



High-order extension of Roe's solver for compressible multicomponent real gas flows

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Introduction

Inflammable gas dynamics in confined environment

- Storage of flammable gas
- Release of hydrogen in core reactor during nuclear accident

Dynamic behaviour of the flame

- Flame acceleration/transition to detonation
- Onset of Detonation
- Influence of concentration gradients¹, complex geometry, turbulence, shock waves...

Experimental Setup 2





- Figure 1 Shadowgraph sequence of DDT inside obstacle with vertical concentration gradient 1
- 1. L. R. Boeck et al. "Detonation propagation in hydrogen-air mixtures with transverse concentration gradients". In : *Shock Waves* 26 (2016), p. 181-192.
- 2. R. Scarpa et al. "Influence of initial pressure on hydrogen/air flame acceleration during severe accident in NPP". In : International Journal of Hydrogen Energy 44.17 (2019). Special issue on The 7th International Conference on Hydrogen Safety (ICHS 2017), 11-13 September 2017, Hamburg, Germany, p. 9009 -9017.

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Flame acceleration and transition to detonation

Numerical challenges

- Compressible effects
 - Hydrodynamic instabilities
 - Interaction with turbulence
 - Chemical reaction
 - Detonation structure...
- Large variation of temperature

- ⇒ Numerical discontinuities
- ⇒ Multiscales in time and space
- \Rightarrow Realistic Thermodynamic models



Figure 2 - Representation of the dependence of heat capacities on temperature with NASA polynomials

Construction of a solver to manage these problematics

Numerical tools : MR CHORUS solver

Navier-Stokes equation

$$\mathbf{w}_t + \nabla \cdot (\mathbf{F}^{\mathcal{E}}(\mathbf{w}) - \mathbf{F}^{\mathcal{V}}(\mathbf{w}, \nabla \mathbf{w})) = \mathbf{S}(\mathbf{w}), \text{ with } \mathbf{w} = (\rho, \rho \mathbf{u}, \rho \mathcal{E})^{\mathcal{T}}$$
(1)

Multiresolution³

• Splitting algorithm on operators and dimensions

$$w_j^{n+1} = \mathcal{L}_{\delta t/2}^{S} \mathcal{L}_{\delta t/2}^{E} \mathcal{L}_{\delta t}^{V} \mathcal{L}_{\delta t/2}^{E} \mathcal{L}_{\delta t/2}^{S} w_j^{n}$$

• Dynamic Refinement

Approximated Riemann Solver

- Classical Roe solver for single calorically perfect gas
- High order extension with limiters to avoid Gibbs phenomenon (spurious oscillations) : OSMP scheme

Objective

Extent existing solver to reactive multicomponent real gas flows with no assumption on the equation of state



Figure 3 – Shock/boundary layer interaction. Adapted grid and contour of the density gradient²

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^{3.} Christian Tenaud, Olivier Roussel et Linda Bentaleb. "Unsteady compressible flow computations using an adaptive multiresolution technique coupled with a high-order one-step shock-capturing scheme". In : *Computers & Fluids* 120 (2015), p. 111 -125.

Numerical model

Roe Approximate Riemann Solver

Roe Solver⁴

Roe's approach replace the Jacobian matrix evaluated at the intersection $\underline{\underline{A}}(w) = \partial F^{E}(w)/\partial w$ by a constant Jacobian matrix evaluated at the Roe average state \overline{w} combination of left w_{L} and right states w_{R}

$$\underline{\underline{A}}(\overline{\mathbf{w}}) = \underline{\underline{A}}(\mathbf{w}_L, \mathbf{w}_R) \tag{3}$$



With a general equation of state

$$\underline{\underline{A}}(\overline{\mathbf{w}}) = \underline{\underline{A}}(\overline{\rho}, \overline{Y}_1, ..., \overline{Y}_{ns}, \overline{\mathbf{u}}, \overline{h}, \overline{\chi}_1, ..., \overline{\chi}_{ns}, \overline{\kappa})$$
(4)

with compressibility factors

$$\chi_{i} = \left(\frac{\partial p}{\partial \rho_{i}}\right)_{\tilde{\epsilon}, \rho_{k, k \neq i}} \quad \text{and} \quad \kappa = \left(\frac{\partial p}{\partial \tilde{\epsilon}}\right)_{\rho_{k}} \tag{5}$$

Flux expression

$$\mathsf{F}_{i+\frac{1}{2}}^{Roe} = \frac{1}{2}(\mathsf{F}_{L} + \mathsf{F}_{R}) - \frac{1}{2}\sum_{i=1}^{m}\delta\overline{\alpha}_{i}|\overline{\lambda}_{i}|\mathbf{\bar{r}}^{(i)} \tag{6}$$

with $\overline{\lambda_i}$, $\overline{\mathbf{r}}^{(i)}$ and $\overline{\alpha}_i$ eigenvalues, eigenvectors and Riemann invariants of $\underline{\mathbf{A}}(\overline{\mathbf{w}})$

^{4.} P.L Roe. "Approximate Riemann solvers, parameter vectors, and difference schemes". In : Journal of Computational Physics 43.2 (1981), p. 357 - 372.

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Rule for the construction of the Roe Average State

$$\underline{\underline{A}}(\overline{\mathbf{w}})(\mathbf{w}_{L} - \mathbf{w}_{R}) = \mathbf{F}(\mathbf{w}_{L}) - \mathbf{F}(\mathbf{w}_{R})$$
(7)

^{5.} Marcel Vinokur et Jean-Louis Montagné. "Generalized flux-vector splitting and Roe average for an equilibrium real gas". In : Journal of Computational Physics 89.2 (1990), p. 276 -300.

^{6.} Jian-Shun Shuen, Meng-Sing Liou et Bram Van Leer. "Inviscid flux-splitting algorithms for real gases with non-equilibrium

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Roe average operator for primitive/conservatives variables

$$[\rho, Y_k, \mathbf{u}, h] \quad \Rightarrow \quad \overline{(\cdot)} = \theta(\cdot)_L + (1 - \theta)(\cdot)_R \quad \text{with} \quad \theta = \frac{\sqrt{\rho_L}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \tag{8}$$

^{5.} Vinokur et Montagné, "Generalized flux-vector splitting and Roe average for an equilibrium real gas".

^{6.} Shuen, Liou et Leer, "Inviscid flux-splitting algorithms for real gases with non-equilibrium chemistry".

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Treatment of the compressibility factors χ_i and κ

$$\underbrace{\underline{\underline{A}}}_{[\overline{\mathbf{w}})}(\mathbf{w}_{L} - \mathbf{w}_{R}) = \mathbf{F}(\mathbf{w}_{L}) - \mathbf{F}(\mathbf{w}_{R}) \\ + \\ \boxed{\text{Roe average operator}} \qquad \Rightarrow \quad \Delta \rho = \sum_{i=0}^{ns} \overline{\chi}_{i} \Delta \rho_{i} + \overline{\kappa} \Delta \tilde{\epsilon}$$
(9)

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(9)

Approximation of the compressibility factors with Vinokur and Montagné⁵ (approximation of integrals) or Liou⁶ (thermodynamic properties) approximations :

$$\hat{\kappa} = \int_0^1 \kappa[\rho(t), \tilde{\epsilon}(t)] dt \qquad \hat{\chi}_i = \int_0^1 \chi_i[\rho(t), \tilde{\epsilon}(t)] dt \qquad (10)$$

^{5.} Vinokur et Montagné, "Generalized flux-vector splitting and Roe average for an equilibrium real gas".

^{6.} Shuen, Liou et Leer, "Inviscid flux-splitting algorithms for real gases with non-equilibrium chemistry".

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Treatment of the compressibility factors χ_i and κ

$$\frac{\underline{\underline{A}}(\overline{\mathbf{w}})(\mathbf{w}_{L} - \mathbf{w}_{R}) = \mathbf{F}(\mathbf{w}_{L}) - \mathbf{F}(\mathbf{w}_{R})}{+} \qquad \Rightarrow \quad \Delta \rho = \sum_{i=0}^{n_{S}} \overline{\chi}_{i} \Delta \rho_{i} + \overline{\kappa} \Delta \tilde{\epsilon}$$
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Orthogonal projection on the ns - 1 dimension hyperplane defined by (9)

$$\overline{\kappa} = \mathcal{P}(\hat{\kappa}) \qquad \overline{\chi}_i = \mathcal{P}(\hat{\chi}_i)$$
(11)

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^{5.} Vinokur et Montagné, "Generalized flux-vector splitting and Roe average for an equilibrium real gas".

^{6.} Shuen, Liou et Leer, "Inviscid flux-splitting algorithms for real gases with non-equilibrium chemistry".

High order extension with OSMP scheme

One step monotonocity preserving (OSMP) scheme⁷

New system of advection equations

$$\frac{\partial \overline{\alpha}_i}{\partial t} + \overline{\lambda}_i \frac{\partial \overline{\alpha}_i}{\partial x} = 0 \quad \text{with} \quad \Lambda = (u, ..., u, u - \overline{c}_s, u + \overline{c}_s)^T$$
(12)

Increase order in time and space with Lax-Wendroff procedure

$$\mathsf{F}_{j+1/2}^{o} = \mathsf{F}_{j+1/2}^{Roe} + \frac{1}{2} \sum_{k} (\Phi^{o} \mathsf{r})_{k,j+1/2}$$
(13)

Flux limiter : Monotonicity preserving scheme (TVD scheme with improvement near extrema)

$$\Phi^{o-MP} = \max(\Phi^{\min}, \min(\Phi^o, \Phi^{\max}))$$
(14)

Riemann invariants recombination

Possible recomposition of the equations (12) with the same eigenvector u to improve flux limiter

$$\overline{\alpha}_{1}^{bis} = \sum_{i=1}^{ns} \overline{\alpha}_{i} \left(\overline{E}_{c} - \frac{\overline{\chi}_{i}}{\overline{\kappa}} \right) = \Delta(\rho E) + \overline{E}_{c} \Delta \rho - \overline{H} \frac{\Delta P}{\overline{c}^{2}}$$
(15)

^{7.} V.Daru et C. Tenaud. "High order one-step monotonicity-preserving schemes for unsteady compressible flow calculations". In : Journal of Computational Physics 193 (2004), p. 563-594.

Numerical experiments

Numerical results : Sod shock tube problem

 $T_1P_1Y_1 \mid T_2P_2Y_2$

Properties

- Sod shock tube with R22 gas, 640 cells and OSMP scheme of 7th order
- Species data with thermodynamic NASA polynomials

	$0 \le x \le 25$	$25 < x \le 50$
P (bar)	1	0.1
$\rho(kg/m^3)$	1	0.125
N ₂ (%)	75.55	23.16
R ₂₂ (%)	23.16	75.55
O ₂ (%)	1.29	1.29
γ	1.38	1.32

Table 1 - initial conditions



Figure 4 - Density, velocity and temperature profiles at t = 20ms

Numerical results : Sod shock tube problem

 $T_1P_1Y_1 \mid T_2P_2Y_2$

Properties

- Sod shock tube with R22 gas, 640 cells and OSMP scheme of 7th order
- Species data with thermodynamic NASA polynomials
- OSMP adapted with combination of Riemann invariants (15)

	$0 \le x \le 25$	$25 < x \le 50$
P (bar)	1	0.1
$\rho(kg/m^3)$	1	0.125
N ₂ (%)	75.55	23.16
R ₂₂ (%)	23.16	75.55
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γ	1.38	1.32





Figure 4 - Density, velocity and temperature profiles at t = 20ms with recombination

Shock-bubble R22 interaction

Reproduction of the computation of Denner and Wachem, 2019 from the experimental test described in Hass, 1984. The numerical results of the article are obtained with the Minmod scheme.



Figure 5 – Computational setup of the two-dimensional R22 bubble in air interacting with a shock wave with Mach number $M_s = 1.22$

Parameters

- $p_{II} = 1.01325 \times 10^5 Pa$, $T_{II} = 351.82K$, $M_s = 1.22$
- OSMP 7th order, adaptive refinement with maximum of 1280 \times 128 cells

Shock-bubble R22 interaction



Figure 6 - Temperature without and with Riemann invariants combination



Figure 7 – Mesh and density gradient at $\tau = ta_{II,R22}/d_0 = 1.15$ for 256 cells in initial bubble diameter

⇒ Capture of Richtmyer–Meshkov instabilities (possible onset of detonation)

Shock/Bubble R22 interaction



Figure 8 – Profiles of the density gradient along the x-axis at different dimensionless time $\tau = ta_{II,R22}/d_0^{\,8}$

Validation of the compressible scheme for non reactive real gas flows

^{8.} Fabian Denner et Berend G. M. van Wachem. "Numerical modelling of shock-bubble interactions using a pressure-based algorithm without Riemann solvers". In : Experimental and Computational Multiphase Flow 1.4 (2019), p. 271-285.

Reactive mixture

Reactive mixture : Detonation front

1D ZND structure



Respect stability criterion (heat release, induction length, overdriven velocity...) 9

2D detonation cells 10



- 9. H. D. Ng et al. "Numerical investigation of the instability for one-dimensional Chapman–Jouguet detonations with chain-branching kinetics". In : Combustion Theory and Modelling 9.3 (2005), p. 385-401.
- Anne Bourlioux et Andrew J. Majda. "Theoretical and numerical structure for unstable two-dimensional detonations". In : Combustion and Flame 90.3 (1992), p. 211 -229.

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Reactive mixture : 2D Detonation

Detonation initiation by reflected shock with two-step chemistry

$$\overrightarrow{M} = 2.5 \quad (flame) \quad \begin{array}{c} T = 300K \\ P = 1atm \\ \Phi = 1 \end{array}$$



Reactive mixture : 2D Detonation

Detonation structure





Carbuncle effect

- Appears when strong shock aligned with the grid : Probably due to insufficient cross-flow dissipation
- Specific to Complete Riemann solver
- Amplified phenomena with heat release



Figure 9 - Detonation front with hydrogen chemistry

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Conclusion

High order compressible solver

- Extension of the approximate Riemann solver of Roe for multicomponent real gas flow (with no assumption on the equation of state)
 - Approximation of compressibility factor χ_i and κ at Roe average state
 - Orthogonal projection on the consistency hyperplane
- OSMP scheme : apply to a particular combination of Riemann invariants to capture correctly the contact wave

Realisation

- Validation for non-reactive flows/1D-2D detonation cases
- Carbuncle instabilities with strong detonation case

Objective : Realized a complete case of flame acceleration in 3D

Thank you for your attention

Bibliography i

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