The reactive Riemann solver for thermally perfect gases and its application to the modeling of combustion in large geometries

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Outline

- Introduction

- Hypotheses and governing equations

- Reactive piston problem solution

- 1D reactive Riemann problem solution

- DEM (Discrete Equation Method)
  UDCS (Upwind Downwind-Controlled Splitting)

- Numerical experiments

- Conclusion

Introduction

- **Problem**. We want to investigate hydrogen-air deflagrations and detonations in large scale geometries, for instance in a nuclear reactor containment during a postulated Loss of Coolant Accident (LOCA).

- In slow deflagration regime, the flame propagation in a premixed mixture is due to thermal and species diffusion from the burnt to the unburnt gases.

- If thermal diffusion is less important than species one, a slow plane flame can be unstable (**intrinsic instability**). Its wrinkling accelerates the flame itself and we can have transition from laminar to turbulent regime.

Introduction (2)

- **Characteristic dimensions**.
  - In a EPR (European Pressurized Reactor), $V = 75000$ m^3 ($\approx$ (40 m)^3).
  - Reaction zone in a laminar deflagration at atmospheric condition can vary from about 1 mm ($X_{\mathrm{H}_2} \approx 0.296$) to 10 mm ($X_{\mathrm{H}_2} \approx 0.1$)

- $\Rightarrow$ Direct modelling of flame acceleration is impossible in so large geometries.

- **Our approach**.
  - We consider the flame as infinitely thin.
  - We neglect the diffusion phenomena and model their effects by directly imposing the flame speed.

Introduction (2bis)

- TONUS, COM3D and other CFD codes implement the **CREBCOM algorithm** to solve reacting flows in deflagration regime, in which the chemical reaction is supposed infinitely fast.

- This combustion model is very simple.
  The flame surface is not reconstructed.

- It involves a parameter which has the dimension of a speed (but it is not the flame speed).

- It involves a **criterion function** which says if a cell burns or not.
  In some applications, in which the flame speed is not important, the criterion function can generate important oscillations which strongly affect the numerical solution.

Introduction (3)

- **Problem**: is there a combustion model which keeps the simplicity of CREBCOM (no flame surface reconstruction) but does not involve the combustion criterion?

- The **Reactive Discrete Equation Method** [LeMetayer 2005] solves the Reactive Euler Equations.
  - ☺ Eulerian approach (ALE extension is possible)
  - ☺ Conservative
  - ☺ No flame surface reconstruction
  - ☺ No operator splitting
  - ☹ In each cell, we have to compute the conservative variables for the burnt and unburnt mixture
  - ☹ We have to solve a **reactive Riemann problem**
  - ☺ It can be used for both deflagration and detonation.

Reactive Riemann problem solution

- [Teng 1982].
  - In deflagration regime, the visible flame speed is imposed.
  - There is not the Taylor wave behind a CJDF **(dramatic for Deflagration-to-Detonation Transition)**.

- [Zhang 1989].
  - The temperature ahead of the reactive shock is equal to the so-called ignition temperature **(difficult to use in a large scale approach)**.
  - There is the Taylor wave behind a CJDF.

- **This work**.
  - In deflagration regime, the fundamental flame speed is given.
  - There is the Taylor wave behind a CJDF.

  $\Rightarrow$ A detonation can be computed as limit case of a deflagration wave. (**Transition occurs continuously**).
  - Thermally perfect gases are considered.

Hypotheses

- We restrict our attention to **ideal gases** mixtures containing H_2, O_2, H_2O and N_2.

- The chemical evolution is supposed to be governed by the **irreversible**, **infinitely fast**, global chemical reaction

$$\mathrm{H_2} + \frac{1}{2}\mathrm{O_2} \to \mathrm{H_2O}.$$

- We **neglect the species** and temperature **diffusion**
$\Rightarrow$ In each elementary control volume,

$$Y_{\mathrm{j,u}}(\vec{r}, t) = Y_{\mathrm{j,u}}(\vec{r}_0), \quad j = \mathrm{H_2},\ \mathrm{O_2},\ \ldots$$

u standing for unburnt, $\vec{r}_0$ being the initial position of the control volume.

∞

Governing equations

- Under these hypotheses, we can write

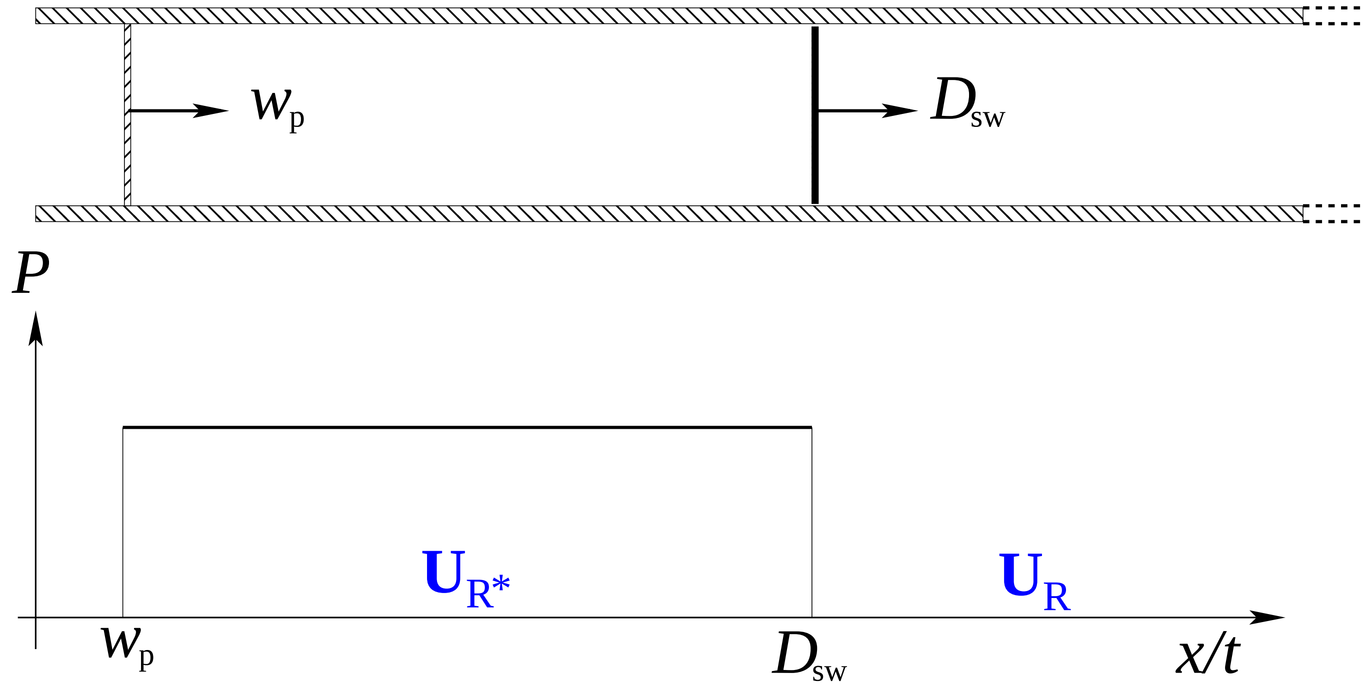
$$\begin{cases} \frac{\partial}{\partial t}\rho + \vec{\nabla}\cdot(\rho\vec{w}) = 0 \\ \frac{\partial}{\partial t}(\rho\vec{w}) + \vec{\nabla}\cdot(\rho\vec{w}\otimes\vec{w} + P) = 0 \\ \frac{\partial}{\partial t}(\rho\tilde{e}_t) + \vec{\nabla}\cdot(\rho\vec{w}\tilde{h}_t) = 0 \\ \frac{\partial}{\partial t}\xi + \vec{D}\cdot\vec{\nabla}\xi = 0 \\ \frac{\partial}{\partial t}(\rho Y_{j,u}) + \vec{\nabla}\cdot(\rho\vec{w}Y_{j,u}) = 0 \quad j = \mathrm{H_2},\ \mathrm{O_2},\ \mathrm{H_2O} \\ \dots \end{cases}$$

$$P = \rho\left(\sum_j Y_j \frac{R^*}{M_j}\right)T, \quad \tilde{e}_t = \frac{1}{2}w^2 + \sum_j Y_j h_j^0 + \int_0^T \left\{\sum_j Y_j c_{v,j}(\alpha)\right\} \mathrm{d}\alpha$$

ξ is the progress variable (1 in the burnt gas, 0 elsewhere)

$$\underbrace{\vec{D}}_{\text{Flame speed}} = \underbrace{\vec{w}}_{\text{unburnt gas}} + K_0 \underbrace{\vec{n}}_{\text{burnt}\to\text{unburnt}}.$$

Piston problem

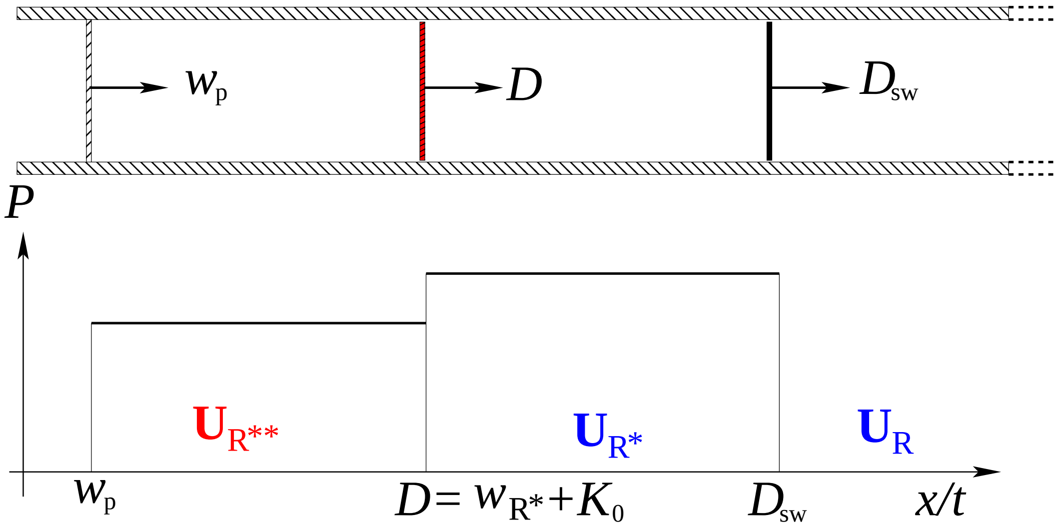


- For a calorically perfect gas, the non-dimensional solution is

$$\mathbf{U} = \mathbf{U}\left(\frac{x}{t w_{\text{ref}}}, \frac{w_{\text{p}}}{w_{\text{ref}}}, \gamma\right), \qquad w_{\text{ref}} = \sqrt{\frac{P_{\text{R}}}{\rho_R}}.$$

- Left GNL wave (shock or rarefaction wave).
- Note that $w_p < D_{\text{sw}}$.

Reactive piston problem



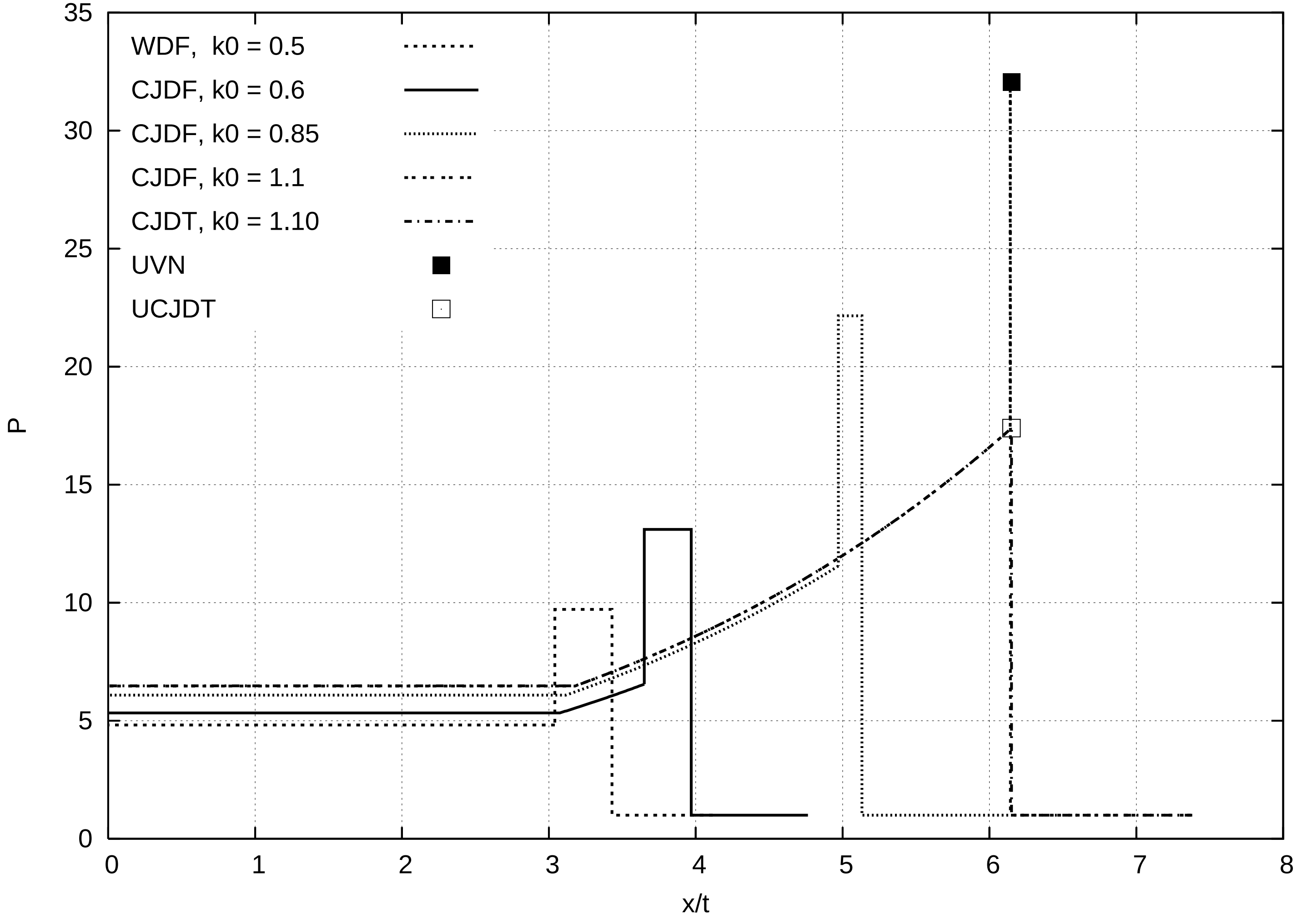
- For a calorically perfect gas, the non-dimensional solution is

$$\mathbf{U} = \mathbf{U}\left(\frac{x}{t w_{\text{ref}}}, \frac{w_{\text{p}}}{w_{\text{ref}}}, \gamma_u, \gamma_b, \frac{q}{w_{\text{ref}}^2}, \frac{K_0}{w_{\text{ref}}}\right), \qquad w_{\text{ref}} = \sqrt{\frac{P_{\text{R}}}{\rho_R}}.$$

- Note that $w_p < D$, $w_p < D_{\text{sw}}$.
  $D \leq D_{\text{sw}}$ for physical reasons.

- Left structure of the reactive Riemann problem (unburnt gas in the right).

Reactive piston problem (2)



Thermally perfect stoichiometric H_2-air. Ambient conditions. $w_p = 0$.

Definition of WDF, CJDF, CJDT, SDT.

Reactive piston problem (3)

- Possible transitions:
  WDF $\to$ CJDF $\to$ CJDT (via K_0)
  WDF $\to$ SDT (via w_p)
  CJDF $\to$ WDF (via w_p)
  CJDT $\to$ SDT (via w_p)

- From a mathematical point of view, the CJ and VN state are limit states for steady deflagrations, as the flame and the precursor shock collapse.
  Continuity does exist and it is necessary.

Reactive Riemann problem

- We specify the following **initial conditions**

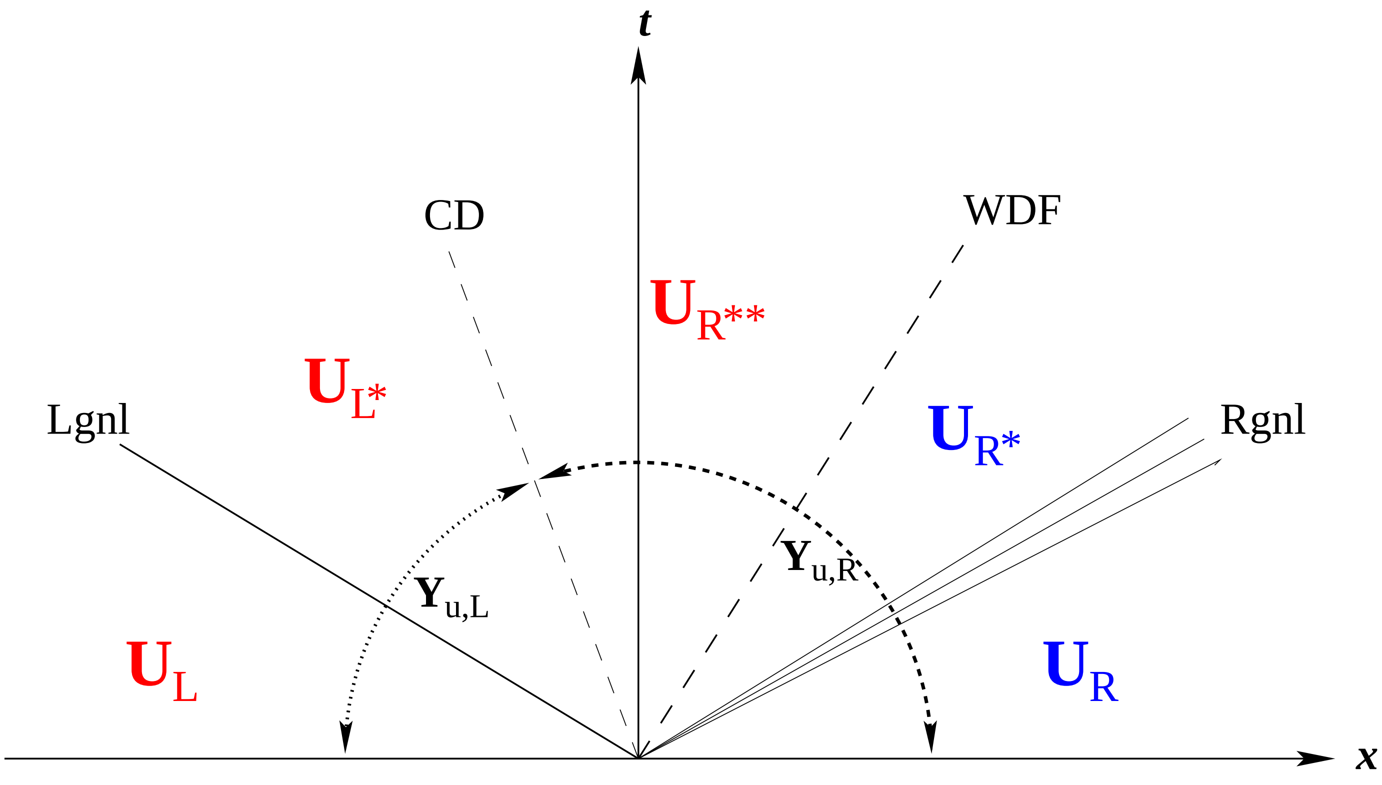
	P	T	w	ξ	$\mathsf{Y_u}$
L	P_L	T_L	w_L	1	$\mathsf{Y_{u,L}}$
R	P_R	T_R	w_R	0	$\mathsf{Y_{u,R}}$

- We also specify the value of the **fundamental flame speed** K_0

- In the case of **deflagration**, K_0 is taken into account.

- If K_0 is larger than the one which corresponds to the collapse of the flame with the precursor shock, we are **in detonation** regime and it is **not taken into account**.

Reactive Riemann problem solution

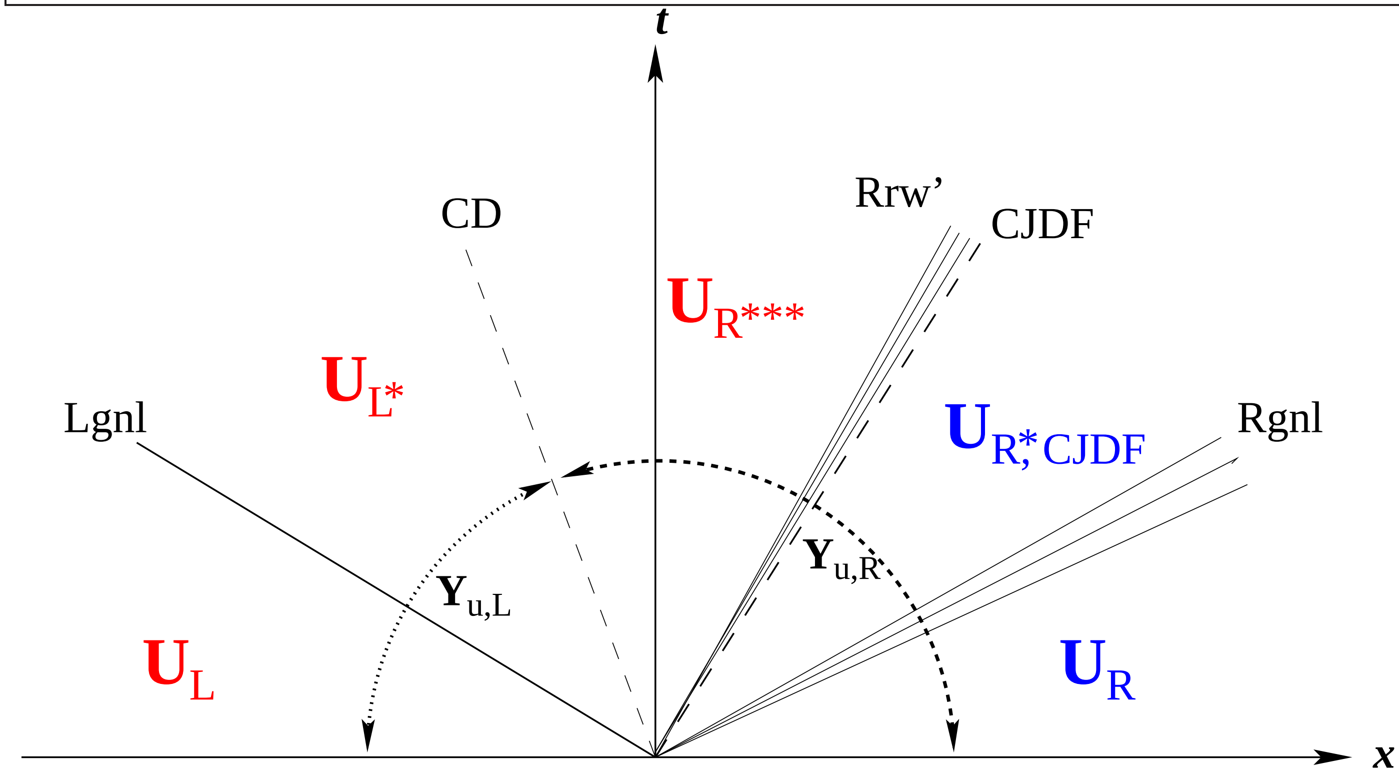


$$U_L \xmapsto{\text{Lgnl}} U_{L^*} \xmapsto{\text{CD}} U_{R^{**}} \xmapsto{\text{WDF}} U_{R^*} \xmapsto{\text{Rgnl}} U_R.$$

$$w_{R^{**}} + c_{R^{**}} > D > w_{R^*} + c_{R^*}$$

$$c_{R^{**}} > D - w_{R^{**}}, \qquad c_{R^*} < D - w_{R^*}$$

Reactive Riemann problem solution (2)

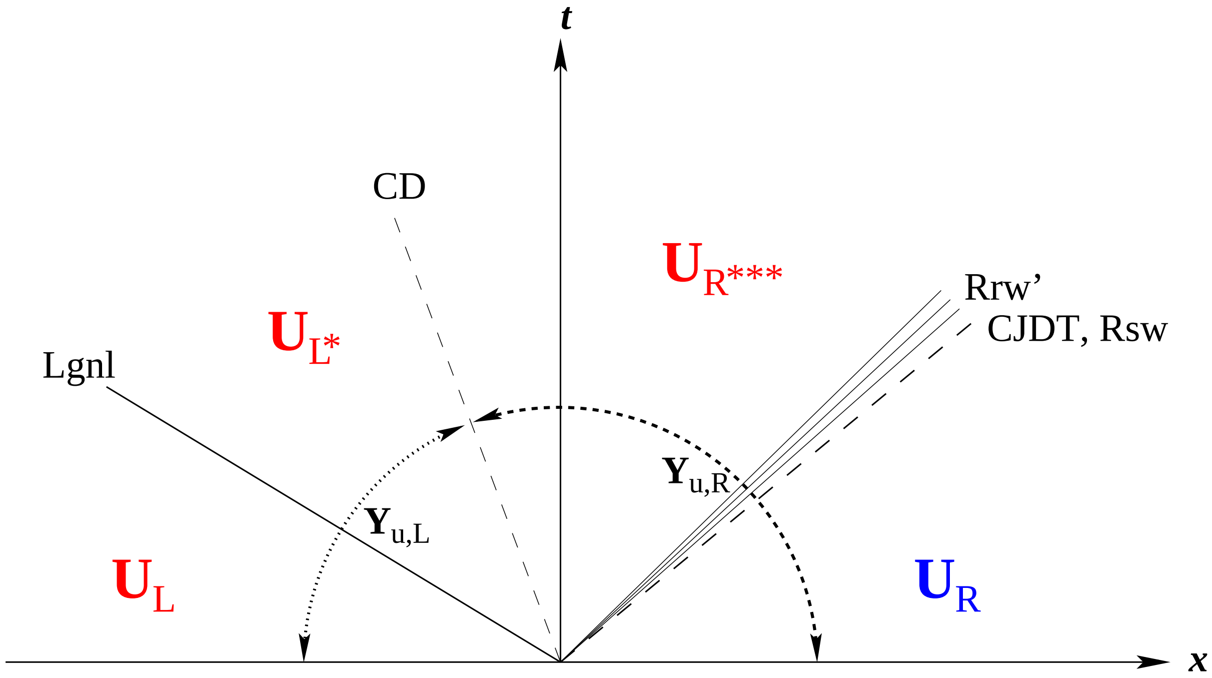


$$\mathbf{U}_{\mathrm{L}} \overset{\mathrm{Lgnl}}{\longmapsto} \mathbf{U}_{\mathrm{L}^*} \overset{\mathrm{CD}}{\longmapsto} \mathbf{U}_{\mathrm{R}^{***}} \overset{\mathrm{Rrw'}}{\longmapsto} \mathbf{U}_{\mathrm{R}^{**},\mathrm{CJDF}} \overset{\mathrm{CJDF}}{\longmapsto} \mathbf{U}_{\mathrm{R}^*,\mathrm{CJDF}} \overset{\mathrm{Rgnl}}{\longmapsto} \mathbf{U}_{\mathrm{R}}.$$

$$w_{\mathrm{R}^{**},\mathrm{CJDF}} + c_{\mathrm{R}^{**},\mathrm{CJDF}} = D > w_{\mathrm{R}^*} + c_{\mathrm{R}^*}$$

$$c_{\mathrm{R}^{**},\mathrm{CJDF}} = D - w_{\mathrm{R}^{**},\mathrm{CJDF}}, \quad c_{\mathrm{R}^*} < D - w_{\mathrm{R}^*}$$

Reactive Riemann problem solution (3)

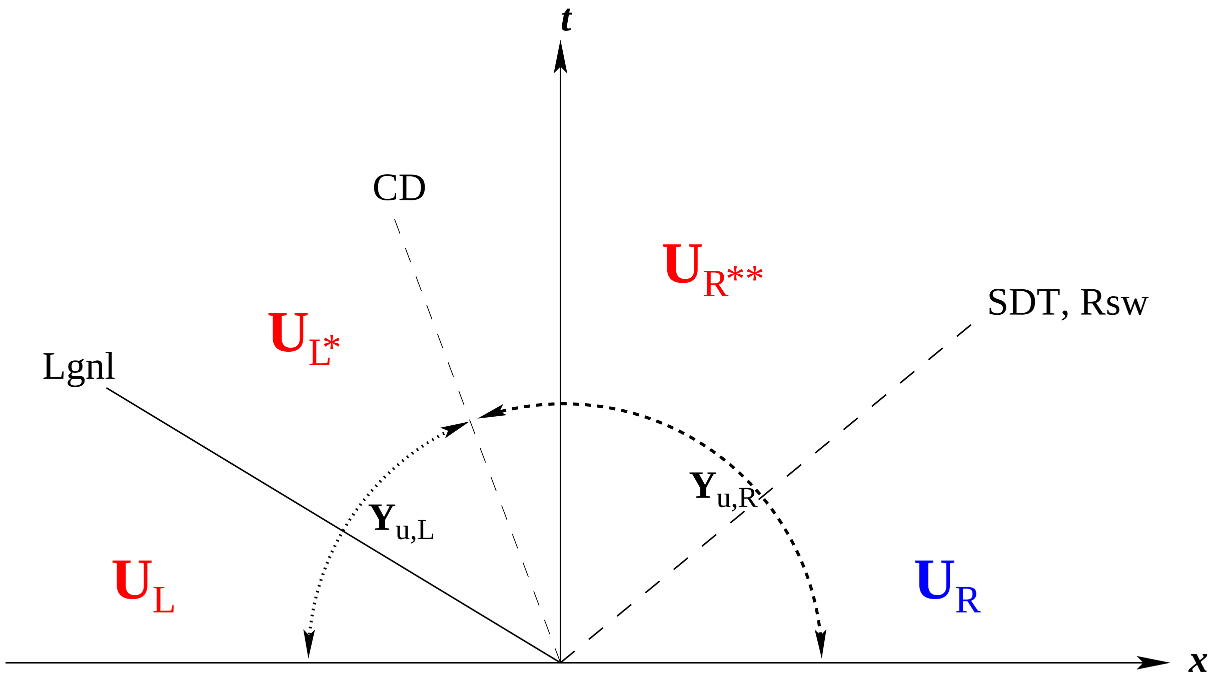


$$U_L \overset{\text{Lgnl}}{\longmapsto} U_{L^*} \overset{\text{CD}}{\longmapsto} U_{R^{***}} \overset{\text{Rrw'}}{\longmapsto} U_{R^{**},\text{CJDT}} \overset{\text{CJDF}}{\longmapsto} U_{R^*,\text{CJDT}} \overset{\text{Rsw}}{\longmapsto} U_R.$$

$$w_{R^{**},\text{CJDT}} + c_{R^{**},\text{CJDT}} = D \Leftrightarrow c_{R^{**},\text{CJDT}} = D - w_{R^{**},\text{CJDT}}$$

$$D - w_{R^*,\text{CJDT}} = K_{0,\text{CJDT}} \leq K_0$$

Reactive Riemann problem solution (4)



$$\mathbf{U}_{\mathsf{L}} \overset{\mathsf{Lgnl}}{\longmapsto} \mathbf{U}_{\mathsf{L}*} \overset{\mathsf{CD}}{\longmapsto} \mathbf{U}_{\mathsf{R}**} \overset{\mathsf{WDF}}{\longmapsto} \mathbf{U}_{\mathsf{R}*} \overset{\mathsf{Rsw}}{\longmapsto} \mathbf{U}_{\mathsf{R}}.$$

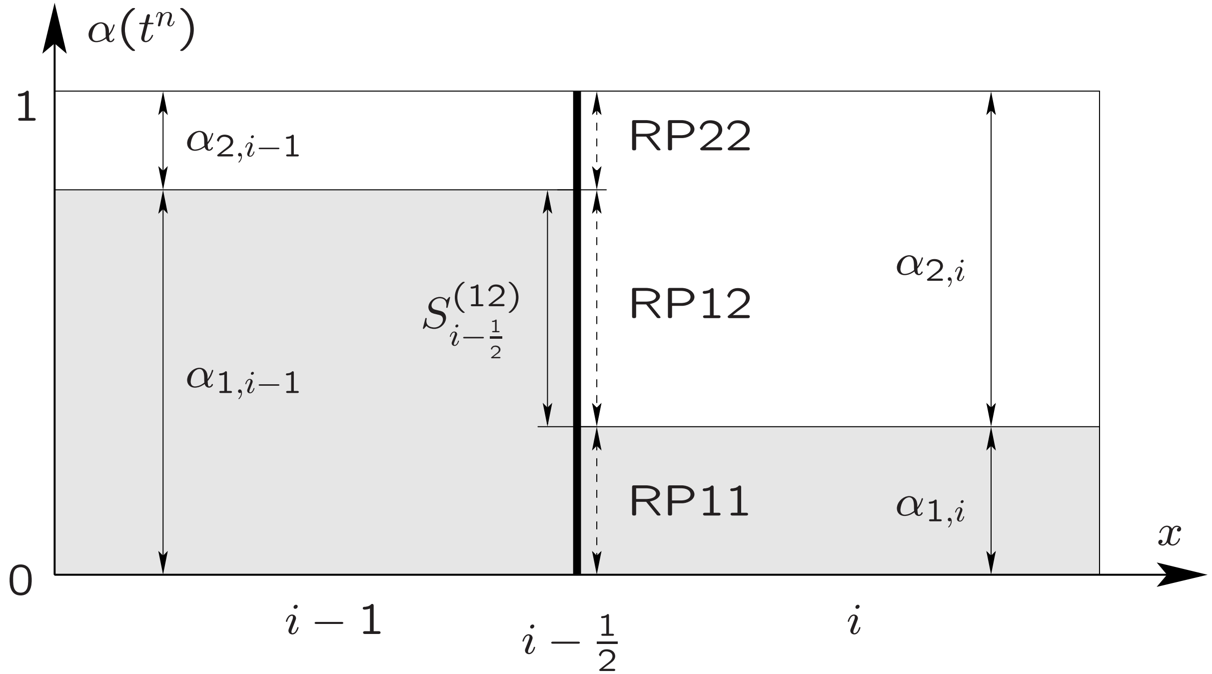
$$w_{\mathsf{R}**} + c_{\mathsf{R}**} > D \Leftrightarrow c_{\mathsf{R}**} > D - w_{\mathsf{R}**}$$

$$D - w_{\mathsf{R}*} = K_{0,\mathsf{SDT}} \leq K_0$$

DEM/RDEM approach

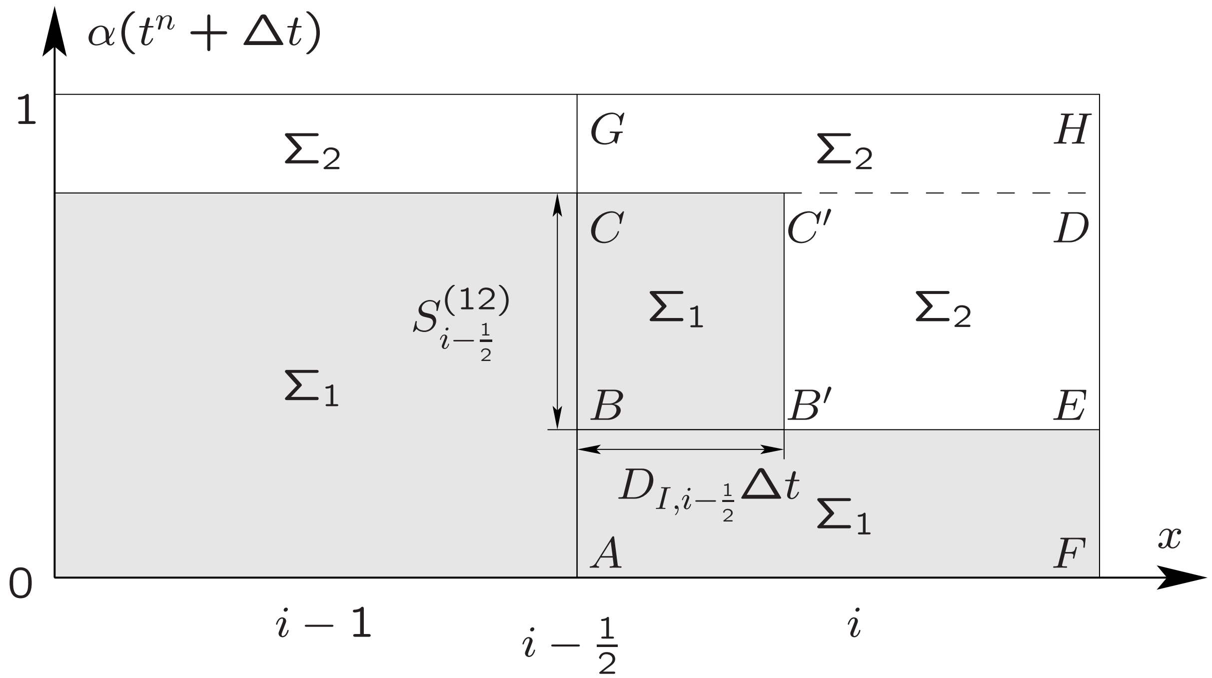
- The discrete equation method is an **Eulerian approach**.
- It is used to study **multiphase mixtures**, in which global averaging of a variable in a control cell would lead to unacceptable numerical errors. In this approach, **each phase has its own variables**.
- It has been introduced in [Abgrall 2003].
- It has been modified (RDEM) and used, **coupled with a reactive solver**, to study **evaporation front propagation** and **detonation propagation** in [LeMetayer 2005].
- In the conclusion of [LeMetayer 2005], it is written:
  "...we believe that **the same approach can be used to propagate flame fronts** ..."

Intercell surface partition at t^n



- The two phases Σ_1 and Σ_2 have their own variables.
- The phase interface is numerically smeared.
- $\alpha_{1,i-1} > \alpha_{1,i} \Rightarrow \Sigma_1$ is on the left, Σ_2 on the right.
- The unitary surface is divided into three parts:
  - RP11 involving Σ_1 and Σ_1
  - RP22 involving Σ_2 and Σ_2
  - RP12 involving Σ_1 and Σ_2

Volume partition at $t^{n+1} = t^n + \Delta t$

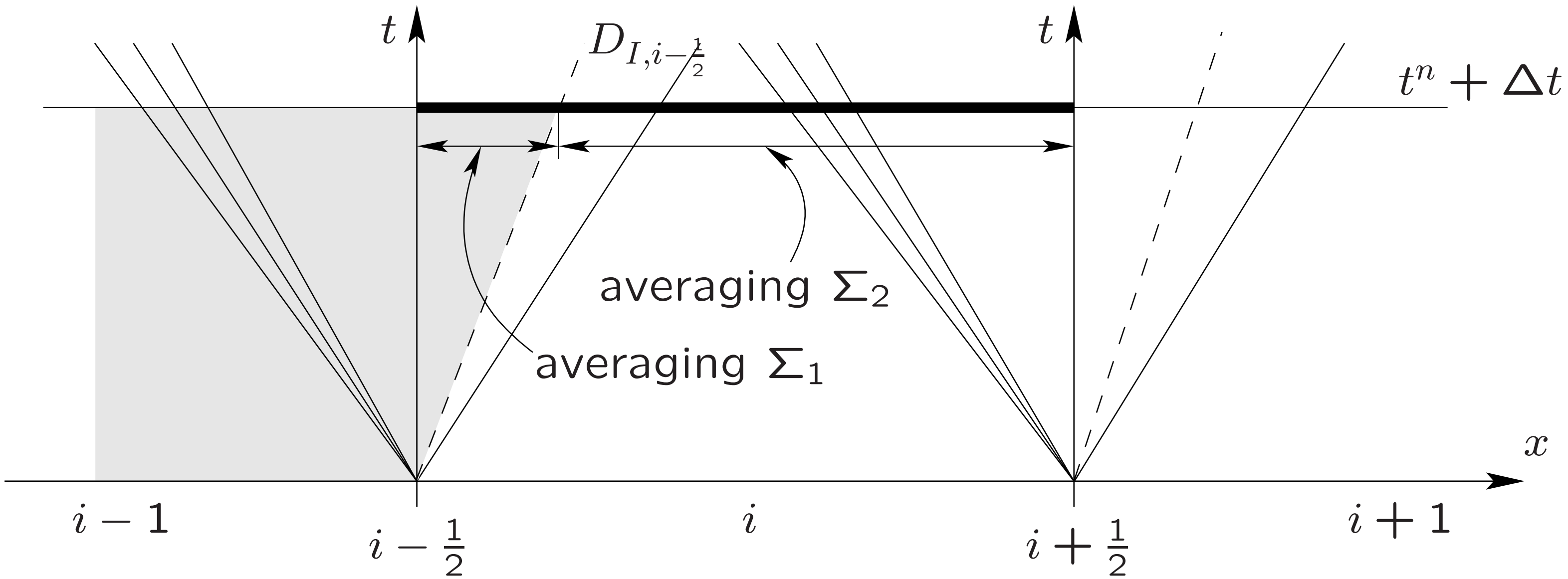


- The two-phase interface RP12 moves with a velocity $D_{I,i-\frac{1}{2}}$.
- Cell i is penetrated by phase Σ_1 in a region with a volume fraction

$$\frac{D_{I,i-\frac{1}{2}}\Delta t S^{(12)}_{i-\frac{1}{2}}}{\Delta x} = \Delta t \underbrace{\left(\frac{D_{I,i-\frac{1}{2}}(\alpha_{1,i-1} - \alpha_{1,i})}{\Delta x}\right)} = \frac{|BB'C'C|}{|AFHG|}.$$

(first-order upwind approximation of $D_I\frac{\partial \alpha_1}{\partial x}$).

Riemann problems and space average-updating



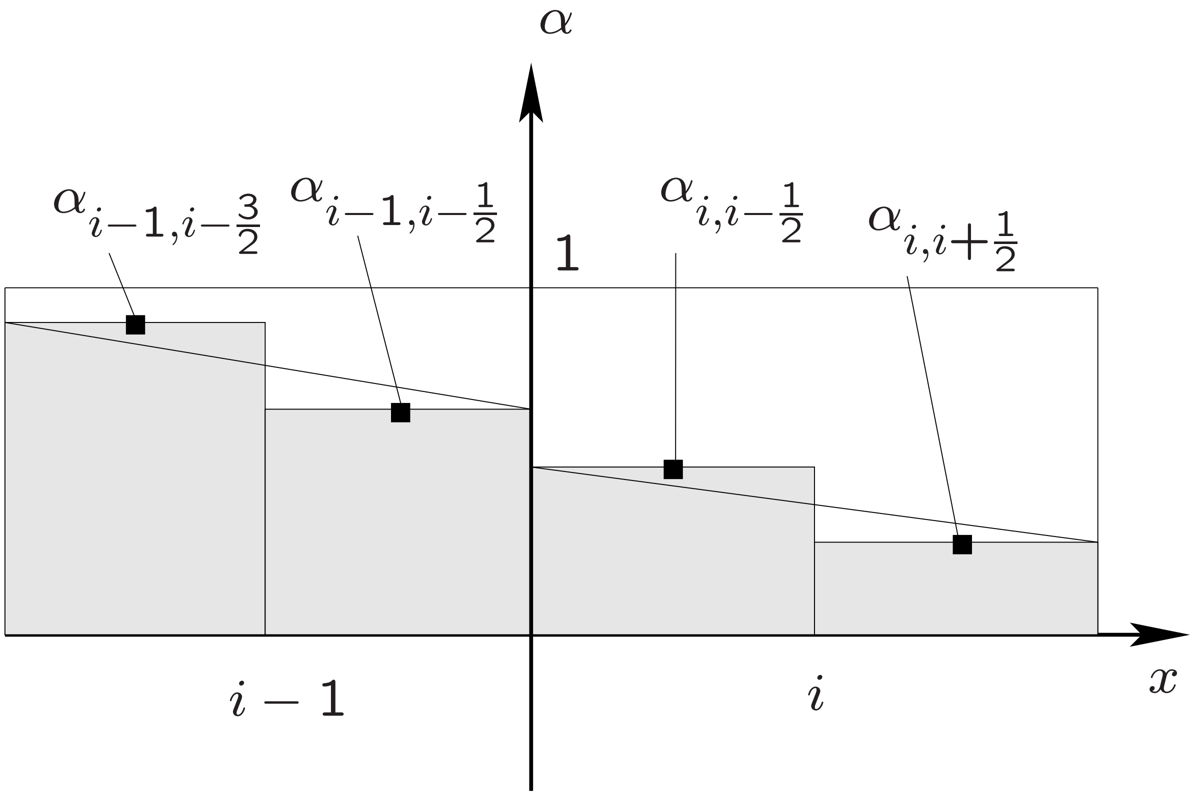
- We restrict our attention to the region BEDC.
- We evaluate the conservative variables by considering the intercell Riemann problems at $x_{i-\frac{1}{2}}$ and at $x_{i+\frac{1}{2}}$.
- We proceed in the same manner for AFEB and CDHG.
- After having obtained the conserved variables of each phase in each partitioned region, we are able to evaluate the conserved variables at t^{n+1} for both phases.

Riemann problems and space average-updating (2)

- From a compuational point of view, the new **space average** of single phases conservative variables is evaluated, as in a classical single phase finite volume approach, by computing the contribution of the **intercell numerical fluxes.**

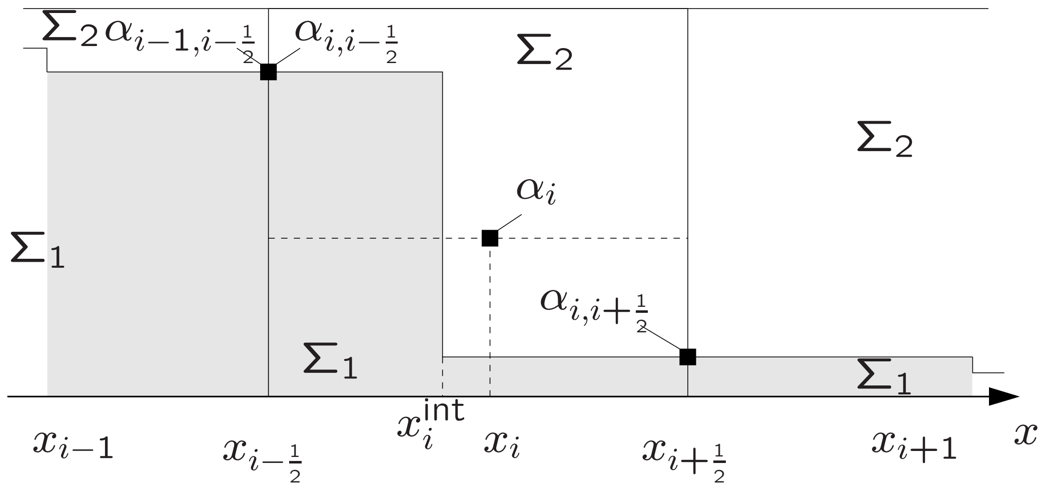
High-order reconstruction for volume fractions

- In DEM/RDEM, high-order reconstruction for volume fractions requires the solution of internal Riemann problems.



(1) Piecewise linear reconstruction.

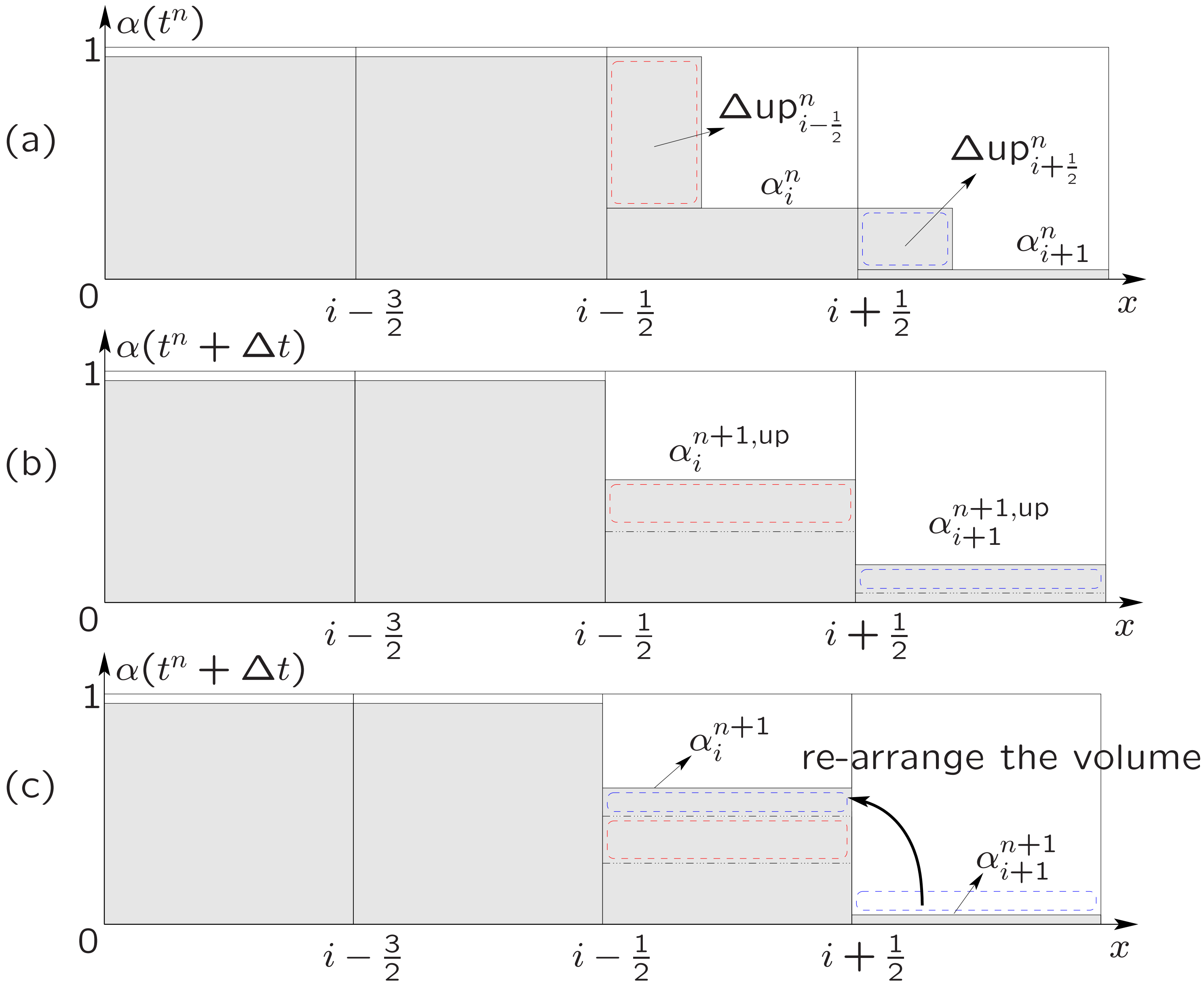
High-order reconstruction for volume fractions (2)



(2) Anti-diffusive reconstruction of Després-Lagoutière.

- Reduction of CFL condition in case (1).
- Dramatic reduction of CFL condition in case (2).
- Large Time Step (LTS) wave propagation method of Leveque has allowed to overcome the problem but too difficult in unstructured meshes.

Upwind Downwind-Controlled Splitting (UDCS)



Upwind Downwind-Controlled Splitting (2)

1. 1st order upwinding,
   (a) Computation of interface RP solutions.
   (b) Computation of (1st order) conserved variables.

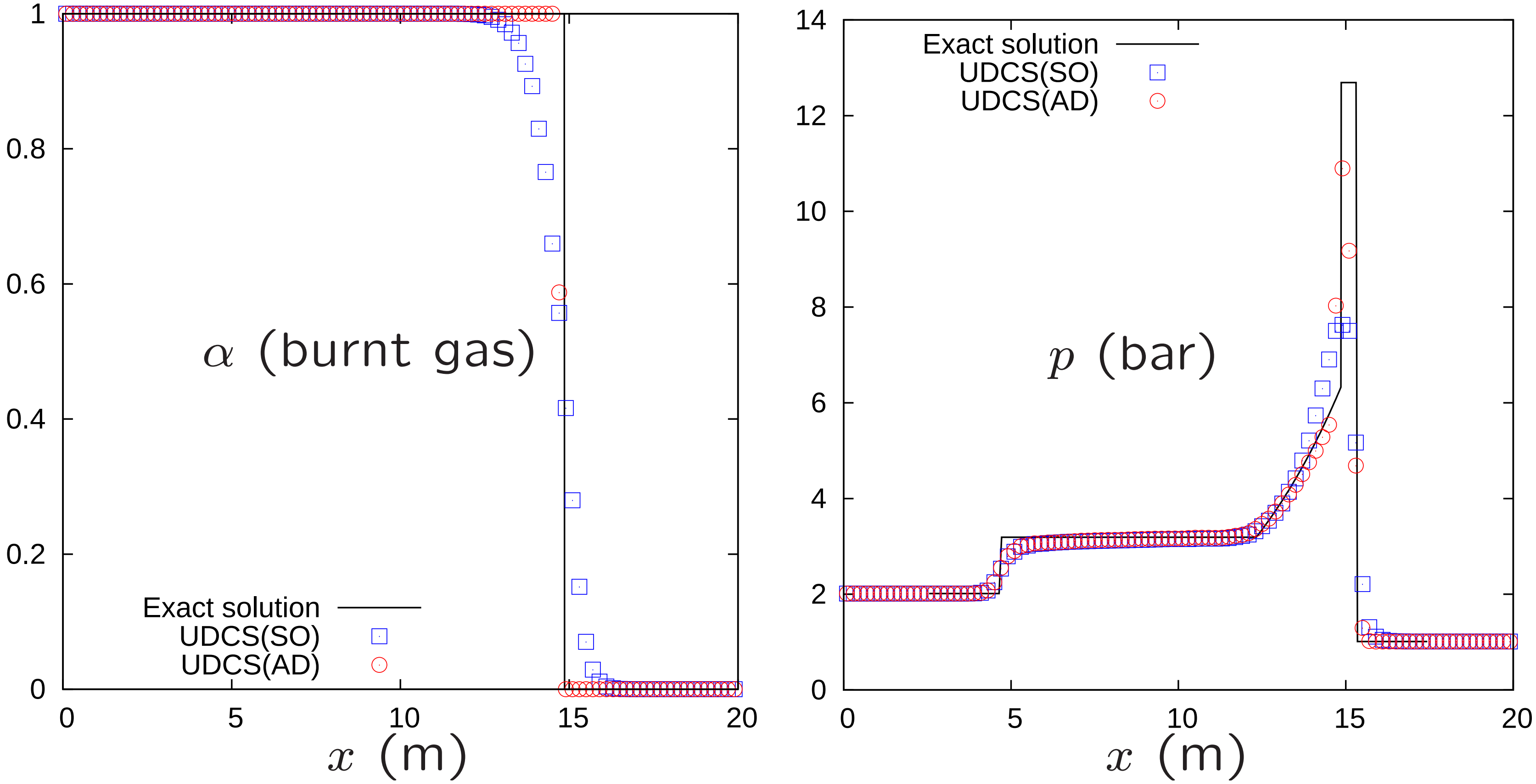
2. Volume downwind (c), according to the reconstruction and computation of conserved variables .
   The **volume to downwind** is equal to
   (1st order upwinded one) - (high-order upwinded one).

- **Advantages**
  - As robust as **first order**.
  - More accurate than first order.
  - Less "two phase-flow" region than in first order.
    Reduction of the CPU cost.
  - As accurate as **"classic" high order approach**.
  - Much more robust than "classic" high order approach.
  - No internal Riemann problems.
    Reduction of the CPU cost.

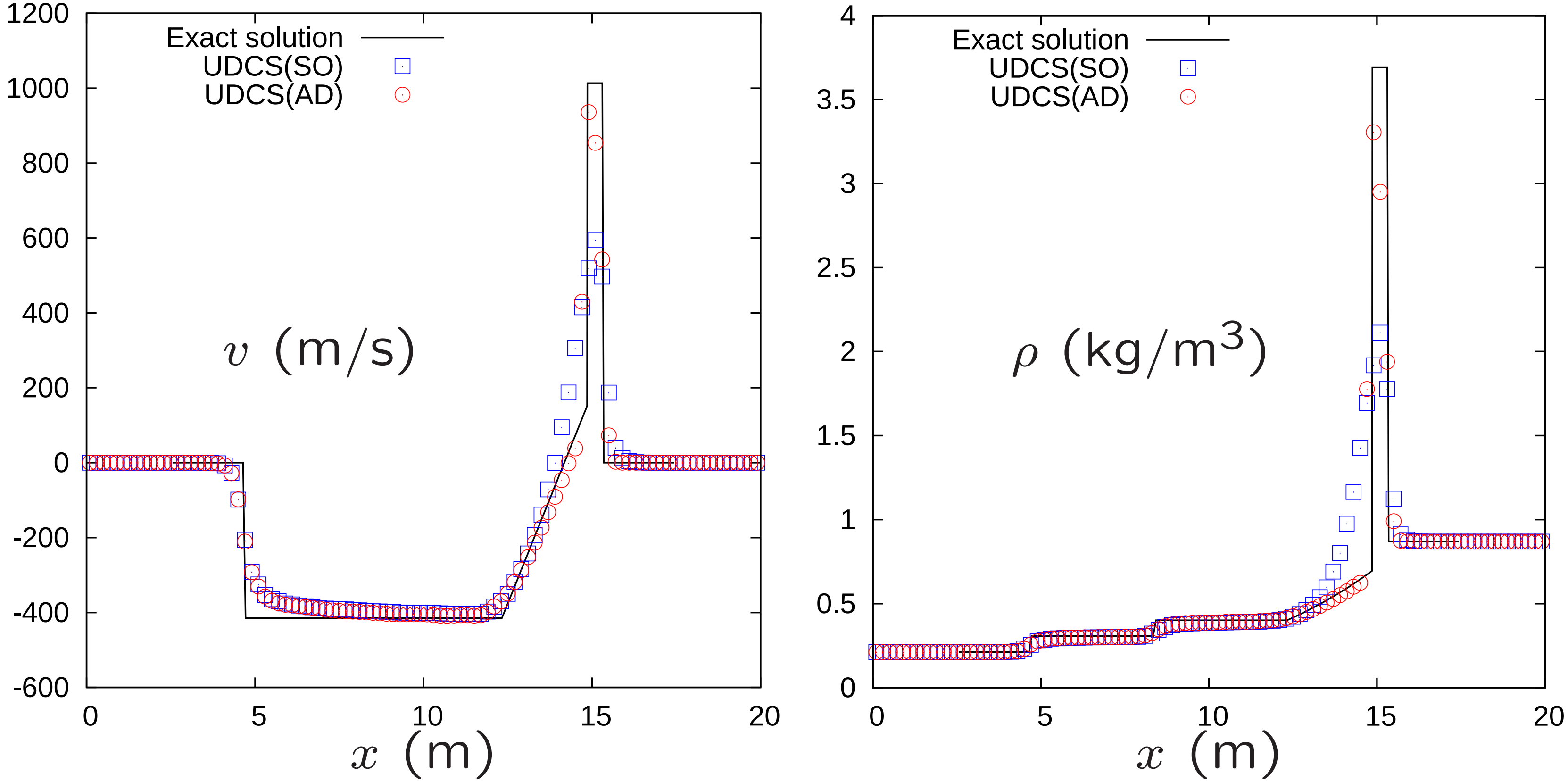
Shock tube at CJDF regime

- Purpose of this test case:
  to show how **the poor accuracy of the numerical solution in the flame region can strongly affect the accuracy of the computed precursor shock**.
- "All shock" reactive and non-reactive solver with entropy fix.
- Minmod reconstruction on primitive variables.
- RK2
- 100 elements
- CFL=0.9
- $\varepsilon = 10^{-8}$

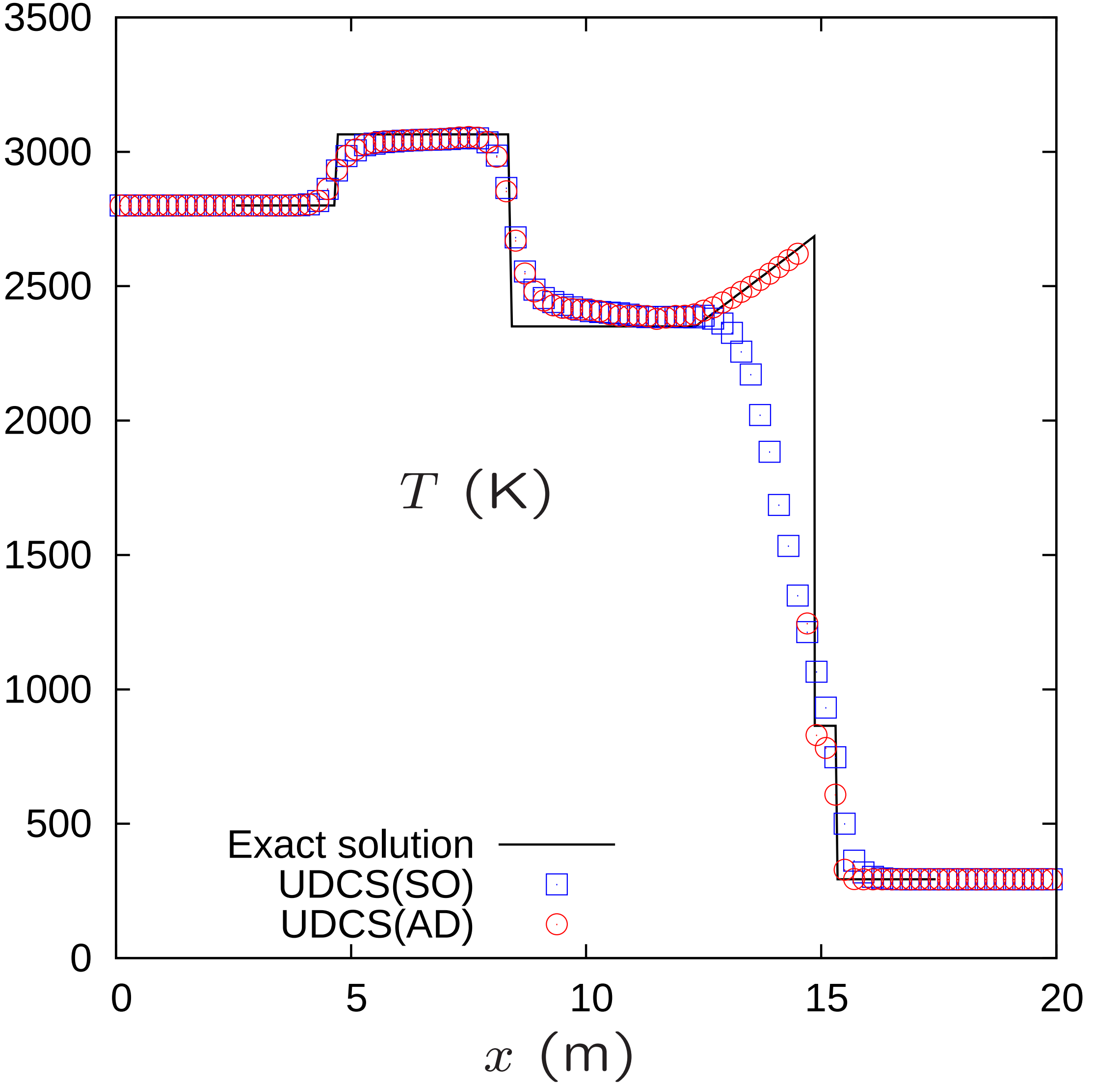
Shock tube at CJDF regime (2)



Shock tube at CJDF regime (3)



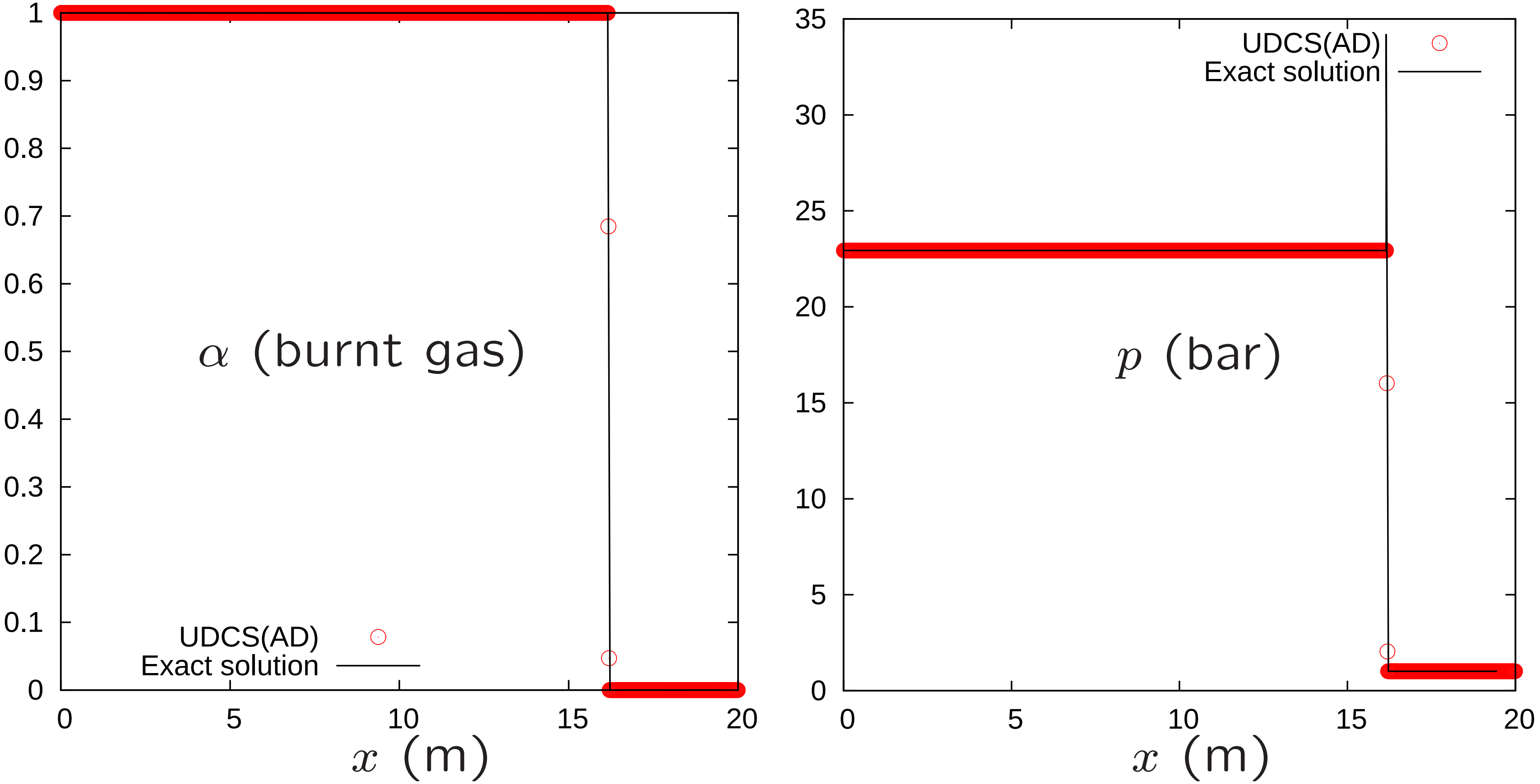
Shock tube at CJDF regime (4)



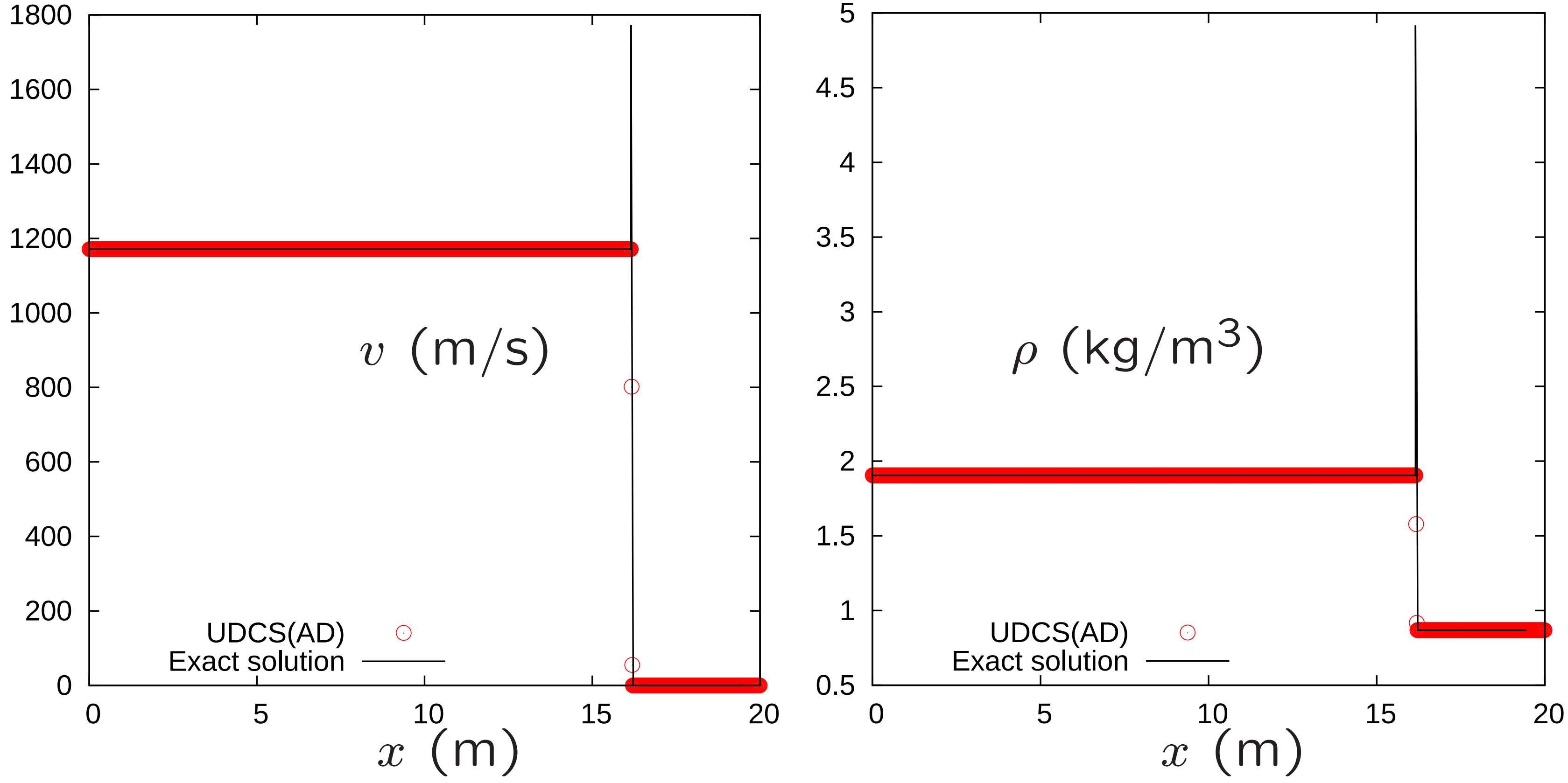
SDT propagation

- Purpose of this test case:
  to show that UDCS(AD) allows **to propagate a reactive shock wave with 1 or 2 intermediate zones** at worst.
- "All shock" reactive and non-reactive solver with entropy fix.
- Minmod reconstruction on primitive variables.
- RK2
- 1000 elements
- CFL=1.0
- $\varepsilon = 10^{-8}$
- $t = 7.5$ ms, i.e. $n_{\text{iter}} = 1110$.

SDT propagation (2)



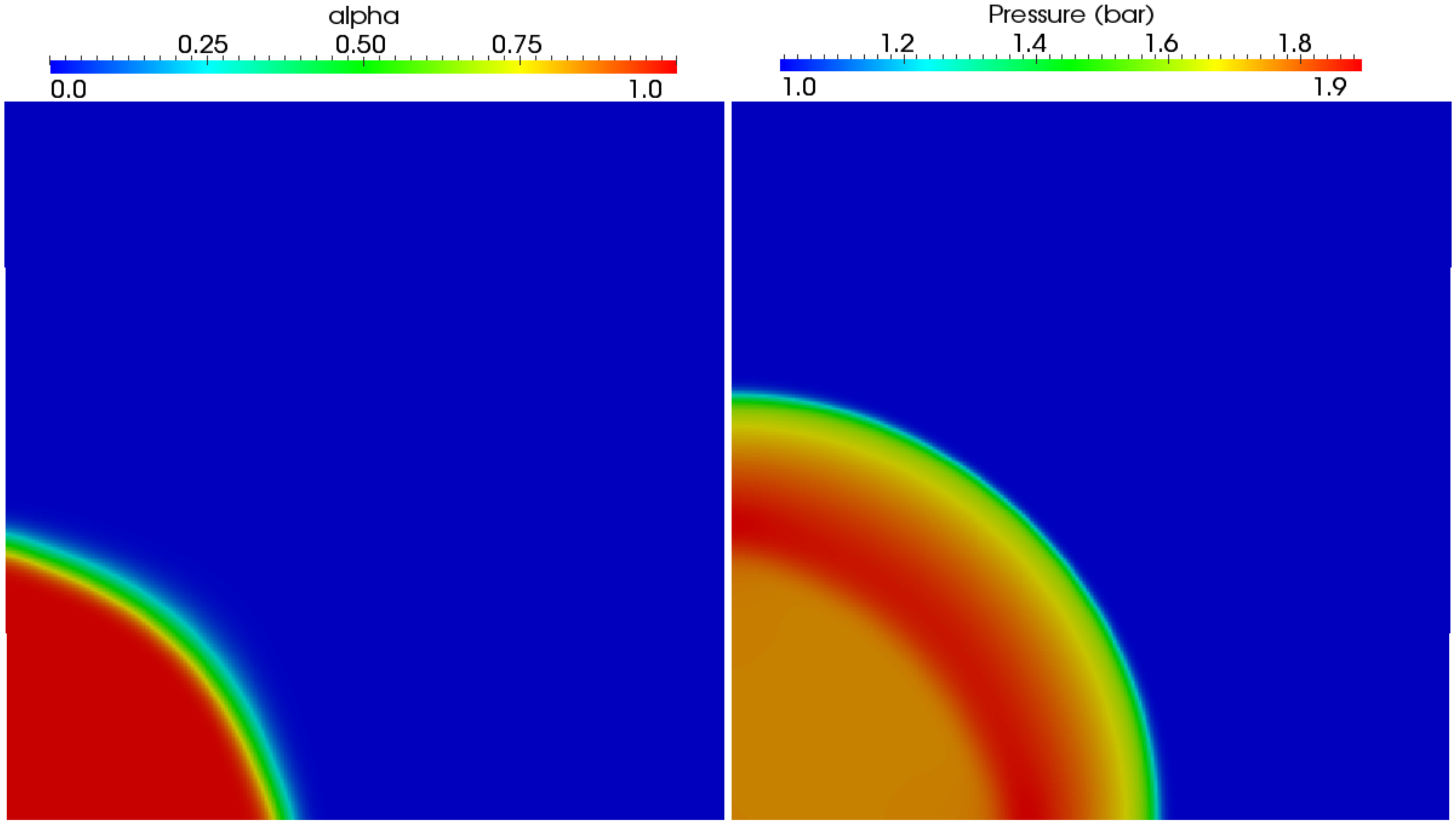
SDT propagation (3)



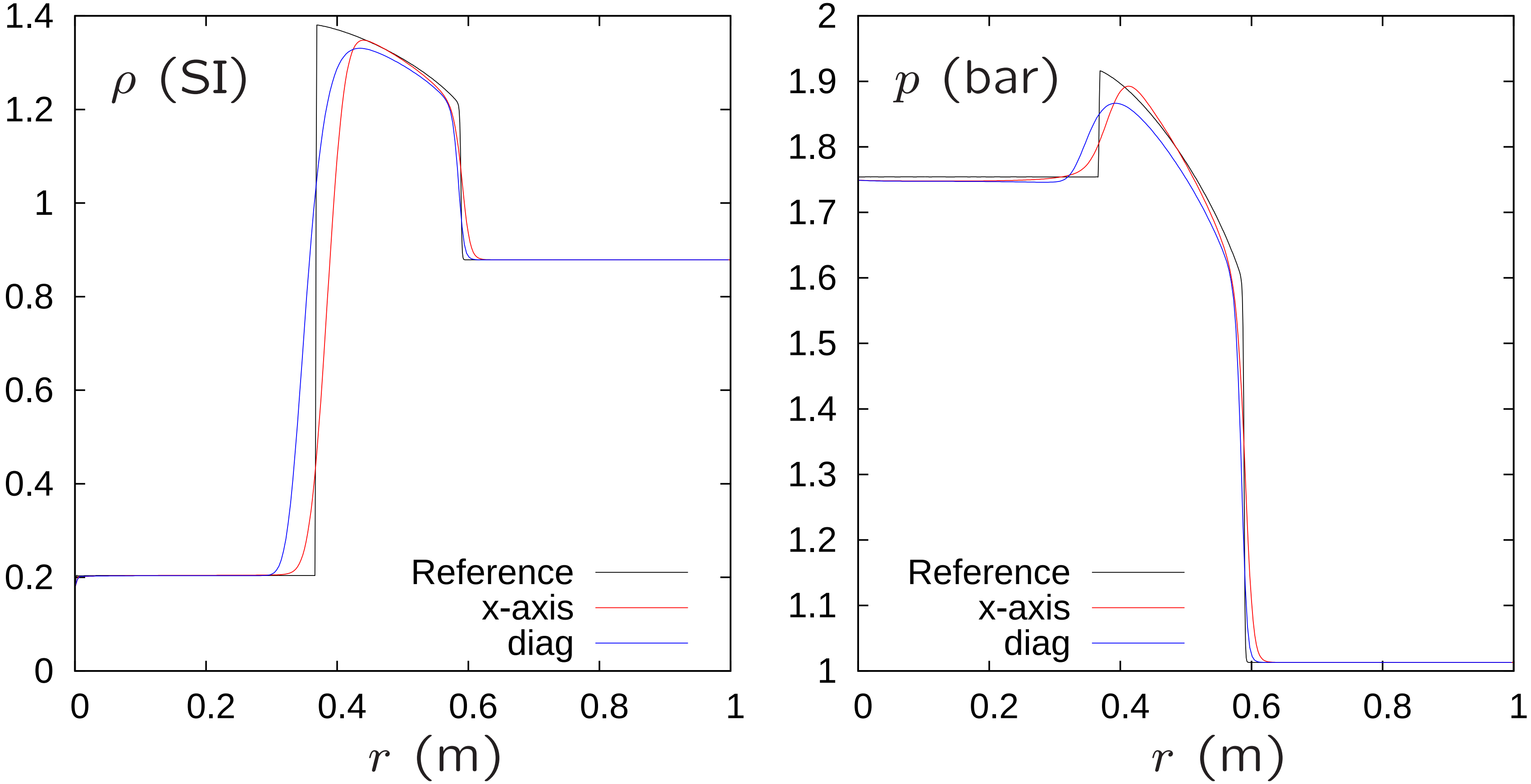
2D cylindrical WDF

- Purpose of this test case:
  to show the capability and the problems of UDCS in propagating a multi-dimensional **reactive shock wave**.
- "All shock" reactive and non-reactive solver with entropy fix.
- 400x400 elements
- CFL=0.4
- $\varepsilon = 10^{-8}$
- $t = 1.2$ ms

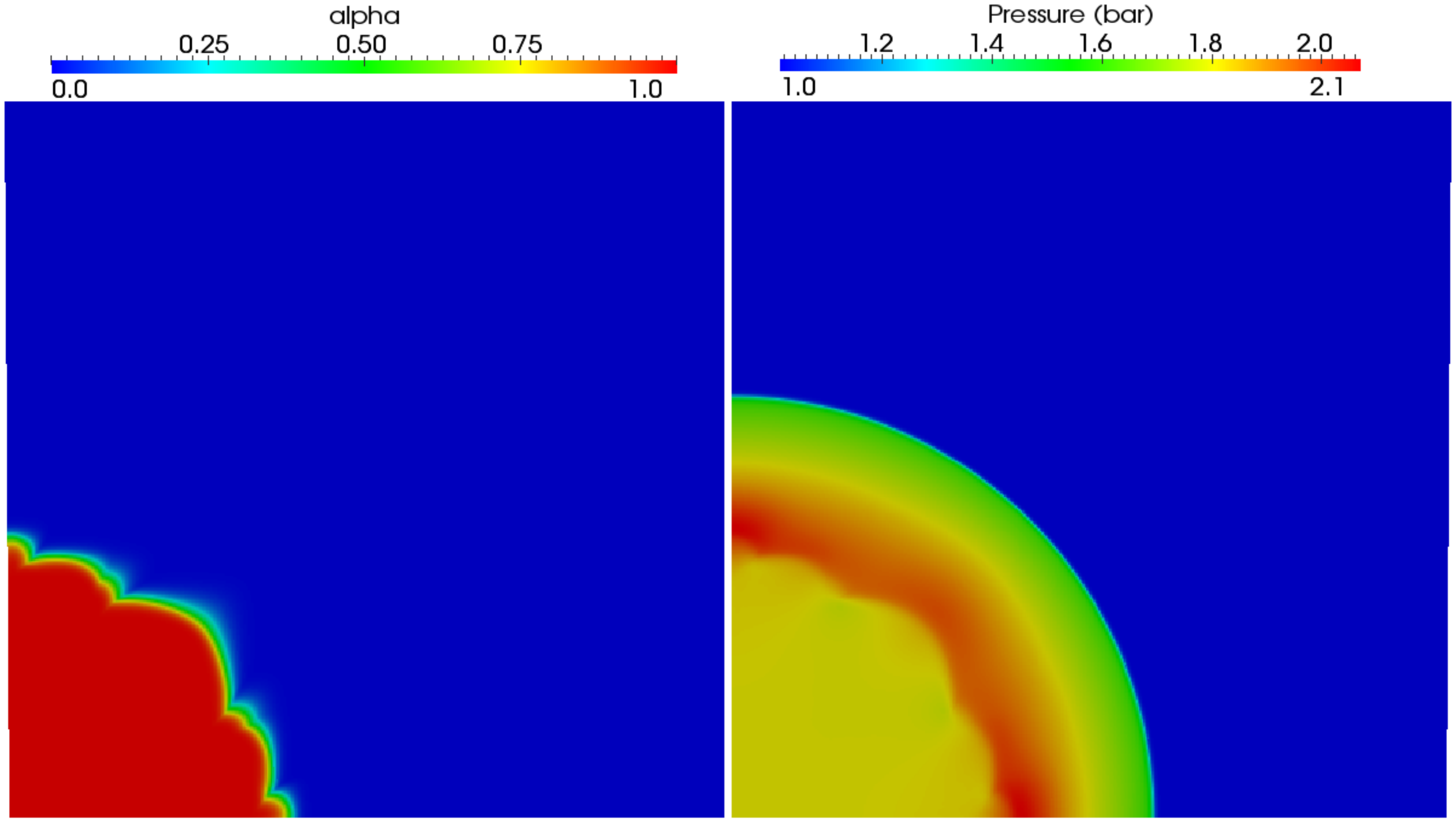
2D cylindrical WDF (2)



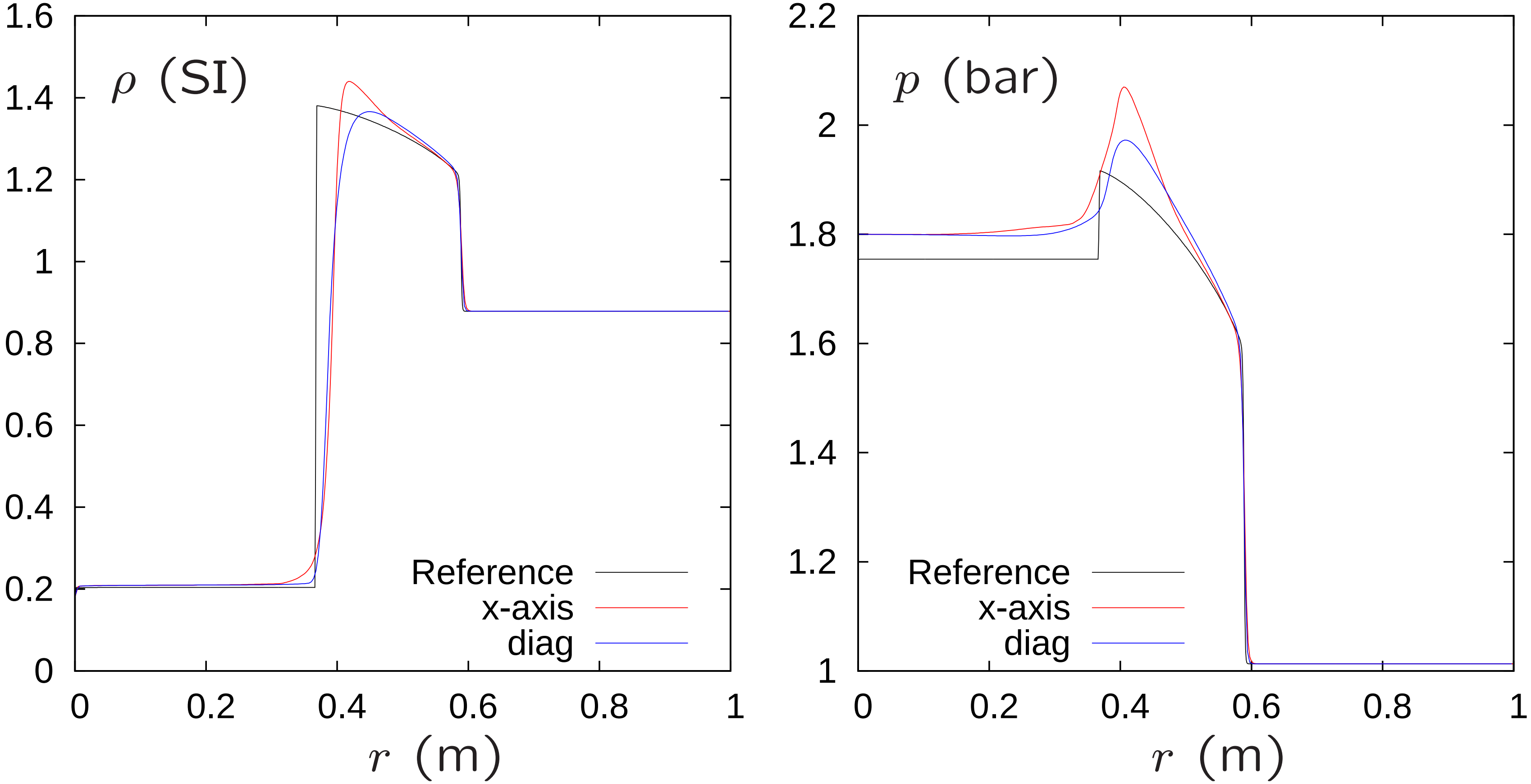
2D cylindrical WDF (3)



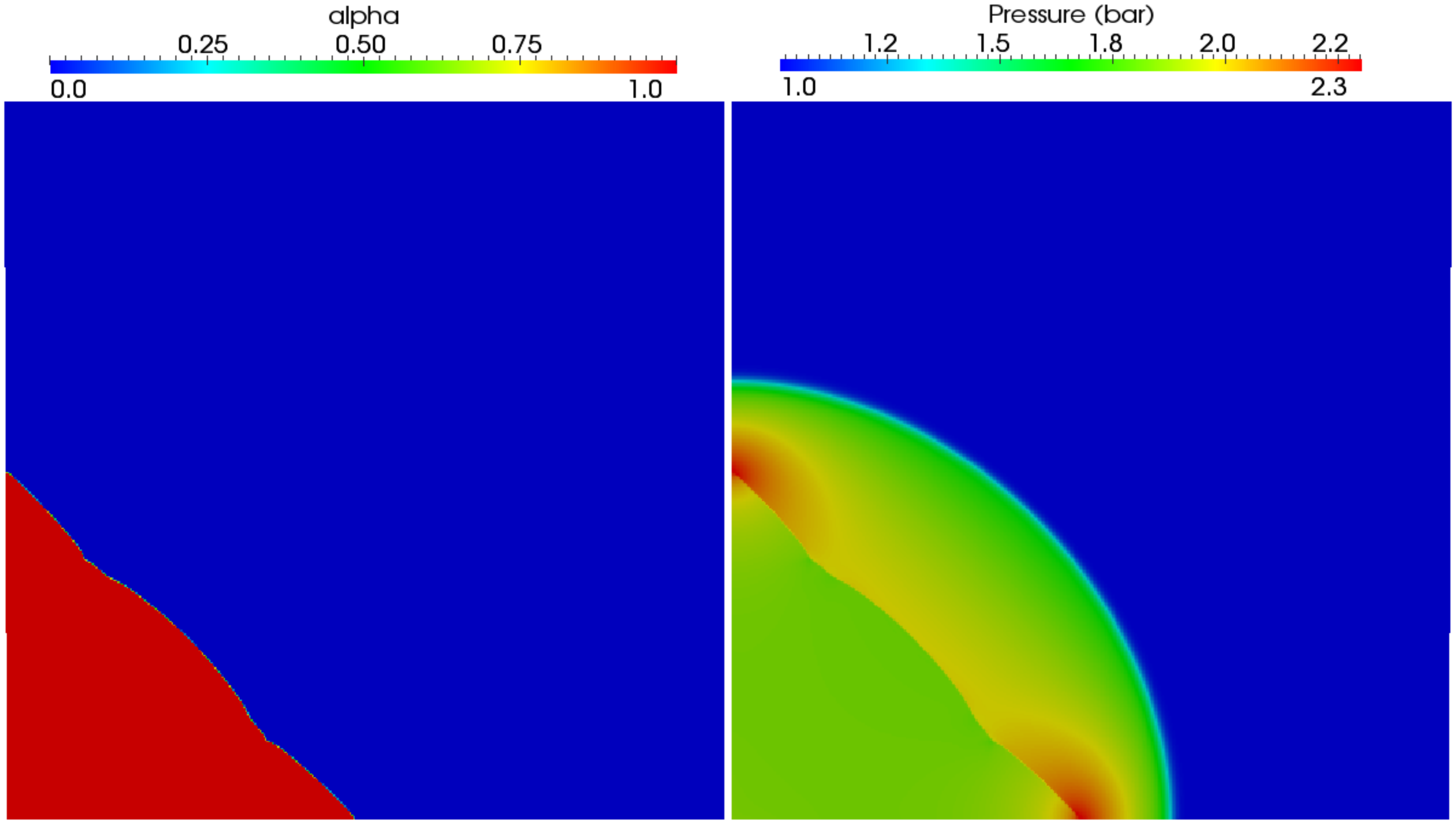
2D cylindrical WDF (4)



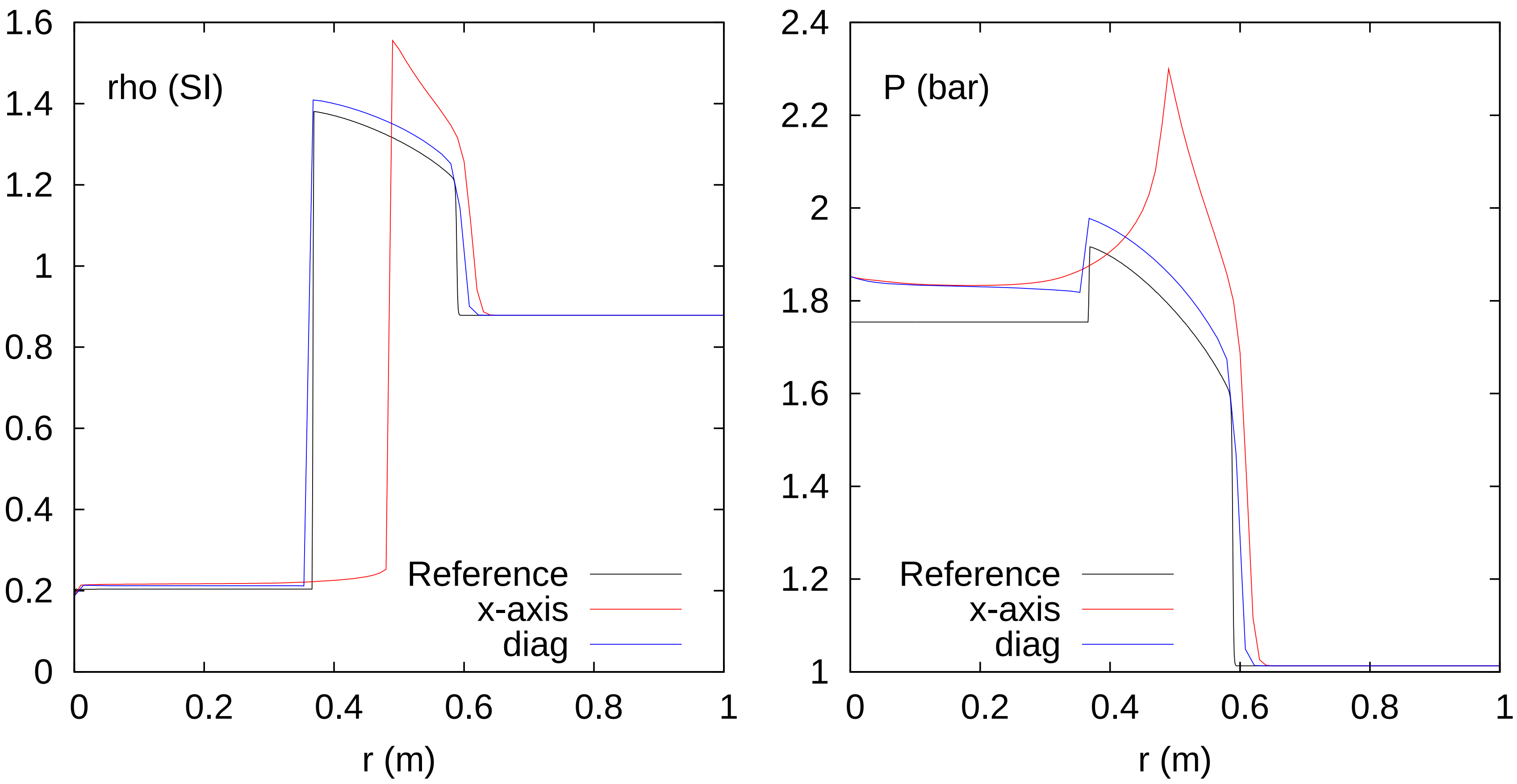
2D cylindrical WDF (5)



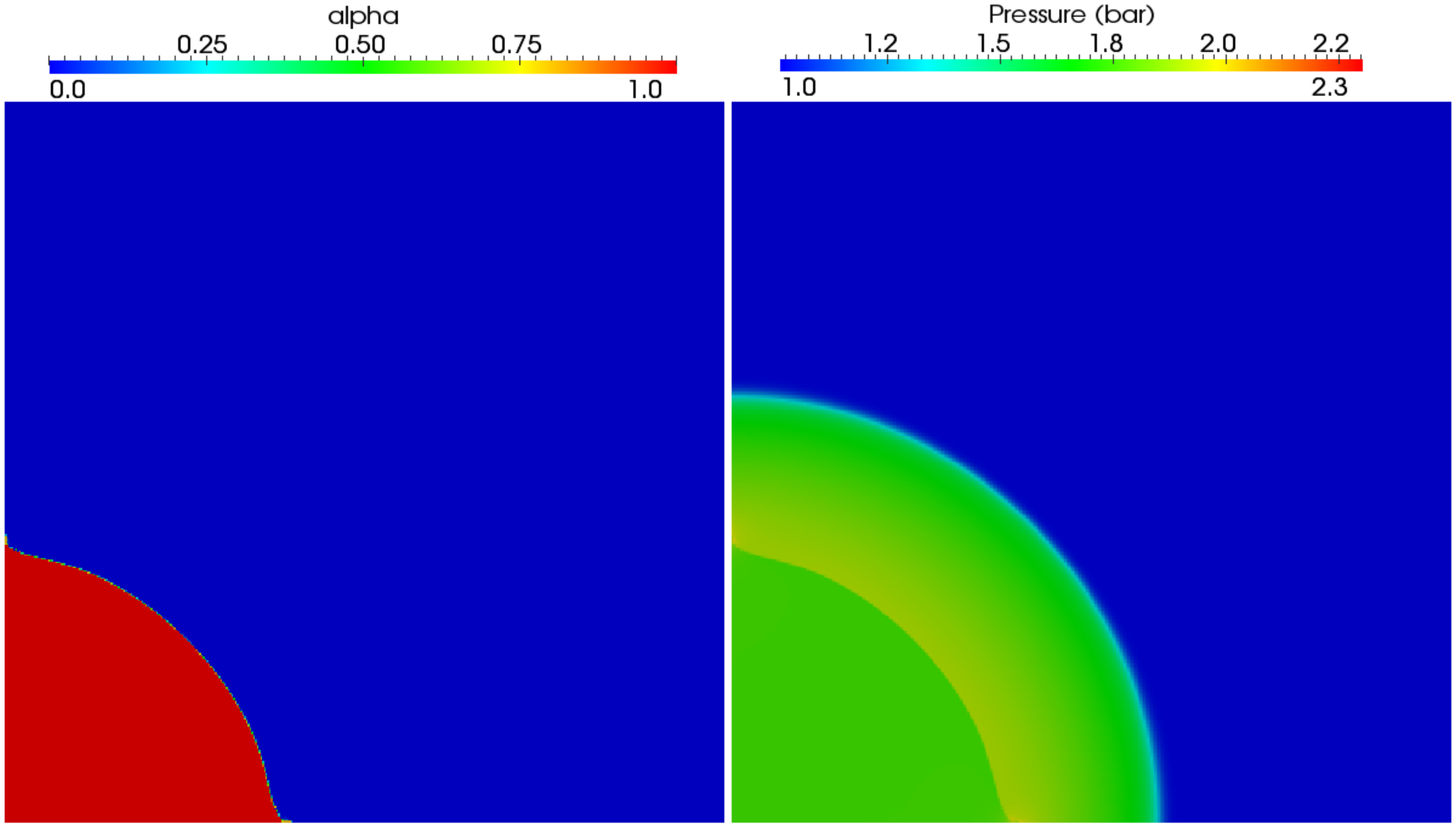
2D cylindrical WDF (6)



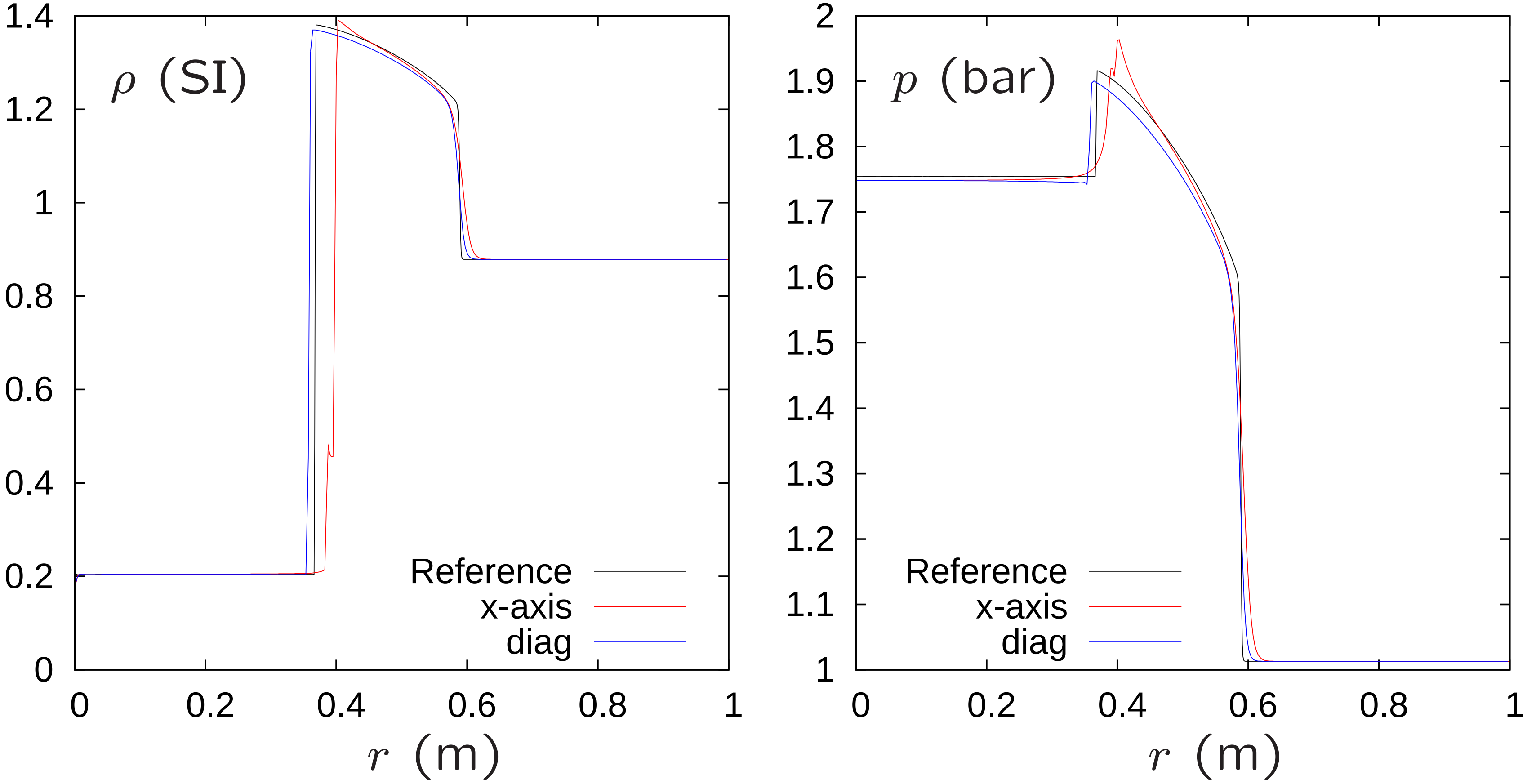
2D cylindrical WDF (7)



2D cylindrical WDF (8)



2D cylindrical WDF (9)



Summary, conclusion and future work

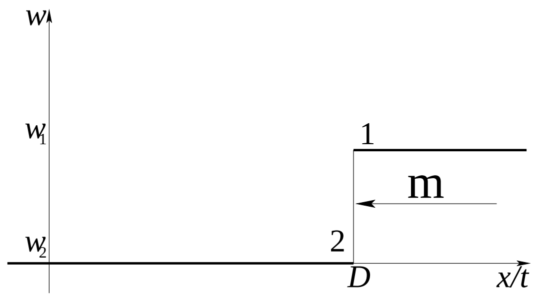
- The Riemann problem has been investigated in the case of thermally perfect ideal gases in deflagration and detonation regime.
- An algorithm is proposed for its solution.
- An **"all shock" reactive Riemann solver** has been developed and used in RDEM.
- Accuracy, robustness, CPU time consumption have been improved via UDCS.
- 1D plane-symmetric, line-symmetric and point-symmetric numerical test cases have successfully been computed in all combustion regimes and compared with Sedov solutions [Sedov 1959, Kuhl 1973].

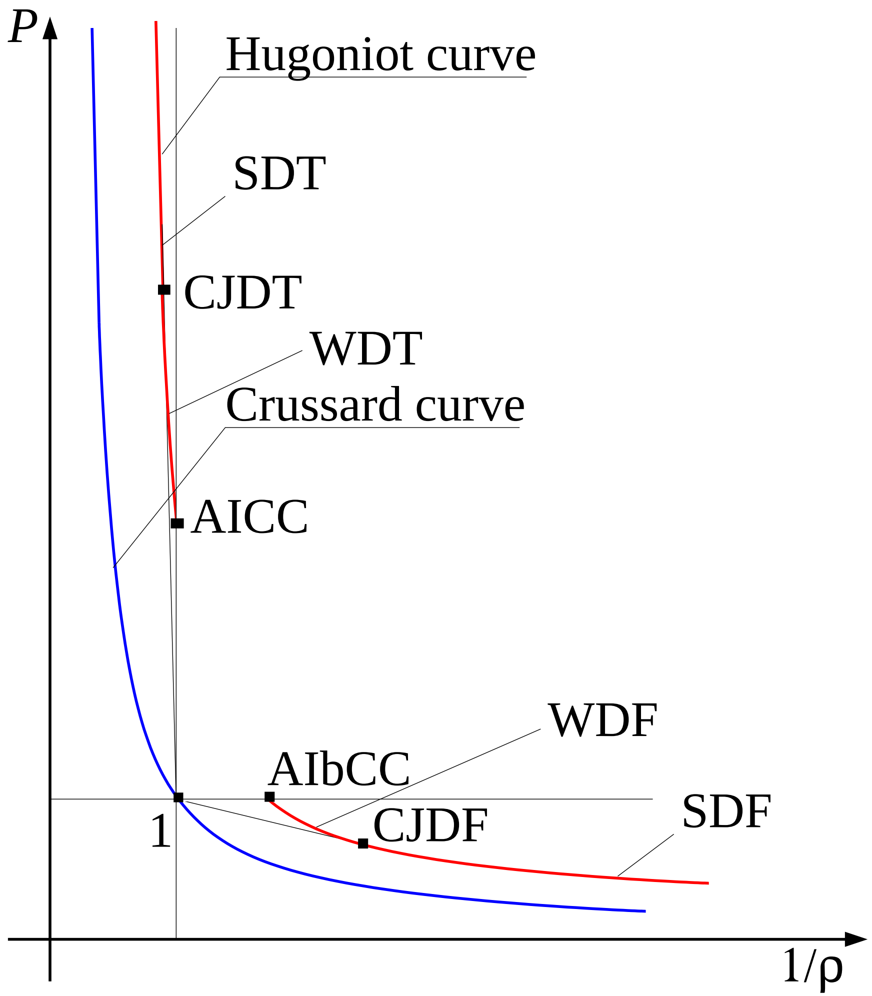
Summary, conclusion and future work (2)

- 2D numerical investigation has shown that UDCS(AD) must be improved.
- In reactor scale application, the value of K_0 is obtained via a phenomenological law [Velikorodny 2013], validated on large scale experiments existing in the literature (fast deflagration, DDT, detonations)
- The complete algorithm is implemented in Europlexus, on ALE grids, to compute the effects of high speed combustion on the mechanical structure.

Questions ?

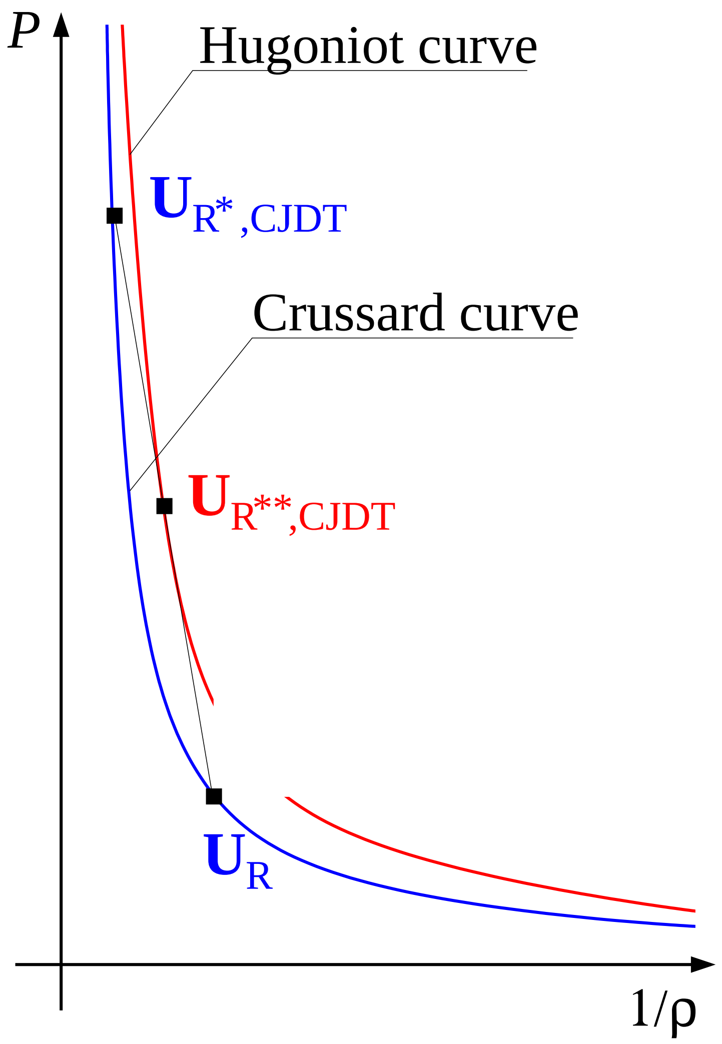
Reactive shock. Hypotheses





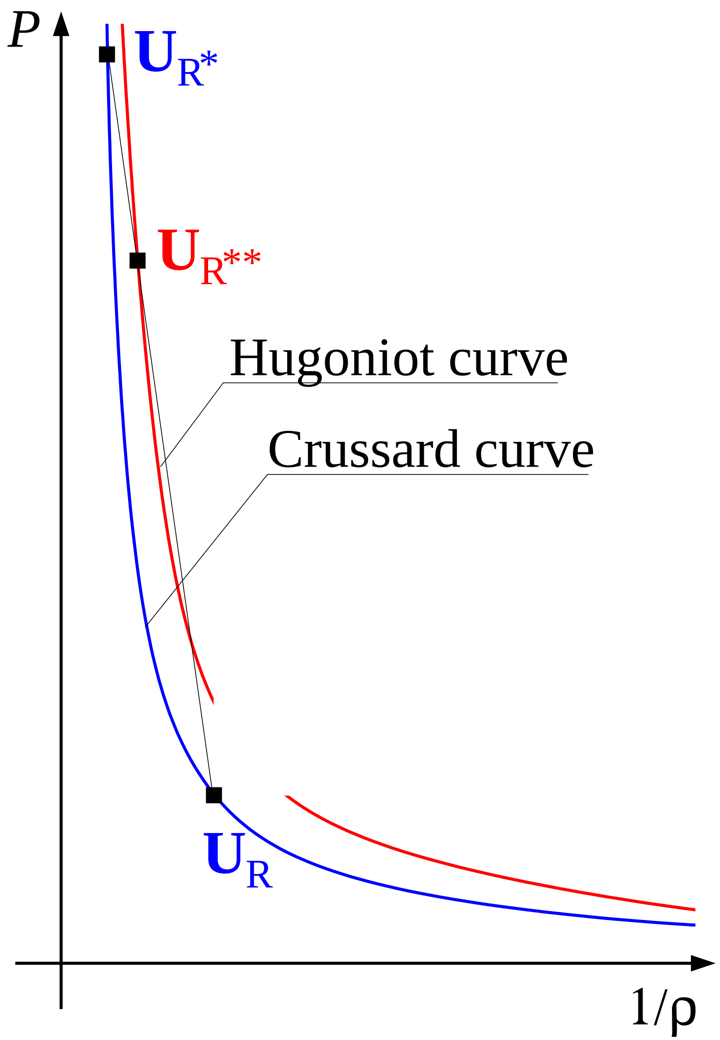
- Hugoniot curve is above the Crussard one
- WDF, CJDF, (SDT, CJDT) only are possible

Reactive Riemann problem solution (3bis)



$$\mathbf{U}_{R^{**},CJDT} \overset{CJDT}{\longmapsto} \mathbf{U}_R = \mathbf{U}_{R^{**},CJDT} \overset{CJDF}{\longmapsto} \mathbf{U}_{R^*,CJDT} \overset{Rsw}{\longmapsto} \mathbf{U}_R.$$

Reactive Riemann problem solution (4bis)



$$\mathbf{U}_{R^{**}} \overset{\text{SDT}}{\longmapsto} \mathbf{U}_R = \mathbf{U}_{R^{**}} \overset{\text{WDF}}{\longmapsto} \mathbf{U}_{R^*} \overset{\text{Rsw}}{\longmapsto} \mathbf{U}_R.$$

1D plane steady flame

- We consider a calorically perfect stoichiometric mixture of H_2 and air.

- We take as initial conditions

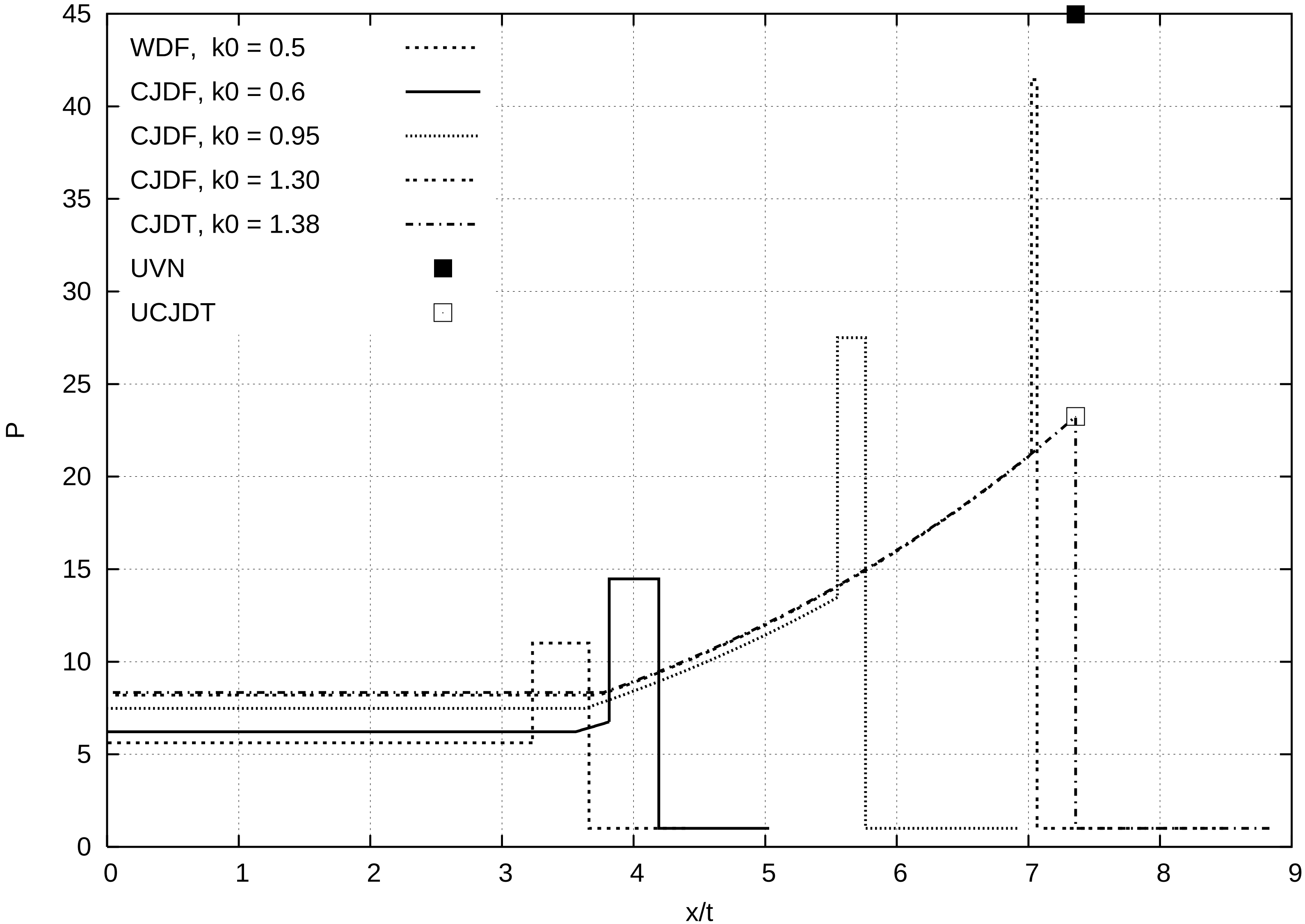
	P (Pa)	ρ (kg/m^3)	w (m/s)	ξ
R	100000.0	0.867268	0.0	0

- We look for the 1D plane-symmetric steady flame [Sedov 1959, Kuhl 73].

- We take as reference scales P_{R}, ρ_{R}, t.

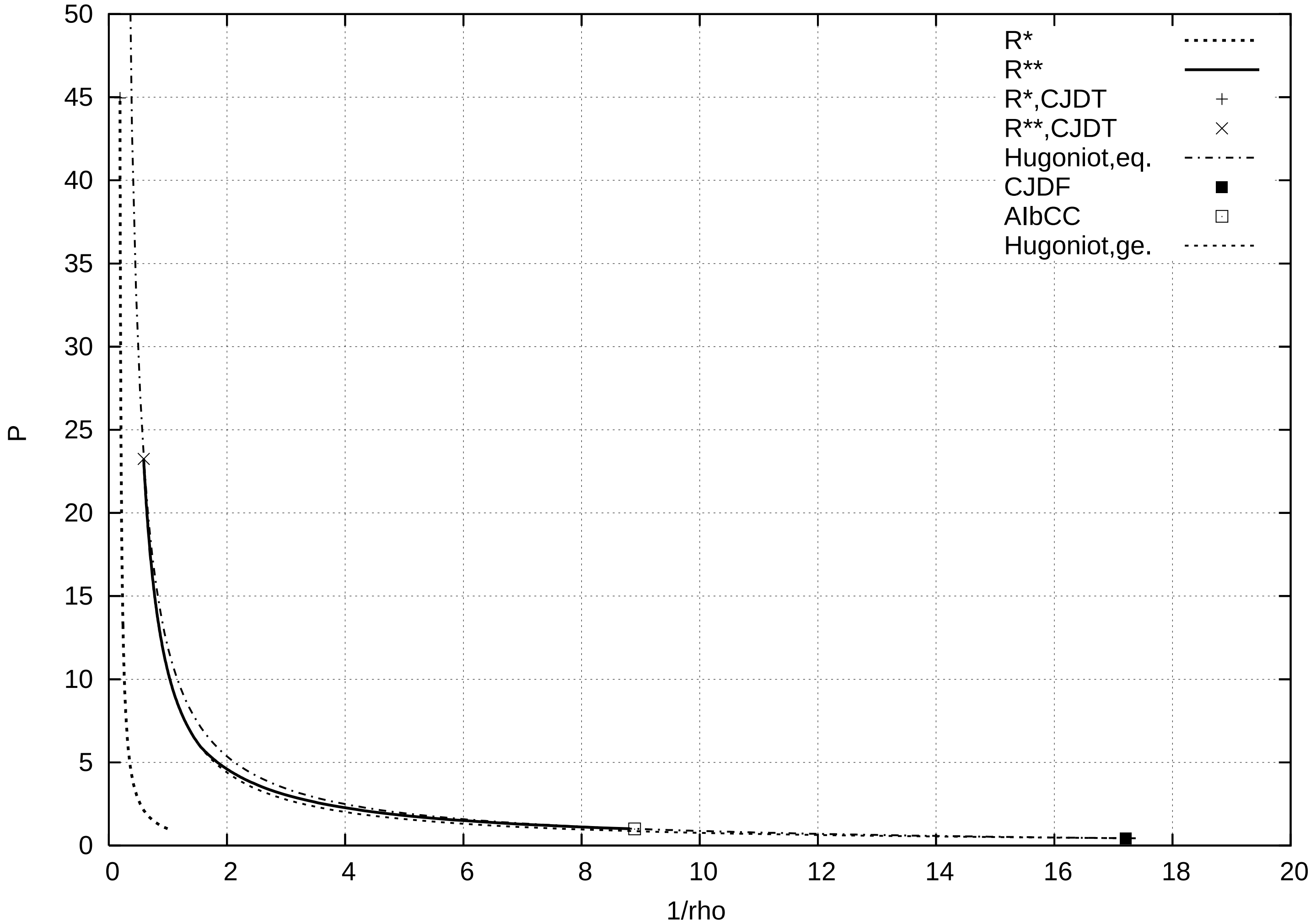
- Let us presents how the solution varies by varying $\tilde{K}_0$. We impose that the velocity in the burnt region is 0 (WDF→CJDF→CJDT).

1D plane steady flame (2)



Calorically perfect case. Non-dimensional values.

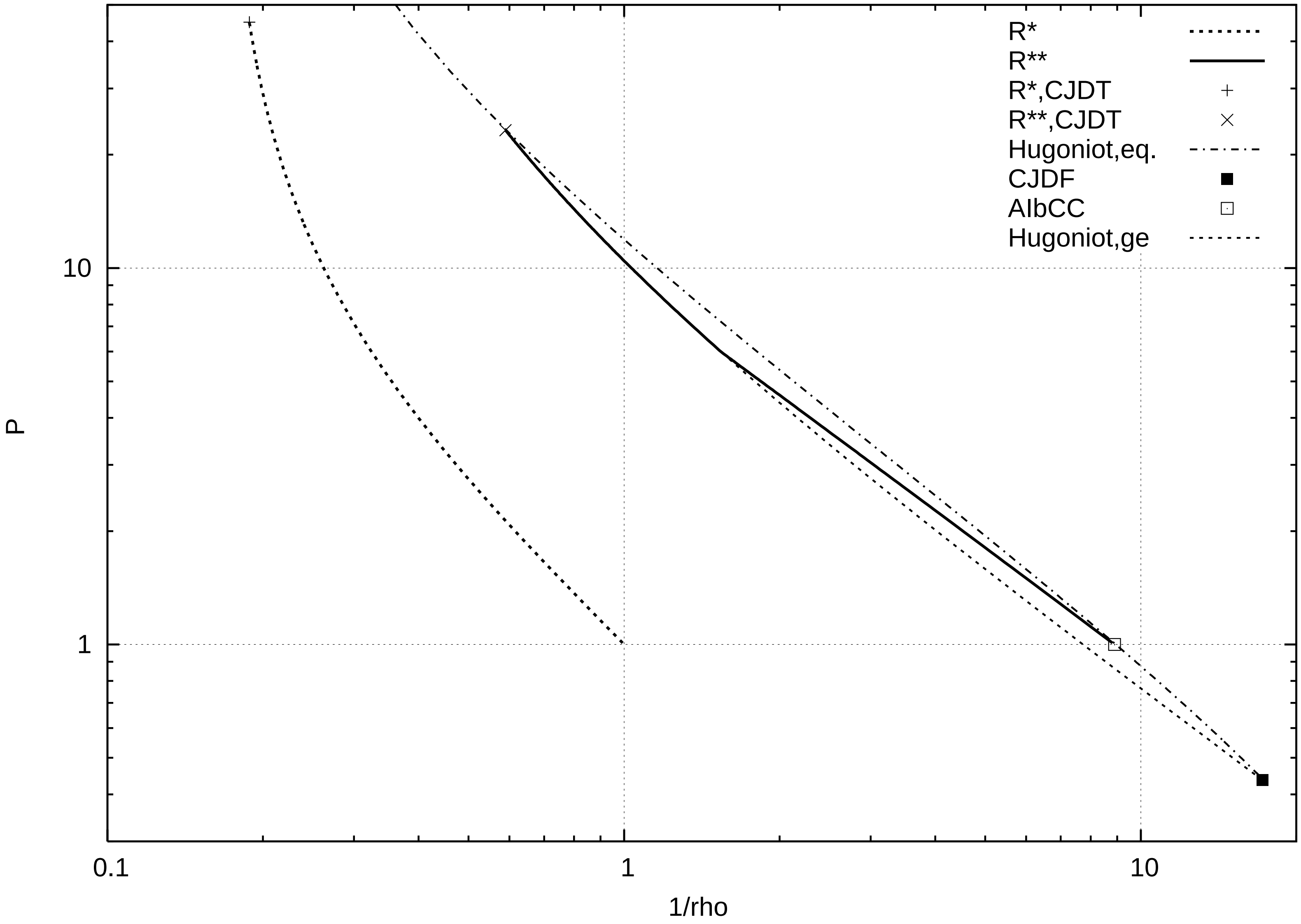
1D plane steady flame (2bis)



$$\text{Hugoniot,ge} = \{\mathbf{U}_{\text{R}^{**},\text{CJDF}} : \mathbf{U}_{\text{R}^{**},\text{CJDF}} \overset{\text{CJDF}}{\longmapsto} \mathbf{U}_{\text{R}^{*},\text{CJDF}} \overset{\text{Rgnl}}{\longmapsto} \mathbf{U}_{\text{R}}, \forall K_0 > 0\}$$

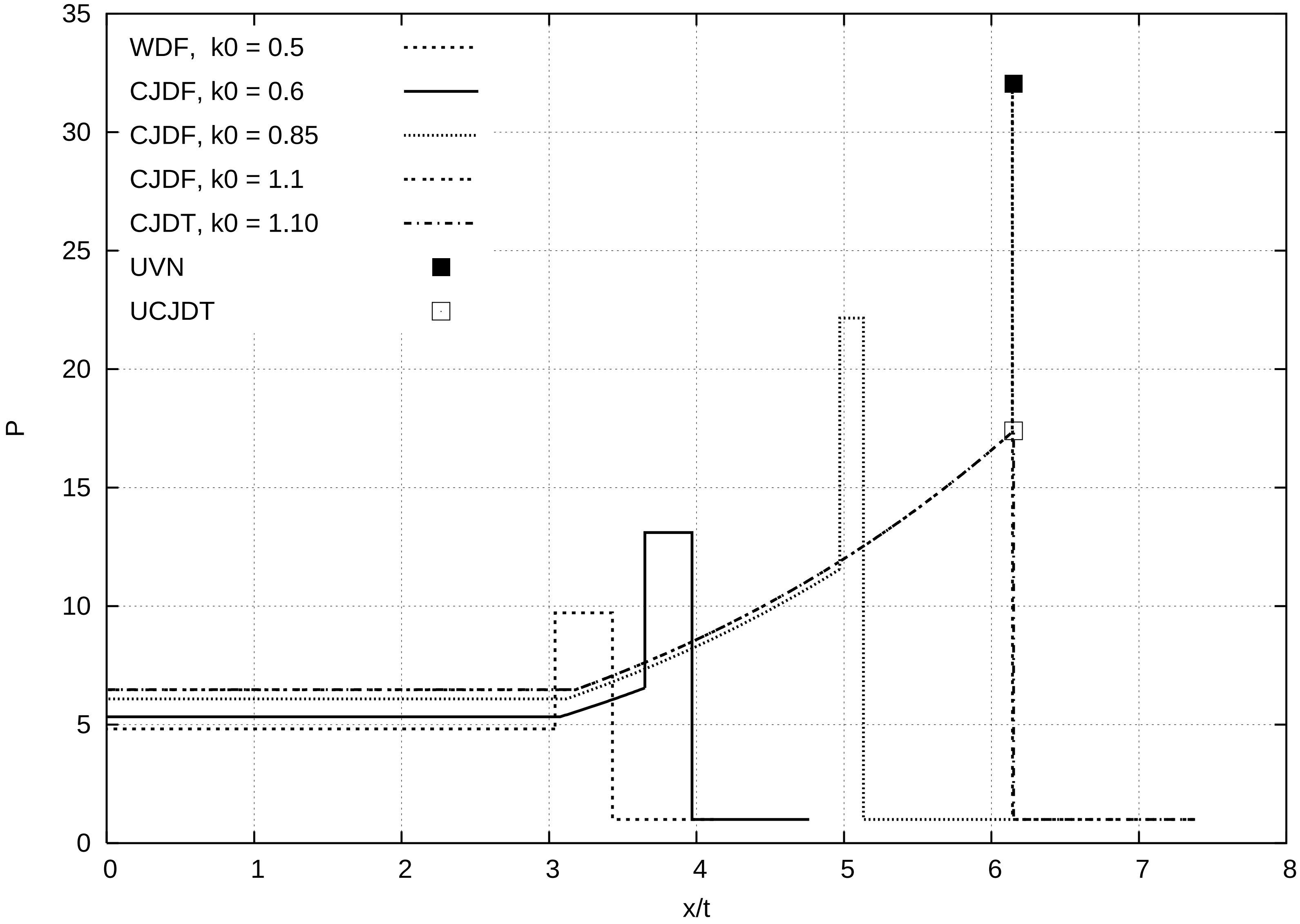
Non-dimensional values. (See also [Ciccarelli 2008], [Oppenheim 1953]).

1D plane steady flame (2ter)



Non-dimensional values. (See also [Ciccarelli 2008], [Oppenheim 1953]).

1D plane steady flame (3)



Non-dimensional values. Thermally-perfect mixture.

RDEM approach

- The discrete equation method is an **Eulerian approach**.
- It is used to study **multiphase mixtures**, in which global averaging of a variable in a control cell would lead to unacceptable numerical errors. In this approach, **each phase has its own variables**.
- It has been introduced in [Abgrall 2003].
- It has been modified (RDEM) and used, **coupled with a reactive solver**, to study **evaporation front propagation** and **detonation propagation** in [LeMetayer 2005].
- In the conclusion of [LeMetayer 2005], it is written:
  "... we believe that **the same approach can be used to propagate flame fronts** ..."

RDEM approach (2)

- For the sake of simplicity, we describe the approach in 1D.

- The 1D Euler equations can be written in compact form as

$$\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} = 0$$

$U = (1, \rho, \rho w, \rho \tilde{e}_t)^T$
$F = (0, \rho, \rho w^2 + P, \rho w \tilde{h}_t)^T.$

- We consider our combustion problem as a two phase problem.
  Phase 1 = unburnt mixture.
  Phase 2 = burnt one.

$$\frac{\partial \chi_k}{\partial t} + D \frac{\partial \chi_k}{\partial x} = 0, \;\; k = 1, 2$$

χ_1 is 0 in the burnt mixture and 1 in the unburnt one.
χ_2 is 1 in the burnt mixture and 0 in the unburnt one.
D is the propagation speed of the flame front.

RDEM approach (3)

- If we multiply the Euler equations by χ_k, we find

$$\chi_k \frac{\partial U}{\partial t} + \chi_k \frac{\partial F}{\partial x} = 0, \;\; k = 1, 2.$$

i.e. we double the number of equations to deal with.

- After some manipulations we find that

$$\frac{\partial \chi_k U}{\partial t} + \frac{\partial \chi_k F}{\partial x} = F^{\mathsf{Lag}} \frac{\partial \chi_k}{\partial x}, \;\; k = 1, 2 \qquad (1)$$

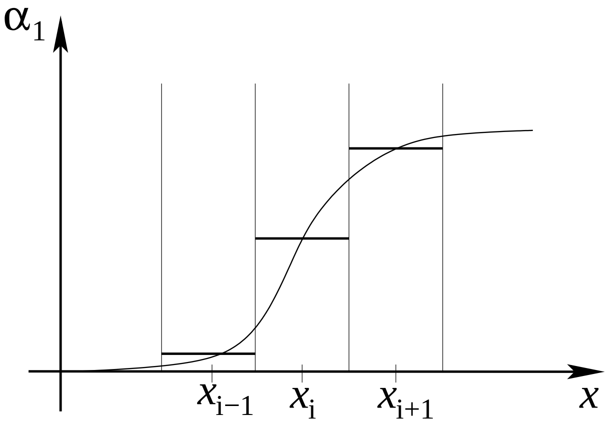
- We define the average value of the conservative variable for each phase

$$\{U_k\} = \frac{1}{V_k} \int_{\Omega_{\mathsf{K}}} U \mathrm{d}V, \;\; k = 1, 2.$$

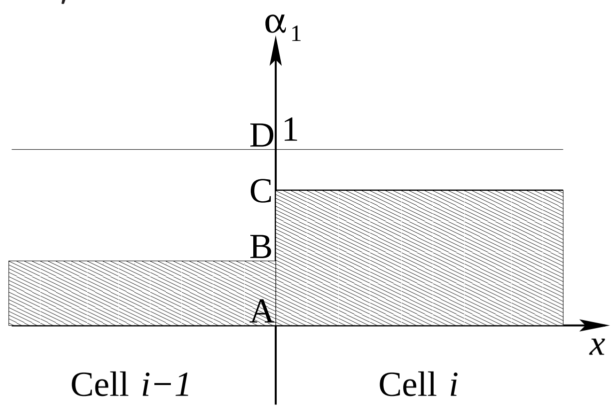
- We perform a partition our computational domain into several cells. We integrate equation (1) over a generic control cell and over time.
- The new vector of variables is $(\chi_k \{U_k\})$, $k = 1, 2$.

RDEM approach (4)

- Because of the numerical diffusion, the propagating flame front is smeared.



- **Each interface is partitioned** according to the values of the volume fraction of the two phases on the left and on the right. For instance, we consider the interface $i - 1/2$.

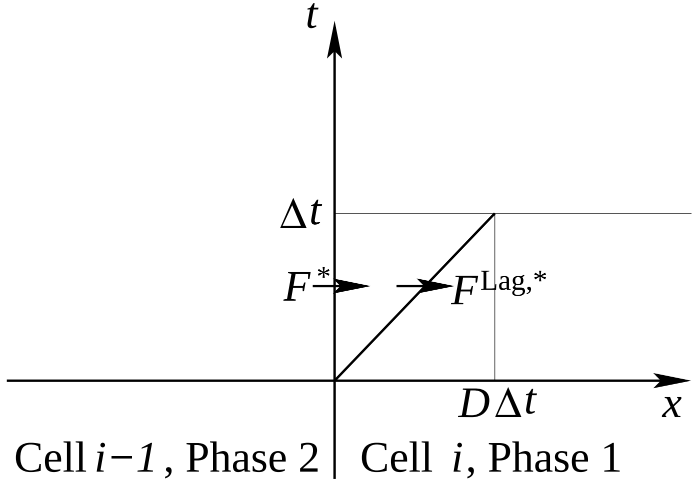


RDEM approach (4bis)

- The (unitary) interface $i-1/2$ is partitioned in **three parts**.
  - **AB**, $S_{k,(1,1),i-1/2}$, with a Riemann problem involving the phase 1 on both sides (**non-reactive Riemann problem** in our case).
  - **CD**, $S_{k,(2,2),i-1/2}$, with a Riemann problem involving the phase 2 on both sides (**non-reactive Riemann problem** in our case).
  - **BC**, $S_{k,(2,1),i-1/2}$, with a Riemann problem involving the phase 2 on the left and the phase 1 on the right (**reactive Riemann problem** in our case).
  - The Riemann problem involving the phase 1 on the left and 2 on the right is not considered since physically non-sense.

RDEM approach (5)

- Let us consider, in the interface $i-1/2$, the Riemann problem involving 2 on the left and 1 on the right. We suppose that the deflagration wave has positive velocity ($D > 0$).



- Because of the Riemann problem (2,1) at this interface,

$$\Delta(V_1\{U_1\})_{i-1} = 0$$

$$\Delta(V_1\{U_1\})_i = \Delta t \cdot S_{1,(12),i-1/2} F^{\mathrm{Lag},*}_{i-1/2}$$

$$\Delta(V_2\{U_2\})_{i-1} = -\Delta t \cdot S_{2,(12),i-1/2} F^{*}_{i-1/2}$$

$$\Delta(V_2\{U_2\})_i = \Delta t \cdot S_{2,(12),i-1/2} \left(F^{*}_{i-1/2} - F^{\mathrm{Lag},*}_{i-1/2} \right)$$

RDEM approach (6)

i.e. if we divided by the cell volume

$$\Delta(\alpha_1\{U_1\})_{i-1} = 0$$

$$\Delta(\alpha_1\{U_1\})_i = \frac{\Delta t}{\Delta x_i} \cdot S_{1,(12),i-1/2} F^{\mathrm{Lag},*}_{i-1/2}$$

$$\Delta(\alpha_2\{U_2\})_{i-1} = -\frac{\Delta t}{\Delta x_{i-1}} \cdot S_{2,(12),i-1/2} F^{*}_{i-1/2}$$

$$\Delta(\alpha_2\{U_2\})_i = \frac{\Delta t}{\Delta x_i} \cdot S_{2,(12),i-1/2} \left(F^{*}_{i-1/2} - F^{\mathrm{Lag},*}_{i-1/2} \right).$$

- In exact algebra, $S_{1,(lm),i-1/2} = S_{2,(lm),i-1/2}$.
- There is a term involving $F^{\mathrm{Lag},*}$ which is **non-conservative** for each single phase. **Nevertheless**, what is taken from one phase is given to the other.

RDEM approach (7)

- In compact form, for the cell i we can write

$$\frac{(\alpha_k\{U_k\})_i^{n+1} - (\alpha_k\{U_k\})_i^n}{\Delta t} +$$
$$\frac{1}{\Delta x_i}\left(\sum_{l,m}(S_k\chi_k^* F^*)_{(lm),i+1/2} - \sum_{l,m}(S_k\chi_k^* F^*)_{(lm),i-1/2}\right) +$$
$$\frac{1}{\Delta x_i}\left(\sum_{l,m}\left\{S_{k,(lm),i+1/2}(F_{i+1/2}^{\mathrm{Lag},*}(\chi_{k,i+1/2}^* - \chi_{k,i}))_{(l,m)}\right\} - \right.$$
$$\left.\sum_{l,m}\left\{S_{k,(lm),i-1/2}(F_{i-1/2}^{\mathrm{Lag},*}(\chi_{k,i-1/2}^* - \chi_{k,i}))_{(l,m)}\right\}\right)$$
$$= 0.$$

Bibliography

- [Abgrall 2003]. R Abgrall, R Saurel. Discrete equations for physical and numerical compressible multiphase mixtures. Journal of Computational Physics vol. 186. 2003.

- [Ciccarelli 2008]. G Ciccarelli and S Dorofeev. Flame acceleration and transition to detonation in ducts. Progress in Energy and Combustion Science. 2008

- [Kuhl 1973]. AL Kuhl, MM Kamel, AK Oppenheim. Pressure Waves Generated by Steady Flames. Fourteenth Symposium (International) on Combustion, The Combustion Institute, pages 1201–. 1973

- [LeMetayer 2005]. O Le Métayer, J Massoni, R Saurel. Modelling evaporation fronts with reactive Riemann solvers. Journal of Computational Physics vol. 205. 2005.

Bibliography (2)

- [Oppenheim 1953]. AK Oppenheim. gasdynamic analysis of the development of gaseous detonation and its hydraulic analogy. Proc Combust Inst, vol. 4. 1953

- [Sedov 1959]. LI Sedov. Similarity and Dimensional Methods in Mechanics. Academic Press. 1959

- [Teng 1982]. ZH Teng, AJ Chorin, TP Liu. Riemann Problems for Reacting Gas, with Applications to Transition. SIAM J Appl Math vol. 42. 1982

- [Tang 2012]. K Tang. Combining Discrete Equations Method and Upwind Downwind-Controlled Splitting for Non-Reacting and Reacting Two-Fluid Computations. PhD thesis, University of Grenoble, 2012.

Bibliography (3)

- [Velikorodny 2013]. A. Velikorodny, E. Studer, S. Kudriakov, A. Beccantini. Combustion modeling in large scale volumes. In ICHS 2013 - International Conference on Hydrogen Safety, September 9-11, 2013, Brussels - Belgium.

- [Zhang 1989]. T Zhang, Y Zheng. Riemann Problems in Gasdynamics Combustion. Journal of Differential Equations vol. 77. 1989