27]).

The path conservative scheme [21, 28] could be written in the form:

\[
Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} (\mathbf{D}^+_{i-1/2} - \mathbf{D}^-_{i+1/2})
\] (12)

where \( \mathbf{D}^+ \) and \( \mathbf{D}^- \) are two continuous functions (fluctuations) of left and right states \( Q_L \) and \( Q_R \), satisfying:

\[
\mathbf{D}^\pm(Q, Q) = 0
\] (13)

and

\[
\mathbf{D}^+(Q_L, Q_R) + \mathbf{D}^-(Q_L, Q_R) = \int_0^1 A(\Psi(s, Q_L, Q_R)) \frac{\partial \Psi}{\partial s}(s, Q_L, Q_R) ds
\] (14)

In order to compute the numerical fluctuations at the cell interface, the Riemann problem for equation (7) has to be solved:

\[
\begin{cases}
\partial_t Q + A(Q)\partial_x Q = 0 \\
Q(x, 0) = \begin{cases} Q_L \text{ if } x < 0 \\
Q_R \text{ if } x > 0 \end{cases}
\end{cases}
\] (15)

As finding the exact solution of the Riemann problem of Baer-Nunziato equations was beyond the scope of this work, only approximate solvers were considered, specifically the HLL solver and its derivation – HLLI, and the DOT solver, which is an extension of the Osher-Solomon method. Both HLLI and DOT solvers are complete Riemann solvers, as they use the whole eigenstructure of the system matrix in order to include into solution every existing intermediate wave. This important feature is valuable for building an accurate numerical scheme, despite increasing computing time.

3.1. Path-conservative HLL and HLLI schemes

The HLL is a universal, positivity preserving and entropy enforcing Riemann solver [25]. An approximate solution to the Riemann problem in this method is given by:

\[
Q\left(\xi = \frac{x}{\Delta x} = 0\right) = \begin{cases} Q_L \text{ if } \xi \leq S_L \\
\left(Q^\ast - Q_L\right) \frac{\xi}{S_L} + Q_L \text{ if } S_L < \xi < S_R \\
Q_R \text{ if } \xi \geq S_R \end{cases}
\] (16)

Here \( S_L \) and \( S_R \) are estimates of the two fastest, respectively left and right going waves [25]:

\[
S_L = \min\left(0, \Lambda(Q_L, \bar{Q})\right), \quad S_R = \max\left(0, \Lambda(Q_R, \bar{Q})\right)
\] (17)

where the mean state \( \bar{Q} \) is defined by an arithmetic or Roe average of the left and right state of vector \( Q \), and \( \Lambda \) is the matrix of eigenvalues.

For non-conservative system (5) the expression for intermediate state \( Q^\ast \) is [25]:

\[
Q^\ast = \frac{1}{(S_R - S_L)} \left[ (S_R Q_R - S_L Q_L) - (F_R - F_L) - \tilde{B}(Q_L, Q^\ast)(Q^\ast - Q_L) - \tilde{B}(Q^\ast, Q_L)(Q_R - Q^\ast) \right]
\] (18)

where matrix \( \tilde{B} \) is computed using path-integral:
\[ \bar{B}(Q_a, Q_b) = \int_{0}^{1} B(\psi(s, Q_a, Q_b)) \, ds \]  

(19)

Here, \( \bar{B} \) is evaluated using three-point Gauss-Legendre quadrature, then \( Q^* \) is obtained using iterative scheme, as proposed in [25].

The scheme based on HLL generalised Riemann problem solver of higher order of accuracy, in this case the second order in both space and time, could be written as [29]:

\[ Q^{n+1}_i = Q^n_i - \Delta t A(Q^n_i)(\partial_x Q^n_i) - \frac{\Delta t}{\Delta x} \left( D^{-;n+1/2}_{HLL;i+1/2} + D^+;n+1/2_{HLL;i-1/2} \right) \]  

(20)

where \( D^{-;n+1/2}_{HLL;i+1/2} \) and \( D^+;n+1/2_{HLL;i-1/2} \) are time-centred, spatially and temporally second-order fluctuations at cell boundaries given by equations [29]:

\[ D^{-;n+1/2}_{HLL;i+1/2} = D^{-;n}_{HLL;i+1/2} - \frac{\Delta t}{2} \left( A(Q^n_{i+1/2}) \right)^2 \left( \partial_x Q^n_i \right) \]  

(21)

\[ D^+;n+1/2_{HLL;i-1/2} = D^+;n_{HLL;i-1/2} + \frac{\Delta t}{2} \left( A(Q^n_{i-1/2}) \right)^2 \left( \partial_x Q^n_i \right) \]  

(22)

and spatially second-order accurate fluctuations \( D^n;\pm 1/2_{HLL;i} \) are [29]:

\[ D^n;\pm 1/2_{HLL;i} = S_{\pm;1/2} \left[ Q^n_i \mp \frac{1}{2} \left( \partial_x Q^n_i \right) \Delta x \right] \]  

(23)

\[ D^n;\pm 1/2_{HLL;i} = S^*_{\pm;1/2} \left[ Q^n_i \mp \frac{1}{2} \left( \partial_x Q^n_i \right) \Delta x \right] \]  

(24)

In order to extend the method to the HLLI solver and include the whole family of intermediate waves, it is necessary to provide the time-centred anti-diffusive contributions to equations (23) and (24) [29]. By denoting the matrix of eigenvalues associated with intermediate waves by \( \Lambda'(Q) \) and associated matrices of left and right eigenvectors by \( L'(Q) \) and \( R'(Q) \) respectively [25], the expression for time-centred fluctuations could be written as:

\[ D^{\pm;\pm 1/2}_{HLL} = D^{\pm;\pm 1/2}_{HLL} \pm \varphi \frac{S_L S_L}{S_R - S_L} \delta^* \left[ L^* \left( Q^{n+1/2}_R - Q^{n+1/2}_L \right) \right] R^* \]  

(25)

Here \( \varphi \) is a flattener function [30] and \( \delta^* \) is a diagonal matrix controlling the amount of anti-diffusion, defined by:

\[ \delta^*(\bar{Q}) = I - \frac{\Lambda^*_{\pm}(\bar{Q})}{S_L} - \frac{\Lambda^*_{\pm}(\bar{Q})}{S_R} \]  

(26)

where \( I \) is an identity matrix and \( \Lambda^*_{\pm}(\bar{Q}) \) the abbreviation of the expression [25]:

\[ \Lambda^*_{\pm}(\bar{Q}) = \frac{1}{2} \left( \Lambda^*(\bar{Q}) \pm |\Lambda^*(\bar{Q})| \right) \]  

(27)

By using the whole eigenstructure of intermediate waves in equation (25), the resulting solution of the Riemann problem becomes complete.

### 3.2 Path-conservative DOT scheme

The Osher-Solomon scheme is a well-known, nonlinear, entropy-enforcing and complete Riemann solver for hyperbolic systems of equations [31]. Its extension to non-conservative systems was proposed by Dumbser and Toro in [24]. The second order Total Variation Diminishing (TVD) scheme based on the DOT solver could be written as [20]:

\[ \text{IC-MSQUARE 2021} \]

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\[ Q_{i}^{n+1} = Q_{i}^{n} - \frac{\Delta t}{\Delta x} (f_{i+1/2} - f_{i-1/2}) - \frac{\Delta t}{\Delta x} (D_{i+1/2} + D_{i-1/2}) - \Delta t B \left( Q_{i}^{n+1/2} \right) \partial_x Q_{i}^{n} \]  

(28)

Here, the Osher numerical flux function \( f \) is \([20, 24]:\)

\[ f_{i+1/2} = \frac{1}{2} \left( f \left( Q_{i+1/2}^{n+1/2} \right) + f \left( Q_{i+1/2}^{n-1/2} \right) \right) - \frac{1}{2} \left[ \int_{0}^{1} A \left( \psi \left( s, Q_{i+1/2}^{n-1/2}, Q_{i+1/2}^{n+1/2} \right) \right) ds \right] \left( Q_{i+1/2}^{n-1/2} - Q_{i+1/2}^{n+1/2} \right) \]  

(29)

where the first term of the equation (29) is a centred part of the numerical flux and the second is the numerical viscosity \([24].\) By denoting the matrix of eigenvalues of \( A \) in absolute values by \( |A|, \) the matrix of corresponding right eigenvectors by \( R \) and by \( R^{-1} \) its inverse, the absolute value operator of the matrix \( A \) could be defined as:

\[ |A| = R |\Lambda| R^{-1} \]  

(30)

The path-integral in equation (29) is evaluated using three-point Gauss-Legendre quadrature.

In this case the terms \( D_{i \pm 1/2} \) in equation (28) represents the jump due to non-conservative products and are obtained using expression \([20]:\)

\[ D_{i \pm 1/2} = \frac{1}{2} \int_{0}^{1} B \left( \psi \left( s, Q_{i+1/2}^{n-1/2}, Q_{i+1/2}^{n+1/2} \right) \right) ds \]  

(31)

which is, again, evaluated using Gauss-Legendre quadrature.

The time-centred and/or boundary extrapolated values \( Q_{i \pm 1/2}^{n+1/2} \) and \( Q_{i}^{n+1/2} \) are obtained using piecewise linear space-time reconstruction polynomial \([20]:\)

\[ Q(x, t) = Q_{i}^{n} + \partial_s Q_{i}^{n} (x - x_i) + \partial_t Q_{i}^{n} (t - t^n) \]  

(32)

where the space derivative approximation \( \partial_s Q \) is obtained using minmod slope limiter \([7]:\)

\[ \partial_s Q_{i}^{n} = \text{minmod} \left( \frac{Q_{i+1}^{n} - Q_{i}^{n}}{\Delta x}, \frac{Q_{i}^{n} - Q_{i-1}^{n}}{\Delta x} \right) \]  

(33)

and the time derivative approximation \( \partial_t Q \) is defined as \([20]:\)

\[ \partial_t Q_{i}^{n} = -f \left( Q_{i}^{n} + \frac{\Delta x}{2} \partial_s Q_{i}^{n} \right) - f \left( Q_{i}^{n} - \frac{\Delta x}{2} \partial_s Q_{i}^{n} \right) - B(Q_{i}^{n}) \partial_s Q_{i}^{n} \]  

(34)

4. Test problems

To verify and compare chosen schemes, numerical tests were performed and the results checked against the exact solution. Table 1 presents initial conditions for chosen test cases \([32].\) Each of the Riemann problems was solved in the spatial domain \([0, 1]\) using 300 mesh cells and CFL number set to 0.9 for both the HLLI-based and DOT-based schemes. For simplicity, the ideal gas equation of state was assumed for both phases \( k: \)

\[ e_k = \frac{p_k}{\gamma_k (\gamma_k - 1)} \]  

(35)

with \( \gamma_k = 1.4. \) For the HLLI-based scheme, the flattener \( \varphi \) was set to 0.97, as in \([25].\) The exact solution was obtained using CONSTRUCT code \([33].\) In every test case, the discontinuity was located at 0.5.
Table 1. Initial values for test problems

| Phase | \(\alpha_{\text{SL}}\) | \(p_{\text{SL}}\) | \(u_{\text{SL}}\) | \(p_{\text{LR}}\) | \(\alpha_{\text{LR}}\) | \(p_{\text{LR}}\) | \(u_{\text{LR}}\) | \(p_{\text{LR}}\) |
|-------|----------------|-------------|-------------|----------------|----------------|-------------|-------------|-------------|
| RP1   |                |             |             |                |                |             |             |             |
| 1     | 0.8            | 2           | 0.3         | 5              | 0.3            | 2           | 0.3         | 12.8567     |
| 2     | 0.2            | 1           | 2           | 1              | 0.7            | 0.1941      | 2.8011      | 0.1         |
| RP2   |                |             |             |                |                |             |             |             |
| 1     | 0.1            | 0.9123      | 1.6305      | 1.5666         | 0.9            | 0.8592      | -0.0129     | 1.1675      |
| 2     | 0.9            | 2.6718      | -0.050      | 1.5            | 0.1            | 1.3359      | 0.5438      | 1.5         |
| RP3   |                |             |             |                |                |             |             |             |
| 1     | 0.5            | 2           | -1          | 2              | 0.1            | 1           | -1          | 8.3994      |
| 2     | 0.5            | 0.2702      | -3.4016     | 0.1            | 0.9            | 0.4666      | -2.6667     | 0.2148      |

Figures 1, 2 and 3 presents the numerical solutions of the respective Riemann problems at time \(t = 0.1\). As it could be seen in figures, numerical solutions obtained using both solvers converge to the exact solution. However, the results of the DOT-based scheme are visibly more accurate than those obtained using HLLI-based scheme.

5. Conclusions

The aim of this work was the review of numerical methods, that could be used to develop one-dimensional numerical scheme of high order accuracy for interior ballistic simulations in the finite volume framework. As the shot event and the interactions between projectile, gun tube, propellant and combustion gases are very complex phenomena, thus the two-phase flow model of Baer-Nunziato was chosen for its mathematical representation. To achieve the high accuracy, spatially and temporally second-order accurate schemes utilising complete Riemann solvers were used, specifically the HLLI and DOT solvers. Moreover, chosen numerical schemes had to be able to deal with non-conservative products of the mathematical model.

The results obtained utilising chosen methods were satisfying. Therefore, these methods could be effectively used to develop the numerical scheme for interior ballistics simulations. However, in future work it is needed to implement the numerical source terms into the scheme, representing propellant burning and projectile motion among others. The resulting scheme would be then verified by simulating the AGARD test gun [12]. Moreover, in order to further improve the accuracy, the methods to achieve higher than second order accuracy would be examined, although the research on these are still being conducted, as developing the high-order path-conservative scheme is a challenging task [34]. Furthermore, other two-phase flow mathematical models, based on the system (1), should be examined, for example [35] and [36], as well as more complex equations of state, that could better model the behaviour of the solid and gas phases in the context of interior ballistics.
Figure 1. Numerical results for RP1
Figure 2. Numerical results for RP2
Figure 3. Numerical results for RP3
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