Optimisation topologique et LBM :
application aux problèmes couplés convectif-diffusif-réactif

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plan

Laboratoire de Thermique et d Énergie de Nantes

- 36 permanents (29+7) et 35 contractuels
- dominante en transferts thermiques et systèmes énergétiques
- structuré en 2 axes:
- TTMI Transferts Thermiques dans les Matériaux et aux Interfaces ⇒ procédés/mise en œuvre matériaux composites, micro-nano thermique, rayonnement...
- TFSE Transferts dans les Fluides et les Systèmes Énergétiques ⇒ fluides et écoulements complexes, modélisation systèmes....
- depuis 6 ans⇒ optimisation topologique + LBM 2 permanents + 2 (1+1) doctorants

cibles visées ?

systèmes énergétiques: échangeurs, réacteurs..

- échangeurs thermiques
- stockage d'énergie thermique
- systèmes de conversion (PaCo...)
- ...

problématique multiphysique

- transferts de chaleur couplés: conduction + convection....voire rayonnement
- transferts de masse - écoulement et diffusion
- changement d'état
- réactions chimiques
- milieux poreux
- ...

pourquoi la LBM ?

approche classique: solveurs EF/VF des équations de transports macro (NS, TT..)⇒ complexe ET concurrentiel...

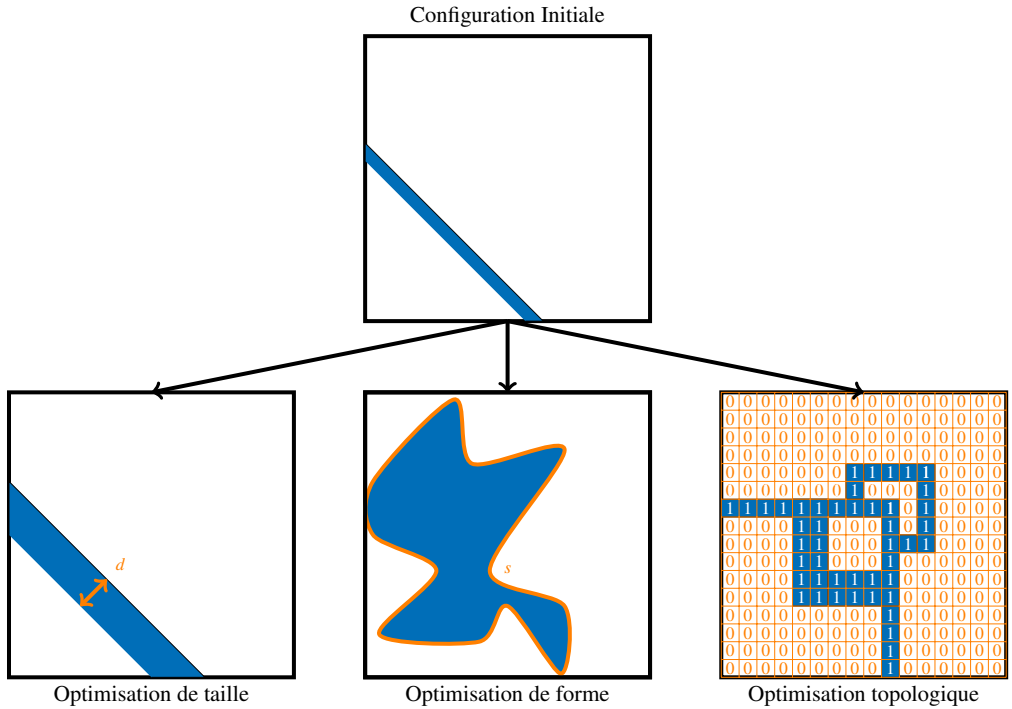
- intérêt évident: méthode "nouvelle" (nous) et "récente" (communauté)
- approche générique multiphysique (solveur unique FW et BW !!)
- ...

état des lieu:

- NS ⇒ LBM +MRT +d2Q9 (d3Q15)
- TT ⇒ champ scalaire passif 2 p.d.f. f et g
- réactif ⇒ idem
- num ⇒ GPU + CUDA
- multiphasique et poreux ⇒ Shan and Chen SCMP +EDM...+micro struture complète / hwbb
- changement d'état ⇒ SC SCMP + terme source (Ping Cheng et al, IJHMT, 2013)
- ...

optimisation topologique = optimisation géométrique...

...ou comment répartir une propriété de manière "optimale": ici allocation optimale de la matière...mais pas uniquement!!

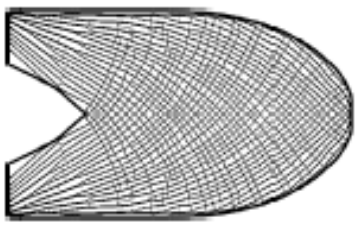


N paramètres: taille (1..10) ⇒ forme (<50)⇒ topo : nx*ny (40000 ci après)!!!

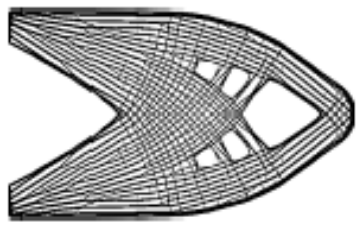
optimisation topologique: applications

premiers résultats en mécanique du solide/ structure
ici minimisation de la déformation avec différentes contraintes de masse (porosité)(Wu et Al, CMAME, 2017)

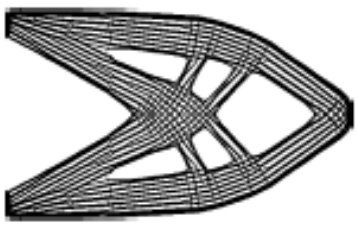
Figure 10: The design domain and boundary condition of the cantilever beam.



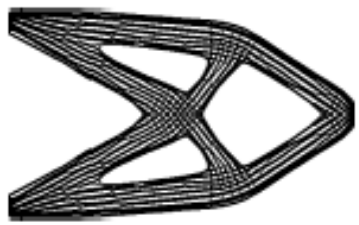
(a) $\gamma = 0.4$, $v = 0.285$, $c = 181.43$



(b) $\gamma = 0.5$, $v = 0.309$, $c = 144.69$



(c) $\gamma = 0.6$, $v = 0.337$, $c = 125.40$

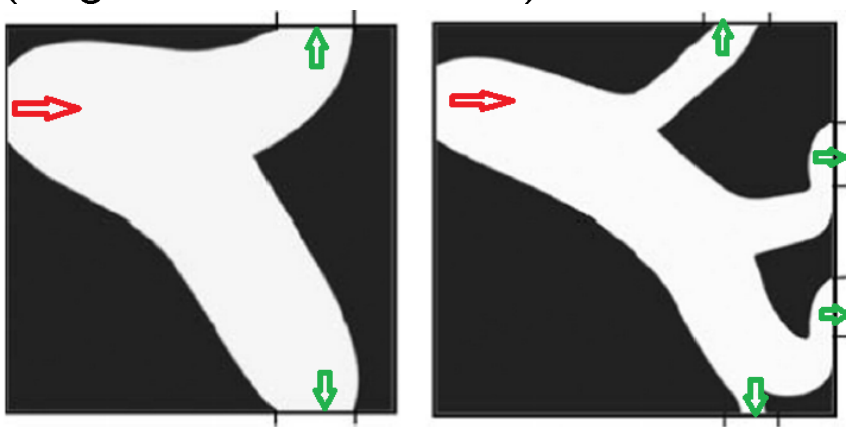


(d) $\gamma = 0.7$, $v = 0.353$, $c = 115.97$

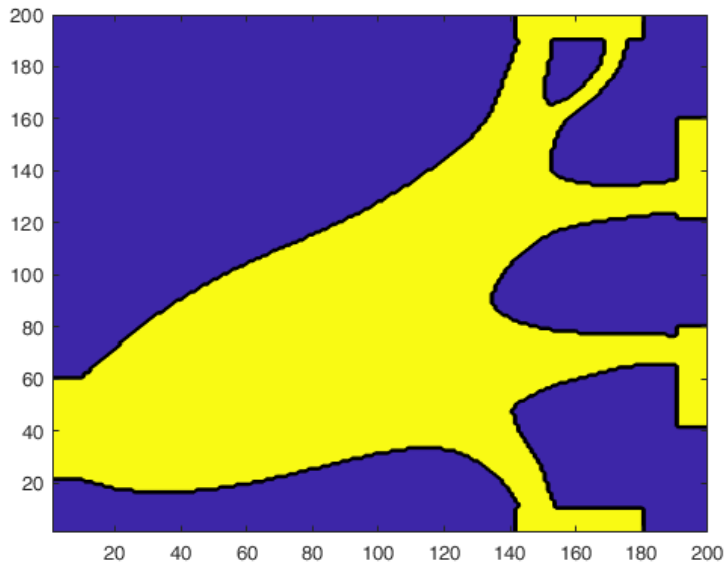
optimisation topologique: applications

puis problèmes purement fluidiques : minimisation de la perte de charges dans un distributeur ne et ns avec débits imposés

(Aage et Al, SMO, 2008)

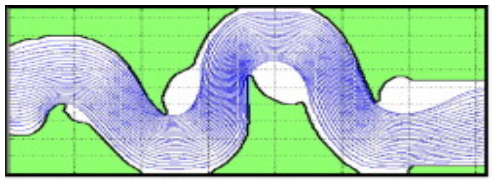


(non publiée)

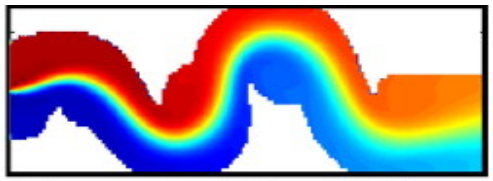


optimisation topologique: applications

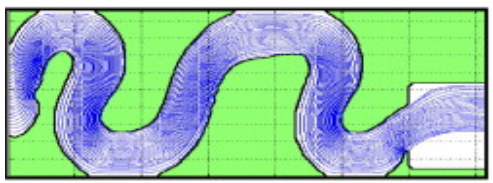
là un mélangeur de 2 fluides newtoniens(Makhija et Al, C & F, 2012)



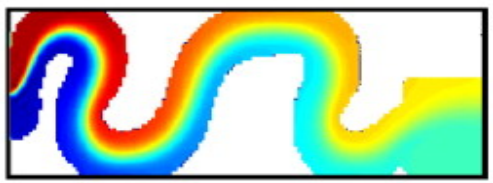
(a) Structure for $K = 0.5$, $\mathscr{F}_1 = -0.2019$.



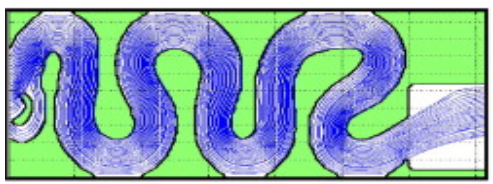
(b) Concentration for $K = 0.5$, $\mathscr{F}_1 = -0.2019$.



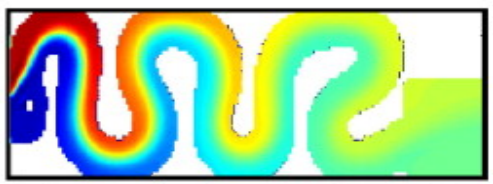
(c) Structure for $K = 2$, $\mathscr{F}_1 = -0.2386$.



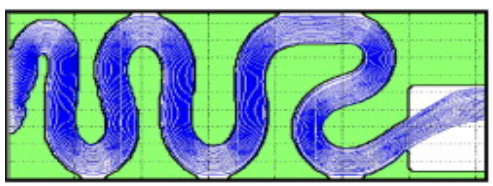
(d) Concentration for $K = 2$, $\mathscr{F}_1 = -0.2386$.



(e) Structure for $K = 5$, $\mathscr{F}_1 = -0.2472$.



(f) Concentration for $K = 5$, $\mathscr{F}_1 = -0.2472$.

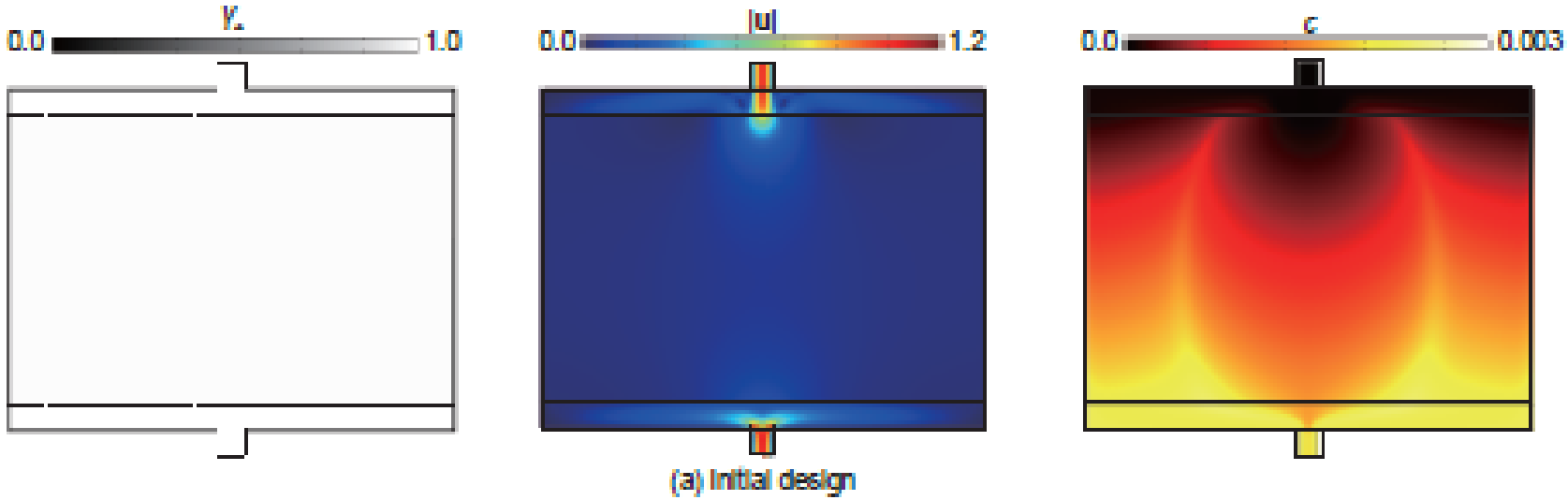


(g) Structure for $K = 12$, $\mathscr{F}_1 = -0.2481$.

(h) Concentration for $K = 12$, $\mathscr{F}_1 = -0.2481$.

optimisation topologique: applications

et des systèmes réactifs (Yaji et Al, SMO, 2017)
ici maximisation de la réaction au sein d'une batterie redox flow : LBM +SIMP



paramétrisation de la matière: densité vs level-set

représentation du solide ? $\Rightarrow \alpha(x)$ variable de design (fw et bw)

méthode à densité

- terme de forçage LBM (pseudo poreux)
- propriétés $\rho = f(\alpha) \Rightarrow$ dérivable
- $\alpha = 0 \leq \alpha \leq \alpha = 1$
- matériau intermédiaire ((Lazarov et Al, IJNME, 2011)$\Rightarrow$ filtres
- biais diffusif

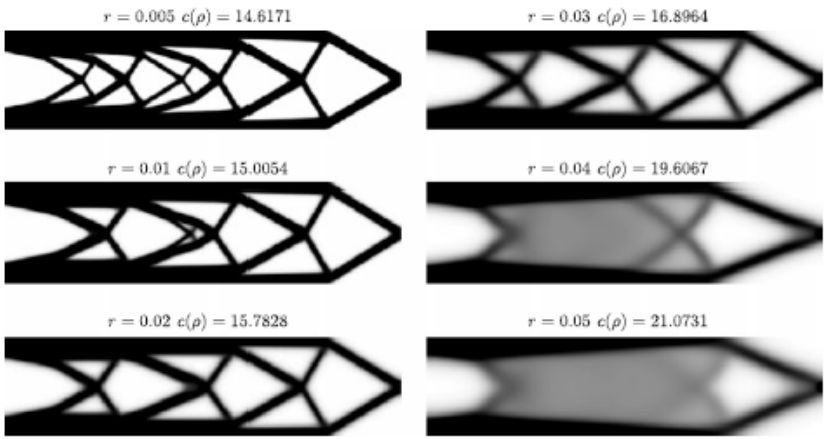


Figure 9. Helmholtz PDE isotropic sensitivity filtering—mesh 100×400 cells for cantilever beam with dimensions 1×4.

méthode à lignes de niveau (LS)

- champ $\Psi/\alpha = 0$ si $\Psi < 0$ ou $\alpha = 1$ si $\Psi > 0 \Rightarrow$ dérivable $/\Psi$
- interface claire $\Rightarrow$ bounce-back
- dérivation $/\alpha$? (cf suite)
- méthode retenue

1. LBM-based model (semi-discretized version):

$$R_i(f_1, \ldots, f_n, \alpha) = \frac{\partial f_i}{\partial t} + \boldsymbol{c}_i \cdot \nabla f_i + \frac{1}{\tau}\left(f_i - f_i^{\mathrm{eq}}\right) = 0 \quad \forall i = 1, \ldots, n,$$

with

$$f_i^{\mathrm{eq}}(f_1, \ldots, f_n, \alpha) = \omega_i \rho \left(1 + 3\alpha \boldsymbol{c}_i \cdot \boldsymbol{u} + \alpha \frac{9}{2}\left(\boldsymbol{c}_i \cdot \boldsymbol{u}\right)^2 - \alpha \frac{3}{2}\boldsymbol{u}^2\right),$$

and

$$\rho = \sum_i f_i,$$

$$\rho \boldsymbol{u} = \sum_i \boldsymbol{c}_i f_i.$$

with also:

- initial condition;
- boundary conditions.

2. cost function formulation

Example (maximization of the reaction)

which is equivalent to the minimization of the product of the velocity with the concentration, at the outlet of the domain. Mathematically, this is written as:

$$\mathcal{J} = \frac{1}{|\partial\mathcal{D}_{\mathbf{out}}|} \int_{\partial\mathcal{D}_{\mathbf{out}}} \boldsymbol{u}\cdot\boldsymbol{n}\; c_A \; + D\nabla c_A \cdot \boldsymbol{n}\; \mathrm{d}\boldsymbol{x},$$

where $\boldsymbol{n}$ is the outward unit normal vector to the boundary, the first term of the integral is the convective part of the reactant flux while the second term represents the diffusive component.

$$\mathcal{J}^+ = \mathcal{J} + \ell\mathcal{J}_1 \quad \text{with} \quad \mathcal{J}_1 = \Delta p_{\max} \exp\left(\frac{\Delta p}{\Delta p_{\max}}\right),$$

The cost function is to be re-written in terms of the lattice Boltzmann variables

- Taking into account of the following relationships between the primal variables and the lattice Boltzmann variables:

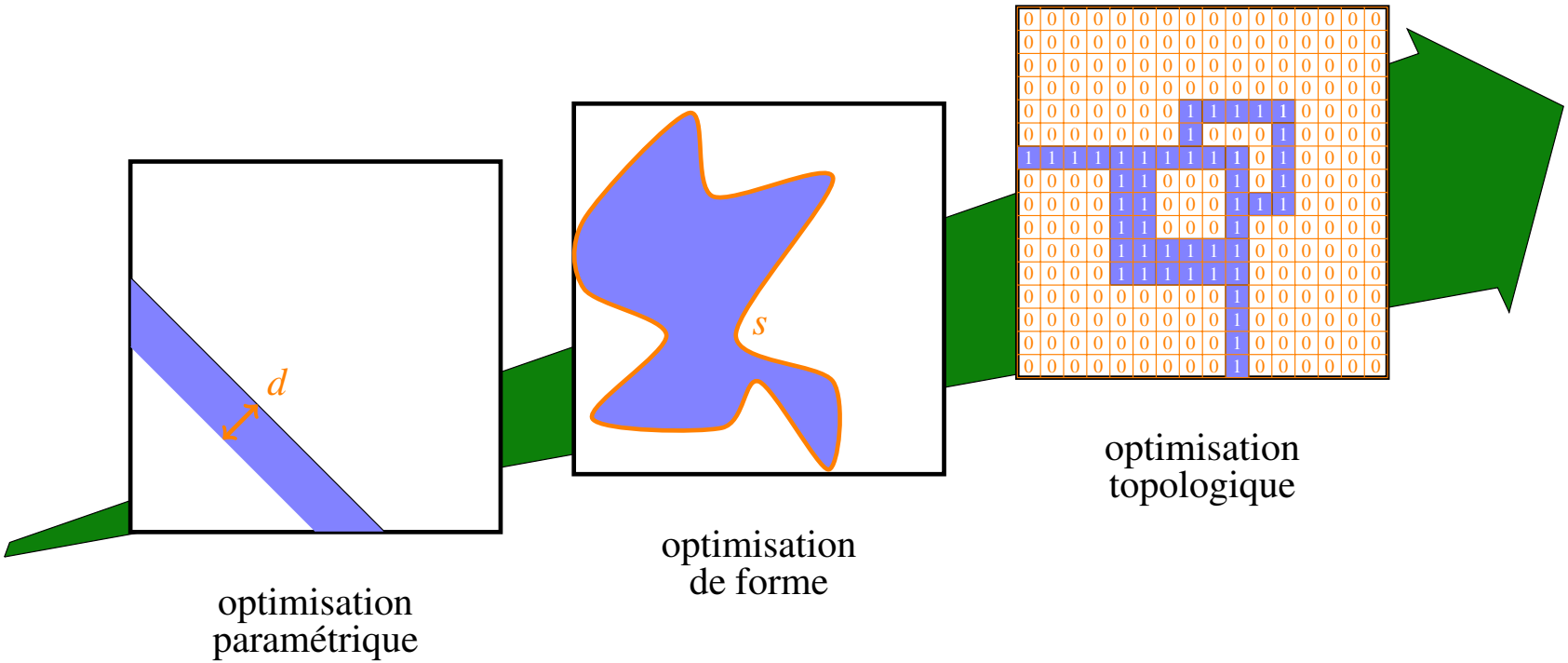
$$\boldsymbol{u} = \sum_{i=0}^{8} \boldsymbol{c}_i f_i(\boldsymbol{x}, t)$$
$$c_A = \sum_{i=0}^{8} g_i(\boldsymbol{x}, t)$$
$$\Delta p = \frac{1}{|\partial \mathcal{D}_{\mathbf{in}}|} \left[\frac{1}{3} \int_{\partial \mathcal{D}_{\mathbf{in}}} \sum_{i=0}^{8} f_i \ \mathrm{d}\boldsymbol{x} - \frac{1}{3} \int_{\partial \mathcal{D}_{\mathbf{out}}} \sum_{i=0}^{8} f_i \ \mathrm{d}\boldsymbol{x} \right],$$

- the cost function that is, finally, to be minimized is:

$$\widehat{\mathcal{J}}^{+}(\boldsymbol{f}, \boldsymbol{g}) = \frac{1}{|\partial \mathcal{D}_{\mathbf{out}}|} \int_{\partial \mathcal{D}_{\mathbf{out}}} \sum_{i=0}^{8} \boldsymbol{c}_i f_i \cdot \boldsymbol{n} \sum_{i=0}^{8} g_i \ \mathrm{d}\boldsymbol{x}$$
$$+ \ell \Delta p_{\max} \exp\left(\frac{\frac{1}{3} \int_{\partial \mathcal{D}_{\mathbf{in}}} \sum_{i=0}^{8} f_i \ \mathrm{d}\boldsymbol{x}}{|\partial \mathcal{D}_{\mathbf{in}}| \, \Delta p_{\max}} \right).$$

- Note that the pressure term at the outlet is not involved here. This one being considered as prescribed, the pressure difference is only driven by the modification of the inlet pressure during the optimization.

3. parameterization



Topology optimization:

- can give complex geometries, with holes
- dim ψ may be large (if pixelization/voxelization)

$$\alpha(\boldsymbol{x}) = \begin{cases} 1 : \text{élément fluide} \\ 0 : \text{élément solide} \end{cases}$$

set-up the optimization problem

optimization problem formulation

$$\min_{\Psi} \widehat{\mathcal{T}}^{+}(\boldsymbol{f}, \boldsymbol{g})$$

optimization problem formulation

$$\min_{\Psi} \widehat{\mathcal{T}}^{+}(\boldsymbol{f}, \boldsymbol{g})$$

méthode à gradient

- optimisation continue ($/!\backslash\ \alpha = \{0, 1\}$)
- rapide wrt gradient-free
- approche locale
- mise en œuvre délicate

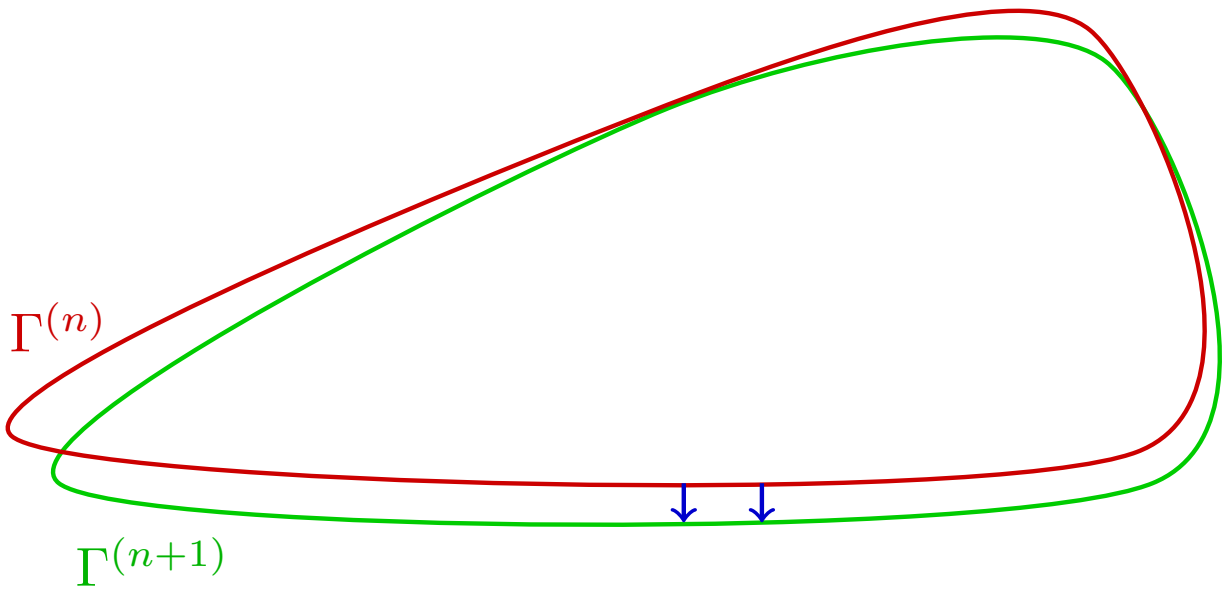
evolution of the domain

- shape derivative:

$$J'(\Omega)(\theta) = \int_\Gamma j(\cdot)\theta \cdot \boldsymbol{n} \, \mathrm{d}\boldsymbol{s}$$

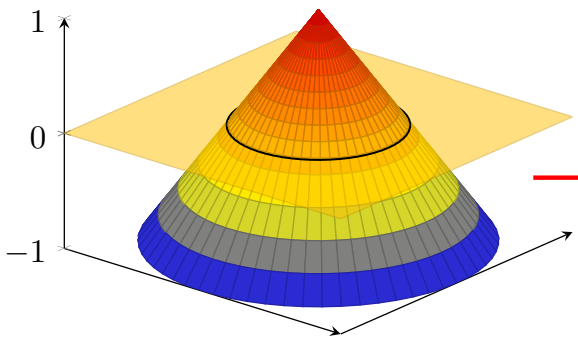
  that gives a direction of descent θ
- transport the domain towards θ with step size τ:

$$\Omega^{n+1} = (I_d + \tau\theta)(\Omega^n)$$

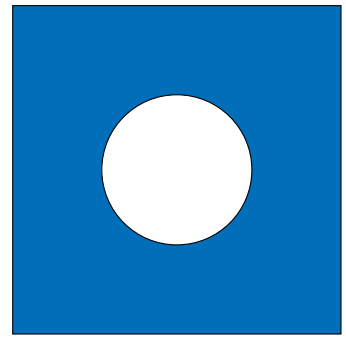


set-up the optimization problem

level-set : optimisation discrète $\Rightarrow$ optimisation continue



Fonction Level-Set



Géométrie Fluide/Solide

clear interface with:

$$\alpha(\Psi(\boldsymbol{x})) = \frac{1}{2}\left(1 + \mathrm{sign}\Psi(\boldsymbol{x})\right), \text{ such that } \alpha(\boldsymbol{x}) = \begin{cases} 0 & \text{if } \Psi(\boldsymbol{x}) < 0; \\ 1 & \text{if } \Psi(\boldsymbol{x}) > 0. \end{cases}$$

différentiable version:

$$\alpha_\epsilon(\Psi(\boldsymbol{x})) = \frac{1}{2} + \frac{1}{\pi}\arctan\frac{\Psi}{\epsilon}$$

Hamilton–Jacobi

The boundary

$$\Gamma(t) := \{\boldsymbol{x} \mid \Psi(t, \boldsymbol{x}) > 0\}$$

evolves in time with normal velocity $v(t, \boldsymbol{x})$. Then, differentiating

$$\Psi(t, \boldsymbol{x}(t)) = 0$$

gives

$$\frac{\partial \Psi}{\partial t} + vn \cdot \nabla \Psi = 0.$$

With $n = \nabla \Psi / |\nabla \Psi|$:

$$\frac{\partial \Psi}{\partial t} + v|\nabla \Psi| = 0.$$

[Allaire, JCP 2004 (194)]

méthode de gradient

Evolution of the discrete level-set function $\Psi(\boldsymbol{x}) \in \mathbb{R}^N$:

$$\Psi^{(n+1)}(\boldsymbol{x}) = \Psi^{(n)}(\boldsymbol{x}) - \mathsf{P}^{(n)} \nabla_\Psi \mathcal{J}^{+(n)}(\boldsymbol{x})$$

where P is the iteration matrix (ideally a good approximation of the inverse of the Hessian matrix, $\mathsf{P} \approx \widetilde{\mathsf{H}}^{-1}$), and $\nabla_\Psi \mathcal{J}^+$ is the augmented cost function gradient.

[Dugast, JCP 2018 (365)]

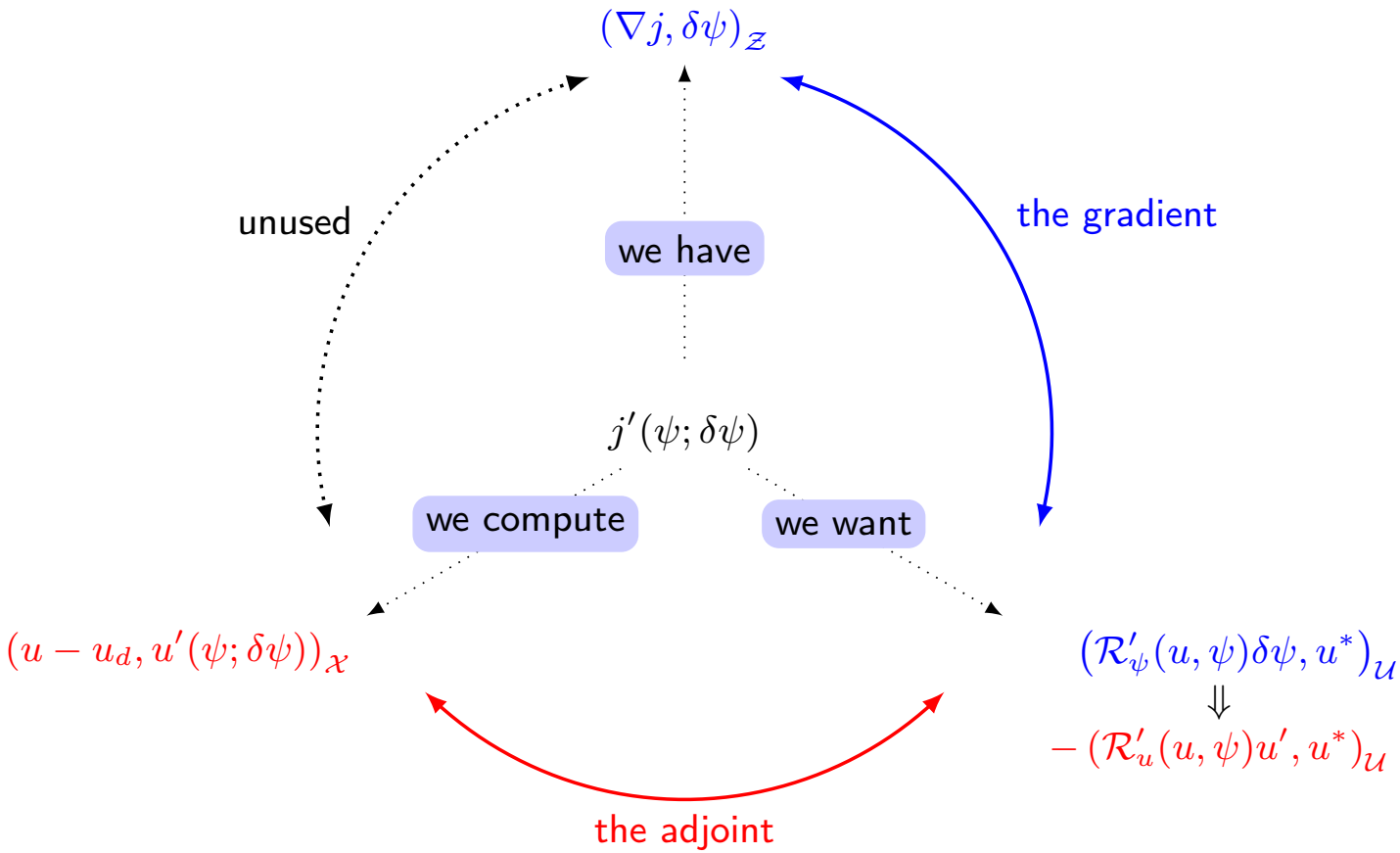
iii) adjoint-state method

main features

- only one "adjoint" system to access the full gradient
- theory of optimal control, 70's
- theory of optimization, 70's
- lots of ways for the method presentation

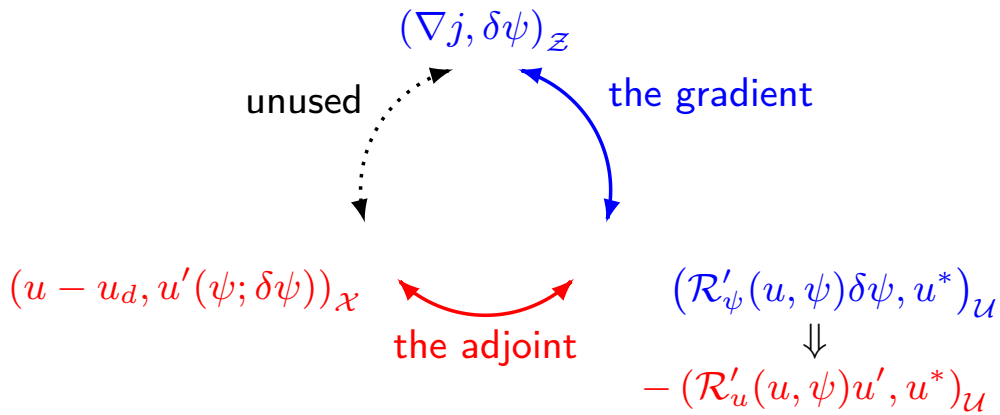
[Favennec, CNRS Metti school 2015]

iii) adjoint-state method



[Favennec, CNRS Metti school 2015]

iii) adjoint-state method



gradient

$$\begin{aligned}(\nabla j, \delta\psi)_{\mathcal{Z}} &= \left(\mathcal{R}'_\psi(u,\psi)\delta\psi, u^*\right)_{\mathcal{U}} \qquad \forall\psi \\ &= \left(\mathcal{R}^*_\psi(u,\psi)u^*, \delta\psi\right)_{\mathcal{U}} \qquad \forall\psi\end{aligned}$$

adjoint

$$\begin{aligned}(u - u_d, u'(\psi;\delta\psi))_{\mathcal{X}} &= -\left(\mathcal{R}'_u(u,\psi)u', u^*\right)_{\mathcal{U}} \qquad \forall u' \\ &= -\left(\mathcal{R}^*_u(u,\psi)u^*, u'\right)_{\mathcal{U}} \qquad \forall u'\end{aligned}$$

[Favennec, CNRS Metti school 2015]

states

- fw state:

$$\frac{\partial f_i}{\partial t} + \boldsymbol{c}_i \cdot \nabla f_i + \frac{1}{\tau}\left(f_i - f_i^{\mathrm{eq}}\right) = 0$$

- bw state:

$$-\frac{\partial f_i^*}{\partial t} - \boldsymbol{c}_i \cdot \nabla f_i^* + \frac{1}{\tau}\left(f_i^* - \sum_j \frac{\partial f_j^{\mathrm{eq}}}{\partial f_i} f_j^*\right) = 0$$

BC:: e.g. BB on south

- fw state:

$$\begin{cases} P_{\mathrm{bb}(1)} = P_2 = f_2 - f_4 \\ P_{\mathrm{bb}(2)} = P_5 = f_5 - f_7 \\ P_{\mathrm{bb}(3)} = P_6 = f_6 - f_8 \end{cases}$$

- bw state:

$$\begin{cases} P^*_{\mathrm{bb}(1)} = P^*_2 = f^*_2 - f^*_4 = 0 \\ P^*_{\mathrm{bb}(2)} = P^*_5 = f^*_5 - f^*_7 = 0 \\ P^*_{\mathrm{bb}(3)} = P^*_6 = f^*_6 - f^*_8 = 0 \end{cases}$$

algorithmic trick

- The adjoint-state eq. is written in reverse way both for time and advection.

- the forward solver can be re-used with:

$$t^* = t_f - t$$

and

$$\boldsymbol{c}_i^* = -\boldsymbol{c}_i$$

- Doing so, the adjoint-state is rewritten as:

$$\frac{\partial f_i^*}{\partial t^*} + \boldsymbol{c}_i^* \cdot \nabla f_i^* + \tau^{-1} f_i^* - \tau^{-1} \sum_j \frac{\partial f_j^{\mathbf{eq}}}{\partial f_i} f_j^* = 0$$

and the initial condition (at $t^* = 0$) is well defined, and boundary conditions are given for entrant directions $c_i^* \cdot \boldsymbol{n} < 0$, ie for $c_i \cdot \boldsymbol{n} > 0$.

gradient

The adjoint-states being computed, the cost function gradient is finally computed through

$$\nabla_{\Psi}\widehat{\mathcal{J}}^{+}\left(\boldsymbol{f},\boldsymbol{g},\boldsymbol{f}^{*},\boldsymbol{g}^{*}\right) =$$

$$-\alpha'(\Psi)\int_{0}^{t_f}\sum_{i=0}^{8}\omega_i f_i^{*}\left(\mathsf{M}^{-1}\mathsf{S}\mathsf{M}\left(3\,\boldsymbol{c}_j\cdot\boldsymbol{u}+\frac{9}{2}(\boldsymbol{c}_j\cdot\boldsymbol{u})^2-\frac{3}{2}\boldsymbol{u}^2\right)\right)_i \,\mathrm{d}t$$

$$-\alpha'(\Psi)\int_{0}^{t_f}\sum_{i=0}^{8}\frac{3\,\omega_i\,g_i^{*}\,c_A\,\boldsymbol{c}_i\cdot\boldsymbol{u}}{\tau_g}\,\mathrm{d}t.$$

NB: comes from differentiation of equilibrium distribution functions

Rem. on bias model/gradient

- expression of the gradient:

$$\nabla_{\Psi}\widehat{\mathcal{J}}^{+}(\cdot) = -{\alpha_{\epsilon}}'(\Psi)\int_{0}^{t_f}\sum_{i=0}^{8}\omega_i f_i^{*}\left(\mathsf{M}^{-1}\mathsf{S}\mathsf{M}\left(3\,\boldsymbol{c}_j\cdot\boldsymbol{u}+\ldots\right)\right)_i \;\mathrm{d}t\ldots$$

- actualization of the LS:

$$\Psi^{(n+1)}(\boldsymbol{x}) = \Psi^{(n)}(\boldsymbol{x}) - \mathsf{P}^{(n)}\nabla_{\Psi}\mathcal{J}^{+(n)}(\boldsymbol{x})$$

- choice for the iteration matrix:

$$\mathsf{P}^{(n)} = \frac{\delta}{{\alpha_{\epsilon}}'(\Psi)}\mathsf{I}$$

Algorithm 1: General topology optimization algorithm

Input: Level-set function $\Psi^{(0)}$;

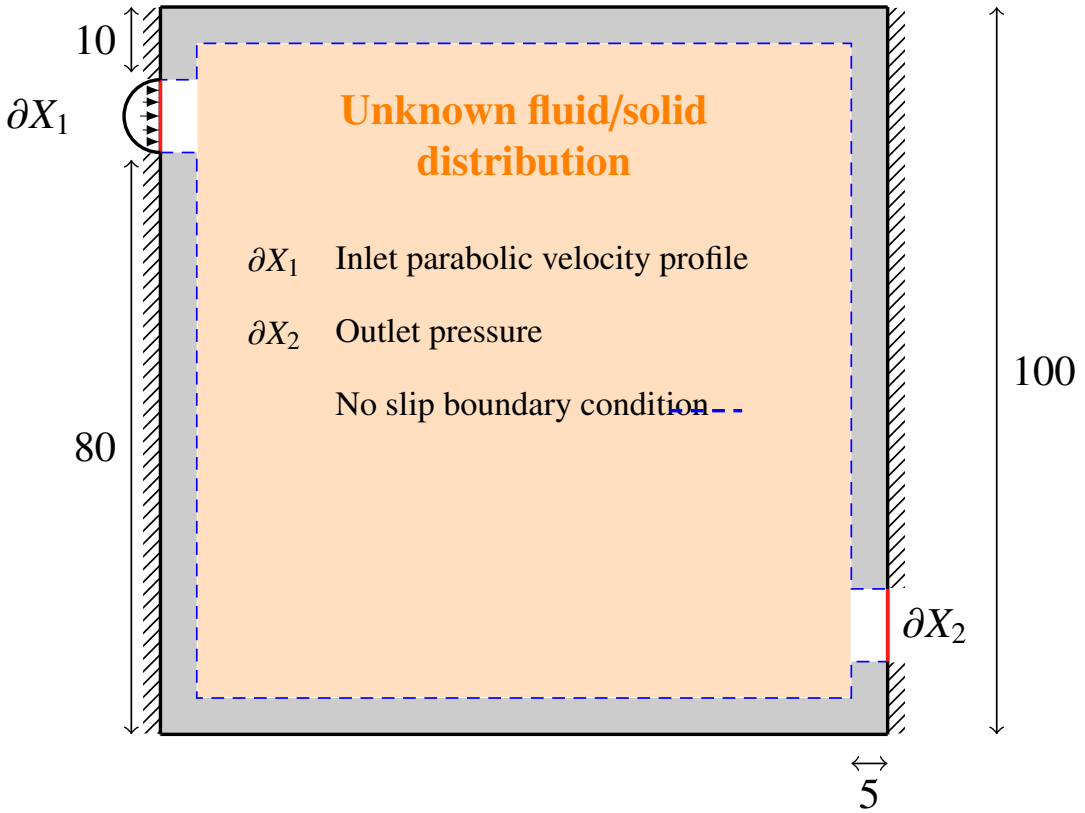
Topology $\mathcal{T}^{(0)}$ through $\alpha^{(0)}$ along with the smooth version ;

while *criterion not satisfied* **do**

- Compute the Boltzmann variables $\boldsymbol{f}$ and $\boldsymbol{g}$ solving the forward problem;
- Compute the cost function value $\widehat{\mathcal{J}}^{+}(\boldsymbol{f}, \boldsymbol{g})$;
- Compute the adjoint Boltzmann variables $\boldsymbol{f}^{*}$ and $\boldsymbol{g}^{*}$ solving the adjoint-state problem;
- Compute the cost function gradient $\nabla_{\Psi}\widehat{\mathcal{J}}^{+}$ from the simple inner product;
- Update of the geometry : actualization of the level-set function;

return *Optimal topology* $\mathcal{T}^{(*)}$;

problème d'optimisation



- Nombre de Reynolds : 10 à 1000
- Fluide : Pe=2000
- discrétisation: 200x200
- Terme réactif : r=10 et k=2.10-5
- réaction a lieu au sein de l'écoulement

Objectif : **max. de la réaction = min. du flux de C en sortie**

Contrainte : **limitation sur les pertes de charge :**

$$\Delta p_{max} = 2\Delta p_{ini}$$

problème couplé d'advection-diffusion-réaction

Champ de concentration C $\Leftrightarrow$ efficacité d'une réaction chimique

$$\nabla \cdot \mathbf{u} = 0,$$

$$(\mathbf{u} \cdot \nabla)\,\mathbf{u} + \frac{1}{\rho}\nabla p - \nu \nabla^2 \mathbf{u} = 0,$$

$$\mathbf{u} \cdot \nabla C - D\nabla^2 C + k\,(1 - \exp(-rC)) = 0.$$

$$\frac{\partial f_i}{\partial t} + \boldsymbol{c_i} \cdot \nabla f_i + M_{ij}^{-1} S_j M_{ij} (f_j - f_j^{eq}) = 0$$

$$\frac{\partial g_i}{\partial t} + \boldsymbol{c_i} \cdot \nabla g_i + \frac{1}{\tau_g}\,(g_i - g_i^{eq}) + S_i = 0$$

$$S_i = \omega_i k \left(1 - \exp(-r \sum_i g_i)\right)$$

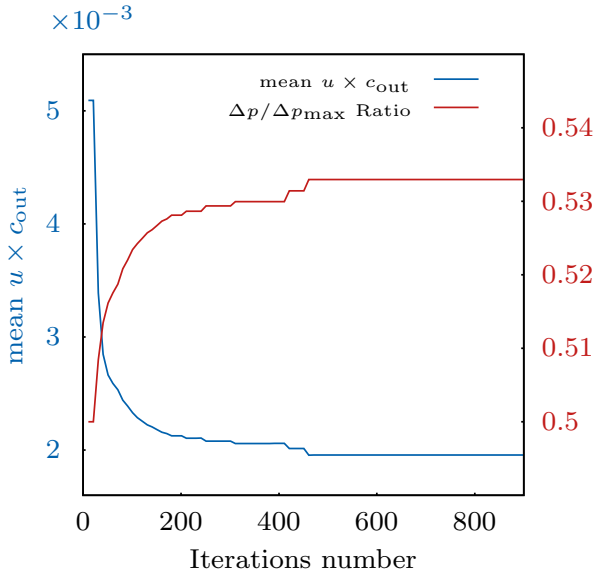
Re=20.mp4

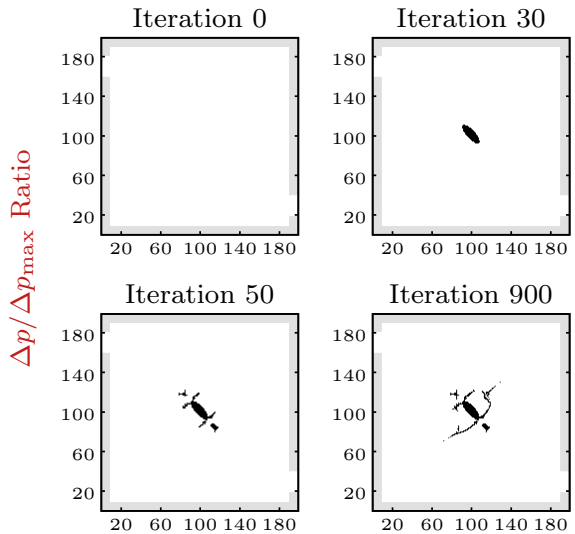
Re=1000.mp4

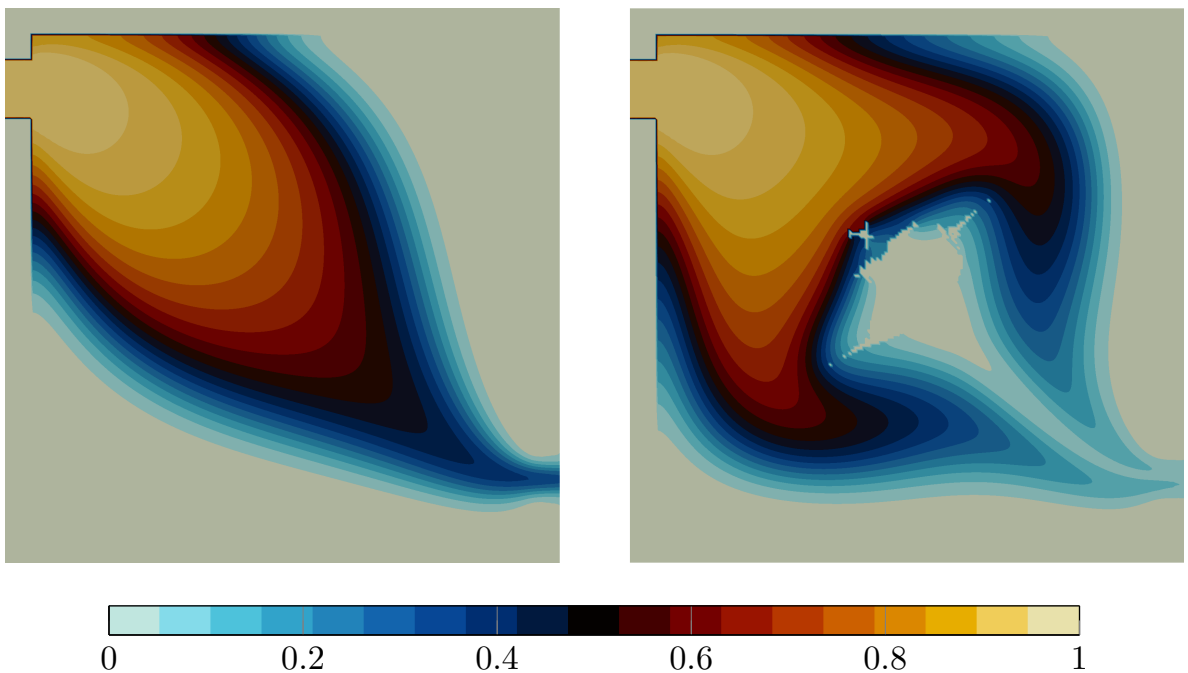
biblio résultats:

- Dugast et al. *Topology optimization of thermal fluid flows with an adjoint Lattice Boltzmann Method Journal of Computational Physics*,Vol 365, 2018
- Dugast et al. *Reactive fluid flow topology optimization with the multi-relaxation time lattice Boltzmann method and a level-set function* Journal of Computational Physics,Vol 429, 2020

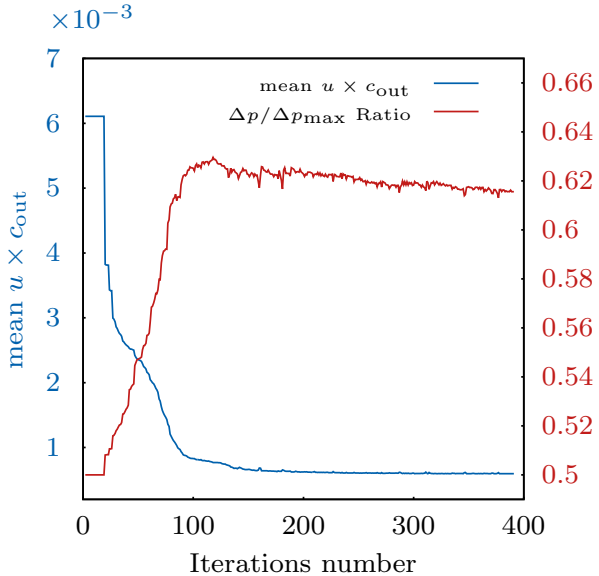
résultats Re=10 et Pe=2000

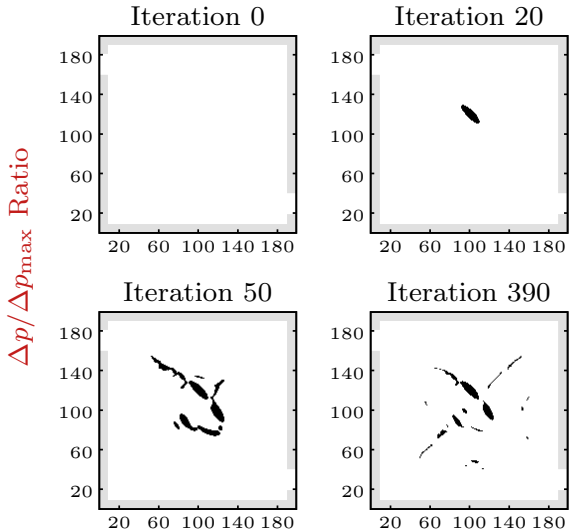


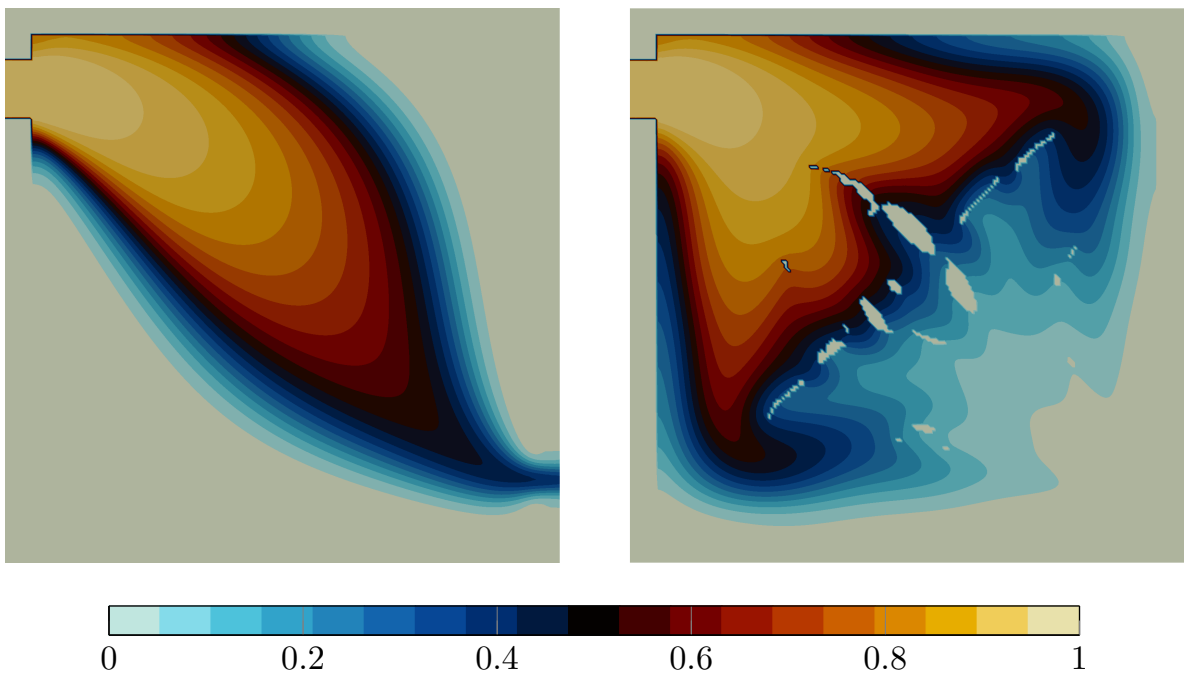




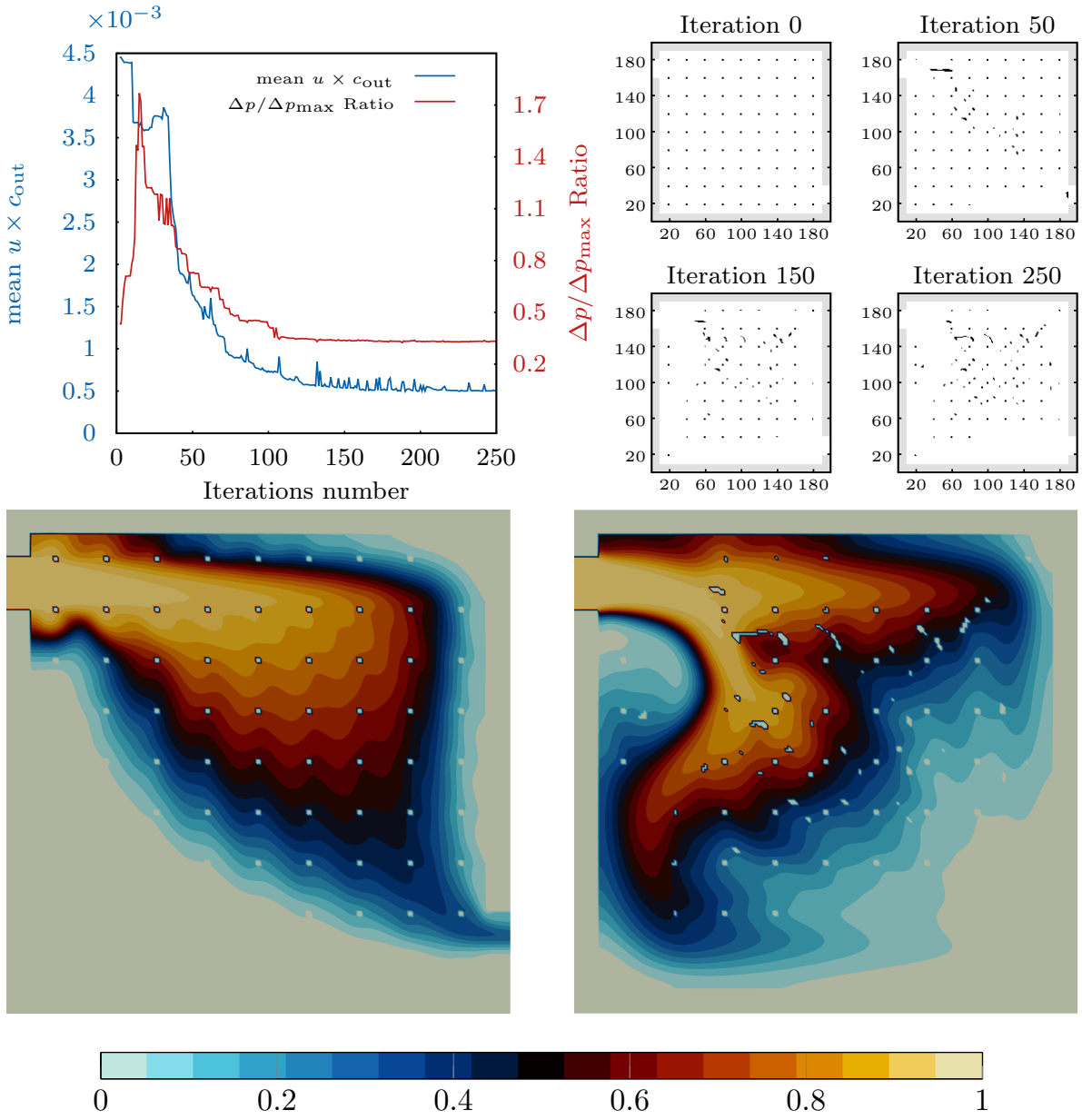
résultats Re=100 et Pe=2000







résultats Re=1000 et Pe=2000



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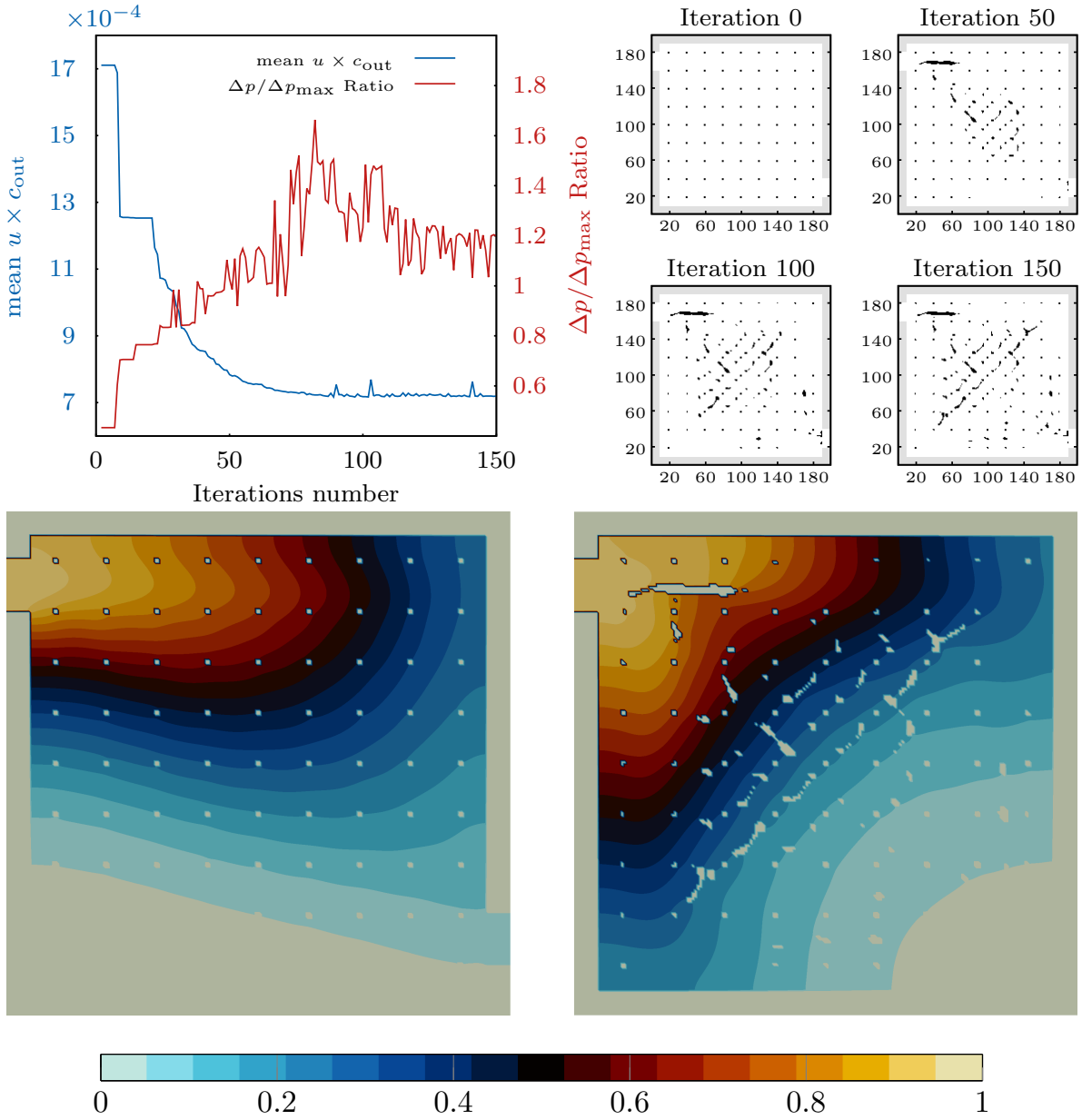
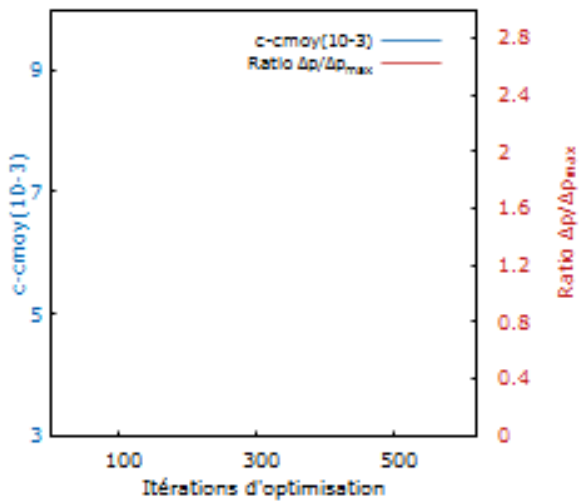
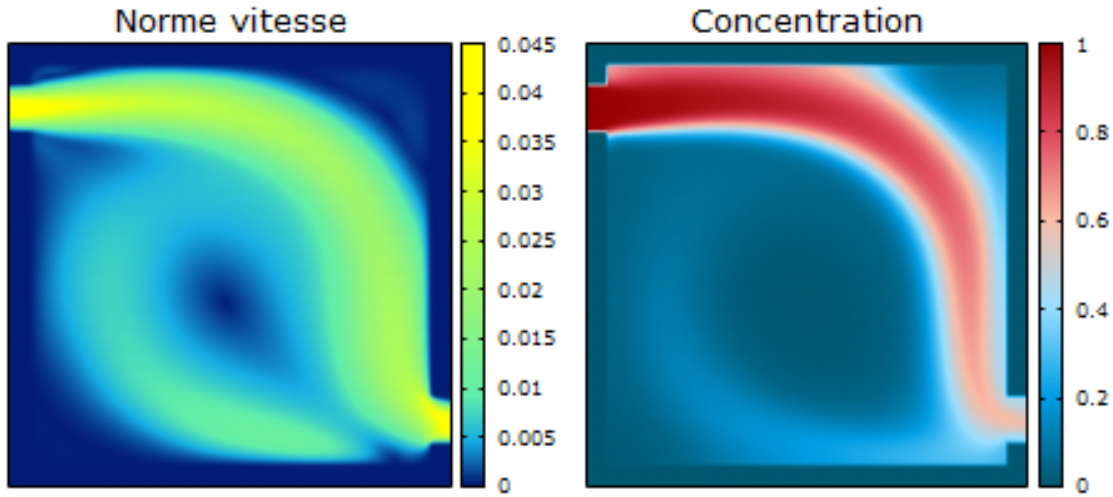
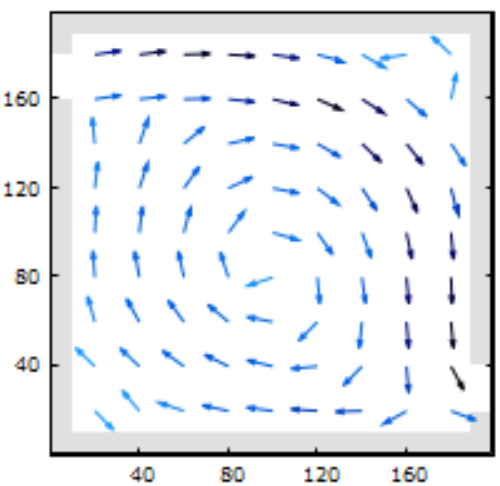


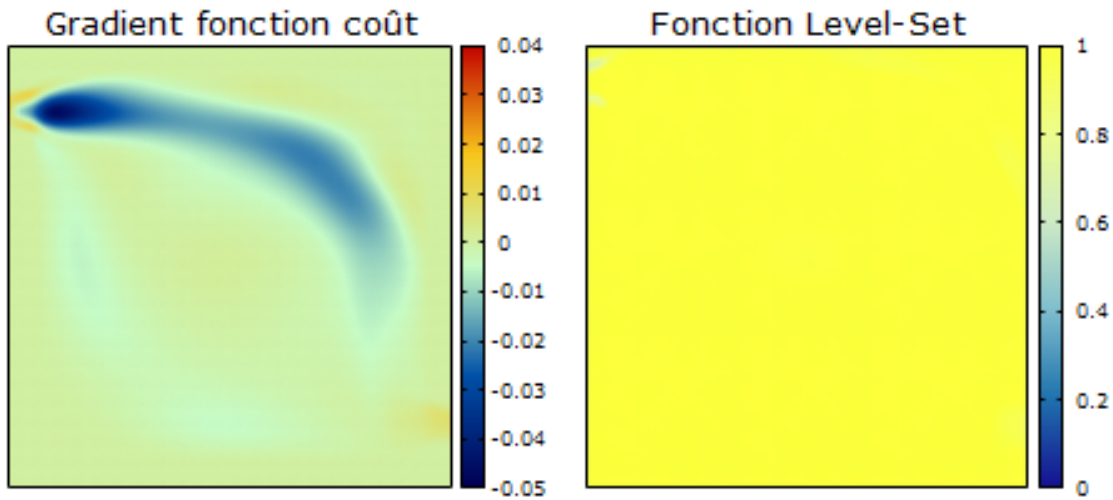
Homogénéisation de la concentration

Itération 0



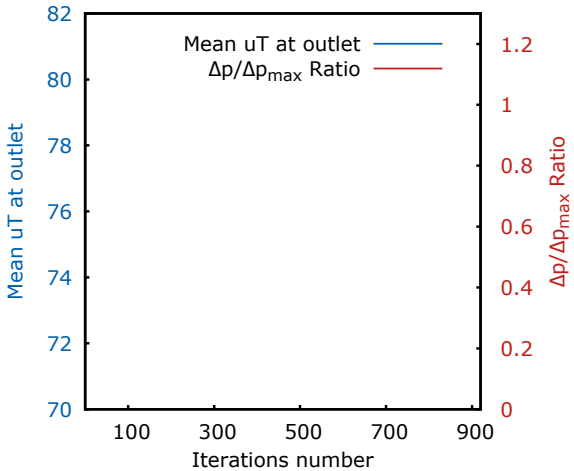


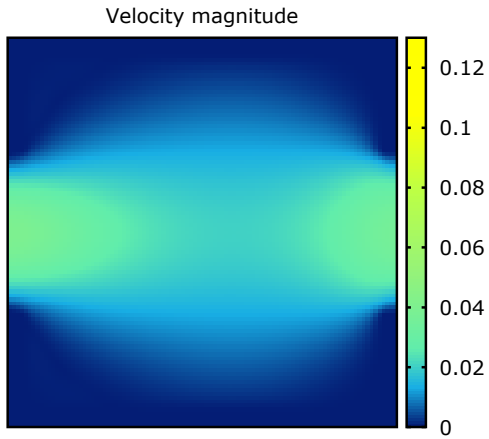


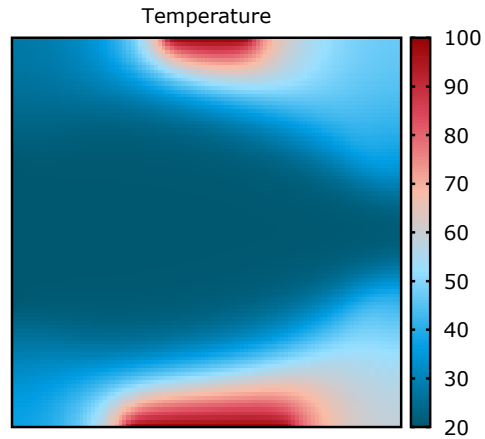


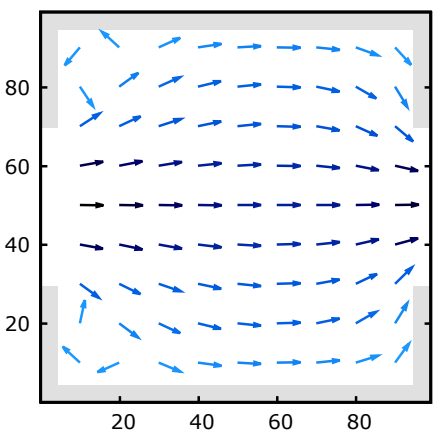
transferts thermiques convecto-conductif 2D

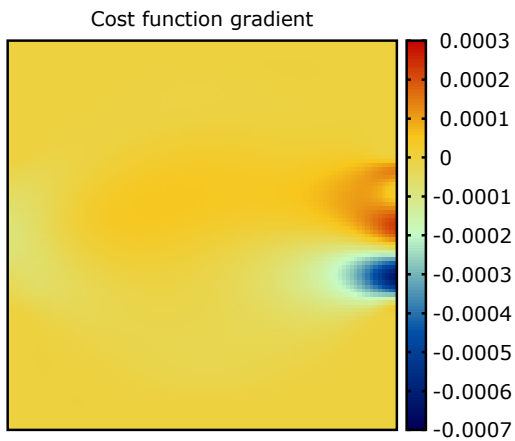
Iteration 0

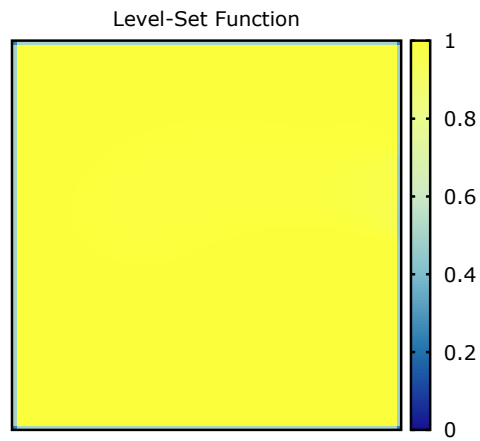












merci de votre attention...

...des questions ?