HLLC solver for hyperbolic non-equilibrium two-phase flows

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Motivations and importance

Build a 3D // unstructured code to solve multiphase mixture flows and interfaces.
Design a very robust scheme able to deal with very strong shocks (mega-bar) and vacuum (1 Pa) for cavitating flows.
Design a method simpler than the DEM (Abgrall and Saurel, 2003) and more robust.
Two-phase flow model

\[ \frac{\partial \alpha_1}{\partial t} + u_i \frac{\partial \alpha_1}{\partial x} = \mu(p_1 - p_2) \]  

Baer and Nunziato (1986)

\[ \frac{\partial (\alpha \rho)_1}{\partial t} + \frac{\partial (\alpha \rho u)_1}{\partial x} = 0 \]

\[ \frac{\partial (\alpha \rho u)_1}{\partial t} + \frac{\partial (\alpha \rho u^2 + \alpha p)_1}{\partial x} = p_i \frac{\partial \alpha_1}{\partial x} + \lambda (u_2 - u_1) \]

\[ \frac{\partial (\alpha \rho E)_1}{\partial t} + \frac{\partial (u(\alpha \rho E + \alpha p))_1}{\partial x} = p_i u_i \frac{\partial \alpha_1}{\partial x} - \mu \ p_i ' (p_1 - p_2) + \lambda \ u_i ' (u_2 - u_1) \]

+ Symmetric system for phase 2

\[ u_i = \frac{Z_1 u_1 + Z_2 u_2}{Z_1 + Z_2} + \text{sgn} \left( \frac{\partial \alpha_1}{\partial x} \right) \frac{(p_2 - p_1)}{Z_1 + Z_2} \]

\[ p_i = \frac{Z_1 p_2 + Z_2 p_1}{Z_1 + Z_2} + \text{sgn} \left( \frac{\partial \alpha_1}{\partial x} \right) \frac{(u_2 - u_1)Z_1Z_2}{Z_1 + Z_2} \]

These symmetric estimates are given in Saurel et al. 2003 and extended in Saurel et al. 2014 to granular mixtures.

The symmetric variant involves 7 waves instead of 6 \( \rightarrow \) very important for the two-phase RP.
Conventional Riemann problem

- 6 or 7 waves,
- many states to compute,
- linear solver not robust enough,
- Roe solver useless (non conservative terms) and difficult to build (shocks),
- regularization needed for the volume fraction wave (Schendeman, Kapila),
- this regularization is not robust enough (shock interface interaction),
- extension to N phases: 10 waves (3 fluids), 14 waves (4 fluids), …
Discrete Equations Method (DEM)

Abgrall and Saurel, JCP, 2003
Saurel, Gavrilyuk and Renaud, JFM, 2003
Chinnayya, Daniel and Saurel, JCP, 2004
Le Metayer, Massoni and Saurel, JCP, 2005
Berry, Saurel, Le Metayer, NED, 2010

→ Solves non conservative products (even with shocks)
→ Computes accurately two-phase fluxes with Euler Riemann solvers

(but complicate for a 3D unstructured code)
Characteristic function

\[ X_k = \begin{cases} 
1 & \text{if the point belongs to the phase} \ k \\
0 & \text{otherwise} 
\end{cases} \]

\[ X_k \text{ obeys } \frac{\partial X_k}{\partial t} + \vec{u}_i \cdot \nabla X_k = 0 \]

\[ u_i \] represents the local interface velocity
The method starts as conventional averaging methods

We start from:

\[ \frac{\partial X_k}{\partial t} + u_i \frac{\partial X_k}{\partial x} + v_i \frac{\partial X_k}{\partial y} = 0 \]

\[ \frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0 \]  \hspace{1cm} \text{(pure fluid = Euler for example)}

Fluid selection \( X_k \times \text{Euler} = 0 \)

\[ \frac{\partial X_k U_k}{\partial t} + \frac{\partial X_k F_k}{\partial x} + \frac{\partial X_k G_k}{\partial y} = (F_k - u_i U_k) \frac{\partial X_k}{\partial x} + (G_k - v_i U_k) \frac{\partial X_k}{\partial y} \]

The equations are then integrated over volume and time.
The input with this method is the flow topology

Stratified flow

Bubbly flow

Given the flow topology we are going to integrate over space and time the Riemann problem solutions at each interface inside the 2D control volume and at its boundaries
Finite volume type integration

\[
\frac{\partial X_k U_k}{\partial t} + \frac{\partial X_k F_k}{\partial x} + \frac{\partial X_k G_k}{\partial y} = (F_k - u_i U_k) \frac{\partial X_k}{\partial x} + (G_k - v_i U_k) \frac{\partial X_k}{\partial y}
\]

For the sake of time restrictions and importance we focus on the non-conservative term

\[
\int_0^{\Delta t} \int_{c_{ij}} \left( \frac{\partial X_k U_k}{\partial t} + \frac{\partial X_k F_k}{\partial x} + \frac{\partial X_k G_k}{\partial x} \right) \, dx \, dy \, dt
\]
At a given cell boundary

- The contact length for each pair of fluids are computed

- In this example

\[ S_{11} = H \min(\alpha_{1,i-1}, \alpha_{1,i}) \]
\[ S_{22} = H \min(\alpha_{2,i-1}, \alpha_{2,i}) \]

\[ S_{12} = H - S_{11} - S_{22} \]

- At each contact (11), (12), (22) the Riemann problem is solved
- The fluxes and non conservative terms are integrated along each contact
Focus on non-conservative terms

We have to compute

\[ \int_0^{\Delta t} \int_{C_{ij}} \left( (F - uU) \frac{\partial X_k}{\partial x} \right) \, dx \, dy \, dt \]

\( X_k \) is discontinuous at the interfaces.

But at the interfaces the Lagrangian flux is precisely **locally constant**:

The product \( (F - uU) \frac{\partial X}{\partial x} \) is thus well defined!

\[ F_{\text{Lagrange}} = F - uU = \begin{pmatrix} 0 \\ p \\ pu \end{pmatrix} \]

\( p_I = \text{cst} \), \( u_I = \text{cst} \)

\( p \) Shock \hspace{1cm} Interface
Non conservative terms are thus integrated easily: 

\[
\int_0^{\Delta t} \int_{C_{ij}} \left( (F - u_i U) \frac{\partial X_j}{\partial x} \right) \, dx \, dy \, dt = \Delta t \left( S_{11} X^*_{1,11} F^*_{11}^{\text{Lagrange}} + S_{22} X^*_{2,22} F^*_{22}^{\text{Lagrange}} + S_{12} X^*_{1,12} F^*_{12}^{\text{Lagrange}} \right) 
\]

\[
\int_0^{\Delta t} \int_{C_{ij}} \left( (F - u_i U) \frac{\partial X_j}{\partial x} \right) \, dx \, dy \, dt = \begin{cases} 
- \Delta t S_{22} F^*_{12}^{\text{Lagrange}} & \text{if } u^*_{12} > 0 \\
0 & \text{otherwise}
\end{cases}
\]
$\frac{\alpha_{i,1}^{n+1} U_{i,1}^{n+1} - \alpha_{i,1}^{n} U_{i,1}^{n}}{\Delta t} + \left[ \frac{XF_{1,i+1/2}}{\Delta x} \right]_{1,1} - \left[ \frac{XF_{1,i-1/2}}{\Delta x} \right]_{1,1} = \left( F - u_i U \right) \frac{\partial X}{\partial x} \right)_{i,1} + \text{Relaxation} \}

\{ XF_{1,i-1/2} = \sum \text{segment length} \times \text{charact. func.} \times \text{Riemann flux} \}_{\text{cellboundar}}

\{ (F - u_i U) \frac{\partial X}{\partial x} \}_{i,1} = \sum \text{segment length} \times \text{charact. func.} \times \text{jump} \times \text{Lagrangian Rieman flux} \}_{\text{cellboundar}}

Need to store Eulerian fluxes and Lagrangian fluxes. Not exactly a finite volume method $\rightarrow$ complexity at first order, increasing complexity at second order (extra NC terms appear) etc.

Stiff source terms, vacuum and complex thermodynamic are present too.

A simplified method is needed with enhanced robustness (genuine positivity).
HLLC two-phase (Furfaro and Saurel, C&F 2015)

Key points:
- each subsystem of PDE’s for a given phase can be decoupled of the overall system
- 4 waves only are present (instead of 7),
- a locally conservative formulation is available.
Flow model for a given phase without source terms

\[
\frac{\partial \alpha_1}{\partial t} + \bar{u}_i \frac{\partial \alpha_1}{\partial x} = 0
\]

\[
\frac{\partial (\alpha \rho)}{\partial t} + \frac{\partial (\alpha \rho u)}{\partial x} = 0
\]

\[
\frac{\partial (\alpha \rho u)}{\partial t} + \frac{\partial (\alpha \rho u^2 + \alpha p)}{\partial x} = \bar{p}_i \frac{\partial \alpha_1}{\partial x}
\]

\[
\frac{\partial (\alpha \rho E)}{\partial t} + \frac{\partial (u(\alpha \rho E + \alpha p))}{\partial x} = p_i \bar{u}_i \frac{\partial \alpha_1}{\partial x}
\]

+ interfacial variables given by Euler-Euler Riemann solvers based on left and right initial data

\[
u_i = \frac{Z_1 u_1 + Z_2 u_2}{Z_1 + Z_2} + \text{sgn} \left( \frac{\partial \alpha_1}{\partial x} \right) \left( p_2 - p_1 \right) \]

\[
p_i = \frac{Z_1 p_2 + Z_2 p_1}{Z_1 + Z_2} + \text{sgn} \left( \frac{\partial \alpha_1}{\partial x} \right) \left( u_2 - u_1 \right) \frac{Z_1 Z_2}{Z_1 + Z_2}
\]

These two interfacial variables are thus locally constant.

The phases are coupled only through the NC terms. But \( p_i \) and \( u_i \) are local constants.
Local conservative formulation

\[
\frac{\partial \alpha_1}{\partial t} + \frac{\partial \bar{u}_1 \alpha_1}{\partial x} = 0
\]

\[
\frac{\partial (\alpha \rho)}{\partial t} + \frac{\partial (\alpha \rho u)}{\partial x} = 0
\]

\[
\frac{\partial (\alpha \rho u)}{\partial t} + \frac{\partial \alpha_i \rho_i u_i^2 + \alpha_i (p_i - \bar{p}_i)}{\partial x} = 0
\]

\[
\frac{\partial (\alpha \rho E)}{\partial t} + \frac{\partial (u(\alpha \rho E + \alpha p))}{\partial x} - \bar{p}_i \bar{u}_i \alpha_1 = 0
\]

HLLC with 4 waves (not so simple a priori).
Wave speeds estimates

\[ S_{R,k} = \text{Max}(u_{L,k} + c_{L,k}, u_{R,k} + c_{R,k}) \]

\[ S_{L,k} = \text{Min}(u_{L,k} - c_{L,k}, u_{R,k} - c_{R,k}) \]

\[ S_{M,k} = \frac{\alpha_{R,k} (\rho u^2 + p)_{R,k} - \alpha_{L,k} (\rho u^2 + p)_{L,k} + S_{L,k} (\alpha \rho u)_{L,k} - S_{R,k} (\alpha \rho u)_{R,k} + (\alpha_{L,k} - \alpha_{R,k})p_l}{(\alpha \rho u)_{R,k} - (\alpha \rho u)_{L,k} + S_{L,k} (\alpha \rho)_{L,k} - S_{R,k} (\alpha \rho)_{R,k}} \]

Combining the 4 RH systems across the 4 waves results in:

\[ u_{R,k}^* = \frac{[(\alpha \rho)_{R,k} - (\alpha \rho)_{L,k} + (\alpha_{L,k} - \alpha_{R,k})p_l]S_{R,k} - (\alpha \rho)_{R,k} (u_{R,k} - S_{R,k})(u_{I,S_{M,k}} - S_{R,k}u_{R,k})}{(\alpha \rho)_{R,k} (u_{R,k} - S_{R,k})(S_{R,k} - u_{I} - S_{M,k} + u_{R,k}) + (\alpha \rho)_{L,k} - (\alpha \rho)_{L,k} + (\alpha_{L,k} - \alpha_{R,k})p_l} \]

And a miracle occurs ...

\[ u_{R,k}^* = S_{M,k} \quad \text{(all velocities in star state are equal)} \]
## HLLC summary

<table>
<thead>
<tr>
<th>$W_{L,k}^*$</th>
<th>$W_{R,k}^*$</th>
<th>$W_k^{**}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_{L,k}^* = a_{L,k}$</td>
<td>$a_{R,k}^* = a_{R,k}$</td>
<td>$a_{k}^{**} = a_{L,k}$</td>
</tr>
<tr>
<td>$\rho_{L,k}^* = \rho_{L,k} \frac{u_{L,k} - S_{L,k}}{S_{M,k} - S_{L,k}}$</td>
<td>$\rho_{R,k}^* = \rho_{R,k} \frac{u_{R,k} - S_{R,k}}{S_{M,k} - S_{R,k}}$</td>
<td>$(\alpha \rho)<em>k^{**} = (\alpha \rho)</em>{R,k}^*$</td>
</tr>
<tr>
<td>$u_{L,k}^* = S_{M,k}$</td>
<td>$u_{R,k}^* = S_{M,k}$</td>
<td>$u_k^{**} = S_{M,k}$</td>
</tr>
<tr>
<td>$E_{L,k}^* = E_{L,k} + \frac{(pu)<em>{L,k} - p</em>{L,k}^* S_{M,k}}{\rho_{L,k} (u_{L,k} - S_{L,k})}$</td>
<td>$E_{R,k}^* = E_{R,k} + \frac{(pu)<em>{R,k} - p</em>{R,k}^* S_{M,k}}{\rho_{R,k} (u_{R,k} - S_{R,k})}$</td>
<td>$E_k^{**} = E_{R,k} - \frac{\alpha_{L,k} - \alpha_{R,k}}{(\alpha \rho)_{R,k}^*} p_1$</td>
</tr>
<tr>
<td>$p_{L,k}^* = p_{L,k} + \rho_{L,k} (u_{L,k} - S_{L,k}) (u_{L,k} - S_{M,k})$</td>
<td>$p_{R,k}^* = p_{R,k} + \rho_{R,k} (u_{R,k} - S_{R,k}) (u_{R,k} - S_{M,k})$</td>
<td>$p_k^{**} = p_{L,k}^*$</td>
</tr>
</tbody>
</table>

The solver is explicit.
Its extension to an arbitrary number of fluids is straightforward.
It is entropy preserving (Furfaro and Saurel, 2015) and genuinely positive.
Godunov type scheme

\[
\frac{\partial U_k}{\partial t} + \frac{\partial F_k}{\partial x} + \alpha_k \frac{\partial H_k}{\partial x} = 0
\]

\[
U_k = \begin{pmatrix}
\alpha_k \\
(\alpha \rho)_k \\
(\alpha \rho u)_k \\
(\alpha \rho E)_k
\end{pmatrix}
\]

\[
F_k = \begin{pmatrix}
\alpha_k u_1 \\
(\alpha \rho u)_k \\
\alpha_k (\rho u^2 + p)_k - \alpha_k p_1 \\
\alpha_k (\rho E + p)_k u_k - \alpha_k p_1 u_1
\end{pmatrix}
\]

\[
H_k = \begin{pmatrix}
-u_1 \\
0 \\
p_1 \\
p_1 u_1
\end{pmatrix}
\]

\[
U_{k,i}^{n+1} = U_{k,i}^n - \frac{\Delta t}{\Delta x} \left[ F_{k,i+\frac{1}{2}}^* - F_{k,i-\frac{1}{2}}^* + \alpha_{k,i}^n \left( H_{k,i+\frac{1}{2}}^* - H_{k,i-\frac{1}{2}}^* \right) \right]
\]

\[
H_{k,i}^{*,\pm\frac{1}{2}} = \left[ - (u_1)_{k,i+\frac{1}{2}}, 0, (p_1)_{k,i+\frac{1}{2}}, (p_1 u_1)_{k,i+\frac{1}{2}} \right]^T
\]

This simple method merges with the more sophisticated DEM method.

Warning: When dealing with higher order extensions, extra NC terms appear.
1D test problem: Shock tube with volume fraction discontinuity

Job done by NC terms. No pressure velocity relaxation is needed to fulfill interface conditions.
Double expansion

Lines = DEM results
Symbols = HLLC
3D computations

- Nearly pure dense gas (1500 kg / m³)
- HP chamber (7000 MPa)
- Nearly pure water (1000 kg / m³)
- Atmospheric pressure (0.1 MPa)
- Nearly pure gas (1 kg / m³)
- Atmospheric pressure (0.1 MPa)
Latter times
Thank you for your attention

Announce: There is an open permanent research position at RS2N (small private company) for a young doctor in CFD, see CFD ONLINE or www.rs2n.eu in France, close to Marseille and Aix-en-Provence.
Lagrangian fluxes at internal interfaces

\[ \left\{ (F - u_i U) \frac{\partial X}{\partial x} \right\}_{\text{internal interfaces}} = \Delta t N_a \left( F_{\text{Lag}^*}(2,1) - F_{\text{Lag}^*}(1,2) \right)_{ij} \]

The differences between interface variables inside the control volume result in relaxation terms.