An Explicit Second Order Scheme on Staggered Finite Volume Meshes for Reactive Flows with Stiff Kinetics

Chady ZAZA*, Jean-Claude LATCHÉ *{chady.zaza, jean-claude.latche}@irsn.fr*

Institute for Radiological Protection and Nuclear Safety – IRSN/PSN-RES/SA2I/LIE

INTRODUCTION

■ Simulating hydrogen-oxygen explosions in ISIS/P2REMICS code:

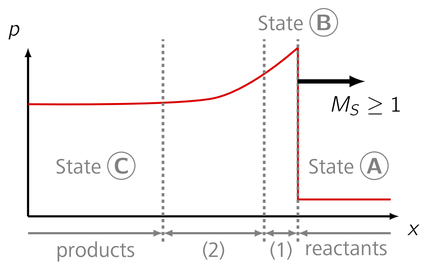
Mixing (Low-Mach, Low speed) → *Ignition* → **Deflagration** (Subsonic, High speed) → *DDT* → **Detonation** (Supersonic, High speed)

Projection scheme — *Explicit scheme*

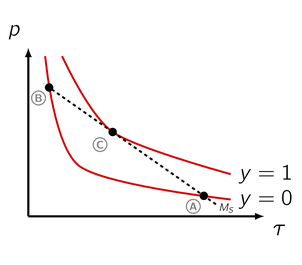
Common Staggered Finite-Volume Mesh

■ The Zeldovich-von Neumann-Döring (ZND) model for detonation:

- Steady 1D combustion wave: inert shock wave + chemical reaction (1) with finite rate
- Self-sustained: shock wave brings reactants to ignition while expansion of products (2) drives shock forward



ZND states on pressure profile



ZND states on Hugoniot curves

■ Unimolecular reaction of a perfect gas with reaction rate defined by Arrhenius law:

$$R \to P \qquad \gamma_R = \gamma_P = \gamma \qquad \kappa(T) = \kappa_0 \exp\left(\frac{-E_A}{RT}\right)$$

■ Equation of state:

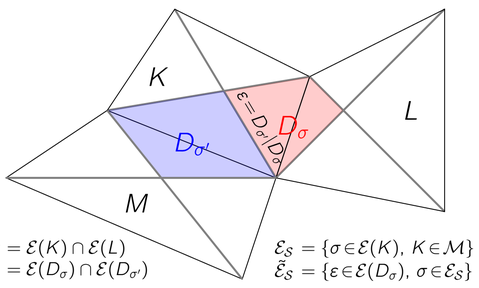
$$e = \frac{p\tau}{\gamma - 1} + q_0 y$$

■ Conservation equations:

$$\partial_t \rho + \operatorname{div}(\rho \underline{u}) = 0$$
$$\partial_t(\rho \underline{u}) + \underline{\operatorname{div}}(\rho \underline{u} \otimes \underline{u}) + \nabla p = 0$$
$$\partial_t(\rho E) + \operatorname{div}(\rho E \underline{u}) + \operatorname{div}(p \underline{u}) = 0$$
$$\partial_t(\rho y) + \operatorname{div}(\rho y \underline{u}) = -\rho y \kappa(T)$$

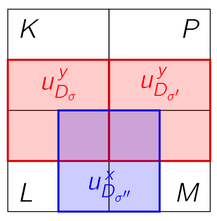
FINITE VOLUME SCHEME

■ Staggered Finite Volume meshes:



$\sigma = \mathcal{E}(K) \cap \mathcal{E}(L)$
$\varepsilon = \mathcal{E}(D_\sigma) \cap \mathcal{E}(D_{\sigma'})$
$\mathcal{E}_\mathcal{S} = \{\sigma \in \mathcal{E}(K),\ K \in \mathcal{M}\}$
$\tilde{\mathcal{E}}_\mathcal{S} = \{\varepsilon \in \mathcal{E}(D_\sigma),\ \sigma \in \mathcal{E}_\mathcal{S}\}$

Rannacher-Turek/Crouzeix-Raviart grids



$\sigma, \sigma' \in \mathcal{E}_\mathcal{S}^{(y)}$; $\sigma'' \in \mathcal{E}_\mathcal{S}^{(x)}$
$u^x_\varepsilon = u^x_{D_{\sigma|D_{\sigma'}}} = \frac{1}{2}\left[u^x_{D_{K|P}} + u^x_{D_{L|M}}\right]$

MAC grid

with unknowns:

- *Primal grid*: ρ_K, p_K, e_K, y_K $\quad \forall K \in \mathcal{M}$
- *Dual grid*: $u^{(i)}_{D_\sigma}$ $\quad \forall \sigma \in \mathcal{E}_\mathcal{S}^{(i)}$, $1 \leq i \leq d$

■ Explicit scheme:

(1) Hydrodynamic step (continuity, mass fraction, internal energy)

$$\rho_K^{n+1} = \rho_K^n - \delta t \operatorname{div}_K(\rho^n \underline{u}^n)$$

$$\bar{y}_K^{n+1} = \frac{1}{\rho_K^{n+1}}\left[\rho_K^n y_K^n - \delta t \operatorname{div}_K(\rho^n \underline{u}^n y^n)\right]$$

$$e_K^{n+1} = \frac{1}{\rho_K^{n+1}}\left[\rho_K^n e_K^n - \delta t(\operatorname{div}_K(e^n \rho^n \underline{u}^n) + p_K^n \operatorname{div}_K(\underline{u}^n) + \frac{1}{|K|}\mathbf{S_K^n})\right]$$

(2) Chemistry step

$$y_K^{n+1} = \bar{y}_K^{n+1} \exp(-\kappa(p_K^n/\rho_K^n)\delta t)$$

(3) Equation of state

$$p_K^{n+1} = (\gamma - 1)\rho_K^{n+1}(e_K^{n+1} - q_0 y_K^{n+1})$$

(4) Hydrodynamic step (momentum)

$$u^{(i)n+1}_\sigma = \frac{1}{\rho^{n+1}_{D_\sigma}}\left[\rho^n_{D_\sigma} u^{(i)n}_\sigma - \delta t\left(\operatorname{div}_{D_\sigma}(\rho^n \underline{u}^n u^{(i)n}) + (\nabla p^{n+1})^{(i)}_\sigma\right)\right]$$

■ Finite volume discretization:

- On the dual grid, ρ_{D_σ} and $u^{(i)}_\varepsilon = u^{(i)}_{D_\sigma|D_{\sigma'}}$ are interpolated as (Trung, 2012):

$$|D_\sigma|\rho_{D_\sigma} = |D_{K,\sigma}|\rho_K + |D_{L,\sigma}|\rho_L$$

$$u^{(i)}_\varepsilon = \begin{cases} u^{(i)}_\sigma \text{ if } F_{\sigma,\varepsilon} \geq 0 \\ u^{(i)}_{\sigma'} \text{ otherwise} \end{cases}$$

- Convection fluxes:

$$\operatorname{div}_K(\rho \underline{u} z) = \frac{1}{|K|}\sum_{\sigma \in \mathcal{E}(K)} F_{K,\sigma} z_\sigma \text{ with } F_{K,\sigma} = |\sigma|\rho_\sigma\left(\sum_{i=1}^d u^{(i)}_\sigma n^{(i)}_{K,\sigma}\right)$$

Dual grid fluxes $F_{\sigma,\varepsilon}$ calculated such that a mass balance holds on the dual grid as well (Ansanay-Alex–Babik–Latché–Vola, 2010):

$$\operatorname{div}_{D_\sigma}(\rho \underline{u} z) = \frac{1}{|D_\sigma|}\sum_{\varepsilon \in \mathcal{E}(D_\sigma)} F_{\sigma,\varepsilon} z_\varepsilon \text{ with } \frac{|D_\sigma|}{\delta t}\left(\rho^{n+1}_{D_\sigma} - \rho^n_{D_\sigma}\right) + \sum_{\varepsilon \in \mathcal{E}(D_\sigma)} F^n_{\sigma,\varepsilon} = 0$$

- Discrete pressure gradient defined such that a discrete duality property holds:

$$\sum_{K \in \mathcal{M}} |K| p_K \operatorname{div}_K \underline{u} + \sum_{i=1}^d \sum_{\sigma \in \mathcal{E}_\mathcal{S}^{(i)}} |D_\sigma| u^{(i)}_\sigma (\nabla p)^{(i)}_\sigma = 0$$

- Second order interpolation : ρ_σ, e_σ are computed using MUSCL interpolation with a limitation procedure such that contact waves are preserved (Therme, 2015)

$$p_\sigma = \beta p_K + (1 - \beta) p_L, \quad \beta \in [0, 1]$$

- $\mathbf{S_K}$ defined to compensate the source term appearing in the following discrete kinetic energy balance (Therme, 2015)

$$\frac{1}{2}\frac{1}{\delta t}\left(\rho^{n+1}_{D_\sigma}\left(u^{(i)n+1}_\sigma\right)^2 - \rho^n_{D_\sigma}\left(u^{(i)n}_\sigma\right)^2\right) + \frac{1}{2}\operatorname{div}_{D_\sigma}(\rho \underline{u} \cdot |\underline{u}|^2) + (\nabla p^{n+1})^{(i)}_\sigma u^{(i)n}_\sigma = -\frac{1}{|D_\sigma|} R^{(i)n+1}_\sigma$$

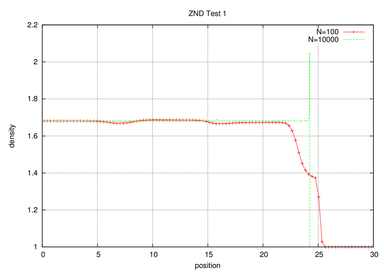
with for all test function φ, when $h, \delta t \to 0$:

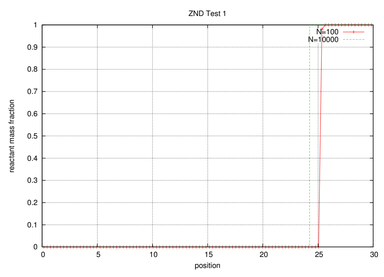
$$\sum_{n \geq 0} \delta t \left(\sum_{K \in \mathcal{M}} S^n_K \varphi^{n+1}_K - \sum_{i=1}^d \sum_{\sigma \in \mathcal{E}_\mathcal{S}^{(i)}} R^{(i)n+1}_\sigma \varphi^{n+1}_\sigma\right) = 0$$

NUMERICAL RESULTS

1D Test: CJ detonation on $\Omega = [0, 30]$ with Arrhenius law, $q_0 = 25$, $\kappa_0 = 164180$, $E_A = 25$.
Problem 2 of (Helzel–LeVeque–Warnecke, 2000).

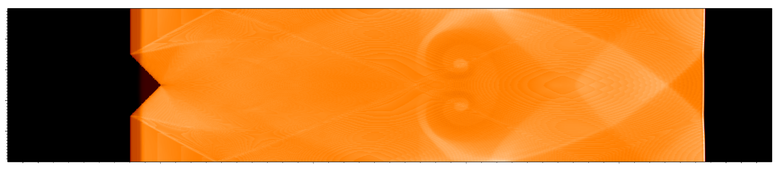
■ Pressure and mass fraction at $t = 2$:



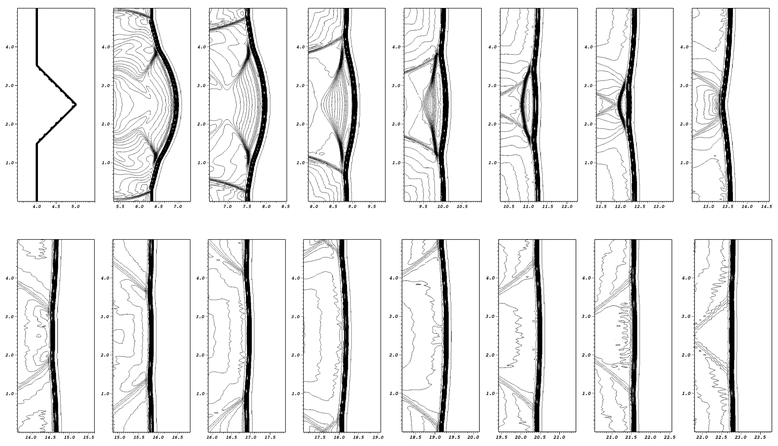


2D Test: stable detonation with overdrive $f = 1.18$ on $\Omega = [0, 0.025] \times [0, 0.005]$ with Heaviside law, $q_0 = 5.2 \times 10^{-11}$, $\kappa_0 = 5.8 \times 10^9$, $E_A = 0.12$.
Problem 5.1 of (Bao–Jin, 2000).

■ Total chemical energy released at $t = 1.6 \times 10^{-7}$:



■ Transverse displacement of the triple points : density contours in the local frame between $t = 0$ and $t = 1.6 \times 10^{-7}$



UNDERRESOLVED DETONATIONS

■ Objective: advance chemistry locally, pointwise instead of cellwise using a local reconstruction of the temperature. One dimensional procedure:

(1) Identify set of transition cells $\mathcal{T}$ across the shock :

$$\mathcal{T} = \{K \in \mathcal{M},\ \eta < y_K < 1 - \eta\}, \quad \eta \ll 1$$

(2) Define the stencils of ENO polynomials π_L and π_R for every cell in $\mathcal{V} = \{K \in \mathcal{M}\ ;\ K \cap L \neq \emptyset,\ L \in \mathcal{T},\ L \neq K\}$ intended for the extrapolation of the solution inside $\mathcal{T}$.

(3) Estimate shock position using Harten's Subcell Resolution technique : solve for x_d the non-linear integral equation

$$\int_{x_1}^{x_d} \pi_L(w_K, x)\,dx + \int_{x_d}^{x_2} \pi_R(w_K, x)\,dx = \sum_{K \in \mathcal{T}} |K| w_K$$

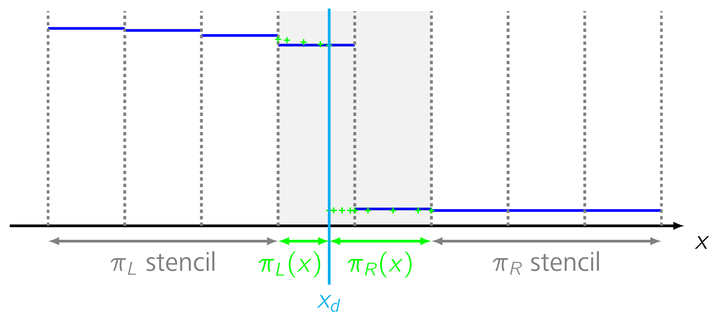
with $[x_1, x_2] = \cup_{K \in \mathcal{T}} K$ and $w_K = \rho_K y_K$.

(4) Define in every transition cells Gauss-Lobatto integration nodes ; in the cell splited by the discontinuity, two distinct stencils are used.

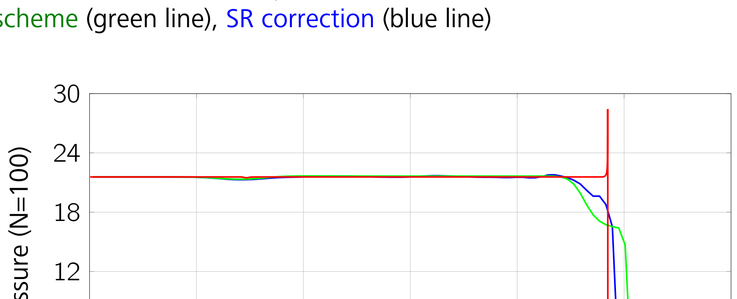
(5) Extrapolate temperature values at every Gauss-Lobatto node using π_L if $x < x_d$, π_R otherwise.

(6) Compute the local mass fraction update using chemistry kinetics at each integration node.

(7) Update mass fraction cell average for $K \in \mathcal{T}$ using Gauss-Lobatto quadrature.



Temperature profile near combustion front



Mass fraction after hydrodynamic step and cell-wise (blue) vs point-wise (green) chemistry step in $\mathcal{T}$

■ CJ detonation with $K_0 = 164180$: reference (red line), standard scheme (green line), SR correction (blue line)