Model order reduction for complex ocular simulations inside the human eyeball

Séminaire Jeunes Chercheurs de Reims

Thomas Saigre[1], Christophe Prud'homme[1], Marcela Szopos[2]

[1]Institut de Recherche Mathématique Avancée, UMR 7501 Université de Strasbourg et CNRS
[2]Université Paris Cité, CNRS, MAP5, F-75006 Paris, France

1st December 2022

Introduction

Eye2brain project: develop a reliable and efficient mathematical and computational framework to simulate and predict the functioning and the connection between the eye and the brain

Introduction

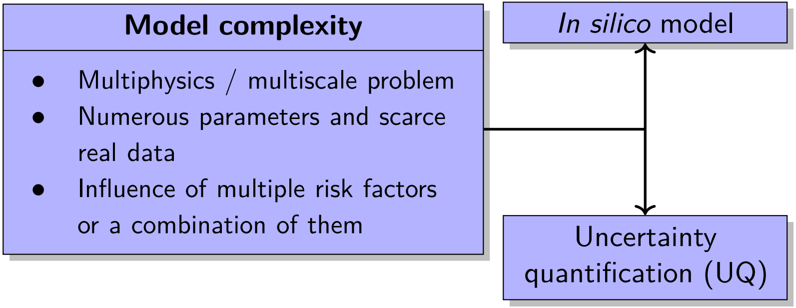
Eye2brain project: develop a reliable and efficient mathematical and computational framework to simulate and predict the functioning and the connection between the eye and the brain

Model complexity

- Multiphysics / multiscale problem
- Numerous parameters and scarce real data
- Influence of multiple risk factors or a combination of them

Introduction

Eye2brain project: develop a reliable and efficient mathematical and computational framework to simulate and predict the functioning and the connection between the eye and the brain



Introduction

Eye2brain project: develop a reliable and efficient mathematical and computational framework to simulate and predict the functioning and the connection between the eye and the brain

Model complexity

- Multiphysics / multiscale problem
- Numerous parameters and scarce real data
- Influence of multiple risk factors or a combination of them

In silico model

Prohibitive cost in 3D

Uncertainty quantification (UQ)

Introduction

Eye2brain project: develop a reliable and efficient mathematical and computational framework to simulate and predict the functioning and the connection between the eye and the brain

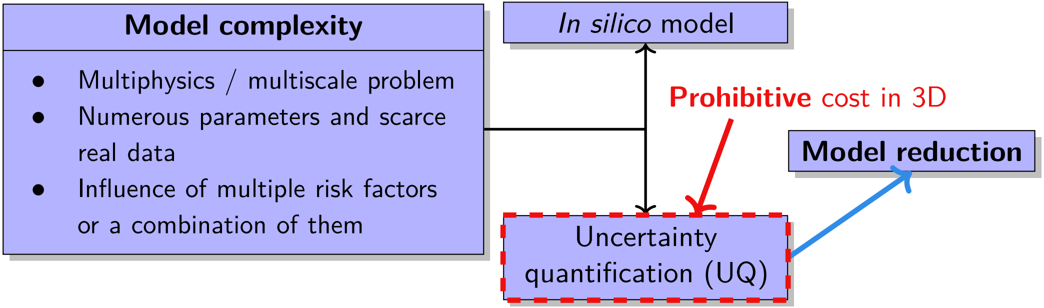
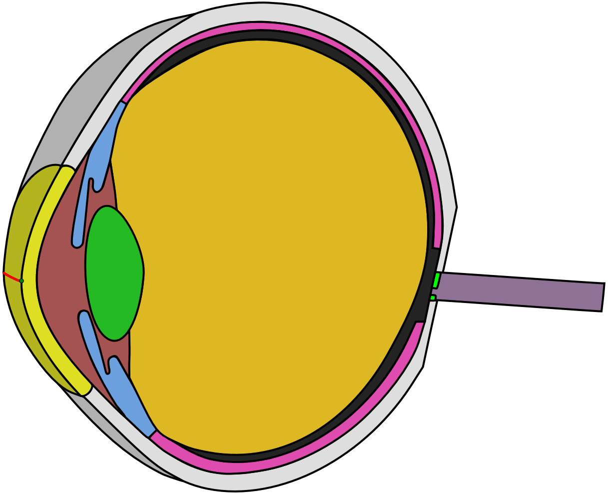


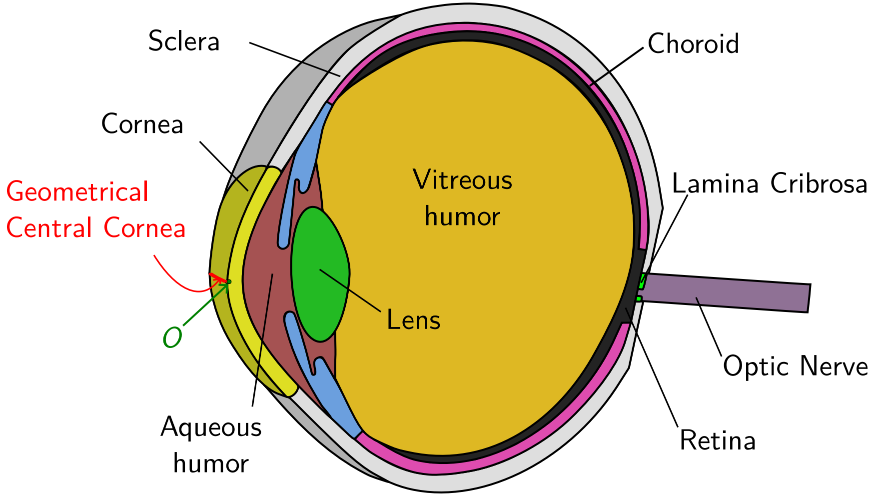
Table of contents

Model

Geometrical model



Geometrical model



Physical model[1]

$$\rho_i C_{p,i} \frac{\partial T_i}{\partial t} + \nabla \cdot (k_i \nabla T_i) = 0 \qquad \text{over } \Omega_i \tag{2.1}$$

where :

- i is the volume index (Cornea, VitreousHumor...),
- T_i [K] is the temperature in the volume i,
- t [s] is the time,
- k_i [$\mathrm{W\,m^{-1}}K^{-1}$] is the thermal conductivity, ρ_i [$\mathrm{kg\,m^{-3}}$] is the density and $C_{p,i}$ [$\mathrm{J\,kg^{-1}}K^{-1}$] is the specific heat.

[1] J.A. Scott. “A finite element model of heat transport in the human eye”. In: *Physics in Medicine and Biology* 33.2 (1988), pp. 227–242; Ng, E.Y.K. and Ooi, E.H. “FEM simulation of the eye structure with bioheat analysis”. In: *Computer Methods and Programs in Biomedicine* 82.3 (2006), pp. 268–276.

Physical model : Boundary conditions

- Robin condition :

$$-k\frac{\partial T}{\partial \underline{n}} = h_{\mathrm{bl}}(T - T_{\mathrm{bl}}) \tag{2.2}$$

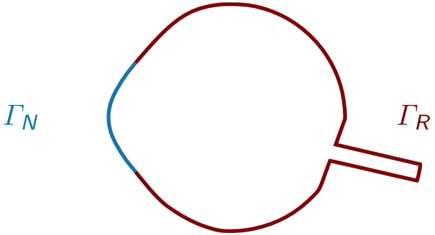


Figure 1: Desciption of the boundary conditions of the domain

Physical model : Boundary conditions

- Neumann conditions :

$$-k_i \frac{\partial T_i}{\partial \underline{n}} = h_{\mathrm{amb}}(T_i - T_{\mathrm{amb}}) + \sigma\varepsilon(T_i^4 - T_{\mathrm{amb}}^4) + E \tag{2.2}$$

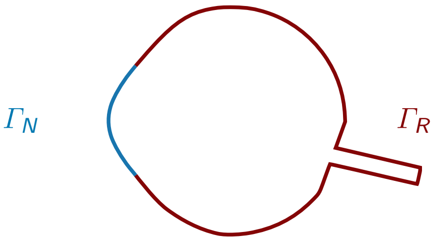


Figure 1: Desciption of the boundary conditions of the domain

Physical model : Boundary conditions

$$-k_i \frac{\partial T_i}{\partial \underline{n}} = h_{\text{amb}}(T_i - T_{\text{amb}}) + \sigma\varepsilon(T_i^4 - T_{\text{amb}}^4) + E \tag{2.3}$$

[2] J.A. Scott. "A finite element model of heat transport in the human eye". In: *Physics in Medicine and Biology* 33.2 (1988), pp. 227–242.

Physical model : Boundary conditions

$$-k_i \frac{\partial T_i}{\partial \underline{n}} = h_{\text{amb}}(T_i - T_{\text{amb}}) + h_r(T_i - T_{\text{amb}}) + E \tag{2.3}$$

with $h_r = 6\ \mathrm{W\,m^{-2}} K^{-1}$, from[2]

[2] J.A. Scott. "A finite element model of heat transport in the human eye". In: *Physics in Medicine and Biology* 33.2 (1988), pp. 227–242.

Physical model : interface conditions

$$\left\{\begin{array}{rcl} T_i & = & T_j \\ k_i(\nabla T_i \cdot \underline{n}_i) & = & -k_j(\nabla T_j \cdot \underline{n}_j) \end{array}\right. \text{ over } \partial\Omega_i \cap \partial\Omega_j \tag{2.4}$$

Parameter-dependant model

Symbol	Name	Dimension	baseline value
T_{amb}	Ambiant temperature	[K]	298
T_{bl}	Blood temperature	[K]	310
h_{amb}	Ambiant air convection coefficient	$[\mathrm{W\,m^{-2}}K^{-1}]$	10
h_{bl}	Blood convection coefficient	$[\mathrm{W\,m^{-2}}K^{-1}]$	65
E	Evaporation rate	$[\mathrm{W\,m^{-2}}]$	40
k_{lens}	Lens conductivity	$[\mathrm{W\,m^{-1}}K^{-1}]$	0.4

Table 1: Parameters involved in the model

Methodologies

Variationnal formulation

$$\sum_i k_i \int_{\Omega_i} \nabla T_i \cdot \nabla v + \int_{\Gamma_N} \left[h_{\text{amb}}(T - T_{\text{amb}}) + h_r(T - T_{\text{amb}}) + E\right] v + \int_{\Gamma_R} \left[h_{\text{bl}}(T - T_{\text{bl}})\right] v = 0$$

Variationnal formulation

$$\sum_i k_i \int_{\Omega_i} \nabla T_i \cdot \nabla v + \int_{\Gamma_N} \left[h_{\text{amb}}(T - T_{\text{amb}}) + h_r(T - T_{\text{amb}}) + E \right] v + \int_{\Gamma_R} \left[h_{\text{bl}}(T - T_{\text{bl}}) \right] v = 0$$

$$\sum_i k_i \int_{\Omega_i} \nabla T_i \cdot \nabla v + \int_{\Gamma_N} \left[h_{\text{amb}} T + h_r T \right] v + \int_{\Gamma_R} h_{\text{bl}} T v = \int_{\Gamma_N} \left[h_{\text{amb}} T_{\text{amb}} + h_r T_{\text{amb}} + E \right] v + \int_{\Gamma_R} h_{\text{bl}} T_{\text{bl}} v$$

Variationnal formulation

$$\sum_i k_i \int_{\Omega_i} \nabla T_i \cdot \nabla v + \int_{\Gamma_N} [h_{\text{amb}}(T - T_{\text{amb}}) + h_r(T - T_{\text{amb}}) + E]\, v + \int_{\Gamma_R} [h_{\text{bl}}(T - T_{\text{bl}})]\, v = 0$$

$$\sum_i k_i \int_{\Omega_i} \nabla T_i \cdot \nabla v + \int_{\Gamma_N} [h_{\text{amb}} T + h_r T]\, v + \int_{\Gamma_R} h_{\text{bl}} T v = \int_{\Gamma_N} [h_{\text{amb}} T_{\text{amb}} + h_r T_{\text{amb}} + E]\, v + \int_{\Gamma_R} h_{\text{bl}} T_{\text{bl}} v$$

$$a(T, v; \mu) = f(T; \mu)$$

where $\mu \in D^\mu \subset \mathbb{R}^d$.

Variationnal formulation

Lax Milgram thoerem.

Let V be a Hilbert space and a a bilinear form on $V \times V$ which is

- contiunous : $\forall u, v \in V, |a(u,v)| \leqslant C\|u\|_V\|v\|_V$,
- coercive : $\forall u \in V, a(u,u) \geqslant \alpha\|u\|_V^2$,

Let f be a continuous linear form on V.
There exist a unique $u \in X$ such that

$$a(u,v) = f(v) \text{ for all } v \in V$$

Variationnal formulation

Lax Milgram thoerem.

Let V be a Hilbert space and a a bilinear form on $V \times V$ which is

- contiunous : $\forall u, v \in V, |a(u,v)| \leqslant C\|u\|_V\|v\|_V$,
- coercive : $\forall u \in V, a(u,u) \geqslant \alpha\|u\|_V^2$,

Let f be a continuous linear form on V.
There exist a unique $u \in X$ such that

$$a(u,v) = f(v) \text{ for all } v \in V$$

Definition

The solution u of the variational problem is called *weak solution*.

Variationnal formulation

Lax Milgram thoerem.

Let V be a Hilbert space and a a bilinear form on $V \times V$ which is

- contiunous : $\forall u, v \in V, |a(u, v)| \leqslant C\|u\|_V\|v\|_V$,
- coercive : $\forall u \in V, a(u, u) \geqslant \alpha\|u\|_V^2$,

Let f be a continuous linear form on V.
There exist a unique $u \in X$ such that

$$a(u, v) = f(v) \text{ for all } v \in V$$

Definition

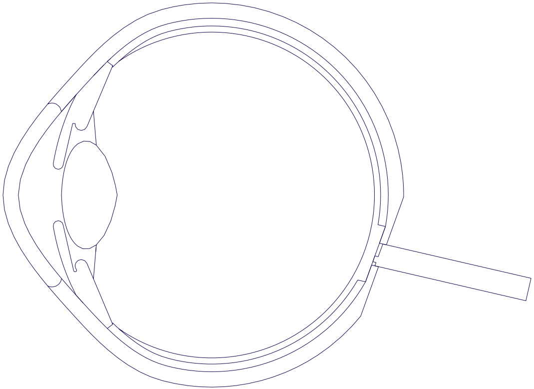
The solution u of the variational problem is called *weak solution*.

Using an argument of density, we show that u is a solution of the original PDE problem, almost everywhere.

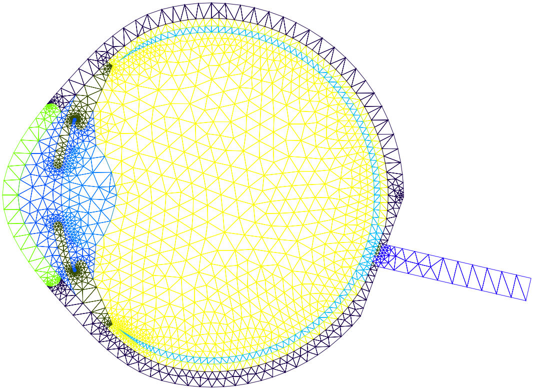
Ritz-Galerkine method

$$a(u, v) = f(v) \text{ for all } v \in X \Leftrightarrow AU = F \tag{3.1}$$

Finite element method

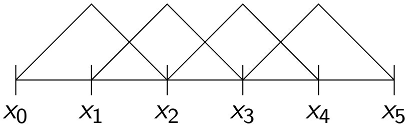


Finite element method



Finite element method

The space V_h is the space of piecewise linear functions on the mesh.



« We » can construct the basis associated to the space V_h, and therefore the matrices A and F, from the problem.

Model Order Reduction

Example of execution of the 3D model :

	$\mathbb{P}_1$	$\mathbb{P}_2$
$\mathcal{N}$	207 845	1 580 932
t_{exec}	21.221s	123.92s

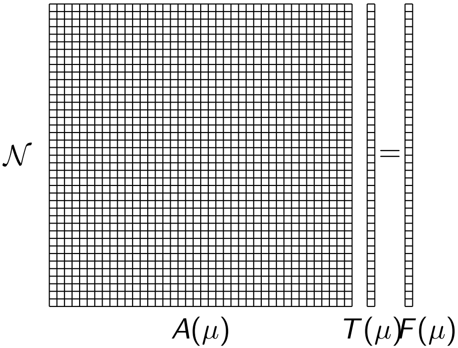
Model Order Reduction : Reduced basis

For $\mu \in D^{\mu}$, we want to solve $\nabla \cdot (k_i \nabla T(\mu)) = 0$ (+BC).
We introduce an *output* quantity : $s(\mu) = \ell(T(\mu); \mu)$

Variational formulation : Find $T(\mu)$ such that $a(T(\mu), v; \mu) = f(T(\mu); \mu), \forall v \in H$.

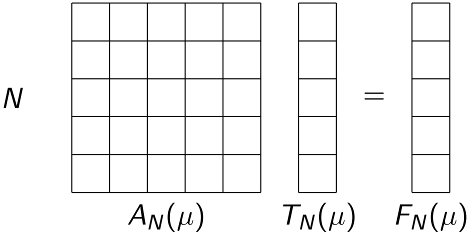
Model Order Reduction : Reduced basis

Variational formulation : Find $T(\mu)$ such that $a(T(\mu), v; \mu) = f(T(\mu); \mu), \forall v \in H$.
Problem to solve : $A(\mu)T(\mu) = F(\mu)$, the output is $s_N(\mu) = L(\mu)^T T(\mu)$



Model Order Reduction : Reduced basis

Variational formulation : Find $T(\mu)$ such that $a(T(\mu), v; \mu) = f(T(\mu); \mu), \forall v \in H$.
Reduced problem : $A_N(\mu) T_N(\mu) = F_N(\mu)$, with $\mathcal{N} \gg N$, the output is $s_N(\mu) = L_N(\mu)^T T_N(\mu)$



Reduced basis

To generate the basis, we take snapshots for different values of μ : $\mu_1, \cdots, \mu_N$, and define the matrix

$$\mathbb{Z}_N = [\xi_1, \cdots, \xi_N] \in \mathbb{R}^{\mathcal{N},N} \tag{3.2}$$

where ξ_i is the solution of $A(\mu_i)\xi_i = F(\mu_i)$. $\mathbb{Z}_N$ is orthonormalized.

Reduced basis

To generate the basis, we take snapshots for different values of μ : $\mu_1, \cdots, \mu_N$, and define the matrix

$$\mathbb{Z}_N = [\xi_1, \cdots, \xi_N] \in \mathbb{R}^{\mathcal{N},N} \tag{3.2}$$

where ξ_i is the solution of $A(\mu_i)\xi_i = F(\mu_i)$. $\mathbb{Z}_N$ is orthonormalized.

Then, $u(\mu) \approx \sum_{i=1}^{N} u_{N,i}(\mu)\xi_i = \mathbb{Z}_N u_N$, so the reduced problem is

$$\underbrace{\mathbb{Z}_N^T A(\mu)\mathbb{Z}_N}_{:=A_N(\mu)\in\mathbb{R}^{N\times N}} u_N(\mu) = \underbrace{\mathbb{Z}_N^T(\mu)F(\mu)}_{:=F_N(\mu)\in\mathbb{R}^N} \tag{3.3}$$

$$s_N(\mu) = \underbrace{L^T(\mu)\mathbb{Z}_N}_{:=L_N^T(\mu)\in\mathbb{R}^N} u_N(\mu) \tag{3.4}$$

Affine decomposition

Issue : compute efficiently $A_N(\mu) = \mathbb{Z}_N^T A(\mu) \mathbb{Z}_N$.

Solution : decompose $A(\mu) \approx \sum_{q=1}^{Q_A} \beta_A^q(\mu) A^q$, with A^q *independant* of μ

Affine decomposition

Issue : compute efficiently $A_N(\mu) = \mathbb{Z}_N^T A(\mu) \mathbb{Z}_N$.

Solution : decompose $A(\mu) \approx \sum_{q=1}^{Q_A} \beta_A^q(\mu) A^q$, with A^q *independant* of μ

$$A_N(\mu) = \mathbb{Z}_N^T A(\mu) \mathbb{Z}_N = \sum_{q=1}^{Q_A} \beta_A^q(\mu) \underbrace{\mathbb{Z}_N^T A^q \mathbb{Z}_N}_{:= A_N^q} \tag{3.5}$$

Terms that can be computed only once (*offline stage*)

Idem for $F(\mu) = \sum_{p=1}^{Q_f} \beta_F^q(\mu) F^p$

Affine decomposition

$$a(T, v; \mu) = \sum_{q=1}^{3} \beta_A^q(\mu) a^q(T, v) \quad (3.5)$$

with

$$\beta_A^1(\mu) = k_{\text{lens}} \qquad a^1(T, v) = \int_{\Omega_{\text{lens}}} \nabla T \cdot \nabla v$$

$$\beta_A^2(\mu) = h_{\text{amb}} + h_{\text{bl}} \qquad a^2(T, v) = \int_{\partial\Omega} Tv$$

$$\beta_A^3(\mu) = 1 \qquad a^3(T, v) = \int_{\Gamma_N} h_r Tv + \sum_{i \neq \text{lens}} \int_{\Omega_i} k_i \nabla T \nabla v$$

Affine decomposition

$$f(v;\mu) = \sum_{p=1}^{2} \beta_F^p(\mu) f^p(v)$$

with

$$\beta_F^1(\mu) = h_{\text{amb}} T_{\text{amb}} + h_r T_{\text{amb}} + E \qquad f^1(v) = \int_{\Gamma_N} v$$

$$\beta_F^2(\mu) = h_{\text{bl}} T_{\text{bl}} \qquad f^2(v) = \int_{\Gamma_R} v$$

How to choose the snapshots ?

Residual error

Let $\mu \in D^{\mu}$. We set $u(\mu)$ the FEM solution, and $u_N(\mu)$ the reduced solution.
We define the residual error as $e(\mu) = u(\mu) - u_N(\mu)$ that satisfies

$$(e(\mu), v)_V = f(v) - a(u_N(\mu), v; \mu) \qquad \forall v \in V$$

How to choose the snapshots ?

Residual error

Let $\mu \in D^\mu$. We set $u(\mu)$ the FEM solution, and $u_N(\mu)$ the reduced solution.
We define the residual error as $e(\mu) = u(\mu) - u_N(\mu)$ that satisfies

$$(e(\mu), v)_V = f(v) - a(u_N(\mu), v; \mu) \qquad \forall v \in V$$

$$\widehat{e}(\mu) = \sum_p \beta_F^p(\mu)\mathcal{S}^p + \sum_q \sum_n \beta_A^q(\mu) u_N^n(\mu)\mathcal{L}^{n,q} \tag{3.5}$$

with :

$$\begin{aligned} (\mathcal{S}^p, v) &= f^p(v) && \forall v \in X, \forall p \in [\![1, Q_F]\!] \\ (\mathcal{L}^{n,q}, v) &= -a^q(\xi^n, v) && \forall v \in X, \forall n \in [\![1, N]\!], \forall q \in [\![1, Q_A]\!] \end{aligned} \tag{3.6}$$

Norm of the residual error

$$\|\widehat{e}(\mu)\|_X^2 = (\widehat{e}(\mu), \widehat{e}(\mu))_X$$
$$= \left(\sum_p \beta_F^p S^p + \sum_q \sum_n \beta_A^q u_N^n \mathcal{L}^{n,q}, \sum_p \beta_F^p S^p + \sum_q \sum_n \beta_A^q u_N^n \mathcal{L}^{n,q} \right)_X$$

$$\|\widehat{e}(\mu)\|_X^2 = \sum_p \sum_{p'} \beta_F^p \beta_F^{p'} (\mathcal{S}^p, \mathcal{S}^{p'})_X + 2 \sum_p \sum_q \sum_n \beta_F^p \beta_A^q u_N^n (\mathcal{S}^p, \mathcal{L}^{n,q})_X$$
$$+ \sum_q \sum_n \sum_{q'} \sum_{n'} \beta_A^q \beta_A^{q'} u_N^n u_N^{n'} (\mathcal{L}^{n',q'}, \mathcal{L}^{n,q})_X$$

Greedy algorithm

Algorithm 1: Greedy algorithm

Input: $\mu_0 \in D^\mu$ and $\Xi_{\text{train}} \subset D^\mu$

$S \leftarrow [\mu_0]$

while $\Delta_N^{max} > \varepsilon$ **do**

$\mu^\star \leftarrow \underset{\mu \in \Xi_{\text{train}}}{\arg\max} \|\widehat{e}(\mu)\|_V^2$ (and $\Delta_N^{\max} \leftarrow \max_{\mu \in \Xi_{\text{train}}} \|\widehat{e}(\mu)\|_V^2$)

Append $\mu^\star$ to S

$u(\mu^\star) \leftarrow$ FE solution, using S as generating sample

$\mathbb{Z}_N \leftarrow \{\xi = u(\mu^\star)\} \cup \mathbb{Z}_{N-1}$

end

Output: sample S, reduced basis $\mathbb{Z}_N$

Time of execution

	$\mathbb{P}_1$	$\mathbb{P}_2$	Online
$\mathcal{N}$	207 845	1 580 932	$N = 10$
t_{exec}	21.221s	123.92s	0.140 60s

Validation

Execution of the full model

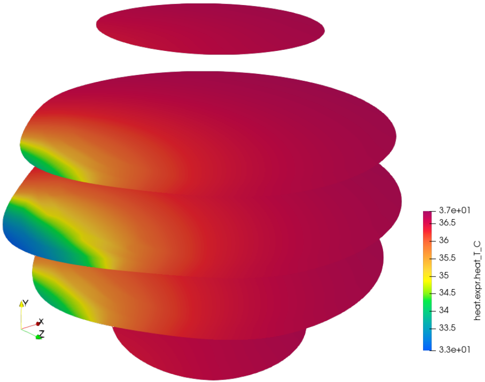


Figure 2: Temperature of the eye (in °C)

Execution of the full model

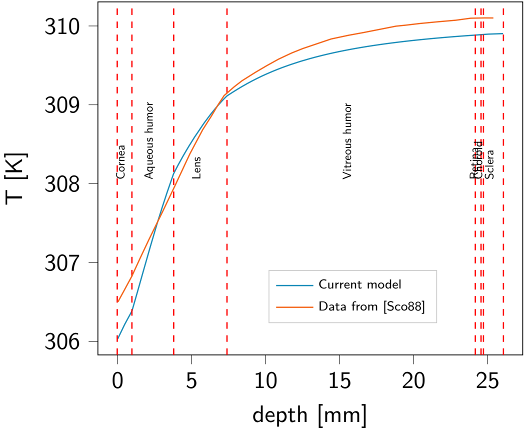
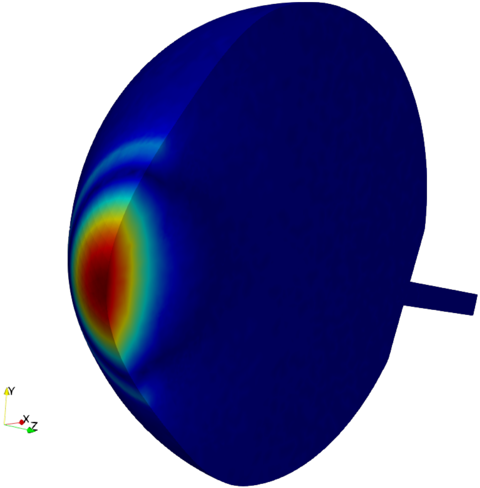


Figure 2: Temperature over an horizontal line

Linearization



Convergence

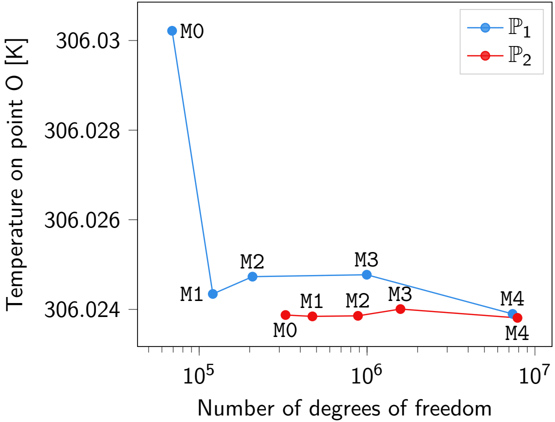


Figure 4: Temperature on the center of the cornea depending on the fineness of the mesh

Validation

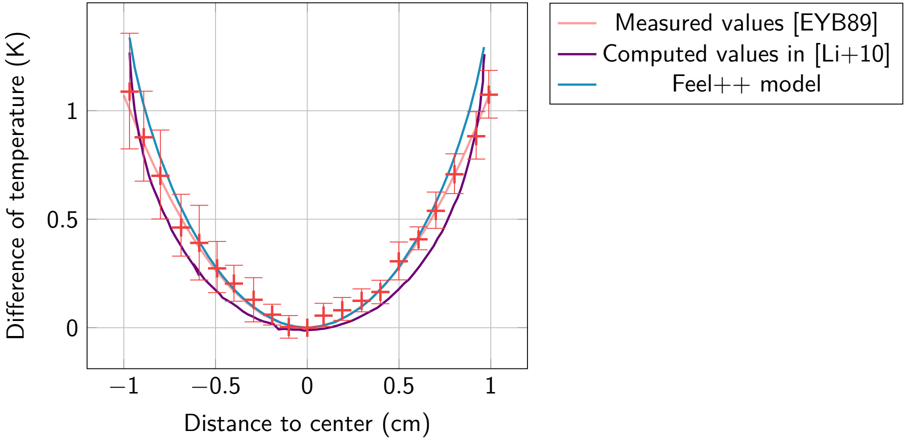


Figure 5: Temperature on the GCC

Sensitivity analysis

Output of interest

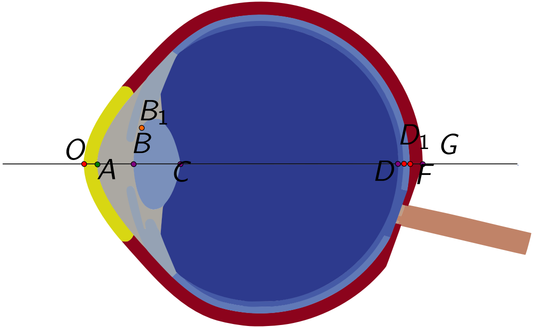


Figure 6: Featured geometrical locations for the output of interest (temperature)

Deterministic sensitivity analysis

- We choose one parameter among the 6 parameters of the model,
- We fix the other one to their nominal value,
- We make the selected parameter vary to study the impact of this single parameter on the output of the model.

Deterministic sensitivity analysis

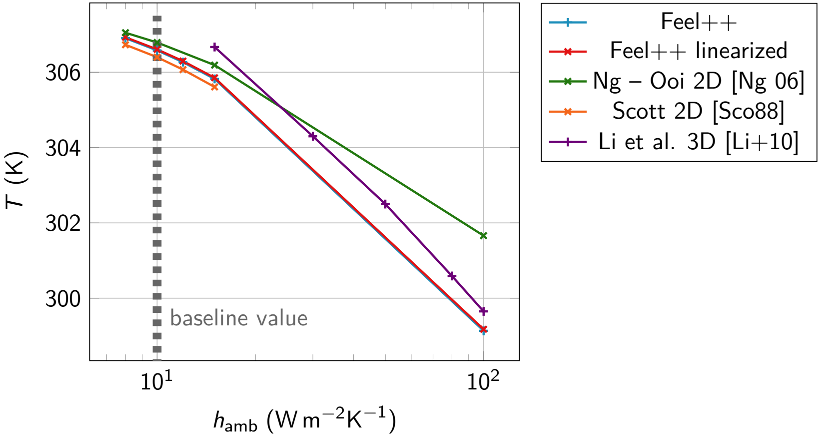


Figure 7: Effect of h_{amb} at point O

Deterministic sensitivity analysis

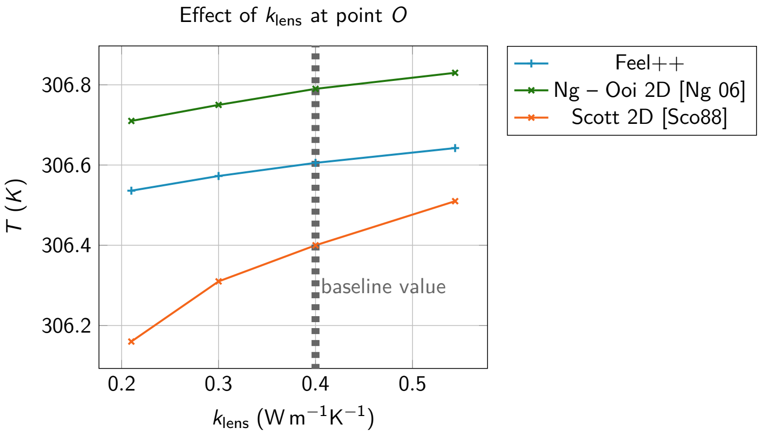
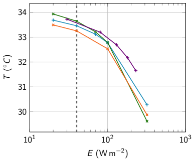
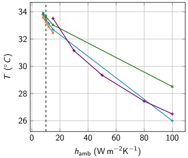


Figure 7: Effect of k_{lens} at point O

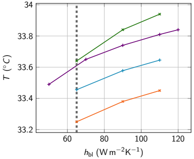
Deterministic sensitivity analysis



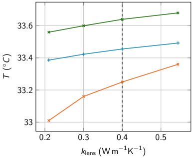
(a) E



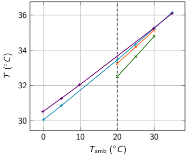
(b) h_{amb}



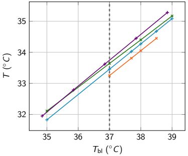
(c) h_{bl}



(d) k_{lens}



(e) T_{amb}



(f) T_{bl}

Figure 7: Point O (Feel++ model, [Ng 06], [Sco88], [Li+10])

Deterministic sensitivity analysis

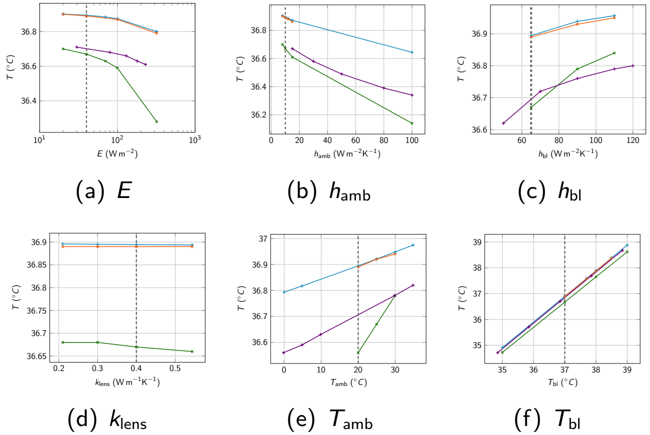
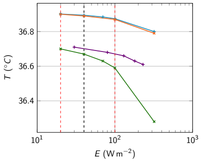
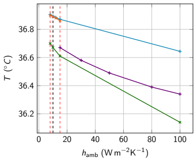


Figure 7: Point G (Feel++ model, [Ng 06], [Sco88], [Li+10])

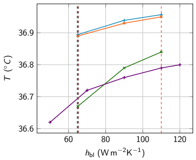
Deterministic sensitivity analysis



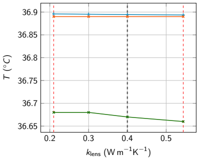
(a) E



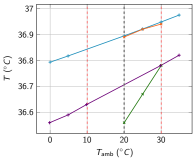
(b) h_{amb}



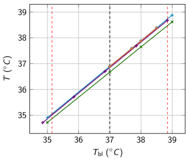
(c) h_{bl}



(d) k_{lens}



(e) T_{amb}



(f) T_{bl}

Figure 7: Point G (Feel++ model, [Ng 06], [Sco88], [Li+10])

Sobol indices

- $\mu = (\mu_1, \ldots, \mu_n) \in D^\mu$,
- $\mu_i \sim X_i$ where $(X_i)_i$ is a familly of independent random variables,
- Output $s_N(\mu) \sim Y = f(X_1, \ldots, X_n)$,

Sobol indices

- **First-order indices**:

$$S_j = \frac{\mathrm{Var}\left(\mathbb{E}\left[Y|X_j\right]\right)}{\mathrm{Var}(Y)} \tag{5.1}$$

- **Total-order indices**:

$$S_j^{\text{tot}} = \frac{\mathrm{Var}\left(\mathbb{E}\left[Y|X_{(-j)}\right]\right)}{\mathrm{Var}(Y)} \tag{5.2}$$

where $X_{(-j)} = (X_1, \ldots, X_{j-1}, X_{j+1}, \ldots, X_n)$.

Sobol indices

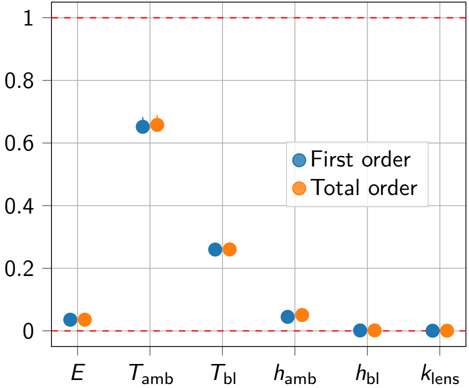


Figure 8: Sobol indices for the output on point O.

Conclusion

- Thanks the RBM, we can run quickly a big number of simulations to run sensitivity analysis,
- In the model, some parameter have a greater impact on some outputs

Conclusion

- Thanks the RBM, we can run quickly a big number of simulations to run sensitivity analysis,
- In the model, some parameter have a greater impact on some outputs

Next steps :

- Use the reduced model method on more complex models :
  - Account aqueous humor flow (for heat transfer model),
  - Darcy coupled problem (3D + 0D)

References

[EYB89] Nathan Efron, Graeme Young, and Noel A Brennan. "Ocular surface temperature.". In: *Current eye research* 8 9 (1989), pp. 901–6.

[Li+10] Eric Li et al. "Modeling and simulation of bioheat transfer in the human eye using the 3D alpha finite element method (αFEM)". In: *International Journal for Numerical Methods in Biomedical Engineering* 26.8 (2010), pp. 955–976.

[Ng 06] Ng, E.Y.K. and Ooi, E.H. "FEM simulation of the eye structure with bioheat analysis". In: *Computer Methods and Programs in Biomedicine* 82.3 (2006), pp. 268–276.

[Sco88] J.A. Scott. "A finite element model of heat transport in the human eye". In: *Physics in Medicine and Biology* 33.2 (1988), pp. 227–242.

Thanks for your attention !