Relative entropy for the finite volume approximation of hyperbolic systems

Hélène Mathis

Supported by LRC Manon, CEA, UPMC Paris 6 and

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Motivations: model adaptation

Join work with: C. Cancès, F. Coquel, E. Godlewski, N. Seguin

Simulation of compressible water flows in pressurized water reactor

- Several models of two-phase flows
- Local properties of the flow $\rightsquigarrow$ appropriate model
- Models linked by asymptotic limits $\rightsquigarrow$ relaxation
  - Fine model: complex system of equations, stiff source term
  - Coarse model: simplified equations
- Coupling technics at interface

Optimal position of the coupling interface

- Minimize the use of the fine model (reference solution)
- Minimize global error due to coupling

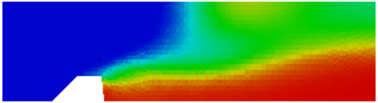
Dynamical model adaptation

Model adaptation, an example

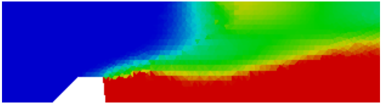
Phase transition model in 2D

- Fine model: thermodynamical equilibrium not reached
  (Euler equations + mass fraction evolution + closure law)
- Coarse model: thermodynamical equilibrium
  (Euler equations + closure law)
- Legend: blue = liquid, red=gas

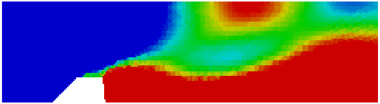
Fine



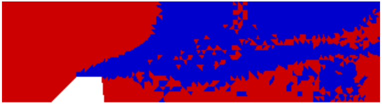
Adapted



Coarse



Indicator (blue=fine, red=coarse)



Simulation

Determine an error indicator

Error indicator to perform adaptation

- U_f solution of the fine model, U_c solution of the coarse model, U_c^h finite volume approximation of U_c

$$Indicator = \|U_f - U_c^h\| \leq \|U_f - U_c\| + \|U_c - U_c^h\|$$

$Indicator(t)$ controlled by U_f^0, U_c^0 and $U_c^{h,0}$

State of art

- Scalar case [Kruzhkov 70 ; Kuznetsov 76 ; Lucier 86 ; Bouchut, Perthame 98 ; Kröner, Ohlberger 00]
- System case
  - Chapman-Enskog expansion (adaptation [Mathis, Seguin 11])
  - Relative entropy [Di Perna 79, Dafermos 05, Tzavaras 05,...]

Fine and coarse models

- **Fine model**: hyperbolic system with relaxation
  [Chen, Levermore, Liu 94]

$$\begin{cases} \partial_t w + \sum_{\alpha=1}^{d} \partial_\alpha F_\alpha(w) = \frac{1}{\varepsilon} R(w), \quad t > 0, \ x \in \mathbb{R}^d \\ w(x,0) = w_0(x), \quad x \in \mathbb{R}^d \end{cases} \qquad (\mathcal{M}_f)$$

- $w = (u, v)^T \in \mathbb{R}^n$, $u \in \mathbb{R}^m$, $n > m$
- F, R smooth enough
- Stiff source term R:

$$R(w) = 0 \Leftrightarrow w = w_{eq}(u)$$

- Map w_{eq} (assumed to be $L_{w_{eq}}-$Lipschitz continuous)

Fine and coarse models

- **Coarse model**: in the limit $\varepsilon \to 0$, hyperbolic system

$$\begin{cases} \partial_t \overline{u} + \sum_{\alpha=1}^{d} \partial_\alpha g_\alpha(\overline{u}) = 0, & t > 0,\ x \in \mathbb{R}^d \\ \overline{u}(x,0) = \overline{u}_0(x), & x \in \mathbb{R}^d \end{cases} \qquad (\mathcal{M}_c)$$

where $g(\overline{u}) = \mathbb{P}F(w_{eq}(\overline{u}))$

- $\mathbb{P} \in \mathbb{M}^{n\times m}$ such that

$$\begin{aligned} \mathbb{P}R(w) &= 0, \quad \forall w \in \mathbb{R}^n \\ \mathbb{P}w &= u, \quad \forall w \in \mathbb{R}^n \\ \mathbb{P}w_{eq}(u) &= u, \quad \forall u \in \mathbb{R}^m \end{aligned} \qquad \text{(Hyp 1)}$$

Error indicator

Error indicator

$$\textit{Indicator} = \|w - w_{eq}(\overline{u}^h)\|^2 \leq 2\|w - w_{eq}(\overline{u})\|^2 + 2L_{w_{eq}}\|\overline{u} - \overline{u}^h\|^2$$

Outline

1. Modeling error estimate $\|w - w_{eq}(\overline{u})\|$
   - estimate in ε between smooth solutions of $(\mathcal{M}_f)$ and $(\mathcal{M}_c)$, relative entropy, [Tzavaras 06]
2. Numerical error estimate $\|\overline{u} - \overline{u}^h\|$
   - FV scheme, convergence towards entropy solution, error estimate [Chainais 99 ; Eymard, Gallouët, Herbin 00], relative entropy
3. Conclusion and prospects

Modeling error estimate: assumptions [Tzavaras 06]

- Non-degeneracy

$$\begin{aligned} \dim \operatorname{Ker}(\nabla_w R(w_{eq}(u))) &= m \\ \dim \operatorname{Im}(\nabla_w R(w_{eq}(u))) &= n - m \end{aligned} \quad \text{(Hyp 2)}$$

- The system $(\mathcal{M}_f)$ is endowed with a β-convex entropy $\eta : \mathbb{R}^n \to \mathbb{R}$

$$\nabla \eta(w)^T \nabla_w F(w) = \nabla_w \xi(w)^T \quad \text{(Hyp 3)}$$

where $\xi_\alpha : \mathbb{R}^n \to \mathbb{R}$, $\alpha = 1, \dots, d$ is the entropy flux

- The pair $\eta - \xi$ satisfy

$$\partial_t \eta(w) + \sum_{\alpha=1}^{d} \partial_\alpha \xi_\alpha(w) = \frac{1}{\varepsilon} \nabla_w \eta(w) * R(w)$$

where $*$ denotes the scalar product in $\mathbb{R}^n$

Modeling error estimate: assumptions [Tzavaras 06]

- Entropy dissipation

$$\nabla_w \eta(w) * R(w) \leq 0 \qquad \text{(Hyp 4)}$$

- Entropy-entropy flux for $(\mathcal{M}_c)$: restriction of $\eta - \xi$ on $\{w \in \mathbb{R}^n, R(w) = 0\}$ induces

$$\nabla_u \overline{\eta}(u)^T \nabla_u g(u) = \nabla_u \overline{\xi}(u)^T \qquad \text{(Hyp 5)}$$

where $g(u) = \mathbb{P}F(w_{eq}(u))$

- For $u \in \mathbb{R}^m$ regular solution of $(\mathcal{M}_c)$, the pair $\overline{\eta} - \overline{\xi}$ satisfies

$$\partial_t \overline{\eta}(u) + \sum_{\alpha=1}^{d} \partial_\alpha \overline{\xi}_\alpha(u) = 0$$

Modeling error estimate

Theorem ([Tzavaras 06])

Assume hypothesis (Hyp 1)-(Hyp 5). *Let* (w^ε) *be a family of regular solutions of* $(\mathcal{M}_f)$ *and* $\overline{u}$ *a regular solution of* $(\mathcal{M}_c)$ *on* $\mathbb{R}^d \times [0, T]$ *with initial conditions* (w_0^ε) *and* $\overline{u}_0$. *Assume that* w^ε, $w_{eq}(u^\varepsilon)$ *and* $w_{eq}(\overline{u})$ *are in* $B_{w_{eq}} \subset \mathbb{R}^n$. *Assume it exists* $\nu = \nu(w_{eq})$ *such that*

$$-(\nabla_w \eta(w) - \nabla_w \eta(w_{eq}(u))) * (R(w) - R(w_{eq}(u))) \geq \nu |w - w_{eq}(u)|^2 \quad \text{(Hyp 6)}$$

for $w, w_{eq}(u) \in B_{w_{eq}}$ *with* $u = \mathbb{P}w$.
Then for $r > 0$ *it exists* A, B, s *such that:*

$$\int_{|x|<r} |w - w_{eq}(\overline{u})|^2 dx \leq A \left(\int_{|x|<r+st} |w(x,0) - w_{eq}(\overline{u}(x,0)|^2 dx + B\varepsilon \right)$$

Modeling error estimate: relative entropy

Let $w \in \mathbb{R}^m$ be a regular solution of $(\mathcal{M}_f)$
Let $\overline{u} \in \mathbb{R}^n$ be a regular solution of $(\mathcal{M}_c)$

- The relative entropy $H : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is given by

$$H(w, w_{eq}(\overline{u})) = \eta(w) - \eta(w_{eq}(\overline{u})) - \nabla_w \eta(w_{eq}(\overline{u})) * (w - w_{eq}(\overline{u}))$$

- Relative entropy flux $H_\alpha : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$

$$Q(w, w_{eq}(\overline{u})) = \xi(w) - \xi(w_{eq}(\overline{u})) - \nabla_w \eta(w_{eq}(\overline{u})) * (F(w) - F(w_{eq}(\overline{u})))$$

- Relative entropy positive definite (convexity of η)

$$H(w, w_{eq}(\overline{u})) \geq \frac{\beta}{2} |w - w_{eq}(\overline{u})|^2$$

Modeling error estimate: main lines of the proof

- Relative entropy identity

$$\partial_t H(w, w_{eq}(u)) + \sum_{\alpha=1}^{d} \partial_\alpha Q_\alpha(w, w_{eq}(u)) + \frac{1}{\varepsilon} D = J_1 + J_2$$

where

$$J_1 = - \sum_{\alpha=1}^{d} \nabla_u^2 \overline{\eta}(\overline{u}) \partial_\alpha \overline{u} \cdot \left[g_\alpha(u) - g_\alpha(\overline{u}) - \nabla_u g_\alpha(\overline{u}) \cdot (u - \overline{u}) \right]$$

$$J_2 = - \sum_{\alpha=1}^{d} \nabla_u^2 \overline{\eta}(\overline{u}) \partial_\alpha \overline{u} \cdot \mathbb{P} \left[F_\alpha(w) - F_\alpha(w_{eq}(u)) \right]$$

$$D = (\nabla_w \eta(w) - \nabla_w \eta(w_{eq}(u))) * (R(w) - R(w_{eq}(u)))$$

Modeling error estimate: main lines of the proof

- Consider the weak form of the relative entropy identity (Kruzhkov procedure)
- Let $r > 0$, $t > 0$, s such that $sH + Q\frac{x}{|x|} > 0$

$$\int_{|x|<r} H(w, w_{eq}(\overline{u}))dx + \frac{1}{\varepsilon}\int_0^t \int_{|x|<r+s(t-\tau)} D\, dxd\tau$$
$$\leq \int_{|x|<r+st} H(w_0, w_{eq}(\overline{u}_0))dx + \int_0^t \int_{|x|<r+s(t-\tau)} J_1 + J_2\, dxd\tau$$

- Use assumption (Hyp 6) and the $\beta-$convexity of η
- Control of the terms $|J_1|$ and $|J_2|$

$$|J_1| \leq C(\overline{\eta}, F, w_{eq}, \partial_\alpha \overline{u})|w - w_{eq}(\overline{u})|^2 \quad |J_2| + \frac{1}{\varepsilon} D \leq \varepsilon C(\overline{\eta}, F, w_{eq}, \partial_\alpha \overline{u})$$

- Conclude via a Gronwall Lemma

Remark: $\partial_\alpha \overline{u}$ known *a priori* (initial data)

Numerical error estimate

Numerical error estimate $\|\overline{u} - \overline{u}^h\|$

- Scalar case: FV scheme, convergence towards entropy solution, error estimate [Chainais 99 ; Eymard, Gallouët, Herbin 00 ; Kröner, Ohlberger 00],
- System case: relative entropy

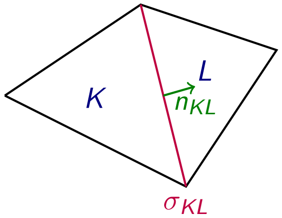
$$\begin{cases} \partial_t u + \sum_{\alpha=1}^{d} \partial_\alpha g_\alpha(u) = 0 \\ u(x,0) = u_0(x) \end{cases} \qquad (\mathcal{M}_c)$$

1. $u_0 \in L^\infty(\mathbb{R}^d)$
2. g Lipschitz continuous
3. Entropy-entropy flux $\overline{\eta} - \overline{\xi}$, $\overline{\eta}$ $\beta-$convex

Finite volume scheme

Mesh $\mathcal{T}$

- $h = \sup\{\text{diam}(K), K \in \mathcal{T}\} < \infty$
- $ah^d \leq m(K)$
- $\mathcal{E}$: set of interfaces
- $\mathcal{N}(K)$: neighbouring cells of K



Time step: $t^n = n\Delta t, \ \forall n \in \mathbb{N}$

Numerical scheme

$$u_K^0 = \frac{1}{m(K)} \int_K u_0$$

$$u_K^{n+1} = u_K^n - \frac{\Delta t}{m(K)} \sum_{L \in \mathcal{N}} G_{KL}(u_K^n, u_L^n) \qquad (\mathcal{S})$$

$$u^h(x,t) = u_K^n, \ \text{if } x \in K, \ t^n \leq t \leq t^{n+1}$$

Numerical flux: assumptions

Numerical flux: $G_{KL} \in C(\mathbb{R}^m \times \mathbb{R}^m, \mathbb{R}^m) : (u, v) \to G_{KL}(u, v)$

- Lipschitz continuous, conservative, stable under CFL condition, consistant
$$\frac{1}{m(\sigma_{KL})} G_{KL}(u, u) = g(u) \cdot n_{KL}$$
- Entropy flux $\overline{\xi}_{KL}(u, v)$, conservative
- Entropy inequality by interface [Harten, Lax, Van Leer 83 ; Bouchut 04]
$$\overline{\xi}_{KL}(u_K, u_L) - m(\sigma_{KL})\overline{\xi}(u_K) \cdot n_{KL} \leq -\frac{1}{\lambda}\big(\overline{\eta}\big(u_K - \lambda\big[G_{KL}(u_K, u_L) - m(\sigma_{KL})G(u_K) \cdot n_{KL}\big]\big) - \overline{\eta}(u_K)\big)$$

Numerical solution: $(u_K^n) \in \mathcal{O} \subset \mathbb{R}^m$, $\mathcal{O}$ open bounded subset

- Weak BV estimate [Eymard, Gallouët, Herbin, 00]
$$\sum_n \sum_{\mathcal{E}} \Delta t \, |G_{KL}(u_K^n, u_L^n) - m(\sigma_{KL}) g(u_K^n) \cdot n_{KL}| \leq \frac{C_{WBV}}{\sqrt{h}}$$

Numerical entropy flux

Lemma

Under assumptions on the numerical flux G_{KL} and $\overline{\eta}$ properties, the numerical entropy flux $\overline{\xi}_{KL}$ satisfies the following properties:

1. *Consistance:* $\overline{\xi}_{KL}(u,u) = m(\sigma_{KL})\overline{\xi}(u) \cdot n_{KL}$
2. *Lipschitz continuity*
3. *Discrete entropy inequality*

$$\frac{m(K)}{\Delta t}(\overline{\eta}(u_K^{n+1}) - \overline{\eta}(u_n^k)) + \sum_{L \in \mathcal{N}} \overline{\xi}_{KL}(u_K^n, u_L^n) \leq 0$$

4. *Weak BV estimate*

$$\sum_k \sum_{\mathcal{E}} \Delta t \left| \overline{\xi}_{KL}(u_K^n, u_L^n) - m(\sigma_{KL})\overline{\xi}(u_K^n) \cdot n_{KL} \right| \leq \frac{\tilde{C}_{WBV}}{\sqrt{h}}$$

Relative entropy

Let $u \in \mathbb{R}^m$ be a regular solution of $(\mathcal{M}_c)$ and u^h its approximation.

- The relative entropy $\overline{H} : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$ is given by

$$\overline{H}(u, u^h) = \overline{\eta}(u^h) - \overline{\eta}(u) - \nabla_u \overline{\eta}(u) \cdot (u^h - u)$$

- Relative entropy flux $\overline{Q}_\alpha : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}$

$$\overline{Q}(u^h, u) = \overline{\xi}(u^h) - \overline{\xi}(u) - \nabla_u \overline{\eta}(u) \cdot (g(u^h) - g(u))$$

- Link between relative entropy and $\mathcal{E}_m$:

$$\overline{H}(u, u^h) \geq \frac{\beta}{2} |u - u^h|^2$$

Relative entropy inequality

Theorem

Let u *be a classical solution of* $(\mathcal{M}_c)$ *and* u^h *an approximate solution defined by* $(\mathcal{S})$. *Then,* $\forall \varphi \in C_c(\mathbb{R}^d \times \mathbb{R}^+)$

$$\int_{\mathbb{R}^d\times\mathbb{R}^+} H(u^h,u)\partial_t\varphi dxdt + Q(u^h,u)div\varphi + \int_{\mathbb{R}^d} H(u_0^h,u_0)\varphi(x,0)dx \geq$$

$$-\int_{\mathbb{R}^d\times\mathbb{R}^+} |div\varphi| + |\partial_t\varphi| d\mu - \int_{R^d} \varphi(x,0)d\mu_0$$

$$-\int_{\mathbb{R}^d\times\mathbb{R}^+} |div(\nabla_u\eta(u)\varphi)| + |\partial_t(\nabla_u\eta(u)\varphi)| d\overline{\mu} - \int_{\mathbb{R}^d} \nabla_u\eta(u_0)\varphi(x,0)d\overline{\mu}_0$$

$$-\int_{\mathbb{R}^d\times\mathbb{R}^+} \varphi \sum_{\alpha=1}^{d} \partial_\alpha u^T Z_\alpha(u^h,u)dxdt$$

where $Z_\alpha(u^h,u) = (g_\alpha(u^h) - g_\alpha)\nabla_u^2\eta(u) - \nabla_u g_\alpha(u)(u^h - u)$

Main lines of the proof

- It exists $\mu_K, \overline{\mu_K} \in \mathcal{M}(\mathbb{R}^d \times \mathbb{R}^+)$ and $\mu_0, \overline{\mu_0} \in \mathcal{M}(\mathbb{R}^d)$ such that for $\varphi \in C_c^\infty(\mathbb{R}^d \times \mathbb{R}^+, \mathbb{R}^+)$

$$\int_{\mathbb{R}^d \times \mathbb{R}^+} \eta(u^h)\partial_t\varphi + \xi(u^h) div\varphi dxdt + \int_{\mathbb{R}^d} \eta(u_0^h)\varphi(x,0)dx \geq - \int_{\mathbb{R}^d \times \mathbb{R}^+} \left(|div\varphi| + |\partial_t\varphi|\right) d\mu - \int_{R^d} \varphi(x,0)d\mu_0$$

and

$$\int_{\mathbb{R}^d \times \mathbb{R}^+} u^h\partial_t\varphi + g(u^h) div\varphi dxdt + \int_{\mathbb{R}^d} u_0^h\varphi(x,0)dx \geq - \int_{\mathbb{R}^d \times \mathbb{R}^+} (|div\varphi| + |\partial_t\varphi|)d\overline{\mu} - \int_{\mathbb{R}^d} \varphi(x,0)d\overline{\mu_0}$$

Main lines of the proof

- The measures μ and μ_0 verify the following properties
  1. If $u_0 \in BV(\mathbb{R}^d)$
  $$\mu_0(\mathbb{R}^d) \leq C(u_0, a)h$$
  $$\overline{\mu_0}(\mathbb{R}^d) \leq C(u_0, a)h$$
  2. $\forall r > 0, \;\; T > 0$
  $$\mu(B(0,r) \times [0,T]) \leq C(G_{KL}, C_{WBV}, u_0, r, T)\sqrt{h}$$
  $$\overline{\mu}(B(0,r) \times [0,T]) \leq C(g, u_0, r, T)\sqrt{h}$$
- Weak BV estimates and the numerical scheme definition $(\mathcal{S})$

Numerical error estimate

Theorem

Let u be a classical solution of $(\mathcal{M}_c)$ on $[0, T]$ taking values in a convex compact subset $\mathcal{D} \subset \mathbb{R}^m$, with initial data u_0. Let u^h be an approximate solution of $(\mathcal{M}_c)$ defined by $(\mathcal{S})$.
Then

$$\int_{|x|<r} |u^h - u|^2 dx \leq Ce^D \int_{|x|<r+st} |u_0^h - u_0|^2 dx$$

holds for any $r > 0$ and $t \in [0, T]$ with positive constant s, $C(\overline{\eta}, \mathcal{D})$ and $D(\overline{\eta}, \mathcal{D}, \partial_\alpha u)$

Main lines of the proof

- Consider relative entropy inequality (Kruzhkov procedure)
- Gronwall Lemma

Global estimate

Corollary

Assume hypothesis (Hyp 1)-(Hyp 6). *Let* w *be a regular solution of* $(\mathcal{M}_f)$ *with initial conditions* w_0. *Let* $\overline{u}$ *be a classical solution of* $(\mathcal{M}_c)$ *on* $[0, T]$ *taking values in a convex compact subset* $\mathcal{D} \subset \mathbb{R}^m$, *with initial data* $\overline{u}_0$. *Let* $\overline{u}^h$ *be an approximate solution of* $(\mathcal{M}_c)$ *defined by* $(\mathcal{S})$.
Then

$$\int_{|x|<r} |w - w_{eq}(\overline{u}^h)|^2 dx \leq A \left(\int_{|x|<r+st} |w_0 - w_{eq}(\overline{u}_0)|^2 dx + B\varepsilon \right) + Ce^D \int_{|x|<r+st} |\overline{u}_0^h - \overline{u}_0|^2 dx$$

holds for any $r > 0$ *and* $t \in [0, T]$

Conclusion and prospects

Conclusions

- Error estimate between hyberbolic system with relaxation and finite volume approximation of the hyperbolic limit
- Use of relative entropy

Prospects

- Specify the regularity hypothesis
  - existence of solution of $(\mathcal{M}_f)$ [Yong 99 ; Hanouzet, Natalini 03]
  - existence of solution of $(\mathcal{M}_c)$ [Dafermos 10]
- Get precisely the constants [Kröner, Ohlberger 99]
- Use this estimate to perform adaptation