



École Doctorale 146

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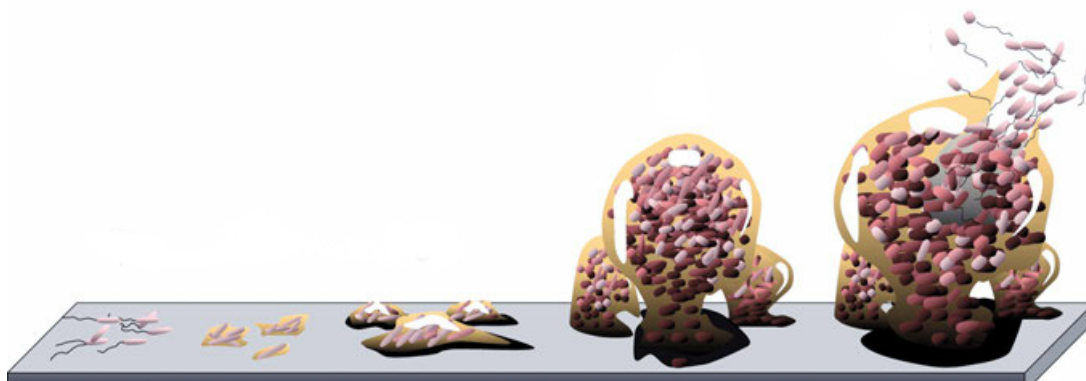
pour obtenir le grade de docteur délivré par

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Spécialité doctorale “*Mathématiques appliquées*”

Méthodes d'éléments finis pour des systèmes d'EDP non linéaires avec interface. Application à un modèle de croissance de biofilm

présentée publiquement par **DINH Anh-Thi**



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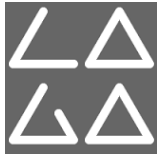
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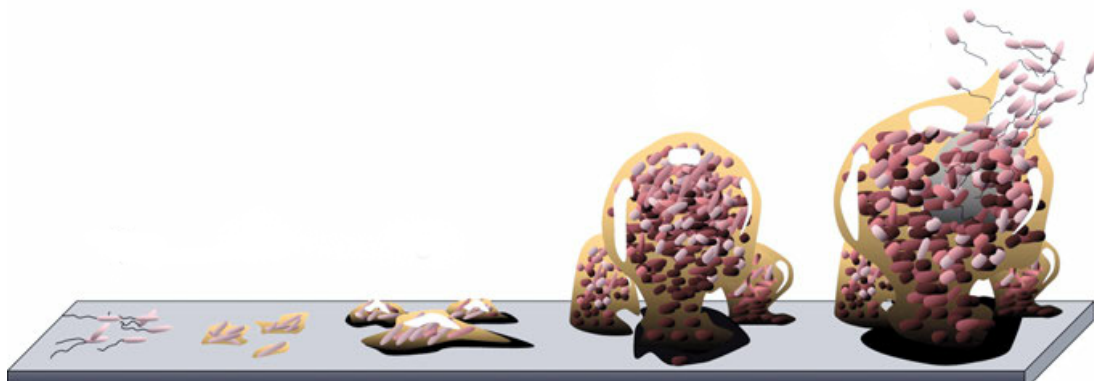
submitted for obtaining the degree of Doctor from

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Finite Element Methods for nonlinear interface problems. Application to a biofilm growth model

presented by **DINH Anh-Thi**



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Résumé

In French.

Mots clés: *NXFEM, Nitsche-Extended Finite Element Method, problème d'interface, méthode de lignes de niveau, biofilm.*

Abstract

In English.

Keywords: *NXFEM, Nitsche-Extended Finite Element Method, interface problem, level set method, biofilm, unfitted mesh.*

Acknowledgements

In English.

En français.

Bằng tiếng Việt.

From a friend, a brother, a son and a Vietnamese guy.

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Glossaries, notations and symbols

In this section, I list all of the acronyms, operators and notations I will use throughout this thesis. There may be ones that are only defined here and used later without recall the definition at the place they appear.

Acronyms

Initials	Meaning
1D	Dimension 1 or 1 dimensional
2D	Dimension 2 or 2 dimensional
aprx	Approximate
DDM	Domain Decomposition Method
DGM, DG	Discontinuous Galerkin Method
EPS	Extracellular Polymeric Substances
FEM	Finite Element Method
FMM	Fast Marching Method
IIM	Immersed Interface Method
ips	intersection points

Initials	Meaning
LHS	Left Hand Side
LSM	Level Set Method
NFEM	Nitsche Finite Element Method
NXFEM	Nitsche-Extended Finite Element Method
RHS	Right Hand Side
SDFEM	Streamline Diffusion Finite Element Method
SUPG	Streamline Upwinding Petrov-Galerkin method
w.r.t	with respect to
XFEM	Extended Finite Element Method

Notations

Notations	Meaning	Page
$\mathcal{T}_h, \mathcal{T}_h^i$	conforming triangulation of domain Ω and it subset which covers subdomain Ω_i .	ix, 11
\mathbf{n}, \mathbf{n}_F	unit normal vector at a given point on interface or on edge F (its direction will be precised when needed or be chosen arbitrarily).	ix, 11

Operators

Operators	Meaning	Page
$\langle u, v \rangle_K$	inner product on a convex set or on a line.	ix, 11
$\{ \{ u \} \}$	average condition on an interface or on an edge of the mesh's element, cf. Definition ??.	ix, 11
$[[u]]$	jumb condition on an interface or on an edge of the mesh's element, cf. Definition ??.	ix, 11



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1. Example chapter

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In this chapter, we take you from the start of biofilm problem to the methods and the motivation of this thesis. We also present a general idea about biofilm and methods people have used for recent years to solve interface problems which are the focus in a biofilm model.

1.1 Example of section

1.2 Example of subsection

An example of subject of multiple paragraphs. This is the content of this subject. This is the content of this subject. This is the content of this subject. This is the content of this subject. This is the content of this subject. This is the content of this subject.

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1.3 Example of enumerate and itemize

A *mathematical model* is a description of a system of natural phenomena using mathematical concepts and language. The process of developing a mathematical model is termed *mathematical modelling*. In this work, we develop a mathematical model describing the growth of a biofilm model under some affects. A good understanding of this phenomenon is in accordance with a good model and inversely. Using and creating a mathematical model require six steps [10]:

1. *The important variables and processes acting in the system must be identified.* In our problem, necessary components are substrates, bacteria, fluid flows, biomass flows and some antimicrobial.
2. *Performing processes as mathematical expressions.* In our case, this is the system of two partial differential equations describing the evolution of substrates and bacteria. They can be represented by Monod's law (Section ??) and diffused by Fick's law.
3. *The mathematical expressions are combined appropriately in equations.* We will discuss the meaning of a biofilm model in Chapter ??.
4. *The parameters involved in the mathematical expressions are given values.* In our model, parameters come from real experiments and from some others' works.
5. *Approximate the solution of the system by numerical methods.* If a problem has a solution, then we approximate it by a numerical scheme. We based on the biofilm model to work with an interface problem. From that, we choose the NXFEM method to treat a such problem. See more detail in Part I.

6. *The properties of the system are explored via the solution of the model.* After doing maths on the biofilm models, we give comments on the results and play with them. See more in Part II.

The thesis is divided into two main parts. The first one is for the NXFEM method and the second one contains the way we apply this method to researching a biofilm growth model. The manuscript is organized as follows:

Chapter ?? In this chapter, I am going to recall the main idea of NXFEM and some principle results which first proposed by A. Hansbo & P. Hansbo [4] and later developed by some other authors. I start with the idea of Nitsche method on a non interface problem and then give details of NXFEM on an interface problem which borrows its idea.

Chapter ?? In this chapter, I will give in details about algorithms and guide to use `NXFEM toolbox` developed by myself. I build it based on the idea of space proposed by Hansbo in Section ??, coming from the idea of implementing Standard FEM in Matlab. In other point of view, this chapter is also used to implement NXFEM in other programming language instead of being used only in Matlab.

Chapter ?? Under the motivation of modeling a biofilm model, we introduce a system of semilinear unsteady interface problem. We also propose a technique of decoupling a semilinear problem and apply the NXFEM method to prove the existence and uniqueness of solutions and their convergent properties. In order to prove the convergence of NXFEM discrete solutions to the continuous ones, we apply the idea of proofs in Discontinuous Galerkin Method proposed by Ern & Di Pietro [1]. Their work relied on techniques inspired by the Finite Volume literature given in the work of Eymard et al. [3]. Noting that, Ern & Di Pietro worked on the discontinuity on each side of element mesh whereas we only work on the discontinuity of functions on the interface.

Chapter ?? As mentioned in Section ??, we need to track the interface's position on a fixed mesh from time to time. The *Level Set Method* helps us to do that. In this chapter, I present a general idea of LSM, as well as its advantages, its inherent drawback and the way we couple it with NXFEM in solving an evolution problem. Some numerical test cases are also given.

Chapter ?? This last chapter provides a way we use the NXFEM method and the toolbox NXFEM in solving biofilm growth models. The models we use are introduced in literatures, but the methods are different. We also have comments on the dependence of the model on parameters.

As mentioned in Section ??, the choice of parameters is very important. With two previous test cases, we give some interesting results about the choice of values for:

- The penalty coefficient λ and the value of $\hat{\lambda}$ which are given in Section ??.
- The values of γ_1, γ_2 when we work with the Ghost Penalty mentioned in Section ??.
- The choice of using or not using Ghost Penalty.

- The *very contrast* problem where the diffusion coefficients take very different values in each subdomain Ω_i .

1.4 Example of algorithms

Algorithm 1.1. Determine intersection points on a cut triangle (**getiPs**).

Input : ϕ_i for $i = 1, 3$ at three vertices x_i of cut triangle.

Output **CT.iPs** of size 2 coordinates $\times 2$ intersections $\times N_{CTs}$.

:

for $1 \leq \tau \leq N_{CTs}$ **do**

$r = 0$;

if $\phi_1 \times \phi_2 < 0$ **then**

CT.iPs $(:, r, \tau) = \text{getiPsonE}(x_1, x_2, \phi_1, \phi_2)$;

$r = r + 1$;

if $\phi_2 \times \phi_3 \leq 0$ **then**

CT.iPs $(:, r, \tau) = \text{getiPsonE}(x_2, x_3, \phi_2, \phi_3)$;

$r = r + 1$;

if $\phi_3 \times \phi_1 \leq 0$ and $r < 2$ **then**

CT.iPs $(:, r, \tau) = \text{getiPsonE}(x_3, x_1, \phi_3, \phi_1)$;

$r = r + 1$;

1.5 Insert figures

Living environment. Biofilm is, generally, observed in aqueous media or in a medium exposed to moisture. They can grow on any natural or artificial surface. This surface may be mineral (rock interfaces, air-liquid,...) or organic (skin, plants,...), industrial (pipes, oil, waste-water,...) or medical (prosthesis, catheters,...),...

1.6 Example of tables

¹Credit: Modification of work by Klaus D. Peter (ear) and bacteriality.com (teeth).

²Credit: skfaquatics.com.

³Credit: *The strange case of a biofilm-forming strain of Pichia fermentans, which controls Monilinia brown rot on apple but is pathogenic on peach fruit* - Sara Giobbe et al.

⁴Credit: P. Dirckx, Center for Biofilm Engineering, Montana State University, Bozeman.

⁵Credit: Courtesy of the Montana State University Center for Biofilm Engineering, P. Dirckx.

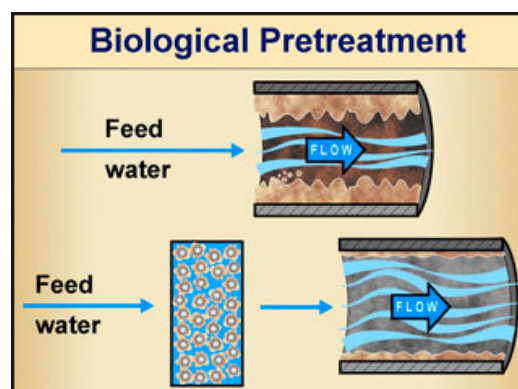
a. On human body¹.b. In nature².c. In food³.d. Water filter⁴.

Figure 1.1. Biofilm appears everywhere in human life.

Figure 1.2. Stages of the biofilm life cycle⁵.

Figure 1.3. Interface cuts triangle at positions which close to its vertex.

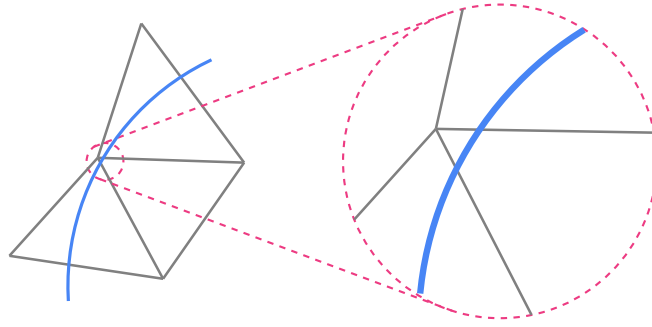
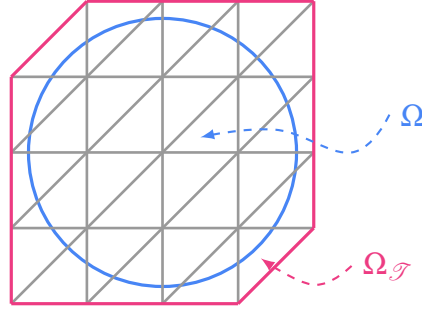


Figure 1.4. An illustration of a fictitious domain $\Omega_{\mathcal{T}}$ of a physical domain Ω .



1.7 Example of mathematics expression

$$\begin{aligned} \langle \nabla u, \nabla v \rangle_{\Omega} - \underbrace{\langle \nabla_{\mathbf{n}} u, v \rangle_{\partial \Omega}}_{\text{consistency}} - \underbrace{\langle \nabla_{\mathbf{n}} v, u \rangle_{\partial \Omega}}_{\text{symmetry}} + \underbrace{\lambda \langle u, v \rangle_{\partial \Omega}}_{\text{stabilization}} \\ = \langle f, v \rangle_{\Omega} - \langle g, \nabla_{\mathbf{n}} v \rangle_{\partial \Omega} + \lambda \langle g, v \rangle_{\partial \Omega}, \quad \forall v \in H^1(\Omega). \end{aligned} \quad (1.1)$$

$$\|v\|_N := \|v\|_{H^1(\Omega)}^2 + \sum_{E \in G_h} h_E^{-1} v^2 dx, \quad (1.2)$$

$$\begin{cases} -\nabla \cdot (k \nabla u) = f & \text{on } \Omega_1 \cup \Omega_2, \\ \llbracket u \rrbracket = 0 & \text{on } \Gamma, \\ \llbracket k \nabla_{\mathbf{n}} u \rrbracket = g & \text{on } \Gamma, \\ u = 0 & \text{on } \partial \Omega, \end{cases} \quad (1.3)$$

1.8 Example of theorem styles

1.8.1 Assumption

Assumption 1.1 We assume that $f \in L^2(\Omega)$, $g \in H^{1/2}(\Gamma)$ and k is constant in Ω_i with $\alpha_i > 0$ for $i = 1, 2$.

1.8.2 Remarks

Som texts.

h	$\ u_h - u_{\text{ex}}\ _{L^2}$	order	$\ u_h - u_{\text{ex}}\ _H$	order
9.52×10^{-2}	7.3×10^{-3}		0.51	
4.88×10^{-2}	1.7×10^{-3}	1.82	0.32	0.7
2.47×10^{-2}	3.91×10^{-4}	2.01	0.17	0.9
1.24×10^{-2}	9.97×10^{-5}	1.93	0.08	1.1

Table 1.1. $L^2, \|\cdot\|_H$ norm errors of the solutions with different mesh sizes in Barrau's test case.

Remark 1.1 — Cut triangle. A triangle is called a *cut triangle* if the Assumption 1.1 is satisfied and at least one cut point is not the vertex of this triangle. Some special cases of cut or not-cut triangles are given in Figure 1.3. Note that, we are considering a \mathbb{P}^1 - finite element space so Γ on each triangle is actually a line segment, that why we see all three cases a, b and c in Figure 1.3 are the same. That is the reason why in the triangulation \mathcal{T}_h , there is some triangle we see that it is cut by interface but it is still considered as a not-cut triangle (Figure 1.3).

1.8.3 Theorem, proposition and definition

Definition 1.1 We use notation of function space $H^k(\Omega_{12})$ as follows,

$$H^k(\Omega_1 \cup \Omega_2) = \{v \in L^2(\Omega) : v_i \in H^k(\Omega_i) \text{ for } i = 1, 2\},$$

for $k = 0, 1, 2$ where $v_i = v|_{\Omega_i}$ and H^0 stands for L^2 .

Theorem 1.1 Let I_h^* be the interpolation operator defined in (1.2), then

$$\|u - I_h^* u\|_H \leq Ch \|u\|_{2, \Omega_{12}}, \forall u \in H_0^1(\Omega) \cap H^2(\Omega_{12}).$$

Proposition 1.1 With the jump and average operators defined in Definition 1.1 and u, v two discontinuous functions across Γ , we have,

$$\begin{aligned} \llbracket uv \rrbracket &= \llbracket u \rrbracket \{v\} + \{u\} \llbracket v \rrbracket + (\kappa_2 - \kappa_1) \llbracket u \rrbracket \llbracket v \rrbracket \text{ and} \\ \{uv\} &= \{u\} \{v\} + \kappa_1 \kappa_2 \llbracket u \rrbracket \llbracket v \rrbracket. \end{aligned}$$

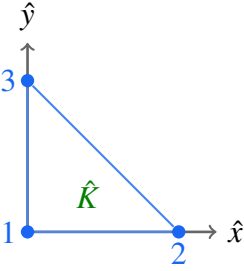
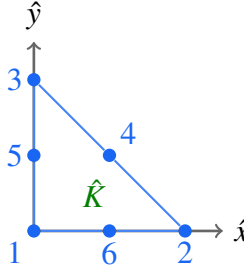
\mathbb{P}^1 -FE	\mathbb{P}^2 -FE
	
$N_1(\hat{x}, \hat{y}) = 1 - \hat{x} - \hat{y},$ $N_2(\hat{x}, \hat{y}) = \hat{x},$ $N_3(\hat{x}, \hat{y}) = \hat{y}.$	$N_1(\hat{x}, \hat{y}) = 1 - 3\hat{x} - 3\hat{y} + 2\hat{x}^2 + 4\hat{x}\hat{y} + 2\hat{y}^2,$ $N_2(\hat{x}, \hat{y}) = 2\hat{x}^2 - \hat{x},$ $N_3(\hat{x}, \hat{y}) = 2\hat{y}^2 - \hat{y},$ $N_4(\hat{x}, \hat{y}) = 4\hat{x}\hat{y},$ $N_5(\hat{x}, \hat{y}) = 4\hat{y} - 4\hat{x}\hat{y} - 4\hat{y}^2,$ $N_6(\hat{x}, \hat{y}) = 4\hat{x} - 4\hat{x}\hat{y} - 4\hat{x}^2.$
function <code>getP1shapes</code> in the toolbox	function <code>getP2shapes</code> in the toolbox

Table 1.2. Local shape functions defined on reference triangle \hat{K} where $N_i(x_j) = \delta_{ij}$.

Proof. Denote $u_i = u|_{\Omega_i}$, $v_i = v|_{\Omega_i}$ for $i = 1, 2$,

$$\begin{aligned}
\llbracket uv \rrbracket &= u_1 v_1 - u_2 v_2 = \sum \kappa_i u_1 v_1 + \sum \kappa_i u_2 v_2 \\
&= 2\kappa_1 u_1 v_1 - 2\kappa_2 u_2 v_2 + (\kappa_2 - \kappa_1)(u_1 v_1 + u_2 v_2) \\
&= 2\kappa_1 u_1 v_1 - 2\kappa_2 u_2 v_2 + (\kappa_2 - \kappa_1)(u_1 v_2 + u_2 v_1) + (\kappa_2 - \kappa_1)\llbracket u \rrbracket \llbracket v \rrbracket \\
&= \kappa_1 u_1 v_1 + \kappa_2 u_1 v_2 - \kappa_1 u_2 v_1 - \kappa_2 u_2 v_2 \\
&\quad + \kappa_1 u_1 v_1 - \kappa_1 u_1 v_2 + \kappa_2 u_2 v_1 - \kappa_2 u_2 v_2 + (\kappa_2 - \kappa_1)\llbracket u \rrbracket \llbracket v \rrbracket \\
&= \llbracket u \rrbracket \llbracket v \rrbracket + \llbracket u \rrbracket \llbracket v \rrbracket + (\kappa_2 - \kappa_1)\llbracket u \rrbracket \llbracket v \rrbracket.
\end{aligned}$$

We also have

$$\begin{aligned}
\llbracket u \rrbracket \llbracket v \rrbracket + \kappa_1 \kappa_2 \llbracket u \rrbracket \llbracket v \rrbracket &= (\kappa_1 u_1 + \kappa_2 u_2)(\kappa_1 v_1 + \kappa_2 v_2) + \kappa_1 \kappa_2 (u_1 - u_2)(v_1 - v_2) \\
&= \kappa_1^2 u_1 v_1 + \kappa_2^2 u_2 v_2 + \kappa_1 \kappa_2 u_1 v_1 + \kappa_1 \kappa_2 u_2 v_2 \\
&= \llbracket uv \rrbracket.
\end{aligned}$$

■

We can call Theorem 1.1 or Theorem 1.1. For others, Propotion 1.1 and Defini-
tion 1.1.

Type 0	Type 2	Type 4

Table 1.3. Example of determining intersections between cut triangle $i-j-k$ (in that order) and interface Γ_h . They are all stored in $CT.iPs$ in order of $[A, B]$.

1.9 Example of bibliography

There are 3 types of bibliography (articles [2, 5], thesis [11, 12] and books [7, 9]). You even can do this [6, Section 3].

1.10 Example of Index

You can use an index or a group of indexes,

1.11 Example of glossaries

, , , , ,

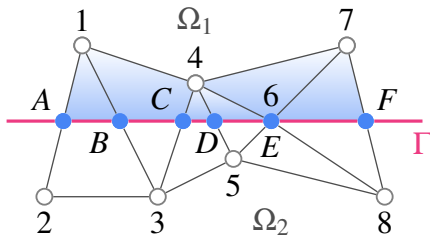
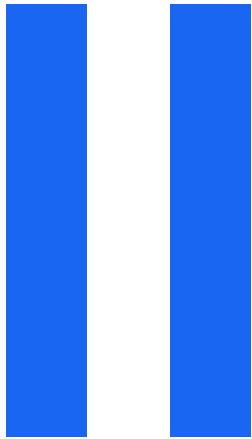
figure		cut triangles					
		i	1	3	3	6	6
		j	2	4	5	4	8
		k	3	1	4	5	7
		CT.type	4	2	4	0	0
		CT.iPs	[A,B]	[C,B]	[D,C]	[D,E]	[F,E]
		CT.uN [⊥]	[B,A]	[C,B]	[D,C]	[E,D]	[F,E]

Table 1.4. Example of determining unit normal vectors CT.uN based on intersections CT.iPs . This result follows Algorithm 1.1. Note that, CT.uN^\perp is an orthogonal vector of CT.uN .



nx fem with biofilms

appendix

A. Implementation and NXFEM toolbox

Contents

A.1 Some principles of quadrature

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A.1 Some principles of quadrature

Definition A.1 — Quadrature. [8] Let D be a non-empty, Lipschitz, compact, connected subset of \mathbb{R}^n . Let l_q be an integer. A quadrature is an approximation of the definite integral of a function. It's usually stated as a weighted sum of function values at specific points within domain of integration. So, a quadrature on D with l_q points consists of

- (i) A set of l_q real numbers $\{\omega_1, \dots, \omega_q\}$ called *quadrature weights*.
- (ii) A set of l_q points $\{\xi_1, \dots, \xi_q\}$ in D called *Gaussian points* or *quadrature nodes*.

The largest integer k such that

$$\forall g \in \mathbb{P}_k, \int_D g(x) \, dx = \sum_{q=1}^{l_q} \omega_q g(\xi_q),$$

is called the *quadrature order* and is denoted by k_q .

In this thesis, I will use an n -point *Gaussian quadrature rule* which is a quadrature rule constructed to yield *an exact* result for polynomials of degree $2n - 1$ or less by using suitable couples $\{\omega_q, \xi_q\}$ for $q = 1, \dots, n$. More specifically, I apply Gaussian quadrature only for type of domain which is a segment (in dimension 1) or a triangle (in dimension 2). Note that, n -point Gaussian quadrature is corresponding to quadrature order $k_q = 2n + 1$ (see the proof in [8, Proposition 8.2]).

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Titre: Méthodes d'éléments finis pour des systèmes d'EDP non linéaires avec interface. Application à un modèle de croissance de biofilm.

Mots clés: NXFEM, Nitsche-Extended Finite Element Method, problème d'interface, méthode de lignes de niveau, biofilm.

Résumé: Un biofilm est un ensemble de micro-organismes tels que les bactéries, les champignons ou encore les algues qui vivent en communauté. Les biofilms ont la capacité d'être présents en tout lieu. Ils sont observés dans les milieux aqueux ou humides. Ils peuvent se développer sur n'importe quel type de surface naturelle ou artificielle, qu'elle soit minérale (roche, interfaces air-liquide...) ou organique (peau, tube digestif, racines et feuilles des plantes), industrielle (canalisations, coques des navires) ou médicale comme les prothèses et les cathéters. Cette ubiquité est à l'origine de nombreuses infections bactériennes. Les infections nosocomiales contractées dans les hôpitaux sont un exemple majeur. Certaines de ces infections pouvant être mortelles. Le traitement médical des biofilms est souvent inefficace pour lutter contre ce type d'infection. Il est donc important de comprendre les mécanismes de croissance d'un biofilm. Telle est la motivation de la présente thèse.

Afin de réaliser des simulations numériques d'un modèle décrivant la croissance d'un biofilm, nous combinons différentes méthodes de calcul basées sur la méthode Nitsche-Extended Finite Element Method (NXFEM) ainsi que sur la méthode des lignes de niveau. Ces méthodes nous permettent d'étudier des modèles complexes dans lesquels l'interface entre le biofilm et son environnement est capable de se déformer tout en dépendant du temps. Ceci permet de considérer une discrétisation à l'aide d'un maillage ne coïncidant pas avec l'interface biofilm/environnement. Nous présentons également une technique de découplage d'un système d'équations aux dérivées partielles semi-linéaires et la façon dont nous appliquons la méthode NXFEM pour résoudre un tel problème. Ce système est en relation avec le modèle de croissance du biofilm qui est traité dans cette thèse.

Pour l'implémentation, une boîte à outils NXFEM, développée en Matlab, a été entièrement conçue pour résoudre un tel problème. Nous donnons dans ce document les détails des algorithmes et techniques numériques utilisés afin que chacun puisse utiliser cette boîte à outils pour ses propres projets.

Title: Finite Element Methods for nonlinear interface problems. Application to a biofilm growth model.

Keywords: NXFEM, Nitsche-Extended Finite Element Method, interface problem, level set method, biofilm, unfitted mesh.

Abstract: A biofilm is a collective of living, reproducing microorganisms, such as bacteria, that stick together as a colony, or community. They appear everywhere in human life and have some impacts on our environment. Biofilm modeling, together with laboratory experiments, has risen as a means of producing quantitative tools for scientists to better understand the biofilm's growth. This thesis is motivated to research on this subject.

A combination of computational methods which are based on *Nitsche-Extended Finite Element Method* (NXFEM), *Level Set Method* and some other stabilized techniques are used to solve and simulate a biofilm growth model. These methods allow us to work with a complex scheme in which the interface between the biofilm and its environment is allowed to change with time and on an unfitted mesh. We also present a technique of decoupling a system of semilinear differential equations and how we apply the NXFEM method to solve such a problem. This system has a relation to a model of biofilm's growth which will be examined carefully in the work.

For the implementations, *NXFEM toolbox* which is a Matlab based toolbox is built for solving such a problem. We give also the details of all algorithms and numerical techniques so that everyone can use this toolbox for their own projects.