Computational Methods in Biomechanics and Physics

A Dissertation

Presented to

the Faculty of the Department of Mathematics

University of Houston

In Partial Fulfillment

of the Requirements for the Degree

Doctor of Philosophy

By

Serguei Lapin

May 2005
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ABSTRACT

This dissertation considers the numerical solution of linear and non-linear wave propagation problems and numerical modeling of blood flow in compliant vessels.

We consider the solution of the linear wave equation with discontinuous coefficients by a domain decomposition method. A time explicit finite difference scheme combined with a piecewise linear finite element method in space is used on semimatching grids. We apply a boundary supported Lagrange multiplier technique on the interface between the subdomains.

We examine the numerical solution of the wave scattering problem via a fictitious domain method. We use a mixed variational formulation to construct a discrete problem, which is explicit in time along with a boundary supported Lagrange multipliers to enforce the boundary condition on the interface.

The next problem deals with the solution of a vector-valued constrained nonlinear wave equation. We use a methodology based on the penalty treatment of the constraint. The numerical scheme combines the use of a continuous piecewise linear finite element approximation along with an implicit in time discretization. The stability and uniqueness results are provided for the aforementioned problems.

The goal of the next problem is to develop an efficient methodology for the numerical simulation of blood flow in bifurcated human arteries. The model is derived using an asymptotic reduction of the Navier-Stokes equations to model the blood, with Navier equation for the wall. We use Riemann invariants analysis in order to describe the continuity of pressure and momentum at the bifurcation point. We calculate shear stress rates for several different prostheses data and obtain results that indicate high shear stress rates in graft limbs where thrombosis is typically observed. Based on our findings, we suggest the optimal design of endovascular prostheses for endoluminal treatment of an aortic abdominal aneurysm.
Contents

1 Introduction 1
   1.1 Numerical methods for solving partial differential equations 1
   1.2 Fictitious domain methods 3
   1.3 Domain decomposition methods 4
   1.4 Absorbing boundary conditions 5
   1.5 Fluid-structure interaction: hemodynamics applications 6
   1.6 Thesis outline 7

2 A Lagrange multiplier based domain decomposition method for wave propagation in heterogeneous media 10
   2.1 Introduction 10
   2.2 Problem formulation 11
   2.3 Time discretization 14
   2.4 Fully discrete scheme 14
   2.5 Energy inequality 18
   2.6 Numerical experiments 20

3 Solution of a wave equation by a mixed finite element - fictitious domain method 37
   3.1 Introduction 37
   3.2 Formulation of the problem 38
3.3 Discretization of the problem. Energy inequality ........................................ 40
3.4 A fictitious domain method with boundary supported Lagrange multiplier 44
3.5 Numerical experiments. ........................................................................... 47

4 A penalty approach to the numerical simulation of a constrained wave motion 53
4.1 Introduction ......................................................................................... 53
4.2 Problem formulation ........................................................................... 53
4.3 Discretization of the problem ............................................................. 58
4.4 Solution method for the fully discrete problem ................................. 65
4.5 Numerical results .............................................................................. 66

5 Mathematical modeling of blood flow in compliant arteries 71
5.1 Introduction ......................................................................................... 71
5.1.1 Background of the problem .......................................................... 71
5.1.2 Mathematical model ....................................................................... 73
5.2 Effective model derivation ................................................................. 73
5.2.1 The 3-D fluid-structure interaction problem ................................. 73
5.2.2 Weak formulation and a priori estimates ......................................... 76
5.2.3 Asymptotic reduction of the model ............................................... 79
5.2.4 The reduced two-dimensional problem ....................................... 81
5.2.5 Derivation of the one-dimensional reduced model ..................... 82
5.3 Conditions at the bifurcation point .................................................... 83
5.4 Numerical method ............................................................................ 87
5.5 Numerical experiments ..................................................................... 88

Bibliography 100
List of Figures

2.1 Computational domain. ................................................. 11
2.2 Semimatching mesh on $\gamma$. ........................................ 15
2.3 Space $\Lambda$ is the space of the piecewise constant functions defined on every union of half-edges with common vertex. ........................................ 16
2.4 Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$ (bottom) meters. Incident wave coming from the left. ................. 23
2.5 Energy behavior versus time for $L = 0.5$ (top) and $L = 0.25$ (bottom). . . 24
2.6 Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$ (bottom) meters. Incident wave coming from the left. ................. 25
2.7 Energy behavior versus time for $L = 0.5$ (top) and $L = 0.25$ (bottom). . . 26
2.8 Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$ (bottom) meters. Incident wave coming from the lower left corner with an angle of 45 degrees. ................................................. 27
2.9 Contour plot of the real part of the solution for $L = 0.5$ meters. .......... 29
2.10 Contour plot of the real part of the solution for $L = 0.25$ meters. .......... 29
2.11 Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$ (bottom). Incident wave coming from the left. ......................... 30
2.12 Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$ (bottom). Incident wave coming from the lower left corner with an angle of 45 degrees. ................................................. 31
2.13 Energy behavior for $L = 0.5$ meters. ........................................... 32
2.14 Energy behavior for $L = 0.25$ meters. ........................................... 32
2.15 Obstacle in a form of an airfoil with a coating. ................................. 33
2.16 Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$
(bottom). Incident wave coming from the left. ................................. 34
2.17 Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$
(bottom). Incident wave coming from the left lower corner with a 45 degree
angle. ........................................................................................................ 35
2.18 Energy behavior versus time for $L = 0.5$ (top) and $L = 0.25$ (bottom). 36

3.1 Computational domain. ............................................................... 38
3.2 Degrees of freedom for $p$ ............................................................ 42
3.3 Shaded rectangulars are boundary elements $T_T$ ............................. 45
3.4 Initial function $u$ ........................................................................... 48
3.5 Domain without an obstacle, time=0.5. ........................................... 48
3.6 Domain without an obstacle, time=0.7. ........................................... 49
3.7 Domain without an obstacle, time=1. ............................................ 49
3.8 Domain with a circular obstacle, time=0.2. ....................................... 50
3.9 Domain with a circular obstacle, time=0.4. ....................................... 50
3.10 Domain with a circular obstacle, time=0.6. ....................................... 51
3.11 Domain with a circular obstacle, time=0.8. ....................................... 51
3.12 Domain with a circular obstacle, time=1. ........................................ 52
3.13 Energy dissipation for $\Delta t = 1/250, h = 1/50$ (dashed line) and $\Delta t =$
$1/500, h = 1/100$ (solid line). ............................................................... 52

4.1 Energy behavior (left) and $\max_x ||u||^2 - 1$ (right) for $\varepsilon = 10^{-3}, h =$
$1/50, \Delta t = 1/100$. ........................................................................ 67
4.2 Energy behavior (left) and \( \max_x |u|^2 - 1 \) (right) for \( \varepsilon = 10^{-4}, h = 1/50, \Delta t = 1/100. \) ................................. 68
4.3 Energy behavior (left) and \( \max_x |u|^2 - 1 \) (right) for \( \varepsilon = 10^{-5}, h = 1/50, \Delta t = 1/100. \) ................................. 68
4.4 \( u_3 \) component of \( u \) at \( t = 1/4 \) (left) and \( t = 1/2 \) (right) for \( \varepsilon = 10^{-3}, h = 1/50, \Delta t = 1/100. \) ................................. 69
4.5 \( u_3 \) component of \( u \) at \( t = 3/4 \) (left) and \( t = 1 \) (right) for \( \varepsilon = 10^{-3}, h = 1/50, \Delta t = 1/100. \) ................................. 69
4.6 \( u_3 \) component of \( u \) at \( t = 1/4 \) (left) and \( t = 1/2 \) (right) for \( \varepsilon = 10^{-5}, h = 1/50, \Delta t = 1/100. \) ................................. 70
4.7 \( u_3 \) component of \( u \) at \( t = 3/4 \) (left) and \( t = 1 \) (right) for \( \varepsilon = 10^{-5}, h = 1/50, \Delta t = 1/100. \) ................................. 70

5.1 Abdominal aorta with and without aneurysm. ................................. 72
5.2 Computational domain. ......................................................... 73
5.3 Blood flow through abdominal aorta (A.A) and iliac arteries (I.A.(1) and I.A.(2)). ......................................................... 84
5.4 Aneurysmal abdominal aorta and iliac arteries with inserted bifurcated stent. 88
5.5 Oscillatory Shear Index. ......................................................... 89
5.6 AneuRx bifurcated stent. ......................................................... 90
5.7 Oscillatory Shear Index for AneuRx stent-graft with limb diameter equal to 12 mm and main body diameter 23 mm. ......................................................... 91
5.8 Oscillatory Shear Index for AneuRx stent-graft with limb diameter equal to 16 mm and main body diameter 28.5 mm. ......................................................... 92
5.9 Oscillatory Shear Index for Wallstent stent with limb diameter equal to 14.5 mm and main body diameter 20 mm. ......................................................... 93
5.10 Shear Stress Rates for AneuRx stent-graft with limb diameter equal to 12 mm and main body diameter 23 mm. .......................... 94
5.11 Shear Stress Rates for AneuRx stent-graft with limb diameter equal to 16 mm and main body diameter 28.5 mm. ...................... 95
5.12 Oscillatory Shear Index for ”optimal” stent with limb diameter equal to 20 mm and main body diameter 28.5 mm. ......................... 96
5.13 Shear Stress Rates for the AneuRx stent-graft with a limb diameter equal to 14.5 mm and a main body diameter 28.5 mm. ..................... 97
5.14 Shear Stress Rates for the AneuRx stent-graft with a limb diameter equal to 14.5 mm and a main body diameter 23 mm. ....................... 98
5.15 Shear Stress Rates for the Wallstent endoprosthesis with a limb diameter equal to 20 mm and a main body diameter of 28 mm. ................. 98
5.16 Shear Stress Rates for an ”optimal” stent with a limb diameter equal to 20 mm and a main body diameter of 28.5 mm. ......................... 99
5.17 Shear Stress Rates for the AneuRx stent-graft with a limb diameter equal to 20 mm and a main body diameter of 28.5 mm. ......................... 99
Chapter 1

Introduction

The numerical modeling of many physical phenomena leads to the solution of differential and integral equations. Using computer-implemented mathematical models it is possible to analyze complicated systems in science and engineering.

An important aspect of many physical areas is the ability to simulate accurately wave phenomena in bounded and unbounded domains. For most applications closed form solutions of the underlying partial differential equations (PDEs) either do not exist or are intractable; therefore, numerical simulation is the only way to solve these PDEs.

One of the applications where numerical mathematics has been focusing on recently is biomechanics. In particular, the modeling of circulatory system of human beings is of a great interest nowadays. The numerical modeling of blood flow leads to the so-called fluid structure interaction problems.

1.1 Numerical methods for solving partial differential equations

There are many different approaches for the numerical approximation of partial differential equations. Some of the most popular schemes are the finite difference based ones, and also
finite volume and finite element methods [1, 16, 93].

The theory of finite difference method can be traced back to the fundamental theoretical paper by Courant, Friedrichs and Lewy [15]. The intensive development of the finite difference methods began at the end of the 1940s and the beginning of the 1950s. It was stimulated by the necessity to deal with the complex problems of science and technology.

Major works of that time belong to J. von Neumann [61] and F. John [40]. Some of the main contributors to the development of finite difference methods in 1950s and 1960s were J. Douglas [20], A. A. Samarskii [74, 73] and O. Widlund [91, 92]. At the end of this period the theory for initial boundary value problems in one space dimension was reasonably well developed and complete. On the contrary, the situation for multidimensional problems on general domains was much less satisfactory. One of the main reasons is the fact that finite difference methods rely on the values of the solution at the points of a uniform mesh, which do not necessarily fit the domain.

In order to deal with this complication scientists developed methods based on variational formulations of the boundary value problems. One of these approaches, the Finite Element Method, is better suited for complex geometries.

The first efforts to use piecewise continuous functions defined over triangular domains appear in applied mathematics literature with the work of Courant [16] in 1943. The actual solution of plane stress problems by means of triangular elements was first introduced by M. J. Turner and R. W. Clough in the presentation given at a meeting on Aeronautical Sciences in New York in 1953, this work was published in 1956 [83]. The current name Finite Element Method appeared only in 1960 in the paper by R. W. Clough [14]. Since its early development the Finite Element Method has become one of the most popular variational methods for solving partial differential equations. Many different variants and extensions of the classical Finite Element Method have been developed. Let us mention here, as examples, fundamental contributions in this area by Babuška and Strouboulis [2], Brezzi and Fortin [8] and Zienkiewicz [93].
1.2 Fictitious domain methods

Fictitious domain methods have a long history; to the best of our knowledge they were first introduced by Hyman [38]. Fictitious domain methods were then discussed in works by Saul’yev [75, 76] (who in fact coined the term ”fictitious domain”), and by Buzbee, Dorr, George and Golub [10]. The basic principle of these methods is the following: suppose that we have to solve a problem in a domain whose shape is complicated, so we are unable to use standard finite difference methods directly. One way to overcome this difficulty is to use finite element methods. Another way is to use a fictitious domain method which will allow us to enjoy the advantages of finite difference methods, e.g. simplicity of discretization and existence of fast numerical solvers. The idea is to extend a problem taking place on a geometrically complex domain to a larger domain of a simpler shape.

Many different realizations of the fictitious domain concept exist. Fictitious domain methods for Dirichlet problems with boundary conditions enforced via Lagrange multiplier are discussed in detail in the work by Glowinski [27]. These methods use structured regular meshes over the extended domain. An example of a non-Lagrange multiplier based fictitious domain method can be found in the immersed boundary method by Peskin [65, 66, 67] and Peskin and McQueen [68] for the simulation of incompressible viscous flow in the presence of elastic moving boundaries. Auxiliary Domain Method is another example of the fictitious domain method; it uses a penalty as an alternative to Lagrange multipliers [48], [57], [31]. The works by Kuznetsov and Matsokin [45], Kuznetsov [44] and Finogenov and Kuznetsov [24] also contributed substantially to the field of fictitious domain methods.
1.3 Domain decomposition methods

Among the methods providing a good and relatively easy way to implement numerical algorithms on complex domains while having a very rich mathematical foundation are Domain Decomposition Methods (DDM). The origin of the Domain Decomposition Methods extends back to the XIX century when H.A. Schwarz introduced the so-called alternating method bearing his name [77].

Nowadays DDM are quite popular. The main goal of DDM is to look for the solution of partial differential equations defined on domains with complicated geometries. DDM’s allow to decompose a given problem into subproblems with simpler and smaller geometries. This approach allows the use of different solvers on each subdomain along with some procedure (iterative in general) to match solutions at the interfaces.

Some of the main reasons making DDM so popular are as follows:

- DDM are well suited to parallel computations,
- allow the use of the different numerical schemes for each subdomain,
- have solid theoretical foundation,
- they can be combined with other methods like local mesh refinement and multigrid methods.

Conferences devoted to Domain Decomposition Methods are held regularly; they allow the presentation of new results and applications. The most recent conferences in this series took place in Berlin in 2003 [42] and in New York in 2005.

While the first domain decomposition algorithms were mostly developed and analyzed for linear, self-adjoint, positive definite elliptic model problems with two subdomains, current applications of the DDM field concerns more complicated problems with more than two subdomain decompositions.
In his work H.A. Schwarz relied on the maximum principle to prove convergence results. In 1936 S. L. Sobolev gave a variational formulation based proof allowing the use of the Schwarz method without the maximum principle [81]. This approach was extended by P.L. Lions for the case of multiple subdomains. [50, 51, 52].

1.4 Absorbing boundary conditions

The effective modeling of waves on unbounded domains by numerical methods depends on the particular boundary condition used to truncate the computational domain. One type of boundary condition used for this purpose is radiating or absorbing boundary conditions (ABC) [3, 22]. The quest for an ABC that produces negligible reflections has been, and continues to be, an active area of research. Most of the popular ABC’s can be classified as those that are derived from differential equations or those that employ an absorbing material. Differential-based ABC’s are generally obtained by factoring the wave equation and allowing a solution which permits only outgoing waves. Material-based ABC’s, on the other hand, are constructed so that fields are dampened as they propagate into an absorbing medium. Other techniques which may be used are exact formulations and superabsorption.

Early techniques used to truncate the computational domain have included differential-based ABC’s, such as those proposed by Merewether [56], Engquist and Majda [22], Lindman [47], and Mur [59]. These early techniques were considerably improved in the mid-1980’s by formulations proposed by Higdon [35, 36] and Keys [41]. Many other extensions of these differential-based ABC’s have been introduced since then.

The idea of using a material-based absorbing boundary condition has existed for some time [37]. However, early material ABC’s did not provide a sufficiently low level of boundary reflection, because the characteristic impedance of the material boundary was matched to the characteristic impedance of free space only at normal incidence. In the early 1990’s, Rappaport et al. [70, 71] proposed a new ABC named the sawtooth anechoic chamber
ABC. This ABC employs pyramidally-shaped absorbing materials similar to those which are often found in anechoic chambers. The most recent advance in material-based ABC’s was put forward by Berenger [6]. His ABC, termed the perfectly matched layer (PML) absorbing boundary condition, appears to yield a major improvement in the reduction of boundary reflections.

1.5 Fluid-structure interaction: hemodynamics applications

The dynamic interaction between a fluid and a structure is a mechanism that is seen in many different physical phenomena: plane wings, suspended and cable-stayed bridges or tall buildings, vibrations in water pipes induced by a water hammer and, among others, blood flow in arteries.

The common aspect in all these phenomena is the energy exchange between the fluid, be it air or water, and the structure; fluid and structure dynamics influence each other. The structure deforms under the load of a fluid, and the fluid follows the displacement of the structure. In the case where the deformation of the structure can be neglected, one can take a fixed domain and the presence of a structure can be treated by appropriate boundary conditions. In this case standard approaches and numerical approximation schemes can be employed. For those situations where the structure displacement is non negligible, one has to solve the fluid equations in a moving domain. This is the case in hemodynamics, where the diameter of an artery may vary up to 10% of its unstressed state.

Analytical solutions are available only to very simple fluid-structure interaction problems. Therefore, in general, different numerical approaches have to be employed in order to solve the problem. Let us mention here the Arbitrary Lagrangian Eulerian formulation [19], the space time approach [55], coupled finite element-boundary element technique [39, 23], the fictitious domain method [31, 32] and the immersed boundary method
One of the fluid-structure interaction problems having received a lot of attention in recent years is the problem arising in hemodynamics applications. In large arteries, the mechanical interaction between blood and the arterial wall plays an important role in the control of blood flow in the circulatory system.

In large arteries blood can be considered a homogeneous and incompressible fluid, and thus can be modeled using the Navier-Stokes equations. One approach to describe the behavior of the arterial wall is to use the Navier equation for the linearly elastic membrane [69, 60, 53]. This equation describes the "effective response" of the arterial walls to the forces induced by the pulsatile blood flow. The mathematical and numerical study of the underlying fluid-structure interaction is a difficult task. Various numerical methods have been successfully proposed to study fluid-structure interactions arising in cardiovascular problems, see e.g. [27, 64, 69]. Nevertheless, they are rather complicated and time-consuming whenever large three-dimensional sections of the cardiovascular system are simulated. This is why simplified, one-dimensional effective models are introduced. These models have been used, for example, in the computation of blood flow through the aorta and coupled to 3D and lumped models to simulate the entire human vascular system [25]; using a "structured tree" to model the "arterial tree" [62]; assuming variable Young’s modulus this model has been used in [84, 86, 87] to study the properties of blood flow and the optimal design of stents (prostheses) in the endovascular treatment of an aortic abdominal aneurysm; in [4] a variable Young’s modulus with the one-dimensional equations have been implemented to study endovascular treatment of a stenosis.

1.6 Thesis outline

Chapter 2 is dedicated to the solution of a linear wave equation with discontinuous coefficients by domain decomposition. We use an explicit in time finite difference scheme...
combined with a piecewise linear finite element method in space on semimatching grids. We apply a boundary supported Lagrange multiplier technique on the interface between subdomains. The resulting "saddle-point" system of linear equations is solved by a conjugate gradient method.

In Chapter 3 we consider the numerical solution of the scattering problem via a fictitious domain method. The main advantage of this method is that a problem can be discretized on a uniform mesh, independent of the obstacle boundary. This approach also involves the use of boundary supported Lagrange multipliers to enforce the boundary condition on the boundary of the obstacle. We use a mixed variational formulation to construct a discrete problem, which is explicit in time. The resulting system of linear algebraic equations is of the "saddle-point" type and is solved effectively using a conjugate gradient method. We also show the stability estimate and prove the uniqueness of the solution.

In Chapter 4 we discuss the numerical solution of a vector-valued constrained nonlinear wave equation. The numerical methodology relies on the penalty treatment of the constraint and on an energy preserving time discretization leading to a scheme which is essentially unconditionally stable and second order accurate. We use a globally continuous piecewise linear finite element approximation for space discretization of the problem. At each time step of the time discretization we use a quasi-Newton method to solve the resulting nonlinear elliptic system. We also provide a proof of the existence and uniqueness of the solution.

Numerical simulation of blood flow in medium-to-large arteries is considered in Chapter 5. As we already mentioned, the blood in large arteries is modeled by the Navier-Stokes equations and we use the Navier equation for the elastic membrane to model the arterial wall behavior. Since the numerical simulation of the resulting system is quite involved and costly we apply asymptotic reduction to obtain a set of reduced 1D equations. We employ Riemann invariants to derive the conditions at the bifurcation point of the artery. The second order Lax-Wendroff scheme is employed for the numerical solution of the resulting
model. Based on our numerical results we present suggestions for the optimal design of the bifurcated prosthesis.

The results of Chapter 3 and Chapter 4 were published [30, 28, 29]. The main results of Chapter 5 were accepted for publication [87].
Chapter 2

A Lagrange multiplier based domain decomposition method for wave propagation in heterogeneous media

2.1 Introduction

The main goal of this chapter is to address the numerical solution of a wave equation with discontinuous coefficients by a finite element method using domain decomposition and semimatching grids. A wave equation with absorbing boundary conditions is considered, the coefficients in the equation essentially differ in the subdomains. The problem is approximated by an explicit in time finite difference scheme combined with a piecewise linear finite element method in the space variables on a semimatching grid. The matching condition on the interface is taken into account by means of Lagrange multipliers. The resulting system of linear equations of the saddle-point form is solved by a conjugate gradient method.
2.2 Problem formulation

Let $\Omega \subset \mathbb{R}^2$ be a rectangular domain with sides parallel to the coordinate axes and boundary $\Gamma_{ext}$ (see Fig. 2.1). Now let $\Omega_2 \subset \Omega$ be a proper subdomain of $\Omega$ with a curvilinear boundary and $\Omega_1 = \Omega \setminus \Omega_2$. We consider the following linear wave problem:

$$\begin{cases}
\varepsilon \frac{\partial^2 u}{\partial t^2} - \nabla \cdot (\mu^{-1} \nabla u) = f \text{ in } \Omega \times (0, T), \\
\sqrt{\varepsilon \mu^{-1}} \frac{\partial u}{\partial t} + \mu^{-1} \frac{\partial u}{\partial n} = 0 \text{ on } \Gamma_{ext} \times (0, T), \\
u(x, 0) = n(x, 0) = 0.
\end{cases} \tag{2.1}$$

Here $\nabla u = \left( \frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2} \right)$, $n$ is the unit outward normal vector on $\Gamma_{ext}$; we suppose that $\mu_i = \mu|_{\Omega_i}$, $\varepsilon_i = \varepsilon|_{\Omega_i}$ are positive constants $\forall i = 1, 2$ and, $f_i = f|_{\Omega_i} \in C(\bar{\Omega}_i \times [0, T])$.

Let $\varepsilon(x) = \{\varepsilon_1 \text{ if } x \in \Omega_1, \varepsilon_2 \text{ if } x \in \Omega_2\}$ and $\mu(x) = \{\mu_1 \text{ if } x \in \Omega_1, \mu_2 \text{ if } x \in \Omega_2\}$. We define a weak solution of problem (2.1) as a function $u$ such that

$$u \in L^\infty(0, T; H^1(\Omega)), \frac{\partial u}{\partial t} \in L^\infty(0, T; L^2(\Omega)), \frac{\partial u}{\partial t} \in L^2(0, T; L^2(\Gamma_{ext})) \tag{2.2}$$
for a.a. $t \in (0, T)$ and for all $w \in H^1(\Omega)$ satisfying the equation
\begin{equation}
\int_\Omega \varepsilon(x) \frac{\partial^2 u}{\partial t^2} \, dx + \mu^{-1}(x) \nabla u \cdot \nabla w \, dx + \sqrt{\varepsilon_1 \mu_1^{-1}} \int_{\Gamma_{\text{ext}}} \frac{\partial u}{\partial t} \, w \, d\Gamma = \int_\Omega f \, w \, dx \tag{2.3}
\end{equation}
with the initial conditions
\[
u(x, 0) = \frac{\partial u}{\partial t}(x, 0) = 0.
\]
Note that the first term in (2.3) means the duality between $(H^1(\Omega))^*$ and $H^1(\Omega)$.

Now using a Faedo-Galerkin method (as in [17]) one can prove the following

**Theorem 2.1.** Under the assumptions (2.2) there exists a unique weak solution of problem (2.1).

Let
\[
E(t) = \frac{1}{2} \int_\Omega \varepsilon(x) \left( \frac{\partial u}{\partial t} \right)^2 \, dx + \frac{1}{2} \int_\Omega \mu^{-1}(x) |\nabla u|^2 \, dx
\]
be the energy of the system. We take $w = \frac{\partial u}{\partial t}$ in (2.3) and obtain:
\[
\frac{dE(t)}{dt} + \sqrt{\varepsilon_1 \mu_1^{-1}} \int_{\Gamma_{\text{ext}}} (\frac{\partial u}{\partial t})^2 \, d\Gamma = \int_\Omega f \frac{\partial u}{\partial t} \, dx \leq \|f\|_{L^2(\Omega)} \|\frac{\partial u}{\partial t}\|_{L^2(\Omega)},
\]
since $E(0) = 0$, the following stability inequality holds:
\[
E(t) \leq \text{const} T \|f\|_{L^2(\Omega \times (0, T))}, \quad \forall t \in (0, T).
\]

In order to use a structured grid in a part of the domain $\Omega$, we introduce a rectangular domain $R$ with sides parallel to the coordinate axes, such that $\Omega_2 \subset R \subset \Omega$ with $\gamma$ the boundary of $R$ (Fig. 2.1).

Define $\tilde{\Omega} = \Omega \setminus R$ and let the subscript 1 of a function $v_1$ mean that this function is defined over $\tilde{\Omega} \times [0, T]$, while $v_2$ is a function defined over $R \times [0, T]$.

Now we formulate problem (2.3) variationally as follows:

Let
\[
W_1 = \{ v \in L^\infty(0, T; H^1(\tilde{\Omega})), \quad \frac{\partial v}{\partial t} \in L^\infty(0, T; L^2(\tilde{\Omega})), \quad \frac{\partial v}{\partial t} \in L^2(0, T; L^2(\Gamma_{\text{ext}})) \},
\]
\[ W_2 = \{ v \in L^\infty(0,T;H^1(R)), \quad \frac{\partial v}{\partial t} \in L^\infty(0,T;L^2(R)) \}, \]

Find a pair \((u_1, u_2) \in W_1 \times W_2\), such that \(u_1 = u_2\) on \(\gamma \times (0,T)\) and for a.a. \(t \in (0,T)\)

\[
\begin{aligned}
&\int_\Omega \varepsilon_1 \frac{\partial^2 u_1}{\partial t^2} w_1 dx + \int_\Omega \mu_1^{-1} \nabla u_1 \cdot \nabla w_1 dx + \int_\Omega \varepsilon(x) \frac{\partial^2 u_2}{\partial t^2} w_2 dx \\
&+ \int_R \mu_1^{-1}(x) \nabla u_2 \cdot \nabla w_2 dx + \int_\Gamma_{\text{ext}} \frac{\partial u_1}{\partial t} w_1 d\Gamma = \int_\Omega f_1 w_1 dx + \int_R f_2 w_2 dx
\end{aligned}
\]  

(2.4)

for all \((w_1, w_2) \in H^1(\tilde{\Omega}) \times H^1(R)\) such that \(w_1 = w_2\) on \(\gamma\),

\[ u(x, 0) = \frac{\partial u}{\partial t}(x, 0) = 0. \]

Now, introduce the interface supported Lagrange multiplier \(\lambda\) (a function defined over \(\gamma \times (0,T)\)), problem (2.4) can be written in the following way:

Find a triple \((u_1, u_2, \lambda) \in W_1 \times W_2 \times L^\infty(0,T;H^{-1/2}(\gamma))\), which for a.a. \(t \in (0,T)\)

satisfies

\[
\begin{aligned}
&\int_\Omega \varepsilon_1 \frac{\partial^2 u_1}{\partial t^2} w_1 dx + \int_\Omega \mu_1^{-1} \nabla u_1 \cdot \nabla w_1 dx + \int_\Omega \varepsilon(x) \frac{\partial^2 u_2}{\partial t^2} w_2 dx \\
&+ \int_R \mu_1^{-1}(x) \nabla u_2 \cdot \nabla w_2 dx + \int_\Gamma_{\text{ext}} \frac{\partial u_1}{\partial t} w_1 d\Gamma + \int_\gamma \lambda(w_2 - w_1) d\gamma = 0\cr
&\int_\Omega f_1 w_1 dx + \int_R f_2 w_2 dx \quad \text{for all } w_1 \in H^1(\tilde{\Omega}), \ w_2 \in H^1(R);\cr
&\int_\gamma \zeta(w_2 - w_1) d\gamma = 0 \quad \text{for all } \zeta \in H^{-1/2}(\gamma),
\end{aligned}
\]  

(2.5)

(2.6)

and the initial conditions from (2.1).

\textbf{Remark 2.1.} We selected the time dependent approach to capture harmonic solutions since it substantially simplifies the linear algebra of the solution process. Furthermore, there exist various techniques to speed up the convergence of transient solutions to periodic ones (see, e.g. [9]).
2.3 Time discretization

In order to construct a finite difference approximation in time of problem (2.5), (2.6) we partition the segment $[0, T]$ into $N$ intervals using a uniform discretization step $\Delta t = T/N$. Let $u^n_i \approx u_i(n \Delta t)$ for $i = 1, 2, \lambda^n \approx \lambda(n \Delta t)$. The explicit in time semidiscrete approximation to problem (2.5), (2.6) reads as follows:

\[ u^n_0 = u^n_1 = 0; \]

for $n = 1, 2, \ldots, N - 1$ find $u^{n+1}_1 \in H^1(\bar{\Omega})$, $u^{n+1}_2 \in H^1(R)$ and $\lambda^{n+1} \in H^{-1/2}(\gamma)$ such that

\[
\int_{\bar{\Omega}} \varepsilon_1 \frac{u^{n+1}_1 - 2u^n_1 + u^{n-1}_1}{\Delta t^2} w_1 dx + \int_{\bar{\Omega}} (\varepsilon(x) \frac{u^{n+1}_2 - 2u^n_2 + u^{n-1}_2}{\Delta t^2} w_2 dx + \int_{\bar{R}} \mu^{-1}(x) \nabla u^n_2 \cdot \nabla w_2 dx
\]

\[ + \int_{\Gamma_{ext}} \frac{\varepsilon_1 \mu^{-1}}{2\Delta t} u^n_1 w_1 d\Gamma + \int_{\gamma} \lambda^{n+1}(w_2 - w_1) d\gamma = \int_{\bar{\Omega}} f^n_1 w_1 dx + \int_{\bar{R}} f^n_2 w_2 dx \quad \text{for all } w_1 \in H^1(\bar{\Omega}), w_2 \in H^1(R); \]

\[ \int_{\gamma} \zeta(u^{n+1}_2 - u^{n+1}_1) d\gamma = 0 \quad \text{for all } \zeta \in H^{-1/2}(\gamma). \]  

Remark 2.2. The integral over $\gamma$ is written formally; the exact formulation requires the use of the duality pairing $\langle \cdot, \cdot \rangle$ between $H^{-1/2}(\gamma)$ and $H^{1/2}(\gamma)$.

2.4 Fully discrete scheme

To construct a fully discrete space-time approximation to problem (2.5), (2.6) we will use a lowest order finite element method on two grids semimatching on $\gamma$ (Fig. 2.2) for the space discretization. Namely, let $T_{1h}$ and $T_{2h}$ be triangulations of $\bar{\Omega}$ and $R$, respectively. Further we suppose that both triangulations are regular in the sense that $\frac{r(e)}{h(e)} \leq q = \text{const}$ for all $e \in T_{1h}$ and $e \in T_{2h}$, where $q$ does not depend on $e$; $r(e)$ is the radius of the circle inscribed in $e$, while $h(e)$ is the diameter of $e$. 

14
We denote by $\mathcal{T}_{1h}$ a coarse triangulation, and by $\mathcal{T}_{2h}$ a fine one. Every edge $\partial e \subset \gamma$ of a triangle $e \in \mathcal{T}_{1h}$ is supposed to consist of $m_e$ edges of triangles from $\mathcal{T}_{2h}$, $1 \leq m_e \leq m$ for all $e \in \mathcal{T}_{1h}$.

Moreover, let a triangulation $\mathcal{T}_{2h}$ be such that the curvilinear boundary $\partial \Omega_2$ is approximated by a polygonal line consisting of the edges of triangles from $\mathcal{T}_{2h}$ whose vertices belong to $\partial \Omega_2$. Further, we say that a triangle $e \in \mathcal{T}_{2h}$ lies in $\Omega_2$ if its larger part lies in $\Omega_2$, i.e. $\text{meas}(e \cap \Omega_2) > \text{meas}(e \cap (R \setminus \Omega_2))$, otherwise this triangle lies in $R \setminus \Omega_2$.

Let $V_{1h} \subset H^1(\tilde{\Omega})$ be the space of the functions globally continuous, and affine on each $e \in \mathcal{T}_{1h}$, i.e. $V_{1h} = \{ u_h \in H^1(\tilde{\Omega}) : u_h \in P_1(e) \ \forall e \in \mathcal{T}_{1h} \}$. Similarly, $V_{2h} \subset H^1(R)$ is the space of the functions globally continuous, and affine on each $e \in \mathcal{T}_{2h}$.

For approximating the Lagrange multipliers space $\Lambda = H^{-1/2}(\gamma)$ we proceed as follows. Assume that on $\gamma$, $\mathcal{T}_{1h}$ is two times coarser than $\mathcal{T}_{2h}$; then let us divide every edge $\partial e$ of a triangle $e$ from the coarse grid $\mathcal{T}_{1h}$, which is located on $\gamma$ ($\partial e \subset \gamma$), into two parts using its midpoint. Now, we consider the space of the piecewise constant functions, which are constant on every union of half-edges with a common vertex (see Fig. 2.3).

Further, we use quadrature formulas for approximating the integrals over the triangles from $\mathcal{T}_{1h}$ and $\mathcal{T}_{2h}$, as well as over $\Gamma_{\text{ext}}$. For a triangle $e$ we set

$$\int_e \phi(x)dx \approx \frac{1}{3} \text{meas}(e) \sum_{i=1}^3 \phi(a_i) \equiv S_e(\phi)$$
Figure 2.3: Space $\Lambda$ is the space of the piecewise constant functions defined on every union of half-edges with common vertex.

where the $a_i$’s are the vertices of $e$ and $\phi(x)$ is a continuous function on $e$. Similarly,

$$\int_{\partial e} \phi(x)dx \approx \frac{1}{2} \text{meas}(\partial e) \sum_{i=1}^{2} \phi(a_i) \equiv S_{\partial e}(\phi),$$

where $a_i$’s are the endpoints of the segment $\partial e$ and $\phi(x)$ is a continuous function on this segment.

We use the notations:

$$S_i(\phi) = \sum_{e \in T_h} S_e(\phi), \quad i = 1, 2, \quad \text{and} \quad S_{\Gamma_{\text{ext}}}(\phi) = \sum_{\partial e \in \Gamma_{\text{ext}}} S_{\partial e}(\phi).$$

Now, the fully discrete problem reads as follows:

Let $u_{1h}^0 = u_{2h}^1 = 0$, $i = 1, 2$;

for $n = 1, 2, \ldots, N - 1$ find $(u_{1h}^{n+1}, u_{2h}^{n+1}, \lambda_h^{n+1}) \in V_{1h} \times V_{2h} \times \Lambda_h$ such that

$$\left\{ \begin{array}{l}
\frac{\varepsilon_1}{\Delta t^2} S_1((u_{1h}^{n+1} - 2u_{1h}^{n} + u_{1h}^{n-1})w_{1h}) + S_1(\mu^{-1} \nabla u_{1h}^{n} \cdot \nabla w_{1h}) \\
+ \frac{1}{\Delta t^2} S_2(\varepsilon(x)(u_{2h}^{n+1} - 2u_{2h}^{n} + u_{2h}^{n-1})w_{2h}) + S_2(\mu^{-1}(x) \nabla u_{2h}^{n} \cdot \nabla w_{2h}) \\
+ \sqrt{\varepsilon_1 \mu^{-1}} \frac{1}{2\Delta t} S_{\Gamma_{\text{ext}}}((u_{1h}^{n+1} - u_{1h}^{n-1})w_{1h}) + \int_{\gamma} \lambda_h^{n+1}(w_{2h} - w_{1h})d\gamma = \\
S_1(f_1^n w_{1h}) + S_2(f_2^n w_{2h}) \quad \text{for all } w_{1h} \in V_{1h}, w_{2h} \in V_{2h};
\end{array} \right.$$  \hspace{1cm} (2.9)

$$\int_{\gamma} \zeta_h(u_{2h}^{n+1} - u_{1h}^{n+1})d\gamma = 0 \quad \text{for all } \zeta_h \in \Lambda_h.  \hspace{1cm} (2.10)$$

16
Note that in \( S_2(\varepsilon(x)(u_{2h}^{n+1} - 2u_{2h}^n + u_{2h}^{n-1})w_{2h}) \) we take \( \varepsilon(x) = \varepsilon_2 \) if a triangle \( e \in T_{2h} \) lies in \( \Omega_2 \) and \( \varepsilon(x) = \varepsilon_1 \) if it lies in \( R \setminus \Omega_2 \), and similarly for \( S_2(\mu^{-1}(x)\nabla u_{2h}^n \nabla w_{2h}) \).

Denote by \( u_1, u_2 \) and \( \lambda \) the vectors of the nodal values of the corresponding functions \( u_{1h}, u_{2h} \) and \( \lambda_h \). Then in order to find \( u_{1h}^{n+1}, u_{2h}^{n+1} \) and \( \lambda^{n+1} \) for a fixed time \( t^{n+1} \) we have to solve a system of linear equations such as

\[
Au + B^T \lambda = F, \tag{2.11}
\]

\[
Bu = 0, \tag{2.12}
\]

where matrix \( A \) is diagonal, positive definite and defined by

\[
(Au, w) = \frac{\varepsilon_1}{\Delta t^2} S_1(u_{1h}w_{1h}) + \frac{1}{\Delta t^2} S_2(\varepsilon(x)u_{2h}w_{2h}) + \frac{\sqrt{\varepsilon_1 \mu_1^{-1}}}{2\Delta t} S_{\Gamma_{ext}}(u_{1h}w_{1h}),
\]

and where the rectangular matrix \( B \) is defined by

\[
(Bu, \lambda) = \int_{\gamma} \lambda_h(u_{2h} - u_{1h}) d\Gamma,
\]

and vector \( F \) depends on the nodal values of the known functions \( u_{1h}^n, u_{2h}^n, u_{1h}^{n-1} \) and \( u_{2h}^{n-1} \).

Eliminating \( u \) from equation (2.11) we obtain

\[
BA^{-1}B^T \lambda = BA^{-1}F, \tag{2.13}
\]

with a symmetric matrix \( C = BA^{-1}B^T \). Let us prove that \( C \) is positive definite. Obviously, \( \text{Ker} C = \text{Ker} B^T \). Suppose, that \( B^T \lambda = 0 \), then a function \( \lambda_h \in \Lambda_h \) corresponding to vector \( \lambda \) satisfies

\[
I \equiv \int_{\gamma} \lambda_h u_h d\gamma = 0
\]

for all \( u_h \in V_{1h} \). Choose \( u_h \) equal to \( \lambda_h \) in the nodes of \( T_{1h} \) located on \( \gamma \). Direct calculations give

\[
I = \frac{1}{2} \sum_{i=1}^{N_h} \left[ h_i + h_{i+1} \frac{\lambda_i^2}{2} + h_{i+1} \frac{\lambda_i + \lambda_{i+1}}{2} \right],
\]

17
where \( N_\lambda \) is the number of edges of \( T_{1h} \) on \( \gamma \), \( h_i \) is the length of \( i \)-th edge and \( h_{N_\lambda+1} \equiv h_1 \), \( \lambda_{N_\lambda+1} \equiv \lambda_1 \). Thus, the equality \( I = 0 \) implies that \( \lambda = 0 \), i.e. \( \text{Ker} \, B^T = \{0\} \). As a consequence we have

**Theorem 2.2.** Problem (2.9), (2.10) has a unique solution \((u_h, \lambda_h)\).

**Remark 2.3.** A closely related domain decomposition method applied to the solution of linear parabolic equations is discussed in [27].

### 2.5 Energy inequality

**Theorem 2.3.** Let \( h_{\text{min}} \) denote the minimal diameter of the triangles from \( T_{1h} \cup T_{2h} \). There exists a positive number \( c \) such that the condition

\[
\Delta t \leq c \min\{\sqrt{\varepsilon_1 \mu_1}, \sqrt{\varepsilon_2 \mu_2}\} \, h_{\text{min}}
\]  

ensures the positive definiteness of the quadratic form

\[
\mathcal{E}^{n+1} = \frac{1}{2} \varepsilon_1 S_1\left(\frac{u_{1h}^{n+1} - u_{1h}^n}{\Delta t}\right)^2 + \frac{1}{2} S_2\left(\frac{u_{2h}^{n+1} - u_{2h}^n}{\Delta t}\right)^2 +
\]

\[
\frac{1}{2} S_1(\mu_1^{-1}|\nabla\left(\frac{u_{1h}^{n+1} + u_{1h}^n}{2}\right)|^2) + \frac{1}{2} S_2(\mu^{-1}|\nabla\left(\frac{u_{2h}^{n+1} + u_{2h}^n}{2}\right)|^2)
\]

\[
- \frac{\Delta t^2}{8} S_1(\mu_1^{-1}|\nabla\left(\frac{u_{1h}^{n+1} - u_{1h}^n}{\Delta t}\right)|^2) - \frac{\Delta t^2}{8} S_2(\mu^{-1}|\nabla\left(\frac{u_{2h}^{n+1} - u_{2h}^n}{\Delta t}\right)|^2),
\]

which we call the discrete energy.

System (2.9), (2.10) satisfies the energy identity

\[
\mathcal{E}^{n+1} - \mathcal{E}^n + \frac{\sqrt{\varepsilon_1 \mu_1^{-1}}}{4 \Delta t} S_{\text{ext}}((u_{1h}^{n+1} - u_{1h}^{n-1})^2) =
\]

\[
\frac{1}{2} S_1(f_1^n(u_{1h}^{n+1} - u_{1h}^{n-1})) + \frac{1}{2} S_2(f_2^n(u_{2h}^{n+1} - u_{2h}^{n-1}))
\]

(2.16)

and the numerical scheme is stable: there exists a positive number \( M = M(T) \) such that

\[
\mathcal{E}^n \leq M \Delta t \sum_{k=1}^{n-1} (S_1((f_1^k)^2) + S_2((f_2^k)^2)) \forall n
\]

(2.17)
Proof. Let $n \geq 1$; from equation (2.10) written for $t_{n+1}$ and $t_{n-1}$ we obtain

$$\int_\gamma \zeta_h((u_{2h}^{n+1} - u_{2h}^{n-1}) - (u_{1h}^{n+1} - u_{1h}^{n-1}))d\gamma = 0 \text{ for all } \zeta_h \in \Lambda_h$$  \hspace{1cm} (2.18)

Choosing $w_{1h} = \frac{u_{1h}^{n+1} - u_{1h}^{n-1}}{2}$, $w_{2h} = \frac{u_{2h}^{n+1} - u_{2h}^{n-1}}{2}$ in (2.9) and $\zeta_h = -\frac{\lambda_{n+1}^{n+1}}{2}$ in (2.18) we add these equalities. Using the identities

$$(u_{ih}^{n+1} - 2u_{ih}^n + u_{ih}^{n-1})(u_{ih}^{n+1} - u_{ih}^{n-1}) = (u_{ih}^{n+1} - u_{ih}^n)^2 - (u_{ih}^n - u_{ih}^{n-1})^2$$

and

$$u_{ih}^n u_{ih}^{n+1} = \frac{1}{4}((u_{ih}^{n+1} + u_{ih}^n)^2 - (u_{ih}^n - u_{ih}^{n-1})^2)$$

after several technical transformations we obtain

$$\mathcal{E}^{n+1} - \mathcal{E}^n = \sqrt{\frac{\varepsilon_1 \mu_1^{-1}}{4\Delta t}} S_{\text{ext}}((u_{1h}^{n+1} - u_{1h}^{n-1})^2) =$$

$$\frac{1}{2} S_1(f_1^n(u_{1h}^{n+1} - u_{1h}^{n-1})) + \frac{1}{2} S_2(f_2^n(u_{2h}^{n+1} - u_{2h}^{n-1})).$$

Therefore

$$\mathcal{E}^{n+1} \leq \mathcal{E}^n + \frac{1}{2} \Delta t S_1^{1/2}((f_1^n)^2)(S_1^{1/2}((u_{1h}^{n+1} - u_{1h}^{n-1})^2) + S_1^{1/2}((u_{1h}^{n+1} - u_{1h}^n)^2))$$

$$+ \frac{1}{2} \Delta t S_2^{1/2}((f_2^n)^2)(S_2^{1/2}((u_{2h}^{n+1} - u_{2h}^{n-1})^2) + S_2^{1/2}((u_{2h}^{n+1} - u_{2h}^n)^2)).$$  \hspace{1cm} (2.19)

Now, we will show that under condition (2.14) the quadratic form $\mathcal{E}^n$ is positive definite; more precisely, that there exists a positive constant $\delta$ such that

$$\mathcal{E}^n \geq \delta \left(S_1\left((u_{1h}^{n+1} - u_{1h}^n)^2\right) + S_2\left((u_{2h}^{n+1} - u_{2h}^n)^2\right)\right).$$  \hspace{1cm} (2.20)

Obviously, it is sufficient to prove the inequality

$$4\varepsilon_e \mu_e S_e(v_h^2) \geq \Delta t^2 S_e(|\nabla v_h|^2) \ \forall e \in T_{1h} \cup T_{2h}, \ \forall v_h \in P_1(e),$$  \hspace{1cm} (2.21)

where $\varepsilon_e$ and $\mu_e$ are defined by $\varepsilon_e = \varepsilon_1$ or $\varepsilon_e = \varepsilon_2$ (respectively, $\mu_e = \mu_1$ or $\mu_e = \mu_2$). It is known that for a regular triangulation

$$S_e(|\nabla v_h|^2) \leq 1/c_1^2 h_e^{-2} S_e(v_h^2)$$  \hspace{1cm} (2.22)
with a positive constant $c_1$, universal for all triangles $e$, where $h_e$ is the minimal length of the sides of $e$. Combining (2.21) and (2.22) we observe that the time step $\Delta t$ should satisfy the inequality

$$\Delta t \leq c \sqrt{\varepsilon h_e}, \quad (c = \sqrt{2c_1}),$$

(2.23)

for all $e \in T_{1h} \cup T_{2h}$. Evidently, (2.14) ensures the validity of (2.23).

Further, using the relation (2.20), $\mathcal{E}^1 = 0$ and summing the inequalities (2.19), one obtains the stability inequality (2.17):

$$\mathcal{E}^n \leq M \Delta t \sum_{k=1}^{n-1} (S_1((f_1^k)^2) + S_2((f_2^k)^2)), \quad \forall n.$$ 

\[ \square \]

### 2.6 Numerical experiments

In order to solve the system of linear equations (2.11)-(2.12) at each time step we use a Conjugate Gradient Algorithm in the form given by Glowinski and LeTallec [33]:

1. $\lambda^0$ given,

2. $Au^0 = F - B\lambda^0$;

3. $g^0 = -B^T u^0$,

   if $||g^0|| \leq \varepsilon_0$ take $\lambda = \lambda^0$, 

   else

4. $w^0 = g^0$.

   For $m \geq 0$, assuming that $\lambda^m, g^m, w^m$ are known

5. $Au^m = Bw^m$.

6. $\bar{g}^m = B^T \bar{u}^m$. 

20
7. $\rho_m = \frac{|g_m|^2}{\langle g_m, w^m \rangle}$,

8. $\lambda^{m+1} = \lambda^m - \rho_m w^m$.

9. $u^{m+1} = u^m + \rho_m \hat{v}^m$.

10. $g^{m+1} = g^m - \rho_m g^m$,

    if $\frac{g^{m+1} \cdot g^{m+1}}{g^m \cdot g^m} \leq \varepsilon$ then take $\lambda = \lambda^{m+1}$,

    else

11. $\gamma_m = \frac{g^{m+1} \cdot g^{m+1}}{g^m \cdot g^m}$.

12. $w^{m+1} = g^{m+1} + \gamma_m w^m$,

    do $m = m + 1$ and go to 5.

We consider problem (2.9)-(2.10) with a source term given by the harmonic planar wave:

$$u^{inc} = -e^{ik(t-a \cdot x)}$$

where $\{x_j\}^2_{j=1}$, $\{a_j\}^2_{j=1}$, $k$ is the angular frequency and $|a| = 1$.

For our numerical simulation we consider two cases: the first with the frequency of the incident wave $f = 0.6$ GHz and the second with $f = 1.2$ GHz, which gives us wavelengths $L = 0.5$ meters and $L = 0.25$ meters respectively.

First, we consider the scattering by a perfectly reflecting obstacle. For the first experiment we have chosen $\Omega_2$ to be a perfectly reflecting disk with diameter $d = 0.5$ meters, and $\Omega$ is a 2 meter $\times$ 2 meter rectangle. Figure 2.4 shows the contour plot of the real part of the scattered solution for wavelength $L = 0.5$ meters and $L = 0.25$ meters.

The second experiment shows the wave propagation through the domain $\Omega$ with an obstacle in form of an airfoil for wavelengths $L = 0.5$ meters and $L = 0.25$ meters. Figure 2.6 shows the contour plot for the case when the incident wave is coming from the left and Figure 2.8 shows the case when the incident wave is coming from the lower left corner.
with an angle of 45°. For all the experiments we chose the time step to be $\Delta t = T/50$, where $T = 1/f = 1.66 \times 10^{-9}$ sec is a time period corresponding to $L = 0.5$ meters and $T = 1/f = 0.83 \times 10^{-9}$ sec for $L = 0.25$ meters. We present the energy decay after the source term was set to zero in Figure 2.5 (for an obstacle in the form of a disk) and Figure 2.7 (for an obstacle in the form of an airfoil).
Figure 2.4: Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$ (bottom) meters. Incident wave coming from the left.
Figure 2.5: Energy behavior versus time for $L = 0.5$ (top) and $L = 0.25$ (bottom).
Figure 2.6: Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$ (bottom) meters. Incident wave coming from the left.
Figure 2.7: Energy behavior versus time for $L = 0.5$ (top) and $L = 0.25$ (bottom).
Figure 2.8: Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$ (bottom) meters. Incident wave coming from the lower left corner with an angle of 45 degrees.
The next set of numerical experiments contains the simulations of wave propagation through a domain with an obstacle completely consisting of a coating material. We have taken the coating material coefficients to be $\varepsilon_2 = 1$ and $\mu_2 = 9$, implying that the speed of propagation in the coating material is three times slower than in the air. As before $\Omega$ is a 2 meter $\times$ 2 meter rectangle and we ran our simulations for two different shapes of $\Omega_2$:

1. $\Omega_2$ is a disk with diameter $d = 0.5$ meters, and

2. $\Omega_2$ has the shape of an airfoil.

For the solution of this problem for an incident frequency $f = 0.6$ GHz we have used a mesh with a total of 8435 nodes and 16228 elements. The time step was taken to be $\Delta t = T/50$, where $T = 1/f = 1.66 \times 10^{-9}$ sec is a time period. We used a mesh consisting of 20258 nodes (39514 elements) for solving the problem for an incident wave with the frequency $f = 1.2$ GHz. The time step was equal to $T/50$, $T = 1/f = 0.83 \times 10^{-9}$ sec.

In Figures 2.9 and 2.10 we present the contour plot of the real part of the solution for the incident frequency $L = 0.5$ and $L = 0.25$ respectively.

Figures 2.13 and 2.14 show the energy decay after four time periods when we set the source term equal to zero.
Figure 2.9: Contour plot of the real part of the solution for $L = 0.5$ meters.

Figure 2.10: Contour plot of the real part of the solution for $L = 0.25$ meters.
Figure 2.11: Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$ (bottom). Incident wave coming from the left.
Figure 2.12: Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$ (bottom). Incident wave coming from the lower left corner with an angle of 45 degrees.
Figure 2.13: Energy behavior for $L = 0.5$ meters.

Figure 2.14: Energy behavior for $L = 0.25$ meters.
We also performed numerical computations for the case when the obstacle is an airfoil with a coating (Figure 2.15). The coating region is moon shaped and, as before, $\varepsilon_2 = 1$ and $\mu_2 = 9$.

We show in Figure 2.16 the contour plot of the real part of the solution for the incident frequency $L = 0.5$ meters and $L = 0.25$ meters for the case when the incident wave is coming from the left.

Figure 2.17 presents the contour plot of the real part of the solution for incident frequency, $L = 0.5$ meters and $L = 0.25$ meters for the case when incident wave is coming from the lower left corner with angle equal to $45^0$.

One can observe the energy decay in Figure 2.18 when the source term has been set equal to zero.

A crucial observation for all of the numerical experiments mentioned is that despite the fact that a mesh discontinuity takes place over $\gamma$ together with a weak forcing of the matching conditions, we do not observe a discontinuity of the computed fields.
Figure 2.16: Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$ (bottom). Incident wave coming from the left.
Figure 2.17: Contour plot of the real part of the solution for $L = 0.5$ (top) and $L = 0.25$ (bottom). Incident wave coming from the left lower corner with a 45 degree angle.
Figure 2.18: Energy behavior versus time for $L = 0.5$ (top) and $L = 0.25$ (bottom).
Chapter 3

Solution of a wave equation by a mixed finite element - fictitious domain method

3.1 Introduction

In this chapter we discuss the numerical solution of a linear wave equation using a combined fictitious domain – mixed finite element methodology. We consider a linear wave equation with constant coefficient in a domain which is a rectangle containing a circular obstacle (Figure 3.1). Dirichlet boundary conditions are imposed on the obstacle boundary, while absorbing boundary conditions are prescribed on the external part of the boundary. We use a mixed variational formulation to construct a discrete problem. This discrete scheme is "explicit" in time and is of the lowest order finite element approximation in space. To avoid difficulties concerning the implementation of a discrete scheme in a curvilinear domain, we construct a finite element approximation of the mixed problem in a rectangular domain containing the original domain (see e.g. [5]) . The interface conditions are treated by Lagrange multipliers.

A conjugate gradient algorithm (discussed in [33], [18]) is used for solving the resulting system of linear algebraic equations (of the "saddle-point" type).
3.2 Formulation of the problem

Let $\Omega$ be a bounded domain in $\mathbb{R}^2$ with boundary $\Gamma_{ext}$. We consider the following wave problem:

\[
\frac{1}{c^2} \frac{\partial^2 u}{\partial t^2} - \Delta u = 0 \quad \text{in} \quad \Omega \times (0, T),
\]

with the absorbing boundary condition

\[
\frac{1}{c} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial n} = 0 \quad \text{on} \quad \Gamma_{ext} \times (0, T),
\]

and the initial conditions

\[
u(0) = u_0, \quad u_t(0) = u_1.
\]

Here $\mathbf{n}$ is the outward unit normal vector on $\Gamma_{ext}$.

We define a weak solution of problem (3.1) – (3.3) as a function $u$ such that

$u \in L^\infty(0, T; H^1(\Omega)), \frac{\partial u}{\partial t} \in L^\infty(0, T; L^2(\Omega)), \frac{\partial u}{\partial \mathbf{n}} \in L^2(0, T; L^2(\Gamma_{ext})), \quad \text{and for a.a.} \ t \in (0, T) \ \text{and for all} \ w \in H^1(\Omega) \ \text{satisfies the equation}

\[
\frac{1}{c^2} \int_\Omega \frac{\partial^2 u}{\partial t^2} w \, dx + \int_\Omega \nabla u \cdot \nabla w \, dx + \frac{1}{c} \int_{\Gamma_{ext}} \frac{\partial u}{\partial \mathbf{n}} w \, d\Gamma = 0
\]
and initial conditions (3.3).

As in [17] one can prove the following

**Theorem 3.1.** Let $u_0 \in H^1(\Omega)$, $u_1 \in L^2(\Omega)$. Then there exists a unique weak solution of problem (3.1) – (3.3).

Now, let us consider an equivalent approach based on a mixed formulation. We introduce the new variables:

$$
p = \nabla u, \quad v = \frac{\partial u}{\partial t}. \quad (3.5)
$$

Clearly, $p$ and $v$ satisfy the following equations:

$$\frac{\partial p}{\partial t} = \nabla v \quad \text{and} \quad \frac{\partial v}{\partial t} = c^2 \nabla \cdot p \quad \text{in} \quad \Omega \times (0, T), \quad (3.6)$$

$$v + cp \cdot n = 0 \quad \text{on} \quad \Gamma_{ext} \times (0, T), \quad (3.7)$$

$$p(0) = \nabla u_0, \quad v(0) = u_1. \quad (3.8)$$

Multiplying the first equation in (3.6) by $q \in H(\Omega, \text{div}) = \{ q \in (L^2(\Omega))^2 : \nabla \cdot q \in L^2(\Omega) \}$, the second equation by $w \in L^2(\Omega)$, and then applying the divergence theorem we obtain the following variational formulation of problem (3.6)-(3.8):

$$\int_{\Omega} \frac{\partial p}{\partial t} \cdot q dx + \int_{\Omega} v \cdot q dx + c \int_{\Gamma_{ext}} (p \cdot n)(q \cdot n) d\Gamma = 0, \quad \forall q \in H(\Omega, \text{div}), \quad (3.9)$$

$$\int_{\Omega} \frac{\partial v}{\partial t}wdx - c^2 \int_{\Omega} \nabla \cdot pwdx = 0, \quad \forall w \in L^2(\Omega), \quad (3.10)$$

$$p(0) = \nabla u_0, \quad v(0) = u_1. \quad (3.11)$$

**Lemma 3.1.** Problem (3.6)-(3.8) satisfies the energy dissipation property.

**Proof.** Let us denote by

$$E(t) = \frac{1}{2} \int_{\Omega} |p(x, t)|^2 dx + \frac{1}{2} c^2 \int_{\Omega} v^2(x, t) dx$$

39
the energy of the system at time $t > 0$. We multiply the first equation in (3.6) by $p$ and the second equation by $v$, add them and then integrate over $\Omega$:

$$
\int_{\Omega} \frac{\partial p}{\partial t} \cdot pdx + \frac{1}{c^2} \int_{\Omega} \frac{\partial v}{\partial t} vdx = \int_{\Omega} \nabla v \cdot pdx + \int_{\Omega} \nabla \cdot pvdx = 0.
$$

Using the divergence theorem we have:

$$
\frac{1}{2} \frac{d}{dt} \int_{\Omega} (p^2 + \frac{1}{c^2}v^2)dx = \int_{\Gamma} v \cdot n d\Gamma
$$

Clearly $dE/dt$ satisfies the inequality

$$
\frac{dE(t)}{dt} = -c \int_{\Gamma_{ext}} (p \cdot n)^2 d\Gamma \leq 0,
$$

therefore we have a dissipation of the energy. \(\square\)

### 3.3 Discretization of the problem. Energy inequality

In order to get a fully discrete problem which will be easy to implement, we first construct an "explicit" in time semi-discrete problem.

Let $\Delta t > 0$, be the time step and let $p^n \approx p(n\Delta t)$, $v^{n+1/2} \approx v((n + 1/2)\Delta t)$ for $n = 0, 1, 2, \ldots$ approximate the corresponding functions $p(t)$ and $v(t)$. The time discretization of problem (3.9)-(3.11) reads as follows:

For $n \geq 1$, find $(p^n, v^{n+1/2}) \in H(\Omega, div) \times L^2(\Omega)$ such that

$$
\int_{\Omega} \frac{p^n - p^{n-1}}{\Delta t} \cdot q dx + \int_{\Omega} v^{n-1/2} \nabla \cdot q dx + c \int_{\Gamma_{ext}} (\frac{p^n + p^{n-1}}{2} \cdot n)(q \cdot n) d\Gamma = 0, \quad (3.13)
$$

$$
\forall q \in H(\Omega, div),
$$

$$
\int_{\Omega} v^{n+1/2} - v^{n-1/2} \frac{\Delta t}{2} w dx - c^2 \int_{\Omega} \nabla \cdot p^n w dx = 0, \quad \forall w \in L^2(\Omega),
$$

$$
p^0 = \nabla u_0, \quad \frac{v^{1/2} - v^0}{\Delta t/2} = c^2 \nabla \cdot p^0.
$$

40
Now, we construct a fully discrete problem.

For convenience, we set $\Omega$ to be a rectangular domain with boundaries parallel to the coordinate axes, namely $\Omega = (0, x_L) \times (0, y_L)$. We define $R_x : 0 = x_0 < x_1 < \ldots < x_{N_x} = x_L$ and $R_y : 0 = y_0 < y_1 < \ldots < y_{N_y} = y_L$ to be partitions of $[0, x_L]$ and $[0, y_L]$, respectively, and denote by $\Delta_{i,j}$ a mesh cell – rectangle $[x_i, x_{i+1}] \times [y_j, y_{j+1}]$. We use $\mathcal{T} = \{\Delta_{i,j}\}$ to denote the corresponding partition of $\Omega$.

Let $P_h$ be a finite dimensional subspace of $H(\Omega, \text{div})$ constructed via the lowest order Raviart-Thomas finite element method, namely,

$$P_h = \{p_h \in H(\Omega, \text{div}) : p_h = (p_{1h}, p_{2h}) \in P_{1,0} \times P_{0,1} \text{ for each } \Delta_{i,j} \in \mathcal{T}\},$$

where $P_{k,l}$ is the space of polynomials of degree $k$ in $x$ and $l$ in $y$. By $V_h \subset L_2(\Omega)$ we denote the space of piecewise constant functions, which are constant on every $\Delta_{i,j}$.

Further, let $\Delta_{i,j} \in \mathcal{T}$, then we denote by

$$a_{i,j}^- = (x_i, \frac{1}{2}(y_j + y_{j+1})), \quad a_{i,j}^+ = (x_{i+1}, \frac{1}{2}(y_j + y_{j+1})),
$$
$$b_{i,j}^- = (\frac{1}{2}(x_i + x_{i+1}), y_j), \quad b_{i,j}^+ = (\frac{1}{2}(x_i + x_{i+1}), y_{j+1})$$

the mid–points of the corresponding edges (see Figure 3.2). The values of the fluxes, $p_h \cdot n$, at the mid–points of the finite elements $\Delta_{i,j} \in \mathcal{T}$ are taken as degrees of freedom for $p_h \in P_h$. Thus, for rectangular elements they are $p_{1h}(a_{i,j}^-), p_{2h}(b_{i,j}^-)$ etc. For $v_h \in V_h$ the values at the center of the cells $\Delta_{i,j} \in \mathcal{T}$ are taken as the degrees of freedom.

Further we denote by $P_h$ and $V_h$ the vectors whose components are the degrees of freedom for the corresponding functions $p_h \in P_h$ and $v_h \in V_h$.

We use the following quadrature formula to approximate $\int_\Omega p_h \cdot q_h \, dx$:

$$S_\Delta(p_h \cdot q_h) = \frac{1}{4} \text{meas } \Delta_{i,j} \left( p_{1h}(a_{i,j}^-)q_{1h}(a_{i,j}^-) + p_{1h}(a_{i,j}^+)q_{1h}(a_{i,j}^+) ight.
$$
$$+ p_{2h}(b_{i,j}^-)q_{2h}(b_{i,j}^-) + p_{2h}(b_{i,j}^+)q_{2h}(b_{i,j}^+)),$$
The integral above is then approximated by

\[ S_\Omega(p_h \cdot q_h) = \sum_{\Delta_i,j \in T} S_\Delta(p_h \cdot q_h). \]

The space discretized formulation of problem (3.13)-(3.15) involves the pair \((p_h^n, v_h^{n+1/2}) \in P_h \times V_h\) satisfying

\[
S_\Omega(p_h^n - p_h^{n-1} \cdot \Delta t) + \int_\Omega v_h^{n-1/2} \nabla \cdot q_h \, dx \\
\quad + c \int_{\Gamma_{ext}} \left( \frac{p_h^n + p_h^{n-1}}{2} \cdot n \right) (q_h \cdot n) \, d\Gamma = 0; \quad \forall q_h \in P_h, \tag{3.16}
\]

\[
\int_\Omega \frac{v_h^{n+1/2} - v_h^{n-1/2}}{\Delta t} w_h \, dx - c^2 \int_\Omega \nabla \cdot p_h^n w_h \, dx = 0; \quad \forall w_h \in V_h, \tag{3.17}
\]

with initial conditions

\[ p_h^0 = (\nabla u_0)_h, \quad \frac{v_h^{1/2} - v_h^0}{\Delta t/2} = c^2 \nabla \cdot p_h^0, \tag{3.18} \]

where \((\nabla u_0)_h\) is an appropriate \(P_h\)-approximation of \((\nabla u_0)\).
Vector \((p_h^n, v_h^{n+1/2})\) can be found recurrently from a system of linear algebraic equations, namely

\[
M_p P_h = G_1, \\
M_v V_h = G_2,
\]

where \(M_p\) and \(M_v\) are diagonal matrices defined by

\[
(M_p P_h, Q) = S_\Omega (\frac{p_h^n \cdot q_h}{\Delta t}) + c \int_{\Gamma_{ext}} (\frac{p_h^n \cdot n}{2} (q_h \cdot n)) d\Gamma \quad \forall p_h \in P_h, \forall q_h \in P_h,
\]

\[
(M_v V_h, W) = \frac{1}{c^2} \int_\Omega \frac{v_h^{n+1/2}}{\Delta t} w_h dx \quad \forall v_h \in V_h, \forall w_h \in V_h.
\]

Obviously, matrices \(M_p\) and \(M_v\) are positive definite; thus, there exists a unique solution \((p_h^n, v_h^{n+1/2})\) of problem (3.16), (3.17).

**Theorem 3.2.** Let \(h_{\min}\) denote the minimal mesh step size. Then the condition

\[
\Delta t \leq \frac{1}{2c} h_{\min}
\]

ensures the positive definiteness of the quadratic form

\[
\mathcal{E}^{n+1} = \frac{1}{2} S_\Omega (p_h^n)^2 + \frac{1}{2} c^2 \int_\Omega (v_h^{n+1/2})^2 dx - \frac{\Delta t}{2} \int_\Omega \nabla \cdot p_h^n v_h^{n+1/2} dx,
\]

which we call the discrete energy. System (3.16)-(3.18) satisfies the discrete energy identity

\[
\mathcal{E}^{n+1} - \mathcal{E}^n = -c \Delta t \int_{\Gamma_{ext}} (\frac{p_h^n + p_h^{n-1}}{2} \cdot n)^2 d\Gamma.
\]

Thus,

\[
\mathcal{E}^{n+1} \leq \mathcal{E}^n, \quad \forall n,
\]

and the discrete problem (3.16)-(3.18) is stable.
Proof. Let us choose \( q = \Delta t \frac{p_h^n + p_h^{n-1}}{2} \) in equation (3.16) and \( w_h = \Delta t \frac{v_h^{n+1/2} + v_h^{n-1/2}}{2 c^2} \) in equation (3.17). By adding these equalities we obtain the identity (3.21).

Now, by direct calculations we obtain the inequality
\[
\int_{\Delta_{i,j}} |\nabla \cdot p_h|^2 dx \leq \frac{16}{h_{\min}^2} S_{\Delta_{i,j}}(|p_h|^2)
\]
for any \( p_h \in P_h \) and any \( \Delta_{i,j} \). From here we derive the estimate
\[
\left| \int_{\Omega} \nabla \cdot p_h^n v_h^{n+1/2} dx \right| \leq \frac{4}{h_{\min}} (S_{\Delta_{i,j}}(|p_h|^2))^{1/2} \left( \int_{\Omega} v_h^{n+1/2} dx \right)^{1/2},
\]
thus, under condition (3.19) we get the positive definiteness of \( E^n \) for all \( n \).

\[\Box\]

### 3.4 A fictitious domain method with boundary supported Lagrange multiplier

Now we consider a domain \( \omega \subset \Omega \) with a piecewise smooth boundary \( \gamma \). Let equation (3.1) and initial conditions (3.3) be valid in \( \Omega \setminus \tilde{\omega} \) and problem (3.1) - (3.3) to be completed by the following Dirichlet boundary condition on \( \gamma \):
\[
u = 0 \quad \text{on} \quad \gamma \times (0, T).
\]

As before, we introduce the new functions \( p \) and \( v \), and get an initial boundary-value problem similar to (3.6) - (3.8) with the additional boundary condition
\[
v = 0 \quad \text{on} \quad \gamma \times (0, T).
\]

Now, let the spaces \( P_h \) and \( V_h \) be defined as above and let \( \Lambda_\eta \) be a finite dimensional subspace of \( L_2(\gamma) \), which is defined below.

First, let us define a family \( T_\gamma \) of the cells \( \Delta \in T \), which we call "boundary elements". In \( T_\gamma \) the following cells \( \Delta \) are included:
• $\Delta$ such that $\gamma \cap \hat{\Delta} \neq \emptyset$;

• if $\gamma \cap \hat{\Delta} = \emptyset$, but $\gamma \cap \partial \Delta \neq \emptyset$, then we include $\Delta$ in $T_\gamma$ only if $\Delta \in \omega$ (Figure 3.3).

Now, let $\gamma = \{ \delta \gamma_i \}$ be a partitioning of $\gamma$ such that every interval $\delta \gamma_i$ contains at least one interval $\gamma \cap \Delta$ of the intersection of $\gamma$ with a cell $\Delta$ from $T_\gamma$. Below we denote by $\Lambda_\eta$ a space of piecewise constant functions which are constant on every $\delta \gamma_i$.

We also denote by $\Pi_\gamma w_h$ a "trace" of $w_h \in V_h$ on $\gamma$ which is defined as a function piecewise constant on $\gamma$, which is equal to $w_h$ on each $\gamma \cap \Delta$ for $\Delta \in T_\gamma$.

A fully discrete problem reads as follows: find a triple $(p^n_h, v^{n+1/2}_h, \lambda^n_\eta) \in P_h \times V_h \times \Lambda_\eta$ satisfying

\begin{align}
S_\Omega\left( \frac{p^n_h - p^{n-1}_h}{\Delta t} \cdot q_h \right) + \int_\Omega v^{n-1/2}_h \nabla \cdot q_h \, dx \\
+ c \int_{\Gamma_{ext}} \left( \frac{p^n_h + p^{n-1}_h}{2} \cdot n \right) (q_h \cdot n) \, d\Gamma = 0, \quad \forall q_h \in P_h,
\end{align}

(3.24)

\begin{align}
\int_\Omega \frac{v^{n+1/2}_h - v^{n-1/2}_h}{\Delta t} w_h \, dx - c^2 \int_\Omega \nabla \cdot p^n_h w_h \, dx + c^2 \int_\gamma \lambda^n_\eta \Pi_\gamma w_h \, dx = 0, \quad \forall w_h \in V_h,
\end{align}

(3.25)
\[
\int_{\gamma} \mu_\eta \Pi_\gamma v_h^{n+1/2} \, d\gamma = 0, \quad \forall \mu_\eta \in \Lambda_\eta, \quad (3.26)
\]

\[
P_h^n = (\nabla u_0)_h, \quad \frac{v_h^{1/2} - v_h^0}{\Delta t/2} = c^2 \nabla \cdot p_h^0. \quad (3.27)
\]

Denote by \( \tilde{P}_h, \tilde{V}_h \) and \( \tilde{\lambda}_h \) the vectors whose components are the degrees of freedom for the corresponding functions \( p_h \in P_h, v_h \in V_h \) and \( \lambda_\eta \in \Lambda_\eta \).

Then for a fixed time \( t_n = n\Delta t \) the first equation (3.24) is a system of linear algebraic equations with a mass matrix \( M_p \) defined above, while for \( \tilde{V}_h \) and \( \tilde{\lambda}_h \) we obtain a system of linear algebraic equations:

\[
\begin{cases}
M \tilde{V}_h + B^T \tilde{\lambda}_h = F, \\
B \tilde{V}_h = 0
\end{cases}
\quad (3.28)
\]

with \( M_\nu \) defined above and the rectangular matrix \( B \) defined by

\[
(BW, \Lambda_h) = \int_{\gamma} \lambda_\eta \Pi_\gamma w_h \, dx \quad \forall \lambda_\eta \in \Lambda_\eta, \, w_h \in V_h.
\]

**Theorem 3.3.** System (3.28) has a unique solution \((\tilde{V}_h, \tilde{\lambda}_h)\).

**Proof.** Since \( M_\nu \) is a regular matrix it is enough to prove that \( \text{Ker} B^T = \{0\} \). Suppose \( B^T \tilde{\lambda}_h = 0 \), i.e.,

\[
\int_{\gamma} \lambda_\eta \Pi_\gamma w_h \, dx = 0 \quad \forall w_h \in V_h.
\]

Let us take \( w_h \in V_h \) such that \( \Pi_\gamma w_h = 1 \) for one \( \Delta_{i,j} \in T_\gamma \), while it equals zero in other cells \( \Delta \). Then \( \lambda_\eta = 0 \) for a \( \delta \gamma_k \) which contains \( \gamma \cap \Delta_{i,j} \). Because each \( \delta \gamma_k \) contains at least one interval \( \gamma \cap \Delta \) with \( \Delta \in T_\gamma \), then \( \tilde{\lambda}_h \equiv 0 \). \( \square \)

**Theorem 3.4.** Let assumption (3.19) hold, then the system (3.24)-(3.26) satisfies the energy identity (3.21), where the discrete energy \( E^{n+1} \) is defined by (3.12). Therefore, problem (3.24)-(3.26) is stable for \( \Delta t \leq \frac{1}{2c} h_{\text{min}} \).

46
Proof. We proceed as in the proof of Theorem 3.2. Namely, let us choose \( q = \Delta t \frac{p_h^n + p_h^{n-1}}{2} \) in equation (3.24), \( w_h = \Delta t \frac{v_h^{n+1/2} + v_h^{n-1/2}}{2 c^2} \) in equation (3.25) and \( \mu_n = \lambda_h^n \) in equation 

\[
\int_{\gamma} \mu_n(\Pi_\gamma v_h^{n+1/2} + \Pi_\gamma v_h^{n-1/2}) d\gamma = 0.
\]

Adding these equalities we get identity (3.21). Now, the rest of the proof is the same as in Theorem 3.2. \(\square\)

In order to solve the system of linear equations (3.28) at each time step we use the conjugate gradient algorithm in the form given in [33].

3.5 Numerical experiments.

For our numerical experiments we have taken \( \Omega = (0, 1) \times (0, 1) \). The initial condition for the function \( u \) (Figure 3.4) has been set to

\[
u_0(x, y) = \begin{cases} 
\cos^2 2\pi r, & \text{if } r \leq 1/4, \\
0, & \text{otherwise}, 
\end{cases}
\]

\( u_1 = 0 \),

where \( r = \sqrt{(x - 1/2)^2 + (y - 1/2)^2} \). We have considered the following cases:

1. A wave problem in the domain \( \Omega \) without an obstacle (Figures 3.5-3.7). For \( \{ h, \Delta t \} \) we took \( h_x = h_y = 1/100 \) and \( \Delta t = 1/500 \).

2. A wave problem in the domain \( \Omega \) with \( \omega \) the quarter of a disc in the right-lower corner. We have taken \( h_x = h_y = 1/100 \) and \( \Delta t = 1/500 \). The radius of the disk has been set to \( R(\omega) = 2/5 \). We divided the boundary of \( \omega \) into 25 intervals, i.e. \( \delta_\gamma = \frac{1}{25} \). The fictitious domain method described in Section 4 has been used. Figures 3.8-3.12 show the wave propagation from the initial state (Figure 3.4) and its reflection from the obstacle. We observe a very good agreement of energy dissipation curves for different mesh and time step sizes in Figure 3.13.
Figure 3.4: Initial function $u$.

Figure 3.5: Domain without an obstacle, time=0.5.
Figure 3.6: Domain without an obstacle, time=0.7.

Figure 3.7: Domain without an obstacle, time=1.
Figure 3.8: *Domain with a circular obstacle, time=0.2.*

Figure 3.9: *Domain with a circular obstacle, time=0.4.*
Figure 3.10: Domain with a circular obstacle, time=0.6.

Figure 3.11: Domain with a circular obstacle, time=0.8.
Figure 3.12: Domain with a circular obstacle, time=1.

Figure 3.13: Energy dissipation for $\Delta t = 1/250, h = 1/50$ (dashed line) and $\Delta t = 1/500, h = 1/100$ (solid line).
Chapter 4

A penalty approach to the numerical simulation of a constrained wave motion

4.1 Introduction

The main goal of this chapter is to discuss the solution of a constrained wave system which has applications in theoretical and applied physics. The numerical methodology relies on the penalty treatment of the constraint and an energy preserving time discretization leading to a scheme which is essentially unconditionally stable and second order accurate; both techniques are combined with a globally continuous piecewise linear finite element approximation. The results of numerical experiments illustrate the properties of the computational methods discussed here, particularly energy and length preservation.

4.2 Problem formulation

Let $\Omega$ be a bounded domain in $\mathbb{R}^2$ with a piecewise smooth boundary $\partial \Omega$ and let $u(x, t) : \Omega \times (0, T) \rightarrow \mathbb{R}^3$. We consider the following constrained wave problem

$$\frac{\partial^2 u}{\partial t^2} - \Delta u + \lambda u = 0, \quad |u|^2 = 1 \quad \text{in} \; \Omega \times (0, T)$$

(4.1)
with Dirichlet boundary conditions
\[ u(x, t) = g(x, t) \quad \text{on } \partial \Omega \times (0, T), \]  
and initial conditions
\[ u(x, 0) = u_0(x), \quad \frac{\partial u}{\partial t}(x, 0) = u_1. \]  

Further we suppose that \( g = g(x) \) and
\[ \left\{ \begin{array}{l}
u_0(x) \cdot u_1(x) = 0, \quad |u_0(x)|^2 = 1 \quad \text{for a.a. } x \in \Omega, \\
g(x) \text{ is the trace of } u_0(x) \text{ on } \partial \Omega. \end{array} \]  

**Remark 4.1.** The function \( \lambda \) is clearly a Lagrange multiplier associated to the constraint \( |u|^2 = 1 \).

We approximate the constrained wave equation (4.1) by the following wave equation with a penalty term:
\[ \frac{\partial^2 u}{\partial t^2} - \Delta u + \frac{1}{\varepsilon}(|u|^2 - 1)u = 0, \]  
namely a kind of "Ginzburg-Landau wave equation" (for more information on Ginzburg-Landau type models see, e.g. [7]).

**Theorem 4.1.** For every fixed \( \varepsilon > 0 \) problem (4.5), (4.2), (4.3) has a unique solution such that \( u \in L^\infty(0, T; H^1(\Omega)^3) \), \( \frac{\partial u}{\partial t} \in L^\infty(0, T; L^2(\Omega)^3) \), provided that \( u_0 \in H^1(\Omega)^3 \), \( u_1 \in L^2(\Omega)^3 \) and the assumptions (4.4) are fulfilled.

If, moreover, \( u_0 \in H^2(\Omega)^3 \) and \( u_1 \in H^1_0(\Omega)^3 \), then the solution \( u \in L^\infty(0, T; H^1(\Omega)^3) \), \( \frac{\partial u}{\partial t} \in L^\infty(0, T; L^2(\Omega)^3) \) and \( \frac{\partial^2 u}{\partial t^2} \in L^\infty(0, T; L^2(\Omega)^3) \).

**Proof.** We give a proof which uses the Faedo-Galerkin method and is based on a proof given in [49] for a similar problem.

1) First, the initial conditions given in (4.3) make sense for a function \( u \in L^\infty(0, T; H^1(\Omega)^3) \), such that \( \frac{\partial u}{\partial t} \in L^\infty(0, T; L^2(\Omega)^3) \). In fact, \( u \in C([0, T]; L^2(\Omega)^3) \), i.e. it is continuous from \([0, T]\) in \( L^2(\Omega)^3 \). Further, from equation (4.5) it follows that \( \frac{\partial^2 u}{\partial t^2} \in L^\infty(0, T; (H^1(\Omega)^3)^3) \),
and together with \( \frac{\partial u}{\partial t} \in L^\infty(0, T; L^2(\Omega)^3) \) it gives \( \frac{\partial u}{\partial t} \in C([0, T]; (H^1(\Omega)^*)^3) \) (here \( (H^1(\Omega)^*)^3 \) is dual to \( H^1(\Omega)^3 \)).

2) Let \( V_0 = H^1_0(\Omega)^3 \) and \( \{w_1, \ldots, w_n, \ldots\} \) be a linear independent basis in \( V_0 \). We find an approximate solution in the form

\[
 u_n(t) = \sum_{i=1}^{n} g_{in}(t) w_i + u_0,
\]

where \( g_{in}(t) \) satisfies the system of equations

\[
\begin{align*}
\int_{\Omega} u_{n}''(t) \cdot w_j dx + \int_{\Omega} \nabla u_n(t) : \nabla w_j dx \\
+ \frac{1}{\varepsilon} \int_{\Omega} (|u_n|^2 - 1) u_n \cdot w_j dx = 0, \quad j = 1, \ldots, n,
\end{align*}
\]

(4.6) completed by initial conditions

\[
 u_n(0) = u_0; \quad u_n'(0) = u_{1n},
\]

(4.7)

with \( u_{1n} \to u_1 \) in \( L^2(\Omega)^3 \) as \( n \to \infty \). (Hereafter we use notation \( u' = \frac{\partial u}{\partial t} \) and similar for second order derivatives).

Owing to general results for non-linear system of ordinary differential equations problem (4.6), (4.7) has a solution in the interval \( (0, t_n) \) and due to a priori estimates obtained below \( t_n = T \).

3) To get the a priori estimates we multiply the \( j \)-th equation in (4.6) by \( g_{jn}(t) \) and sum these equations. Then taking into account the equality \( u_n'(t) = \sum_{i=1}^{n} g_{in}'(t) w_i \), we obtain

\[
\frac{1}{2} \frac{d}{dt} \int_{\Omega} |\partial u_n/\partial t|^2 dx + \frac{1}{2} \frac{d}{dt} \int_{\Omega} |
abla u_n|^2 dx + \frac{1}{4\varepsilon} \frac{d}{dt} \int_{\Omega} (|u_n|^2 - 1)^2 dx = 0.
\]

(4.8)

It follows from (4.8) that the sequence \( \{u_n\} \) is bounded in \( L^\infty(0, T; H^1(\Omega)^3) \) while \( \{u_n'\} \) is bounded in \( L^\infty(0, T; L^2(\Omega)^3) \) and as a consequence, the sequence \( \{u_n\} \) is bounded in \( H^1(\Omega \times (0, T))^3 \). Recall also, that \( H^1(\Omega \times (0, T))^3 \subset L^q(\Omega \times (0, T))^3 \) compactly for any
\( q < \infty \ (\Omega \subset \mathbb{R}^2) \). This means that there exists a subsequence (we keep the same notation for it) such that

\[
\begin{align*}
\mathbf{u}_n &\to \mathbf{u}^* \quad \text{weakly in } L^\infty(0, T; H^1(\Omega)^3), \\
\mathbf{u}_n' &\to \mathbf{u}'^* \quad \text{weakly in } L^\infty(0, T; L^2(\Omega)^3), \\
\mathbf{u}_n &\to \mathbf{u} \quad \text{strongly in } L^\infty(0, T; L^q(\Omega)^3) \forall q < \infty \text{ almost everywhere.}
\end{align*}
\]

(4.9)

Similar to [49] one can prove that

\[
(|\mathbf{u}_n|^2 - 1) \mathbf{u}_n \to (|\mathbf{u}|^2 - 1) \mathbf{u} \quad \text{weakly in } L^q(\Omega \times (0, T))^3, \forall q < \infty.
\]

(4.10)

Using (4.9) and (4.10) we pass to the limit as \( n \to \infty \) in (4.6) for a fixed \( j \) and obtain

\[
\frac{d^2}{dt^2} \int_\Omega \mathbf{u}(t) \cdot \mathbf{w}_j dx + \int_\Omega \nabla \mathbf{u}(t) : \nabla \mathbf{w}_j dx + \frac{1}{\varepsilon} \int_\Omega (|\mathbf{u}|^2 - 1) \mathbf{u} \cdot \mathbf{w}_j dx = 0
\]

and then, in view of the density of the basis \( \{\mathbf{w}_1, \ldots, \mathbf{w}_n, \ldots\} \), we get

\[
\frac{d^2}{dt^2} \int_\Omega \mathbf{u}(t) \cdot \mathbf{w}_j dx + \int_\Omega \nabla \mathbf{u}(t) : \nabla \mathbf{w}_j dx + \frac{1}{\varepsilon} \int_\Omega (|\mathbf{u}|^2 - 1) \mathbf{u} \cdot \mathbf{w}_j dx = 0, \ \forall \mathbf{w} \in V_0.
\]

The last equation means that the limit function \( \mathbf{u} \) is a weak solution of (4.5). By standard methods one can prove that \( \mathbf{u}'(0) = \mathbf{u}_1 \).

4) To prove the uniqueness we take two solutions \( \mathbf{u} \) and \( \mathbf{v} \) and let \( z = \mathbf{u} - \mathbf{v} \). Then

\[
\begin{align*}
\frac{\partial^2 z}{\partial t^2} - \Delta z &= \frac{1}{\varepsilon} (|\mathbf{v}|^2 - 1) \mathbf{v} - \frac{1}{\varepsilon} (|\mathbf{u}|^2 - 1) \mathbf{u}, \\
z(0) &= z'(0) = 0, \\
z(t) &\in L^\infty(0, T; H^1_0(\Omega)^3), \ z'(t) \in L^\infty(0, T; L^2(\Omega)^3).
\end{align*}
\]

(4.11)

Multiplying (formally) the first equation in expression (4.11) by \( z' \) we get

\[
\frac{1}{2} \frac{d}{dt} \int_\Omega |z'(t)|^2 dx + \frac{1}{2} \frac{d}{dt} \int_\Omega |
abla z|^2 dx = \frac{1}{\varepsilon} \int_\Omega ((|\mathbf{v}|^2 - 1) \mathbf{v} - (|\mathbf{u}|^2 - 1) \mathbf{u}) z' dx \quad (4.12)
\]

For the right-hand side we have the following estimate (\( H^1(\Omega)^3 \subset L^q(\Omega)^3 \) for any \( q < \infty \)):

\[
\frac{1}{\varepsilon} \int_\Omega ((|\mathbf{v}|^2 - 1) \mathbf{v} - (|\mathbf{u}|^2 - 1) \mathbf{u}) z' dx \leq c(\varepsilon) \int_\Omega (1 + |\mathbf{v}|^2 + |\mathbf{u}|^2) |z||z'| dx
\]

56
For this we use the traditional approach. Namely, we let independent basis in

\[ z(t) \] can be found, for example, in [49].

From here we derive the estimate

\[ (4.12) \quad \text{and} \quad (4.13) \]

Therefore, we have

\[ \| z'(t) \|^2_{L^2(\Omega)^3} + \| z(t) \|^2_{H^1(\Omega)^3} \leq 2c(\varepsilon) \int_0^t \left( \| z'(\sigma) \|^2_{L^2(\Omega)^3} + \| z(\sigma) \|^2_{H^1(\Omega)^3} \right) d\sigma, \]

hence \( z = 0 \).

The justification of this formal transformation (multiplication of equation (4.11) by \( z' \)) can be found, for example, in [49].

5) The last point is the proof of the regularity of the solution for more regular data. For this we use the traditional approach. Namely, we let \( \{ w_1, \ldots, w_n, \ldots \} \) be a linearly independent basis in \( V_0 \cap H^2(\Omega)^3 \). Differentiating equation (4.6) by \( t \) and multiplying it by \( g_{jn}(t) \) we get

\[
\frac{1}{2} \frac{d}{dt} \int_\Omega \left| \frac{\partial u_n''}{\partial t} \right|^2 dx + \frac{1}{2} \frac{d}{dt} \int_\Omega \left| \nabla u_n' \right|^2 dx = -\frac{1}{\varepsilon} \int_\Omega \left( (|u_n|^2 - 1)u_n'u_n'' + 2(u_n'u_n)(u_n'u_n'') \right) dx.
\]

The right-hand side is estimated above by

\[
\left| \frac{1}{\varepsilon} \int_\Omega \left( (|u_n|^2 - 1)u_n'u_n'' + 2(u_n'u_n)(u_n'u_n'') \right) dx \right| \leq c(\varepsilon) \| u_n'' \|_{L^2(\Omega)^3} \| u_n' \|_{H^1(\Omega)^3} \| u_n' \|_{H^1(\Omega)^3} \leq c(\varepsilon) \| u_n'' \|_{L^2(\Omega)^3} \| u_n' \|_{H^1(\Omega)^3},
\]

thus,

\[
\frac{1}{2} \frac{d}{dt} \left( \| u_n'' \|^2_{L^2(\Omega)^3} + \| u_n' \|^2_{H^1(\Omega)^3} \right) \leq c(\varepsilon) \| u_n'' \|_{L^2(\Omega)^3} \| u_n' \|_{H^1(\Omega)^3},
\]

From here we derive the estimate

\[
\| u_n''(t) \|^2_{L^2(\Omega)^3} + \| u_n'(t) \|^2_{H^1(\Omega)^3} \leq c(\varepsilon)(1 + \int_0^t \left( \| u_n''(\sigma) \|^2_{L^2(\Omega)^3} + \| u_n'(\sigma) \|^2_{H^1(\Omega)^3} \right) d\sigma)
\]

and the boundness

\[
\{ u_n' \} \text{ in } L^\infty(0, T; H^1_0(\Omega)^3), \quad \{ u_n'' \} \text{ in } L^\infty(0, T; L^2(\Omega)^3).
\]

57
Thus, the limit function (solution to the problem) is such that \( u' \in L^\infty(0, T; H^1_0(\Omega)^3) \) and \( u'' \in L^\infty(0, T; L^2(\Omega)^3) \).

Remark 4.2. Model (4.5), (4.2), (4.3) is energy preserving. Namely, by passing to a limit as \( n \to \infty \) in equation (4.8) we get

\[
\frac{1}{2} \int_\Omega \left| \frac{\partial u(t)}{\partial t} \right|^2 dx + \frac{1}{2} \int_\Omega |\nabla u|^2 dx + \frac{1}{4\varepsilon} \int_\Omega (|u|^2 - 1)^2 dx = 0,
\]

which implies that the energy

\[
E(t) = \frac{1}{2} \int_\Omega |u_1|^2 dx + \int_\Omega |\nabla u_0|^2 dx
\]

of the system is constant in time. Due to the assumption that \( |u_0(x)|^2 = 1 \) the energy \( E(0) \) does not depend upon the penalty parameter \( \varepsilon \) and reduces to

\[
E(0) = \frac{1}{2} \left( \int_\Omega |u_1|^2 dx + \int_\Omega |\nabla u_0|^2 dx \right).
\]

This equality and the energy conservation imply the following estimate for any \( t > 0 \)

\[
\int_\Omega (|u|^2 - 1)^2 dx \leq 2\varepsilon \left( \int_\Omega |u_1|^2 dx + \int_\Omega |\nabla u_0|^2 dx \right). \tag{4.14}
\]

4.3 Discretization of the problem

First, we construct a semidiscrete problem by approximating the time derivative in equation (4.5). Let \( \Delta t > 0 \) be a time step and set \( u^n \approx u(n\Delta t) \) for \( n = 1, 2, \ldots \). Then, we consider the following time discretization scheme:

\[
\frac{u^{n+1} + u^{n-1} - 2u^n}{\Delta t^2} - \Delta \left( \frac{u^{n+1} + 2u^n + u^{n-1}}{4} \right) + \frac{1}{2\varepsilon} \left( \left| \frac{u^n + u^{n+1}}{2} \right|^2 + \left| \frac{u^n + u^{n-1}}{2} \right|^2 - 2 \right) \left( \frac{u^{n+1} + 2u^n + u^{n-1}}{4} \right) = 0, \tag{4.15}
\]

with corresponding boundary conditions. Scheme (4.15) is initialized with

\[
\begin{cases}
  u^0 = u_0, & u^1 - u^{-1} = 2\Delta t u_1, \\
  u^1 - 2u^0 + u^{-1} = \Delta t^2 \Delta u^0.
\end{cases} \tag{4.16}
\]
The semidiscrete problem keeps (in some sense) the energy preserving property of the initial problem. Approximate the energy $E$ at $t = (n + 1/2)\Delta t$ by

$$E_{e}^{n+1/2} = \frac{1}{2} \int_{\Omega} \left| \frac{u^{n+1} - u^{n}}{\Delta t} \right|^2 dx + \frac{1}{2} \int_{\Omega} \left| \nabla \frac{u^{n+1} + u^{n}}{2} \right|^2 dx$$

$$+ \frac{1}{4e} \int_{\Omega} \left( \left| \frac{u^{n+1} + u^{n}}{2} \right|^2 - 1 \right)^2 dx; \quad (4.17)$$

multiplying (4.15) by $(u^{n+1} - u^{n-1})/2$ and integrating in $x$ over $\Omega$ we obtain

$$E_{e}^{n+1/2} = E_{e}^{n-1/2} \forall n. \quad (4.18)$$

The basis of the previous formal calculations will be shown below, where the existence of a weak solution to problem (4.15), (4.16) and its corresponding regularity will be proved.

We construct a finite dimensional approximation of the semidiscrete scheme (4.15) via the finite element method; the simplest quadrature formulas (based on the trapezoidal rule) are used to avoid non-diagonal mass matrices.

Let $T_h$ be a regular triangulation of $\Omega$, that we assume to be polygonal. For simplicity we denote by $e$ the generic element of triangulation $T_h$. By $V_h \subset (H^1(\Omega))^3$ we denote the finite element space: \{ $v_h = (v_{1h}, v_{2h}, v_{3h})$, $v_{ih} \in C^0(\Omega)$, $v_{ih} \mid e \in P_1(e)$ for all $i$ and for all $e \in T_h$ \}. For simplicity, let the function $g(x)$ be continuous, i.e. $g(x) \in (H^{1/2}(\partial \Omega) \cap C^0(\partial \Omega))^3$ and let $g_h$ be it’s piecewise linear interpolate: $g_h(x) = g(x)$ at the boundary vertices.

We introduce the space $V_h^g = \{ v_h \in V_h : v_h = g_h$ on $\partial \Omega \}$ and a test function space $V_h^0 = (H^1_0(\Omega))^3 \cap V_h$. Further $\{ a_i \}_{i=1}^3$ will be the vertices of an element $e \in T_h$ of measure $|e|$. For any function $\phi(x) \in C^0(\bar{e})$, we use the quadrature formulas

$$\int_{e} \phi(x)dx \approx S_e(\phi) \equiv \frac{1}{3}|e| \sum_{i=1}^3 \phi(a_i).$$

For a function $\phi \in C^0(\bar{\Omega})$ we use $S_h(\phi) = \sum_{e \in \Omega} S_e(\phi)$. 

59
Now a discretization scheme for problem (4.5), (4.2), (4.3) can be written as follows: find \( u^h \in V^g_h \), such that for all \( v_h \in V^0_h \) and all \( n = 1, 2, \ldots \)

\[
S_h \left( \frac{u^{n+1}_h - u^n_h}{\Delta t} \cdot v_h \right) + \int_{\Omega} \nabla u^{n+1}_h + \frac{2}{4} (u^n_h + u^{n-1}_h) : \nabla v_h \, dx +
\]

\[
\frac{1}{2} \varepsilon S_h \left( \left( \left| \frac{u^{n+1}_h + u^n_h}{2} \right|^2 + \left| \frac{u^n_h + u^{n-1}_h}{2} \right|^2 \right) - 2 \left( \frac{u^{n+1}_h + 2u^n_h + u^{n-1}_h}{4} \right) \cdot v_h \right) = 0,
\]

(4.19)

with the discrete analogue of (4.16):

\[
\begin{cases}
  u^n_h = u^n_0, \\
  S_h (u^n_h \cdot v_h) = S_h ((u^n_0 + \Delta t u^n_1) \cdot v_h) \\
  -\frac{\Delta t^2}{2} \int_{\Omega} \nabla u^n_0 : \nabla v_h \, dx \ \forall v_h \in V^0_h.
\end{cases}
\]

(4.20)

Here, \( u^n_0 \in V^g_h \) and \( u^n_1 \in V^0_h \) approximate in some sense \( u^n_0 \) and \( u^n_1 \), respectively.

**Remark 4.3.** Higher order finite element methods can be also employed; the technique discussed below would still apply.

The fully discrete scheme (4.19), (4.20) inherits the energy preserving property of the continuous and semidiscrete problems: if the discrete energy is defined by

\[
E^{n+1/2}_h = \frac{1}{2} S_h \left( \left( \frac{u^{n+1}_h - u^n_h}{\Delta t} \right)^2 \right) + \frac{1}{2} \int_{\Omega} \left( \left| \frac{u^{n+1}_h + u^n_h}{2} \right|^2 \right) \, dx +
\]

\[
\frac{1}{4 \varepsilon} S_h \left( \left( \left| \frac{u^{n+1}_h + u^n_h}{2} \right|^2 - 1 \right)^2 \right),
\]

(4.21)

then

\[
E^{n+1/2}_h = E^{1/2}_h
\]

(4.22)

for all \( n \geq 1 \). To prove it, take \( v_h = \frac{1}{2} (u^{n+1}_h - u^{n-1}_h) \in V^0_h \) in (4.19).

**Theorem 4.2.** 1) The fully discrete problem (4.19) has a solution for any \( h, \Delta t \) and \( \varepsilon > 0 \).
2) If \( u_1 \in L_p(\Omega)^3 \) and \( \Delta u_0 \in L_p(\Omega)^3 \) for a \( p > 2 \), and \( \Delta t \leq 2\sqrt{\varepsilon} \), then the semidiscrete problem (4.15) has a solution, such that \( u^n \in L_p(\Omega)^3 \) and \( \frac{u^{n+1} + 2u^n + u^{n-1}}{4} \in H^1(\Omega)^3 \) for \( n = 1, 2, \ldots \).

3) If \( u_1 \in H^1(\Omega)^3 \) and \( \Delta u_0 \in H^1(\Omega)^3 \), then problem (4.15) has a solution, such that \( u^n \in H^1(\Omega)^3 \) for all \( n = 1, 2, \ldots \).

Proof. 1) To prove the existence of the solution for the fully discrete problem (4.19) we use the following variant of the Brouwer theorem [49]:

Let \( V \) be a finite dimensional linear space endowed with an inner product \((\cdot, \cdot)\) and norm \( ||\cdot||\). Let \( P : V \to V \) be a continuous mapping with the following property: there exists \( \rho > 0 \) such that \( (P\xi, \xi) \geq 0 \) on the sphere \( ||\xi|| = \rho \). Then there exists a vector \( \xi^*, ||\xi^*|| \leq \rho \) such that \( P\xi^* = 0 \).

We equip the space \( V^0_h \) with the inner product \((v_h, w_h)_h = S_h(v_h \cdot w_h)\) and the corresponding norm \( ||v_h||_h = S^{1/2}_h(v_h \cdot v_h)\). For a fixed \( n \geq 1 \) let \( \xi_h = \frac{1}{2}(u^n_h - u^{n-1}_h) \in V^0_h \) and operator \( P : V^0_h \to V^0_h \) be defined by the left-hand side of (4.19). In other words, we write (4.19) in the form \( (P\xi_h, v_h)_h = 0 \ \forall v_h \in V^0_h \). The operator \( P \) is obviously continuous. Now, if we take \( v_h = \xi_h \) in (4.19), then

\[
(P\xi_h, \xi_h)_h = E_h^{n+1/2} - E_h^{n-1/2}.
\]  

(4.23)

Let \( c_n \) be a generic constant depending on \( u^n_h \) and \( u^{n-1}_h \) (we recall that \( u^n_h \) and \( u^{n-1}_h \) are supposed to be known). Then obviously,

\[
E_h^{n-1/2} \leq c_n
\]

and

\[
E_h^{n+1/2} \geq \frac{1}{2(\Delta t)^2} S_h(|u^n_h - u^{n-1}_h|^2) - c_n \geq \frac{1}{4(\Delta t)^2} S_h(\xi_h \cdot \xi_h) - c_n.
\]

Hence,

\[
(P\xi_h, \xi_h)_h \geq \frac{1}{4(\Delta t)^2} S_h(\xi_h \cdot \xi_h) - c_n
\]

61
and for \(|\|\xi_h||_h\) large enough we have \((P\xi_h, \xi_h)_h \geq 0\), implying that problem (4.19) has a solution from the variant of the Brouwer theorem above.

2) Now we study the solvability of the semidiscrete problem (4.15), using the limit as \(h \to 0\) in the fully discrete problem. As it was mentioned in Remark 4.3, the previous existence result holds also for a fully discrete problem with high order finite element approximation in space variables (Lagrange or Hermit finite elements). Further we suppose in this the case, in particular, that \(|\|\Delta u_{0h} - \Delta u_0||_{L_p} \to 0\).

Let us introduce, for \(n \geq 1\) fixed, \(z^n = 1/4(u^{n+1} + 2u^n + u^{n-1})\). We then have the following weak formulation of the problem (4.15):

find \(u^{n+1} \in L_p(\Omega)^3\) with \(p > 2\), such that \(z^n \in H^1(\Omega)^3\) and

\[
\int_{\Omega} \frac{4}{\Delta t^2} z^n \eta \, dx + \int_{\Omega} \nabla z^n \nabla \eta \, dx + \int_{\Omega} \frac{1}{2\varepsilon} \left( \frac{|u^n + u^{n+1}|^2}{2} - 2 \right) z^n \, dx = \int_{\Omega} \frac{4}{\Delta t^2} u^n \eta \, dx, \quad \forall \eta \in H^1_0(\Omega)^3. \tag{4.24}
\]

Under the assumptions \(u^n, u^{n-1} \in L_p(\Omega)^3\), and for \(z^n, \eta \in H^1(\Omega)^3\), the integral

\[
\int_{\Omega} \left( \left| \frac{u^n + u^{n+1}}{2} \right|^2 + \left| \frac{u^n + u^{n-1}}{2} \right|^2 \right) z\eta \, dx
\]

is well-defined, because of the Hölder inequality (\(\int uvw \leq ||u||_{L_{p_1}} ||v||_{L_{p_2}} ||w||_{L_{p_3}}, 1/p_1 + 1/p_2 + 1/p_3 = 1\)) and the continuous embedding of \(H^1(\Omega) \subset L_q(\Omega)\) for any \(q < \infty\).

From equation (4.16) we have that \(u^1 = u_0 + \Delta t u_1 + 1/2\Delta t^2 \Delta u_0\); if \(u_1 \in L_p(\Omega)^3\) and \(\Delta u_0 \in L_p(\Omega)^3\), then \(u^0, u^1 \in L_p(\Omega)^3\).

Let \(|\|\Delta u_{0h} - \Delta u_0||_{L_p} \to 0\) and \(|\|u_{1h} - u_1||_{L_p} \to 0\) as \(h \to 0\). This ensures the uniform boundness in \(h\) in the \(L_p\)-norm of sequences \(\{u_{1h}\}_h\) and \(\{\Delta u_{0h}\}_h\).

Now, choose \(v_h = z^n_h\) for (4.19) and we obtain

\[
\left( \frac{4}{\Delta t^2} - \frac{1}{\varepsilon} \right) S_h(|z^n_h|^2) + ||\nabla z^n_h||_0^2 \leq \frac{4}{\Delta t^2} S_h(|u^n_h||z^n_h|).
\]

62
Under the induction assumption \( ||u_h^n||_{L^p} \leq c \neq c(h) \) (using the inequality \( \Delta t \leq 2\sqrt{\varepsilon} \)) we get the uniform estimate in \( h \)

\[
||\nabla z^n_h||_0 \leq c \neq c(h).
\]

Using this estimate and the induction assumptions \( ||u_h^{n-1}||_{L^p}, ||u_h^n||_{L^p} \leq c \neq c(h) \) we can choose from the sequence \( \{u_h^{n+1}\}_h \) a subsequence (we keep the same notation for it) such that

\[
z_h^{n+1} \rightharpoonup z^{n+1} = 1/4(u^{n+1} + 2u^n + u^{n-1}) \quad \text{weakly in } H^1(\Omega)^3,
\]

\[
u_h^{n+1} \to u^{n+1} \quad \text{strongly in } L^p(\Omega)^3.
\]

(4.25)

Now, passing to the limit as \( h \to 0 \) in equation (4.19) with \( v_h \to v \) strongly in \( H^1(\Omega)^3 \), we derive the weak form of equation (4.15).

3) Under the assumptions of this section we prove that the sequences \( \{||u_h^0||_1\}_h \) and \( \{||u_h^1||_1\}_h \) are uniformly bounded in \( h \). So, \( E_h^{1/2} \leq c \neq c(h) \) and as a consequence of (4.22) \( E_h^{n+1/2} \leq c \neq c(h, n) \) for any \( n \). This means that \( ||u_h^n||_1 \leq c \neq c(h, n) \) and we can choose the subsequences of \( \{u_h^n\}_h \), which converge weakly in \( H^1(\Omega)^3 \) for any \( n \). The rest of the proof is the same as in the previous case.

\[\square\]

Remark 4.4. When \( u_1 \in H^1(\Omega)^3 \) and \( \Delta u_0 \in H^1(\Omega)^3 \) the energy \( E^n \) in (4.17) is well defined and the energy preserving property (4.18) holds for any \( n \). Direct calculations show that

\[
E_{\varepsilon/2} = \frac{1}{2} \int_{\Omega} \frac{|u_1 - u_0|}{\Delta t}^2 \, dx + \frac{1}{2} \int_{\Omega} \left| \nabla \frac{u_1 + u_0}{2} \right|^2 \, dx + \frac{1}{\varepsilon} c_1 \Delta t^4 =
\]

\[
\int_{\Omega} |u_1|^2 \, dx + \int_{\Omega} |\nabla u_0|^2 + \frac{1}{\varepsilon} (c_2 \Delta t^4 + c_3 \Delta t)
\]

(4.26)

with constants \( c_1, c_2 \) and \( c_3 \) depending on the \( H^1(\Omega)^3 \)-norms of \( u_1 \) and \( \Delta u_0 \). As a consequence of (4.18) and (4.26) we have the following estimate

\[
\int_{\Omega} \left( \frac{|u^{n+1} + u^n|^2}{2} - 1 \right)^2 \, dx \leq 2\varepsilon \left( \int_{\Omega} \frac{|u_1 - u_0|}{\Delta t}^2 \, dx + \int_{\Omega} \left| \nabla \frac{u_1 + u_0}{2} \right|^2 \, dx \right) + O(\Delta t^4)
\]

63
\[ = 2\varepsilon \left( \int_{\Omega} |u_1|^2 \, dx + \int_{\Omega} |\nabla u_0|^2 \, dx \right) + O(\Delta t) \text{ for all } n \geq 2. \quad (4.27) \]

**Remark 4.5.** The energy preserving properties (4.18) and (4.22) ensure the unconditional stability of schemes (4.15) and (4.19) respectively.

It follows from the proof of Lemma 4.2 that a solution of the semidiscrete problem (4.15) is a weak limit when $h \to 0$ of solutions of the fully discrete problem (4.19).

When the assumptions $u_1 \in H^1(\Omega)^3$ and $\Delta u_0 \in H^1(\Omega)^3$ hold, we get from (4.18) the uniform boundness in $\Delta t$ (or, equivalently, in $n$) of the sequences $\{ || u^{n+1} - u^n ||_0 / \Delta t \}$ and $\{ || \nabla u^{n+1} + u^n ||_0 / 2 \}$. Using this result, we can prove that a solution of problem (3.7) – (4.5) is a weak limit (in the corresponding norms) of a subsequence of solutions to problem (4.15).

**Theorem 4.3.** Let $u^1 \in H^1(\Omega)^3$ and $\Delta u_0 \in H^1(\Omega)^3$. There exists a constant $\tilde{c}$, independent of $\Delta t$ and $\varepsilon$, such that for $\Delta t \leq \tilde{c}\varepsilon$ problems (4.15) and (4.19) have unique solutions.

**Proof.** We prove the uniqueness result only for problem (4.15), the proof for (4.19) is similar.

Let $u_1^{n+1}$ and $u_2^{n+1}$ be two solutions of (4.15), and $w = u_1^{n+1} - u_2^{n+1}$; assume that $u_1^k = u_2^k$ for all $k \leq n$. From (4.15) we obtain

\[ \frac{1}{\Delta t^2} || w ||^2_0 + || \nabla w ||^2_0 \leq \frac{1}{\varepsilon} || w ||^2_0 + \frac{c}{\varepsilon} \int_{\Omega} |w|^2 (u_1^{n+1} + u_2^{n+1} + 2u_1^n ||u_1^{n+1} + u_2^{n+1} + 2u_2^n|dx \quad (4.28) \]

We estimate the right-hand side of (4.28) (denoted by $S$) by using the Hölder inequality, the continuous embedding $H^1(\Omega) \subset L_q(\Omega)$, $\forall q < +\infty$, and the uniform boundness in $n$ of the $H^1(\Omega)^3$-norms for the solutions of (4.15):

\[ S \leq \frac{1}{\varepsilon} || w ||^2_0 + \frac{c}{\varepsilon} \max_k (|| u_1^k ||^2_1 + || u_1^k ||^2_1) || w ||_0 || w ||_1 \]

\[ \leq \frac{c}{\varepsilon^2} || w ||^2_0 + || w ||^2_1 \]

64
Here \( c \) is a generic constant independent of \( n \) and \( \varepsilon \). Now it is easy to see that for \( \Delta t \leq \tilde{c}\varepsilon \) with appropriate \( \tilde{c} \), we have \( \|w\|_0^2 \leq 0 \). 

4.4 Solution method for the fully discrete problem

We solve equation (4.19) for \( n \geq 1 \). Hereafter we drop the index \( h \) from the functions. Let us introduce at each time step the auxiliary variable \( z = (u^{n+1} + 2u^n + u^{n-1})/4 \), then problem (4.19) can be written as follows

\[
(4z - 4u^n) - \Delta t^2 \Delta_h z + \frac{\Delta t^2}{2\varepsilon} (|2z - u^{-1/2}|^2 + |u^{n-1/2}|^2 - 2) z = 0,
\]

where \( u^{-1/2} = (u^n + u^{n-1})/2 \), and \( -\Delta_h \) is the discrete Laplace operator. Equation (4.29) is completed by Dirichlet boundary conditions. Let us now denote the left-hand side of (4.29) by \( F(z) \). Obviously, function \( F(z) \) is differentiable and

\[
F'(z)w = 4w - \Delta t^2 \Delta_h w + \frac{\Delta t^2}{2\varepsilon} (|2z - u^{-1/2}|^2 + |u^{n-1/2}|^2 - 2) w
+ \frac{2}{\varepsilon} \Delta t^2 (2z - u^{-1/2}, w) z,
\]

where \((.,.)\) is the inner product in \( \mathbb{R}^3 \) and matrix \( F'(z) \) has the form

\[
(4 + \frac{\Delta t^2}{2\varepsilon} (|2z - u^{-1/2}|^2 + |u^{n-1/2}|^2 - 2)) I - \Delta t^2 \Delta_h
+ \frac{4\Delta t^2}{\varepsilon} zz^T - \frac{2}{\varepsilon} \Delta t^2 z (u^{-1/2})^T,
\]

with the unit matrix \( I \). Under the assumption \( \Delta t \leq 2\sqrt{\varepsilon} \), the matrix \( F'(z) \) is positive definite but not symmetric due to the term \((2/\varepsilon)\Delta t^2 z (u^{-1/2})^T\). In order to solve the equation \( F(z) = 0 \) we use the following Quasi-Newton method

\[
F'_0(z^k)(z^{k+1} - z^k) + F(z^k) = 0, \quad k = 0, 1, 2, ...
\]

where

\[
F'_0(z) = (4 + \frac{\Delta t^2}{2\varepsilon} (|2z - u^{-1/2}|^2 + |u^{n-1/2}|^2 - 2)) I - \Delta t^2 \Delta_h + \frac{2\Delta t^2}{\varepsilon} zz^T,
\]

65
which is obviously positive definite for $\Delta t \leq 2\sqrt{\varepsilon}$. Clearly, $F'_0(z)$ differs from $F'(z)$ by the term $\frac{2}{\varepsilon}\Delta t^2 z(z - u^{n-1/2})^T$ which is equal to

$$
\frac{1}{\varepsilon} \Delta t^3 \left( \frac{u^{n+1} + 2u^n + u^{n-1}}{4} \right) \left( \frac{u^{n+1} - u^{n-1}}{2\Delta t} \right)^T
$$

at the exact solution and is expected to be "small" enough when starting from a "good" initial guess. To solve problem (4.31) at each time step we use a conjugate gradient algorithm.

### 4.5 Numerical results

We have performed numerical experiments for problem (4.2)-(4.5) in $\Omega = (0, 1) \times (0, 1)$ by using finite difference in space for (4.15) with a uniform mesh step size $h$. This difference scheme can be treated as a finite element scheme with $P_1$-interpolation and trapezoidal quadrature formulas to approximate the integrals. We considered different input data and different mesh and time step sizes $h$ and $\Delta t$, and penalty parameter $\varepsilon > 0$. We have found that our numerical results agree very well with the constrained verification estimate (4.27). Moreover, our calculations showed that the discrete scheme is stable and that the iterative method (4.31) is convergent with a high rate of convergence under much less restrictive conditions between $h$, $\Delta t$ and $\varepsilon$ than those given by the developed theory.

The following graphs show the energy and $\max_x ||u||^2 - 1|$ behavior in time, the shape of the $u_3$ component of $u$ for different values of $\varepsilon$ with the initial data defined as follows

$$
\begin{align*}
  u_1^0 &= \frac{x - x^*}{r}, & u_2^0 &= \frac{y - y^*}{r}, & u_3^0 &= \frac{\cos(\pi x - \pi y)}{r}, \\
  u_1 &= 0,
\end{align*}
$$

and boundary data given by:

$$
\begin{align*}
  g_1 &= \frac{x - x^*}{r}, & g_2 &= \frac{y - y^*}{r}, & g_3 &= \frac{\cos(\pi x - \pi y)}{r},
\end{align*}
$$

with $r = \sqrt{(x - x^*)^2 + (y - y^*)^2 + \cos^2(\pi x - \pi y)}$ and $(x^*, y^*) = (1.1, 1.1)$.  

66
Figure 4.1: *Energy behavior (left) and $\max_x \|u\|^2 - 1\| (right)$ for $\varepsilon = 10^{-3}, h = 1/50, \Delta t = 1/100$.*

**Remark 4.6.** In both graphs in Figure 4.1 (which show the history of the discrete energy and deviation from the constraint $|u|^2 = 1$), we observe oscillations taking place at the beginning of the evolution. These oscillations damped out as $t$ increases. In order to reduce this unwanted phenomenon we have modified scheme (4.15), (4.16) as follows:

- We started (4.15) from $n = 0$, instead of $n = 1$.
- We used $u^0 = u_0$ and $u^1 - u^{-1} = 2\Delta t u_1$ as initial conditions.

This modification slightly improves the numerical result (level of oscillations at the start is reduced by about 10%).
Figure 4.2: Energy behavior (left) and $\max_x |u|_2^2 - 1$ (right) for $\varepsilon = 10^{-4}$, $h = 1/50$, $\Delta t = 1/100$.

Figure 4.3: Energy behavior (left) and $\max_x |u|_2^2 - 1$ (right) for $\varepsilon = 10^{-5}$, $h = 1/50$, $\Delta t = 1/100$. 
Figure 4.4: $u_3$ component of $u$ at $t = 1/4$ (left) and $t = 1/2$ (right) for $\varepsilon = 10^{-3}$, $h = 1/50$, $\Delta t = 1/100$.

Figure 4.5: $u_3$ component of $u$ at $t = 3/4$ (left) and $t = 1$ (right) for $\varepsilon = 10^{-3}$, $h = 1/50$, $\Delta t = 1/100$. 
Figure 4.6: $u_3$ component of $u$ at $t = 1/4$ (left) and $t = 1/2$ (right) for $\varepsilon = 10^{-5}$, $h = 1/50$, $\Delta t = 1/100$.

Figure 4.7: $u_3$ component of $u$ at $t = 3/4$ (left) and $t = 1$ (right) for $\varepsilon = 10^{-5}$, $h = 1/50$, $\Delta t = 1/100$. 
Chapter 5

Mathematical modeling of blood flow in compliant arteries

5.1 Introduction

5.1.1 Background of the problem

In this chapter we consider a problem of modeling blood flow in the human arteries. The focus is on numerical simulation of the flow through branching arteries with an inserted prostheses called stents and stent-grafts. Both the arteries and the stents are assumed to be elastic. The Young’s modulus of elasticity for arteries was obtained from [60]. The Young’s modulus of elasticity of stents was obtained from the measurements by K. Ravi-Chandar and R. Wang [88, 89]. The underlying problem consists of modeling the flow through the human aorta branching into iliac arteries (see Figure 5.1), that suffers from an 
aortic abdominal aneurysm (AAA).

An aneurysm can be described as a bulging of the human aorta (Figure 5.1). There is a 90% mortality rate associated with AAA rupture. Treatment of AAA consists of either surgical interventions or nonsurgical AAA repair for high-risk patients. Non-surgical repair
entails inserting a prosthesis (either a stent or a stent-graft) inside the diseased aorta to redirect the flow of blood and lower the pressure to the aneurysmal walls, thereby lowering the probability of rupture.

Stents and stent-grafts are tube-like devices made of stainless steel or nitinol with a mesh (stent) that can be covered with polyester or Dacron grafts. In a bifurcated aneurysm, bifurcated stent-grafts are typically used for AAA-repair.

There are various complications associated with this procedure, they include stent-graft migration, occlusion of the graft limbs and formation of new aneurysms near the anchoring sites [82].

The purpose of the study presented here is to use mathematical modeling and numerical simulations to understand some of the hemodynamic factors that might be responsible for the complications listed above, and suggest an improved prosthesis design that might minimize some of the problems. More details will be presented in section 5.5.
5.1.2 Mathematical model

We use a reduced, one dimensional model, together with the special conditions derived via Riemann invariants, to simulate the flow through the branching arteries. The model is derived using an asymptotic reduction of the Navier-Stokes equations modeling blood with the Navier equation for the wall.

The resulting set of equations is used to study the optimal prostheses design by investigating the impact of shear stress rates on the initiation of focal atherogenesis.

5.2 Effective model derivation

In this section we follow the derivation of effective equations given in detail in [85].

5.2.1 The 3-D fluid-structure interaction problem

We consider the unsteady axisymmetric flow of a Newtonian incompressible fluid in a thin elastic cylinder whose radius is small with respect to its length. We define the ratio $\varepsilon = R/L$, where $R$ is the radius and $L$ is the length of the cylinder. Now, for every fixed $\varepsilon > 0$ we introduce the computational domain (Figure 5.2)

$$\Omega_\varepsilon(t) = \{ x \in \mathbb{R}^3; x = (rcos\Theta, rsin\Theta, x), r < R + \eta(x,t), 0 < x < L \}$$
This domain is filled with fluid modeled by the incompressible Navier-Stokes equations. We assume that the angular velocity is zero, then the problem in an Eulerian framework in cylindrical coordinates in \( \Omega_\varepsilon(t) \times \mathbb{R}_+ \) reads as follows

\[
\rho \left[ \frac{\partial v^r_\varepsilon}{\partial t} + v^r_\varepsilon \frac{\partial v^r_\varepsilon}{\partial r} + v_x^\varepsilon \frac{\partial v^r_\varepsilon}{\partial x} \right] - \mu \left[ \frac{\partial^2 v^r_\varepsilon}{\partial r^2} + \frac{1}{r} \frac{\partial v^r_\varepsilon}{\partial r} + \frac{\partial^2 v^r_\varepsilon}{\partial x^2} - \frac{v^r_\varepsilon}{r^2} \right] + \frac{\partial p^\varepsilon}{\partial r} = 0, \quad (5.1)
\]

\[
\rho \left[ \frac{\partial v_x^\varepsilon}{\partial t} + v^r_\varepsilon \frac{\partial v_x^\varepsilon}{\partial r} + v_x^\varepsilon \frac{\partial v_x^\varepsilon}{\partial x} \right] - \mu \left[ \frac{\partial^2 v_x^\varepsilon}{\partial r^2} + \frac{1}{r} \frac{\partial v_x^\varepsilon}{\partial r} + \frac{\partial^2 v_x^\varepsilon}{\partial x^2} \right] + \frac{\partial p^\varepsilon}{\partial x} = 0, \quad (5.2)
\]

\[
\frac{\partial v^r_\varepsilon}{\partial r} + \frac{\partial v_x^\varepsilon}{\partial x} + \frac{v^r_\varepsilon}{r} = 0. \quad (5.3)
\]

Further we assume that the lateral wall of the cylinder \( \Sigma_\varepsilon(t) = \{r = R + \eta_\varepsilon(x, t)\} \times (0, L) \) is elastic and allows only radial displacement. We can describe its motion (in Lagrangian coordinates) using the Navier equations for a linearly elastic membrane.

The radial contact force is given by

\[
F_r = -\frac{h(\varepsilon)E(\varepsilon) \eta^\varepsilon}{1 - \sigma^2} \frac{\eta^\varepsilon}{R^2} + h(\varepsilon)G(\varepsilon)k(\varepsilon) \frac{\partial^2 \eta^\varepsilon}{\partial x^2} - \rho_w h(\varepsilon) \frac{\partial^2 \eta^\varepsilon}{\partial t^2}, \quad (5.4)
\]

where \( F_r \) is the radial component of external forces (coming from the stresses induced by the fluid), \( \eta^\varepsilon \) is the radial displacement from the reference state \( \Sigma_\varepsilon^0 := \Sigma_\varepsilon(0) \), \( h = h(\varepsilon) \) is the membrane thickness, \( \rho_w \) is the wall volumetric mass, \( E = E(\varepsilon) \) is the Young’s modulus, \( 0 < \sigma \leq 0.5 \) is the Poisson ratio, \( G = G(\varepsilon) \) is the shear modulus and \( k = k(\varepsilon) \) is the Timoshenko shear correction factor ([69, 72]).

The fluid equations are coupled with the membrane equation through the lateral boundary conditions requiring the continuity of velocity and balance of forces. We require that the fluid velocity evaluated at the deformed interface \( (R + \eta^\varepsilon, x, t) \) equals the Lagrangian velocity of the membrane

\[
v^r_\varepsilon(R + \eta^\varepsilon, x, t) = \frac{\partial \eta^\varepsilon}{\partial t}(x, t) \text{ on } (0, L) \times \mathbb{R}_+ \quad (5.5)
\]

\[
v^\varepsilon_x(R + \eta^\varepsilon, x, t) = 0 \text{ on } (0, L) \times \mathbb{R}_+ \quad (5.6)
\]
Now we consider the balance of forces, namely we set the radial contact force equal to the radial component of the force exerted by the fluid.

The fluid contact force is given in Eulerian coordinates as,

\[ F_f = ((p^e - p_{ref})I - 2\mu D(v^e))ne_r, \]

where \( D(v^e) \) is the symmetrized gradient of velocity defined by,

\[ D(v^e) = \frac{1}{2}(\nabla v^e + (\nabla v^e)^T). \]

We need the Jacobian of the transformation from Eulerian to Lagrangian coordinates in order to perform the coupling. We consider Borel subsets \( B \) of \( \Sigma_0^e \) and require that

\[
\int_B ((p^e - p_{ref})I - 2\mu D(v^e))ne_r(R + \eta^e(x,t)) \sqrt{1 + \left(\frac{\partial \eta^e}{\partial x}\right)^2} \, dx = \int_B -F_r R \, dx, \tag{5.7}
\]

for all \( B \in \Sigma_0^e \), where \( J = \sqrt{1 + \left(\frac{\partial \eta^e}{\partial x}\right)^2} \) is the Jacobian determinant of the transformation from \( dx \) to \( d\Sigma_0^e/(2\pi R) \). Pointwise we have

\[
-F_r = ((p^e - p_{ref})I - 2\mu D(v^e))ne_r(1 + \frac{\eta^e}{R}) \sqrt{1 + \left(\frac{\partial \eta^e}{\partial x}\right)^2} \text{ on } \Sigma_0^e \times \mathbb{R}_+. \tag{5.8}
\]

The initial data are given by,

\[
\eta^e = \frac{\partial \eta^e}{\partial t} = 0 \text{ and } v^e = 0 \text{ on } \Sigma_0^e(0) \times \{0\}. \tag{5.9}
\]

We assume that the end-points of the tube are fixed and that the problem is driven by a time-dependent pressure drop between the inlet and outlet boundary. Therefore, we have the following inlet-outlet boundary conditions:

\[
v^e_r = 0, p^e + \rho(v^e_x)^2/2 = P_1(t) + p_{ref} \text{ on } (\partial \Omega_x(t) \cap \{x = 0\}) \times \mathbb{R}_+, \tag{5.10}
\]

\[
v^e_r = 0, p^e + \rho(v^e_x)^2/2 = P_2(t) + p_{ref} \text{ on } (\partial \Omega_x(t) \cap \{x = L\}) \times \mathbb{R}_+, \tag{5.11}
\]

\[
\eta^e = 0 \text{ for } x = 0, \eta^e = 0 \text{ for } x = L \text{ and } \forall t \in \mathbb{R}_+. \tag{5.12}
\]

We will assume that the pressure drop, \( A(t) = P_1(t) - P_2(t) \in C_0^\infty(0, +\infty) \).
Table 5.1: Parameter values

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\varepsilon$</td>
<td>0.002-0.06</td>
</tr>
<tr>
<td>Characteristic radius: $R_0$</td>
<td>0.0025-0.012 m</td>
</tr>
<tr>
<td>Characteristic length: $L$</td>
<td>0.065-0.2 m</td>
</tr>
<tr>
<td>Young’s modulus: $E$</td>
<td>$10^5 - 10^6$ Pa [60]</td>
</tr>
<tr>
<td>Wall thickness: $h$</td>
<td>$1 - 2 \times 10^{-3}$ m</td>
</tr>
<tr>
<td>Blood density: $\rho$</td>
<td>1050 kg/m$^3$</td>
</tr>
<tr>
<td>Reference pressure: $p_0$</td>
<td>13000 Pa = 97.5 mmHg</td>
</tr>
</tbody>
</table>

5.2.2 Weak formulation and a priori estimates

In this section we will introduce the variational formulation of the problem (5.1)-(5.3), (5.5)-(5.12) and a priori solution estimates, which are necessary for the reduced model derivation.

We proceed, first, by introducing the following norms

$$
||P_{12}(q, T)||^2_v = \max\{||P_1^2||_\infty, ||P_2^2||_\infty\}
+ 4q^2T^2\frac{1}{T}\int_0^T \max\{P_1^2(q, \tau), P_2^2(q, \tau)\} d\tau,
$$

(5.13)

$$
||A(q, T)||^2_{\text{aver}} = \frac{1}{T}\int_0^T |A(q, \tau)|^2 d\tau,
$$

(5.14)

$$
\mathcal{P} \equiv ||P_{12}(q, T)||^2_v + 24\pi^2T^2||A(q, T)||^2_{\text{aver}},
$$

(5.15)

where $q$ is the frequency of oscillations.

Further, we have the following bounds for the velocities $v^\varepsilon$ and radial displacements $\eta^\varepsilon$,
\[
\sup_{0 \leq t \leq T} \left\{ \frac{h(\varepsilon)E(\varepsilon)}{R(1 - \sigma^2)} \left| \eta^\varepsilon(t) \right|^2_{L^2(0,L)} + \frac{h(\varepsilon \rho_w R)}{2} \left| \frac{\partial \eta^\varepsilon}{\partial t}(t) \right|^2_{L^2(0,L)} \\
+ \frac{h(\varepsilon)G(\varepsilon) R}{2} \left| \frac{\partial \eta^\varepsilon}{\partial t}(x) \right|^2_{L^2(0,L)} \right\} \leq 2 \frac{R^3 L(1 - \sigma^2)}{h(\varepsilon)E(\varepsilon)} p^2,
\]
(5.16)

\[
\frac{2\mu}{\pi} \int_0^T \left| D(v^\varepsilon)(\tau) \right|^2_{L^2(\Omega_\varepsilon(\tau))} d\tau + \frac{\rho}{2\pi} \sup_{0 \leq t \leq T} \left| v^\varepsilon(\tau) \right|^2_{L^2(\Omega_\varepsilon(\tau))} \leq 2 \frac{R^3 L(1 - \sigma^2)}{h(\varepsilon)E(\varepsilon)} p^2.
\]
(5.17)

See [85] for more details.

Now, we are ready to introduce the solution and tests spaces.

Let the space \( \Gamma \) consists of all the functions \( \gamma \in L^\infty(0, T; H^1(0, L)) \cap W^{1,\infty}(0, T; L^2(0, L)) \) such that \( \gamma(t, 0) = \gamma(t, L) = 0 \) and such that the bound (5.16) is satisfied.

The space \( U \) consists of all the functions \( u = (u_r, u_x) \in L^2(0, T; H^{1/2-\delta}(\Omega_{R_{\max}})) \times H^1(\Omega_{R_{\max}}) \cap L^\infty(0, T; L^2(\Omega_{R_{\max}}))^2 \) for some \( \delta > 0 \), such that \( \nabla \cdot u = 0 \) in \( \Omega_{R_{\max}} \times \mathbb{R}_+ \), \( u_r = 0 \) for \( x = 0, L \) and the bound (5.17) is satisfied.

Let

\[
\Omega_\gamma(t) = \{(r, x)| 0 < r < R + \gamma(t, x), x \in (0, L)\}
\]

and \( \Sigma_\gamma(t) = \{r = R + \gamma(t, x)\} \times (0, L) \).

The set of solution candidates \( K \) consists of all the functions \( (\gamma, u) \), where the \( u \)'s are axially symmetric, such that

\[
K = \{(\gamma, u) \in \Gamma \times U | u_r(r, x, t) = \frac{\partial \gamma}{\partial t} \text{ for } R + \gamma(t, x) \leq r \leq R_{\max}, \\\n\text{ } u_r \in H^1(\Omega_\gamma(t)) | u_x(r, x, t) = 0 \text{ for } R + \gamma(t, x) \leq r \leq R_{\max}\}.
\]
(5.18)

Let us now define the space

\[
V(\Omega_\gamma(t)) = \{\varphi = \varphi_r e_r + \varphi_x e_x \in H^1(\Omega_\gamma(t)) | \varphi_r(r, 0) = \varphi_x(r, L) = 0, \\\n\varphi_x(R + \gamma(x, t), x) = 0 \text{ and } \nabla \cdot \varphi = 0 \text{ in } \Omega_\gamma(t) \text{ a.e.}\},
\]
(5.19)
then the test space is the space $H^1(0, T; V(\Omega_\gamma(t)))$

The weak formulation of the problem (5.1)-(5.3) and (5.5)-(5.12) is the following

For a given $(\gamma, u) \in K$ find $(\eta^\varepsilon, v^\varepsilon_r, v^\varepsilon_x) \in K$ such that $\forall \varphi \in H^1(0, T; V(\Omega_\gamma(t)))$ we have

\[
2\mu \int_{\Omega_\gamma(t)} D(v^\varepsilon) : D(\varphi) r \, dr \, dx + \rho \int_{\Omega_\gamma(t)} \{\frac{\partial \eta^\varepsilon}{\partial t} + (u(t) \nabla) v^\varepsilon\} \varphi \, r \, dr \, dx \\
+ R \int_0^L \{h(\varepsilon)G(\varepsilon)k(\varepsilon) \frac{\partial^2 \eta^\varepsilon}{\partial x^2} \frac{\partial}{\partial x} \varphi_r (R + \gamma(x, t), x, t) + \frac{h(\varepsilon)\rho(\varepsilon)}{1-\sigma^2} \eta^\varepsilon \varphi_r (R + \gamma(x, t), x, t)\} \, dx \\
+ R \rho h \int_0^L \frac{\partial^2 \eta^\varepsilon}{\partial x^2} \varphi_r (R + \gamma(x, t), x, t) \, dx = - \int_0^R \{P_2(qt) - \frac{\rho}{2}(u_x v_x^\varepsilon)|_{x=L}\} \varphi_x|_{x=L} \, r \, dr \\
+ \int_0^R \{P_1(qt) - \frac{\rho}{2}(u_x v_x^\varepsilon)|_{x=0}\} \varphi_x|_{x=0} \, r \, dr,
\]

and

\[
\eta^\varepsilon = \frac{\partial \eta^\varepsilon}{\partial t} = 0 \text{ on } (0, L) \times \{0\} \text{ and } v^\varepsilon (r, x, 0) = 0.
\]

**Remark 5.1.** Integrals involving scalar products with $\frac{\partial \eta^\varepsilon}{\partial t}$ and $\frac{\partial^2 \eta^\varepsilon}{\partial x^2}$ in fact are duality pairings.

Now, we present a priori solution estimates for the problem (5.20)-(5.21). The a priori estimates are important for determining an asymptotically reduced model (for the detailed derivation of these estimates see [85]).

**Theorem 5.1.** The following are the a priori solution estimates for the fluid-structure interaction problem defined above

\[
\frac{1}{L} ||\eta^\varepsilon(t)||^2_{L^2(O, L)} \leq 4 \frac{R^4(1 - \sigma^2)^2}{h(\varepsilon)^2 E(\varepsilon)^2} p^2,
\]

\[
||v^\varepsilon(t)||^2_{L^2(O, L)} \leq 4\pi \frac{R^3 L(1 - \sigma^2)}{\rho h(\varepsilon) E(\varepsilon)} p^2,
\]

78
\[
\int_0^t \left\{ \left\| \frac{\partial v^\varepsilon}{\partial r} \right\|^2_{L^2(\Omega_c(\tau))} + \left\| \frac{\partial v^\varepsilon}{\partial x} \right\|^2_{L^2(\Omega_c(\tau))} + \left\| \frac{\partial v^\varepsilon}{\partial x} \right\|^2_{L^2(\Omega_c(\tau))} \right\} d\tau \\
\leq \frac{R^2}{2\mu} \sqrt{\frac{R(1-\sigma^2)}{\rho h(\varepsilon)E(\varepsilon)\rho}} \mathcal{P}^2, \quad (5.24)
\]

\[
\int_0^t \left\{ \left\| \frac{\partial v^\varepsilon}{\partial r} \right\|^2_{L^2(\Omega_c(\tau))} + \left\| \frac{\partial v^\varepsilon}{\partial x} \right\|^2_{L^2(\Omega_c(\tau))} \right\} d\tau \leq \frac{R^2}{2\mu} \sqrt{\frac{R(1-\sigma^2)}{\rho h(\varepsilon)E(\varepsilon)\rho}} \mathcal{P}^2. \quad (5.25)
\]

5.2.3 Asymptotic reduction of the model

In order to represent the equations (5.1)-(5.3) in nondimensional form we introduce the independent variables \( \tilde{r}, \tilde{x} \) and \( \tilde{t} \)

- \( r = R\tilde{r} \),
- \( x = L\tilde{x} \),
- \( t = \frac{1}{\omega^e} \tilde{t} \), where \( \omega^e = \frac{1}{L} \sqrt{\frac{hE}{R(1-\sigma^2)}} \).

Based on the \textit{a priori} estimates (5.22) - (5.25) we introduce the following asymptotic expansions

\[
v^\varepsilon = V \{ v^0 + \varepsilon v^1 + \ldots \}, \quad \text{with} \quad V = \sqrt{\frac{R(1-\sigma^2)}{\rho hE}} \mathcal{P}, \quad (5.26)
\]

\[
\eta^\varepsilon = \Xi \{ \eta^0 + \varepsilon \eta^1 + \ldots \}, \quad \text{with} \quad \Xi = \frac{R^2(1-\sigma^2)}{hE} \mathcal{P}, \quad (5.27)
\]

\[
p^\varepsilon = \rho V^2 \{ p^0 + \varepsilon p^1 + \ldots \}. \quad (5.28)
\]

After ignoring the terms of order \( \varepsilon^2 \) and smaller the momentum equations and the incompressibility condition become
\begin{align}
Sh & \frac{\partial \tilde{v}_x^e}{\partial t} + \tilde{v}_x^e \frac{\partial \tilde{v}_x^e}{\partial x} + \tilde{v}_r^e \frac{\partial \tilde{v}_x^e}{\partial r} - \frac{1}{Re} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial \tilde{v}_x^e}{\partial r} \right) \right] = 0, \tag{5.29} \\
\frac{\partial \tilde{p}}{\partial r} &= 0, \tag{5.30} \\
\frac{\partial}{\partial r} (\tilde{r} \tilde{v}_r^e) + \frac{\partial}{\partial x} (\tilde{r} \tilde{v}_x^e) &= 0, \tag{5.31}
\end{align}

where \( Sh = \frac{Le}{\nu} \) and \( Re = \frac{\nu R^2}{\mu L} \).

The leading order Navier equations read

\[-F_r = \mathcal{P} \left[ \tilde{\eta} - \frac{G(\varepsilon)k(1 - \sigma^2)\varepsilon}{E(\varepsilon)} \frac{\partial^2 \tilde{\eta}}{\partial x^2} \right] + O(\varepsilon^2). \tag{5.32} \]

Since \( G = E/(2(1 + \sigma)) \) and \( k = O(1) \), the second term on the right-hand side can also be neglected.

The asymptotic form of the contact force derived from (5.4) becomes

\[ ((\tilde{p}^e - \tilde{p}_{ref})I - 2\mu D(v^e))n e_r = \rho V^2 (\tilde{p}^e - \tilde{p}_{ref} + O(\varepsilon^2)) \left( 1 + \frac{\Xi}{R} \tilde{\eta} \right). \]

Therefore, we obtain the following leading order relationship between the pressure and the radial displacement

\[ (\tilde{p}^e - \tilde{p}_{ref}) = \frac{\mathcal{P}}{\rho V^2} \frac{\tilde{\eta}}{1 + \frac{\Xi}{R} \tilde{\eta}} = \frac{\mathcal{P}}{\rho V^2 \Xi} \frac{\Xi}{R} \tilde{\eta} \left( 1 - \frac{\Xi}{R} \tilde{\eta} + \ldots \right) = \frac{\mathcal{P} R}{\rho V^2 \Xi} \left( \frac{\Xi}{R} \tilde{\eta} - \left( \frac{\Xi}{R} \tilde{\eta} \right)^2 \ldots \right). \tag{5.33} \]

We assume that \( \Xi/R \) is of order \( \varepsilon \) so the last term on right-hand side of (5.33) can be ignored and we obtain

\[ \tilde{p}^e - \tilde{p}_{ref} = \frac{\mathcal{P} R}{\rho V^2} \tilde{\eta}, \tag{5.34} \]

which in dimensional variables gives us the Law of Laplace,

\[ \tilde{p}^e - \tilde{p}_{ref} = \frac{Eh}{(1 - \sigma^2)R \tilde{R}} \frac{\eta}{R}. \tag{5.35} \]
5.2.4 The reduced two-dimensional problem

Now, having the results of the previous section in hand, we proceed by introducing the reduced two-dimensional model written in non-dimensional variables.

We define the domain (scaled)

\[ \tilde{\Omega}(\bar{t}) = \{(\tilde{x}, \tilde{r}) \in \mathbb{R}^2 | \tilde{r} < 1 + \frac{\Xi}{R} \eta(\tilde{x}, \bar{t}), 0 < \tilde{x} < 1\}, \]

and the lateral boundary \( \tilde{\Sigma}(\bar{t}) = \{\tilde{r} = 1 + \frac{\Xi}{R} \eta(\tilde{x}, \bar{t})\} \times (0, 1) \).

Now we formulate the two-dimensional problem in the following way,

**Find a triple** \((\tilde{v}_x, \tilde{v}_r, \tilde{\eta})\) **satisfying**

\[
Sh \frac{\partial \tilde{v}^e_x}{\partial \bar{t}} + \tilde{v}^e_x \frac{\partial \tilde{v}^e_x}{\partial \bar{x}} + \tilde{v}^e_r \frac{\partial \tilde{v}^e_x}{\partial \bar{r}} + \frac{\partial \tilde{p}}{\partial \bar{x}} = \frac{1}{Re} \left[ \frac{1}{\tilde{r}} \frac{\partial}{\partial \tilde{r}} \left( \tilde{r} \frac{\partial \tilde{v}_x^e}{\partial \bar{r}} \right) \right],
\]

\( (\tilde{p}^e - \tilde{p}_{ref}) = \frac{PR}{\rho V^2 \tilde{\eta}}, \)

\[
\tilde{v}_r(\tilde{x}, 1 + \frac{\Xi}{R} \eta(x, t), \bar{t}) = \frac{\partial \tilde{\eta}}{\partial \bar{t}}, \quad \tilde{v}_x = 0,
\]

with the initial and boundary conditions given by

\[
\tilde{\eta} = \frac{\partial \tilde{\eta}}{\partial \bar{t}} = 0 \text{ at } \bar{t} = 0,
\]

\[
\tilde{v}_r^e = 0, \quad \tilde{p} = (P_1(\bar{t}) + p_{ref})/(\rho V^2) \text{ on } (\partial \Omega_x(\bar{t}) \cap \{\tilde{x} = 0\}) \times \mathbb{R}_+,
\]

\[
\tilde{v}_r^e = 0, \quad \tilde{p} = (P_2(\bar{t}) + p_{ref})/(\rho V^2) \text{ on } (\partial \Omega_x(\bar{t}) \cap \{\tilde{x} = 1\}) \times \mathbb{R}_+,
\]

\[
\tilde{\eta} = 0 \text{ for } \tilde{x} = 0, \quad \tilde{\eta} = 0 \text{ for } \tilde{x} = 1 \text{ and } \forall \bar{t} \in \mathbb{R}_+.
\]

81
The model defined above is a free-boundary degenerate hyperbolic system with parabolic regularization. This system, though already simplified, is still quite complex. The theoretical analysis and numerical simulation of (5.36)-(5.43) is a difficult task; that is why we will proceed further in order to obtain a simplified one-dimensional reduced model.

### 5.2.5 Derivation of the one-dimensional reduced model

In order to derive a simplified one-dimensional model we express the two-dimensional equations in terms of the averaged quantities across the cross-sectional area.

Let us introduce 
\[ \bar{A} = (1 + \frac{\bar{\varepsilon}}{R} \tilde{\eta})^2 \] and 
\[ \bar{m} = \bar{A} \bar{U} \] where

\[ \bar{U} = \frac{2}{\bar{A}} \int_0^{1 + \frac{\bar{\varepsilon}}{R} \tilde{\eta}} \bar{v}_x \bar{r} d\bar{r}, \] (5.44)

\[ \bar{\alpha} = \frac{2}{\bar{A}U^2} \int_0^{1 + \frac{\bar{\varepsilon}}{R} \tilde{\eta}} 2 \bar{v}_x^2 \bar{r} d\bar{r}. \] (5.45)

Now we integrate the equations (5.36)-(5.37) from \( \bar{r} = 0 \) to \( \bar{r} = 1 + \frac{\bar{\varepsilon}}{R} \tilde{\eta} \) and then express them in terms of the averaged quantities. Using the no-slip condition at the lateral boundary we obtain

\[ \frac{\partial \bar{A}}{\partial \bar{t}} + \frac{\Xi}{R} \frac{\partial \bar{m}}{\partial \bar{x}} = 0, \] (5.46)

\[ Sh \frac{\partial \bar{m}}{\partial \bar{t}} + \frac{\partial}{\partial \bar{x}} \left( \frac{\bar{A} \bar{m}^2}{\bar{A}} \right) + \bar{A} \frac{\partial \bar{\rho}}{\partial \bar{x}} = \frac{2}{\bar{A}} \sqrt{\bar{A}} \left[ \frac{\partial \bar{v}_x}{\partial \bar{r}} \right]_\Sigma. \]

The next step is to specify the axial velocity profile \( \bar{v}_x \) in terms of the averaged quantities. The typical approximation (corresponding to Poiseuille flow [90]) is

\[ \bar{v}_x = \frac{\gamma + 2}{\gamma} \bar{U} \left[ 1 - \left( \frac{\bar{r}}{1 + \frac{\bar{\varepsilon}}{R} \tilde{\eta}} \right)^\gamma \right]. \] (5.47)

We assume that \( \gamma = 9 \), which corresponds to the non-Newtonian flow of blood [78, 79]. We calculate \( \alpha \) and obtain \( \alpha = 1.1 \).
After plugging (5.47) into (5.43) the right hand side becomes

\[
\frac{-2(\gamma + 2) \tilde{m}}{Re \ \overline{A}}
\]

Using \( A_0 \) to denote the non-stressed area \( R^2 \) we obtain a one-dimensional system written in dimensional variables

\[
\frac{\partial A}{\partial t} + \frac{\partial m}{\partial x} = 0, \quad (5.48)
\]

\[
\frac{\partial m}{\partial t} + \frac{\partial}{\partial x} \left( \frac{\alpha m^2}{A} \right) + \frac{A \partial p}{\rho \partial x} = -\frac{2\mu}{\rho} (\gamma + 2) \frac{m}{\overline{A}}, \quad (5.49)
\]

\[
p := p - p_{ref} = \left( \frac{Eh}{(1 - \sigma^2)R} \left( \sqrt{\frac{A}{A_0}} - 1 \right) \right). \quad (5.50)
\]

We use \( \sigma = 0.5 \), so equation (5.50) reduces to

\[
p = G_0 \left( \sqrt{\frac{A}{A_0}} - 1 \right), \quad (5.51)
\]

with \( G_0 = \frac{4Eh}{3R} \).

### 5.3 Conditions at the bifurcation point

We use the system of equations (5.48)-(5.49) and (5.51) to model blood flow through the abdominal aorta branching into the iliac arteries (Fig.5.3).

One of the important questions here is how to model the flow at the branching point. We use the continuity of pressure and conservation of mass condition to couple the flow exiting the abdominal aorta with the flow entering the iliac arteries [62]. It was shown in [54] that the 1-D approximation to the flow at the branching point for the fixed geometry provides \( \varepsilon^{1/2} \) accuracy to the 3-D flow for small to moderate Reynolds numbers. The analysis demonstrating the accuracy of the 1-D approximation on compliant branching points remains an open problem.
We calculate the continuity of pressure and conservation of mass condition at the branching point using the concept of Riemann invariants for a hyperbolic system. More precisely, let us write the system (5.48)-(5.49) and (5.51) in quasilinear form:

$$
\begin{pmatrix}
A_t \\
m_t
\end{pmatrix} + \begin{pmatrix}
0 & 1 \\
-\frac{m^2}{A^2} + \frac{1}{\rho} Ap(A) & \frac{2m}{A}
\end{pmatrix} \begin{pmatrix}
A_x \\
m_x
\end{pmatrix} = \begin{pmatrix}
0 \\
-2 \frac{\alpha}{\alpha - 1} \nu m
\end{pmatrix}
$$

(5.52)

The eigenvalues of (5.52) are

$$\lambda = \frac{m}{A} - \sqrt{\frac{1}{2} \frac{G_0}{\rho} \left( \frac{A}{A_0} \right)^{1/2}}, \quad \mu = \frac{m}{A} + \sqrt{\frac{1}{2} \frac{G_0}{\rho} \left( \frac{A}{A_0} \right)^{1/2}}.
$$

(5.53)

Let us further use the following notation: \(\bar{c} = \sqrt{\frac{1}{2} \frac{G_0}{\rho} A_0^{-1/2}}\).

One can show that the right eigenvectors corresponding to \(\lambda\) and \(\mu\) are given by

$$r_\lambda = \begin{pmatrix} 1 \\ \lambda \end{pmatrix}, \quad r_\mu = \begin{pmatrix} 1 \\ \mu \end{pmatrix}.
$$

(5.54)

Consider Riemann invariants \(w\) and \(z\) corresponding to the eigenvalues \(\lambda\) and \(\mu\) respectively. Then \(w\) and \(z\) satisfy the following equations [80]:

$$\nabla w \cdot r_\lambda = 0, \quad \nabla z \cdot r_\mu = 0,
$$

(5.55)
Direct calculations give us

\[
w = \frac{m}{A} + 4\sqrt{\frac{1}{2} \frac{G_0}{\rho} \left( \frac{A}{A_0} \right)^{1/2}}, \quad (5.56)
\]

\[
z = \frac{m}{A} - 4\sqrt{\frac{1}{2} \frac{G_0}{\rho} \left( \frac{A}{A_0} \right)^{1/2}}. \quad (5.57)
\]

Now, we assume that the bifurcation occurs at a point and that there is no leakage at the bifurcation. Then the outflow from the abdominal aorta ("parent" vessel) should be balanced by the inflow into the iliac arteries ("daughter" vessels) [62]:

\[m_p = m_{d1} + m_{d2}, \quad (5.58)\]

which describes conservation of mass. We also assume the continuity of pressure

\[p_p = p_{d1} = p_{d2}, \quad (5.59)\]

here subscript \(p\) corresponds to the "parent" vessel and \(d1, d2\) correspond to the "daughter" vessels.

The Riemann invariants for the "parent" and the two "daughter" vessels read as follows:

\[w_p = \frac{m_p}{A_p} + \tilde{c}_p A_p^{1/4}, \quad (5.60)\]

\[z_{d1} = \frac{m_{d1}}{A_{d1}} - \tilde{c}_{d1} A_{d1}^{1/4}, \quad (5.61)\]

\[z_{d2} = \frac{m_{d2}}{A_{d2}} - \tilde{c}_{d2} A_{d2}^{1/4}. \quad (5.62)\]

Recalling the pressure-area relationship (5.51) and assuming that \(G_0\) at the branching point is the same for the "parent" vessel and the "daughter" vessels we can rewrite (5.59)
in terms of the cross-sectional areas:

\[ \frac{A_p}{A_{0p}} = \frac{A_{d1}}{A_{0d1}}, \]

\[ \frac{A_p}{A_{0p}} = \frac{A_{d2}}{A_{0d2}}. \]

Adding (5.61) and (5.62) and using (5.58) we have

\[ m_p = m_{d1} + m_{d2} = A_{d1}z_{d1} + \bar{c}_{d1}A_{d1}^{5/4} + 4A_{d2}z_{d2} + \bar{c}_{d2}A_{d2}^{5/4}. \]

Further, the use of equations (5.60) and (5.63) gives us

\[ A_p w_p - \bar{c}_p A_p^{5/4} = \frac{A_p A_{0d1}}{A_{0p}} z_{d1} + \bar{c}_{d1}A_{d1}^{5/4} \left( \frac{A_p A_{0d1}}{A_{0p}} \right)^{5/4} \]
\[ + \frac{A_p A_{0d2}}{A_{0p}} z_{d2} + \bar{c}_{d2}A_{d2}^{5/4} \left( \frac{A_p A_{0d1}}{A_{0p}} \right)^{5/4}. \]

Let us introduce auxiliary variables \( b_1 = \frac{A_{d1}}{A_{0p}} \) and \( b_2 = \frac{A_{d2}}{A_{0p}} \). Then we have the following nonlinear equation for \( A_p \):

\[ (w_p - b_1 z_{d1} - b_2 z_{d2}) A_p - 4(\bar{c}_p + \bar{c}_{d1}b_1^{5/4} + \bar{c}_{d2}b_2^{5/4}) A_p^{5/4} = 0. \]

Due to physical reasons we assume that \( A_p \neq 0 \), hence \( A_p \) can be determined through

\[ A_p^{1/4} = \frac{w_p - b_1 z_{d1} - b_2 z_{d2}}{4 (\bar{c}_p + \bar{c}_{d1}b_1^{5/4} + \bar{c}_{d2}b_2^{5/4})}. \]

Now using equations (5.63) and (5.61)-(5.62) it is easy to evaluate \( A_{d1}, A_{d2}, m_p, m_{d1} \)
and \( m_{d2} \).

Thus, using Riemann invariants and conditions (5.58) and (5.59) we can calculate \( A_p \),
\( A_{d1}, m_p, m_{d1} \) and \( m_{d2} \) in terms of the Riemann invariants \( w_p, z_{d1} \) and \( z_{d2} \). The "forward"
Riemann invariant \( w_p \) and the "backward" Riemann invariants \( z_{d1} \) and \( z_{d2} \) are known from
the initial conditions and the inlet and outlet boundary data.
5.4 Numerical method

In order to solve equations (5.48)-(5.49) and (5.51) we rewrite them first in conservation form. We take into account that $A_0$ can depend on $x$ and write the equations in conservation form as follows

$$\frac{\partial}{\partial t} U + \frac{\partial}{\partial x} F = S,$$

where

$$U = \begin{bmatrix} A \\ m \end{bmatrix}, \quad F(U) = \begin{bmatrix} m \\ \frac{\alpha m^2}{A} + \frac{G_0}{3\rho} \left( \frac{A}{A_0} \right)^{3/2} A_0 \end{bmatrix},$$

and

$$S(U) = \begin{bmatrix} 0 \\ -2 \frac{\alpha}{\alpha - 1} \frac{m}{A} + \frac{G_0}{3\rho} \left( \frac{A}{A_0} \right)^{3/2} A_0 \end{bmatrix}.$$

For the numerical solution of the problem stated above we apply the two-step Lax-Wendroff method [46]. We assume here that the grid is uniform, with $\Delta x$ denoting the mesh step size and $\Delta t$ the time step, then we define $U^n_m$ to be the approximation of the solution at $(m\Delta x, n\Delta t)$. The method takes the following form

$$U^{n+1}_m = U^n_m - \frac{\Delta t}{\Delta x} (F(U^{n+1/2}_{m+1/2}) - F(U^{n+1/2}_{m-1/2})) + \frac{\Delta t}{2} (S(U^{n+1/2}_{m+1/2}) + S(U^{n+1/2}_{m-1/2}))$$

where

$$U^{n+1/2}_j = \frac{U^n_{j+1/2} + U^n_{j-1/2}}{2} + \frac{\Delta t}{\Delta x} \left( -\frac{F(U^n_{j+1/2}) - F(U^n_{j-1/2})}{\Delta x} + \frac{S(U^n_{j+1/2}) + S(U^n_{j-1/2})}{2} \right)$$

for $j = m + 1/2$ and $j = m - 1/2$.

The method is stable if the CFL condition

$$\max |\lambda, \mu| \frac{\Delta t}{\Delta x} = \max \left| \frac{\alpha m}{A} \pm \sqrt{\alpha(\alpha - 1)} \left( \frac{m}{A} \right)^2 + \frac{G_01}{2\rho} \left( \frac{A}{A_0} \right)^{1/2} \right| \frac{\Delta t}{\Delta x} < 1,$$

is satisfied.
Figure 5.4: Aneurysmal abdominal aorta and iliac arteries with inserted bifurcated stent.

5.5 Numerical experiments

We use the numerical method described above to study blood flow through the aneurysmal prostheses (see Figure 5.4). We considered two kinds of prostheses:

- Fabric covered "rigid" stent-grafts, such as AneuRx™.
- Highly compliant bare stents, such as Wallstent.

Presently, bare stents are no longer in use. We considered stents in this study because they have drastically different elastic properties than stent-grafts such as AneuRx™. One of the goals of this study was to understand the influence of the elastic properties of the prosthesis on the stresses exerted by the prostheses to the walls of the native aorta. In particular we were interested in understanding what hemodynamic factors are related to the occlusion of graft limbs, observed in patients and reported in [13, 12, 63, 82].

Many researchers have shown that the wall shear stress has a significant influence on blood coagulation and thrombosis, endothelial cell structure and function. For instance, C.G. Caro et al. [11] stated that low wall shear stress could produce an area of low mass transfer. On the contrary, D. L. Fry [26] showed that wall shear stress in excess of 400 dyn/cm² can damage endothelial cell layer.

C.K. Zarins et al.([43],[58]) proposed a method called Oscillatory Shear Index (OSI) to quantify the degree of oscillation in shear direction. OSI can be calculated using the
Figure 5.5: Oscillatory Shear Index.

following formula:

\[
OSI = \frac{|A_{neg}|}{|A_{pos}| + |A_{neg}|},
\]

where \( A_{neg} \) and \( A_{pos} \) are the areas under the shear stress vs. time when the shear stress is negative and positive respectively (see Figure 5.5).

M. Haidekker, C. White and J.A. Frangos suggested that the spatial and temporal gradients of the shear stress must be separated in order to identify which one is the primary cause of atherosclerotic plaque. In their paper [34], they presented a study implicating high shear stress rate (or the temporal gradient of shear stress) as the main hemodynamic factor responsible for the initiation of focal atherogenesis.

We studied the Oscillatory Shear Index and the shear stress rate to detect possible causes for graft limb occlusion.

The following two parameters were varied in our study:

- prostheses flexibility (Young’s modulus),
- prostheses diameter.
Figure 5.6: *AneuRx bifurcated stent.*

We have used the following data in our computations:

- Young’s modulus $E_c = 8700 \text{Pa}$ and $E_r = 217500 \text{Pa}$ for compliant and rigid stents respectively

- Young’s modulus of a human aorta $E_a = 10^5 \text{Pa}$

First, we present the results of the numerically computed OSI for two different prostheses flexibility parameters and different diameters of ”parent”(main body) and ”daughter” (limb) components.

On each of the Figures 5.7-5.9 the solid curve shows the Oscillatory Shear Index for the main body component from the anchoring site to the bifurcation point and the ”solid-star” curve presents the OSI corresponding to the limb component from the bifurcation point downstream to the distal anchoring site.

The Young’s modulus of the prostheses shown in Figures 5.7- 5.8 corresponds to the one of AneuRx stent-graft, the main body diameters are 23 mm and 28.5 mm and the limb
Figure 5.7: Oscillatory Shear Index for AneuRx stent-graft with limb diameter equal to 12 mm and main body diameter 23 mm.

diameters are 12 mm and 16 mm. We observed that the smaller the diameter of the prosthesis the higher the OSI. We also tested a flexible prosthesis with a Young’s modulus corresponding to a Wallstent endoprosthesis. The diameter of the main body for this case was taken to be 20 mm and the limb diameter is 14.5 mm. The amplitude of the Oscillatory Shear Index drastically increased for this case, indicating a much higher probability for occlusion.

Although the OSI showed that the smaller the diameter of the limbs the higher the OSI, it did not capture the patient-observed prosthesis characteristics that show higher probability for thrombosis at the distal site and not typically at the proximal site of the prosthesis. In contrast, the shear stress rate of the bifurcated prostheses did show to be higher at the distal anchoring site thereby conforming better to the complications observed in patients.

Figures 5.10-5.16 present the temporal gradient of shear stress at the systolic peak for different prostheses data. Each figure has two curves:
Figure 5.8: Oscillatory Shear Index for AneuRx stent-graft with limb diameter equal to 16 mm and main body diameter 28.5 mm.

- one curve corresponding to the shear stress rate along the "parent" prosthesis part (main modular element) from the proximal anchoring site to the bifurcation point.

- the second curve corresponding to the shear stress rate along the graft limb from the bifurcation point downstream to the distal anchoring site.

The Young’s modulus of the AneuRx stent-graft shown in Figure 5.6 was used in the numerical experiments to describe the flexibility of the prosthesis. Several different stent-graft designs were tested for shear stress rates. The parent (main body) diameter ranged from 23 mm to 28.5 mm and the limbs ranged in diameter from 12 mm to 14.5 mm for smaller prostheses, and from 12 mm to 16 mm for larger prostheses.

Figures 5.10 and 5.11 show the shear stress rates corresponding to the two extreme cases: the prosthesis with the smaller limb diameter (12 mm) and the prosthesis with the largest limb diameter (16 mm), respectively. We observe that the smaller the diameter of the limbs the larger the shear stress rate, indicating a higher chance for occlusion. The
Figure 5.9: Oscillatory Shear Index for Wallstent stent with limb diameter equal to 14.5 mm and main body diameter 20 mm.

worst performance was obtained for the smallest prostheses (Figure 5.10) and the best performance was for prostheses with a limb diameter equal to 16 mm (Figure 5.11).

We also observed that the size of the diameter of the main body influences the magnitude of the shear stress rate. Figures 5.13 and 5.14 show the comparison between two prostheses with the same limb diameters, but with different sizes for the main body: one with a main body diameter of 23 mm and the second one with a main body diameter of 28.5 mm. We can see an improvement in the shear stress rates for the larger main body prosthesis.

We calculated the shear stress rates for a bifurcated prosthesis with a compliancy corresponding to the Wallstent endoprosthesis. The Young’s modulus of the Wallstent was measured \[88, 89, 87\] and is equal to 8700 \(N/m^2\), which is about ten times more elastic than the wall of the human aorta \[87\]. As in the previous experiments for the ”stiff” stent, we assumed that the diameter of the main modular component ranged from 23 mm to 28.5
Figure 5.10: Shear Stress Rates for AneuRx stent-graft with limb diameter equal to 12 mm and main body diameter 23 mm.

mm, and that the limbs diameter is between 12 mm and 16 mm. Figure 5.15 presents the results of the numerical computations which indicate that the shear stress rates are drastically higher than for the case of stiff prosthesis.

The results presented above indicate that the magnitude of the shear stress rate is affected mainly by the size of the limbs and by the prostheses elasticity. In an attempt to obtain an optimal design minimizing shear stress rates we tested different prosthesis structures varying the limb diameter and elasticity parameters. We have found that the shear stress rate is minimized for the prosthesis with the following two characteristic:

- The diameter of the prosthesis limbs should be around $\sqrt{2}/2$ of the diameter of the main body component: if $D_p$ denotes the diameter of the parent (main body) component and $D_d$ denotes the diameter of the daughter (limb) component, then we obtained numerically that the lowest shear stress rates in the limbs are observed when $D_d = \frac{\sqrt{2}}{2} D_p$. This relationship is a consequence of the conservation of mass princi-
Figure 5.11: *Shear Stress Rates for AneuRx stent-graft with limb diameter equal to 16 mm and main body diameter 28.5 mm.*

- **Variable elasticity:** The prosthesis which is stiffer in the central section, where there is no support to the prosthesis walls by the walls of native aorta, and softer at the overlap with the iliac arteries, showed best performance. In this test we used the fact that the stiffness of the composit prosthesis/vessel structure is equal to the combined stiffness of each structure, \[21\]. Hence, the smaller the stiffness of the prosthesis in the overlap anchoring region, the smaller the difference between the stiffness of the native vessel and prosthesis.

Figure 5.16 shows the behavior of the shear stress rates for the ”optimal” prosthesis with characteristics obtained from the suggestions above:

- **Young’s modulus in the overlap region** \(E_{\text{overlap}} = 8700 \text{Pa}\) (corresponds to \textit{Wallstent} elasticity),
Figure 5.12: Oscillatory Shear Index for "optimal" stent with limb diameter equal to 20 mm and main body diameter 28.5 mm.

- Young’s modulus of the prosthesis in the aneurysm sac region is equal to 100000 Pa, i.e. equal to AneuRx Young’s modulus,
- diameter of the main body component is $D_{mb} = 28.5 \text{ mm}$,
- diameter of the limbs is $D_l = 20 \text{ mm}$ (which is about $\sqrt{2} D_{mb}$).

We observed a drastic improvement in the limb shear stress rates with respect to the previous prosthesis structures.

We also calculated the Oscillatory Shear Index for the "optimal prosthesis" described above (see Figure (5.12)). The results also showed a much smaller amplitude of OSI compared to the cases given in Figures (5.7)-(5.9).

For a comparison, we tested the shear stress rates for a bifurcated AneuRx stent-graft prosthesis with uniform stiffness, with a main body diameter of 28.5 mm and a limb diameter of 20 mm. The results are presented in Figure 5.17. We can see that this prosthesis...
Figure 5.13: *Shear Stress Rates for the AneuRx stent-graft with a limb diameter equal to 14.5 mm and a main body diameter 28.5 mm.*

design produces shear stress rates that are close to optimal.
Figure 5.14: Shear Stress Rates for the AneuRx stent-graft with a limb diameter equal to 14.5 mm and a main body diameter 23 mm.

Figure 5.15: Shear Stress Rates for the Wallstent endoprosthesis with a limb diameter equal to 20 mm and a main body diameter of 28 mm.
Figure 5.16: *Shear Stress Rates for an "optimal" stent with a limb diameter equal to 20 mm and a main body diameter of 28.5 mm.*

Figure 5.17: *Shear Stress Rates for the AneuRx stent-graft with a limb diameter equal to 20 mm and a main body diameter of 28.5 mm.*
Bibliography


