– Geometrical optimization of a reactor's core of gen IV using FreeFem++–

joint-work [1] between SINETICS department at EDF *R&D*, Clamart and CMAP, Ecole Polytechnique

1. PEPS agreement

Introduction
Goals of the internship

Aims and context

- Apply a shape optimization method to the conception of a nuclear reactor of generation IV having a reduced sodium void effect
- Implement the method with the finite element software FreeFem++
- Show to what extent the method could be applied in this context

Modeling of the reactor

Description of the core

- We assume the reactor can be simplified to a cylinder and that we have an axisymetric geometry $\Omega = [0, R] \times [0, h]$
- $\Omega = \cup_{i=1}^{4} \Omega_i$ is defined as the reunion of 4 regions having some averaged physical properties, each of them being characterized by a set of homogenized coefficients (D, Σ_a, Σ_f)
- The active core is composed by 3 different materials : we denote by Ω_f the fissile material
- The last region is the reflector surrounding the active core : absorbing region made of steel material

1-group energy diffusion model

State equation

- Using the notations : $\partial\Omega_D = \{(r,z) \in \partial\Omega;\ r \neq 0\}$, $\partial\Omega_N = \{(r,z) \in \partial\Omega;\ r = 0\}$ and u the neutrons flux
- We consider the simplified 1 group energy diffusion equation formulated on the space $X = \{\phi \in H^1(\Omega); \phi_{|\partial\Omega_D} = 0\}$ on a bounded domain $\Omega = \cup_i \Omega_i$:

$$\begin{cases} -D \triangle u + \Sigma_a u = \lambda \nu \Sigma_f u & in\ \Omega_i \\ \text{transmissions conditions} & on\ \partial\Omega_i \cap \partial\Omega_j \\ u = 0 & on\ \partial\Omega_D \cap \partial\Omega_i \\ \dfrac{\partial u}{\partial n} = 0 & on\ \partial\Omega_N \cap \partial\Omega_i \end{cases} \tag{1}$$

Remark : With this convention for λ, we have $\lambda = \frac{1}{k_{eff}}$

k_{eff} is a key parameter linked to the neutronic equilibrium of the core (generaly close to 1)

Variational form

The state equation represents an equilibrium between the reactions describing the behaviour of neutrons at steady states :

$$\underbrace{-D \triangle u}_{\text{leakage rate}} + \underbrace{\Sigma_a u}_{\text{absorption rate}} = \underbrace{\nu \Sigma_f u}_{\text{production rate}} \tag{2}$$

Variational form

We are looking for weak solutions of the variational form :
Find $u \in X$ such that :

$$\int_\Omega Dr\nabla u \cdot \nabla v + r\Sigma_a uv\, dx = \lambda \int_\Omega r\nu\Sigma_f uv\, dx \;\forall v \in X$$

In the following we write :

$$\begin{aligned} a(u,v) &= \int_\Omega Dr\nabla u \cdot \nabla v + r\Sigma_a uv\, dx \\ b(u,v) &= \int_\Omega r\nu\Sigma_f uv\, dx. \end{aligned} \tag{3}$$

Cost function

Estimation of the sodium void effect

We want to determine the first eigenvalue of this problem, which is simple, since this is the only to have a physical meaning (eigenvector keep the same sign over Ω)

- By considering two set of homogenized coefficients for this equation in a nominal state (with index "n") and a peturbated one (index "v"), we calculate the sodium void effect as $\delta\rho_{Na} = \lambda_n - \lambda_v$

Our cost function is :

$$J(\Omega_f) = \qquad + \qquad + \tag{4}$$

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The last term is not differentiable so we approximate it by the following quantity :

$$V(\Omega_f)^{1-\frac{1}{s}} \left(\int_{\Omega_f} r \Sigma_{fn} u_n \, drdz \right)^{-1} \left| \int_{\Omega_f} r (\Sigma_{fn} u_n)^s \, drdz \right|^{1/s} \tag{5}$$

What the algorithm does

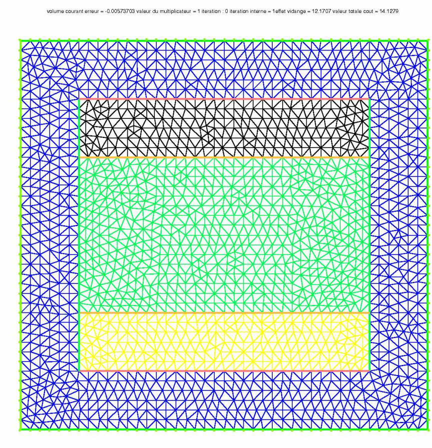

Figure: Initial shape

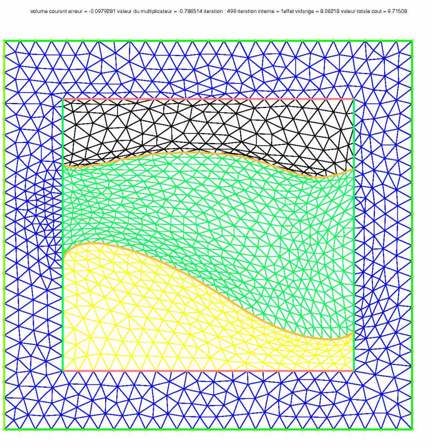

Figure: Shape after 500 iterations

Admissible shape transformation of the bounded set Ω

- We move the shape during a time t with a lipschitzian velocity field satisfying $\|t\theta_n\|_\infty \leq 1$ moving the points with the following equation :

$$x \to x + t\ \theta_n(x)$$

Thus, we have $\Omega_{n+1} = (I_d + t\ \theta_n)(\Omega_n)$

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- We impose $\theta \cdot n = 0$ on $\partial\Omega$ and on the external boundary of the active core
- The volume constraint expresses as $vol(T(\Omega_f)) = vol(\Omega_f)$

$T = Id + t\ \theta$

Gradient method

- The optimization variable is the velocity field θ_n
- We characterize the optimal shape by first order optimality conditions
- We define the shape derivative in Ω of the function $J(\Omega)$ as the derivative at the point 0 of the application :

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- That is also the linear form on $W^{1,\infty}(\Omega_f, \mathbb{R}^2)$ such that :

$$J((Id + t\ \theta)(\Omega_f)) = J(\Omega_f) + \langle J'(\Omega_f), \theta \rangle + \circ(\theta) \qquad (6)$$

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$$\forall \theta \ \in \ H^1(\Omega_f, \mathbb{R}^2) : J'(\Omega_f)(\theta) + \langle \theta_n, \theta \rangle = 0 \tag{7}$$

for the scalar product on $X \times X$, it gives $J'(\Omega_f)(\theta_n) = -\|\theta_n\|^2$

Lagrangian associated to the minimization problem

- J does not depend explicitly on the shape Ω
- Use of the adjoint method
- We introduce the Lagrangian $\mathcal{L}$ that transforms the initial problem into a new one without constraints on the variables :

$$\mathcal{L}(\Omega, \hat{u}_n, \hat{u}_v, \hat{p}_n, \hat{p}_v, \hat{\lambda}_n, \hat{\lambda}_v) = \underbrace{\hat{\lambda}_n - \hat{\lambda}_v}_{\text{sodium void effect}} + \underbrace{(\hat{\lambda}_n - \lambda_0)^2}_{\text{target reactivity}}$$

$$+ \underbrace{vol(\Omega_f)^{1-\frac{1}{s}} \frac{\left(\int_{\Omega_f} r \, (\Sigma_{fn}\hat{u}_n)^s \, drdz\right)^{\frac{1}{s}}}{\int_{\Omega_f} r \, \Sigma_{fn}\hat{u}_n \, drdz}}_{\text{shape factor}}$$

$$+ \underbrace{\sum_{k=n,v} a_k(\Omega, \hat{u}_k, \hat{p}_k) - \hat{\lambda}_k b_k(\Omega, \hat{u}_k, \hat{p}_k)}_{\text{states equations}}$$

Adjoint method

- Let (u_k, λ_k) be the solution of the state equation in the state k
- We have the relation :

$$J(\Omega) = \mathcal{L}(\Omega, u_n, u_v, \lambda_n, \lambda_v, p, q) \ \forall \ (p, q) \ \in X^2 \tag{8}$$

- By composed derivation, we get :

$$\langle \frac{\partial J}{\partial \Omega}, \theta \rangle \ = \ \sum_k (\langle \frac{\partial \mathcal{L}}{\partial \hat{p}_k}, \hat{p}'_k(\theta) \rangle + \langle \frac{\partial \mathcal{L}}{\partial \hat{u}_k}, \hat{u}'_k(\theta) \rangle + \langle \frac{\partial \mathcal{L}}{\partial \hat{\lambda}_k}, \hat{\lambda}'_k(\theta) \rangle) + \langle \frac{\partial \mathcal{L}}{\partial \Omega}, \theta \rangle$$

- The adjoint state is defined in the following manner :

$$\begin{cases} \dfrac{\partial \mathcal{L}}{\partial \hat{\lambda}_k}(u_k, p_k, \lambda_k) = 0 \\ \langle \dfrac{\partial \mathcal{L}}{\partial \hat{u}_k}, \phi \rangle (u_k, p_k, \lambda_k) = 0 \ \forall \ \phi \ \in X \end{cases} \iff p_k := \text{adjoint state of } \ u_k \tag{9}$$

Finally, we obtain :

$$\langle \frac{\partial J}{\partial \Omega}, \theta \rangle = \langle \frac{\partial \mathcal{L}}{\partial \Omega}, \theta \rangle \tag{10}$$

The two studied configurations

$$J(\Omega, e) = \alpha_1 \ J_1 + \alpha_2 \ J_2 + \alpha_3 \ J_3 \tag{11}$$

- We consider two cases : one with the same weights for the parametric and geometric optimization, another one with distinct weights taking into account the physical dependency of each criterium J_i to e and Ω
- With an admissible error on the volume of 10% and an initial value of $e_{Pu} = 20\%$ on Ω_f
- Thanks to a program given by O. PANTZ we apply a change of topology of the mesh when needed.

We look at the following quantities to asses the convergence :
For e : $\|e^n - e^{n-1}\| = \int_{\Omega_f} r(e^n(r,z) - e^{n-1}(r,z))^2 drdz$
For Ω : $\frac{J'(\Omega_n)(\theta_n)}{J'(\Omega_0)(\theta_0)}$

The behaviour of our algorithm in images

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After a first step (1)

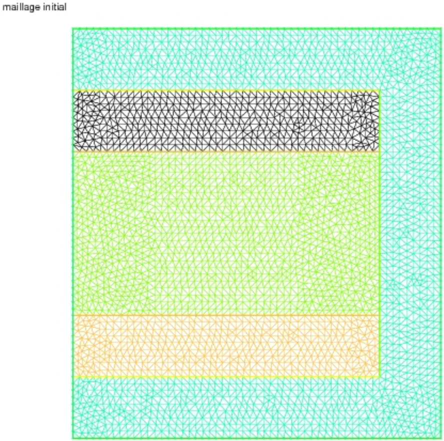


Figure: Initial condition

After a first step (2)

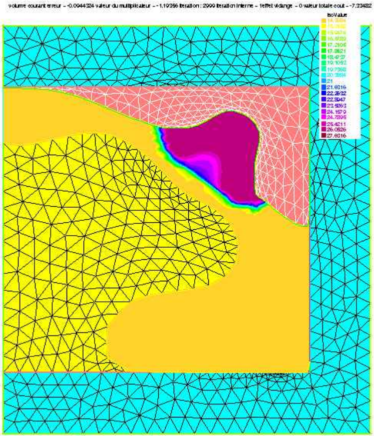


Figure: Case 1 : $\delta\rho_{Na} = -29,06pcm$

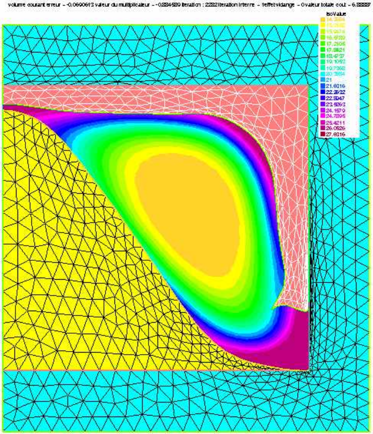


Figure: Case 2 : $\delta\rho_{Na} = 5,88pcm$

Cost function

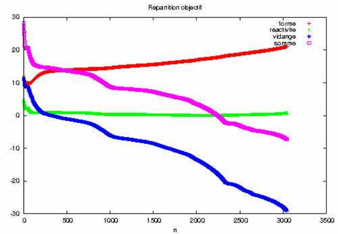


Figure: $J = \alpha_i \ J_i$

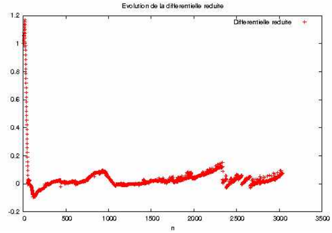
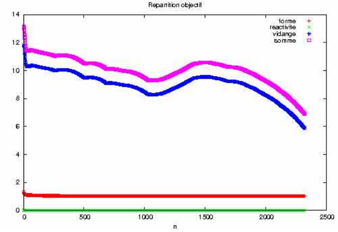
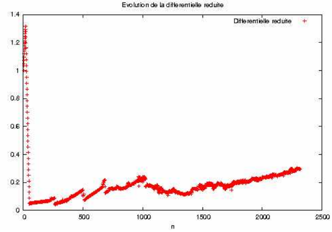
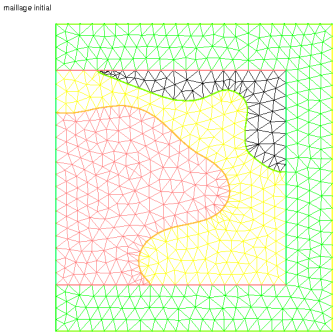


Figure: $\dfrac{J'(\Omega_n)(\theta_n)}{J'(\Omega_0)(\theta_0)}$





After having changed the topology



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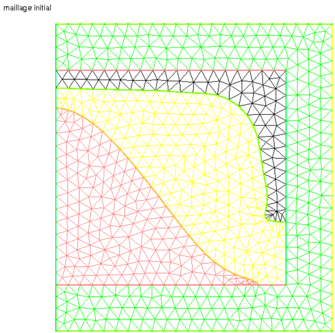


Figure: Case 2

After a second step (1)

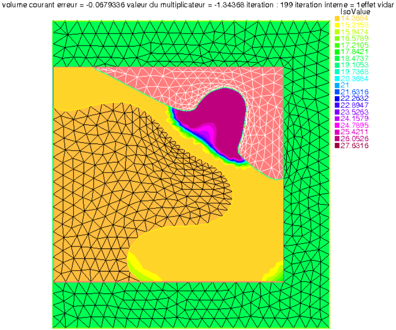


Figure: Case 1 : $\delta\rho_{Na} = -35pcm$

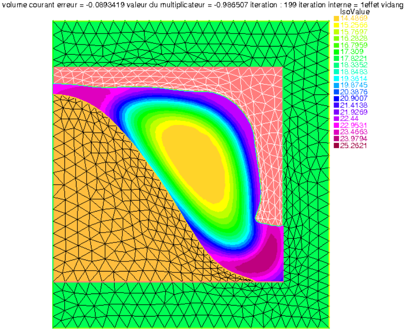
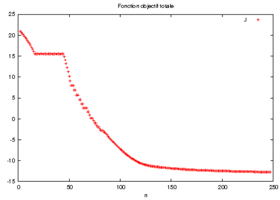


Figure: Case 2 : $\delta\rho_{Na} = 4pcm$

Convergence indexes



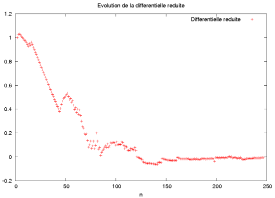
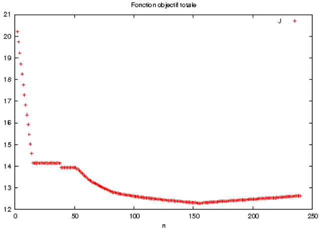
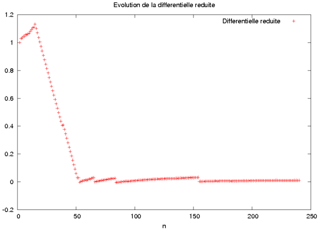


Figure: $J = \alpha_i \ J_i$

Figure: $\dfrac{J'(\Omega_n)(\theta_n)}{J'(\Omega_0)(\theta_0)}$





Conclusion and perspectives

- Simulation must still be done with the 2 groups energy diffusion model
- Initialize with different shape to check the robustness of the algorithm
- Generalize the remeshing with Level-Set to much more complex situations
- Apply a penalization step to obtain feasible design

Thank you for your attention