A Mixing Model for multimaterial computations in fluid dynamics: Remapping and ALE

Raphaël Loubère, Mikhail J. Shashkov
Theoretical Division, T-7, Los Alamos National Laboratory
MS-B284, Los Alamos, NM, 87545, USA
loubere@lanl.gov, shashkov@lanl.gov
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1 Introduction

This report is an extension of the previous reports [1] and [2] dealing with a new model for mixed cell introduced by B.Després and F.Lagoutiére in [9]. In these reports we presented the mixing model and it implementation into a 1D Lagrangian code. The present report extends the idea of having mixed cells to the context of Arbitrary-Lagrangian-Eulerian (ALE) simulations in 1D.

We first review the mixing model (section 2), then present it implementation as a stand-alone solver (section 3). then the Lagrangian scheme, rezone and remap phases in presence of mixed cell are described (sections 4, 5, 6). We focus our attention to the three step remap stage (gather, remap, scatter) as it is the most difficult part in this context of mixed cells. The entire process is therefore much detailed.

Finally in section 7, we present some numerical results to prove that the implementation of these ideas into the 1D ALE code described in [11] does not produce any numerical artifacts or parasital oscillations.

2 Presentation of the Mixing Model (MM)

The 1D Euler equations for one fluid, in Eulerian coordinates are given by

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 & \text{(mass)}, \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0 & \text{(momentum)}, \\ \partial_t(\rho e) + \partial_x(\rho u e + p u) = 0 & \text{(total energy)}, \\ \partial_t \rho S + \partial_x(\rho u S) \geq 0, & \end{cases} \tag{2.1}$$

knowing the second principle of the thermodynamic $TdS = d\varepsilon + pd\tau = \delta Q$.
In the previous equations ρ is the density, u the velocity, p the pressure (given by an Equation Of State EOS), e the total energy, ε the internal energy, S the mathematical entropy, T the temperature and $\tau = 1/\rho$ the specific volume.

The principle we are going to follow to develop the model states that: *The multi-material model should satisfy the entropy inequality.*

The 1D Euler equation for m fluids can be written as

$$\begin{cases} \partial_t(\rho c_i) + \partial_x(\rho c_i u) = 0, & \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0, & \text{(momentum)}, \\ \partial_t(\rho e) + \partial_x(\rho u e) = 0, & \text{(total energy)}, \end{cases} \tag{2.2}$$

where c_i is the concentration of fluid i and $0 \leq c_i \leq 1$. Clearly the concentrations fulfill

$$\sum_{i=1}^{m} c_i = 1, \tag{2.3}$$

The variables are linked to each other thanks to $\rho = \frac{1}{\tau}$ and $e = \varepsilon + \frac{1}{2}u^2$. Moreover

$$\tau = \sum_{i=1}^{m} c_i \tau_i, \tag{2.4}$$

$$\varepsilon = \sum_{i=1}^{m} c_i \varepsilon_i. \tag{2.5}$$

Even if these equations are natural the system is ill-posed because we have more unknowns than equations. Therefore a compatibility principle has to be chosen in order to close such a system. This principle states that each fluid has its own thermodynamic characteristics

$$p_i = p(\tau_i, \varepsilon_i), \tag{2.6}$$

$$T_i dS_i = d\varepsilon_i + p_i d\tau_i, \tag{2.7}$$

and the principle will enforce

$$T\mathrm{D}_t S = \mathrm{D}_t \varepsilon + p\mathrm{D}_t \tau, \tag{2.8}$$

where $\mathrm{D}_t = \partial_t + u\partial_x$ is the particle derivative and the total entropy is given by

$$S = \sum_{i=1}^{m} c_i S_i. \tag{2.9}$$

This principle will actually be enough to close the system, indeed let's write the sum for all fluids using (2.7) into

$$\sum_{i=1}^{m} c_i \left(T_i \mathrm{D}_t S_i\right) = \sum_{i=1}^{m} c_i (\mathrm{D}_t \varepsilon_i + p_i \mathrm{D}_t \tau_i) \tag{2.10}$$

$$= \mathrm{D}_t \varepsilon + \sum_{i=1}^{m} c_i p_i \mathrm{D}_t \tau_i, \tag{2.11}$$

(recall that $\mathrm{D}_t c_i = 0$) but $\mathrm{D}_t \varepsilon = T\mathrm{D}_t S - p\mathrm{D}_t \tau$, then

$$\sum_{i=1}^{m} c_i \left(T_i \mathrm{D}_t S_i\right) = T\sum_{i=1}^{m} c_i \mathrm{D}_t S_i + \sum_{i=1}^{m} c_i p_i \mathrm{D}_t \tau_i - p\sum_{i=1}^{m} c_i \mathrm{D}_t \tau_i, \tag{2.12}$$

equivalently written into

$$\sum_{i=1}^{m} c_i \left(T_i \mathrm{D}_t S_i\right) - T\sum_{i=1}^{m} c_i \mathrm{D}_t S_i = \sum_{i=1}^{m} c_i p_i \mathrm{D}_t \tau_i - p\sum_{i=1}^{m} c_i \mathrm{D}_t \tau_i. \tag{2.13}$$

The right hand side of the previous equation is constructed only with "temperature" terms. On the other hand, the left hand side of the previous equation is constructed only with "pressure" terms. Philosophically we can state that considerations on "pressure" and "temperature" are different and, arbitrarily, split the previous equation into to two equations, each of them set to zero, that is

$$\sum_{i=1}^{m} c_i T_i \mathrm{D}_t S_i - T\sum_{i=1}^{m} c_i \mathrm{D}_t S_i = 0, \tag{2.14}$$

$$\sum_{i=1}^{m} c_i p_i \mathrm{D}_t \tau_i - p\sum_{i=1}^{m} c_i \mathrm{D}_t \tau_i = 0. \tag{2.15}$$

A closure model has then to be chosen to link T to T_i and p to p_i to solve (2.14–2.15). The most simple and common closure is the isobaric-isothermal one, stating that $p = p_i$ (isobaric) and $T = T_i$ (isothermal). With such a choice equations (2.14–2.15) are clearly true. However our closure choice will be different. First of all the isobaric closure is kept because pressures often relax to equilibrium and keeping $p_i = p$ seems reasonable. On the other hand we don't want to keep the isothermal closure because it needs the knowledge of $(c_v)_i$, the specific heats in the EOS for each fluid. Instead we are going to use

$$T_i \mathrm{D}_t S_i = T_j \mathrm{D}_t S_j, \tag{2.16}$$

for any pair of fluids i and j. Equation (2.16) can be rewritten into

$$\mathrm{D}_t \varepsilon_i + p_i \mathrm{D}_t \tau_i = \mathrm{D}_t \varepsilon_j + p_j \mathrm{D}_t \tau_j, \tag{2.17}$$

the value of total temperature T being given by

$$\frac{1}{T} = \sum_{i=1}^{m} \frac{c_i}{T_i}. \tag{2.18}$$

In order to simplify the notations we will consider only two fluids denoted by script 1 and 2. The model we are considering can be written formally into

$$\begin{aligned}
\partial_t \rho + \partial_x(\rho u) + \partial_y(\rho v) &= 0, && (2.19)\\
\partial_t(\rho c_1) + \partial_x(\rho u c_1) &= 0, && (2.20)\\
\partial_t(\rho c_2) + \partial_x(\rho u c_2) &= 0, && (2.21)\\
\partial_t(\rho u) + \partial_x(\rho u^2 + p) &= 0, && (2.22)\\
\partial_t(\rho e) + \partial_x(\rho u e + p u) &= 0, && (2.23)\\
c_1\tau_1 + c_2\tau_2 = \tau = 1/\rho, & && (2.24)\\
e = c_1\varepsilon_1 + c_2\varepsilon_2 + \frac{1}{2}|\vec{u}|^2, & && (2.25)\\
p_1 = p_2 = p, & && (2.26)\\
\mathrm{D}_t\varepsilon_1 + p_1\mathrm{D}_t\tau_1 = \mathrm{D}_t\varepsilon_2 + p_2\mathrm{D}_t\tau_2. & && (2.27)
\end{aligned}$$

Remark that the isobaric-isothermal model would have been the same, only the last equation would have been replaced by $T_1 = T_2 = T$. This mixing model is hyperbolic (as is the isobaric-isothermal model). A second property of this model is that, for smooth solutions, every fluid fulfills

$$\mathrm{D}_t S_i = 0. \tag{2.28}$$

The mathematical accuracy of (2.19–2.27) is clear for smooth flows. For discontinuous flows, a clear interpretation of (2.27) is deduced form the discretised form.

3 Implementation of the mixing model

The Lagrangian scheme we use is a staggered scheme with a compatible discretisation using a classical artificial viscosity. Such a scheme increments the fluid variables (cell-centered density, nodal velocity and cell-centered specific internal energy) and the mesh position at every time step. The time discretisation is performed with a predictor-corrector scheme.

Consider a domain split into three parts: a pure area of fluid 1, one mixed cell and a pure area of fluid 2. Assume that the numerical scheme provides at time $t = t_n$ the following set of data for the mixed cell:

c_1^{ini}, c_2^{ini}	:	concentrations,
$\tau_1^{ini}, \tau_2^{ini}$	:	specific volumes,
$\varepsilon_1^{ini}, \varepsilon_2^{ini}$	:	specific internal energies,
τ^{ini}	:	total specific volume,
ε^{ini}	:	total specific internal energy.

The point is to be able to compute a total pressure p in the mixed cell, and deduce $\varepsilon_1, \varepsilon_2$, and τ_1, τ_2. The concentrations c_1, c_2 will not evolve during this step so $c_1 = c_1^{ini}$ and $c_2 = c_2^{ini}$.
During the Lagrangian step one needs to solve the following system

$$\begin{aligned}
c_1^{ini}\tau_1 + c_2^{ini}\tau_2 &= \tau^{ini}, && (3.1)\\
c_1^{ini}\varepsilon_1 + c_2^{ini}\varepsilon_2 &= \varepsilon^{ini}, && (3.2)\\
p_1(\tau_1,\varepsilon_1) &= p_2(\tau_2,\varepsilon_2), && (3.3)\\
\varepsilon_1 - \varepsilon_1^{ini} + p_1(\tau_1 - \tau_1^{ini}) &= \varepsilon_2 - \varepsilon_2^{ini} + p_2(\tau_2 - \tau_2^{ini}), && (3.4)
\end{aligned}$$

This system has four equations and four unknowns $\tau_1, \tau_2, \varepsilon_1, \varepsilon_2$ and has an exact solution for a perfect EOS[1]. This solution can be computed by choosing $p = p_1 = p_2$ as the principal unknown. The perfect EOS leads to

$$p = (\gamma - 1)\frac{\varepsilon}{\tau} \quad \Longrightarrow \quad \varepsilon + p\tau = \gamma\varepsilon, \tag{3.5}$$

and equation (3.4) can be rewritten into

$$\gamma_1\varepsilon_1 - \gamma_2\varepsilon_2 = a + bp \tag{3.6}$$

where $a = \varepsilon_1^{ini} - \varepsilon_2^{ini}$ and $b = \tau_1^{ini} - \tau_2^{ini}$. The 2×2 linear system on $\varepsilon_1, \varepsilon_2$ is given by

$$\begin{aligned}
c_1\varepsilon_1 + c_2\varepsilon_2 &= \varepsilon^{ini}, && (3.7)\\
\gamma_1\varepsilon_1 - \gamma_2\varepsilon_2 &= a + bp. && (3.8)
\end{aligned}$$

The determinant of this system $D = c_1\gamma_2 + c_2\gamma_1 \neq 0$, then this system is always invertible and its solution is

$$\begin{aligned}
\varepsilon_1 &= \alpha_1 + \beta_1 p, && (3.9)\\
\varepsilon_2 &= \alpha_2 + \beta_2 p, && (3.10)
\end{aligned}$$

where the coefficients $\alpha_1, \alpha_2, \beta_1, \beta_2$ are given by

$$\begin{aligned}
\alpha_1 &= \frac{1}{D}\left(\gamma_2\varepsilon^{ini} + c_2(\varepsilon_1^{ini} - \varepsilon_2^{ini})\right), && (3.11)\\
\alpha_2 &= \frac{1}{D}\left(\gamma_1\varepsilon^{ini} - c_1(\varepsilon_1^{ini} - \varepsilon_2^{ini})\right), && (3.12)\\
\beta_1 &= \frac{1}{D}\left(\tau_1^{ini} - \tau_2^{ini}\right), && (3.13)\\
\beta_2 &= -\frac{1}{D}\left(\tau_1^{ini} - \tau_2^{ini}\right). && (3.14)
\end{aligned}$$

The specific volumes are given by the EOS

$$\begin{aligned}
\tau_1 &= (\gamma_1 - 1)\frac{\varepsilon_1}{p} = (\gamma_1 - 1)\left(\frac{\alpha_1}{p} + \beta_1\right), && (3.15)\\
\tau_2 &= (\gamma_2 - 1)\frac{\varepsilon_2}{p} = (\gamma_2 - 1)\left(\frac{\alpha_2}{p} + \beta_2\right). && (3.16)
\end{aligned}$$

The linear relation (3.1) between τ_1 and τ_2 becomes

$$c_1(\gamma_1 - 1)\left(\frac{\alpha_1}{p} + \beta_1\right) + c_2(\gamma_2 - 1)\left(\frac{\alpha_2}{p} + \beta_2\right) = \tau^{ini}, \tag{3.17}$$

the value of the pressure p is deduced from the previous equations as

$$p = \frac{c_1(\gamma_1 - 1)\alpha_1 + c_2(\gamma_2 - 1)\alpha_2}{\tau^{ini} - c_1(\gamma_1 - 1)\beta_1 - c_2(\gamma_2 - 1)\beta_2}. \tag{3.18}$$

[1] For non perfect EOS a local Newton algorithm can be used to solve the system.

Once p is known then τ_1, τ_2 and $\varepsilon_1, \varepsilon_2$ are deduced. As previously noticed the concentrations c_1, c_2 are not evolving during the Lagrangian step. This finalizes the mixing model implementation for one Lagrangian step.

The Mixing Model (MM) can be viewed as a solver that takes $\left(\rho^{ini}, \varepsilon^{ini}, \tau_1^{ini}, \tau_2^{ini}, \varepsilon_1^{ini}, \varepsilon_2^{ini}, c_1^{ini}, c_2^{ini}\right)$ as input data and returns the mixed cell pressure p_{mix} *via* equation (3.18) and the updated values of $\tau_1, \tau_2, \varepsilon_1, \varepsilon_2$. It can be sketched as:

$$p_{mix} = \mathrm{MM}\left(\rho^{ini}, \varepsilon^{ini}, \tau_1^{ini}, \tau_2^{ini}, \varepsilon_1^{ini}, \varepsilon_2^{ini}, c_1^{ini}, c_2^{ini}; \tau_1, \tau_2, \varepsilon_1, \varepsilon_2\right). \tag{3.19}$$

We showed in a previous report that such a mixing model behaves nicely on 1D Riemann problems like Sod, Le Blanc problems in pure Lagrangian simulation where only one cell is treated as a mixed cell but with the same gammas . In a more recent report we also showed that on more advanced problems (Collela-Woodward blastwave and a modification to take into account two ratios of specific heats γ) the model encounters some difficulties.

4 Lagrangian scheme in presence of mixed cell

The staggered Lagrangian predictor-corrector scheme in 1D with the mixed model is described in this section.
Let's assume a 1D mesh is given with N_c cells and $N_p = Nc + 1$ points, which position are denoted X_i, $\forall 1 \le i \le N_p$. Each cell $C_{i+1/2}$ is split into two subcells: $S_i^+ = [X_i; X_{i+1/2}]$ and $S_{i+1}^- = [X_{i+1/2}; X_{i+1}]$ where initially $X_{i+1/2} = \frac{1}{2}(X_i + X_{i+1})$. In this discretization zone /point mass $M_{i+1/2}, M_i$ are constant in time as well as subzonal mass m_i^+, m_{i+1}^-. In our discretization we assume that subcell are always pure, meaning that in a mixed cell we have: $S_i^+ = [X_i; X_{intf}]$ and $S_{i+1}^- = [X_{intf}; X_{i+1}]$, where X_{intf} is the real interface position.

Assume the given data at t_n are: a time step Δt, zone density $\rho_{i+1/2}^n$, zone specific internal energy $\varepsilon_{i+1/2}^n$, nodal velocity u_i^n, nodal position X_i^n, zone pressure $p_{i+1/2}^n$ and for the mixing model the energies in the mixed cell $\varepsilon_1^n, \varepsilon_2^n$, the specific volumes τ_1^n, τ_2^n, the concentrations c_1^n, c_2^n and the pressure in the mixed cell p_{mix}^n. (Remark that the pressure in the mixed cell comes from the application of the Mixed Model MM on the previous time step.)

The Lagrangian scheme solves the following set of equations:

Predictor.

$$\begin{aligned}
M_i \frac{u_i^* - u_i^n}{\Delta t} &= -(p_{i+1/2}^n - p_{i-1/2}^n), && (4.1)\\
X_i^* &= X_i + \Delta t \left(\frac{u_i^* + u_i^n}{2}\right), && (4.2)\\
V_{i+1/2}^* &= X_{i+1}^* - X_i^*, && (4.3)\\
\rho_{i+1/2}^* &= \frac{M_{i+1/2}}{V_{i+1/2}^*}, && (4.4)\\
M_{i+1/2} \frac{\varepsilon_{i+1/2}^* - \varepsilon_{i+1/2}^n}{\Delta t} &= -p_{i+1/2}^n \left[\left(\frac{u_{i+1}^* + u_{i+1}^n}{2}\right) - \left(\frac{u_i^* + u_i^n}{2}\right)\right], && (4.5)
\end{aligned}$$

$$\begin{aligned}
\text{Pure cell} \quad \rightarrow \quad p_{i+1/2}^* &= \mathrm{EOS}\left(\rho_{i+1/2}^*, \varepsilon_{i+1/2}^*\right), && (4.6)\\
\text{Mixed cell} \quad \rightarrow \quad p_{mix}^* &= \mathrm{MM}\left(\rho_{i+1/2}^*, \varepsilon_{i+1/2}^*, \tau_1^n, \tau_2^n, \varepsilon_1^n, \varepsilon_2^n, c_1^n, c_2^n; \tau_1^*, \tau_2^*, \varepsilon_1^*, \varepsilon_2^*\right) && (4.7)
\end{aligned}$$

Pressures are recomputed using the Equation of State (EOS) or the Mixed Model (MM). We do not want to update $\tau_1^n, \tau_2^n, \varepsilon_1^n, \varepsilon_2^n$ in the mixed cell by the MM call for the predictor step. This call only produces the predicted mixed cell pressure: p^*_{mix}.

Corrector.

$$
\begin{aligned}
M_i \frac{u_i^{n+1} - u_i^n}{\Delta t} &= -(p^*_{i+1/2} - p^*_{i-1/2}), &(4.8)\\
X_i^{n+1} &= X_i + \Delta t \left(\frac{u_i^{n+1} + u_i^n}{2} \right), &(4.9)\\
V_{i+1/2}^{n+1} &= X_{i+1}^n - X_i^n, &(4.10)\\
\rho_{i+1/2}^{n+1} &= \frac{M_{i+1/2}}{V_{i+1/2}^{n+1}}, &(4.11)\\
M_{i+1/2} \frac{\varepsilon_{i+1/2}^{n+1} - \varepsilon_{i+1/2}^n}{\Delta t} &= -p^*_{i+1/2} \left[\left(\frac{u_{i+1}^{n+1} + u_{i+1}^n}{2} \right) - \left(\frac{u_i^{n+1} + u_i^n}{2} \right) \right], &(4.12)
\end{aligned}
$$

$$
\begin{aligned}
\text{Pure cell} \quad \rightarrow \quad p_{i+1/2}^{n+1} &= \text{EOS}\left(\rho_{i+1/2}^{n+1}, \varepsilon_{i+1/2}^{n+1} \right), &(4.13)\\
\text{Mixed cell} \quad \rightarrow \quad p_{mix}^{n+1} &= \text{MM}\left(\rho_{i+1/2}^{n+1}, \varepsilon_{i+1/2}^{n+1}, \tau_1^n, \tau_2^n, \varepsilon_1^n, \varepsilon_2^n, c_1^n, c_2^n; \tau_1^{n+1}, \tau_2^{n+1}, \varepsilon_1^{n+1}, \varepsilon_2^{n+1} \right), &(4.14)\\
c_1^{n+1} &= c_1^n, &(4.15)\\
c_2^{n+1} &= c_2^n. &(4.16)
\end{aligned}
$$

The MM call results not only in updating the mixed cell pressure p_{mix}^{n+1} but to the update of the mixed cell quantities: $\tau_1^{n+1}, \tau_2^{n+1}, \varepsilon_1^{n+1}, \varepsilon_2^{n+1}$. The last two equations are trivial and express the fact that the concentrations are not changing during the Lagrangian cycle. The complete the Lagrangian cycle one needs to define a time step for the next cycle using the CFL function

$$
\Delta t = CFL \left(\rho_{i+1/2}^{n+1}, \varepsilon_{i+1/2}^{n+1}, p_{i+1/2}^{n+1}, p_{mix}^{n+1} \right), \tag{4.17}
$$

this completes the scheme.

5 Rezone in presence of mixed cell

The rezoning in presence of mixed cell does not change besides the fact that we have to track the interface position. This position can be computed at the end of the Lagrangian step by considering the concentration in the mixed cell:

$$
\begin{aligned}
c_1 &= \frac{m_i^+}{M_{i+1/2}}, &(5.1)\\
&= \frac{V_i^+ \rho_i^+}{M_{i+1/2}}, &(5.2)\\
&= \frac{1}{\tau_1} \frac{V_i^+}{M_{i+1/2}}, &(5.3)\\
&= \frac{1}{\tau_1} \frac{X_{intf} - X_i}{M_{i+1/2}}, &(5.4)
\end{aligned}
$$

as well as

$$
c_2 = \frac{1}{\tau_2} \frac{X_{i+1} - X_{intf}}{M_{i+1/2}}. \tag{5.5}
$$

Therefore the formula to compute the interface position at time t_{n+1} is

$$
X_{intf}^{n+1} = X_i^{n+1} + c_1^{n+1} \tau_1^{n+1} M_{i+1/2} = X_{i+1}^{n+1} - c_2^{n+1} \tau_2^{n+1} M_{i+1/2}. \tag{5.6}
$$

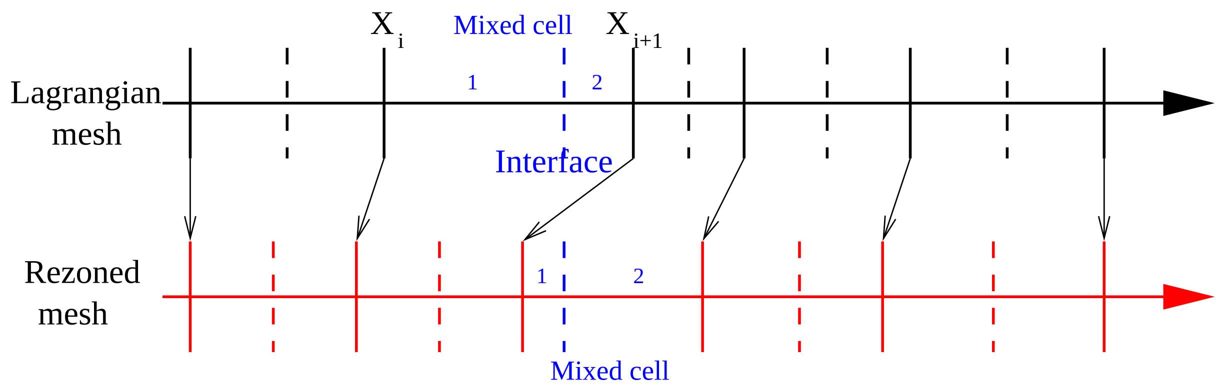

Figure 1: Rezoning in presence of a mixed cell. The mixed cell is in blue (the subcells are denoted as $1, 2$). The blue interface position does not change during the rezoning but this interface can be in another cell. Therefore the red cell on the left of the mixed cell is pure in the rezoned mesh. The black cell in the Lagrangian mesh on the right of the mixed cell becomes mixed in the rezoned mesh.

If the interface is in the same cell in the Lagrangian and rezoned meshes then nothing has to be done except that the boundary between the two subcells of the mixed cell is X_{intf}^{n+1}. On the other hand if the interface is not in the same cell anymore, see Fig.1, then X_{intf} becomes the new position separating the two subcells of the new mixed cell. In any pure cell, the position separating two subcells is the center of the cell.

6 Remap in presence of mixed cell

The remapping is a three step process: (i) a gathering of conservative quantity on subcell, (ii) a subcell remapping, (iii) a scattering to retrieve nodal velocity, cell-centered energy and density.

6.1 Gathering

Mass. Subcell masses are already given: $m_i^{+,n+1}, m_{i+1}^{-,n+1}$ in pure and mixed cells. (Remark that mixed cell densities are given by $\rho_i^{+,n+1} = 1/\tau_1^{n+1}, \rho_{i+1}^{-,n+1} = 1/\tau_2^{n+1}$.)

Momentum Subcell velocities are gathered thanks to the linear system

$$\begin{pmatrix} u_i^{+,n+1} \\ u_{i+1}^{-,n+1} \end{pmatrix} = \begin{pmatrix} \frac{2m_i^{+,n+1}+m_{i+1}^{-,n+1}}{M_{i+1/2}} & \frac{m_{i+1}^{-,n+1}}{M_{i+1/2}} \\ \frac{m_i^{-,n+1}}{M_{i+1/2}} & \frac{m_i^{+,n+1}+2m_{i+1}^{-,n+1}}{M_{i+1/2}} \end{pmatrix} \begin{pmatrix} u_i^{n+1} \\ u_{i+1}^{n+1} \end{pmatrix}, \tag{6.1}$$

and the subcell momentum are given by:

$$\mu_i^{+,n+1} = m_i^{+,n+1}\, u_i^{+,n+1}, \tag{6.2}$$
$$\mu_{i+1}^{-,n+1} = m_{i+1}^{-,n+1}\, u_{i+1}^{-,n+1}. \tag{6.3}$$

Energy. The kinetic energy is gathered the same way as the velocity

$$\begin{pmatrix} k_i^{+,n+1} \\ k_{i+1}^{-,n+1} \end{pmatrix} = \begin{pmatrix} \frac{2m_i^{+,n+1}+m_{i+1}^{-,n+1}}{M_{i+1/2}} & \frac{m_{i+1}^{-,n+1}}{M_{i+1/2}} \\ \frac{m_i^{-,n+1}}{M_{i+1/2}} & \frac{m_i^{+,n+1}+2m_{i+1}^{-,n+1}}{M_{i+1/2}} \end{pmatrix} \begin{pmatrix} \left(u_i^{n+1}\right)^2/2 \\ \left(u_{i+1}^{n+1}\right)^2/2 \end{pmatrix}, \tag{6.4}$$

and the subcell kinetic energy is

$$K_i^{+,n+1} = m_i^{+,n+1} k_i^{+,n+1}, \tag{6.5}$$
$$K_{i+1}^{-,n+1} = m_{i+1}^{-,n+1} k_{i+1}^{-,n+1}. \tag{6.6}$$

A linear reconstruction per pure cell is computed for the internal energy $(\rho\varepsilon)^{n+1}(x)$ and this linear function is integrated on each of the two subcells to get the total specific internal energy: $\mathcal{E}_i^{+,n+1}, \mathcal{E}_{i+1}^{-,n+1}$.

$$\mathcal{E}_i^{+,n+1} = \int_{X_i^{n+1}}^{\frac{1}{2}(X_i^{n+1}+X_{i+1}^{n+1})} (\rho\varepsilon)^{n+1}(x)dx, \tag{6.7}$$

$$\mathcal{E}_{i+1}^{-,n+1} = \int_{\frac{1}{2}(X_i^{n+1}+X_{i+1}^{n+1})}^{X_{i+1}^{n+1}} (\rho\varepsilon)^{n+1}(x)dx. \tag{6.8}$$

For the mixed cell we simply set

$$\mathcal{E}_i^{+,n+1} = m_i^{+,n+1}\varepsilon_1^{n+1}, \tag{6.9}$$

$$\mathcal{E}_{i+1}^{-,n+1} = m_{i+1}^{+,n+1}\varepsilon_2^{n+1}. \tag{6.10}$$

It is easy to show that conservation of mass, momentum and total energy is preserved by this step.

6.2 Remapping

The remapping is not affected by the presence of mixed cell as it is subcell-based. We only need to have a remapping by exact intersection instead of a donor-based remapping. After the remap one gets new subcell variables (denoted with a tilde.)

$$\widetilde{m_i^{+,n+1}}, \widetilde{m_{i+1}^{-,n+1}}, \widetilde{\mu_i^{+,n+1}}, \widetilde{\mu_{i+1}^{-,n+1}}, \widetilde{K_i^{+,n+1}}, \widetilde{K_{i+1}^{-,n+1}}, \widetilde{\mathcal{E}_i^{+,n+1}}, \widetilde{\mathcal{E}_{i+1}^{-,n+1}}. \tag{6.11}$$

This step is conservative as well.

6.3 Scattering

The scattering of physical variables writes:

Density. Density is simply computed as:

$$\widetilde{\rho_i^{+,n+1}} = \widetilde{m_i^{+,n+1}}/\widetilde{V_i^{+,n+1}}, \tag{6.12}$$

$$\widetilde{\rho_{i+1}^{-,n+1}} = \widetilde{m_{i+1}^{-,n+1}}/\widetilde{V_{i+1}^{-,n+1}}, \tag{6.13}$$

and cell density is given by

$$\widetilde{\rho_{i+1/2}^{n+1}} = \frac{\widetilde{M_{i+1/2}}}{\widetilde{V_{i+1/2}^{n+1}}}, \tag{6.14}$$

where new cell mass and volumes are:

$$\widetilde{M_{i+1/2}} = \widetilde{m_i^{+,n+1}} + \widetilde{m_{i+1}^{-,n+1}} \tag{6.15}$$

$$\widetilde{V_{i+1/2}^{n+1}} = \widetilde{V_i^{+,n+1}} + \widetilde{V_{i+1}^{-,n+1}}. \tag{6.16}$$

Nodal velocity. First one computes one-sided velocities:

$$\begin{pmatrix} \widetilde{u_i^{+,n+1}} \\ \widetilde{u_{i+1}^{-,n+1}} \end{pmatrix} = \begin{pmatrix} \frac{2\widetilde{m_i^{+,n+1}}+\widetilde{m_{i+1}^{-,n+1}}}{\widetilde{M_{i+1/2}}} & \frac{\widetilde{m_{i+1}^{-,n+1}}}{\widetilde{M_{i+1/2}}} \\ \frac{\widetilde{m_i^{-,n+1}}}{\widetilde{M_{i+1/2}}} & \frac{\widetilde{m_i^{+,n+1}}+2\widetilde{m_{i+1}^{-,n+1}}}{\widetilde{M_{i+1/2}}} \end{pmatrix}^{-1} \begin{pmatrix} \frac{\widetilde{\mu_i^{+,n+1}}}{\widetilde{m_i^{+,n+1}}} \\ \frac{\widetilde{\mu_{i+1}^{-,n+1}}}{\widetilde{m_{i+1}^{-,n+1}}} \end{pmatrix}, \tag{6.17}$$

then the nodal velocity is finally computed thanks to

$$\widetilde{u_i^{n+1}} = \frac{1}{\widetilde{M_{i+1/2}}} \left(\widetilde{m_i^{+,n+1}} \widetilde{u_i^{+,n+1}} + \widetilde{m_i^{+,n+1}} \widetilde{u_{i+1}^{-,n+1}} \right) \tag{6.18}$$

Cell specific internal energy. By taking into account the discrepancy of kinetic energy one gets

$$\widetilde{\mathcal{E}_{i+1/2}^{n+1}} = \widetilde{\mathcal{E}_i^{+,n+1}} + \widetilde{\mathcal{E}_{i+1}^{-,n+1}} + \left\{ \widetilde{K_i^{+,n+1}} + \widetilde{K_{i+1}^{-,n+1}} - \widetilde{K_{i+1/2}^{n+1}} \right\}, \tag{6.19}$$

where $\widetilde{K_{i+1/2}^{n+1}}$ is the kinetic energy in the cell after remapping:

$$\widetilde{K_{i+1/2}^{n+1}} = \frac{1}{2} \left(\widetilde{m_i^{+,n+1}} \left(\widetilde{u_i^{n+1}} \right)^2 + \widetilde{m_{i+1}^{-,n+1}} \left(\widetilde{u_{i+1}^{n+1}} \right)^2 \right). \tag{6.20}$$

Finally

$$\widetilde{\varepsilon_{i+1/2}^{n+1}} = \frac{\widetilde{\mathcal{E}_{i+1/2}^{n+1}}}{\widetilde{M_{i+1/2}^{n+1}}}. \tag{6.21}$$

6.4 Mixed cell variables

The mixed cell variables to be used to re-initialize the Mixed Model are

$$\widetilde{\tau_1^{ini}} = \frac{1}{\widetilde{\rho_i^{+,n+1}}}, \tag{6.22}$$

$$\widetilde{\tau_2^{ini}} = \frac{1}{\widetilde{\rho_{i+1}^{-,n+1}}}, \tag{6.23}$$

$$\widetilde{\varepsilon_1^{ini}} = \frac{1}{\widetilde{m_i^{+,n+1}}} \left(\widetilde{\mathcal{E}_i^{+,n+1}} + \widetilde{K_i^{+,n+1}} - \frac{1}{2} \widetilde{m_i^{+,n+1}} \left(\widetilde{u_i^{n+1}} \right)^2 \right), \tag{6.24}$$

$$\widetilde{\varepsilon_2^{ini}} = \frac{1}{\widetilde{m_{i+1}^{-,n+1}}} \left(\widetilde{\mathcal{E}_{i+1}^{-,n+1}} + \widetilde{K_{i+1}^{-,n+1}} - \frac{1}{2} \widetilde{m_{i+1}^{-,n+1}} \left(\widetilde{u_{i+1}^{n+1}} \right)^2 \right). \tag{6.25}$$

Moreover the new concentrations are given by the formula

$$\widetilde{c_1^{n+1}} = \frac{\widetilde{m_i^{+,n+1}}}{\widetilde{M_{i+1/2}^{n+1}}}, \tag{6.26}$$

$$\widetilde{c_2^{n+1}} = \frac{\widetilde{m_{i+1}^{-,n+1}}}{\widetilde{M_{i+1/2}^{n+1}}}. \tag{6.27}$$

These mixed cell values are consistent with the mixed model because:

$$\widetilde{c_1^{n+1}} + \widetilde{c_2^{n+1}} = 1, \tag{6.28}$$

$$\widetilde{c_1^{n+1}} \widetilde{\tau_1^{ini}} + \widetilde{c_2^{n+1}} \widetilde{\tau_2^{ini}} = \frac{\widetilde{m_i^{+,n+1}}}{\widetilde{M_{i+1/2}^{n+1}}} \frac{1}{\widetilde{\rho_i^{+,n+1}}} + \frac{\widetilde{m_{i+1}^{-,n+1}}}{\widetilde{M_{i+1/2}^{n+1}}} \frac{1}{\widetilde{\rho_{i+1}^{-,n+1}}} = \frac{1}{\widetilde{\rho_{i+1/2}^{n+1}}}, \tag{6.29}$$

$$\widetilde{c_1^{n+1}} \widetilde{\varepsilon_1^{ini}} + \widetilde{c_2^{n+1}} \widetilde{\varepsilon_2^{ini}} = \widetilde{\varepsilon_{i+1/2}^{n+1}}. \tag{6.30}$$

The last step of the algorithm is to apply the mixed model and the equation of state to define the pressures and the mixed cell variables at t_{n+1}:

$$\begin{aligned} \text{Pure cell} \quad \rightarrow \quad \widetilde{p_{i+1/2}^{n+1}} \quad &= \quad \text{EOS}\left(\widetilde{\rho_{i+1/2}^{n+1}}, \widetilde{\varepsilon_{i+1/2}^{n+1}}\right), \\ \text{Mixed cell} \quad \rightarrow \quad \widetilde{p_{mix}^{n+1}} \quad &= \quad \text{MM}\left(\widetilde{\rho_{i+1/2}^{n+1}}, \widetilde{\varepsilon_{i+1/2}^{n+1}}, \widetilde{\tau_1^{ini}}, \widetilde{\tau_2^{ini}}, \widetilde{\varepsilon_1^{ini}}, \widetilde{\varepsilon_2^{ini}}, \widetilde{c_1^{n+1}}, \widetilde{c_2^{n+1}}; \widetilde{\tau_1^{n+1}}, \widetilde{\tau_2^{n+1}}, \widetilde{\varepsilon_1^{n+1}}, \widetilde{\varepsilon_2^{n+1}}\right), \end{aligned} \tag{6.31}$$

the mixed model produces the new mixed cell variables: $\widetilde{\tau_1^{n+1}}, \widetilde{\tau_2^{n+1}}, \widetilde{\varepsilon_1^{n+1}}, \widetilde{\varepsilon_2^{n+1}}$.

All variables have been remapped and scattered for pure and mixed cells, a new Lagrangian step can be performed.

7 Numerical results

In this section we present some numerical tests showing the efficiency of this model of the Sod Riemann problem and the Le Blanc Riemann problem.
The Lagrangian scheme in ALE INC is a staggered grid scheme with artificial viscosity and a predictor-corrector time discretisation (see [4],[5],[6],[7]). The rezoning method is the so-called Reference-Jacobian-Rezone-Strategy in 1D [10], the remapping method is described in [3].

Two γs Riemann problem. We are going to compare several pure Eulerian calculations, as Lagrange+Remap with a Lagrangian computation performed with a mixed cell initially containing the interface. Then the remapping is performed onto the original grid at each time step. The interface jumps from cell to cell and therefore the mixed model is applied to different cell as the time goes. the remapping method produces the physical global quantities (density, velocity, energy), as well as the local-mixed quantities ($\varepsilon_1, \varepsilon_2, \tau_1\, tau_2$).

A coarse mesh (100 cells) and a refined one (500 cells) are used. The reference solutions are computed with the Lagrangian scheme on very fine grids.
The domain is $\Omega = [0:1]$, the interface is initially at $X = 1/2$ and the final time is $T = 0.14$.
In Figure 2-3-4 are gathered the results when two different fluids are initiated ($\gamma_1 = 1.4, \gamma_2 = 2.0$) with a Lagrangian run with a mixed cell around the interface and the Lagrange+Remap run. The results show that the remapping does not produce any paras-ital oscillation on this problem.

8 Conclusion

In this paper we have presented a mixing model developed by B.Després and F.Lagoutiere and its extension to 1D Arbitrary-Lagrangian-Eulerian framework. In this framework the rezone is not really affected by the presence of mixed cells, however the remapping part is. The extra-variables brought by the mixing model, namely $\varepsilon_1, \varepsilon_2, \tau_1, \tau_2$, have to be remapped as well. This 1D code can now perform such a remapping of mixed cell as proven by the numerical results.

The future work will be to test much difficult test cases (Blastwave, Le Blanc) is order to understand the impact of the remapping of the mixed cell values on the accuracy and stability of the results. Moreover in this code one might need to develop a repair method (to cure pathological unphysical variables) adapted to multi-component simulations.

Acknowledgment

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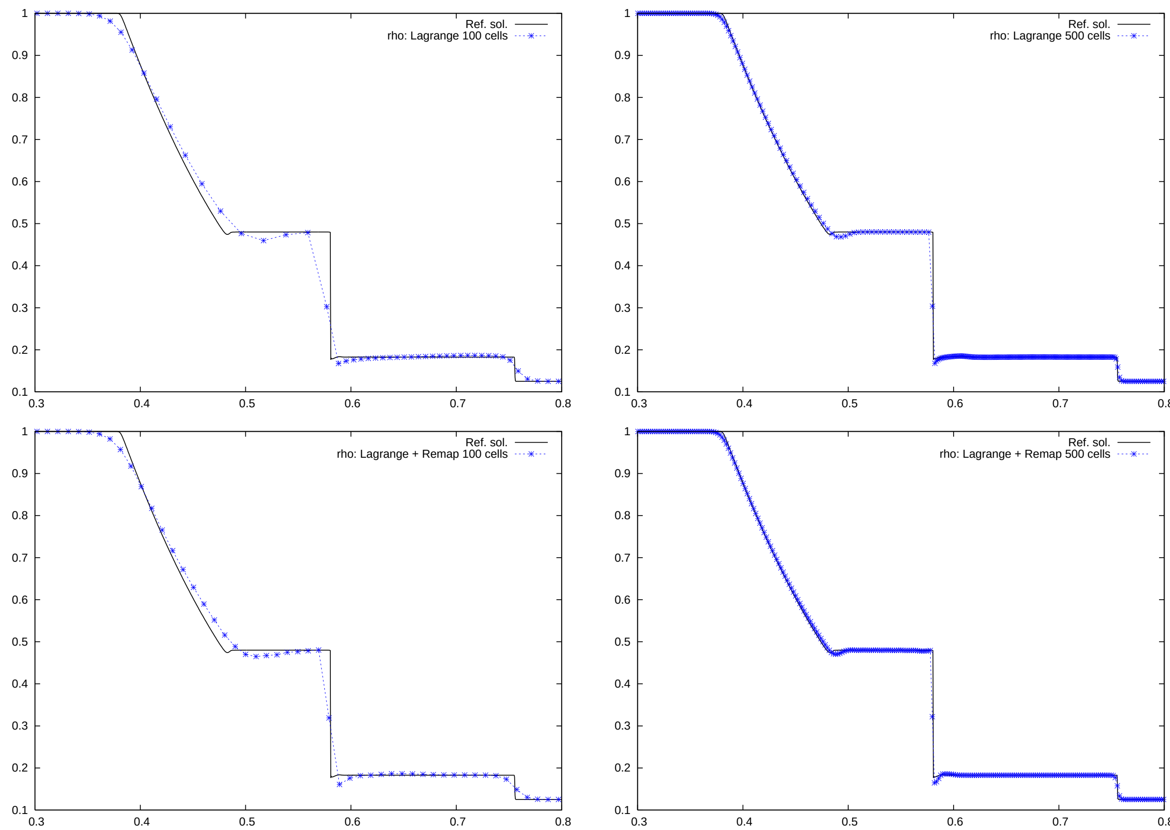

Figure 2: ALE INC code results — Density of the two-fluids Sod Riemann problem — Top: Lagrange plus mixing model (one mixed cell), Bottom: Lagrange+Remap plus mixing model.

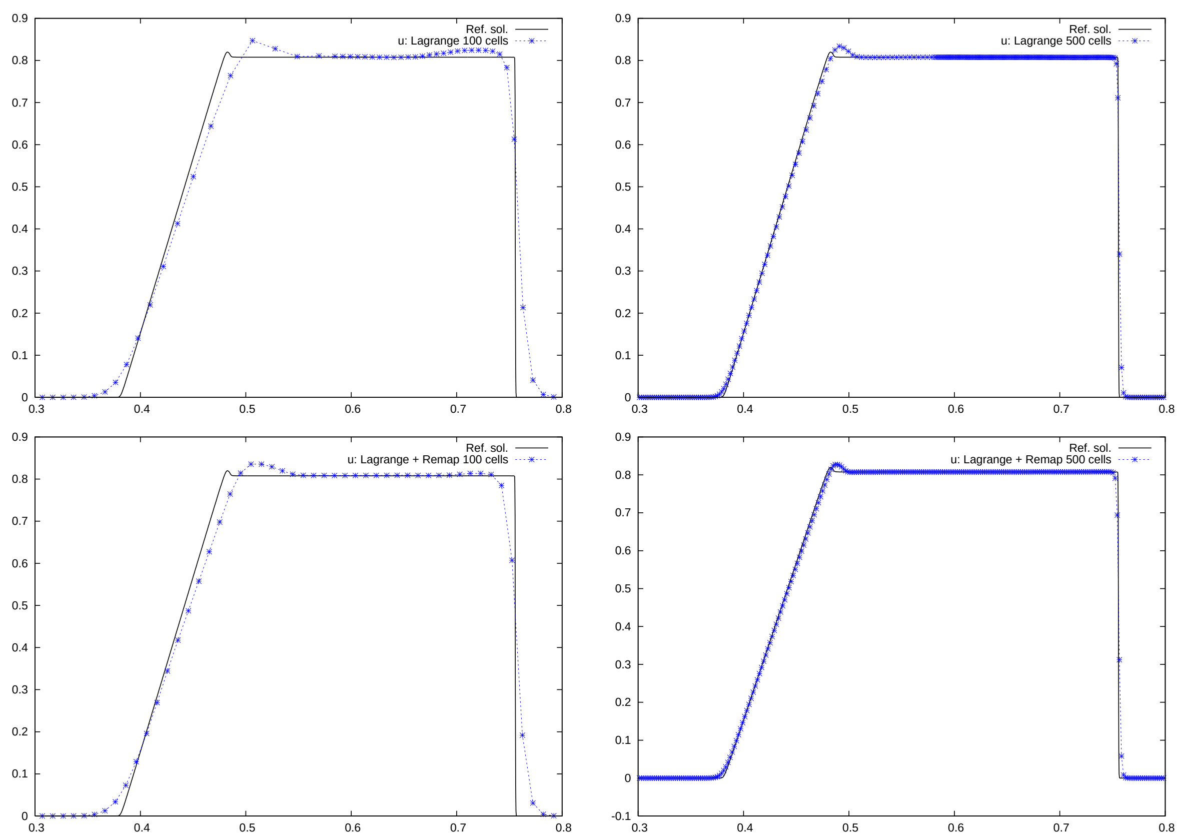

Figure 3: ALE INC code results — Velocity of the two-fluids Sod Riemann problem — Top: Lagrange plus mixing model (one mixed cell), Bottom: Lagrange+Remap plus mixing model.

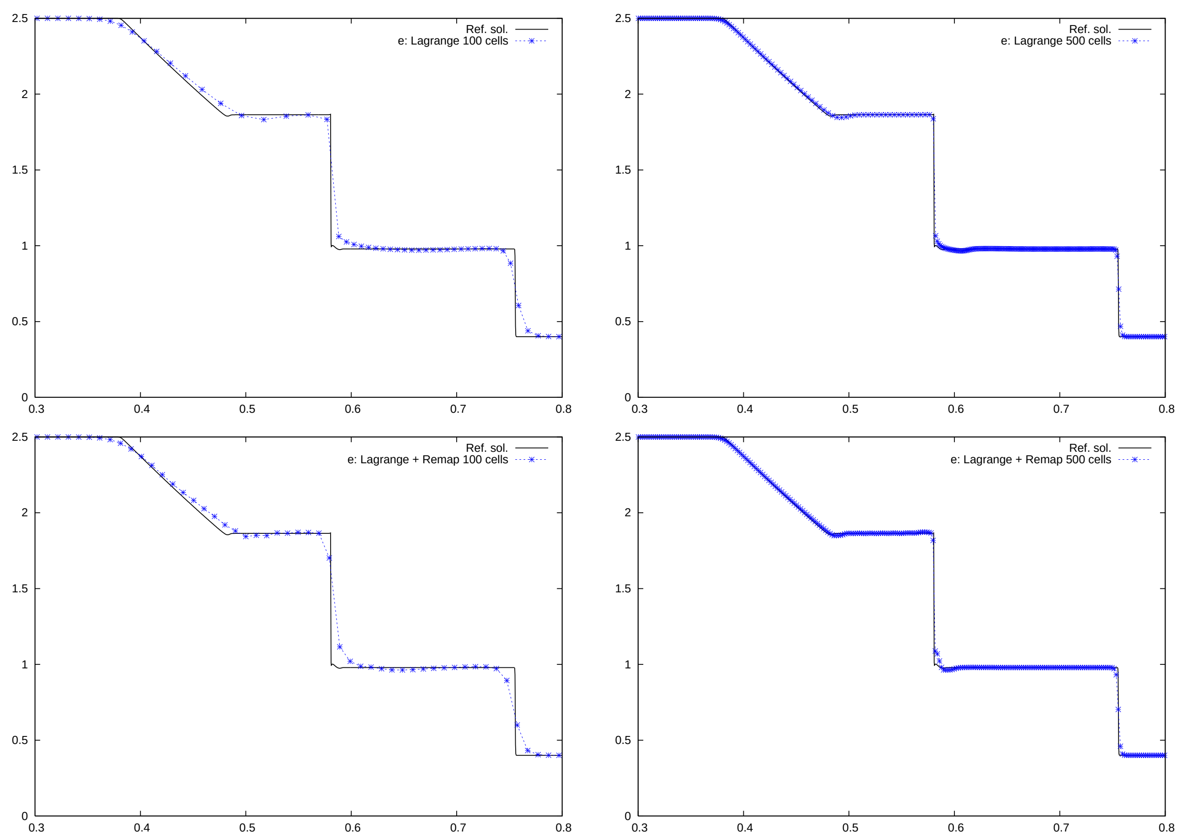

Figure 4: ALE INC code results — Specific internal energy of the two-fluids Sod Riemann problem — Top: Lagrange plus mixing model (one mixed cell), Bottom: Lagrange+Remap plus mixing model.

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