Some tools for model adaptation in the context of fluid flows

Edwige Godlewski

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collaborations

Frédéric Coquel (CMAP, Ecole Polytechnique)
Clément Cancès
Hélène Mathis (LMJL, U. Nantes)
Nicolas Seguin

LRC MANON

Introduction

Model adaptation, multiscale modeling

- Duality based methods, linked to a goal oriented strategy:

output functional $J(u)$ (example drag computation, pressure point value). *Rannacher (2009); Oden, Prudhomme et al (2006)*; *Braack, Ern (2003)*

$u \in V, \quad a(u)(\phi) + d(u)(\phi) = (f, \phi), \ \forall \phi \in V$

$u_m \in V, \ a(u_m)(\phi) = (f, \phi), \ \forall \phi \in V$

estimate the influence of neglecting $d(u)$ on $J(u)$.

- Heterogeneous Multiscale Method, *W. E, Engquist et al.(2007)*

capture the macroscale behavior of a system with the help of microscale models.

- In between, multiscale kinetic-fluid solver: kinetic-fluid regions and coupled model. Fluid model everywhere, localized kinetic upscaling *P. Degond, G. Dimarco, L. Mieussens 2010*: micro-macro decomposition $f = E[\varrho] + g$ (local equilibrium + deviation part). Localization of fluid-kinetic transition and dynamic coupling.

Introduction

- Domain decomposition
  - and geometrical multiscale modeling *Formaggia, Gerbeau, Nobile, Quarteroni (2001)* for flows in compliant vessels or *Malleron, Zaoui, Goutal, Morel (2011)* Efficient model coupling in hydroinformatics (dynamic coupling of existing 2D-1D codes).
  - *Shi Jin, Jian-guo Liu and Li Wang Math. Comp. (2013)* A domain decomposition method for semilinear hyperbolic systems with two-scale relaxations; provides a rigourous analysis in the linear case (solution by Laplace transform).

- We follow the strategy developed in *Braack, Ern (2003)*: " achieve compromise between accuracy of the model and computational costs by increasing adaptivity.
- next step: change locally the model or the mesh size; balancing model and mesh size." by adding posteriori error control *Kröner, Ohlberger 1999* and adaptivity *M. Ohlberger (2009)* (scalar case)

Application

Context (LRC)

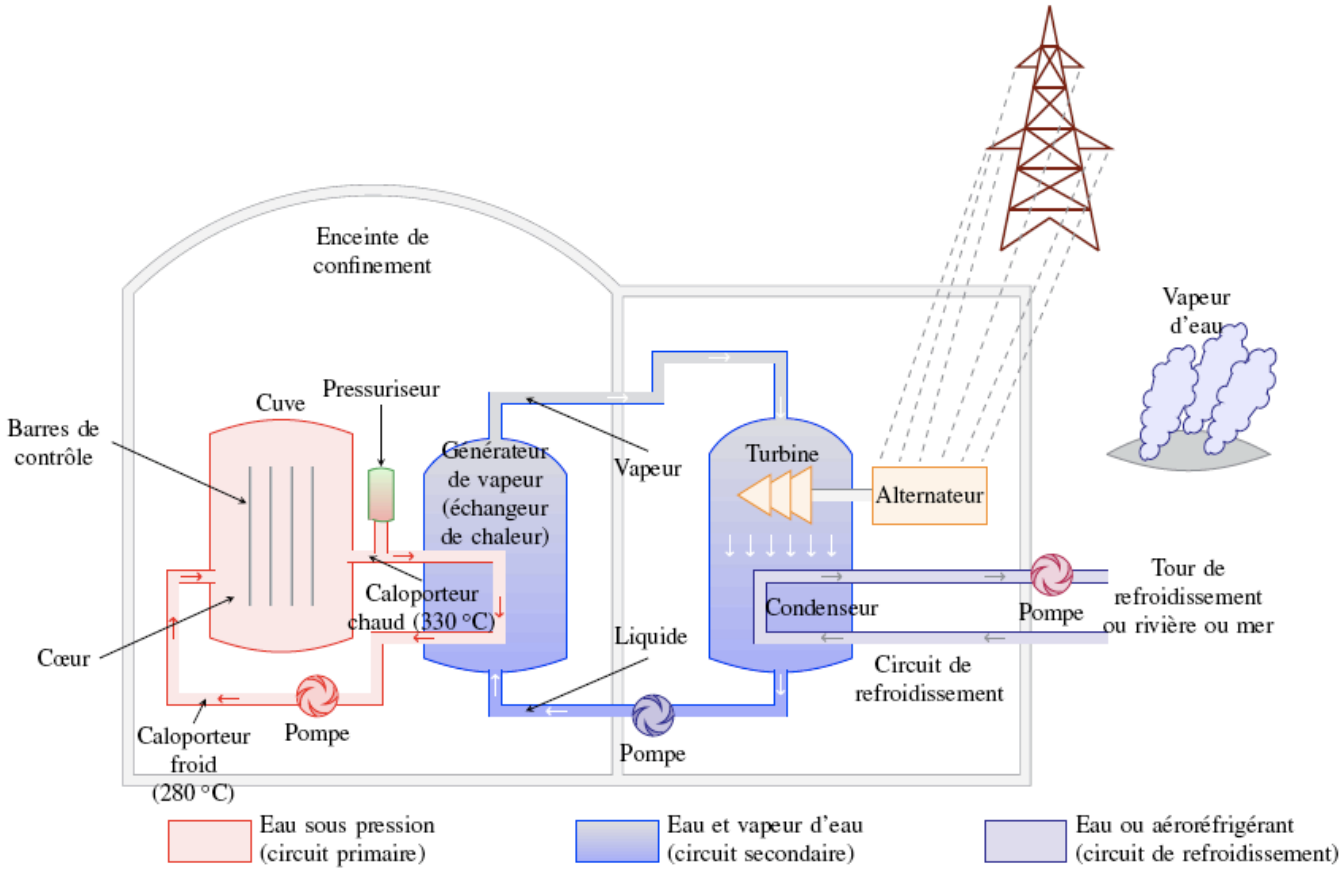


FIGURE 1 – Schéma simplifié d'un réacteur nucléaire à eau sous pression

Introduction

Simulation of multiphase flow in nuclear energy industry (CEA): coolant circuits are formed by different components, each one with its associated specific model for the coolant flow. The coolant is a two-phase fluid.
There exists a wide variety of models (mixture, drift, homogeneous or not, two-fluid, multi-field models...):
- according to the main features of the flow (immiscible, dispersed, 3D effects, ...)
- according to what one is interested in (fluid velocity / acoustic waves,...)
- more or less costly to implement (number of variables, complex pressure laws,...)
- more or less *accurate* (thermal, mechanical, dynamical equilibria).
$\rightarrow$ Build a (numerical) strategy to choose the "right" one at the "right" place: adaptative procedure.
Begin by some academic case: 2 models, linked by some hierarchy.

Outline

Model adaptation

- Framework
- Relaxation / equilibrium models
- Adaptation procedure in the relaxation framework
- A toy model (theoretical validation)

Our framework for model adaptation

In the context of two-phase flows: many (numerical) models.
We assume there exists a fine / accurate / expensive model valid everywhere and also a coarse / less accurate / cheaper model.
Goal: build a (numerical) strategy to choose the right one, define the regions where one uses each model.

- fine / coarse models $\mathcal{M}_{fi}/\mathcal{M}_{co}$: a hierarchy between them
- right means a balance between tolerance of less accuracy (measured by an indicator) and cost
- nonlinear approach, non stationary
- domain decomposition: fine / coarse (space) domains D_{fi}/D_{co}
- dynamic adaptation define $D_{fi/co}^{(n)}$ at each time step t_n
- Need to couple $\mathcal{M}_{fi}/\mathcal{M}_{co}$ at a sharp* interface $D_{fi}^n \cap D_{co}^n$ (fixed on $[t_n, t_{n+1}]$)

* regularized for the toy model

Our framework for model adaptation

Hierarchy between the 2 systems given by relaxation (other process: averaging, homogenization, linearization, viscous approximation, low Mach regime, ...)
Assumptions:

- models given by a system of PDE's (conservation laws, hyperbolicity required) linked by relaxation
- $\mathcal{M}_{fi}$ Relaxation system / $\mathcal{M}_{co}$ Equilibrium system

Ex: HRM/HEM (Homogeneous Relaxation/Equilibrium Model)

- here analysis of 1D problems, for simplicity $D_{fi}/D_{co} \subset \mathbb{R}$
- finite volume (conservative) schemes
- balance cost / accuracy: use a *coarse* (less expensive) model whenever acceptable and *fine* model elsewhere: $\overline{D} = \overline{D}_{co} \cup \overline{D}_{fi}$
- use a (sharp) interface coupling model

Theoretical frame: some tools

- Sharp interface coupling model, as general as possible (flux or state coupling): *G-Raviart, (2004), Ambroso et al. (2008)*...
- well understood (theoretical results) on significative examples
- *numerical interface coupling* procedures for general situations
- regularized (thickened) interface for regularity results *Boutin et al. (2011)*

- Hierarchy between systems is linked to a relaxation process: $\mathcal{M}_{fi}$ Relaxation system $\rightarrow \mathcal{M}_{co}$ Equilibrium system as relaxation time $\varepsilon \rightarrow 0$

Again well understood on significative examples:

  - fluid models (theoretical results) *Coquel-G-Seguin (2012)*
  - HRM / HEM (phase transition) *Ambroso et al. (2007)*
  - more complicated: bifluid / drift model; Baer-Nunziato / two-component Euler system *Dellacherie (2003)*

- Hierarchy may be inherited by numerical scheme
- Possible to couple numerically with different schemes

Some principles for model adaptation

• Some issues: which model (coarse/fine)? how do we switch? estimate of modeling error?
Relaxation system considered as *fine, more accurate, more expensive* / equilibrium system as *coarse, cheaper*. Both are given.

• Need of:
- an indicator (involving the relaxation time ε) which measures the *modeling error*
- a tolerance θ for this error
- a dynamic procedure: $u_{ad}(., t_n) \rightarrow u_{ad}(., t_{n+1})$
- a numerical indicator should NOT need compute the fine solution everywhere, only $u_{ad}(., t_n)$

• Validate the approach on
- simpler models: for which hierarchy between models can be proved and with compatible numerical schemes
- numerical extension to more general cases (different schemes)
- a toy model: theoretical results can be obtained

Example of relaxation system

Example of a relaxation model for the equilibrium $p-$system (Suliciu; Chaplygin gas model)

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

$\Pi = \Pi(\tau, \mathcal{T}) = p(\mathcal{T}) + a^2(\mathcal{T} - \tau)$ linearization of the pressure.
Chapman-Enskog expansion: $\mathcal{T} = \tau + \varepsilon \mathcal{T}_1 + \mathcal{O}(\varepsilon^2)$, $\mathcal{T}_1$ corrector

$$\begin{cases} \partial_t \tau - \partial_x u = 0 \\ \partial_t u + \partial_x p(\tau) = \varepsilon \partial_x \Big((p'(\tau) + a^2) \partial_x u \Big) \end{cases}$$

dissipative if $p'(\tau) + a^2 > 0$, *stability criteria*.
Theoretical results *Chalons, Coulombel (2007)* after *Yong*
Use $\varepsilon \mathcal{T}_1 = \varepsilon (p'(\tau) + a^2) \partial_x u$ as indicator

Model adaptation relaxation framework

Simplified presentation
-fine model: system with a relaxation term

$$\begin{cases} \partial_t u + \partial_x f(u,v) = 0 \\ \partial_t v + \partial_x g(u,v) = \frac{1}{\varepsilon}(e(u) - v) \end{cases} \tag{1}$$

as $\varepsilon \to 0$, $(u_\varepsilon, v_\varepsilon) \to (u_{eq}, v_{eq} = e(u_{eq}))$, u_{eq} satisfies the
- coarse *equilibrium* model:

$$\partial_t u + \partial_x f(u, e(u)) = 0 \tag{2}$$

Approximation results *Chen, Levermore, Liu (1994), Yong (1999, 2004)* under stability conditions (entropy extension, structural stability), for 2×2 system *Natalini, Serre* (for Jin-Xin model), for fluid systems *Coquel et al. (2012)*
Intermediate model by Chapman-Enskog expansion

Numerical model adaptation

- Indicator for adaptative procedure: use corrector in the Chapman Enskog expansion $v = e(u) + \varepsilon v_1 + \mathcal{O}(\varepsilon^2)$, set $U_e \equiv (u, e(u))$, $f_e(u) \equiv f(U_e)$; u_ε solution of (1) satisfies at order $\mathcal{O}(\varepsilon^2)$

$$\partial_t u + \partial_x f_e(u) = -\varepsilon \partial_x \Big(\partial_v f(U_e) \big(e'(u) \partial_x f(U_e) - \partial_x g(U_e) \big) \Big)$$

- effective indicator: FV schemes with numerical fluxes $\mathcal{F}, \mathcal{G}$ consistent with f, g and $\mathcal{F}_e$ with f_e and compatible $\mathcal{F}_e(u, \overline{u}) = \mathcal{F}(U_e, \overline{U}_e)$. Discretization of v_1, roughly (precise formula in the preprint) for $e'(u)\partial_x f(U_e) - \partial_x g(U_e)$

$$\sim e'(u_i^n) \frac{\mathcal{F}^n_{e,i+1/2} - \mathcal{F}^n_{e,i-1/2}}{\Delta x} - \frac{\mathcal{G}^n_{i+1/2,eq} - \mathcal{G}^n_{i-1/2,eq}}{\Delta x}$$

then $v_i^n = v_{eq}(u_i^n) + \varepsilon v^n_{1,i} + \mathcal{O}(\varepsilon^2)$

Numerical model adaptation

Given: two models, fine $\mathcal{M}_{fi}$ and coarse $\mathcal{M}_{co}$, associated FV schemes with numerical fluxes $\mathbf{g}_{fi}$, $\mathbf{g}_{co}$; an indicator $\delta^n(x)$ of the 'model error'; a tolerance θ.
The principle is: at each time step, compute the coarse model $\mathcal{M}_{co}$ whenever possible: if solution too far ($\delta > tol\theta$) from equilibrium, use the fine model and at interface one couples the two models.
Numerical model adaptation scheme: compute a piecewise constant solution noted $u_{ad}(., t_n)$ following the algorithm:
on one time step $t_n \to t_{n+1}$, starting from $u_{ad}(., t_n)$

- compute δ^{n+1} everywhere
- determine D_{fi}^n: if $\delta^n(x) \geq \theta$, $x \in D_{fi}^n$
- solve $\mathcal{M}_{fi}$ with $\mathbf{g}_{fi}$ in D_{fi}^n: gives $(u, v)(x, t_{n+1})$, $x \in D_{fi}^n$
- solve $\mathcal{M}_{co}$ with $\mathbf{g}_{co}$ in $D_{co}^n = D \setminus D_{fi}^n$, gives $u(x, t_{n+1})$, $x \in D_{co}^n$, $v = e(u)$
- couple them at interface $\overline{D}_{fi}^n \cap \overline{D}_{co}^n$:

Numerical interface coupling

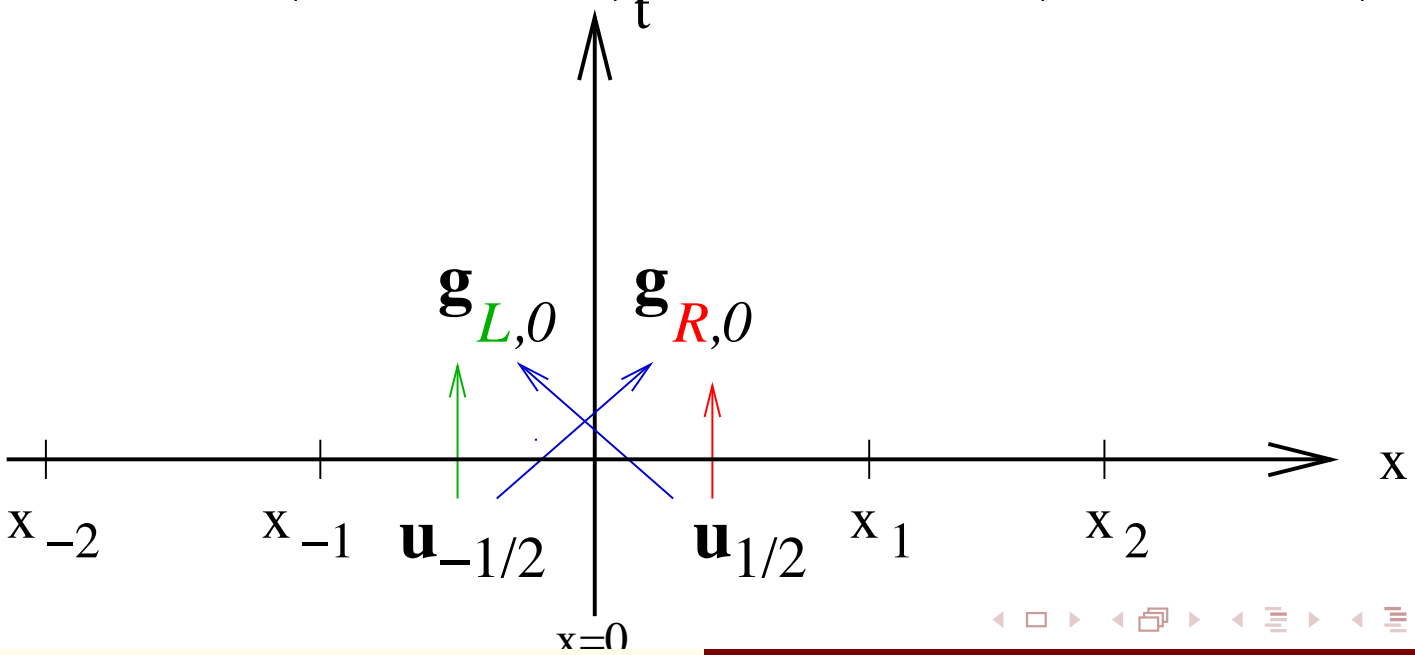
Finite Volume method: interface at $j = 0$, cells $C_{j+1/2} = (x_j, x_{j+1})$

$$\mathbf{u}_{j+1/2}^{n+1} = \mathbf{u}_{j+1/2}^{n} - \frac{\Delta t}{\Delta x}(\mathbf{g}_{\alpha,j+1}^{n} - \mathbf{g}_{\alpha,j}^{n}), j \in \mathbb{Z}$$

with $\alpha = L$ for $j \leq -1, R, j \geq 0$, we have 2 conservative FV schemes, in $x < 0$ and in $x > 0$.

Non conservative approach: TWO fluxes at the interface $x = 0$

$$\mathbf{g}_{L,0}^{n} = \mathbf{g}_{L}\left(\mathbf{u}_{-1/2}^{n}, \mathbf{u}_{+1/2}^{n}\right), \quad \mathbf{g}_{R,0}^{n} = \mathbf{g}_{R}\left(\mathbf{u}_{-1/2}^{n}, \mathbf{u}_{+1/2}^{n}\right)$$



• Theoretical relaxation framework with entropy extension (EE).
scheme for relaxation system: splitting convection / source (implicit)
scheme for equilibrium (coarse) system: deduced with instantaneous relaxation (fine scheme has AP property).
Numerical illustration on a test case satisfying the EE condition.
• Numerical illustration on test cases which do not satisfy the EE:
  • 2D experiment with a phase transition HRM/HEM model (extended entropy is not strictly convex)
  • 1D experiment with Baer Nunziato (7 equations) - bicomponent (4 equations); different (non compatible) schemes: Rusanov for convection + successive splitting of the relaxation terms; with Chapman-Enskog type indicator
cf. Hélène Mathis et al. preprint 2013

a toy scalar example

In order to prove some results (theoretical validation, no CPU gain!) we consider

- fine model: 2×2 system (relaxation)

$$\begin{cases} \partial_t u + \partial_x f(u, v) = 0, \\ \partial_t v = \frac{1}{\varepsilon}(v_{eq}(x) - v), \end{cases} \tag{3}$$

$g = 0$, $e(u) = v_{eq}(x)$, so that we can compute explicitly the ODE for v (decoupled)

- coarse scalar conservation law (equilibrum, $\varepsilon \to 0$)

$$\partial_t u + \partial_x f(u, v_{eq}(x)) = 0$$

Theoretical results are possible: obtained by comparing u_{fi} and u_{ad} respective solution of equation with flux $F_{fi}(u, x, t) = f(u, v_{fi}(x, t))$ ad $F_{ad}(u, x, t) = f(u, v_{ad}(x, t))$, where v_{ad} obtained by the adaptation algorithm.

a toy scalar example

Use results for comparing solution u, v of CL with resp. fluxes f, g, resp. i. d. u_0, v_0: need smooth fluxes $\rightarrow$ a smooth $v_{ad} \rightarrow$ thicken the interface.

Algorithm: steps $t_n \rightarrow t_{n+1}$, $n \geq 0$ with $t_k = k\Delta t_a$, starting from $(u_{ad}^{-1}, v_{ad}^{-1}) = (u_0, v_0)$:

- Indicator: $v_i^{(n)}$ exact solution of (3) with initial data $v_{ad}^{(n-1)}(., t_n)$ (recall that $v_{co} = v_{eq}$)
- $D_{fi}^n = \{x, |v_{eq}(x,t) - v_i^{(n)}(x,t)| > \Delta t_a \Sigma,$
$|\partial_x v_{eq}(x,t) - \partial_x v_i^{(n)}(x,t)| > \Delta t_a \Sigma'$ or $|\partial_{xx} v_i^{(n)}(x,t)| > \Sigma''\}$
- regularized caracteristic function $\chi_\delta(x,t) = 1$ on $D_{fi}^{(n)} = 0$ if distance $d(x, D_f^{(n)}) \geq \delta$.
- Define $v_{ad}^{(n)} = \chi v_i^{(n)} + (1-\chi) v_{eq}$
- Define $u_{ad}^{(n)}$ entropy solution on $(t_n, t_{n+1}]$ of equation with flux $F_{ad} = f(u, v_{ad})$ and data $u_{ad}^{(n-1)}(., t_n)$

a toy scalar example

Assumption: v_{eq} constant outside $(-R, R) \times \mathbb{R}+$, $v_0 = v_{eq}$ outside $(-R, R) \Rightarrow v_{fi} = v_{eq}$ outside $(-R, R) \times \mathbb{R}+ \Rightarrow D_{fi} \subset]-R, R[$

- Bouchut-Perthame

$$||u(., T) - v(., T)||_{L^1(\mathbb{R})} \leq ||u_0 - v_0||_{L^1(\mathbb{R})} + CTV(v_0)\, Tlip(f - g)$$

Extend the result to fluxes depending on x, t to compare the solutions u_{ad}, u_{fi} of equations with different fluxes $F_{fi} = f(u, v_{fi}(x, t))$ and $F_{ad} = f(u, v_{ad}(x, t))$; use BV estimates on entropy solutions (Mercier, Colombo-Mercier-Rosini, Chainais).
Need of estimates on $v_{fi} - v_{ad}$ for estimating $F_{fi} - F_{ad}$
δ buffer size: then $||\partial_x \chi_\delta|| \leq \frac{c}{\delta}$, $||\partial_{xx} \chi_\delta|| \leq \frac{c}{\delta^2}$

- Bound $|v_{ad}(x, t) - v_{fi}(x, t)|$ in terms of Σ (very technical), and $|\partial_x v_{ad} - \partial_x v_{fi}|$ in terms of $\Sigma' + \Sigma/\delta$ (again very technical)
- Bound $||u_{ad}(t) - u_{fi}(t)||_{L^1(\mathbb{R})}$ in terms of $\epsilon, \Sigma/\epsilon, \Sigma/\delta, \Sigma^2/\delta^2, ...$
- Balance between different parameters involved in the error: ϵ, time step Δ_a; tolerance Σ, buffer size δ (thickened interface)

Theorem

$$||u_{ad} - u_{fi}||_{\mathcal{C}([0,T];L^1(\mathbb{R}))} \leq c\Sigma^{1/2}$$

Numerical illustration

cf. preprint C. Cancès et al. (2013)

Conclusion and future work

- Model adaptation
- an original approach involving coupling of existing codes
- indicator well founded in the relaxation framework (Chapman-Enskog)
- some convincing numerical illustrations validate the approach
- theoretical result on a toy problem

- A lot remains to do!
- include numerical error estimate (Chainais, Kröner-Ohlberger)
- extend the formalism to some other criteria (indicator) on model examples; other ε, small parameter (other hierarchy: Mach number, fluctuation,...)
- other models (hyperbolic-parabolic, convection dominated viscous flow)
- link with other approaches (goal oriented)
- ...

Thank you for your attention