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Study of a collocated Lagrange-Remap scheme for multimaterial flows adapted to HPC

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Outline

1. Collocated Lagrange-Remap scheme features
2. Collocated Lagrange scheme and entropy dissipation
3. Collocated Remap scheme and total energy

Context

- The methods presented here are developped in the SHY code platform (Peybernes, Poncet, Motte, Rivoire), dedicated to research in HPC and numerics.
- The goal is to propose a **multimaterial Eulerian scheme** for the next generation of HPC hydrocodes:
  1. Meshes will be refined: the scheme should be robust, second order in time and space and entropic at first order. If the scheme is conservative, it converges to the right solution.
     $\rightarrow$ *Collocated Lagrange+Remap scheme*
  2. Code scalability: the number of MPI parallel synchronisations should be limited and remap should be generic to allow OpenMP parallel loops and vectorization.
     $\rightarrow$ *Direct multidirectional remap scheme*
- This study is restricted to 2D Cartesian orthogonal meshes and multimaterial flows with two materials (sharp interface).

Collocated Lagrange-Remap scheme

Collocated Lagrangian schemes EUCCLHYD (P.-H. Maire et al, 2007) or GLACE (Després et al, 2005) solve this conservative system:

$$
\left\{
\begin{array}{lcl}
\dfrac{d}{dt}\displaystyle\int_{\Omega(t)} 1dV & = & \displaystyle\int_{\Omega(t)} (\vec{\nabla}.\vec{u})(x.t)dV \\
\dfrac{d\vec{x}(t)}{dt} & = & \vec{u}(x,t) \\
\dfrac{d}{dt}\displaystyle\int_{\Omega(t)} \rho(x,t)dV & = & 0 \\
\dfrac{d}{dt}\displaystyle\int_{\Omega(t)} \rho(x,t)\vec{u}(x,t)dV & = & -\displaystyle\int_{\Omega(t)} \vec{\nabla}P(x,t)dV \\
\dfrac{d}{dt}\displaystyle\int_{\Omega(t)} \rho(x,t)E(x,t)dV & = & -\displaystyle\int_{\Omega(t)} \vec{\nabla}.(P(x,t)\vec{u})(x,t)dV \\
P(x,t) & = & P(\rho(x,t), e(x,t))
\end{array}
\right.
$$

with ρ the density, P the pressure, E the specific total energy and $\vec{u}$ the velocity on volume $\Omega(t)$.

Collocated Lagrange scheme

Multimaterial collocated Lagrange scheme steps:

S. Galera, P.-H. Maire, J. Breil. A two-dimensional unstructured cell-centered multimaterial ALE scheme using VOF interface reconstruction, *J. Comput. Phys.*, 229 (2010), 5755-5787.

1) **Acoustic Godunov Riemann problems at nodes** to obtain node velocities and pressures at half edges with constraints:

- -volume and total energy conservation,
- -entropy dissipation (first order).

2) Fluxes are computed with node velocities and half edges pressures, and variables $(\vec{x}, V, \vec{u}, E)$ are updated.

3) In mixed cell i with materials α:

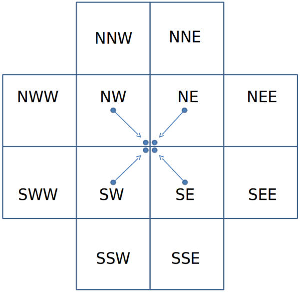
- -velocity is the same for all materials,
- -materials densities evolve considering iso-deformation,
- -mixture pressure is materials pressures volume averaged,
- -specific entropy dissipation rate is the same for all materials:

$$m_\alpha d_t e_\alpha + f_\alpha p_\alpha d_t Vol_i = m_\alpha (T d_t s)_i$$

Collocated Lagrange scheme second order

- Second order in time with predictor-corrector integration.
- Second order in space for node velocities and pressures at half edges, by MUSCL reconstruction at nodes of cell centered variable $P = (u, v, p)$. For instance for SW:

$$P_{SW}^{order2} = P_{SW} + \frac{\varphi(\theta^x_{SW})}{2}(P_{SW} - P_{SWW}) + \frac{\varphi(\theta^y_{SW})}{2}(P_{SW} - P_{SSW})$$



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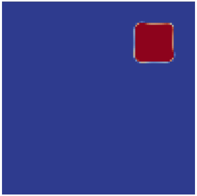
Lagrange Wilkins + Remap: Alternate Directions vs Direct Remap

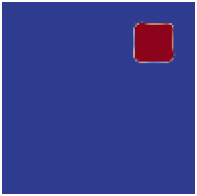
Work with Bastien Chaudet, Master degree training 2014

- Build a Direct remap using the same tools as the ADI remap
- Naive Direct FV remap not very accurate for multimaterial flows → **Direct remap with corner fluxes**
- "Alternate directions" does a good job in many situations.
- Direct remap with corner fluxes is a more complex algorithm, but it could worth when dealing with many cores (scalability).

Direct



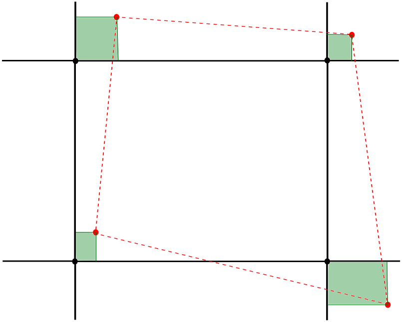
Alternate Directions



Direct Corner Fluxes

Direct Remap with Corner Fluxes

- Lagrangian displacement along all directions,
- Face fluxes, Corner fluxes.



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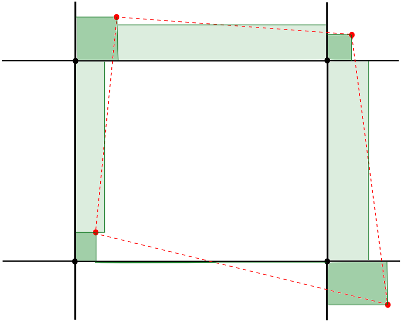

Direct Remap with Corner Fluxes

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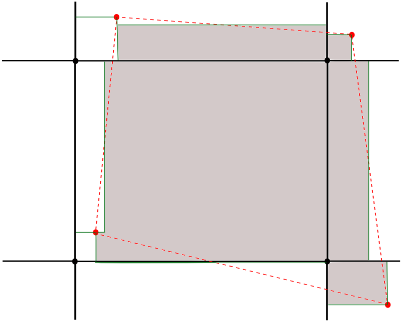


Direct Remap with Corner Fluxes

- Computation of multimaterial faces $dVol_{\alpha f}$ and corners $dVol_{\alpha c}$ volume fluxes,
- Interface positioning with volume fractions (Youngs) and rectangular approximation of the lagrangian cell.

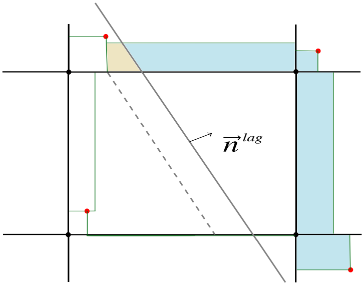
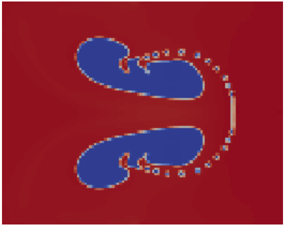


Figure : Intersection between the interface and faces and corners volume fluxes.

Results Wilkins+Remap AD vs Direct with Corner Fluxes

- Interaction between a shock in air and a bubble of Helium. Mesh 1000×90, domain $[0, 1000] \times [0, 9]$cm.

Initial state	Left air state (shock)	Right air state	Bubble
Density ρ (kg.m^3)	1.376363	1	0.18187
Velocity $\mathbf{u}.\mathbf{e}_x$ (m.s^{-1})	124.824	0	0
Pressure p (Pa)	$1.5698\,10^5$	10^5	10^5
Gamma γ	1.4	1.4	1.66



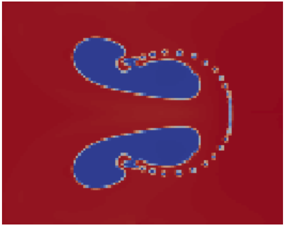


Figure : Zoom, density at final state, $t = 1$ ms. ADI left, DirectCF right.

Results Wilkins+Remap AD vs Direct with Corner Fluxes

- Impact droplet on thin film: Impact of a water drop into air on a water wall. Mesh 320×160, domain $[0,10] \times [0,5]$ cm. Multimaterial, air Perfect Gas, and water Stiffened Gas.

Initial state	Air	Wall	Drop
Density ρ (kg.m^3)	1.29	1000	1000
Velocity $\mathbf{u}.\mathbf{e}_x$ (m.s^{-1})	-1000	0	-1000
Pressure p (Pa)	10^5	10^5	10^5
Gamma γ	1.4	7	7
Pi π (Pa)	0	$2.1\ 10^9$	$2.1\ 10^9$

Results Wilkins+Remap AD vs Direct with Corner Fluxes

- Impact droplet on thin film: Impact of a water drop into air on a water wall. Mesh 320×160, domain $[0, 10] \times [0, 5]$ cm.

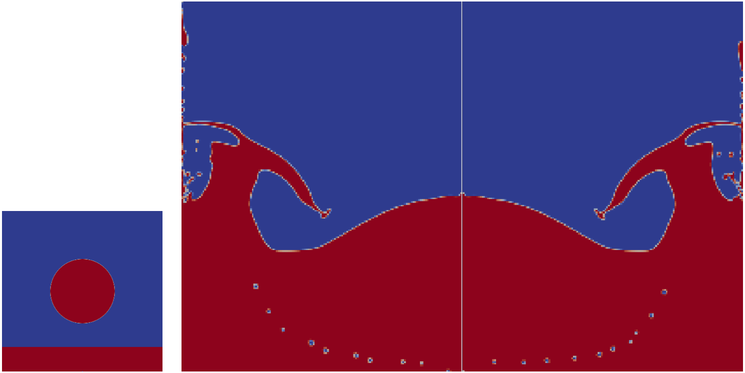


Figure : Volume fraction at initial state, $t = 0$s and $t = 6$s. ADI left, DirectCF right.

Parallelization

Lagrange phase:
$t^n \longrightarrow t^{lag}$

MPI communications between subdomains

Nodal solver	OpenMP loops on nodes
Variables evolution	OpenMP loops on cells

Remap phase:
$t^{lag} \longrightarrow t^{n+1}$

MPI communications between subdomains

Multimaterial Fluxes	OpenMP loops on directions/faces
Variables Remap	OpenMP loops on cells

Figure : Sketch of the hybrid parallelization MPI-OpenMP.

Diminishing entropy dissipation

$\rightarrow$ Good scheme properties (numerics, HPC),

but entropy dissipation: can we diminish it ?

Diminishing entropy dissipation

FRAMEWORK: the time derivative is considered at the discrete level, whatever the time integration scheme:

$$d_t A = \frac{A^{n+1} - A^n}{\Delta t}$$

For a cell i, EUCCLHYD scheme writes:

$$\begin{aligned}
m_i d_t(1/\rho_i) &= \ [\nabla \cdot u]_i &&= \int_{\Omega_i} \nabla \cdot u = \sum_f A_f (u_f \cdot n_f) \\
m_i d_t(u_i) &= - \ [\nabla p]_i &&= \int_{\Omega_i} -\nabla p = -\sum_f A_f p_f n_f \\
m_i d_t(E_i) &= - \ [\nabla \cdot (p \ u)]_i &&= \int_{\Omega_i} -\nabla \cdot (p \ u) = -\sum_f A_f p_f (u_f \cdot n_f)
\end{aligned} \tag{1}$$

Flux terms $[\nabla \cdot u]_i$, $[\nabla p]_i$, $[\nabla \cdot (p \ u)]_i$ computation is detailed in EUCCLHYD literature.

Scheme diffusion of velocity

In 1D, $Vol_i = 1 \cdot \Delta x_i$ and EUCCLHYD is the Godunov acoustic scheme:

$$p_{i+1/2} = \overline{p}_{i+1/2} - \frac{\overline{\alpha}_{i+1/2}}{2}(u_{i+1} - u_i) \tag{2}$$

$$\begin{aligned}\rho_i d_t(u_i) &= -\frac{\overline{p}_{i+1/2} - \overline{p}_{i-1/2}}{\Delta x_i} + \frac{\overline{\alpha}_{i+1/2}(u_{i+1} - u_i) - \overline{\alpha}_{i-1/2}(u_i - u_{i-1}}{2\Delta x_i} \\ &\# - \partial_x(p + q)\end{aligned} \tag{3}$$

with an equivalent linear artificial viscosity $q = \frac{1}{2}\rho c \Delta u$.

Scheme diffusion of pressure

In 1D, $Vol_i = 1 \cdot \Delta x_i$ and EUCCLHYD is the Godunov acoustic scheme:

$$u_{i+1/2} = \overline{u}_{i+1/2} - \frac{p_{i+1} - p_i}{2\overline{\alpha}_{i+1/2}} \tag{4}$$

Considering an isentropic flow, $\dfrac{dp}{d\rho} = c^2$:

$$d_t p_i = -(\rho c^2)_i \frac{\overline{u}_{i+1/2} - \overline{u}_{i-1/2}}{\Delta x_i} + \frac{(\rho c^2)_i}{\Delta x_i} \left(\frac{p_{i+1} - p_i}{2\overline{\alpha}_{i+1/2}} - \frac{p_i - p_{i-1}}{2\overline{\alpha}_{i-1/2}} \right) \tag{5}$$

No equivalent term within the "artificial viscosity" framework.

Diminishing entropy dissipation

We choose an explicit discretization to describe entropy evolution:

$$m_i T_i^n d_t(s_i) \quad = m_i d_t(e_i) + m_i p_i^n d_t(1/\rho_i) \tag{6}$$

Let us compute it in function of fluxes using equations (1):

$$\begin{aligned} m_i d_t(E_i) \quad &= -[\nabla \cdot (p\ u)]_i \\ &= m_i d_t(e_i) + m_i d_t(u_i^2/2) \\ &= m_i T_i^n d_t(s_i) - p_i^n [\nabla \cdot u]_i - u_i^n \cdot [\nabla p]_i \end{aligned} \tag{7}$$

Finally: $m_i T_i^n d_t(s_i) = -[\nabla \cdot (p\ u)]_i + p_i^n [\nabla \cdot u]_i + u_i^n \cdot [\nabla p]_i$

For the EUCCLHYD scheme in 1D, it comes:

$$m_i T_i^n d_t(s_i) = \frac{1}{2} \rho_i c_i \Delta u_i^2 = q[\partial_x u]_i$$

with the equivalent linear artificial viscosity $q = \dfrac{1}{2}\rho c \Delta u$.

Diminishing entropy dissipation

Flows with $u \neq cst$ are computed with an entropy dissipation corresponding to a linear artificial viscosity with coefficient $1/2$:

$$m_i d_t(e_i) + m_i p_i^n d_t(1/\rho_i) = m_i T_i^n d_t(s_i) \;\; \# \;\; \frac{1}{2}\rho_i c_i (\Delta u_i)^2 > 0 \tag{8}$$

Key ideas:

- **We want to reduce EUCCLHYD's entropy dissipation** on isentropic flows.
- **Robustness: same velocity and pressure numerical diffusion** coming from acoustic Godunov solver (no use of Dukowicz solver, A. Burbeau, R. Loubere-P.-H. Maire).
- We allow a trade off with total energy conservation: **quasi-conservation to keep proper shock waves propagation.**

Diminishing entropy dissipation

Thus we introduce a parameter $0 \leq \theta_i \leq 1$ such that:

$$d_t(e_i) + p_i^n d_t(1/\rho_i) = \theta_i T_i^n d_t s_i$$

$$\rightarrow m_i d_t(E_i) = -\theta_i[\nabla \cdot (p\ u)]_i + (1-\theta_i)\left(-u_i^n \cdot [\nabla p]_i - p_i^n[\nabla \cdot u]_i\right)$$

Rough idea:

When dealing with shock waves:
$\theta_i = 1$, *EUCCLHYD, entropic and total energy conservation*

When computing an isentropic flow:
$\theta_i = 0$, *isentropic but non conservative in total energy*

The idea comes from classical schemes with artificial viscosity, and is mentionned in C. Mazeran's PhD thesis 2007 (with B. Després) and D. Chauveheid PhD thesis 2012 (with J.M. Ghidaglia).

Diminishing entropy dissipation

$$R_i = \frac{T_i^n d_t(s_i)}{|p_i^n d_t(1/\rho_i)|} = \frac{-[\nabla \cdot (p\ u)]_i + u_i^n \cdot [\nabla p]_i + p_i^n [\nabla \cdot u]_i}{|p_i^n [\nabla \cdot u]_i|}$$

The analysis of R_i (acoustic Riemann problems, strong shock or rarefaction waves) leads to a proposition for $0 \leq \theta_i \leq 1$:

<u>$T_i^n d_t(s_i) > 0$:</u>

$$\rightarrow [\nabla \cdot u]_i < 0 \ \ (shock\ \ wave)$$
$$\theta_i = \min(1,\ C_q\ R_i)$$

$$\rightarrow [\nabla \cdot u]_i > 0 \ \ (quasi\text{-}conservation\ of\ \ E_{tot}\ \ and\ \ possibly\ \ isentropic)$$
$$\theta_i = \min\left(1,\ \frac{|p_{i+1}^n - 2\ p_i^n + p_{i-1}^n|}{\min(p_{i-1}^n, p_i^n, p_{i+1}^n)}\right)$$

<u>$T_i^n d_t(s_i) \leq 0$:</u>

$$\theta_i = 1 \ \ (EUCCLHYD\ \ scheme).$$

Diminishing entropy dissipation

1D shock wave: $T_i^n d_t(s_i) \geq 0$, $[\nabla \cdot u]_i < 0$ and $\theta_i = C_q R_i < 1$:

$$m_i \left(d_t(e_i) + p_i^n d_t(1/\rho_i) \right) = \frac{C_q \left(\frac{1}{2} \rho_i c_i (\Delta u_i)^2 \right)^2}{p_i^n \Delta u_i} \# q_i [\partial_x u]_i \tag{9}$$

It comes a quadratic artificial viscosity:

$$q_i = C_q \left(\frac{\rho_i (c_i)^2}{4 \ p_i} \right) \rho_i (\Delta u_i)^2 \tag{10}$$

We set $C_q = 4$ because for perfect gases $\rho_i (c_i)^2 / p_i = \gamma_i > 1$ should be a proper value as a quadratic artificial viscosity coefficient.

Diminishing entropy dissipation WILKINS/EUCCLHYD + Remap

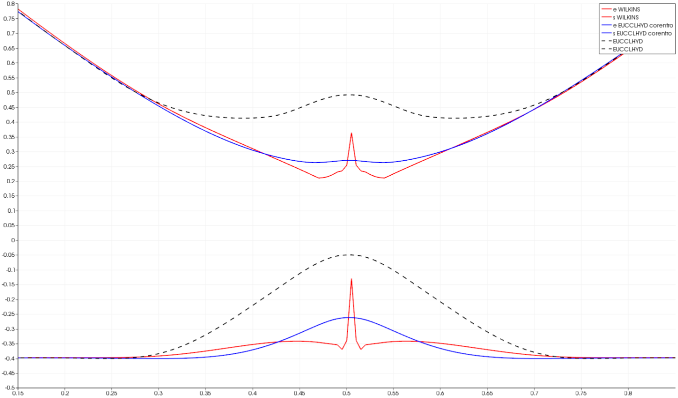


Figure : Double rarefaction wave 1D 200 cells, **internal energy (above), entropy (below)**: EUCCLHYD (black dash), EUCCLHYD quasi-conservation (blue), WILKINS Qquad=2 Qlin=0.1 (red).

Diminishing entropy dissipation EUCCLHYD+Remap

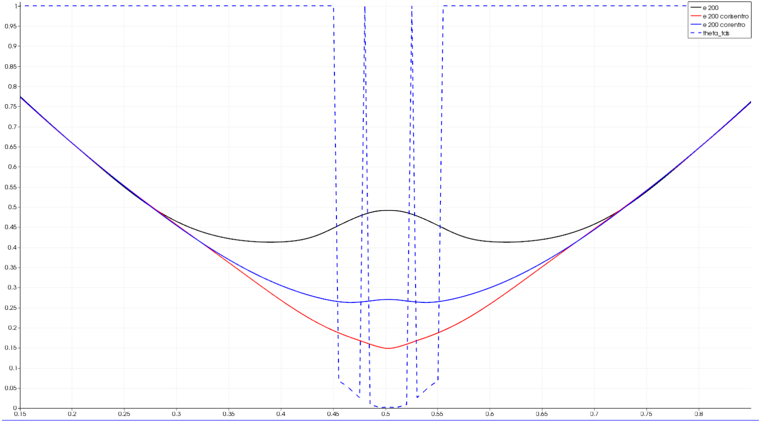


Figure : Double rarefaction wave 1D 200 cells, **internal energy**: EUCCLHYD (black), EUCCLHYD isentropic in rarefaction waves (red) or EUCCLHYD quasi-conservation (blue) with theta (blue dash).

Diminishing entropy dissipation
CONVERGENCE EUCCLHYD + Remap

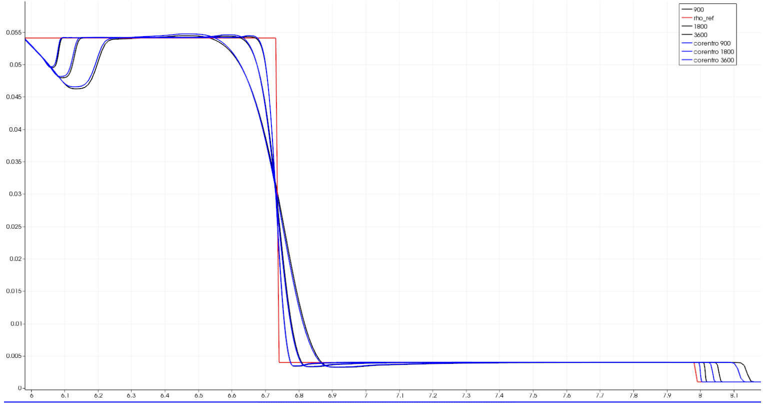


Figure : HELL (LeBlanc Shock tube) 1D 900, 1800 and 3600 cells, **density**: EUCCLHYD (black), EUCCLHYD quasi-conservation (blue).

Diminishing entropy dissipation WILKINS/EUCCLHYD + Remap

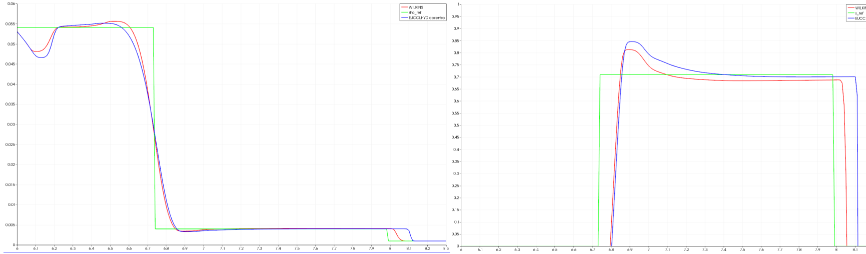


Figure : HELL (LeBlanc Shock tube) 1D 900 cells, **density (left), entropy (right)**: EUCCLHYD quasi-conservation (blue) and WILKINS (red).

Diminishing entropy dissipation WILKINS/EUCCLHYD + Remap

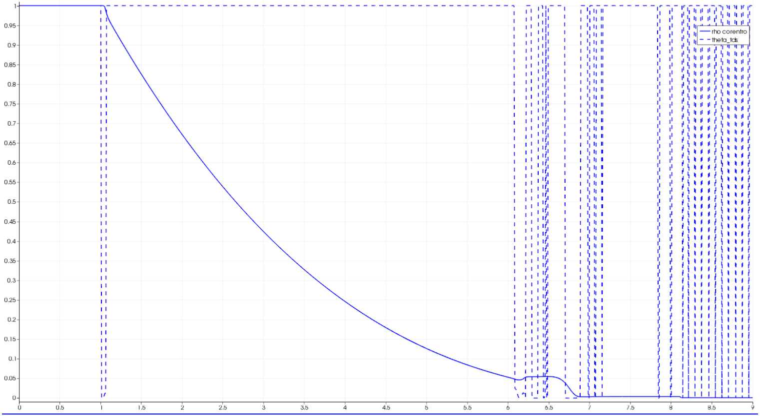


Figure : HELL (LeBlanc Shock tube) 1D 900 cells, **density (blue) and theta (blue dash)** for EUCCLHYD quasi-conservation.

Diminishing entropy dissipation WILKINS/EUCCLHYD + Remap

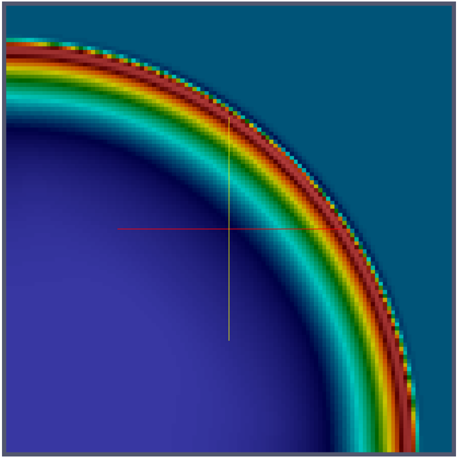


Figure : SEDOV 2D 110x110 cells, **density**.

Diminishing entropy dissipation WILKINS/EUCCLHYD + Remap

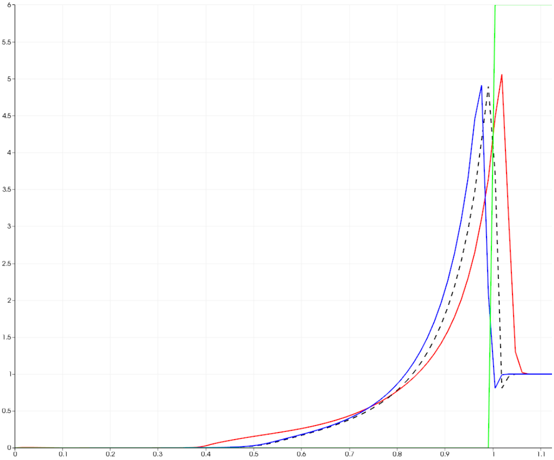


Figure : SEDOV 2D 110x110 cells, **density**: EUCCLHYD (black dash), EUCCLHYD quasi-conservation (blue) or WILKINS (red).

Diminishing entropy dissipation
WILKINS/EUCCLHYD + Remap

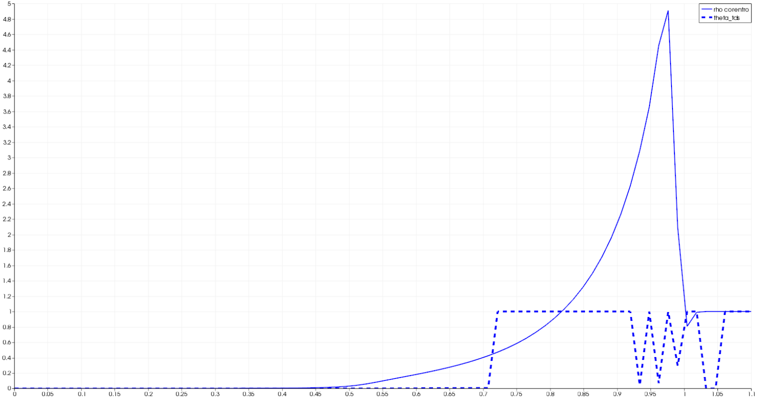


Figure : SEDOV 2D 110x110 cells, **density (blue) with theta (blue dash)** for EUCCLHYD quasi-conservation.

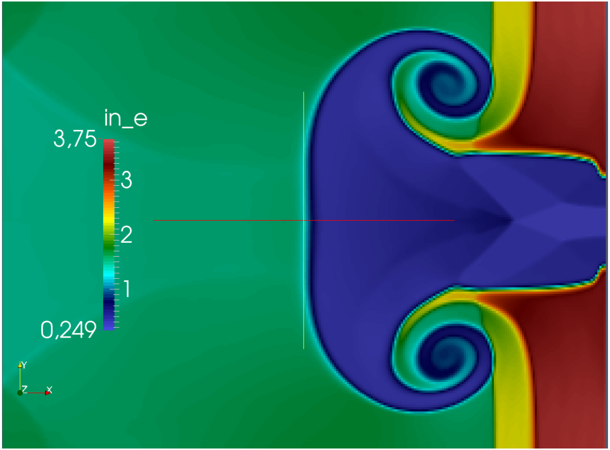


Figure : Triple point 2D 280x120 cells, **internal energy**: EUCCLHYD (top), EUCCLHYD quasi-conservation (bottom).

Diminishing entropy dissipation WILKINS/EUCCLHYD + Remap

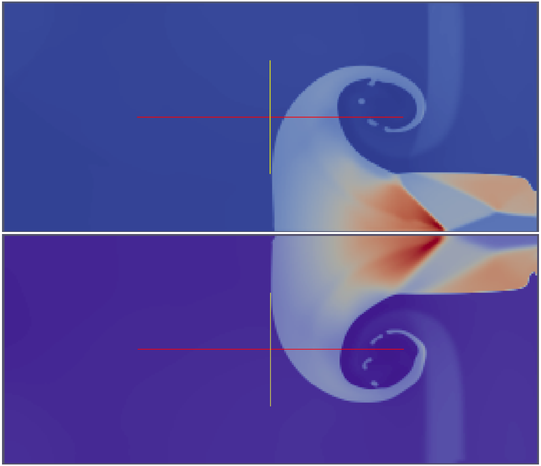


Figure : Multimaterial Triple point 2D 280x120 cells, **density**: EUCCLHYD quasi-conservation (top) and WILKINS (bottom).

Collocated Remap scheme and total energy

$\rightarrow$ Conservative remap of total energy, effect on internal energy.

Collocated Remap scheme

Remap phase is achieved by using a flux scheme, thus is fully conservative:

$$
\begin{cases}
Vol_i & = & Vol_i^{lag} + \sum_f dVol_f \\
m_i & = & m_i^{lag} + \sum_f dm_f \\
u_i & = & \left(u_i^{lag} m_i^{lag} + \sum_f dqu_f \right) / m_i \\
v_i & = & \left(v_i^{lag} m_i^{lag} + \sum_f dqv_f \right) / m_i \\
E_i & = & \left(E_i^{lag} m_i^{lag} + \sum_f dmE_f \right) / m_i \\
e_i & = & E_i - (u_i)^2/2 + (v_i)^2/2
\end{cases}
$$

Collocated Remap scheme

Remap phase is achieved by using a flux scheme, thus is fully conservative:

$$\left\{\begin{array}{lllll} dm_f & = & & \rho_f^{o2} & dVol_f \\ dqu_f & = & \rho_f^{o2} & u_f^{o2} & dVol_f \\ dqv_f & = & \rho_f^{o2} & v_f^{o2} & dVol_f \\ dmE_f & = & \rho_f^{o2} & (e_f^{o2} + k_f^{o2}) & dVol_f \end{array}\right.$$

$$k_f^{o2} = \frac{(u_f^{o2})^2}{2} - \frac{(u_f^{o2} - u_{f\ upw}^{lag})^2}{2} + \frac{(v_f^{o2})^2}{2} - \frac{(v_f^{o2} - v_{f\ upw}^{lag})^2}{2}$$

with at face f:

ρ_f^{o2} the limited linear reconstruction of ρ,

$u_{f\ upw}^{lag}$ the upwind value on the Lagrange mesh.

Collocated Remap scheme

Let us consider a **face** f **between lagrangian cells** i **and** $i+1$:

$$m_i E_i - m_i^{lag} E_i^{lag} + dm_f E_f^{o2} = 0$$

$$\rightarrow m_i e_i - m_i^{lag} e_i^{lag} + dm_f e_f^{o2} = \epsilon_i^x + \epsilon_i^y$$

with

$$\epsilon_i^x = m_i^{lag} k_i^{x\ lag} - m_i k_i^x - dm_f k_f^{x\ o2}$$
$$\epsilon_i^y = m_i^{lag} k_i^{y\ lag} - m_i k_i^y - dm_f k_f^{y\ o2}$$

with $k_i^{lag} = (u_i^{lag})^2/2$ and $k_i = (u_i)^2/2$.

Since we would like an "adiabatic" remap, we should find $k_f^{x\ o2}$ such that $\epsilon_i^x \approx 0$ and $\epsilon_{i+1}^x \approx 0$.

Collocated Remap scheme

Which value for the kinetic energy flux "$dm_f k_f^{x\ o2}$" to obtain $\epsilon_i^x \approx 0$ and $\epsilon_{i+1}^x \approx 0$?

If $k_f^{x\ o2} = (u_f^{o2})^2/2$:

$$\rightarrow \begin{cases} \epsilon_i^x = -\left(\dfrac{dm_f m_i^{lag}}{m_i}\right) \dfrac{(u_f^{o2} - u_i^{lag})^2}{2} < 0 \\ \epsilon_{i+1}^x = \left(\dfrac{dm_f m_{i+1}^{lag}}{m_{i+1}}\right) \dfrac{(u_f^{o2} - u_{i+1}^{lag})^2}{2} > 0 \end{cases}$$

If $k_f^{x\ o2} = (u_f^{o2})^2/2 - (u_f^{o2} - u_i^{lag})^2/2$:

$$\rightarrow \begin{cases} \epsilon_i^x = -\left(\dfrac{(dm_f)^2}{m_i}\right) \dfrac{(u_f^{o2} - u_i^{lag})^2}{2} < 0 \\ \epsilon_{i+1}^x = \left(\dfrac{dm_f}{m_{i+1}}\right) \left(m_{i+1}^{lag} \dfrac{(u_f^{o2} - u_{i+1}^{lag})^2}{2} - m_{i+1} \dfrac{(u_f^{o2} - u_i^{lag})^2}{2}\right) \end{cases}$$

Collocated Remap scheme

Figure : Double rarefaction wave, 200 cells, **internal energy (above) and entropy (below)**, comparison between isentropic schemes: WILKINS q=0 + internal energy remap, EUCCLHYD $\theta = 0$ isentropic + total energy remap, with and without corrected "k".

Conclusion-Perspectives

- Goal: propose a multimaterial scheme adapted to HPC on exascale computers constraints.
- Collocated Lagrange EUCCLHYD-Remap is robust, conservative and entropic (first order).
- Multidirectional direct remap and multimaterial interface sharp reconstruction is classical and robust. An explicit partial pressure relaxation is available.
- The trade off with total energy to reduce entropy error should be further investigated, i.e. quasi-conservation should be proved and quantified.
- The algorithm parallelization efficiency should be evaluated (scalability).