Model adaptation for hyperbolic systems with relaxation

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Introduction

Join work with C. Cancès, F. Coquel, E. Godlewski, N. Seguin
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- Complex flows modeling: compressible two-phase flows (liquid+gas)
  - multi-scales (space and time)
- Couple complex models: coupling of a fine model with a coarser one
- Coupling interface evolves in time
- Aim: compute an modeling error indicator in order to
  - determine dynamically the sub-domains
    - $\mathcal{D}_f(t)$: fine model solved to preserve accuracy (reference model)
    - $\mathcal{D}_c(t)$: coarse model solved (simplify computation)
  - Adapted model on $\mathcal{D} = \mathcal{D}_f \cup \mathcal{D}_c$

Introduction

Algorithm $t^n \to t^{n+1}$:

Let (u_K^n) known $\forall K$ and θ a given threshold

1. Compute the indicator $e_K^n := e(u_K^n)$ in each cell K
2. Define the partition of the computational domain
   - $\mathcal{D}_f^{n\to n+1} = \{K; |e_K^n| > \theta\}$
   - $\mathcal{D}_c^{n\to n+1} = \{K; |e_K^n| < \theta\}$
3. Solve the fine model if $K \in \mathcal{D}_f^{n\to n+1}$
   and the coarse model if $K \in \mathcal{D}_c^{n\to n+1}$
   - Coupling strategies at sub-domains interface

Note : $e_K^n \simeq \|(u_f)_K^{n+1} - (u_c)_K^{n+1}\|$

Introduction

Model error indicator:

- Scalar case [Kruzhkov 70 ; Kuznetsov 76 ; Lucier 86 ; Bouchut, Perthame 98 ; Kröner, Ohlberger 00]
- System case: relative entropy [Di Perna 79, Dafermos 05, Tzavaras 05,...]

✓ Chapman-Enskog expansion

Coupling strategies:

- Thin or diffuse interfaces [Boutin 09, Ambroso *et al* 07, Caetano 06]

✓ Thin coupling, “state coupling”

Outline

Outline

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2. Hyperbolic systems with relaxation
   - Chapman-Enskog expansion

3. Adaptation
   - Discrete indicator and discrete CE
   - Coupling and algorithm

4. Numerical illustrations
   - Suliciu and P-system
   - Phase transition
   - 7 equations and Euler

Structure of relaxation

Hyperbolic systems with source term [Chen, Levermore, Liu 94 ; Serre 09 ; Hanouzet, Natalini 03,...]

$$\partial_t W + \sum_\alpha \partial_\alpha F_\alpha(W) = \frac{1}{\varepsilon} R(W) \tag{1}$$

with $W(0,x) = W_0(x)$

- $W(x,t) : \mathbb{R} \times \mathbb{R}^+ \to \Omega \subset \mathbb{R}^n$, set of admissibles states
- $F, R : \mathbb{R}^n \to \mathbb{R}^n$ regular fluxes, R source term
- ε relaxation parameter
- Relaxation: $R(W) = 0 \Leftrightarrow W$ equilibrium state
    - equilibrium manifold $\Omega_{eq} = \{W \in \Omega : R(W) = 0\}$

Dissipative structure of relaxation systems

It exists $\Phi : \mathbb{R}^n \to \mathbb{R}$ and $\Psi : \mathbb{R}^n \to \mathbb{R}$ such that

$$D_W \Phi D_W \mathcal{F} = D_W \Psi$$

Regular solutions satisfy:

$$\partial_t \Phi(W) + \sum_\alpha \partial_\alpha \Psi_\alpha(W) = -\frac{1}{\varepsilon} D_W \Phi(W) R(W) \leq 0$$

- Φ convex: $D^2_W \Phi$ positive definite on Ω_{eq}
- Dissipative entropy, compatible with the source term [Bouchut 04]

$$D_W \Phi R \geq 0 \text{ in } \mathbb{R}^n$$

System with relaxation source term: fine model

Focus on hyperbolic system with "BGK" source term

Fine model:

$$\begin{aligned}\partial_t u + \sum_\alpha \partial_\alpha f_\alpha(u,v) &= 0\\ \partial_t v + \sum_\alpha \partial_\alpha g_\alpha(u,v) &= \frac{1}{\varepsilon}(v_{eq}(u) - v)\end{aligned} \qquad (\mathcal{M}_f)$$

$\rightsquigarrow$ Relaxation: $(u,v) \in \Omega_{eq} \Leftrightarrow v = v_{eq}(u)$

Coarse model: equilibrium system of conservation laws

$$\partial_t u + \sum_\alpha \partial_\alpha f_\alpha(u, v_{eq}(u)) = 0 \qquad (\mathcal{M}_c)$$

Chapman-Enskog expansion [Chapman, Cowling 60]

Let us consider

$$v^{\varepsilon} = v_{eq} + \varepsilon v_1 + \mathcal{O}(\varepsilon^2)$$

Proposition

Up to ε^2 terms, the smooth solutions of $(\mathcal{M}_f)$ satisfy

$$\partial_t u + \sum_{\alpha} \partial_{\alpha} f_{\alpha}(u, v_{eq}(u)) = -\varepsilon \left(\sum_{\alpha} \partial_{\alpha} \nabla_v f_{\alpha}(u, v_{eq}(u)) \right) v_1, \qquad (Para)$$

where

$$v_1 = -\left[\sum_{\alpha} \partial_{\alpha} g_{\alpha}(u, v_{eq}(u)) - \nabla v_{eq}^T \sum_{\alpha} \partial_{\alpha} f_{\alpha}(u, v_{eq}(u)) \right]$$

Chapman-Enskog

Proof

Let us plug the ansatz

$$v^{\varepsilon} = v_{eq} + \varepsilon v_1 + \mathcal{O}(\varepsilon^2)$$

into the fine model:

$$\partial_t u + \sum_{\alpha} \partial_\alpha f_\alpha(u, v_{eq}) = -\varepsilon \left(\sum_{\alpha} \partial_\alpha \nabla_v f_\alpha(u, v_{eq}) \right) v_1 + \mathcal{O}(\varepsilon^2) \tag{2}$$

$$\partial_t v_{eq} + \sum_{\alpha} \partial_\alpha g_\alpha(u, v_{eq}) = -v_1 + \mathcal{O}(\varepsilon) \tag{3}$$

- *Equation* (2) *is exactly* (*Para*)
- *Multiply* (2) *par* $\nabla v_{eq}(u)^T$ *and combine with* (3)

Remarks

- Second order intermediate model (*Para*):
  - Regular solutions of the fine model solve (*Para*) up to ε^2
  - When $\varepsilon \to 0$, recover the $(\mathcal{M}_c)$
- Second order term dissipative
- Expansion fails near shock, calculus valid only for smooth solutions

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Fine model scheme

Assume the approximation $Z_K^n = (u_K^n, v_K^n)$ is known at time t^n

1. Convective part $t^n \to t^{n+1,-}$:

$$u_K^{n+1,-} = u_K^n - \frac{\Delta t}{|K|} \sum_{L \in \mathcal{N}(K)} |e_{KL}| F(Z_K^n, Z_L^n, n_{KL})$$

$$v_K^{n+1,-} = v_K^n - \frac{\Delta t}{|K|} \sum_{L \in \mathcal{N}(K)} |e_{KL}| G(Z_K^n, Z_L^n, n_{KL})$$

2. Source term $t^{n+1,-} \to t^{n+1}$:

$$\begin{aligned} u_K^{n+1} &= u_K^{n+1,-} \\ v_K^{n+1} &= v_K^{n+1,-} + \frac{\Delta t}{\varepsilon}\left(v_{eq}(u_K^{n+1}) - v_K^{n+1}\right) \end{aligned} \tag{$\mathcal{S}_f$}$$

Coarse model scheme

⇝ When $\varepsilon \to 0$ in $(\mathcal{S}_f)$

1. Convective part $t^n \to t^{n+1,-}$: similar to fine scheme with

$$v_K^n = v_{eq}(u_K^n)$$

2. Source term $t^{n+1,-} \to t^{n+1}$:

$$\begin{aligned} u_K^{n+1} &= u_K^{n+1,-} \\ v_K^{n+1} &= v_{eq}(u_K^{n+1,-}) \end{aligned} \qquad (\mathcal{S}_c)$$

✓ Compatibility between the schemes → simplify adaptation algorithm

Discrete indicator

- ✓ Similar construction as the regular case:

$$v_K^{n+1} = v_{eq}(u_K^{n+1}) + \varepsilon v_{1,K}^{n+1}$$

Proposition

Up to ε^2, one has:

$$v_{1,i}^{n+1} = -\frac{1}{|K|} \sum_{L \in \mathcal{N}(K)} |e_{KL}| \Big[G(Z_{e,K}^n, Z_{e,L}^n, n_{KL}) \\ + \nabla v_{eq}(u_K^n)^T F(Z_{e,K}^n, Z_{e,L}^n, n_{KL}) \Big]$$

where $Z_{e,K}^n = (u_K^n, v_{eq}(u_K^n))^T$

Remarks

- The indicator is $e_K^n = \varepsilon v_{1,K}^{n+1}$, that is

$$e_K^n = v_K^{n+1} - v_{eq}(u_k^{n+1}) \tag{indic}$$

with

$$v_{1,K}^{n+1} = -\frac{1}{|K|} \sum_{L \in \mathcal{N}(K)} |e_{KL}| \\ \left[G(Z_{e,K}^n, Z_{e,L}^n, n_{KL}) + \nabla v_{eq}(u_K^n)^T F(Z_{e,K}^n, Z_{e,L}^n, n_{KL}) \right]$$

✓ At time t^{n+1} the indicator is an explicit function of $(u_K^n)_K$

Adapted model and coupling

Adapted model: $\forall n \in \mathbb{N}$

$$\left\{ \begin{array}{l} (\mathcal{M}_f) \text{ solved in } \mathcal{D}_f^{n\to n+1} \times (t^n, t^{n+1}) \\ (\mathcal{M}_c) \text{ solved in } \mathcal{D}_c^{n\to n+1} \times (t^n, t^{n+1}) \\ \text{Coupling conditions in } \mathcal{D}_f^{n\to n+1} \cap \mathcal{D}_c^{n\to n+1} \times (t^n, t^{n+1}) \end{array} \right.$$

Coupling conditions:
At an interface, consider $(u_f, v_f) \in \mathcal{D}_f^{n\to n+1}$ and $(u_c, v_{eq}(u_c)) \in \mathcal{D}_c^{n\to n+1}$

$$\left\{ \begin{array}{l} u_f \text{ "="}\ u_c \\ v_f \text{ "="}\ v_{eq}(u_c) \end{array} \right. \qquad (\mathit{coupling})$$

- Coupling condition understood in a weak sense [Dubois, LeFloch 88 ; Ambroso, Boutin, Caetano, Chalons, Coquel, Galié, Godlewski, Lagoutière, Raviart, Seguin]

Algorithm

A) $\forall K$, compute e_K^n using $(\textit{indic})$

B) Define the partition of the computational domain

- $\mathcal{D}_f^{n\to n+1} = \{K; |e_K^n| > \theta\}$
- $\mathcal{D}_c^{n\to n+1} = \{K; |e_K^n| < \theta\}$

C) At this stage $\mathcal{D}_f^{n\to n+1} \cup \mathcal{D}_c^{n\to n+1} = \mathbb{R}^d$
$\forall K$:

- If K and its neighbors $\in \mathcal{D}_f^{n\to n+1}$
  - Compute W_K^{n+1} with $(\mathcal{S}_f)$
- If K and its neighbors $\in \mathcal{D}_c^{n\to n+1}$
  - Compute W_K^{n+1} with $(\mathcal{S}_c)$
- Else
  - Compute W_K^{n+1} with $(\textit{coupling})$

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Suliciu and P-system

Fine model: Suliciu system

$$\begin{aligned} \partial_t \tau - \partial_x u &= 0 \\ \partial_t u + \partial_x \Pi &= 0 \\ \partial_t \mathcal{T} &= \frac{1}{\varepsilon}(\tau - \mathcal{T}) \end{aligned}$$

with

$$\Pi(\tau, \mathcal{T}) = p(\mathcal{T}) + a^2(\mathcal{T} - \tau)$$

and

$$a^2 > \max_s(-p'(s)) \quad \text{and} \quad p = p(\tau) = \tau^{-\gamma},\ \gamma > 1$$

$\rightsquigarrow$ Relaxation: equilibrium state $\mathcal{T} = \tau$

Coarse model: barotropic Euler equations

$$\begin{aligned} \partial_t \tau - \partial_x u &= 0 \\ \partial_t u + \partial_x p &= 0 \end{aligned}$$

Suliciu and P-system

Adaptation parameters: $\theta = 5 \times 10^4$, $\varepsilon = 10^{-6}$

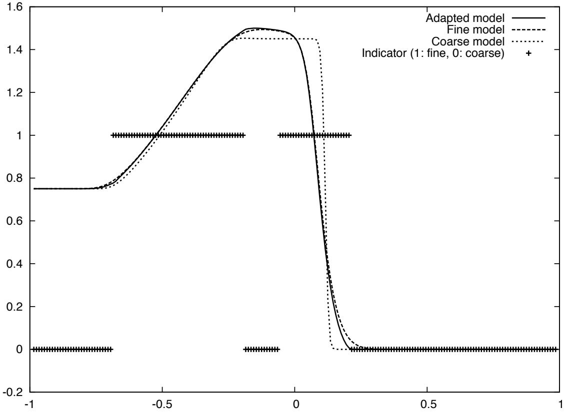


Figure: Velocity u

Phase transition [Helluy, Seguin 06 ; Allaire, Faccanoni, Kokh 12]

Fine model: Euler equations + transport of volume fraction of gas

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0 \\ \partial_t(\rho E) + \partial_x((\rho E + p)u) = 0 \\ \partial_t(\rho \varphi) + \partial_x(\rho u \varphi) = \dfrac{1}{\varepsilon}(\varphi_{eq}(\rho) - \varphi) \end{cases}$$

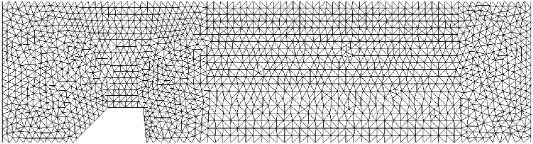
with

$$p(x,t) = p(\rho, e, \varphi) = \begin{cases} (\gamma_1 - 1)\rho e & \text{if } \varphi = 1 \\ (\gamma(\varphi) - 1)\rho e & \text{if } 1 > \varphi > 0 \\ (\gamma_2 - 1)\rho e & \text{if } \varphi = 0 \end{cases}$$

- $\rightsquigarrow$ Relaxation: equilibrium $\varphi = \varphi_{eq}(\rho)$
- $\rightsquigarrow$ Mixture pressure law

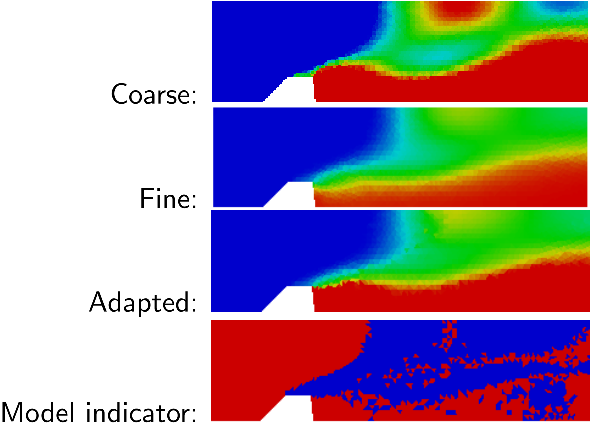
2D test case

Test case: liquid + production of a bubble of gas



Adaptation parameters: $\varepsilon = 10^{-2}$, $\theta = 500$

2D test case



- Mass fraction φ: blue = liquid, red = gas
- Indicator: blue = fine, red = coarse
- Simulation

7 equation model

⇝ Work in progress

Compressible two-phase flows [Baer, Nunziato 86]

$$\begin{cases} \partial_t \alpha_k + u_{\mathcal{I}} \partial_x \alpha_k = \dfrac{1}{\varepsilon_p}(p_k - p_l) \\ \partial_t(\alpha_k \rho_k) + \partial_x(\alpha_k \rho_k u_k) = 0 \\ \partial_t(\alpha_k \rho_k u_k) + \partial_x(\alpha_k \rho_k u_k^2 + \alpha_k p_k) - p_{\mathcal{I}} \partial_x \alpha_k = -\dfrac{1}{\varepsilon_u}(u_k - u_l) \\ \partial_t(\alpha_k \rho_k E_k) + \partial_x((\alpha_k \rho_k E_k + \alpha_k p_k) u_k) - p_{\mathcal{I}} u_{\mathcal{I}} \partial_x \alpha_k = -\dfrac{1}{\varepsilon_T}(T_k - T_l) \\ \qquad\qquad - \dfrac{u_{\mathcal{I}}}{\varepsilon_u}(u_k - u_l) - \dfrac{p_{\mathcal{I}}}{\varepsilon_p}(p_k - p_l) \end{cases}$$

with $k, l = 1, 2$, $l \neq k$ and $\alpha_1 + \alpha_2 = 1$

Fine model: 7 equation model

[Baer, Nunziato 86 ; Gallouët, Hérard, Seguin 04 ; Andrianov, Warnecke 04 ; Ambroso, Chalons, Raviart 11...]

Assumptions:

- Interfacial closure law: $u_{\mathcal{I}} = u_1$, $p_{\mathcal{I}} = p_2$
- Perfect gas law: $p_k = (\gamma_k - 1)\rho_k e_k$ et $T_k = e_k$
- Same relaxation time-scales : $\varepsilon = \varepsilon_u = \varepsilon_p = \varepsilon_T$

Difficulties:

- Non conservative system
- Non strictly hyperbolic
- Non strictly convex entropy
- Non BGK-like source term

Fine model: 7 equation model

Rewrite under the form

$$\begin{aligned}\partial_t U + \partial_x f(U,V) &= 0\\ \partial_t V + \partial_x g(U,V) + h(U,V)\partial_x \alpha_1 &= \frac{1}{\varepsilon} r(U,V)\end{aligned}$$

with $U = \begin{pmatrix} \alpha_1\rho_1 \\ \rho \\ \rho u \\ \rho E \end{pmatrix}$ and $V = \begin{pmatrix} \alpha_1 \\ \alpha_1\rho_1 u_1 \\ \alpha_1\rho_1 u_1 \end{pmatrix}$ where

$$\begin{aligned}\rho &= \alpha_1\rho_1 + \alpha_2\rho_2\\ \rho u &= \alpha_1\rho_1 u_1 + \alpha_2\rho_2 u_2\\ \rho E &= \alpha_1\rho_1 E_1 + \alpha_2\rho_2 E_2\end{aligned}$$

Coarse model: Euler equations

⇝ Equilibrium state: $r(U,V)=0 \Leftrightarrow V_{eq}(U)=V$

$$\begin{aligned} u &= u_1 = u_2 \\ p &= p_1 = p_2 \\ T &= T_1 = T_2 \end{aligned}$$

Coarse model:

$$\begin{cases} \partial_t(\alpha_1\rho_1) + \partial_x(\alpha_1\rho_1 u_1) = 0 \\ \partial_t\rho + \partial_x(\rho u) = 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = 0 \\ \partial_t(\rho E) + \partial_x((\rho E + p)u) = 0 \end{cases}$$

Pressure law: $p = (\gamma(U) - 1)\rho e$ with:

$$\gamma(U) = (\gamma_1 - 1)\frac{\rho_1(U)}{\rho} + 1 \quad et \quad \rho_1(U) = \frac{(\gamma_2 - 1)\rho}{(\gamma_2 - 1)\alpha_1 + (1-\alpha_1)(\gamma_1 - 1)}$$

Chapman-Enskog [Dellacherie 03]

Proposition

Up to ε^2 terms, regular solutions satisfy:

$$\begin{cases} \partial_t(\alpha_1\rho_1) + \partial_x(\alpha_1\rho_1 u_1) = \varepsilon\partial_x A \\ \partial_t\rho + \partial_x(\rho u) = \varepsilon\partial_x B \\ \partial_t(\rho u) + \partial_x(\rho u^2 + p) = \varepsilon\partial_x C \\ \partial_t(\rho E) + \partial_x\left((\rho E + \partial)u\right) = \varepsilon\partial_x D \end{cases}$$

Chapman-Enskog [Dellacherie 03]

Proposition

where

$$\begin{aligned}
A &= \rho (Y_1)^2 Y_2 \left(\frac{\rho}{\rho_1} - 1\right) \partial_x p \\
B &= \rho Y_1 Y_2 \partial_x P \left(Y_1 \left(\frac{\rho}{\rho_1} - 1\right) + Y_2 \left(\frac{\rho}{\rho_2} - 1\right)\right) \\
C &= \frac{T}{\rho^2} \frac{(2\alpha_1\rho_1 - \rho)^2}{\alpha_1\rho_1(\rho - \alpha_1\rho_1)} \partial_x u \\
D &= uC + \partial_x \left(\rho Y_1 Y_2 \partial_x p \left[Y_1 \left(\frac{\rho}{\rho_1} - 1\right) h_1 + Y_2 \left(\frac{\rho}{\rho_2} - 1\right) h_2 \right]\right)
\end{aligned}$$

with $Y_k = \dfrac{\alpha_k \rho_k}{\rho}$

Adaptation for 7 equations

- ✓ Indicator explicit function of $U = (\alpha_1\rho_1, \rho, \rho u, \rho E)^T$
  - Fine model scheme [Gallouët, Hérard, Seguin 04 ; Ambroso, Chalons, Raviart 11]
    - semi-implicit discretization of the relaxation terms
  - Coarse model scheme [Abgrall ; Abgrall, Saurel]
- ✗ No discrete Chapman-Enskog expansion