### RICE UNIVERSITY

### **Optimization of Shell Structure Acoustics**

by

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A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE

Doctor of Philosophy

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#### Abstract

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This thesis analyzes a mathematical model for shell structure acoustics, and develops and implements the adjoint equations for this model. The adjoint equations allow the computation of derivatives with respect to large parameter sets in shape optimization problems where the thickness and mid-surface of the shell are computed so as to generate a radiated sound field subject to broad-band design requirements.

The structure and acoustics are modeled, respectively, via the Naghdi shell equations, and thin boundary integral equations, with full coupling at the shell midsurface. In this way, the three-dimensional structural-acoustic equations can be posed as a problem on the two-dimensional mid-surface of the shell. A wide variety of shapes can thus be explored without re-meshing, and the acoustic field can be computed anywhere in the exterior domain with little additional effort. The problem is discretized using triangular MITC shell elements and piecewise-linear Galerkin boundary elements, coupled with a simple one-to-one scheme.

Prior optimization work on coupled shell-acoustics problems has been focused on applications with design requirements over a small range of frequencies. These problems are amenable to a number of simplifying assumptions. In particular, it is often assumed that the structure is dense enough that the air pressure loading can be neglected, or that the structural motions can be expanded in a basis of low-frequency eigenmodes. Optimization of this kind can be done with reasonable success using a small number of shape parameters because simple modal analysis permits a reasonable knowledge of the parts of the design that will require modification. None of these assumptions are made in this thesis. By using adjoint equations, derivatives of the radiated field can be efficiently computed with respect to large numbers of shape parameters, allowing a much richer space of shapes, and thus, a broader range of design problems to be considered. The adjoint equation approach developed in this thesis is applied to the computation of optimal mid-surfaces and shell thicknesses, using a large shape parameter set, proportional in size to the number of degrees of freedom in the underlying finite element discretization.

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# Chapter 1

# Introduction

# 1.1 Motivation

The aim of this work is to perform shape optimization of elastic shell structures with respect to acoustic characteristics. There is a wide variety of applications for such a technique, which may be divided into two general categories.

The first comprises applications where mechanical, and not acoustic, characteristics are of primary importance. Shell structures are useful in such situations, for when a shell supports a load through membrane stresses, it can be very stiff for a given mass [24]. Example applications include the design of automobiles [91, 93], and buildings [1]. These are interior domain problems where the basic shape of the object in question is already determined by mechanical considerations, and it is of interest to see whether noise can in some sense be reduced by modification of the shell geometry without undue addition of mass.

The second category, on which this work is focused, includes applications where acoustic characteristics are of paramount importance, such as the design of loudspeakers [40] and musical instruments [66]. Here, the main consideration is the radiated acoustic field, potentially into an unbounded domain. Several techniques for characterization of the radiated field are discussed in [41], but as both aforementioned



Figure 1.1: Acoustic transfer functions of Douglas Martin's balsa violin #4 and a violin by Barbieri, as measured by George Bissinger.



Figure 1.2: Coupled problem geometry. The domain  $\Omega^-$  has one "thin" dimension. The response due to spatially localized loading f is measured at the far-field point  $x^*$ .

classes of applications often make use of point-response measurements, which are relatively easy to measure via experiment, I choose to consider optimization of the acoustic transfer function produced by a spatially localized time-harmonic driving force. In general, the performance of the structure is measured over a broad range of frequencies, e.g., for the violin transfer functions shown in figure 1.1. In the next section, the prototypical problem is formally stated.

# **1.2** Coupled Problem Definition

Consider the Lipschitz domain  $\Omega^-$  shown in figure 1.2, with boundary  $\Gamma$ , and outward normal vector n defined almost everywhere. The exterior domain is  $\Omega^+ = \mathbb{R}^3 \setminus \overline{\Omega^-}$ . In the following, Latin indices range from 1 to 3. The equations of linear elasticity for the displacement  $u: \Omega^- \to \mathbb{R}^3$  are

$ ho u_{tt} =  abla \cdot \sigma$	in $\Omega^-$
$\sigma = H : e(u)$	in $\Omega^-$
$\sigma \cdot n = h$	on $\Gamma$ ,

where

- $\rho: \Omega^- \to \mathbb{R}^+$  is the density of the elastic material,
- $H_{ijkl}: \Omega^- \to \mathbb{R}$  are the Cartesian components of the constitutive tensor,
- $\sigma_{ij}: \Omega^- \to \mathbb{R}$  are the Cartesian components of the stress tensor,
- $e(u)_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i)$  are the Cartesian components of the symmetric gradient or strain tensor,
- and  $h_i: \Gamma \to \mathbb{R}$  are the Cartesian components of the boundary traction.

The acoustic wave equation (with Neumann boundary conditions) for the velocity potential  $\varphi : \Omega^+ \to \mathbb{R}$  is

$$\frac{1}{c^2} \frac{\partial^2 \varphi}{\partial t^2} - \Delta \varphi = 0 \qquad \text{in } \Omega^+$$
$$\partial_n \varphi = g \qquad \text{on } \Gamma,$$

where

- c > 0 is the speed of sound in the acoustic medium,
- $\rho_0 > 0$  is the density of the air,
- and  $g_i: \Gamma \to \mathbb{R}$  are the Cartesian components of the prescribed normal velocity.

The elastic boundary traction h is the sum of a driving force f, and the acoustic pressure load: since fluids do not support shear stresses, the force per unit area of the air on the elastic body is purely opposite the surface normal, and is equal to the pressure  $p = -\rho_0 \varphi_t$ , so that

$$h = f + \rho_0 \varphi_t n.$$

The acoustic normal velocity g must match the elastic normal velocity:

$$g = \partial_t u \cdot n.$$

By assuming time-harmonic solutions proportional to  $\exp(-i\omega t)$ , with  $\omega = c\kappa$  and inserting the definitions of g, h, the following coupled equations for  $u, \varphi$  are obtained:

$$-\omega^2 \rho u = \nabla \cdot \sigma \qquad \qquad \text{in } \Omega^- \qquad (1.2.1a)$$

$$\sigma = H : e(u) \qquad \qquad \text{in } \Omega^- \qquad (1.2.1b)$$

$$\sigma \cdot n = f - i\omega \rho_0 \varphi n \qquad \qquad \text{on } \Gamma \qquad (1.2.1c)$$

$$\partial_n \varphi = -i\omega u \cdot n \qquad \qquad \text{on } \Gamma \qquad (1.2.1d)$$

$$\Delta \varphi + \kappa^2 \varphi = 0 \qquad \qquad \text{in } \Omega^+ \qquad (1.2.1e)$$

$$|\nabla \varphi \cdot x/|x| - i\kappa \varphi| = O\left(1/|x|^2\right) \qquad \text{as } |x| \to \infty.$$
 (1.2.1f)

For a unique solution to the Helmholtz problem, it is also necessary to assume that  $\varphi$  satisfies the Sommerfeld radiation condition (1.2.1f).

The response is measured at a point  $x^* \in \Omega^+$ , i.e., given a solution  $u_{\omega}, \varphi_{\omega}$  to the above problem at frequency  $\omega$ , the transfer function is defined as

$$T_{\Gamma}(\omega) = |\varphi_{\omega}(x^*)| / \|f_{\omega}\|_{\Gamma}.$$

Minimization over some admissible set of domain shapes  $\Gamma_{\rm ad}$ 

$$\min_{\Gamma \in \Gamma_{\mathrm{ad}}} \|T_{\Gamma} - T^*\|, \qquad (1.2.2)$$

yields a shape  $\Gamma$  with a transfer function  $T_{\Gamma}$  close to the desired transfer function  $T^*$ . Choice of the norm in which the difference  $T_{\Gamma} - T^*$  is measured is clearly an important issue.

## 1.3 Prior Work

The question of how to model (1.2.1) now arises. The essential considerations are as follows.

- The domain  $\Omega^-$  is "thin."
- The exterior domain  $\Omega^+$  is unbounded.
- The acoustic field need only be known at the measurement point  $x^*$ .

These suggest the use of boundary integral equations (§4.3) for the acoustic equations, in conjunction with shell models (§3.2), or when the middle-surface is flat, plate models (§2.2), for the elastic domain. The whole coupled three-dimensional problem can then be elegantly formulated on a two-dimensional reference domain, removing the need for re-meshing during optimization so long as the design changes are not too large. The boundary integral equations yield solutions exactly satisfying the Sommerfeld radiation condition (1.2.1f), without the need for artificial truncation of the exterior domain, and naturally lend themselves to point-measurement of the external field via an exterior representation formula.

However, the use of these modeling assumptions introduces some problems.

- The boundary integral equations for the exterior Helmholtz problem involves singular kernels that complicate the analysis and the implementation of finite element methods: The boundary element method (BEM) matrix assembly routines must deal with integration of the kernels, and result in dense, complexvalued matrices. For larger problems, it is necessary to use iterative solvers and sophisticated techniques such as fast multipole methods [46], FFT-based methods [34], or heirarchical block decompositions [105] in order to achieve reasonable speed.
- The formulation of shell and plate models reduces 3d elasticity to a 2d problem via a kinematic assumption suitable for small thicknesses. But as the thickness

becomes small relative to the dimensions of the shell or plate, discretizations can behave very badly if the finite element spaces are not carefully chosen in cognizance of the small-thickness asymptotics. This phenomenon is known as "locking." It can be encountered in both simulation and optimization of plates and shells, independent of any coupling. For small thicknesses, the linear systems can also become poorly conditioned, and care must be taken to avoid rounding errors in the assembly procedure.

• For coupled problems, there is typically a substantial disparity between the speed of plate bending waves and acoustic waves (see §2.7). It is useful to be able to consider meshes with rather different length scales, as is done by [63] with mortar elements. However, this complicates the implementation of the coupling, and the solution of the resulting linear systems.

In this section, a review is undertaken of prior work involving modeling and optimization of (1.2.1) using boundary integral equations and shell or plate models. Also mentioned is work on optimization of plates and shells without acoustic coupling, as these raise important issues to be considered in the context of the fully coupled problem.

#### 1.3.1 Coupled Modeling

A review of coupled elastic-acoustic systems can be found in [82]. Mariem and Hamdi [95] solved (1.2.1) using the Kirchhoff plate model and the hypersingular integral equation (4.3.14). Existence and uniqueness of the solutions is not discussed, but several numerical results are given, which are compared with analytic solutions.

Such modeling has since become considerably more sophisticated, as in the work of Gaul and Fischer [62, 63], who also coupled Kirchhoff plates to acoustics, but added several important features:

- Mortar element coupling allows different length scales for the elastic and acoustic meshes;
- Fast multipole methods for solution of boundary element systems;
- Development of iterative solution techniques.

In [67] and [16], the coupled problem is formulated in the time domain.

Modeling of curved shells coupled with boundary integral equations has been done in the context of optimization. In [42], a conical structure is considered, however the optimization parameters are the weights of concentric ring masses, so the shell geometry is unaltered. In [91], optimization of the more general shell shapes of an automobile dashboard is considered. These papers are discussed in more detail in the section on coupled optimization.

#### **1.3.2** Mechanical Optimization

There has been significant work on optimization of plates and shells without acoustic coupling. The addition of acoustics does appear to detract from the importance of the basic issues involved in such optimization: the choice of function spaces for the admissible shapes and objective functionals that guarantee the existence of optimal solutions, and numerical locking under discretization.

The thickness distribution of the plate is often chosen as an optimization variable. Under this framework, static characteristics of the plate are optimized in [75, 76], while optimization of vibrational frequencies was considered for plates in [84] and for shells in [37]. Instead of the thickness, the optimization variables were chosen in [17] to be the material parameters.

Optimization of plates and shells is done in [11], while the papers [36] and [24] focus on optimization of shells and the so-called locking issue in particular. Sprekels et al. also formulate shell optimization problems and consider existence of solutions: [6, 7, 107],[99, Ch. 6].

#### **1.3.3** Coupled Optimization

Excellent review articles on the full coupled problem are [41] and [92].

The first of these, [41], discusses several potential choices of exterior objective functions, namely energy flux (the acoustically radiated power), directivity (integral quantities relative to some benchmark), and the amplitude at some set of points. The differential dependence of acoustic properties on structural design parameters is given the name "acoustic sensitivity." Another article by the same authors, [42], focuses on example problems for axisymmetric structures. Various numerical methods are used. They are validated on the test problem from [3]: a clamped circular plate in an infinite domain. In [40], these techniques are applied to shape optimization of a loudspeaker diaphragm. The optimization is done using finite differences and sequential linear programming.

In the second review article, [92], Marburg reviews the theory of the coupled elastic-acoustic problem, and discusses a "semianalytic" method for calculating objective function derivatives, in which some terms are computed using numerical finite differences. The application is optimization of the transfer function in a car body from an engine mount to the driver's ear. A variety of assumptions are made:

- Geometry modification is small relative to acoustic wavelength;
- Geometry modification is small with respect to the shell dimensions;
- Geometry modification is primarily in the surface normal direction;
- Geometry modification does not affect forcing.

These assumptions eliminate the dependence of various parts of the equations on the parameter set. Marburg points out that in general, quite different length scales may be needed for the elastic and acoustic meshes. The function to be optimized is of the form

$$\frac{1}{\omega_{\max} - \omega_{\min}} \int_{\omega_{\min}}^{\omega_{\max}} \Phi(p(\omega)) \, d\omega,$$

where p is the transfer function, and  $\Phi$  is a weighting function designed to ignore "valleys" in the objective function, and seek improvement by working primarily on the peaks. The strategy is to combine random searches for an initial parameter set with a gradient approach to find local minima. Marburg subsequently wrote a paper [91] discussing the application of [92] to the design of a vehicle dashboard. There is a great deal of manual tweaking done during the optimization process, and the following additional assumptions are made:

- Air pressure does not drive the body (steel is dense relative to air);
- Structural motions are expanded in terms of a few calculated eigenmodes.

Apparently based on this experience, Marburg and Hardtke wrote two more papers entitled "A general concept for design modification of shell meshes in structuralacoustic optimization," I and II. The first of these, [94], emphasizes that there is real practical difficulty if the mesh is directly modified by the optimization scheme, and that there needs to be a way to search a smaller parameter space. The mesh is divided into a modification domain, and its complement, which remains unchanged. In the modification domain, local "modification functions" are parametrized by only a few variables. The second paper, [93], applies these techniques to a floor panel in a car. They find that even with all these assumptions, the technique is still expensive: while it took 5000 function evaluations to drop the objective function by 1.5dB, it took about 50000 (three months' calculation time) to drop it by 2dB.

### 1.4 This Thesis

Given how expensive it is to solve shell-structure optimization problems without derivative information, it is natural to ask why existing work such as [42, 91, 64] has never used adjoint equations. The closest thing I have found is the paper by Sigmund et al. [117], in which adjoint equations are used in the context of topology optimization for a fluid-acoustics problem: density and elastic parameters are used as variables to differentiate between the solid and fluid regions. But this approach is so expensive that it is done only in two spatial dimensions, and with a bounded domain.

It appears that the primary difficulty is that the use of adjoint equations requires considerable knowledge of the workings of the finite element codes, which are themselves quite complex: the development of practical and reliable finite element methods for shell and for boundary integral equations have been active areas of research for over 30 years. For a practitioner who only uses finite element codes written by others, just the implementation would be a daunting task.

I am not aware of any work prior to this thesis in which the basic issues related to well-posedness of the model problem involving shells and boundary integral equations are considered, or in which the adjoint equations for this coupled problem are worked out.

In this work, I formulate the coupled problem using a shell model in place of 3d elasticity, and boundary integral equations for the acoustics, and prove a wellposedness result for the problem (theorem 5.3.2). I implement boundary elements and shell elements, and their shape derivatives, with a simple one-to-one coupling scheme intended to make the implementation as simple as possible. Finally, I formulate the adjoint equations for the coupled problem, with theoretical justification for smooth surfaces (theorem 5.4.1), and discretize them using the above finite elements, so that shape derivatives can be computed efficiently. I then use gradient-based optimization to improve the transfer function via changes in the shape of the structure.

In the following chapters, a review is undertaken of Reissner-Mindlin plates, Naghdi shells, and boundary integral methods, including shape derivatives of the shell and boundary integral operators. Then, the coupling and the optimization problem are presented. Details of the finite element implementation are discussed in the appendices.

# Chapter 2

# Simulation and Optimization of Reissner Mindlin Plates

## 2.1 Introduction

In order to formulate the coupled problem (1.2.1) with shell models and boundary integral equations, and further, to discretize it effectively, much background work is required. It is sensible to begin by focusing on a simpler problem - that of the Reissner-Mindlin plate, which, without the complicating geometric factors involved in shell models, nonetheless serves to illustrate many of the issues that will be important later.

The Reissner-Mindlin plate model results from kinematic and geometric assumptions applied to standard three-dimensional elasticity. The transition to shells in §3.2 then requires only a relaxation of these assumptions. In both cases, it is possible to model a thin three-dimensional body with equations on a two-dimensional coordinate system.

Unfortunately, displacement-based discretizations of the Reissner-Mindlin equations yield poor convergence behavior as the thickness t becomes small relative to the characteristic size of the domain  $\Omega_0$ . This foreshadows a similar problem that exists



Figure 2.1: In general 3d elasticity, the point at x moves to x + u(x), deforming the domain  $\Omega$ .

with the Naghdi shell model. In the case of the plates, reliable and mathematically sound finite element methods have been developed. For the numerics, the focus is on the Mixed Interpolation of Tensorial Components (MITC) method first described in [13]. Numerical examples are presented in §2.6.1.

At the end of the chapter, mechanical junction conditions for plates are discussed in §2.5. The final section is a brief calculation of bending wave speeds in Reissner-Mindlin plates, which gives some indication as to mesh scale requirements for dynamic plate problems.

## 2.2 Derivation of the Reissner-Mindlin Equations

In this section the Reissner-Mindlin plate equations are derived from the equations of 3d linear elasticity. See, e.g., [28, 44, 51].

In linear elasticity, a point  $x \in \Omega \subset \mathbb{R}^3$  is displaced by u(x) (see Figure 2.1). The symmetric stress tensor  $\sigma$  is linearly related to the symmetric strain tensor (the symmetric gradient of the displacement)

$$e(u)(x) = \frac{1}{2} \left( \nabla u(x) + (\nabla u(x))^T \right)$$

through tensor contraction:

$$\sigma(x) = H : e(u)(x).$$

The fourth-rank constitutive tensor H contains the elastic constants. In particular, for homogeneous isotropic materials, it is given by

$$H^{ijkl} = \frac{E}{2(1+\nu)} (\delta^{ik} \delta^{jl} + \delta^{il} \delta^{jk}) + \frac{E\nu}{(1+\nu)(1-2\nu)} \delta^{ij} \delta^{kl}, \quad i, j, k, l = 1, 2, 3, ...$$

where E and  $\nu$  are respectively the Young modulus and Poisson ratio and  $\delta^{ij}$  is the Kronecker delta.

Let  $\Gamma_0 \cup \Gamma_1 \cup \Gamma_F$  be a partition of  $\partial \Omega$  with meas $(\Gamma_0) > 0$ . The portion  $\Gamma_0$  of the boundary is clamped, while boundary traction h is applied to  $\partial \Gamma_1$ . The portion  $\Gamma_F$  is free. For body forcing f, the equilibrium equations are

$-\operatorname{div} \sigma = j$	f	in	Ω

$\sigma = H : e(u)$	in $\Omega$

$$u = 0$$
 on  $\Gamma_0$ 

$$\sigma \cdot n = h \qquad \qquad \text{on } \Gamma_1$$

$$\sigma \cdot n = 0$$
 on  $\Gamma_F$ .

The equivalent weak form is to find

$$u \in \mathcal{U}_0 \equiv \left\{ u \in H^1(\Omega)^3 : u = 0 \text{ on } \Gamma_0 \right\}$$

such that

$$\int_{\Omega} (H(x) : e(u)(x)) : e(v)(x) \, dx = \int_{\Omega} f(x) \cdot v(x) \, dx + \int_{\Gamma_1} h(x) \cdot v(x) \, d\Gamma \qquad (2.2.1)$$

for all  $v \in \mathcal{U}_0$ . For more discussion of 3d elasticity see, e.g., [43].



Figure 2.2: Reissner-Mindlin further assumes that the material line normal to the plate surface is displaced by z(x), and rotates by  $\theta = (\theta_1(x), \theta_2(x))$ .

Next, the Reissner-Mindlin equations are derived from (2.2.1). The following notational conventions are used.

Notation. The following notational convention is used. Latin indices i, j, etc., take their values in the set  $\{1, 2, 3\}$  while Greek indices  $\alpha, \beta$ , etc., take their values in the set  $\{1, 2\}$ . Furthermore, Einstein summation convention is used: repeated appearance of an index in an equation implies summation over that index.

#### Assumptions of the Reissner-Mindlin Model.

• Geometry. The domain  $\Omega$  is assumed to have one thin dimension. Let  $\Omega_0 \subset \mathbb{R}^2$  be bounded, and  $t : \Omega_0 \to (0, \infty)$ . The domain  $\Omega$  is then

$$\Omega \equiv \left\{ (x_1, x_2, x_3) \in \mathbb{R}^3 : (x_1, x_2) \in \Omega_0, \ x_3 \in [-t(x_1, x_2)/2, t(x_1, x_2)/2] \right\}.$$

The domain  $\Omega_0$  is called the middle surface.

• Kinematics. The displacement  $u: \Omega \to \mathbb{R}^3$  takes the specific form

$$u(x_1, x_2, x_3) = (z_1(x_1, x_2) - \theta_1(x_1, x_2)x_3, z_2(x_1, x_2) - \theta_2(x_1, x_2)x_3, z_3(x_1, x_2)).$$
(2.2.2)

The rotation angles  $\theta = (\theta_1, \theta_2)$  and the vertical displacement  $z = (z_1, z_2, z_3)$ depend only on the middle-surface coordinates  $(x_1, x_2) \in \Omega_0$ . The state of a Reissner-Mindlin plate is then described by  $U = (\theta, z)$ . The state space for the rotation angles  $\theta$  is a subspace of  $H^1(\Omega)^2$  and the state space for the vertical displacement z is a subspace of  $H^1(\Omega)^3$ . These subspaces depend on the boundary conditions and will be specified in §2.3.

The test functions v take the form

$$v(x_1, x_2, x_3) = (y_1(x_1, x_2) - \eta_1(x_1, x_2)x_3, y_2(x_1, x_2) - \eta_2(x_1, x_2)x_3, y_3(x_1, x_2)).$$
(2.2.3)

The model trades the integration over the thickness in (2.2.1) that would be required in three-dimensional elasticity for the assumed kinematics of (2.2.2), which imply that a material line normal to the plate is displaced in the normal direction by a distance  $z_3$ , and executes a rotation with components  $\theta_{\alpha}$ . The in-plane motions are given by  $(z_1, z_2)$ .

Note that this allows transverse shearing of the plate, as in general, Reissner-Mindlin does not assume that  $e_{\alpha3}(u) = 0$ , or as shall later be shown to be equivalent, that  $\theta = \nabla z_3$ , i.e., fibers initially normal to the plate need not stay normal to the surface of the deformed plate. Although the material line in Figure 2.2 is shown nearly perpendicular to the deformed middle surface, it is accorded the freedom to rotate independently.

• Mechanics. Stress is planar, i.e.,  $\sigma^{33} = 0$ .

With these assumptions, the elasticity equation (2.2.1) can be rewritten. Since  $H^{333\alpha} = H^{3\alpha\beta\lambda} = 0$ , the stresses can be written

$$\sigma^{\alpha\beta} = H^{\alpha\beta\lambda\mu}e_{\lambda\mu} + H^{\alpha\beta33}e_{33}, \qquad (2.2.4a)$$

$$\sigma^{\alpha 3} = 2H^{\alpha 3\beta 3} e_{\beta 3}, \qquad (2.2.4b)$$

$$\sigma^{33} = H^{33\alpha\beta} e_{\alpha\beta} + H^{3333} e_{33}. \tag{2.2.4c}$$

The planar stress assumption  $\sigma^{33} = 0$  implies via (2.2.4c) that

$$e_{33} = -\frac{H^{33\alpha\beta}}{H^{3333}}e_{\alpha\beta}$$

Plugging  $e_{33}$  back in to (2.2.4a) yields

$$\sigma^{\alpha\beta} = H^{\alpha\beta\lambda\mu}e_{\lambda\mu} - H^{\alpha\beta33}\frac{H^{33\lambda\mu}}{H^{3333}}e_{\lambda\mu}.$$

The reduced constitutive tensors are defined via

$$\begin{split} C^{\alpha\beta\lambda\mu} &= H^{\alpha\beta\lambda\mu} - \frac{H^{\alpha\beta33}H^{33\lambda\mu}}{H^{3333}} \\ &= \frac{E}{2(1+\nu)} \left( \delta^{\alpha\lambda}\delta^{\beta\mu} + \delta^{\alpha\mu}\delta^{\beta\lambda} + \frac{2\nu}{1-\nu}\delta^{\alpha\beta}\delta^{\lambda\mu} \right), \\ D^{\alpha\lambda} &= 4H^{\alpha3\lambda3} = \frac{2E}{(1+\nu)}\delta^{\alpha\lambda}, \end{split}$$

so that

$$\sigma^{\alpha\beta} = C^{\alpha\beta\lambda\mu}e_{\lambda\mu}$$
 and  $\sigma^{\alpha3} = \frac{1}{2}D^{\alpha\lambda}e_{\lambda3}.$  (2.2.5)

Thus, the contraction between stress and strain tensors is written

$$\sigma^{ij}(u)e_{ij}(v) = \sigma^{\alpha\beta}(u)e_{\alpha\beta}(v) + \underbrace{\sigma^{\alpha3}(u)e_{\alpha3}(v) + \sigma^{3\alpha}(u)e_{3\alpha}(v)}_{=2\sigma^{\alpha3}e_{\alpha3}} + \underbrace{\sigma^{33}(u)}_{=0}e_{33}(v)e_{33}(v)$$
$$= C^{\alpha\beta\lambda\mu}e_{\alpha\beta}(v)e_{\lambda\mu}(u) + D^{\alpha\lambda}e_{\alpha3}(v)e_{\lambda3}(u).$$

The in-plane terms can be expanded as

$$\begin{split} C^{\alpha\beta\lambda\mu}e_{\lambda\mu}(u) = & \frac{E}{2(1+\nu)} \left( \underbrace{(\delta^{\alpha\lambda}\delta^{\beta\mu} + \delta^{\alpha\mu}\delta^{\beta\lambda})e_{\lambda\mu}(u)}_{e_{\alpha\beta}(u) + e_{\beta\alpha}(u) = 2e_{\alpha\beta}(u)} + \frac{2\nu}{1-\nu} \underbrace{\delta^{\alpha\beta}\delta^{\lambda\mu}e_{\lambda\mu}(u)}_{(\mathrm{tr}\;e(u))\delta^{\alpha\beta}} \right) \\ = & \frac{E}{1+\nu} \left( e_{\alpha\beta}(u) + \frac{\nu}{1-\nu}(\mathrm{tr}\;e(u))\delta^{\alpha\beta} \right), \end{split}$$

corresponding to the the operator L, which takes any second-rank tensor  $\tau$  to

$$L\tau = D\left[(1-\nu)\tau + \nu \mathrm{tr}(\tau)I\right], \qquad (2.2.6)$$

with the elastic constant

$$D = \frac{E}{1 - \nu^2}.$$
 (2.2.7)

In order to plug (2.2.2) into (2.2.1), the strains

$$e_{\alpha\beta}(u) = \frac{1}{2}(\partial_{\alpha}u_{\beta} + \partial_{\beta}u_{\alpha}) = \frac{1}{2}(\partial_{\alpha}z_{\beta} + \partial_{\beta}z_{\alpha}) - x_{3}\frac{1}{2}(\partial_{\alpha}\theta_{\beta} + \partial_{\beta}\theta_{\alpha}), \qquad (2.2.8a)$$

$$e_{\alpha3}(u) = \frac{1}{2}(\partial_{\alpha}u_3 + \partial_3u_{\alpha}) = \frac{1}{2}(\partial_{\alpha}z_3 - \theta_{\alpha})$$
(2.2.8b)

must be computed. If

$$\bar{z} = (z_1, z_2)$$

and

$$\bar{e}(\bar{z}) = \frac{1}{2} \left( \nabla \bar{z}(x_1, x_2) + (\nabla \bar{z}(x_1, x_2))^T \right) \in \mathbb{R}^{2 \times 2},$$

then the strains in (2.2.8a) can be written as

$$\left(e_{\alpha\beta}(u)\right)_{\alpha,\beta=1,2} = \bar{e}(\bar{z}) - x_3\bar{e}(\theta).$$
(2.2.8c)

The variable  $\bar{y}$  and the strain  $\bar{e}(\bar{y})$  are defined analogously.

By use of (2.2.5) and (2.2.8), the left-hand side of (2.2.1) can be written as

$$\int_{\Omega} (H(x) : e(u)(x)) : e(v)(x) \, dx$$
  
= 
$$\int_{\Omega_0} \frac{t^3}{12} (L\bar{e}(\theta) : \bar{e}(\eta)) + t (L\bar{e}(\bar{z}) : \bar{e}(\bar{y})) + t\lambda (\nabla z_3 - \theta) \cdot (\nabla y_3 - \eta) \, d(x_1, x_2), \quad (2.2.9)$$

where L is defined in (2.2.6) and the elastic constant  $\lambda$  is given by

$$\lambda = \frac{Ek}{2(1+\nu)}.\tag{2.2.10}$$

Here the dimensionless number 0 < k < 1 is called the shear correction factor, and is used to compensate for the fact that in an actual plate, the transverse shear  $e_{\alpha 3}(u)$ cannot really be constant through the thickness, but must vanish on the faces [39, p. 90].

Consider now the right-hand side of (2.2.1). Suppose that f applies no torque (moment) to the middle surface  $\Omega_0$ , i.e.,

$$\int_{-t(x_1,x_2)/2}^{t(x_1,x_2)/2} (0,0,x_3) \times f(x_1,x_2,x_3) \, dx_3 = 0.$$

This implies that

$$\int_{-t(x_1,x_2)/2}^{t(x_1,x_2)/2} x_3 f_1(x_1,x_2,x_3) \, dx_3 = \int_{-t(x_1,x_2)/2}^{t(x_1,x_2)/2} x_3 f_2(x_1,x_2,x_3) \, dx_3 = 0.$$

The resultant pressure on the middle surface is defined as

$$p(x_1, x_2) = \int_{-t(x_1, x_2)/2}^{t(x_1, x_2)/2} f(x_1, x_2, x_3) \, dx_3.$$

Therefore, for v given by (2.2.3),

$$\int_{\Omega} f \cdot v \, dx = \int_{\Omega_0} \int_{-t(x_1, x_2)/2}^{t(x_1, x_2)/2} f_1 y_1 - f_1 \eta_1 x_3 + f_2 y_2 - f_2 \eta_2 x_3 + f_3 y_3 \, dx_3 d(x_1, x_2)$$
$$= \int_{\Omega_0} p \cdot y \, d(x_1, x_2). \tag{2.2.11}$$

To rewrite the integral in (2.2.1) involving h, the boundary of the plate must be more precisely specified. The edges are given by

$$\Gamma_E = \left\{ x \in \mathbb{R}^3 : (x_1, x_2) \in \partial \Omega_0, x_3 \in [-t(x_1, x_2)/2, t(x_1, x_2)/2] \right\}$$

The faces are assumed to be free, and that the forced and clamped parts are purely on the edges, i.e.,

$$\Gamma_0 \cup \Gamma_1 \subset \Gamma_E.$$

The intersections of these with the middle surface are written

$$\gamma_0 = \Gamma_0 \cap \Omega_0, \gamma_1 = \Gamma_1 \cap \Omega_0.$$

These regions are further assumed not to overlap, i.e.,

$$\gamma_0 \cap \gamma_1 = \emptyset.$$

For  $(x_1, x_2) \in \gamma_1$ , the resultant of h is defined via

$$T(x_1, x_2) = \int_{-t(x_1, x_2)/2}^{t(x_1, x_2)/2} h(x_1, x_2, x_3) \, dx_3. \tag{2.2.12}$$

Let  $n \in \mathbb{R}^3$  and  $\tau \in \mathbb{R}^3$  be the unit normal and unit counter-clockwise tangent vector, respectively  $(n \times \tau = e_3 = (0, 0, 1))$  with components

$$h_n = h \cdot n, \quad h_\tau = h \cdot \tau.$$

The boundary moment of h is

$$M = \int_{-t(x_1, x_2)/2}^{t(x_1, x_2)/2} x_3 e_3 \times h \, dx_3$$

given by components

$$M_n(x_1, x_2) = -\int_{-t(x_1, x_2)/2}^{t(x_1, x_2)/2} x_3 h_\tau \, dx_3, \qquad (2.2.13a)$$

$$M_{\tau}(x_1, x_2) = \int_{-t(x_1, x_2)/2}^{t(x_1, x_2)/2} x_3 h_n \, dx_3, \qquad (2.2.13b)$$

with

$$h = h_n n + h_\tau \tau + h_3 e_3.$$

Thus, for v given by (2.2.3),

$$\int_{\Gamma_1} h \cdot v \, dx = \int_{\gamma_1} \int_{-t(x_1, x_2)/2}^{t(x_1, x_2)/2} h_3 y_3 + (h_\tau \tau + h_n n) \cdot (y_1 - \eta_1 x_3, y_2 - \eta_2 x_3, 0) \, dx_3 d(x_1, x_2)$$
$$= \int_{\gamma_1} T_i y_i + M_n \eta_\tau - M_\tau \eta_n \, d(x_1, x_2) \tag{2.2.14}$$

with

$$\eta_n = \eta_1 n_1 + \eta_2 n_2, \quad \eta_\tau = \eta_1 \tau_1 + \eta_2 \tau_2.$$

Now the Reissner-Mindlin equations can be derived from (2.2.1). The state space for the rotation angles  $\theta$  is denoted by  $\mathcal{R}$  and the state space for the vertical replacements z is denoted by  $\mathcal{V}$ . In particular,  $\mathcal{R}$  is a subspace of  $H^1(\Omega_0)^2$  and  $\mathcal{V}$  is a subspace of  $H^1(\Omega_0)^3$ . The notation  $\mathcal{V}_i$  indicates the space for the *i*th displacement component, which is a subspace of  $H^1(\Omega_0)$ . The precise definition of these spaces depends on the boundary conditions applied. The spaces will be specified in §2.3.

Combining (2.2.9) with (2.2.11) and (2.2.14), (2.2.1) can be written as follows: Find  $(\theta, z) \in \mathcal{R} \times \mathcal{V}$  such that

$$\int_{\Omega_0} \frac{t^3}{12} (L\bar{e}(\theta) : \bar{e}(\eta)) + t(L\bar{e}(\bar{z}) : \bar{e}(\bar{y})) + t\lambda(\nabla z_3 - \theta) \cdot (\nabla y_3 - \eta) d(x_1, x_2)$$
  
= 
$$\int_{\Omega_0} p \cdot y \, d(x_1, x_2) + \int_{\gamma_1} T_i y_i + M_n \eta_\tau - M_\tau \eta_n \, d(x_1, x_2)$$
(2.2.15)

for all  $(\eta, y) \in \mathcal{R} \times \mathcal{V}$ .

Thus, (2.2.15) decouples into an in-plane and an out-of-plane problem. In fact, recalling that  $\bar{z} = (z_1, z_2)$ ,  $\bar{y} = (y_1, y_2)$  and setting  $\bar{y} = (y_1, y_2) = (0, 0)$ , then (2.2.15)

reduces to the following problem. Find  $(\theta, z_3) \in \mathcal{R} \times \mathcal{V}_3$  such that

$$\int_{\Omega_0} \frac{t^3}{12} (L\bar{e}(\theta) : \bar{e}(\eta)) + t\lambda(\nabla z_3 - \theta) \cdot (\nabla y_3 - \eta) d(x_1, x_2)$$
(2.2.16a)

$$= \int_{\Omega_0} p_3 y_3 \, dx + \int_{\gamma_1} T_3 y_3 + M_n \eta_\tau - M_\tau \eta_n \, d(x_1, x_2) \tag{2.2.16b}$$

for all  $(\eta, y_3) \in \mathcal{R} \times \mathcal{V}_3$ .

If  $\eta = (0,0)$  and  $y_3 = 0$ , then (2.2.15) reduces to the following problem. Find  $\overline{z} = (z_1, z_2) \in \mathcal{V}_1 \times \mathcal{V}_2$  such that

$$\int_{\Omega_0} t(L\bar{e}(\bar{z}):\bar{e}(\bar{y})) d(x_1, x_2)$$
(2.2.17a)

$$= \int_{\Omega_0} p_{\alpha} y_{\alpha} \, dx + \int_{\gamma_1} T_{\alpha} y_{\alpha} \, d(x_1, x_2). \tag{2.2.17b}$$

The strong form of (2.2.15) is

$$(-t\nabla \cdot Le(z))_{\alpha} = p_{\alpha}$$
 in  $\Omega_0$ , (2.2.18a)

$$-\lambda t \nabla \cdot (\nabla z_3 - \theta) = p_3 \qquad \text{in } \Omega_0, \qquad (2.2.18b)$$

$$\left(-\frac{t^3}{12}\nabla \cdot Le(\theta) - \lambda t(\nabla z_3 - \theta)\right) = 0 \qquad \text{in } \Omega_0 \qquad (2.2.18c)$$

plus boundary conditions. This can easily be checked via integration by parts and addition of the equations. See §2.3 for more details. Equation (2.2.18c) balances the torques applied by f, which have been assumed to vanish.

# 2.3 Existence and Uniqueness of Solutions

Recall the Reissner-Mindlin equations, derived in §2.2. The domain  $\Omega_0 \subset \mathbb{R}^2$  describes the mid-surface of the plate and  $t : \Omega_0 \to (0, \infty)$  is the thickness of the plate. Since the Reissner-Mindlin equations describe the displacement of the plate through functions defined on the midsurface, the coordinates are written

$$x = (x_1, x_2)$$

from now on in this chapter. As before  $\theta : \Omega_0 \to \mathbb{R}^2$  denotes the rotation angles and  $z : \Omega_0 \to \mathbb{R}^3$  denotes the mid-surface displacement. However, the notation  $\overline{z} = (z_1, z_2)$  is still used to indicate the in-plane displacement components. In §2.2, it was necessary to differentiate between the strain e for the displacement in 3d elasticity and the strain  $\overline{e}$  arising for functions defined on  $\Omega_0$ . Since from now on only functions on  $\Omega_0$  are considered, the - can be removed from e: for the vector-valued function  $\theta : \Omega_0 \to \mathbb{R}^2$ , the notation

$$e(\theta) = \frac{1}{2} \left( \nabla \theta(x) + (\nabla \theta(x))^T \right) \in \mathbb{R}^{2 \times 2}$$

is used.

Recall also the elastic constants

$$D = \frac{E}{1 - \nu^2}, \quad \lambda = \frac{Ek}{2(1 + \nu)}, \tag{2.3.1}$$

where E and  $\nu$  are respectively the Young modulus and Poisson ratio and the dimensionless number 0 < k < 1 is the shear correction factor. The operator L takes any second-rank tensor  $\tau$  to

$$L\tau = D\left[(1-\nu)\tau + \nu \mathrm{tr}(\tau)I\right]. \tag{2.3.2}$$

See (2.2.6), (2.2.7), (2.2.10).

#### 2.3.1 The In- and Out-of-Plane Problems

The Reissner-Mindlin equations specify the rotation angles  $\theta$  and the vertical displacement z as the solution of two decoupled systems of PDEs. The out-of-plane problem determines  $\theta$  and  $z_3$ . The in-plane problem determines  $\bar{z} = (z_1, z_2)$ . First, the out-of-plane problem is stated.

#### 2.3.1.1 The Out-of-Plane Problem

The strong form of the out-of-plane problem is given by

$$-\lambda t \nabla \cdot (\nabla z_3 - \theta) = p_3 \qquad \text{in } \Omega_0, \qquad (2.3.3a)$$

$$\left(-\frac{t^3}{12}\nabla \cdot Le(\theta) - \lambda t(\nabla z_3 - \theta)\right) = 0 \qquad \text{in } \Omega_0, \qquad (2.3.3b)$$

plus appropriate boundary conditions, which will be discussed later.

To formally derive the weak form of (2.3.3), the equations are multiplied by test functions  $y_3$  and  $\eta$ , respectively, integrated over  $\Omega$ , and integrated by parts. If  $n \in \mathbb{R}^2$ denotes the unit normal vector on  $\partial \Omega_0$ , then

$$\int_{\Omega_0} \lambda t (\nabla z_3 - \theta) \nabla y_3 - p_3 y_3 \, dx = \int_{\partial \Omega_0} \lambda t \, (\nabla z_3 - \theta) \cdot n \, y_3 \, dx,$$
$$\int_{\Omega_0} \frac{t^3}{12} \, Le(\theta) : e(\eta) \, dx - \int_{\Omega_0} \lambda t (\nabla z_3 - \theta) \eta \, dx = \int_{\partial \Omega_0} \frac{t^3}{12} \, (Le(\theta) \, n) \cdot \eta \, dx.$$

Adding both equations leads to

$$\int_{\Omega_0} \frac{t^3}{12} Le(\theta) : e(\eta) \, dx + \int_{\Omega_0} \lambda t (\nabla z_3 - \theta) (\nabla y_3 - \eta) \, dx$$
$$= \int_{\Omega_0} p_3 y_3 \, dx + \int_{\partial\Omega_0} \lambda t (\nabla z_3 - \theta) \cdot n \, y_3 + \frac{t^3}{12} \left( Le(\theta) \, n \right) \cdot \eta \, dx$$

(cf., (2.2.16)). Using

$$\eta = \eta_n n + \eta_\tau \tau$$
, where  $\eta_n = \eta \cdot n$  and  $\eta_\tau = \eta \cdot \tau$ ,

the right hand side in the previous identity can be expanded to obtain

$$\int_{\Omega_0} \frac{t^3}{12} Le(\theta) : e(\eta) dx + \int_{\Omega_0} \lambda t (\nabla z_3 - \theta) (\nabla y_3 - \eta) dx$$

$$= \int_{\Omega_0} p_3 y_3 dx$$

$$+ \int_{\partial\Omega_0} \lambda t (\nabla z_3 - \theta) \cdot n y_3 + \frac{t^3}{12} (n \cdot Le(\theta) n) \eta_n + \frac{t^3}{12} (\tau \cdot Le(\theta) n) \eta_\tau dx.$$
(2.3.4b)

A useful discussion of boundary conditions can be found in [72]. Let  $n, \tau \in \mathbb{R}^2$  be the unit normal and the unit counter clockwise tangential vector to  $\Omega_0$ . The paper [10] considers the homogeneous boundary conditions

$$\begin{aligned} \theta &= 0, \ z_3 = 0 & \text{(hard clamped)} & (2.3.5a) \\ \theta \cdot n &= \tau \cdot Le(\theta) \ n &= z_3 = 0 & \text{(soft clamped)} & (2.3.5b) \\ \theta \cdot \tau &= n \cdot Le(\theta) \ n &= z_3 = 0 & \text{(hard simply-supported)} & (2.3.5c) \\ n \cdot Le(\theta) \ n &= \tau \cdot Le(\theta) \ n &= z_3 = 0 & \text{(soft simply-supported)} & (2.3.5d) \\ n \cdot Le(\theta) \ n &= \tau \cdot Le(\theta) \ n &= (\nabla z_3 - \theta) \cdot n = 0. & \text{(free)} & (2.3.5e) \end{aligned}$$

It is possible to specify different boundary conditions on different part of the boundary and to specify inhomogeneous boundary conditions.

The different boundary conditions in (2.3.5) lead to different function spaces  $\mathcal{R}, \mathcal{V}_3$ for  $\theta$  and  $z_3$ . The function spaces are given by

$$\mathcal{R} = H_0^1(\Omega_0)^2, \quad \mathcal{V}_3 = H_0^1(\Omega_0) \qquad \text{(hard clamped)} \qquad (2.3.6a)$$
$$\mathcal{R} = \left\{ \eta \in H^1(\Omega_0)^2 : \eta \cdot n = 0 \text{ on } \partial\Omega_0 \right\},$$
$$\mathcal{V}_3 = H_0^1(\Omega_0) \qquad \text{(soft clamped)} \qquad (2.3.6b)$$
$$\mathcal{R} = \left\{ \eta \in H^1(\Omega_0)^2 : \eta \cdot \tau = 0 \text{ on } \partial\Omega_0 \right\},$$
$$\mathcal{V}_3 = H_0^1(\Omega_0) \qquad \text{(hard simply-supported)} \qquad (2.3.6c)$$
$$\mathcal{R} = H^1(\Omega_0)^2, \quad \mathcal{V}_3 = H_0^1(\Omega_0) \qquad \text{(soft simply-supported)} \qquad (2.3.6d)$$

$$\mathcal{R} = H^1(\Omega_0)^2, \quad \mathcal{V}_3 = H^1(\Omega_0) \tag{free} \tag{2.3.6e}$$

For each of the boundary conditions listed in (2.3.5) and the corresponding spaces specified in (2.3.6) the weak form of the out-of-plane problem is given as follows: Find  $(\theta, z_3) \in \mathcal{R} \times \mathcal{V}_3$  such that

$$\int_{\Omega_0} \frac{t^3}{12} Le(\theta) : e(\eta) \, dx + \int_{\Omega_0} \lambda t (\nabla z_3 - \theta) (\nabla y_3 - \eta) \, dx = \int_{\Omega_0} p_3 y_3 \, dx \tag{2.3.7}$$

for all  $(\eta, y_3) \in \mathcal{R} \times \mathcal{V}_3$ .

The bilinear form  $A_t : (\mathcal{R} \times \mathcal{V}_3) \times (\mathcal{R} \times \mathcal{V}_3) \to \mathbb{R}$  $A_t(\theta, z_3; \eta, y_3) = \int_{\Omega_0} \frac{t^3}{12} Le(\theta) : e(\eta) \, dx + \int_{\Omega_0} \lambda t (\nabla z_3 - \theta) (\nabla y_3 - \eta) \, dx$  (2.3.8)
is associated with the out-of-plane problem.

Inhomogeneous boundary conditions can be imposed as well. For example, consider

$$n \cdot Le(\theta) n = M_n, \quad \tau \cdot Le(\theta) n = M_{\tau}, \quad z_3 = 0$$

and the function spaces in (2.3.6d). The weak form of this problem is given as follows: Find  $(\theta, z_3) \in \mathcal{R} \times \mathcal{V}_3$  such that

$$\int_{\Omega_0} \frac{t^3}{12} Le(\theta) : e(\eta) \, dx + \int_{\Omega_0} \lambda t (\nabla z_3 - \theta) (\nabla y_3 - \eta) \, dx \tag{2.3.9a}$$

$$= \int_{\Omega_0} p_3 y_3 \, dx + \int_{\partial \Omega_0} \frac{t^3}{12} M_n \, \eta_n + \frac{t^3}{12} M_\tau \, \eta_\tau \, dx \tag{2.3.9b}$$

for all  $(\eta, y_3) \in \mathcal{R} \times \mathcal{V}_3$ .

Existence and uniqueness results for (2.3.7) with some of the choices for function spaces specified in (2.3.6) can be found, e.g., in [9, 50]. See also [28, § 6] and [61].

#### 2.3.1.2 The In-Plane Problem

Recalling for convenience (2.2.18), the strong form of the in-plane problem is given by

$$(-t\nabla \cdot Le(z))_{\alpha} = p_{\alpha}$$
 in  $\Omega_0$ , (2.3.10a)

plus some boundary conditions remaining to be specified. There could be clamping over one or both components or some portion of the boundary, e.g.,

$$\mathcal{V}_1 = H_0^1(\Omega_0), \quad \mathcal{V}_2 = H_0^1(\Omega_0) \qquad (\text{fully clamped}) \qquad (2.3.11)$$

$$\mathcal{V}_1 = H_0^1(\Omega_0), \quad \mathcal{V}_2 = H^1(\Omega_0) \qquad (z_1 \text{ clamped}) \qquad (2.3.12)$$

$$\mathcal{V}_1 = H^1(\Omega_0), \quad \mathcal{V}_2 = H^1_0(\Omega_0)$$
 (2.3.13)

The weak form of the in-plane problem is given as follows:

Find  $\bar{z} = (z_1, z_2) \in \mathcal{V}_1 \times \mathcal{V}_2$  such that

$$\int_{\Omega_0} t \, Le(\bar{z}) : e(\bar{y}) \, dx = \int_{\Omega_0} p_1 y_1 + p_2 y_2 \, dx \tag{2.3.14}$$

for all  $\bar{y} = (y_1, y_2) \in \mathcal{V}_1 \times \mathcal{V}_2$ .

The bilinear form  $B_t : (\mathcal{V}_1 \times \mathcal{V}_2) \times (\mathcal{V}_1 \times \mathcal{V}_2) \to \mathbb{R}$ 

$$B_t(z_1, z_2; y_1, y_2) = \int_{\Omega_0} t \, Le(\bar{z}) : e(\bar{y}) \, dx \tag{2.3.15}$$

is associated with the in-plane problem, where  $\bar{z} = (z_1, z_2)$  and  $\bar{y} = (y_1, y_2)$ .

### 2.3.2 Rigid-Body Motions and Coercivity

In order to establish existence and uniqueness of solutions to (2.2.16), it must be shown that the Reissner-Mindlin bilinear form is bounded and coercive with respect to the norm  $\|\cdot\|_{\mathcal{U}}$ . At this point, it is necessary to make some assumptions about the thickness function t. Assume that  $t_{\min} > 0$  is a given constant. The set of admissible thickness functions is

$$\mathcal{T} \equiv \left\{ t \in L^{\infty}(\Omega_0) : t(x) \ge t_{\min} \text{ for a.e. } x \in \overline{\Omega_0} \right\},\$$

with the norm

$$\|\cdot\|_{\mathcal{T}} = \|\cdot\|_{L^{\infty}(\Omega_0)}.$$

Boundedness follows easily from the following lemma.

Lemma 2.3.1 (Bounds on Strain Tensors) The following bounds on the terms in (2.2.16) hold:

$$\left| \int_{\Omega_0} Le(\theta) : e(\eta) \, dx \right| \le C_1 \|\theta\|_{H^1(\Omega_0)^2} \|\eta\|_{H^1(\Omega_0)^2}$$
$$\left| \int_{\Omega_0} (\nabla z_3 - \theta) \cdot (\nabla y_3 - \eta) \, dx \right| \le C_2 \|(\theta, z)\|_{\mathcal{U}} \|(\eta, y)\|_{\mathcal{U}}.$$

**Proof:** Straightforward application of the triangle inequality and Cauchy-Schwarz. □

Lemma 2.3.2 (Boundedness of  $A_t, B_t$ ) For any  $t \in L^{\infty}(\Omega_0)$ , there exists  $C = C(||t||_{L^{\infty}(\Omega_0)}) > 0$  such that

$$|A_t(U,V)| \le C ||U||_{\mathcal{U}} ||V||_{\mathcal{U}},$$
  
$$|B_t(U,V)| \le C ||U||_{\mathcal{U}} ||V||_{\mathcal{U}}.$$

**Proof:** Write out the bilinear form and use lemma 2.3.1:

$$|A_{t}(\theta, z; \eta, y)| \leq C_{1} \frac{\|t\|_{T}^{3}}{12} \|\theta\|_{H^{1}(\Omega_{0})^{2}} \|\eta\|_{H^{1}(\Omega_{0})^{2}} + C_{2}\lambda\|t\|_{T} \|(\theta, z)\|_{\mathcal{U}} \|(\eta, y)\|_{\mathcal{U}}$$
$$\leq C'\|(\theta, z)\|_{\mathcal{U}} \|(\eta, y)\|_{\mathcal{U}}.$$

The same argument works for the Le(z) : e(y) term in  $B_t$ . The constant C is then chosen as the larger of those from the  $A_t$  and  $B_t$  bounds.

To show ellipticity, it is necessary to make some assumptions on the boundary conditions.

**Definition 2.3.3 (Rigid-Body Motions)**  $(\theta, z) \in \mathcal{U}$  is called a rigid-body motion if there exist vectors  $a, b \in \mathbb{R}^3$  such that

$$(z_1, z_2) = (a_1 - b_3 x_2, a_2 + b_3 x_1)$$
(2.3.16a)

$$z_3 = a_3 + b_1 x_2 - b_2 x_1, \ \theta = (-b_2, b_1).$$
(2.3.16b)

If (2.3.16a) holds,  $(\theta, z)$  is an in-plane rigid-body motion. If (2.3.16b) holds,  $(\theta, z)$  is a transverse rigid-body motion.

The vector a is a translation; b is an infinitesimal rotation. It will be necessary to exclude such motions from consideration in order to make (2.2.16) well-posed.

Lemma 2.3.4 (Rigid-Body Lemma)  $U = (\theta, z) \in \mathcal{U}$  is an in-plane rigid-body motion if and only if e(z) = 0.  $U = (\theta, z) \in \mathcal{U}$  is a transverse rigid-body motion if and only if  $e(\theta) = 0$  and  $\nabla z_3 - \theta = 0$ .

#### **Proof:**

1. If U is an in-plane rigid-body motion, then

$$e(z)_{11} = e(z)_{22} = 0,$$

and

$$e(z)_{12} = e(z)_{21} = \frac{1}{2}(-b_3 + b_3) = 0.$$

2. If U is a transverse rigid-body motion, then

$$\nabla z_3 - \theta = (-b_2, b_1) - (-b_2, b_1) = 0,$$

and  $e(\theta) = 0$ , as  $\theta$  is independent of x.

3. Under the Reissner-Mindlin kinematic assumption for the plate, the threedimensional strain tensor components are given by

$$e_{\alpha\beta}(u) = e_{\alpha\beta}(z) - x_3 e_{\alpha\beta}(\theta)$$
$$e_{\alpha3}(u) = \frac{1}{2}(\nabla z_3 - \theta)$$
$$e_{33}(u) = 0,$$

and therefore by assumption,  $e_{ij}(u)$  is identically zero. It is shown in [43, Theorem 6.3-4] that this implies the motion is a three-dimensional rigid-body motion, i.e. that the three-dimensional displacement  $u(\cdot): \Omega_0 \ni x = (x_1, x_2) \times$  $[-t(x)/2, t(x)/2] \to \mathbb{R}^3$  takes the form

$$u(x) = a + b \wedge x$$

for some  $a, b \in \mathbb{R}^3$ , matching precisely the assumed form of the rigid body motion for the plate.

The proof is not yet finished, as it was claimed that the transverse or in-plane quantities could independently guarantee transverse or in-plane rigid-body motions. However, the components are entirely independent:

$$a_1, a_2, b_3 \sim \theta_1, \theta_2, z_3; \ b_1, b_2, a_3 \sim z_1, z_2.$$

Therefore, to show that

$$e(\theta) = 0, \nabla z_3 - \theta = 0 \Rightarrow U = \text{ transverse rigid-body motion},$$

it can be assumed that the in-plane components  $z_1, z_2$  satisfy the in-plane rigidbody hypothesis, and then use the 3d theory. Likewise, to show that

$$e(z) = 0 \Rightarrow U =$$
 in-plane rigid-body motion,

it can be assumed that the transverse components  $z_3$ ,  $\theta_1$ ,  $\theta_2$  satisfy the transverse rigid-body hypothesis.

**Lemma 2.3.5 (Coercivity of**  $A_t, B_t$ ) If the choice of  $\mathcal{U} = (\mathcal{R}, \mathcal{V})$  excludes transverse rigid-body motions, then there exists a constant  $c_1(t_{min})$  such that for every  $U \in \mathcal{U}$ ,

$$A_t(U,U) \ge c_1 \|U\|_{\mathcal{U}}.$$

Likewise, if the choice of  $\mathcal{U} = (\mathcal{R}, \mathcal{V})$  excludes in-plane rigid-body motions, then there exists a constant  $c_2(t_{min})$  such that for every  $U \in \mathcal{U}$ ,

$$B_t(U,U) \ge c_2 \|U\|_{\mathcal{U}}.$$

**Proof:** This argument appears in the more general context of Naghdi shells in [39, Prop. 4.3.2].

Putting everything together, the following uniqueness result is obtained.

**Theorem 2.3.6 (Solutions to (2.2.16))** If  $\mathcal{U}$  excludes rigid-body motions, then for any  $t \in \mathcal{T}$ , (2.2.16) has a unique solution  $U[t] = (\theta[t], z[t])$ .

**Proof:** Follows from lemma 2.3.2, lemma 2.3.5, and the Lax-Milgram theorem.  $\Box$ 

# 2.4 Finite Element Discretization of the Reissner-Mindlin Equations

In this section, the finite element discretization of the Reissner-Mindlin equations is discussed. It turns out that the discretization of the out-of-plane problem (2.3.7) requires some care, whereas the finite element discretization of the in-plane problem (2.3.14) is standard. Therefore, in this section only the finite element discretization of the out-of-plane problem (2.3.7) will be considered: in particular, the development of the MITC finite elements for the Reissner-Mindlin plate equations. A good survey of finite element methods for the Reissner-Mindlin equations is given in [61].

For simplicity of the presentation, several additional assumptions are made:

- The boundary conditions are assumed to be clamped (2.3.5a). In particular,  $\mathcal{R} = H_0^1(\Omega_0)^2$  and  $\mathcal{V}_3 = H_0^1(\Omega_0)$ . It is not difficult to include other boundary conditions listed in (2.3.5) through use of the spaces (2.3.6).
- The thickness t is constant, i.e.,  $t \in \mathbb{R}$ , t > 0. The presentation of the classical error analysis done in [33] is much simpler than that of [74], in which the error analysis was extended to the case of non-constant thicknesses.
- To ensure that the limit problem as  $t \to 0$  is well-behaved, assume that the loading  $p_3$  scales as

$$p_3 = t^3 g,$$

i.e., as the plate gets increasingly thin, it is necessary to reduce the applied force in an appropriate manner so as to retain a finite solution.

Define the bilinear forms

$$a(\theta, \eta) = \int_{\Omega_0} \frac{1}{12} (Le(\theta) : e(\eta)) \, dx$$
$$b(\gamma, \varphi) = \int_{\Omega_0} \gamma \cdot \varphi \, dx.$$

The bilinear form (2.3.8) for the out-of-plane problem is now written as

$$A_t(\theta, z_3; \eta, y_3) = t^3 a(\theta, \eta) + \lambda t b(\nabla z_3 - \theta, \nabla y_3 - \eta).$$

## 2.4.1 Naïve FEM Approximation

By Theorem 2.3.6, the Reissner-Mindlin bilinear form is bounded and elliptic, and so standard finite element methods can be applied to the problem. By Céa's Lemma, if  $\mathcal{R}_h \subset \mathcal{R}$  and  $\mathcal{V}_{3h} \subset \mathcal{V}_3$  are used to discretize the rotation and displacement spaces, the approximation error bound

$$\|\theta - \theta_h\|_{H^1(\Omega_0)}^2 + \|z_3 - z_{3h}\|_{H^1(\Omega_0)}^2 \le C_t \inf_{\substack{\zeta_h \in \mathcal{R}_h \\ w_h \in \mathcal{V}_{3h}}} \left\{ \|\theta - \zeta_h\|_{H^1(\Omega_0)}^2 + \|z_3 - w_h\|_{H^1(\Omega_0)}^2 \right\}$$

is obtained. In the above estimate, the constant in the error bound has been labeled  $C_t$ , as it depends on the ratio of the ellipticity and boundedness constants of  $A_t$ , which both depend on t. The trouble is that as t gets small, this constant can grow so fast that finite element discretizations using this approach are not useful in practice. See Figure 2.3 for a numerical example.

### 2.4.2 Locking and the Kirchhoff Limit Problem

Under the assumptions of this section, the out-of-plane problem (2.3.7) becomes

$$a(\theta,\eta) + \lambda t^{-2}b(\nabla z_3 - \theta, \nabla y_3 - \eta) = (g, y_3)_{L^2(\Omega_0)}.$$
(2.4.1)

This is equivalent to finding

$$\min_{\substack{\theta \in \mathcal{R} \\ z_3 \in \mathcal{V}_3}} \frac{1}{2} a(\theta, \theta) + \lambda \frac{t^{-2}}{2} b(\nabla z_3 - \theta, \nabla z_3 - \theta) - (g, z_3)_{L^2(\Omega_0)}.$$
 (2.4.2)

Intuitively, as  $t \to 0$ , the solution should tend to obey  $\theta = \nabla z_3$ , i.e. it will approach the solution to the Kirchhoff problem

$$\min_{\substack{\theta \in \mathcal{R} \\ z_3 \in \mathcal{V}_3}} \frac{1}{2} a(\theta, \theta) - (g, z_3)_{L^2(\Omega_0)},$$
s.t.  $\theta = \nabla z_3.$ 
(2.4.3)



Figure 2.3: In this figure, the  $L^2$  error is shown for the problem described in §2.6, for which an analytic solution is available. The finite element discretization uses a uniform grid of MITC7 elements, but without making use of the reduction operator, so that it is just a displacement-based scheme using six nodes per element for z, and seven nodes for  $\theta_{\alpha}$  (cubics restricted to be quadratic on the edges). The convergence behavior quickly deteriorates as the thickness decreases.

This is discussed in detail in [10] (see also [61]). The solution to the Reissner-Mindlin problem (2.4.2) with thickness t by  $(\theta^t, z_3^t)$ , and the limiting Kirchhoff solution (2.4.3) is denoted  $(\theta^0, z_3^0)$ .

The finite element problem corresponding to (2.4.2) is

$$\min_{\substack{\theta_h \in \mathcal{R}_h \\ z_{3h} \in \mathcal{V}_{3h}}} \frac{1}{2} a(\theta_h, \theta_h) + \lambda \frac{t^{-2}}{2} b(\nabla z_{3h} - \theta_h, \nabla z_{3h} - \theta_h) - (g, z_{3h})_{L^2(\Omega_0)}.$$

A well-behaved finite element discretization of (2.4.1) must use a space which contains an approximation of  $(\theta^0, z^0)$ . As  $t \to 0$ , the solution tends to the best approximation in the finite element space to the Kirchhoff solution, which satisfies  $\nabla z_{3h}^0 = \theta_h^0$ . The set

$$\{(\theta_h, z_{3h}) \in \mathcal{R}_h \times \mathcal{V}_{3h} : \nabla z_{3h} = \theta_h\}$$

must have enough degrees of freedom left to approximate the solution  $(\theta^0, z_3^0)$  to the Kirchhoff limit problem. In the worst case, the set  $\{(\theta_h, z_{3h}) \in \mathcal{R}_h \times \mathcal{V}_{3h} : \nabla z_{3h} = \theta_h\}$  can contain only the zero function. In the case of clamped boundary conditions (2.3.5a), it is not difficult to see that piecewise linear elements would have this problem:  $\theta_h^0$  must be zero on the boundary, and  $\nabla z_{3h}^0$  would be piecewise constant, but must match  $\theta_h^0$ . Thus,  $\theta_h^0 = 0$  and  $z_{3h}^0 = 0$  in this case. In this case the computed displacements  $(\theta_h^t, z_{3h}^t)$  becomes smaller than it should be. The finite elements are said to overestimate the stiffness of the plate, hence the term "locking."

$$t \to 0 \quad \begin{array}{c} \theta_h^t & \xrightarrow{h \to 0} & \theta^t \\ \downarrow & & \downarrow \\ \theta_h^0 & \xrightarrow{h \to 0} & \theta^0 \end{array} \quad t \to 0$$

Figure 2.4: Desired convergence diagram.  $\theta_h^t$  is the rotation component of the solution to the finite element problem with mesh size h, and thickness t.



Figure 2.5: The worst-case scenario is exemplified by piecewise-linear elements, where for fixed h, the finite element solution approaches the zero function as  $t \to 0$ .

#### 2.4.3 The Mixed Form and the Helmholtz Decomposition

Locking-free finite element methods for (2.4.1) are based on mixed formulations. The physically relevant quantity is the transverse shear strain

$$\gamma = \lambda t^{-2} (\nabla z_3 - \theta) \in \mathcal{S},$$

which is treated as an independent variable. The state space for the shear term is denoted by S, with dual space S'. For fixed t, since the components of  $\theta$  and  $z_3$  are in  $H^1(\Omega_0)$ , it holds that  $S = L^2(\Omega_0)^2$ , and the problem (2.4.1) is equivalent to the following: find  $(\theta, z_3, \gamma) \in (\mathcal{R}, \mathcal{V}_3, S)$  such that

$$a(\theta,\eta) + \lambda b(\gamma,\nabla y_3 - \eta) = (g,y_3)_{L^2(\Omega_0)}$$
(2.4.4a)

$$\lambda t^{-2} (\nabla z_3 - \theta, \varphi)_{L^2(\Omega_0)} - (\gamma, \varphi)_{L^2(\Omega_0)} = 0$$
 (2.4.4b)

for all  $(\eta, y_3, \varphi) \in (\mathcal{R}, \mathcal{V}_3, \mathcal{S})$ .

However,  $S = L^2(\Omega_0)$  is not the proper choice in the limiting case of small t: the shear term can exhibit significant boundary layers ([10, §1]), and is unbounded in  $L^2(\Omega_0)$  as  $t \to 0$ . Analysis thus requires more exotic function spaces. First, several definitions.

**Definition 2.4.1** For a scalar field p and a two-component vector field  $q = (q_1, q_2)$ , define

$$rot(p) = (\partial_2 p, -\partial_1 p)$$
  
 $rot(q) = \partial_1 q_2 - \partial_2 q_1.$ 

Furthermore, define the spaces

$$H(\operatorname{rot};\Omega_0) = \left\{ \eta \in L^2(\Omega_0)^2 : \operatorname{rot}(\eta) \in L^2(\Omega_0) \right\}$$
$$H_0(\operatorname{rot};\Omega_0) = \left\{ \eta \in L^2(\Omega_0)^2 : \operatorname{rot}(\eta) \in L^2(\Omega_0), \eta \cdot \tau = 0 \text{ on } \partial\Omega_0 \right\}$$
$$H^{-1}(\operatorname{div};\Omega_0) = \operatorname{completion} \operatorname{of} C^\infty(\Omega_0)^2 w.r.t. \| \cdot \|_{H^{-1}(\Omega_0)} + \|\operatorname{div} \cdot \|_{H^{-1}(\Omega_0)}.$$

For fixed t, the shear term  $\gamma$  is not only in  $L^2(\Omega_0)$  but also in  $H(\operatorname{rot};\Omega_0)$ , while as  $t \to 0$ , only

$$\gamma \in H^{-1}(\operatorname{div}; \Omega_0)$$

holds. In fact,  $H^{-1}(\text{div}; \Omega_0)$  is known to be the proper Lagrange multiplier space for the limiting case of the Kirchhoff plate [28, VI§5]. Thus, (2.4.4b) must hold, with

$$\mathcal{S} = H(\operatorname{rot}; \Omega_0).$$

It holds that

$$(H(\operatorname{rot};\Omega_0))' = H^{-1}(\operatorname{div};\Omega_0).$$

See [28, VI§6] and [31]. The duality pairing between  $H(\operatorname{rot}; \Omega_0)$  and  $H^{-1}(\operatorname{div}; \Omega_0)$ ensures that the necessary inf-sup condition holds. While analysis of the limiting case can proceed with  $S = H^{-1}(\operatorname{div}; \Omega_0)$ , the standard approach is to use the Helmholtz decomposition. This offers a more precise error estimate, and provides the framework in which the analysis of the MITC elements is possible. More detailed discussion appears in [31]; see also [28, VI§6].

**Theorem 2.4.2 (The Helmholtz Decomposition)** Every  $\gamma \in H^{-1}(div; \Omega_0)$  can be uniquely decomposed as

$$\gamma = \nabla s + \operatorname{rot}(q),$$

with  $s \in H_0^1(\Omega_0)$ ,  $q \in L^2(\Omega_0)/\mathbb{R}$ . Furthermore,

$$\gamma \in L^{2}(\Omega_{0}) \Leftrightarrow q \in H^{1}(\Omega_{0})/\mathbb{R}$$
$$\gamma \in H(rot; \Omega_{0}) \Leftrightarrow q \in H^{2}(\Omega_{0})/\mathbb{R}$$
$$\gamma \in H_{0}(rot; \Omega_{0}) \Leftrightarrow q \in H^{2}(\Omega_{0})/\mathbb{R} \text{ and } \nabla q \cdot n = 0 \text{ on } \partial\Omega_{0}.$$

**Proof:** See [32, Proposition VII.3.4]

For future reference, note that the spaces produced through application of the Helmholtz decomposition to the list (2.3.5) of standard boundary conditions: the boundary conditions and the regularity information in theorem 2.4.2 lead to the following specific choices for the shear space S, and the space Q (corresponding to the second component of the Helmholtz decomposition):

$$S = H_0(\operatorname{rot}; \Omega_0),$$
  

$$Q = \left\{ q \in H^2(\Omega_0) / \mathbb{R} : \nabla q \cdot n = 0 \text{ on } \partial \Omega_0 \right\}$$
 (hard clamped) (2.4.5a)

$$S = H(\operatorname{rot}; \Omega_0), Q = H^2(\Omega_0)/\mathbb{R}$$
 (soft clamped) (2.4.5b)

$$S = H_0(\operatorname{rot}; \Omega_0),$$
  

$$Q = \{q \in H^2(\Omega_0) / \mathbb{R} : \nabla q \cdot n = 0 \text{ on } \partial \Omega_0\} \quad (\text{hard simply-supported}) \quad (2.4.5c)$$
  

$$S = H(\operatorname{rot}; \Omega_0), Q = H^2(\Omega_0) / \mathbb{R} \quad (\text{soft simply-supported}). \quad (2.4.5d)$$

The expansion of (2.4.4) via the Helmholtz decomposition also requires the following lemma.

Lemma 2.4.3 (L<sup>2</sup>-orthogonality of the Helmholtz decomposition) Let  $s \in H_0^1(\Omega_0)$ ,  $q \in H(rot; \Omega_0)$ . Then

$$\int_{\Omega_0} \nabla s \cdot \operatorname{rot}(q) = 0.$$

**Proof:** Approximate s with smooth functions and integrate by parts; the zero boundary-condition on s ensures that the resulting boundary terms vanish.

The decompositions of the shear term  $\gamma$  and the test function  $\varphi$  in (2.4.4) are thus written as

$$\gamma = \nabla s + \operatorname{rot}(q)$$
$$\varphi = \nabla r + \operatorname{rot}(p).$$

Making use of this decomposition, the system (2.4.4) becomes

$$a(\theta,\eta) + (\nabla s + \operatorname{rot}(q), \nabla y_3 - \eta)_{L^2(\Omega_0)} = (g, y_3)_{L^2(\Omega_0)}$$
$$(\nabla s + \operatorname{rot}(q), \nabla r + \operatorname{rot}(p))_{L^2(\Omega_0)} - \lambda t^{-2} (\nabla z_3 - \theta, \nabla r + \operatorname{rot}(p))_{L^2(\Omega_0)} = 0,$$

which expands to become the following (to save space, the subscript  $L^2(\Omega_0)$  on the inner products is dropped)

$$\begin{aligned} a(\theta,\eta) + (\nabla s, \nabla y_3) - (\nabla s,\eta) + (\operatorname{rot}(q), \nabla y_3) - (\operatorname{rot}(q),\eta) &= (g,y_3) \\ (\nabla s, \nabla r) + (\nabla s, \operatorname{rot}(p)) + (\operatorname{rot}(q), \nabla r) + (\operatorname{rot}(q), \operatorname{rot}(p)) \\ -\lambda t^{-2} [(\nabla z_3, \nabla r) + (\nabla z_3, \operatorname{rot}(p)) - (\theta, \nabla r) - (\theta, \operatorname{rot}(p))] &= 0. \end{aligned}$$

By lemma 2.4.3, this simplifies to

$$a(\theta,\eta) + (\nabla s, \nabla y_3) - (\nabla s,\eta) - (\operatorname{rot}(q),\eta) = (g,y_3)$$
$$(\nabla s, \nabla r) + (\operatorname{rot}(q), \operatorname{rot}(p)) - \lambda t^{-2}[(\nabla z_3, \nabla r) - (\theta, \nabla r) - (\theta, \operatorname{rot}(p))] = 0.$$

The previous system decouples into the following problem:

Find  $(\theta, z_3, s, q) \in \mathcal{R} \times \mathcal{V}_3 \times H^1_0(\Omega_0) \times \mathcal{Q}$  such that

$$(\nabla s, \nabla y_3) = (g, y_3), \qquad \forall y_3 \in \mathcal{V}_3$$
 (2.4.6a)

$$a(\theta, \eta) - (\nabla s, \eta) - (\operatorname{rot}(q), \eta) = 0,$$
  $\forall \eta \in \mathcal{R}$  (2.4.6b)

$$(\operatorname{rot}(q), \operatorname{rot}(p)) + \lambda t^{-2}(\theta, \operatorname{rot}(p)) = 0, \qquad \forall p \in \mathcal{Q}$$
 (2.4.6c)

$$\lambda t^{-2}[(\nabla z_3, \nabla r) - (\theta, \nabla r)] = (g, r), \qquad \forall r \in H_0^1(\Omega_0) \qquad (2.4.6d)$$

for all  $(\eta, y_3, r, p) \in \mathcal{R} \times \mathcal{V}_3 \times H^1_0(\Omega_0) \times \mathcal{Q}$ .

The system (2.4.6) can be solved sequentially. First one can solve the Poisson problem (2.4.6a) for s. The subproblems (2.4.6b)-(2.4.6c) are like the Stokes problem, but with a penalty term. Finally, given  $\theta$  one can solve the Poisson problem (2.4.6d). Since the Helmholtz decomposition is unique, the following theorem has been proven.

#### Theorem 2.4.4 (Equivalence of the Helmholtz-Decomposed Problem)

Let  $(\theta, z_3) \in \mathcal{R} \times \mathcal{V}_3$  be the solution to (2.4.1). Then with  $(s, q) \in \times H^1_0(\Omega_0) \times \mathcal{Q}$ chosen via the Helmholtz decomposition (theorem 2.4.2),  $(\theta, z_3, s, q)$  solves (2.4.6). Likewise, if  $(\theta, z_3, s, q) \in \mathcal{R} \times \mathcal{V}_3 \times H^1_0(\Omega_0) \times \mathcal{Q}$  is the solution to (2.4.6), then  $(\theta, z_3)$  solves (2.4.1).

The following regularity result is proven in [31, Prop. 2.4]. See also [61, Sec. 5].

**Theorem 2.4.5** Let  $\Omega_0 \subset \mathbb{R}^2$  be a convex polygon. Assume that  $\mathcal{R}, \mathcal{V}_3, \mathcal{Q}$  satisfy the hard-clamped conditions (2.3.6a), (2.4.5a). If  $g \in L^2(\Omega_0)$ , then (2.4.6) has a unique solution  $(\theta_t, z_{3t}, s_t, q_t) \in \mathcal{R} \times \mathcal{V}_3 \times H_0^1(\Omega_0) \times \mathcal{Q}$ . Moreover the solution has the regularity property  $(\theta_t, z_{3t}, s_t, q_t) \in H^2(\Omega_0)^2 \times H^2(\Omega_0)^2 \times H^2(\Omega_0) \times H^2(\Omega_0)$  and obeys

 $\|\theta_t\|_{H^2(\Omega_0)^2} + \|z_{3t}\|_{H^2(\Omega_0)^2} + \|s_t\|_{H^2(\Omega_0)} + \|q_t\|_{H^1(\Omega_0)} + t\|q_t\|_{H^2(\Omega_0)} \le C\|g\|_{L^2(\Omega_0)}.$ 

#### 2.4.4 MITC Finite Elements

The MITC finite elements can be stated in terms of the original problem (2.4.1), but their analysis requires the mixed form introduced in §2.4.3. MITC finite elements discretize the displacement and rotation spaces

$$\mathcal{R}_h \subset \mathcal{R},$$
  
 $\mathcal{V}_{3h} \subset \mathcal{V}_3,$ 

and incorporate the shear space  $S_h \subset S$  into (2.4.2) indirectly via a so-called reduction operator

$$R_h: H(\operatorname{rot}; \Omega_0) \to \mathcal{S}_h.$$

Instead of using the naive discretization

$$a(\theta_h, \eta_h) + \lambda t^{-2} b(\nabla z_{3h} - \theta_h, \nabla y_{3h} - \eta_h)_{L^2(\Omega_0)} = (g, y_{3h})_{L^2(\Omega_0)}.$$
 (2.4.7)

for all  $\eta_h \in \mathcal{R}_h$  and all  $y_{3h} \in \mathcal{V}_{3h}$ , the discretization

$$a(\theta_h, \eta_h) + \lambda t^{-2} b(R_h(\nabla z_{3h} - \theta_h), R_h(\nabla y_{3h} - \eta_h))_{L^2(\Omega_0)} = (g, y_{3h})_{L^2(\Omega_0)}$$
(2.4.8)

for all  $\eta_h \in \mathcal{R}_h$  and all  $y_{3h} \in \mathcal{V}_{3h}$  is used. Often it is assumed that

$$R_h \nabla y_{3h} = \nabla y_{3h} \quad \forall y_{3h} \in \mathcal{V}_{3h}.$$

In this case (2.4.8) can be written as

$$a(\theta_h, \eta_h) + \lambda t^{-2} b(\nabla z_{3h} - R_h \theta_h, \nabla y_{3h} - R_h \eta_h)_{L^2(\Omega_0)} = (g, y_{3h})_{L^2(\Omega_0)}$$
(2.4.9)

for all  $\eta_h \in \mathcal{R}_h$  and all  $y_{3h} \in \mathcal{V}_{3h}$ .

If  $\theta_h^t \in \mathcal{R}_h$ ,  $y_{3h}^t \in \mathcal{V}_{3h}$  is the solution of (2.4.9), then in the limit  $t \to 0$  one expects the condition

$$\nabla z_{3h}^0 - R_h \theta_h^0 = 0$$

to hold. The introduction of the reduction operator introduces more flexibility and allows the previous identity to hold for elements other than  $z_{3h}^0 = 0$  and  $\theta_h^0 = 0$ . Thus the reduction operator "unlocks" the elements by altering the discrete shear term.

According to Braess [28, p. 329], one of the primary reasons that the MITC approach is favored is that it leads to positive definite matrices with fewer unknowns, as it does not actually discretize the shear space. Another motivation is that the use of a reduction operator in this situation has roots in engineering practice (see [32]).

Discrete versions of the spaces  $\mathcal{Q}$ , and  $H_0^1(\Omega_0)$  are also needed for the analysis of MITC, which is based on a mixed formulation related to (2.4.6). Actually, the discrete space  $\mathcal{Q}_h$  is used to discretize both  $\mathcal{Q}$  and  $H_0^1(\Omega_0)$ . In the following discussion, the clamped boundary conditions shall be assumed so as to simplify the exposition.

The assumptions on the spaces  $\mathcal{R}_h$ ,  $\mathcal{V}_{3h}$ ,  $\mathcal{S}_h$ ,  $\mathcal{Q}_h$ , as well as the assumption on the reduction operator  $R_h$  are given as follows (see, e.g., [30], [28, p. 302]).

- (P1)  $\nabla \mathcal{V}_{3h} \subset \mathcal{S}_h$ .
- (P2)  $\operatorname{rot} \mathcal{S}_h \subset \mathcal{Q}_h$ .
- (P3) The inf-sup condition.

$$\inf_{p_h \in \mathcal{Q}_h} \sup_{\eta_h \in \mathcal{R}_h} \frac{(\operatorname{rot}(\eta_h), p_h)}{\|\eta_h\|_1 \|p_h\|_0} = \beta > 0.$$
(2.4.10)

(P4) Let  $P_h$  be the  $L^2$ -projector onto  $\mathcal{Q}_h$ . Then

$$\operatorname{rot} R_h \eta = P_h \operatorname{rot} \eta \quad \forall \eta \in H^1_0(\Omega_0)^2.$$

This is the "commuting diagram property," related to the solution of elliptic problems using mixed methods. It is described as "the pair  $S_h$ ,  $Q_h$  is good for elliptic problems" in [12].

(P5) If  $\eta_h \in S_h$  and  $rot(\eta_h) = 0$ , then  $\eta_h \in \nabla \mathcal{V}_{3h}$ .

It is shown in [33, Lemma 3.1] that MITC properties (P1),(P2),(P4),(P5) (n.b., the properties are not numbered the same in [33] as they are in these notes and many earlier papers) lead to a discrete analog of the Helmholtz decomposition. See also, e.g., [28, p. 303]. Condition (P3) is the standard inf-sup condition required to ensure well-posedness of the Stokes problem (2.4.6b)-(2.4.6c) (see [12]).

The application of the Helmholtz decomposition to the MITC weak form (2.4.9) yields

$$(\nabla s, \nabla y_3) = (g, y), \qquad \forall y_3 \in \mathcal{V}_{3h}$$
 (2.4.11a)

$$a(\theta, \eta) - (\nabla s, R_h \eta) - (\operatorname{rot}(q), R_h \eta) = 0, \qquad \forall \eta \in \mathcal{R}_h \qquad (2.4.11b)$$

$$(\operatorname{rot}(q), \operatorname{rot}(p)) + \lambda t^{-2}(R_h \theta, \operatorname{rot}(p)) = 0, \qquad \forall p \in \mathcal{Q}_h \qquad (2.4.11c)$$

$$\lambda t^{-2}[(\nabla z_3, \nabla r) - (R_h \theta, \nabla r)] = (g, r), \qquad \forall r \in \mathcal{Q}_h.$$
(2.4.11d)

This is analogous to the derivation of (2.4.6). Now, integrate by parts and apply (P4), which shows that

$$(\operatorname{rot}(q), R_h \eta) = (q, \operatorname{rot}(\eta))$$
$$(R_h \theta, \operatorname{rot}(p)) = (\operatorname{rot}(\theta), p).$$

Making these substitutions in (2.4.11b)-(2.4.11c), and further treating rot(p) as an

independent variable  $\alpha$ , with compatibility weakly enforced, (2.4.11) becomes

$$(\nabla s, \nabla y_3) = (g, y_3), \qquad \forall y_3 \in \mathcal{V}_{3h} \qquad (2.4.12a)$$

$$a(\theta,\eta) - (\nabla s, R_h\eta) - (q, \operatorname{rot}(\eta)) = 0, \qquad \forall \eta \in \mathcal{R}_h \qquad (2.4.12b)$$

$$(\operatorname{rot}(\alpha), p) + \lambda t^{-2}(\operatorname{rot}\theta, p) = 0, \qquad \forall p \in \mathcal{Q}_h \qquad (2.4.12c)$$

$$(\alpha, \delta) - (q, \operatorname{rot}(\delta)) = 0,$$
  $\forall \delta \in S_h$  (2.4.12d)

$$\lambda t^{-2}[(\nabla z_3, \nabla r) - (R_h \theta, \nabla r)] = (g, r), \qquad \forall r \in \mathcal{Q}_h, \qquad (2.4.12e)$$

which, except for the presence of  $R_h$ , is equivalent to an ordinary weak formulation of Reissner-Mindlin, in which rot(p) is treated as an independent variable, as above. This introduces a consistency error relative to (2.4.1), but due to the properties of the reduction operator  $R_h$ , it is possible to prove that even with the changes, MITC still converges to the solution of the Reissner-Mindlin problem.

Error estimates are thus based upon the error in the two Poisson problems, and in the penalized Stokes problem, and the result is quite complex: see [33, Thm. 3.2]. For problems with smooth solutions, the following error bound holds for the MITC7 element.

**Theorem 2.4.6 (Error Estimate for MITC7)** Assuming that each component of  $\theta, z, s, q$  from (2.4.11) is in  $H^3(\Omega_0)$ , the error bound

$$\begin{aligned} \|z - z_h\|_{H^1(\Omega_0)} + \|\theta - \theta_h\|_{H^1(\Omega_0)^2} + \|\gamma - \gamma_h\|_{H^{-1}(\Omega_0)} \\ &\leq Ch^2(\|z\|_{H^3(\Omega)} + \|\theta\|_{H^3(\Omega_0)} + \|q\|_{H^2(\Omega_0)} + t\|q\|_{H^3(\Omega_0)}) \end{aligned}$$

holds.

**Proof:** MITC7 uses a Raviart-Thomas reduction operator , allowing application of the result [33, Cor. 3.1], using "Family I" with k = 2.

Additional error estimates can be found, e.g., in [33, 38, 61]. Results for nonconstant thickness functions can be found in [74].



Figure 2.6: Convergence of the hard simply-supported plate described in §2.6 to an analytic solution, cf. figure 2.3, which shows what happens in the same test case, but with the reduction operator switched off, i.e., replaced with the identity. The conditioning of the resulting linear system deteriorates as t becomes small, and in practice, it seems to be this factor which limits the range of problems that can be solved accurately with the MITC elements.

## 2.5 Joints between Reissner-Mindlin Plates

In order to model structures composed of more than one plate or shell, it is necessary to consider junction conditions, as is done in [53, 54]. They arise from limit problems in which the thickness of joined 3d regions tends to zero, along with an appropriately scaled loading. Networks of joined plates were modeled in [85].

Junction conditions between Kirchhoff plates at arbitrary angles were considered in [21], using more of a modeling perspective, in which forces and moments (torques) are matched at the plate junction. In this section, the results are extended to Reissner-Mindlin plates.



Figure 2.7: Plates occupying the domains  $\Omega$ ,  $\tilde{\Omega}$ , joined along a common straight edge. They are endowed with the local coordinate systems  $e_1, e_2, e_3$ , and  $\tilde{e}_1, \tilde{e}_2, \tilde{e}_3$ , respectively. It is assumed that  $-1 < e_3 \cdot \tilde{e}_3 < 1$ , i.e., that the plates do not lie in the same plane.

In §2.2, the Reissner-Mindlin plate equations were derived using the Cartesian coordinate system  $e_1 = (1, 0, 0)^T$ ,  $e_2 = (0, 1, 0)^T$ ,  $e_3 = (0, 0, 1)^T$  and assuming that the plate occupies the region  $\{(x_1, x_2, x_3) : (x_1, x_2) \in \Omega_0, x_3 \in [-t/2, t/2]\}$ . Now it is necessary to represent the plates and their displacements in rotated bases. The first plate has reference coordinates in  $\Omega_0 \subset \mathbb{R}^2$  and orthonormal basis vectors  $e_1, e_2, e_3$ , while the second has reference coordinates in  $\tilde{\Omega}_0 \subset \mathbb{R}^2$  and orthonormal basis vectors  $\tilde{e}_1, \tilde{e}_2, \tilde{e}_3$ . Assume (see figure 2.7) the following:

• The plates occupy the domains

$$\Omega = \{ x_i e_i : (x_1, x_2) \in \Omega_0, x_3 \in [-t/2, t/2] \},\$$
  
$$\tilde{\Omega} = \{ \tilde{x}_i \tilde{e}_i : (\tilde{x}_1, \tilde{x}_2) \in \tilde{\Omega}_0, \tilde{x}_3 \in [-\tilde{t}/2, \tilde{t}/2] \},\$$

respectively, and their displacements take the form

$$u(x) = (z_1(x_1, x_2) - \theta_1(x_1, x_2)x_3)e_1 + (z_2(x_1, x_2) - \theta_2(x_1, x_2)x_3)e_2 + z_3(x_1, x_2)e_3,$$
  
$$\tilde{u}(\tilde{x}) = (\tilde{z}_1(\tilde{x}_1, \tilde{x}_2) - \tilde{\theta}_1(\tilde{x}_1, \tilde{x}_2)\tilde{x}_3)\tilde{e}_1 + (\tilde{z}_2(\tilde{x}_1, \tilde{x}_2) - \tilde{\theta}_2(\tilde{x}_1, \tilde{x}_2)\tilde{x}_3)\tilde{e}_2 + \tilde{z}_3(\tilde{x}_1, \tilde{x}_2)\tilde{e}_3.$$

•  $\partial \Omega_0 \cap \partial \tilde{\Omega}_0 \subset \mathbb{R}^2$  is a line segment along  $x_1 = 0$ ;  $e_2 = \tilde{e}_2$ , i.e., the reference coordinate sets intersect along  $x_1 = 0$ , and the new coordinate axes differ from the old by a rotation about  $e_2$ .

The physical intersection is the straight segment  $\Gamma$  along  $e_2$ :

$$\Gamma \equiv \{x_i e_i : x \in \Omega, x_1 = 0\} = \left\{ \tilde{x}_i \tilde{e}_i : \tilde{x} \in \tilde{\Omega}, \tilde{x}_1 = 0 \right\}.$$

•  $-1 < e_3 \cdot \tilde{e}_3 < 1$ , i.e., the plates do not lie in the same plane.

The vectors  $n, \tau$  denote the normal and counter-clockwise tangent on the boundary of the first plate;  $\tilde{n}, \tilde{\tau}$  are the normal and counter-clockwise tangent vectors for the second plate. The vectors  $e_3 = n \times \tau$  and  $\tilde{e}_3 = \tilde{n} \times \tilde{\tau}$  are normal to the middle surfaces of the respective plates.

The Reissner-Mindlin equations (2.2.16) and (2.2.17) for the second plate, for example, are now written as

$$\int_{\tilde{\Omega}_0} \frac{\tilde{t}^3}{12} (\tilde{L}\tilde{e}(\tilde{\theta}) : \tilde{e}(\tilde{\eta})) + t\lambda(\nabla \tilde{z}_3 - \tilde{\theta}) \cdot (\nabla \tilde{y}_3 - \tilde{\eta}) d(\tilde{x}_1, \tilde{x}_2)$$
$$= \int_{\tilde{\Omega}_0} \tilde{p}_\alpha \tilde{y}_\alpha d(\tilde{x}_1, \tilde{x}_2) + \int_{\tilde{\gamma}_1} \tilde{T}_3 \tilde{y}_3 + \tilde{M}_{\tilde{n}} \tilde{\eta}_{\tilde{\tau}} - \tilde{M}_{\tilde{\tau}} \tilde{\eta}_{\tilde{n}} d(\tilde{x}_1, \tilde{x}_2).$$

and

$$\int_{\tilde{\Omega}_0} \tilde{t}(\tilde{L}\tilde{e}(\tilde{z}_1, \tilde{z}_2) : \tilde{e}(\tilde{z}_1, \tilde{z}_2)) d(\tilde{x}_1, \tilde{x}_2)$$
  
= 
$$\int_{\tilde{\Omega}_0} \tilde{p}_{\alpha} \tilde{y}_{\alpha} d(\tilde{x}_1, \tilde{x}_2) + \int_{\tilde{\gamma}_1} \tilde{T}_{\alpha} \tilde{y}_{\alpha} d(\tilde{x}_1, \tilde{x}_2).$$

The coupling requires a mechanical and a kinematic condition on  $\Gamma$ . The mechanical condition follows from Newton's third law; moments M and forces T (see (2.2.12) and (2.2.13)) across the junction must balance:

$$M + \tilde{M} = 0$$
$$T + \tilde{T} = 0.$$

Expressed in their local coordinate systems,

$$M_n + M_{\tilde{n}} = 0,$$
  
$$M_\tau \tau = -\tilde{M} = -(\tilde{M}_{\tilde{n}}\tilde{n} + \tilde{M}_{\tilde{\tau}}\tilde{\tau}),$$
  
$$T + \tilde{T} = 0.$$

~

Since n and  $\tilde{n}$  point away from their respective domains,

$$M_n = \tilde{M}_{\tilde{n}} = 0.$$

Let  $\phi$  be the (infinitesimal rotation) vector satisfying

$$\theta = \theta_1 e_1 + \theta_2 e_2 = \phi \times e_3.$$

The kinematic condition for a rigid hinge is that

$$z = z_n n + z_\tau \tau + z_3 e_3 = \tilde{z} = \tilde{z}_{\tilde{n}} \tilde{n} + \tilde{z}_{\tilde{\tau}} \tilde{\tau} + \tilde{z}_3 \tilde{e}_3$$
$$\phi \cdot \tau = \tilde{\phi} \cdot \tilde{\tau}.$$

The latter of these implies that

$$\theta_n + \theta_{\tilde{n}} = 0,$$

i.e., that the angle between the plates is preserved during the motion.

To summarize, the coupling conditions are

$$T + \tilde{T} = 0 \tag{2.5.1a}$$

$$M_n = \tilde{M}_{\tilde{n}} = 0 \tag{2.5.1b}$$

$$M_{\tau} - \tilde{M}_{\tilde{\tau}} = 0 \tag{2.5.1c}$$

$$z - \tilde{z} = 0 \tag{2.5.1d}$$

$$\theta_n + \theta_{\tilde{n}} = 0. \tag{2.5.1e}$$

Upon addition of the weak forms for the two plates and insertion of the conditions

(2.5.1), the coupled weak form

$$A_{t}(\theta, z; \eta, y) + \tilde{A}_{\tilde{t}}(\tilde{\theta}, \tilde{z}; \tilde{\eta}, \tilde{y}) + B_{t}(\theta, z; \eta, y) + \tilde{B}_{\tilde{t}}(\tilde{\theta}, \tilde{z}; \tilde{\eta}, \tilde{y})$$

$$= \int_{\Omega_{0}} p \cdot y \, dx + \int_{\tilde{\Omega}_{0}} \tilde{p} \cdot \tilde{y} \, d\tilde{x}$$

$$+ \int_{\gamma_{1} \setminus \Gamma} T \cdot y + M_{n} \eta_{\tau} - M_{\tau} \eta_{n} \, dx + \int_{\tilde{\gamma}_{1} \setminus \Gamma} \tilde{T} \cdot \tilde{y} + \tilde{M}_{\tilde{n}} \tilde{\eta}_{\tilde{\tau}} - \tilde{M}_{\tilde{\tau}} \tilde{\eta}_{\tilde{n}} \, d\tilde{x}$$

$$+ \int_{\Gamma} T \cdot (y - \tilde{y}) - M_{\tau} (\eta_{n} + \tilde{\eta}_{\tilde{n}}) \, dx. \qquad (2.5.2)$$

is obtained. The last integral vanishes due to the kinematic conditions in (2.5.1). This leads to

Problem 1 [Joined Reissner-Mindlin Plates]

Let

$$\mathcal{J} = \left\{ (\theta, z) \in \mathcal{R} \times \mathcal{V}, (\tilde{\theta}, \tilde{z}) \in \tilde{\mathcal{R}} \times \tilde{\mathcal{V}} : (2.5.1d, e) \text{ are satisfied on } \Gamma \right\}.$$

Find  $(\theta, z), (\tilde{\theta}, \tilde{z}) \in \mathcal{J}$  such that for all  $(\eta, y), (\tilde{\eta}, \tilde{y}) \in \mathcal{J}$ ,

$$\begin{aligned} A_t(\theta, z; \eta, y) &+ \tilde{A}_{\tilde{t}}(\tilde{\theta}, \tilde{z}; \tilde{\eta}, \tilde{y}) + B_t(\theta, z; \eta, y) + \tilde{B}_{\tilde{t}}(\tilde{\theta}, \tilde{z}; \tilde{\eta}, \tilde{y}) \\ &= \int_{\Omega_0} p \cdot y \, dx + \int_{\tilde{\Omega}_0} \tilde{p} \cdot \tilde{y} \, d\tilde{x} \\ &+ \int_{\gamma_1 \setminus \Gamma} T \cdot y + M_n \eta_\tau - M_\tau \eta_n \, dx + \int_{\tilde{\gamma}_1 \setminus \Gamma} \tilde{T} \cdot \tilde{y} + \tilde{M}_{\tilde{n}} \tilde{\eta}_{\tilde{\tau}} - \tilde{M}_{\tilde{\tau}} \tilde{\eta}_{\tilde{n}} \, d\tilde{x}. \end{aligned}$$

**Theorem 2.5.1 (Existence and uniqueness of solutions to problem 1)** Assume that rigid body motions are prohibited for at least one of  $\mathcal{R}, \mathcal{V}, \tilde{\mathcal{R}}, \tilde{\mathcal{V}}$ . Then problem 1 has a unique solution.

**Proof:** The result is sketched based on the work of [21, Thm. 3.2.1]. As in the proof of lemma 2.3.5, it is necessary to show that the norm

$$\left(\|\cdot\|_{A}^{2}+\|\cdot\|_{B}^{2}+\|\cdot\|_{\tilde{A}}^{2}+\|\cdot\|_{\tilde{B}}^{2}\right)^{\frac{1}{2}},$$

defined using the strain terms of both the transverse  $(A_t)$  and in-plane  $(B_t)$  components of the bilinear form, is equivalent to the norm on  $(\mathcal{R}, \mathcal{V}) \times (\tilde{\mathcal{R}}, \tilde{\mathcal{V}})$ , provided that rigid-body motions are prohibited. The result then follows from the Lax-Milgram theorem.

## 2.6 Discretization of Joined Plates

In this section, two related plate problems with analytic solutions are presented. The first is a single square plate under transverse sinusoidal load; it is later used to construct an analytic solution for two square plates joined at a right angle.

#### 2.6.1 Square Plate under Sinusoidal Pressure

For some real a > 0, let the domain be given by

$$\Omega_0 = \left\{ (x_1, x_2) \in \mathbb{R}^2 : (x_1, x_2) \in [-a/2, a/2] \times [-a/2, a/2] \right\},\$$

and assume that the displacements and forcing are of the following form:

$$z = A \cos\left(\frac{\pi x_1}{a}\right) \cos\left(\frac{\pi x_2}{a}\right)$$
$$\theta = B \left( \frac{\sin\left(\frac{\pi x_1}{a}\right) \cos\left(\frac{\pi x_2}{a}\right)}{\cos\left(\frac{\pi x_1}{a}\right) \sin\left(\frac{\pi x_2}{a}\right)} \right)$$
$$g = C \cos\left(\frac{\pi x_1}{a}\right) \cos\left(\frac{\pi x_2}{a}\right).$$

To construct an analytic solution, A, B, C must be found so that (2.2.18) is satisfied. The boundary condition (2.3.5c) holds due to the forms assumed; clearly,  $\theta \cdot \tau = z = 0$  on  $\partial \Omega_0$ . It is easy to verify from the following expression that  $M_n = 0$  on  $\partial \Omega_0$ :

$$\begin{split} L\epsilon(\theta) &= D[(1-\nu)\epsilon(\theta) + \nu \mathrm{tr}[\epsilon(\theta)]I] \\ &= D\left[ (1-\nu) \begin{pmatrix} \theta_{1,1} & \frac{1}{2}(\theta_{1,2} + \theta_{2,1}) \\ \frac{1}{2}(\theta_{1,2} + \theta_{2,1}) & \theta_{2,2} \end{pmatrix} + \nu \begin{pmatrix} \theta_{1,1} + \theta_{2,2} & 0 \\ 0 & \theta_{1,1} + \theta_{2,2} \end{pmatrix} \right] \\ &= D\left( \begin{pmatrix} \theta_{1,1} + \nu \theta_{2,2} & \frac{1-\nu}{2}(\theta_{1,2} + \theta_{2,1}) \\ \frac{1-\nu}{2}(\theta_{1,2} + \theta_{2,1}) & \theta_{2,2} + \nu \theta_{1,1} \end{pmatrix} \right) \\ &= \frac{\pi BD}{a} \begin{pmatrix} (1+\nu)\cos\left(\frac{\pi x_1}{a}\right)\cos\left(\frac{\pi x_2}{a}\right) & (\nu-1)\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right) \\ (\nu-1)\sin\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right) & (1+\nu)\cos\left(\frac{\pi x_1}{a}\right)\cos\left(\frac{\pi x_2}{a}\right) \end{pmatrix}. \end{split}$$

The remaining terms appearing in (2.2.18) are:

$$\nabla \cdot L\epsilon(\theta) = \left(\frac{\pi}{a}\right)^2 BD \begin{pmatrix} -(1+\nu)\sin\left(\frac{\pi x_1}{a}\right)\cos\left(\frac{\pi x_2}{a}\right) + (\nu-1)\sin\left(\frac{\pi x_1}{a}\right)\cos\left(\frac{\pi x_2}{a}\right) \\ (\nu-1)\cos\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right) + -(1+\nu)\cos\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right) \end{pmatrix}$$
$$= -2\left(\frac{\pi}{a}\right)^2 D\theta$$
$$\nabla z - \theta = -\frac{\pi}{a} A \begin{pmatrix} \sin\left(\frac{\pi x_1}{a}\right)\cos\left(\frac{\pi x_2}{a}\right) \\ \cos\left(\frac{\pi x_1}{a}\right)\sin\left(\frac{\pi x_2}{a}\right) \end{pmatrix} - \theta = -(1+\frac{\pi}{a}A/B)\theta$$
$$\nabla \cdot (\nabla z - \theta) = -2\left(\frac{\pi}{a}\right) (B + \frac{\pi}{a}A)\cos\left(\frac{\pi x_1}{a}\right)\cos\left(\frac{\pi x_2}{a}\right).$$

Putting everything together yields the following linear system for for A and B:

$$\begin{pmatrix} (\pi/a)^2 & \pi/a \\ 1 & a/\pi + 2t^2 \frac{\pi}{a} \frac{D}{12\lambda} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \frac{Ct^2}{2\lambda} \\ 0 \end{pmatrix}.$$

## 2.6.2 Square Plates Joined at a Right Angle

This example problem is shown in figure 2.8. The idea is to combine two hard simply-supported plates with sinusoidal loading, described in the previous section to get a joined problem satisfying the conditions (2.5.1) with the analytic solution (the



Figure 2.8: The joined hard simply-supported plates. The reference coordinates for plate 1 (on top) are in  $\{(x_1, x_2) : x_1 \in [-a/2, a/2], x_2 \in [-a/2, a/2]\}$ . Likewise, for plate 2 (on the side), the coordinates are  $\{(\tilde{x}_1, \tilde{x}_2) : \tilde{x}_1 \in [-a/2, a/2], \tilde{x}_2 \in [-a/2, a/2]\}$ . The junction is along  $x_2 = -a/2, \tilde{x}_2 = a/2$ .

superscripts signify the number of the plate)

$$z_3^1 = A \cos\left(\frac{\pi x_1}{a}\right) \cos\left(\frac{\pi x_2}{a}\right)$$
$$\begin{pmatrix} \theta_1^1\\ \theta_2^1 \end{pmatrix} = B \begin{pmatrix} \sin\left(\frac{\pi x_1}{a}\right) & \cos\left(\frac{\pi x_2}{a}\right)\\ \cos\left(\frac{\pi x_1}{a}\right) & \sin\left(\frac{\pi x_2}{a}\right) \end{pmatrix}$$
$$z_3^2 = -z_3^1$$
$$\theta^2 = -\theta^1$$
$$0 = z_1^1 = z_2^1 = z_1^2 = z_2^2.$$

Each plate remains clamped with the same conditions as before on its three un-

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joined edges; the combination of the symmetry of the problem and the kinematic coupling conditions allow the solution for the single plate to be used for each of the two joined plates.

## 2.7 Bending Waves in Reissner-Mindlin Plates

In choosing the level of refinement for finite element discretization of plate equations, it is necessary to consider the speed of bending waves. Here, the dispersion relation for bending waves in a Kirchhoff plate is derived. The inertial term for Reissner-Mindlin comes from integration of  $\rho u_{tt}$  against a test function v, viz.

$$-\omega^2 \int_{\Omega} \rho u v \, dx = -\omega^2 \rho \int_{\Omega_0} \int_{-t(x_1, x_2)/2}^{t(x_1, x_2)/2} x_3^2 \theta \cdot \eta + z_3 y_3 \, dx_3 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_3 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_4 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_4 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_4 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_4 \, dx_4 dx = -\omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + t z_3 y_4 \, dx_5 \,$$

Recalling (2.2.16), for bending waves it holds that

$$\int_{\Omega_0} \frac{t^3}{12} (Le(\theta) : e(\eta)) + t\lambda(\nabla z_3 - \theta) \cdot (\nabla y_3 - \eta) \, dx = \omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \theta \cdot \eta + tz_3 y_3 \, dx.$$

Using the Kirchhoff-Love kinematic assumption  $\nabla z_3 = \theta$ , this becomes

$$\int_{\Omega_0} \frac{t^3}{12} (Le(\nabla z_3) : e(\nabla y_3)) \, dx = \omega^2 \rho \int_{\Omega_0} \frac{t^3}{12} \nabla z_3 \cdot \nabla y_3 + t z_3 y_3 \, dx.$$

In the strong form, this reads

$$\frac{t^{3}E}{12(1-\nu^{2})}\Delta^{2}z_{3} = \omega^{2}\rho\left(-\frac{t^{3}}{12}\Delta z_{3} + tz_{3}\right).$$

Assuming a solution proportional to  $\exp(i\kappa \cdot x)$ , this becomes

$$\omega^2 \left( 1 + \frac{(\kappa t)^2}{12} \right) = \frac{(\kappa t)^2}{12} (\nu \kappa)^2,$$

where the characteristic velocity is

$$v = \sqrt{\frac{E}{\rho(1-\nu^2)}}.$$

Assuming that  $\kappa t \ll 1$ ,

$$\omega \approx \kappa^2 t v / \sqrt{12},$$

so that the phase velocity  $v_p=\omega/\kappa$  is

$$v_p \approx \kappa t v / \sqrt{12}.$$

The critical frequency for sound radiation is where  $v_p = c$ , the acoustic sound speed. This is given by

$$\omega_c \approx c^2 \sqrt{12}/(vt).$$

Physically, the idea is that if there is sufficient mismatch between the bending wave speed and the acoustic sound speed, radiation will be inefficient. Although this line of reasoning is not directly applicable to curved shells, the basic intuition it provides is helpful in considering discretization requirements.



Figure 2.9: Error in the joined plate problem as computed with Duran-Liberman plate elements of [56].

## Chapter 3

## Naghdi Shells

## 3.1 Introduction

In this chapter, the Naghdi model for thin curved shells is discussed. It generalizes the kinematic and mechanical assumptions of the Reissner-Mindlin plate model in §2.2 to the case of a curved shell. The shell geometry is given by a mapping called a chart function from reference coordinates onto the physical domain; in the case of plates, this mapping is simply the identity. The derivatives of the chart function form locally varying bases, which are used to represent the shell geometry, the constitutive tensors, and in the classical formulation of the Naghdi model, also the displacement vectors.

In some more recent work [25, 107, 23] a different method is adopted: the vector fields are represented in the Cartesian basis, which turns out to allow more relaxed assumptions on the regularity of the chart function, and is better-suited to the implementation of finite element methods. I follow this approach, but also discuss the classical Naghdi model in §3.4 due to its widespread exposition.

Discretizations of the Naghdi shell model can also suffer from the locking phenomenon exhibited by the Reissner-Mindlin plate model. However unlike the Reissner-Mindlin case, development of finite element methods that satisfy an inf-sup condition analogous to (2.4.10) is an open problem. Practical methods for the alleviation of the locking phenomenon include the use of higher-order transverse terms, such as in [57] and [103]. There has also been some recent work on Discontinuous Galerkin methods [69, 68], and NURBS [79]. Among the earlier work was the paper [8], in which a finite element method that satisfies the inf-sup condition is developed, under restrictive assumptions on the geometric coefficients in the model. The authors speculate that their result may also be true without these assumptions.

This thesis uses the MITC shell elements, which are developed by analogy to the plate elements; a related family of "locking-free" shell elements were also proposed and tested in [23]. Since there is no available proof that the inf-sup condition holds, the authors of [14, 15] develop a numerical test of the inf-sup condition requiring matrix assembly and the solution of an eigenvalue problem. Elements such as the MITC6 shell element, described in [87] are shown to be well-behaved in this sense, and to be a practical solution method for shell problems.

A review of shape optimization methods for Naghdi shells, including the shape derivatives of the shell operators is presented near the end of this chapter, in §3.5. Finally, mechanical junction conditions for shells are discussed in §3.6.

#### 3.1.1 Notation and Preliminaries

- The Einstein summation convention is used throughout: repeated appearance of an index in an equation implies summation over that index. Latin indices range over {1,2,3}, and Greek indices range over {1,2}. When such summation occurs, the repeated index will appear once as a superscript and once as a subscript.
- Parentheses around tensor components denote the matrix given by those components, e.g.,  $(g_{ij})$  denotes the 3 × 3 matrix given by the components  $g_{ij}$ .
- The elastic problem is posed in the physical space  $\mathcal{E}^3 \sim \mathbb{R}^3$ , associated by an

invertible mapping  $\Phi : \mathbb{R}^3 \to \mathcal{E}^3$  with reference coordinates in  $\mathbb{R}^3$ . Elements of  $\mathcal{E}^3$  are merely vectors in  $\mathbb{R}^3$ : the notation  $\mathcal{E}^3$  is used to avoid confusion between the reference and physical coordinates. The distinction between  $\mathcal{E}^3$  and  $\mathbb{R}^3$  is also maintained through the appearance of hats over coordinates in  $\mathcal{E}^3$  and functions whose domains are in  $\mathcal{E}^3$ . Thus, the standard bases for  $\mathbb{R}^3$  and  $\mathcal{E}^3$  are respectively  $\{e_1, e_2, e_3\}$ , and  $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$ . These may also be written with superscripts. The same letter e is also used for the strain tensor, though it always has two subscripts or superscripts.

Partial derivatives of  $\Phi$  with respect to the coordinates in  $\mathbb{R}^3$  will define two local bases for  $\mathcal{E}^3$ : the covariant basis

$$\{g_1(x), g_2(x), g_3(x)\},\$$

and the contravariant basis

$$\{g^1(x), g^2(x), g^3(x)\}.$$

For example, with x and  $\hat{x}$  related as above, a vector field  $v(x) = \hat{v}(\hat{x})$  would be represented as

$$\hat{v}(\hat{x}) = v(x) = v_i(x)g^i(x) = v^i(x)g_i(x) = \hat{v}_i(\hat{x})\hat{e}^i = \hat{v}^i(\hat{x})\hat{e}_i.$$

The functions  $v_i, v^i, \hat{v}_i = \hat{v}^i$  are respectively the covariant, contravariant, and Cartesian components of the vector field.

• The contraction operator : is defined on dyads, which are outer products of vectors. For example, if  $e_i, e_j \in \mathbb{R}^3$ , then the dyad  $e_i e_j$  gives a linear operation defined by

$$e_i e_j \cdot e_k = (e_i \cdot e_k) e_j \in \mathbb{R}^3.$$

Dyads need not consist of only two vectors. Let Lin be the space of linear maps from  $\mathcal{E}^3 \to \mathcal{E}^3$ . The linear operator abcd: Lin  $\to$  Lin (formed from



Figure 3.1: The chart function  $\Phi$  maps  $\Omega \subset \mathbb{R}^3$  to  $\mathcal{E}^3$ . This transformation takes a point x to a vector  $\hat{x}$ .

$$a, b, c, d \in \mathcal{E}^3$$
) acting on  $ef \in \text{Lin}$  (with  $e, f \in \mathcal{E}^3$ ) yields

$$abcd: ef = (a \cdot e)(b \cdot f)cd \in Lin$$

As the dyads  $\hat{e}_i \hat{e}_j \hat{e}_k \hat{e}_l$  form a basis for maps from Lin  $\rightarrow$  Lin, the contraction operation : is defined on general tensors irrespective of basis.

The derivative  $\hat{\nabla}\hat{u}(\hat{x}) \in \text{Lin of the mapping } \hat{u}(\hat{x})$  satisfies

$$\hat{u}(\hat{x} + \delta \hat{x}) - \hat{u}(\hat{x}) = \hat{\nabla} \hat{u}(\hat{x}) \delta \hat{x} + o(\|\delta \hat{x}\|).$$

### 3.1.2 Three-dimensional Differential Geometry

Let  $\Omega \subset \mathbb{R}^3$  be a bounded open set  $\Omega \subset \mathbb{R}^3$ , and  $\Phi : \Omega \to \mathcal{E}^3$  a differentiable function. Recall that for the plate equations, it was not really necessary to maintain the distinction between the reference coordinates in  $\mathbb{R}^3$  and the physical points in  $\mathcal{E}^3$ , as the mapping between the two was the identity. In general, this is not the case. Let  $\Phi$  be an *immersion*, i.e., the matrix  $\nabla \Phi$  exists and is non-singular for every  $x \in \Omega$ .  $\Phi$  is called the *chart function*. From here on, it is assumed that the point  $x \in \Omega$  and  $\hat{x} \in \hat{\Omega}$  are related via

$$\hat{x} = \Phi(x)$$
  
 $x = \Phi^{-1}(\hat{x})$ 

Define  $g_i$  by

 $g_i = \partial_i \Phi.$ 

As  $\Phi$  is differentiable,

$$\Phi(x + \delta x) - \Phi(x) = (\nabla \Phi)\delta x + o(\|\delta x\|).$$

If  $\delta x = \delta t e_i$  ( $e_i \in \mathbb{R}^3$  is column *i* of the 3  $\times$  3 identity matrix), then

$$\Phi(x + \delta x) - \Phi(x) = g_i \delta t + o(|\delta t|).$$

The vectors  $g_i$  form a local basis, and are tangent to the image of lines in the direction of the coordinate axes under action of the chart function. These are the *covariant basis vectors*.

The contravariant basis vectors  $g^i$  are uniquely defined by the relations

$$g^i \cdot g_j = \delta^i_j,$$

where  $\delta$  denotes the Kronecker delta symbol (regardless of the position of its indices). In general, a vector (or tensor) field expressed in terms of the contravariant basis vectors uses functions with lower indices, called the *covariant components*. Likewise, a field expressed in terms of the covariant basis vectors uses functions with upper indices, called the *contravariant components*. When a vector field is expressed in terms of either set of these components, one must know how the basis vectors depend on the coordinates in order to reconstruct the field: without this information, the component functions are meaningless.

Consider the relation between these two bases. Since the  $g_i$  form a basis, each  $g^i$  may be written a priori as a linear combination of the  $g_j$ :

$$g^i = g^{ij}g_j.$$

Now, dot both sides with  $g_k$  to see that

$$\delta_k^i = g^{ij} g_j \cdot g_k = g^{ij} g_{jk}.$$

Therefore, the entries of the 3 by 3 matrices  $(g_{ij}), (g^{ij})$  satisfy

$$(g_{ij}) = (g^{ij})^{-1}$$

These can be used to raise and lower indices:

$$g_i = g_{ij}g^j$$
$$g^i = g^{ij}g_j.$$

To the end of computing lengths, note that

$$|\Phi(x+\delta x) - \Phi(x)|^2 = \delta x^T [(\nabla \Phi)^T (\nabla \Phi)] \delta x + o(||\delta x||^2).$$

It is natural to define the first fundamental form (or metric tensor) through its covariant components by

$$g_{ij} \equiv g_i \cdot g_j.$$

The role of the first fundamental form in converting lengths and volumes is quite clear. For completeness, the formula for converting areas (see e.g. [45]) is also stated:

$$d\hat{l} = \sqrt{\delta x^i g_{ij} \delta x^j}$$
$$d\hat{\Gamma} = \sqrt{g} \sqrt{n_i g^{ij} n_j} d\Gamma$$
$$d\hat{x} = \sqrt{g} dx,$$

where  $g \equiv \det(g_{ij})$ , and the  $n_i$  are components of the unit normal vector.

## 3.1.3 Differential Geometry of Surfaces

Let  $\Omega_0 \subset \mathbb{R}^2$ , and let  $\mathcal{E}^3$  be as before. Consider a chart function  $\phi : \Omega_0 \to \mathcal{E}^3$ . If  $\phi$  is differentiable and the function  $\nabla \phi$  is full-rank, then  $\phi$  is called an *immersion*.

Motivated by the three-dimensional case, the *covariant basis vectors* are defined by

$$a_{\alpha} = \partial_{\alpha} \phi.$$

Again, these basis vectors are tangent to the coordinate directions. The  $a_{\alpha}$  form a basis for the tangent plane to the middle surface  $\phi(\Omega_0) \subset \mathcal{E}^3$ .



Figure 3.2: The chart function  $\phi$  maps a point  $x \in \Omega_0 \subset \mathbb{R}^2$  to a vector  $\hat{x} \in \mathcal{E}^3$ .

Likewise, the change of metric tensor or first fundamental form is defined

$$a_{\alpha\beta} = a_{\alpha} \cdot a_{\beta}.$$

Its role in converting lengths and areas is reminiscent of the role of  $g_{ij}$ :

$$d\hat{l} = \sqrt{\delta x^{\alpha} a_{\alpha\beta} \delta x^{\beta}}$$
$$d\hat{x} = \sqrt{a} dx$$
$$a = \det((a_{\alpha\beta})).$$

The contravariant basis vectors are given by the relations

$$a_{\alpha} \cdot a^{\beta} = \delta_{\alpha}^{\beta}.$$

Again, this is largely analogous to the three-dimensional case:

$$a^{\alpha} = a^{\alpha\beta} a_{\beta}$$
$$a_{\alpha} = a_{\alpha\beta} a^{\beta}.$$

The unit normal vector, given by

$$a_3 = \frac{a_1 \times a_2}{\|a_1 \times a_2\|},$$

is used to represent out-of-plane vector fields.

In the next section, the shell model is derived. Relations between the surface and three-dimensional differential geometry will be essential in the derivation of the Naghdi shell model, in which the thin dimension is integrated away by use of a kinematic assumption.

## 3.2 The Naghdi Elastic Shell Model

This section begins by presenting the basic assumptions of the Naghdi model, and deriving the corresponding bilinear forms, following the model of [25], which is a straightforward reinterpretation of the classical Naghdi model (e.g., [39]). The advantages of this newer approach (similar in spirit to the work of [107, 23]) are several:

- It allows the chart function φ to be in W<sup>2,∞</sup>(Ω<sub>0</sub>) instead of C<sup>3</sup>(Ω<sub>0</sub>), and hence is amenable to the definition of surfaces based on CAD patches ([55]) which may have discontinuous curvatures.
- The presentation is simpler and does not require differential geometric concepts such as covariant derivatives and the second fundamental form.
- It is better suited to finite element implementation than the classical method: in fact, much of [39, Ch. 6] is devoted to going "back" from the classical assumptions to something like the "new" approach in order to prepare for finite element implementation.

Next, convergence theory is given for discretizations of this model. In theory, the discretization error can be made as small as desired by choosing a sufficiently refined mesh. However in practice for a given shell profile, as the shell thickness decreases, the behavior gets worse to the point of making this approach useless for general shell problems.

#### 3.2.1 Derivation

The assumptions made in the Naghdi model are as follows:

For shell models, the surface chart function φ : Ω<sub>0</sub> → E<sup>3</sup> defines the middle surface. The entire shell is then the image of the set

$$\Omega \equiv \{x = (x_1, x_2, x_3) \in \mathbb{R}^3 : (x_1, x_2) \in \Omega_0 \text{ and } |x_3| < t(x_1, x_2)/2\},\$$


Figure 3.3: Naghdi shell geometry: the three-dimensional chart function  $\Phi$  is constructed from the two-dimensional chart  $\phi$ , and the thickness function t.

under the mapping

$$\Phi(x_1, x_2, x_3) \equiv \phi(x_1, x_2) + x_3 a_3, \qquad (3.2.1)$$

where the thickness t of the shell once again lies in the set  $\mathcal{T}$ , as in problem 2.2.16.

Three-dimensional curvilinear coordinates for the region  $\hat{\Omega}$  are thus effected from the two-dimensional coordinate system on the middle surface plus the thickness, obtaining a bona fide system of three-dimensional curvilinear coordinates: it is only when approximations relying on the fact that the shell is thin are desired that the special structure of the chart function  $\Phi$  is needed. It is shown in [45, Thm. 4.1-1] that if  $\phi$  is an immersion and t is sufficiently small, then  $\Phi$  is also an immersion.

The covariant basis vectors are:

$$g_{\alpha} = \partial_{\alpha}(\phi + x_{3}a_{3})$$

$$= a_{\alpha} + x_{3}\partial_{\alpha}a_{3} \qquad (3.2.2a)$$

$$= (\delta_{\alpha}^{\nu} - x_{3}b_{\alpha}^{\nu})a_{\nu}.$$

$$g_{3} = a_{3}. \qquad (3.2.2b)$$

The vectors  $g_{\alpha}$  and  $a_{\alpha}$  coincide on the middle surface, but generally (if the middle surface is curved) in following the  $x_3$  coordinate direction (normal to

the middle surface),  $g_{\alpha}$  differs from  $a_{\alpha}$ . The symbols  $b_{\alpha}^{\nu}$  are mixed components of the second fundamental form, related to the curvature of the middle surface, and discussed in §3.4.2.

• The displacement field satisfies the Reissner-Mindlin kinematic assumption, i.e., the displacement field u of the shell is given by

$$u(x_1, x_2, x_3) = z(x_1, x_2) + x_3 \theta(x_1, x_2).$$
(3.2.3)

The displacement u is composed of the displacement  $z : \Omega_0 \to \mathcal{E}^3$  of the middle surface plus a first-order rotation  $\theta : \Omega_0 \to \mathcal{E}^3, \theta \cdot a_3 = 0$ . This means that material lines normal to the undeformed mid-surface can translate and make a first order rotation in the direction given by  $\theta$ .

- Stress is planar, i.e.,  $\sigma_{33} = 0$  (no force in the normal direction across the middle surface). This simplifies the elastic relationships somewhat.
- The linear strain-displacement relations will include powers of  $x_3$ , the thickness coordinate. These expansions will be truncated to first order.
- The material is homogeneous and isotropic. In this section, the Young modulus E and the Poisson ratio  $\nu$  are used instead of the Lamé parameters  $L_1, L_2$  (usually denoted  $\lambda, \mu$ , but these letters have already been used for tensor indices), which are related to each other as follows:

$$L_{1} = \frac{E\nu}{(1+\nu)(1-2\nu)}$$
$$L_{2} = \frac{E}{2(1+\nu)}.$$

One can allow for more general elastic constitutive relations (say those of an orthotropic material) by specifying more elastic constants than the two required for an isotropic material. This complicates the integration of the assumed displacement form across the thickness, as the material axes of symmetry do not generally align with the vectors  $g_i$ .

In the following, the stress-strain relationship  $\sigma = H : e$  is considered using the basis  $\{g_i\}$ , so that

$$\sigma = \sigma^{ij} g_i g_j$$
$$H = H^{ijkl} g_i g_j g_k g_l$$
$$e = e^{ij} g_i g_j.$$

Due to the form of the transformation  $\Phi$ , the first fundamental form  $g^{ij}$  obeys

$$g^{\alpha 3} = g^{3\alpha} = 0$$
$$g^{33} = 1.$$

Therefore, through (3.4.8),

$$H^{333\alpha} = H^{3\alpha\beta\lambda} = 0,$$

and so the strains are

$$\sigma^{\alpha\beta} = H^{\alpha\beta\lambda\mu}e_{\lambda\mu} + H^{\alpha\beta33}e_{33}$$
$$\sigma^{\alpha3} = 2H^{\alpha3\beta3}e_{\beta3}$$
$$\sigma^{33} = H^{33\alpha\beta}e_{\alpha\beta} + H^{3333}e_{33}.$$

The mechanical assumption  $\sigma^{33} = 0$  implies that

$$e_{33} = -\frac{H^{33\alpha\beta}}{H^{3333}}e_{\alpha\beta}.$$

Plugging  $e_{33}$  back in yields

$$\sigma^{\alpha\beta} = C^{\alpha\beta\lambda\mu} e_{\lambda\mu}$$
$$\sigma^{\alpha3} = \frac{1}{2} D^{\alpha\lambda} e_{\lambda3},$$

where the constitutive tensors C, D are given by

$$C^{\alpha\beta\lambda\mu} = H^{\alpha\beta\lambda\mu} - \frac{H^{\alpha\beta33}H^{\lambda\mu33}}{H^{3333}}$$
$$= \frac{E}{2(1+\nu)} \left( g^{\alpha\lambda}g^{\beta\mu} + g^{\alpha\mu}g^{\beta\lambda} + \frac{2\nu}{1-\nu}g^{\alpha\beta}g^{\lambda\nu} \right)$$
$$D^{\alpha\lambda} = 4H^{\alpha3\lambda3} = \frac{2E}{1+\nu}g^{\alpha\lambda}.$$

Thus, the strain energy is written

$$\frac{1}{2} \int_{\Omega} \left( C^{\alpha\beta\lambda\mu} e_{\alpha\beta}(u) e_{\lambda\mu}(u) + D^{\alpha\lambda} e_{\alpha3}(u) e_{\lambda3}(u) \right) \sqrt{g} \, dx, \qquad (3.2.4)$$

It is worthwhile to note that the Naghdi kinematic assumption implies that  $e_{33} = 0$ , which does not fit with the assumptions made above. See [100] for discussion of this issue.

It is necessary to expand the strain terms appearing in (3.2.4). To simplify the presentation, discussion of the relation between these contravariant tensor components and the standard Cartesian ones is deferred to §3.4.3; the spirit and appearance is none the less very much similar to the derivation of the Reissner-Mindlin plate model in §2.2. The strain tensor is

$$\hat{e}_{ij}\hat{e}^i\hat{e}^j = e_{ij}g^ig^j,$$

with the standard Cartesian components

$$\hat{e}_{ij} = \frac{1}{2}(\hat{\partial}_j \hat{u}_i + \hat{\partial}_i \hat{u}_j),$$

and so the covariant components are (cf. (3.4.9))

$$e_{kl} = \frac{1}{2} (\hat{\partial}_j \hat{u}_i + \hat{\partial}_i \hat{u}_j) [\hat{e}^i \cdot g_k] [\hat{e}^j \cdot g_l]$$
  
$$= \frac{1}{2} (\hat{\partial}_j \hat{u} \cdot g_k [\hat{e}^j \cdot g_l] + \hat{\partial}_i \hat{u} \cdot g_l [\hat{e}^i \cdot g_k])$$
  
$$= \frac{1}{2} (\partial_l u \cdot g_k + \partial_k u \cdot g_l). \qquad (3.2.5)$$

In the above derivation, the chain rule (3.4.2) was used to convert from derivatives  $\hat{\partial}$ in  $\mathcal{E}^3$  to derivatives  $\partial$  in  $\Omega$ . Therefore, using (3.2.2), the strain terms in (3.2.4) can be written

$$\begin{split} e_{\alpha\beta}(u) &= \frac{1}{2} (g_{\alpha} \cdot \partial_{\beta} u + g_{\beta} \cdot \partial_{\alpha} u) \\ &= \frac{1}{2} (a_{\alpha} \cdot (\partial_{\beta} z + x_{3} \partial_{\beta} \theta) + a_{\beta} \cdot (\partial_{\alpha} z + x_{3} \partial_{\alpha} \theta) + \\ & x_{3} \partial_{\alpha} a_{3} \cdot (\partial_{\beta} z + x_{3} \partial_{\beta} \theta) + x_{3} \partial_{\beta} a_{3} (\partial_{\alpha} z + x_{3} \partial_{\alpha} \theta)) \\ &= \frac{1}{2} (a_{\alpha} \cdot \partial_{\beta} z + a_{\beta} \cdot \partial_{\alpha} z) + x_{3} \frac{1}{2} (a_{\alpha} \cdot \partial_{\beta} \theta + a_{\beta} \cdot \partial_{\alpha} \theta + \partial_{\alpha} a_{3} \cdot \partial_{\beta} z + \partial_{\beta} a_{3} \cdot \partial_{\alpha} z) + \\ &\equiv \gamma_{\alpha\beta}(z) \qquad \qquad \equiv \chi_{\alpha\beta}(\theta, z) \\ & x_{3}^{2} \frac{1}{2} (\partial_{\alpha} a_{3} \cdot \partial_{\beta} \theta + \partial_{\beta} a_{3} \cdot \partial_{\alpha} \theta), \\ &\equiv \kappa_{\alpha\beta}(\theta) \\ e_{\alpha3}(u) &= \frac{1}{2} (a_{\alpha} \cdot \theta + a_{3} \cdot (\partial_{\alpha} z + x_{3} \partial_{\alpha} \theta) + \partial_{\alpha} a_{3} \cdot \theta) \\ &= \frac{1}{2} (a_{\alpha} \cdot \theta + a_{3} \cdot \partial_{\alpha} z) + \frac{1}{2} x_{3} \underbrace{(a_{3} \cdot \partial_{\alpha} \theta + \partial_{\alpha} a_{3} \cdot \theta)}_{= \partial_{\alpha}(a_{3} \cdot \theta) = 0} \end{split}$$

Thus with the above definitions, the strains can be written

$$e_{\alpha\beta}(u) = \gamma_{\alpha\beta}(z) + x_3\chi_{\alpha\beta}(\theta, z) + x_3^2\kappa_{\alpha\beta}(\theta)$$
$$e_{\alpha3}(u) = \zeta_{\alpha}(\theta, z).$$

Per the assumptions of the Naghdi model, the term  $\kappa_{\alpha\beta}$  is neglected. Upon plugging in the strain-displacement relations and integrating over  $x_3 \in [-t/2, t/2]$ , the Naghdi strain energy takes the form (cf. (3.4.10))

$$\frac{1}{2} \int_{\Omega_0} \left( \tilde{C}^{\alpha\beta\lambda\mu} \left[ t\gamma_{\alpha\beta}(z)\gamma_{\lambda\mu}(z) + \frac{t^3}{12}\chi_{\alpha\beta}(\theta,z)\chi_{\lambda\mu}(\theta,z) \right] + t\tilde{D}^{\lambda\mu}\zeta_{\lambda}(\theta,z)\zeta_{\mu}(\theta,z) \right) \sqrt{a} \, dx.$$
(3.2.6)

where  $C^{\alpha\beta\lambda\mu}$  is approximated by

$$\tilde{C}^{\alpha\beta\lambda\mu} = \frac{E}{2(1+\nu)} (a^{\alpha\lambda}a^{\beta\mu} + a^{\alpha\mu}a^{\beta\lambda} + \frac{2\nu}{1-2\nu}a^{\alpha\beta}a^{\lambda\mu}),$$

and analogously,

$$\tilde{D}^{\lambda\mu} = \frac{Ea^{\lambda\mu}}{2(1+\nu)}.$$

The approximate constitutive relations (with the tildes) use  $a^{\alpha\beta}$  instead of  $g^{\alpha\beta}$ . These are approximately equal as the thickness of the shell becomes small.

Problem 2 [(The Naghdi Problem)]

Let  $\phi \in W^{2,\infty}(\Omega_0)^3$ , and

$$t \in \mathcal{T} \equiv \left\{ t \in L^{\infty}(\Omega_0) : t(x) \ge t_{\min} \text{ for a.e. } x \in \overline{\Omega_0} \right\}$$

with  $t_{\min} > 0$  a given constant. The Naghdi problem is to find  $U = (\theta, z)$  in

$$\mathcal{U} = \left\{ (\theta, z) \in H^1(\Omega_0)^3 \times H^1(\Omega_0)^3 : \theta \cdot a_3 = 0 \text{ almost everywhere} \right\} \cap \mathcal{BC},$$

such that for all  $V = (\eta, y)$  in  $\mathcal{U}$ ,

$$K(\theta, z; \eta, y) \equiv \int_{\Omega_0} \left( \tilde{C}^{\alpha\beta\lambda\mu} \left[ t\gamma_{\alpha\beta}(z)\gamma_{\lambda\mu}(y) + \frac{t^3}{12}\chi_{\alpha\beta}(\theta, z)\chi_{\lambda\mu}(\eta, y) \right] + t\tilde{D}^{\lambda\mu}\zeta_{\lambda}(\theta, z)\zeta_{\mu}(\eta, y) \right) \sqrt{a} \, dx = F(V)$$
(3.2.7)

The loading is represented by  $F \in \mathcal{U}'$ .  $\mathcal{BC}$  incorporates boundary conditions that prohibit rigid body motions, i.e., those  $U \neq 0 \in \mathcal{U}$  such that K(U, U) = 0.

Later, the inertial term

$$\int_{\Omega} \rho u(x) \cdot v(x) \, dx$$

will also be needed. Under the Naghdi kinematic assumption (3.2.3), it becomes (assuming  $\rho$  is independent of  $x_3$ )

$$M(\theta, z; \eta, y) \equiv \int_{\Omega_0} \rho\left(tz \cdot y + \frac{t^3}{12}\theta \cdot \eta\right) \sqrt{a} \, dx. \tag{3.2.8}$$

Finite element discretization of problem 2 is discussed in §B.1.

# 3.3 Asymptotic Behavior of Naghdi's Model

To understand why the non-uniform convergence (or locking) described in the previous section occurs, it is necessary to study the asymptotic behavior of Naghdi's model. The first step in this direction is to remove the scaling of the thickness profile, t, from the Naghdi bilinear form (3.2.7). It contains a piece proportional to t (the membrane strain energy, composed of transverse shear and stretching of the membrane) and a piece proportional to  $t^3$  (the bending strain energy).

Recall that  $t \in \mathcal{T}$  is uniformly bounded away from 0, so that

$$t_m = \inf_{x \in \overline{\Omega_0}} t(x) \ge t_{\min},$$

and let the number  $\epsilon$  be given by

$$\epsilon = t_m/L,$$

with L some characteristic length of the shell. Then the scaled thickness  $\tilde{t}$  can be defined by

$$\tilde{t} = \frac{t}{t_m} L$$

Equation (3.2.7) can thus be rearranged into

$$K(U,V) = \epsilon^3 K_b(U,V) + \epsilon K_m(U,V) = F(V),$$

where

$$K_m(U,V) = \int_{\Omega_0} \tilde{t} \left\{ \tilde{C}^{\alpha\beta\lambda\mu}\gamma_{\alpha\beta}(z)\gamma_{\lambda\mu}(y) + \tilde{D}^{\lambda\mu}\zeta_{\lambda}(\theta,z)\zeta_{\mu}(\eta,y) \right\} \sqrt{a} \, dx,$$
  
$$K_b(U,V) = \int_{\Omega_0} \frac{\tilde{t}^3}{12} \left\{ \tilde{C}^{\alpha\beta\lambda\mu}\chi_{\alpha\beta}(\theta,z)\chi_{\lambda\mu}(\eta,y) \right\} \sqrt{a} \, dx.$$

 $K_m$  and  $K_b$  are so named because of their respective associations with membrane stretching and bending energy.

Study of the solutions of this problem in the limiting case of  $\epsilon \to 0$  is essential to understanding the practical difficulties encountered with shell finite elements. In this limit, t is no longer assumed to belong to  $\mathcal{T}$  for a fixed  $t_{\min}$ , but for each  $\epsilon$ , t is uniformly bounded away from 0. **Theorem 3.3.1 ((Properties of**  $K_b, K_m$ )) Under the assumptions of Problem 2, The bilinear forms  $K_b$  and  $K_m$  are independent of  $\epsilon$ . K is bounded and coercive in the  $\mathcal{U}$ -norm.

**Proof:** Constant scaling of t does not change  $\tilde{t}$ , and has no effect on any of the other terms in  $K_b$  and  $K_m$ . The rest of the proof is very much like that of lemmas 2.3.2 and 2.3.5 for the plate equations. For specific differences in the classical formulation, see e.g., [39, Prop. 4.3.1,4.3.2]. The extension to  $W^{2,\infty}$  charts (with the strain tensors defined as in §3.2.1) is handled in [25].

Much like (2.2.16), (3.2.7) has a unique solution, and standard finite element discretizations yield error estimates optimal with respect to the approximation capabilities of the finite element spaces (see §2.4.1). However, these discretizations also suffer from the so-called locking phenomenon. In practice, what can happen is that as  $\epsilon$  gets small, the *h*-refinement required to achieve any reasonable level of error is so extreme as to make finite element solution of Naghdi's model impractical, i.e., the convergence is non-uniform in the parameter  $\epsilon$ . There is more subtlety here than for the plate equations.

To study the asymptotic behavior of Naghdi's model, one considers the contents of

$$\mathcal{U}_0 = \{ U \in \mathcal{U} \mid K_m(U, U) = 0 \},\$$

the space of pure bending displacements (since the membrane portion  $K_m$  of the bilinear form is not active). The contents of  $\mathcal{U}_0$  are determined by the geometry of the shell structure, and the boundary conditions.

Allowing  $\epsilon$  to vary, one obtains from problem 2 the following scaled problem: find  $U^{\epsilon} = (\theta^{\epsilon}, z^{\epsilon})$  in

$$\mathcal{U} = \left\{ (\theta, z) \in H^1(\Omega_0)^3 \times H^1(\Omega_0)^3 : \theta \cdot a_3 = 0 \text{ almost everywhere} \right\} \cap \mathcal{BC},$$

such that for all  $V = (\eta, y) \in \mathcal{U}$ ,

$$A(U^{\epsilon}, V) = \epsilon^{3} K_{b}(U^{\epsilon}, V) + \epsilon K_{m}(U^{\epsilon}, V) = F^{\epsilon}(V).$$
(3.3.1)

In order for this problem to be well-posed as  $\epsilon \to 0$ , the forcing  $F^{\epsilon}$  must be of the form

$$F^{\epsilon}(V) = \epsilon^{\rho} G(V),$$

for some real number  $\rho$  and some  $G \in \mathcal{U}'$  independent of  $\epsilon$ . The choice of  $\rho$  determines the nature of (3.3.1), and in fact, whether it has a solution at all. While some more technical details of asymptotically admissible loadings are omitted in the following discussion, it still serves to describe the essential difficulties involved in creating robust shell finite elements, as the two extreme cases are considered.

### 3.3.1 The Membrane-Dominated Case

Suppose that the subspace of pure bending displacements  $\mathcal{U}_0 = \{0\}$ , so that every deformation activates the membrane term. Then if  $\rho=1$ , one would expect that as  $\epsilon \to 0$ , the energy will be dominated by the  $O(\epsilon)$  membrane term. The stiffness of the shell structure is said to be of order  $\epsilon$  in this case.

When  $\mathcal{U}_0 = \{0\}$ , the membrane energy norm can be defined via

$$||U||_m = \sqrt{K_m(U, U)},$$

and find  $U^m \in \mathcal{U}_m$  such that

$$K_m(U^m, V) = G(V), \,\forall V \in \mathcal{U}_m, \tag{3.3.2}$$

where  $\mathcal{U}_m$  is the completion of  $\mathcal{U}$  with respect to  $\|\cdot\|_m$ .

 $\mathcal{U}_m$  is complete with respect to  $\|\cdot\|_m$ , and therefore by the Lax-Milgram theorem, (3.3.2) has a unique solution provided that  $G \in \mathcal{U}'_m$ . This last requirement seems somewhat technical; provided that the loading is nice in this sense (meaning that the structure can control displacements excited by the loading without resorting to bending), (3.3.1) is called membrane-dominated, and  $\rho = 1$  (see [39, Prop. 5.1.3]. Otherwise it is an ill-posed membrane problem (this situation prevails in the case of the Scordelis-Lo roof), and it is possible to show that  $1 < \rho < 3$ , if a solution exists at all.

In membrane-dominated problems, conforming finite elements usually work reasonably well - in fact, there is theory giving (in a slightly weakened sense)  $\epsilon$ -uniform convergence [39, Prop. 7.3.1].

## 3.3.2 The Bending-Dominated Case

The trouble begins in the bending-dominated case, when  $\mathcal{U}_0 \neq \{0\}$ , i.e., there are displacements which do not activate the membrane term. Then, one would expect that with  $\rho = 3$ , as  $\epsilon \to 0$ , equation (3.3.1) can be solved by choosing  $U \in \mathcal{U}_0$ , so as to make the energy look like  $\epsilon^3$ , as in the bending term. In this case, the stiffness of the shell is said to be of order  $\epsilon^3$ .

When  $\mathcal{U}_0 \neq \{0\}$ , the following problem must be considered: find  $U^0 \in \mathcal{U}_0$  such that

$$K_b(U^0, V) = G(V), \,\forall V \in \mathcal{U}_0.$$

$$(3.3.3)$$

Due to theorem 3.3.1,  $K_b$  is coercive on  $\mathcal{U}_0$ , and therefore this problem has a unique solution.

Provided that there exists  $V \in \mathcal{U}_0$  such that  $G(V) \neq 0$ , i.e., that the loading activates some bending mode of the structure, then this is called a bending-dominated problem, and for  $F^{\epsilon}$  to provide an asymptotically admissible loading,  $\rho = 3$  must hold.

It is the bending-dominated case where conforming finite element methods for Naghdi's model usually exhibit shear locking, characterized by ever-worse requirements on the mesh size to achieve a given level of accuracy as the thickness decreases.

### 3.3.3 Numerical Locking

Recall that in the case of the Reissner-Mindlin plate, as the thickness tended towards 0, the solution would approach the solution of the Kirchhoff limit problem (2.4.3), in the space of vanishing shear strains

$$\{U = (\theta, z) \in \mathcal{U} : \nabla z = \theta\}$$

For shells,  $\mathcal{U}_0$  is the analog of this space. The situation is in fact much worse than with plates. The trick of using the Helmholtz decomposition to set up a stable problem no longer works. Consider a discretization of (3.3.3) using the finite element space  $\mathcal{U}_h \subset \mathcal{U}$ . The solution of this problem is no longer in  $\mathcal{U}_0$ , but in  $\mathcal{U}_0 \cap \mathcal{U}_h$ . So  $\mathcal{U}_h$  should be "rich" in  $\mathcal{U}_0$ . However, [39, Prop. 7.3.2] shows that in general for shells, if  $\mathcal{U}_h$  is a space of piecewise polynomial functions, not only does  $\mathcal{U}_h$  fail to be rich in  $\mathcal{U}_0$ , in fact

$$\mathcal{U}_0 \cap \mathcal{U}_h = \{0\}.$$

This means that as the shell gets thinner and the solution  $U^{\epsilon}$  approaches  $U^{0}$ , the finite element solution approaches the zero function! In effect, the finite element procedure increasingly over-estimates the stiffness of shell structure in the bending-dominated case.

MITC shell elements are built analogously to the plate elements. When written in a mixed formulation, there is no theory guaranteeing that the inf – sup condition necessary for  $\epsilon$ -uniform convergence will be satisfied. However, numerical tests have been done, involving the solution of an eigenvalue problem over a variety of meshes that approximates the inf – sup constant in [15]. So in practice, it appears that the MITC shell elements ([87]) work quite well.

## 3.4 The Classical Formulation

The Naghdi model, as formulated in §3.2.1, represents the constitutive tensors  $C^{\alpha\beta\lambda\mu}$ ,  $D^{\alpha\lambda}$  via their contravariant components, and the strain tensor  $e_{ij}(u)$  via its covariant

components, using the curvilinear coordinate system described in §3.1.2,3.1.3. The kinematic assumption (3.2.3) then allows the 3d strain tensor  $e_{ij}(u)$  to be expressed in terms of tensors  $\gamma(z), \chi(\theta, z), \zeta(\theta, z)$ . But the mid-surface displacement z and the rotation vector  $\theta$  are each expressed via Cartesian components. In the classical formulation, they are instead expressed via their covariant components, as  $z = z_i a^i$ ,  $\theta = \theta_{\alpha} a^{\alpha}$ . This means that the condition  $\theta \cdot a_3 = 0$  is automatically satisfied and does not need to be built into the variational space, and that  $\theta$  now has two components instead of three. In order to do this, further tools of differential geometry are required; in fact, some of these were hidden so as to simplify the presentation of §3.2.1.

### 3.4.1 Covariant Differentiation

In order to calculate the components of the strain tensor, it is necessary to differentiate the Euclidean components of the displacement field, i.e. compute things like

$$\hat{\partial}_j \hat{v}_i(\hat{x}_k \hat{e}^k),$$

in terms of the covariant or contravariant basis vectors. In the above,  $\hat{\partial}_j$  denotes differentiation with respect to  $\hat{x}_j$ , and

$$\hat{x} = \hat{x}_k \hat{e}^k.$$

First, relations between the components of a vector field v in the Euclidean and contravariant bases must be determined. Note that

$$v(x) = v_i(x)g^i(x) = \hat{v}_i(\hat{x})\hat{e}^i.$$

By dotting both sides with the right things, the following relations are obtained:

$$v_j(x) = (v_i(x)g^i(x)) \cdot g_j(x) = \hat{v}_i(\hat{x})\hat{e}^i \cdot g_j(x)$$
$$\hat{v}_i(\hat{x}) = (\hat{v}_j(\hat{x})\hat{e}^j) \cdot \hat{e}_i = v_j(x)g^j(x) \cdot \hat{e}_i.$$

By defining the symbols

$$[g^k]_i \equiv g^k \cdot \hat{e}_i$$
$$[g_k]^i \equiv g_k \cdot \hat{e}^i,$$

these may be more succinctly written as

$$v_j(x) = \hat{v}_i(\hat{x})[g_j]^i$$
$$\hat{v}_i(\hat{x}) = v_j(x)[g^j]_i.$$

Application of the chain rule to  $\Phi^{-1}(\Phi(x)) = x$  shows that

$$\nabla \Phi^{-1}(\Phi(x)) = \hat{\nabla}(\Phi^{-1})(\hat{x}) \cdot \nabla \Phi(x) = I.$$
(3.4.1)

This implies that the rows of the matrix  $\hat{\nabla}(\Phi^{-1})$  are given by the components of the vectors  $g^i$ . Therefore, the chain rule can be written:

$$\hat{\partial}_j w(\Phi^{-1}(\hat{x})) = \partial_l w(x) [g^l(x)]_j.$$
 (3.4.2)

The other needed piece of information is how to differentiate the symbols  $[g^i]_j$ . Since the vectors  $g^i$  are a basis, assume a priori that

$$\partial_l g^q = -\Gamma^q_{lk} g^k.$$

Therefore

$$\Gamma^{q}_{lk} = \Gamma^{q}_{lm} \delta^{m}_{k} = \Gamma^{q}_{lm} g^{m} \cdot g_{k}$$
$$= -\partial_{l} g^{q} \cdot g_{k}, \qquad (3.4.3)$$

and

$$\partial_l [g^q]_i = -\Gamma^q_{lk} [g^k]_i.$$

Armed with these facts, the calculation begins.

$$\begin{split} \hat{\partial}_{j} \hat{v}_{i} \left( \hat{x} \right) &= \hat{\partial}_{j} \left( v_{k}(x) [g^{k}]_{i} \right) \\ &= \hat{\partial}_{j} \left( v_{k}(\Phi^{-1}(\hat{x})) [g^{k}]_{i} \right) \\ &= (\hat{\partial}_{j} v_{k}) (\Phi^{-1}(\hat{x})) [g^{k}]_{i} + v_{q}(x) \hat{\partial}_{j} [g^{q}(\Phi^{-1}(\hat{x}))]_{i}. \end{split}$$

Applying them yields

$$= \partial_l v_k(x) [g^k]_i [g^l]_j + v_q(x) \left(\partial_l [g^q]_i\right) [g^l]_j$$
$$= \left(\partial_l v_k(x) - \Gamma^q_{lk} v_q(x)\right) [g^k]_i [g^l]_j.$$

The covariant derivatives  $v_{i||j}$  are thus defined by

$$v_{i||j} = \partial_j v_i - \Gamma^p_{ij} v_p, \qquad (3.4.4)$$

so that

$$\hat{\partial}_j \hat{v}_i \left( \hat{x} \right) = v_{k||l} [g^k]_i [g^l]_j.$$
(3.4.5)

The symbols  $v_{i||j}$  may equivalently be defined by

$$\partial_j(v_i g^i) = v_{i||j} g^i. \tag{3.4.6}$$

## 3.4.2 Covariant Derivatives on Surfaces

Now consider differentiation of the vector field  $\eta = \eta_i a^i$ . Note that this is analogous to the other way the three-dimensional covariant derivatives (cf. equation 3.4.6) can be defined. The derivatives  $\partial_{\alpha} a^i$  must be computed. These will come out in application of the chain rule to the vector field  $\eta$ . These are given by

$$\partial_{\alpha}a^{3} = (\partial_{\alpha}a^{3} \cdot a_{\beta})a^{\beta} \equiv -b_{\alpha\beta}a^{\beta}$$
$$\partial_{\alpha}a^{\beta} = (\partial_{\alpha}a^{\beta} \cdot a_{\sigma})a^{\sigma} + (\partial_{\alpha}a^{\beta} \cdot a_{3})a^{3} \equiv -C^{\beta}_{\alpha\sigma}a^{\sigma} + b^{\beta}_{\alpha}a^{3},$$

wherein the surface Christoffel symbols  $C^{\alpha}_{\beta\gamma}$  have been defined, and the surface curvature tensor or second fundamental form  $b_{\alpha\beta}$ , by its covariant components. To obtain the above, vector fields must be represented by their components, e.g. for a vector field v,

$$v = (v \cdot a_i)a^i = (v \cdot a^i)a_i.$$

In the above, the same thing is done with the components of vector fields like  $\partial_{\alpha}a^{\beta}$ .

Thus, the surface covariant derivatives are defined

$$\eta_{\beta|\alpha} = \partial_{\alpha}\eta_{\beta} - C^{\sigma}_{\alpha\beta}\eta_{\sigma}$$
$$\eta_{3|\alpha} = \partial_{\alpha}\eta_{3},$$

so that

$$\partial_{\alpha}(\eta_i a^i) = (\eta_{\beta|\alpha} - b_{\alpha\beta}\eta_3)a^{\beta} + (\eta_{3|\alpha} + b^{\beta}_{\alpha}\eta_{\beta})a^3.$$
(3.4.7)

There is an important difference between this and the simpler relation which holds in the three-dimensional case: compare (3.4.6) with (3.4.7). Even if the vector field  $\eta$  is always locally in the tangent plane to the surface  $\phi(\Omega_0)$ , i.e.,  $\eta_3 = 0$  everywhere, the derivative still has an out-of-plane component if there is non-zero curvature of the surface.

#### 3.4.3 Linear Elasticity in Curvilinear Coordinates

Consider now the elastic weak form (2.2.1) in Cartesian coordinates over the reference domain  $\Omega$ . To do this, the strain tensor and constitutive relations must be rewritten in terms of the reference coordinates. The following relation on the symbols  $[g^i]_j$  and  $[g_i]^j$  is needed, which again comes from (3.4.1):

$$[g^p]_k [g_p]^i = \delta^i_k.$$

First, the constitutive relations given by the constants  $\hat{H}^{ijkl}$  are considered. The tensor H can be represented as

$$H = \hat{H}^{ijkl} \hat{e}_i \hat{e}_j \hat{e}_k \hat{e}_l = H^{ijkl} g_i g_j g_k g_l$$

Given that  $g_i = [g_i]^j \hat{e}_j$ , so that

$$H = H^{ijkl}[g_i]^m [g_j]^n [g_k]^o [g_l]^p \hat{e}_m \hat{e}_n \hat{e}_o \hat{e}_p.$$

Combining the above,

$$\hat{H}^{mnop} = H^{ijkl}[g_i]^m [g_j]^n [g_k]^o [g_l]^p.$$

For an isotropic material, the Cartesian components of  $\hat{H}$  take the form

$$\hat{H}^{ijkl} = L_1 \delta^{ij} \delta^{kl} + L_2 (\delta^{ik} \delta^{jl} + \delta^{il} \delta^{jk}),$$

where  $L_1, L_2$  are the Lamé parameters characterizing the material. A quick calculation shows that:

$$H^{ijkl} = L_1 g^{ij} g^{kl} + L_2 (g^{ik} g^{jl} + g^{il} g^{jk}).$$
(3.4.8)

Now, return to the strain tensor. With  $\hat{e}^i = \hat{e}_i$ , the tensor  $\hat{e}$  may be represented

$$\hat{e}(\hat{u}(\hat{x})) = \hat{e}_{ij}(\hat{u}(\hat{x}))\hat{e}^i\hat{e}^j = e_{ij}(u(x))g^ig^j = e(u(x)).$$

The formula for covariant differentiation (3.4.5) shows that

$$\hat{e}_{ij} = \frac{1}{2} \left( \hat{\partial}_j \hat{u}_i + \hat{\partial}_i \hat{u}_j \right)$$

can be rewritten as

$$\hat{e}_{ij} = \frac{1}{2} \left( u_{k||l} + u_{l||k} \right) [g^k]_i [g^l]_j.$$

Therefore

$$e_{ij} = \frac{1}{2}(u_{j||i} + u_{i||j}), \qquad (3.4.9)$$

and the above can be put together to rewrite the energy term in (2.2.1) as

$$\int_{\hat{\Omega}} \hat{H}^{ijkl} \hat{e}_{kl}(\hat{u}) \hat{e}_{ij}(\hat{v}) \, d\hat{x} = \int_{\Omega} H^{ijkl} e_{kl}(u) e_{ij}(v) \sqrt{g} \, dx.$$

Other transformations are required to rewrite the forcing terms and boundary conditions, but they shall not be discussed here.

## 3.4.4 Derivation

The kinematic assumption of the classical model differs from (3.2.3) in that  $\theta, z$  are now covariant components, rather than vectors in  $\mathbb{R}^3$ , i.e.,

$$\mathcal{U} = H^1(\Omega_0)^3 \times H^1(\Omega_0)^2 \cap \mathcal{BC},$$

and the kinematic assumption is

$$u(x_1, x_2, x_3) = z_i(x_1, x_2)a^i + x_3\theta_{\alpha}(x_1, x_2)a^{\alpha}.$$

Proceeding once again from (3.2.5) (cf. (3.4.9)) and applying the rules developed in §3.4.2 yields

$$e_{\alpha\beta}(\theta, z) = \gamma_{\alpha\beta}(z) + x_3 \chi_{\alpha\beta}(\theta, z) - x_3^2 \kappa_{\alpha\beta}(\theta),$$
$$e_{\alpha3}(\theta, z) = \zeta_{\alpha}(\theta, z),$$

where

$$\begin{split} \gamma_{\alpha\beta}(z) &= \frac{1}{2} (z_{\alpha|\beta} + z_{\beta|\alpha}) - b_{\alpha\beta} z_3, \\ \chi_{\alpha\beta}(\theta, z) &= \frac{1}{2} (\theta_{\alpha|\beta} + \theta_{\beta|\alpha} - b_{\beta}^{\lambda} z_{\lambda|\alpha} - b_{\alpha}^{\lambda} z_{\lambda|\beta}) + c_{\alpha\beta} z_3, \\ \kappa_{\alpha\beta}(\theta) &= \frac{1}{2} (b_{\beta}^{\lambda} \theta_{\lambda|\alpha} + b_{\alpha}^{\lambda} \theta_{\lambda|\beta}), \\ \zeta_{\alpha}(\theta, z) &= \frac{1}{2} (\theta_{\alpha} + z_{3,\alpha} + b_{\alpha}^{\lambda} z_{\lambda}). \end{split}$$

The third fundamental form  $c_{\alpha\beta}$  is given by

$$c_{\alpha\beta} = b_{\alpha}^{\lambda} b_{\lambda\beta}.$$

As mentioned in the assumptions of the Naghdi model, the term  $\kappa_{\alpha\beta}$  is neglected. Plugging in the strain-displacement relations and integrating over  $x_3 \in [-t/2, t/2]$ , the Naghdi strain energy takes the form

$$\frac{1}{2} \int_{\Omega_0} \left( \tilde{C}^{\alpha\beta\lambda\mu} \left[ t\gamma_{\alpha\beta}(z)\gamma_{\lambda\mu}(z) + \frac{t^3}{12}\chi_{\alpha\beta}(\theta,z)\chi_{\lambda\mu}(\theta,z) \right] + t\tilde{D}^{\lambda\mu}\zeta_{\lambda}(\theta,z)\zeta_{\mu}(\theta,z) \right) \sqrt{a} \, dx.$$
(3.4.10)

The constitutive tensors and the rest of (3.4.10) appear just as in (3.2.6); the difference is in the definition chosen for the strain tensors  $\gamma, \chi, \zeta$ .

## 3.5 Shape Optimization of Naghdi Shells

As is clear from the discussion of finite element methods and locking, the development of shape optimization methods for Naghdi shells is fraught with difficulties. There is significant literature in the engineering community: Bletzinger, Camprubi, et al. solve mechanical shell optimization problems in [24] making use of energy minimization problems related to soap films. Marburg et al. consider optimization of shells coupled to acoustics in [92, 91], with application to design of an automobile dashboard. Since they do not use adjoint equations, and need only a relatively small parameter space to effect the needed sorts of changes to the acoustics, they consider somewhat restrictive parametrizations in [94, 93]; the scheme is further refined in [64]. However in the above papers, the following issues are not fully addressed.

- Locking. Obviously, it should not be expected that a locking finite element formulation should be successful in computing objective function derivatives through the adjoint method. In [36], Bletzinger, Camprubi et al. demonstrate this phenomenon using several simple mechanical optimization problems: due to locking, the shape derivative can even have the wrong sign. They use the so-called DSG elements of [23]. But the spirit of it is still to pick a "good" FEM formulation and hope everything else works out.
- Boundary layers. The optimization problems considered in [36] also serve to demonstrate the importance of resolving boundary layers; this is of course obvious to anyone who routinely solves plate and shell problems.
- Chart function space. In the engineering optimization literature, and even in classical presentations of the Naghdi model, e.g., [39], there is little or no concern paid to the proper space for the chart function φ. Blouza and Le Dret [25] show well-posedness of the Naghdi model (in the vector form as presented in §3.2.1, as opposed to the classical presentation with covariant derivatives

§3.4.4) with  $W^{2,\infty}$  charts. In [55], Le Dret does the some for the Naghdi model with  $G_1$  or "visually  $C^{1}$ " charts, which are related to CAD representations.

• Existence theory. Existence of solutions to shell optimization problems is considered by Sprekels et al. in [7], for a  $C^2$  chart of the form

$$\phi(x_1, x_2) = (x_1, x_2, h(x_1, x_2)),$$

using the generalized Naghdi model of [107]. They do not present numerical results, and do not seem to be aware of the work of Le Dret et al.

I do not address the issues of existence theory and the effect of locking on the computation of derivatives in this thesis, although future work in these directions would be worthwhile. The next section discusses shape differentiation of the Naghdi shell operators, in hopes that with adequate mesh refinement, the derivatives can be computed accurately using MITC elements.

#### 3.5.1 Shape Differentiation of Naghdi Shell Operators

The Naghdi bilinear forms K, M were defined in the usual way in (3.2.7,3.2.8) over the Hilbert space

$$\mathcal{U} = \left\{ (\theta, z) \in H^1(\Omega_0)^3 \times H^1(\Omega_0)^3 : \theta \cdot a_3 = 0 \text{ almost everywhere} \right\} \cap \mathcal{BC}.$$

This is not the right thing to do for shape derivatives, as the condition  $\theta \cdot a_3 = 0$ almost everywhere is incorporated into the space, but depends on the choice of the chart function  $\phi$ . The choice of  $\phi \in W^{2,\infty}(\Omega_0)^3$  allows definition of  $\theta, \eta$  via their covariant components as

$$\theta = \tilde{\theta}_{\alpha} a^{\alpha}, \ \eta = \tilde{\eta}_{\alpha} a^{\alpha}$$

almost everywhere in  $\Omega_0$ . Modified bilinear forms  $\tilde{K}, \tilde{M}$  can then be defined via

$$\begin{split} \tilde{K}(\tilde{\theta}, z; \tilde{\eta}, y) = & K(\tilde{\theta}_{\alpha} a^{\alpha}, z; \tilde{\eta}_{\alpha} a^{\alpha}, y), \\ \tilde{M}(\tilde{\theta}, z; \tilde{\eta}, y) = & M(\tilde{\theta}_{\alpha} a^{\alpha}, z; \tilde{\eta}_{\alpha} a^{\alpha}, y). \end{split}$$

These take the covariant components  $\tilde{\theta}, \tilde{\eta}$ , of  $\theta, \eta$ , and plug them back into the original forms K, M. This is justified since these two representations of the problem are isomorphic [25, Lemma 4.1]; the classical approach requires  $\phi \in C^3(\overline{\Omega}_0)^3$  because it is required by the classical rigid-body lemma: added regularity of the chart is not required just to write down the classical equations.

The shape is given by  $g = (\phi, t) \in \mathcal{G}$ . The shape derivative is written  $D_g$ , with component derivatives  $D_{\phi}$ ,  $D_t$ . The derivatives are stated in the following theorem.

#### Theorem 3.5.1 (Naghdi Shape Derivatives) Assume that the set

$$\mathcal{G} \subset W^{2,\infty}(\Omega_0)^3 \times \left\{ t \in L^{\infty}(\Omega_0) : t(x) \ge t_{\min} \text{ for a.e. } x \in \overline{\Omega_0} \right\}$$

is compact. Then the the bilinear forms  $\tilde{M}$ ,  $\tilde{K}$  are continuously Fréchet differentiable, and the derivatives in the direction  $\delta g = (\delta \phi, \delta t)$  are given by

$$\begin{split} D_{g}\tilde{M}(\tilde{\theta},z;\tilde{\eta},y)\delta g &= \int_{\Omega_{0}} \left( tz \cdot y + \frac{t^{3}}{12}\theta \cdot \eta \right) D_{\phi}\sqrt{a}\delta\phi \, dx + \\ &\int_{\Omega_{0}} \left( \delta tz \cdot y + \delta t \frac{3t^{2}}{12}\theta \cdot \eta \right) \sqrt{a} \, dx + \\ &\int_{\Omega_{0}} \frac{t^{3}}{12} (D_{\phi}\theta \cdot \eta + \theta \cdot D_{\phi}\eta)\delta\phi\sqrt{a} \, dx \\ D_{g}\tilde{K}(\tilde{\theta},z;\tilde{\eta},y)\delta g &= \int_{\Omega_{0}} \left( \tilde{C}^{\alpha\beta\lambda\mu} \left[ t\gamma_{\alpha\beta}(z)\gamma_{\lambda\mu}(y) + \frac{t^{3}}{12}\chi_{\alpha\beta}(\theta,z)\chi_{\lambda\mu}(\eta,y) \right] \\ &+ t\tilde{D}^{\lambda\mu}\zeta_{\lambda}(\theta,z)\zeta_{\mu}(\eta,y) \right) D_{\phi}\sqrt{a}\delta\phi \, dx + \\ &\int_{\Omega_{0}} \left( \tilde{C}^{\alpha\beta\lambda\mu} \left[ \delta t\gamma_{\alpha\beta}(z)\gamma_{\lambda\mu}(y) + \frac{3t^{2}\delta t}{12}\chi_{\alpha\beta}(\theta,z)\chi_{\lambda\mu}(\eta,y) \right] \\ &+ \delta t\tilde{D}^{\lambda\mu}\zeta_{\lambda}(\theta,z)\zeta_{\mu}(\eta,y) \right) \sqrt{a} \, dx + \\ &\int_{\Omega_{0}} \left( D_{\phi}\tilde{C}^{\alpha\beta\lambda\mu} \left[ t\gamma_{\alpha\beta}(z)\gamma_{\lambda\mu}(z) + \frac{t^{3}}{12}\chi_{\alpha\beta}(\theta,z)\chi_{\lambda\mu}(\eta,y) \right] \\ &+ tD_{\phi}\tilde{D}^{\lambda\mu}\zeta_{\lambda}(\theta,z)\zeta_{\mu}(\eta,y) \right) \delta\phi\sqrt{a} \, dx \\ &\int_{\Omega_{0}} \left( \tilde{C}^{\alpha\beta\lambda\mu} \left[ tD_{\phi}(\gamma_{\alpha\beta}(u)\gamma_{\lambda\mu}(v)) + \frac{t^{3}}{12}D_{\phi}(\chi_{\alpha\beta}(\theta,z)\chi_{\lambda\mu}(\eta,y)) \right] \\ &+ t\tilde{D}^{\lambda\mu}D_{\phi}(\zeta_{\lambda}(\theta,z)\zeta_{\mu}(\eta,y)) \right) \delta\phi\sqrt{a} \, dx, \end{split}$$

*i.e.*, the differentiation can be moved inside the integral.

**Proof:** It is necessary to show continuous Fréchet differentiability of the mappings  $\phi \to \sqrt{a}, \phi \to a^{\alpha}$  (appearing through  $\theta, \eta$ ), of  $\phi \to a^{\alpha\beta}$  (appearing through the constitutive tensors), and of  $\phi \to a_i, \phi \to \partial_{\alpha} a_3$  (appearing through the strain tensors). As  $t \to t, t \to t^3$  are continuously Fréchet differentiable with respect to the thickness function, the integrand is continuously Fréchet differentiable with respect to g on the compact set  $\mathcal{G} \times \overline{\Omega_0}$ . This establishes uniform continuity of the integrand, so that integration and differentiation may be interchanged. Most of the following calculations appear again in the discussion of §B.2 on finite element implementation of shell operator shape derivatives.

The mapping

$$\phi \in W^{2,\infty}(\Omega_0)^3 \to a_\alpha \in W^{1,\infty}(\Omega_0)^3$$

of the chart to the tangent basis vectors has Fréchet derivative

$$D_{\phi}a_{\alpha}\delta\phi = \partial_{\alpha}\delta\phi,$$

which can be used to express the derivative of the mapping

$$\phi \in W^{2,\infty}(\Omega_0)^3 \to a_3 \in W^{1,\infty}(\Omega_0)^3$$

of the chart to the normal vector via

$$D_{\phi}a_{3} = \frac{1}{|a_{1} \times a_{2}|} \left( I - a_{3}a_{3}^{T} \right) \left( D_{\phi}a_{1} \times a_{2} + a_{1} \times D_{\phi}a_{2} \right).$$

The mapping

$$\phi \in W^{2,\infty}(\Omega_0)^3 \to a_{\alpha\beta} \in W^{1,\infty}(\Omega_0)$$

of the chart to the covariant components of the metric tensor has Fréchet derivative

$$D_{\phi} \begin{pmatrix} a_{11} \\ a_{12} \\ a_{22} \end{pmatrix} = \begin{pmatrix} 2a_1^T & 0 \\ a_2^T & a_1^T \\ 0 & 2a_2^T \end{pmatrix} D_{\phi} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix},$$

and appears in the computation of the derivatives of  $a^{\alpha\beta}$ ,  $a^{\alpha}$ , and  $\sqrt{a}$ . The Fréchet derivative of the mapping

$$\phi \in W^{2,\infty}(\Omega_0)^3 \to \sqrt{a} \in W^{1,\infty}(\Omega_0)$$

to the change of metric factor is

$$D_{\phi}\sqrt{a} = \frac{1}{2\sqrt{a}}(a_{22}D_{\phi}a_{11} - 2a_{12}D_{\phi}a_{12} + a_{11}D_{\phi}a_{22}).$$

The contravariant components  $a^{\alpha\beta} \in W^{1,\infty}(\Omega)$  have Fréchet derivatives

$$D_{\phi} \begin{pmatrix} a^{11} \\ a^{12} \\ a^{22} \end{pmatrix} = \begin{bmatrix} \frac{1}{\sqrt{a^2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} - \frac{1}{\sqrt{a^4}} \begin{pmatrix} a_{22} \\ -a_{12} \\ a_{11} \end{pmatrix} \begin{pmatrix} a_{22} & -2a_{12} & a_{11} \end{pmatrix} \end{bmatrix} D_{\phi} \begin{pmatrix} a_{11} \\ a_{12} \\ a_{22} \end{pmatrix}.$$

The Fréchet derivatives of the dual basis vectors  $a^{\alpha} \in W^{1,\infty}(\Omega_0)^3$  are determined by solving the four linear equations

$$a_{\alpha}D_{\phi}a^{\beta} + a^{\beta}D_{\phi}a_{\alpha} = 0.$$

The Fréchet derivative of  $\partial_{\alpha}a_3 \in L^{\infty}(\Omega_0)$  (related to surface curvature) follows from differentiation of the formula for  $D_{\phi}a_3$ .

The compactness condition on  $\mathcal{G}$  would typically be established by use of the Arzela-Ascoli theorem [104, Thm. 4.17], via uniform Lipschitz continuity of the chart function and its components, and of the thickness function.

In practice, the approximation of solutions to equations involving these operators is done with general shell elements (§B.1). In that situation, the equations are as above, except for the interchange of  $e^0_{\alpha\beta}(u)$  for  $\gamma_{\alpha\beta}(z)$ ,  $e^1_{\alpha\beta}(u)$  for  $\chi_{\alpha\beta}(\theta, z)$ , and  $e^0_{\alpha3}(u)$ for  $\zeta_{\alpha}(\theta, z)$ . While these are the same in spirit, the basis vectors  $a_i$  are stored at the finite element nodes, and their values interpolated, rather than computed via direct differentiation of the chart function. So as not to introduce large numbers of superfluous optimization variables, it is necessary to specify the dependence of the nodal basis vectors on the chart function. This is discussed in §B.2.

## 3.6 Joints between Naghdi Shells

The paper by Bernadou on plate coupling [21] used Kirchhoff plates, and likewise, his paper [20] on shell coupling focuses on the analogous scenario: Koiter shells. In order to apply the results, one must consider how the relaxation of the Kirchhoff-Love kinematic assumption affects the equations. This extends the discussion of §2.5 to shells. The discussion in this section is less complete than that of §2.5 because the extension is quite straightforward.

Along the edge of the shell, the unit edge normal and tangent vectors are

$$n = n_{\alpha} a^{\alpha},$$
  
$$\tau = a_3 \times n = \tau_{\alpha} a^{\alpha}.$$

Note that unlike the case of a junction between plates, the vectors  $n, \tau, a_3$  need not be constant along the edge of the shell. The force vector T and moment vector Mare then expressed via

$$T = T^i a_i,$$
$$M = M_n n + M_\tau \tau.$$

Analogous to (2.2.15), the weak formulation for a shell with forcing over the edge  $\gamma_1 \subset \partial \Omega_0$  is to find  $(\theta, z) \in \mathcal{U}$  such that for all  $(\eta, y) \in \mathcal{U}$ ,

$$K(\theta, z; \eta, y) = \int_{\Omega_0} f \cdot y \sqrt{a} \, dx + \int_{\gamma_1} \left( T \cdot y + M_n \eta_\tau - M_\tau \eta_n \right) \sqrt{dx^\lambda a_{\lambda\nu} dx^\nu} \, dx.$$

The conditions at the shell junction are the same as (2.5.1):

$$T + \tilde{T} = 0 \tag{3.6.1a}$$

$$M_n = \tilde{M}_{\tilde{n}} = 0 \tag{3.6.1b}$$

$$M_{\tau} - \tilde{M}_{\tilde{\tau}} = 0 \tag{3.6.1c}$$

$$z - \tilde{z} = 0 \tag{3.6.1d}$$

$$\theta_n + \tilde{\theta}_{\tilde{n}} = 0. \tag{3.6.1e}$$

The coupled weak formulation (analogous to [21, (3.6)], (2.5.2)) thus becomes

$$\begin{split} K(\theta, z; \eta, y) + \tilde{K}(\tilde{\theta}, \tilde{z}; \tilde{\eta}, \tilde{y}) &= \int_{\Omega_0} p \cdot y \sqrt{a} \, dx + \int_{\tilde{\Omega}_0} \tilde{p} \cdot \tilde{y} \sqrt{\tilde{a}} \, d\tilde{x} + \\ &\int_{\gamma_1 \setminus \Gamma} \left( T \cdot y + M_n \eta_\tau - M_\tau \eta_n \right) \sqrt{dx^\lambda a_{\lambda\nu} dx^\nu} \, dx + \\ &\int_{\tilde{\gamma}_1 \setminus \Gamma} \left( \tilde{T} \cdot \tilde{y} + \tilde{M}_{\tilde{n}} \tilde{\eta}_{\tilde{\tau}} - \tilde{M}_{\tilde{\tau}} \tilde{\eta}_{\tilde{n}} \right) \sqrt{d\tilde{x}^\lambda \tilde{a}_{\lambda\nu} d\tilde{x}^\nu} \, d\tilde{x} + \\ &\int_{\Gamma} T \cdot (y - \tilde{y}) - M_\tau (\eta_n + \tilde{\eta}_{\tilde{n}}) \sqrt{dx^\lambda a_{\lambda\nu} dx^\nu} \, dx. \end{split}$$

The kinematic conditions once again eliminate the last integral over  $\Gamma$ . Provided that rigid body motions are prohibited by at least one of the spaces  $\mathcal{U}, \tilde{\mathcal{U}}$ , the problem of finding  $(\theta, z), (\tilde{\theta}, \tilde{z})$  in

$$\mathcal{J} = \left\{ (\theta, z) \in \mathcal{U}, (\tilde{\theta}, \tilde{z}) \in \tilde{\mathcal{U}} : (3.6.1 \text{d}, e) \text{ are satisfied on } \Gamma \right\}$$

such that for all  $(\eta, y), (\tilde{\eta}, \tilde{y}) \in \mathcal{J}$ ,

$$\begin{split} K(\theta, z; \eta, y) + \tilde{K}(\tilde{\theta}, \tilde{z}; \tilde{\eta}, \tilde{y}) &= \int_{\Omega_0} p \cdot y \sqrt{a} \, dx + \int_{\tilde{\Omega}_0} \tilde{p} \cdot \tilde{y} \sqrt{\tilde{a}} \, d\tilde{x} + \\ \int_{\gamma_1 \setminus \Gamma} \left( T \cdot y + M_n \eta_\tau - M_\tau \eta_n \right) \sqrt{dx^\lambda a_{\lambda\nu} dx^\nu} \, dx + \\ \int_{\tilde{\gamma}_1 \setminus \Gamma} \left( \tilde{T} \cdot \tilde{y} + \tilde{M}_{\tilde{n}} \tilde{\eta}_{\tilde{\tau}} - \tilde{M}_{\tilde{\tau}} \tilde{\eta}_{\tilde{n}} \right) \sqrt{d\tilde{x}^\lambda \tilde{a}_{\lambda\nu} d\tilde{x}^\nu} \, d\tilde{x} \end{split}$$

has a unique solution [21, Thm. 3.2.1].

# Chapter 4

# Acoustics

# 4.1 Introduction

As a component of (1.2.1), the exterior Helmholtz problem must be solved. While this could be done with 3d finite element methods (for a review, see, e.g., [112]), boundary element methods seem suitable for this application for several reasons.

- They naturally satisfy the Sommerfeld radiation condition (1.2.1f), allowing simulation of the radiated acoustic field without boundary effects.
- Boundary element methods easily give the response at given far-field points.
- When coupled with a shell model, they provide for an essentially two-dimensional discretization of a three-dimensional problem.

However, the use of boundary element methods is not without difficulty. Unlike for the finite element method, the matrices must be generated for each frequency. The matrices are dense and complex; storage can be an issue for large problems, but more seriously, naïve implementation results in  $O(N^2)$  complexity. Speedy evaluation requires some kind of acceleration method, e.g., fast multipole methods [46], FFTbased methods [34], wavelets [58], panel-clustering [70], and the adaptive cross method [111]. These are not discussed in the thesis; rather, the focus is on what can be done in regard to coupling and optimization.

For three-dimensional problems, it is also necessary to overcome the so-called irregular frequency problem, in which solutions of the boundary integral equations lose uniqueness near frequencies corresponding to eigenvalues of an interior adjoint problem. One historically popular way of dealing with this issue was the CHIEF (Combined Helmholtz Integral Equation Formulation) method of [106], which involved solution of a least-squares problem. The Burton-Miller method [35] requires discretization of additional matrix operators, but has a full theoretical justification.

Trouble can ensue when typical boundary element methods are applied to thin structures. For example, a shell structure will have approximately the same normal velocity on either side, so that the pressure jump across the thin dimension is the relevant physical quantity: to store the pressure on both sides doubles the number of variables involved without substantially improving the quality of the solution. But for very thin structures, failure to consider the thin dimension carefully can lead to instability. Basic analysis, including a careful accounting of the geometric approximations involved in translating the equations to the middle surface (say of a shell) are done by Martinez in [96]. The formulation involves the jumps across the surface rather than separately storing the values on either side. The same technique is used in [95] to deal with coupling between a thin elastic structure and boundary integral equations. More practical implementation details are discussed in [115] and [116], the latter paper focusing on cases where the body includes both thick and thin structures. These methods work, but none of these papers provide their theoretical justification. This was done by Stephan in [109] for Helmholtz "screen" problems, which turn out to be exactly the limiting problems obtained by Martinez through various approximations.

In this chapter, I first review the Helmholtz equation, and state the standard representation formula giving the solution in the exterior domain in terms of the boundary data. Taking boundary traces of the representation formula then yields the various integral equations. Well-posedness of these equations is discussed in Sobolev spaces. Next, the process is repeated for thin bodies. At the end of the chapter, shape differentiation of the integral equations for thin bodies is discussed.

# 4.2 The Acoustic Helmholtz Equation

The acoustic wave equations for the pressure p (actually the difference from equilibrium pressure) and the velocity field **v** in an acoustic medium with sound speed c and density  $\rho_0$  are

$$\frac{1}{\rho_0 c^2} \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{v} = 0 \tag{4.2.1a}$$

$$\rho_0 \frac{\partial \mathbf{v}}{\partial t} + \nabla p = 0. \tag{4.2.1b}$$

Time differentiation of the mass conservation equation (4.2.1a) and application of Newton's second law (4.2.1b) yields the wave equation

$$\frac{1}{c^2}\frac{\partial^2 p}{\partial t^2} - \Delta p = 0.$$

See e.g., [28, §I.1.4], for more discussion of the wave equation.

The velocity potential  $\varphi$  is chosen so that  $\nabla \varphi = \mathbf{v}$ , which will be seen to be convenient for matching boundary velocities. Assuming that derivatives can be freely interchanged, equation (4.2.1b) yields

$$\rho_0 \frac{\partial \nabla \varphi}{\partial t} + \nabla p = 0 \Rightarrow p = -\rho_0 \frac{\partial \varphi}{\partial t} + C.$$

Inserting this equation for p and  $\mathbf{v} = \nabla \varphi$  into (4.2.1a) gives the wave equation for the velocity potential  $\varphi$ :

$$\frac{1}{c^2} \frac{\partial^2 \varphi(t, x)}{\partial t^2} - \bigtriangleup \varphi(t, x) = 0 \text{ in } (0, \infty) \times \Omega.$$
(4.2.2)

In the following I assume that time-harmonic waves are of the form

$$\varphi(t,x) = \operatorname{Re}\left(\widetilde{\varphi}(x)e^{-i\omega t}\right),$$
(4.2.3)

where i is the imaginary unit and

$$\widetilde{\varphi}: \Omega \to \mathbb{C}.$$

Inserting (4.2.3) into (4.2.2) gives the Helmholtz equation

$$\Delta \widetilde{\varphi}(x) + \kappa^2 \widetilde{\varphi}(x) = 0 \text{ in } \Omega, \qquad (4.2.4)$$

where  $\kappa = \omega/c$  is the wave number. Since from now on I consider the Helmholtz equation (4.2.4) and not the wave equation (4.2.2), I will drop the  $\sim$  and write  $\varphi$  instead of  $\tilde{\varphi}$ .

# 4.2.1 Exterior Neumann Problem for the Helmholtz Equation



Figure 4.1: The boundary between  $\Omega^+$  and  $\Omega^-$  is denoted  $\Gamma$ , with *n*, the normal on  $\Gamma$ , outward from  $\Omega^-$ .

Throughout this section I assume that  $\Omega^-$  is a bounded, simply-connected Lipschitz domain and  $\Omega^+ = \mathbb{R}^3 \setminus \Omega^-$ . The vector n(x) denotes the unit normal on  $\Gamma$ , outward from  $\Omega^-$ . See figure 4.1. The exterior domain truncated at radius  $\rho$  is written

$$\Omega^{\rho} = \left\{ x \in \Omega^+ : |x| \le \rho \right\}.$$

Since solutions of the time-harmonic wave equation (4.2.4) are complex-valued, the spaces  $L^2(\Omega^-)$ , etc., and the Sobolev spaces  $H^1(\Omega^-)$ , etc., are spaces of complexvalued functions. The inner products on  $L^2(\Omega^-)$  and  $H^1(\Omega^-)$  are given by

$$\langle u, v \rangle_{L^2(\Omega^-)} = \int_{\Omega^-} u(x) \overline{v(x)} dx$$

and

$$\langle u, v \rangle_{H^1(\Omega^-)} = \int_{\Omega^-} u(x)\overline{v(x)} + \nabla u(x) \cdot \nabla \overline{v(x)} dx$$

respectively. Norms and inner products on other Sobolev spaces are also defined in the usual way. See, e.g., [2], [78, § 4], [114]. For the solution of the outer problem, one also needs the space

$$H^1_{\text{loc}}(\Omega^+) \equiv \left\{ u \in H^m(K) : \text{ for every compact set } K \subset \Omega^+ \right\}.$$

The space  $H^1_{\text{loc}}(\Omega^+)$  can also be characterized by the statement

$$u \in H^1_{\text{loc}}(\Omega^+)$$
 if and only if  $\varrho u \in H^1(\Omega^+)$  for every  $\varrho \in C_0^{\infty}(\mathbb{R}^n)$ .

See [78, p. 192].

In relating Sobolev spaces on  $\Omega^{\pm}$  to those on  $\Gamma$ , it will be necessary to use trace operators. Under the assumptions on  $\Omega^{-}$  stated above, there exist bounded linear operators

$$\begin{split} \gamma^- &: H^1(\Omega^-) \to H^{1/2}(\Gamma), \qquad \qquad \partial_n^- : H^1(\Omega^-) \to H^{-1/2}(\Gamma), \\ \gamma^+ &: H^1_{\text{loc}}(\Omega^+) \to H^{1/2}(\Gamma), \qquad \qquad \partial_n^+ : H^1_{\text{loc}}(\Omega^+) \to H^{-1/2}(\Gamma). \end{split}$$

See [48], [78, p. 178], [114, p. 130]. For sufficiently smooth functions,

$$\gamma^{\pm}u(x) = \lim_{x' \in \Omega^{\pm}, x' \to x \in \Gamma} u(x'), \ \partial_n^{\pm}u(x) = \lim_{x' \in \Omega^{\pm}, x' \to x \in \Gamma} n(x) \cdot \nabla_{x'}u(x').$$

Unless otherwise specified, for surfaces other than  $\Gamma$ , *n* indicates the outward normal vector, and the symbols  $\gamma$ ,  $\partial_n$  are used without  $\pm$  superscripts to indicate the trace and outward normal derivative. The exterior Helmholtz Neumann problem is to solve (4.2.4), with Neumann boundary data g used to match the normal component of the velocity at the boundary between the air and the elastic material:

$$\Delta \varphi + \kappa^2 \varphi = 0 \qquad \text{in } \Omega^+ \qquad (4.2.5a)$$

$$\partial_n^+ \varphi = g \qquad \qquad \text{on } \Gamma \qquad (4.2.5b)$$

$$\lim_{\rho \to \infty} \int_{\partial \Omega^{\rho}} \left| \nabla \varphi \cdot \frac{x}{|x|} - i\kappa \varphi \right|^2 dx = 0$$
(4.2.5c)

Condition (4.2.5c) is a weakened version of the classical Sommerfeld radiation condition

$$\left|\nabla\varphi\cdot\frac{x}{|x|}-i\kappa\varphi\right|=O\left(\frac{1}{|x|^2}\right) \text{ as } |x|\to\infty.$$
 (4.2.6)

For sufficiently smooth solutions of (4.2.5), the conditions (4.2.6) and (4.2.5c) are equivalent (see [97, Thm. 9.6]). The Sommerfeld condition requires that waves be strictly out-going at infinity, and is needed in order for uniqueness to hold.

#### Theorem 4.2.1 (Exterior Neumann Problem Existence and Uniqueness)

Given  $g \in H^{-1/2}(\Gamma)$ , there exists a unique  $\varphi \in H^1_{loc}(\Omega^+)$  satisfying (4.2.5). The Helmholtz equation (4.2.5a) is satisfied in the sense of distributions, i.e., for every  $v \in C_0^{\infty}(\mathbb{R}^n)$ ,

$$\int_{\Omega^+} \nabla \varphi \cdot \nabla \overline{v} - \kappa^2 \varphi \overline{v} \, dx = \int_{\Gamma} g \overline{v}.$$

**Proof:** See [97, Thm. 9.11, Ex. 9.5].

#### 4.2.2 Exterior Neumann Problem Representation Formula

Discretization of (4.2.5) is complicated by the fact that the problem is over an infinite domain. Of course, it is also unnecessary to know the solution everywhere: for many applications, knowledge of  $\varphi$  at a small number of points in  $\Omega^+$  will suffice. By using

a fundamental solution for (4.2.5), it is possible to derive a representation formula which given  $\varphi$  and  $\partial_n \varphi$  on  $\Gamma$ , allows for the calculation of  $\varphi$  at points in  $\Omega^+$ . The representation formula can then be used to pose integral equations for  $\varphi$  on the twodimensional boundary  $\Gamma$ .

The usual fundamental solution (Green's function) for the Helmholtz equation is

$$G(x, x') = \frac{\exp(i\kappa |x - x'|)}{4\pi |x - x'|},$$

satisfying

$$\Delta_x G(x, x') + \kappa^2 G(x, x') = 0, \ \forall x \neq x'.$$

Assume that  $\varphi \in C^2(\Omega^+)$  is a strong solution to (4.2.5). This assumption can later be relaxed to work with general  $\varphi \in H^1_{\text{loc}}(\Omega^+)$ .

Lemma 4.2.2 (Green's Identity for the Helmholtz Equation) If  $\Omega$  is a Lipschitz domain, and  $u \in H^2(\Omega)$ ,  $v \in H^1(\Omega)$ , then

$$\int_{\Omega} -(\bigtriangleup u + \kappa^2 u) v \, dx = \int_{\Omega} (\nabla u \cdot \nabla v) - \kappa^2 u v \, dx - \int_{\partial \Omega} \partial_n u \cdot \gamma v \, dx. \tag{4.2.7}$$

**Proof:** See [97, Lemma 4.1].

Fix  $x' \in \Omega^{\rho}$ , and use Green's second identity in the region

$$\Omega^{\rho}_{\epsilon} = \left\{ x \in \Omega^{\rho} : |x - x'| > \epsilon \right\}.$$

Then,

$$\int_{\Omega_{\epsilon}^{\rho}} \varphi(x) \Delta_{x} G(x, x') - G(x, x') \Delta \varphi(x) \, dx = \int_{\partial \Omega_{\epsilon}^{\rho}} \varphi(x) \partial_{n,x} G(x, x') - G(x, x') \partial_{n} \varphi \, dx.$$
(4.2.8)

Since  $\varphi$  satisfies  $\Delta \varphi = -\kappa^2 \varphi$ , the left hand side of (4.2.8) becomes

$$\int_{\Omega_{\epsilon}^{\rho}} \varphi(x) (\Delta_x G(x, x') + \kappa^2 G(x, x')) \, dx = 0$$

and therefore,

$$0 = \int_{\partial \Omega_{\epsilon}^{\rho}} \varphi(x) \partial_{n,x} G(x, x') - G(x, x') \partial_{n} \varphi \, dx.$$
(4.2.9)

The derivative of G on  $|x - x'| = \epsilon$  is

$$\partial_{n,x}G(x,x') = \left(\frac{1}{\epsilon} - i\kappa\right) \frac{\exp(ik\epsilon)}{4\pi\epsilon},$$

and as

$$\lim_{\epsilon \to 0} 4\pi \epsilon^2 \partial_{n,x} G(x, x') = 1,$$

it follows from a simple calculation that

$$\lim_{\epsilon \to 0} \int_{|x-x'|=\epsilon} \varphi(x) \partial_{n,x} G(x,x') - G(x,x') \partial_n \varphi \, dx = \varphi(x'),$$

and therefore, (4.2.9) becomes

$$0 = \varphi(x') + \int_{\partial \Omega^{\rho}} \varphi(x) \partial_{n,x} G(x, x') - G(x, x') \partial_{n} \varphi \, dx,$$

Now, note that Green's formula is written with an outward normal, but the normal on  $\Gamma$  has been taken to be outward to  $\Omega^-$ , so that it is inward to  $\Omega^{\rho}$ . Therefore,

$$\varphi(x') = \int_{\Gamma} \varphi(x) \partial_{n,x}^{+} G(x, x') - G(x, x') \partial_{n}^{+} \varphi \, dx - \int_{|x|=\rho} \varphi(x) \partial_{n,x} G(x, x') - G(x, x') \partial_{n} \varphi \, dx$$
(4.2.10)

It is shown, e.g., in [105, Sec. 1.4] that due to the Sommerfeld condition (4.2.5c), the integral over the outer boundary in (4.2.10) satisfies

$$\lim_{\rho \to \infty} \int_{|x|=\rho} \partial_{n,x} G(x,x') \varphi(x) - \partial_n \varphi(x) G(x,x') \, dx = 0.$$

This yields the representation formula for the exterior domain.

**Theorem 4.2.3 (Exterior Representation Formula)** Let  $\varphi \in C^2(\Omega^+)$  be a solution to (4.2.5). Then for  $x' \in \Omega^+$ ,

$$\varphi(x') = \int_{\Gamma} \partial_{n,x}^{+} G(x,x') \gamma^{+} \varphi(x) - \partial_{n}^{+} \varphi(x) G(x,x') \, dx, \ \forall x' \in \Omega^{+}.$$
(4.2.11)

This result can be extended to more general classes of functions by approximating a solution  $\varphi \in H^1_{\text{loc}}(\Omega^+)$  with smooth functions. See [48, Lemma 3.4].

# 4.3 Boundary Integral Operators

The Green's function and its derivative in (4.2.11) are known, as is the Neumann data, so an integral equation can now be formulated for the unknown Dirichlet data. The idea is to apply the trace operators to (4.2.11). For  $x' \in \Omega^{\pm}$ ,  $\psi \in L^1(\Gamma)$ , and  $\varsigma \in L^1(\Gamma)$ , the single and double-layer potentials are defined via

$$(SL\psi)(x') = \int_{\Gamma} \psi(x)G(x, x') dx$$
$$(DL\zeta)(x') = \int_{\Gamma} \partial_{n,x}^{+} G(x, x')\varsigma(x) dx$$

named after their association with surface distributions of electric monopole and dipole charges. Later, these and related operators will be defined on a larger set of functions than  $L^1(\Gamma)$ .

For sufficiently smooth functions, (4.2.11) can be written using the single and double-layer potentials as follows.

$$\varphi = DL\gamma^+\varphi - SL\partial_n^+\varphi.$$

The results of the application of the trace operators to the potentials are given for more general functions in the following theorem.

**Theorem 4.3.1 (Mapping Properties)** SL and DL give rise to the bounded linear operators

$$\begin{split} \gamma^{\pm}SL : & H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma) \\ \partial_n^{\pm}SL : & H^{-1/2}(\Gamma) \to H^{-1/2}(\Gamma) \\ \gamma^{\pm}DL : & H^{1/2}(\Gamma) \to H^{1/2}(\Gamma) \\ \partial_n^{\pm}DL : & H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma), \end{split}$$

for  $\psi \in H^{-1/2}(\Gamma)$  and  $\varsigma \in H^{1/2}(\Gamma)$  satisfying the jump relations

$$[SL\psi]_{\Gamma} \equiv \gamma^+ SL\psi - \gamma^- SL\psi = 0 \tag{4.3.1a}$$

$$[\partial_n SL\varsigma]_{\Gamma} \equiv \partial_n^+ SL\varsigma - \partial_n^- SL\varsigma = -\varsigma \tag{4.3.1b}$$

$$[DL\psi]_{\Gamma} \equiv \gamma^{+} DL\psi - \gamma^{-} DL\psi = \psi \qquad (4.3.1c)$$

$$[\partial_n DL\varsigma]_{\Gamma} \equiv \partial_n^+ DL\varsigma - \partial_n^- DL\varsigma = 0 \tag{4.3.1d}$$

**Proof:** See [48, Thm. 1].

It turns out that the integral operators resulting from application of the trace and normal derivative can be expressed in terms of

$$V \equiv \gamma^{\pm} SL : \quad H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$$
$$K \equiv (\gamma^{+} DL + \gamma^{-} DL) / 2 : \quad H^{1/2}(\Gamma) \to H^{1/2}(\Gamma)$$
$$D \equiv -\partial_{n}^{\pm} DL : \quad H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma).$$

Combining these definitions with the jump relations in theorem 4.3.1, and the duality relations of [97, Thms. 6.15,6.17] yields the following expressions for the traces and normal derivatives of the potentials

$$\gamma^{\pm}SL\psi = V\psi \tag{4.3.2a}$$

$$\gamma^{\pm}DL\varsigma = \left(\pm \frac{1}{2}I + K\right)\varsigma \tag{4.3.2b}$$

$$\partial_n^{\pm} SL\psi = \left(\mp \frac{1}{2}I + K^*\right)\psi \tag{4.3.2c}$$

$$\partial_n^{\pm} DL\varsigma = -D\varsigma. \tag{4.3.2d}$$

An integration kernel k(x, y) that is continuous for  $x \neq y$  is called weakly singular if there exist positive constants M and  $\alpha \in (0, 2]$  such that

$$|k(x,y)| \le M|x-y|^{\alpha-2}.$$

Otherwise, it is called strongly singular. Integral representations of V, K, D, are given in the following theorem.

**Theorem 4.3.2 (Integral Representations)** Let  $\chi \in L^{\infty}(\Gamma)$ ,  $\psi, \varsigma \in \mathcal{D}(\Gamma)$ . The representation formula

$$V\chi(x) = \int_{\Gamma} \chi(y)G(x,y) \, dy$$

holds for  $x \in \Gamma$ .  $D\psi$  can be evaluated against a test function via

$$\langle D\psi,\varsigma\rangle_{\Gamma} = \langle V(n\times\nabla\psi), n\times\nabla\varsigma\rangle_{\Gamma} - \kappa^2 \langle V(\psi n),\varsigma n\rangle_{\Gamma}.$$

If  $\Gamma$  has a tangent plane at x, then

$$K\varsigma(x) = \lim_{\epsilon \to 0} \int_{\Gamma \setminus B_{\epsilon}(x)} \partial_{n,y} G(x,y)\varsigma(y) \, dy$$
$$K^*\psi(x) = \lim_{\epsilon \to 0} \int_{\Gamma \setminus B_{\epsilon}(x)} \partial_{n,x} G(x,y)\psi(y) \, dy.$$

**Proof:** The integrand in V is weakly singular. In fact, it satisfies

$$\int_{\Gamma \cap B_{\epsilon}(x)} |G(x,y)| \, dy \le C\epsilon.$$

The integrands for  $K, K^*$  are strongly singular, and in the absence of added surface regularity, the integrals exist only in the Cauchy principal value sense. See [97, Thm. 7.4].

The integrand for D is called hypersingular, and can be evaluated as a finite-part integral if  $\Gamma$  is  $C^2$ . For general Lipschitz surfaces, it can be evaluated as above (see [97, Thm. 7.4, Thm. 9.15]).

## 4.3.1 Boundary Integral Equations

Consider now the exterior Neumann problem, in which  $\partial_n^+ \varphi = g \in H^{-1/2}(\Gamma)$ . One seeks the unknown Dirichlet data  $\gamma^+ \varphi = \varphi_{\Gamma} \in H^{1/2}(\Gamma)$ . Upon application of  $\gamma^+$ , (4.2.11) becomes

$$\left(-\frac{1}{2}I + K\right)\varphi_{\Gamma} = Vg, \qquad (4.3.3)$$

while  $\partial_n^+$  yields

$$D\varphi_{\Gamma} = -\left(\frac{1}{2}I + K^*\right)g. \tag{4.3.4}$$

The following theorem establishes the correspondence between solutions to (4.3.4) and (4.2.5).

#### Theorem 4.3.3 (Integral Equations and Exterior Helmholtz)

If  $\varphi \in H^1_{loc}(\Omega^+)$  is the solution to (4.2.5), then the trace  $\varphi_{\Gamma} = \gamma^+ \varphi \in H^{1/2}(\Gamma)$  is a solution of (4.3.4). Moreover,  $\varphi$  has the representation

$$\varphi(x') = \int_{\Gamma} \partial_{n,x}^+ G(x,x')\varphi_{\Gamma}(x) - g(x)G(x,x')\,dx, \ \forall x' \in \Omega^+.$$
(4.3.5)

Conversely, if  $\varphi_{\Gamma} \in H^{1/2}(\Gamma)$  is a solution of (4.3.4), then (4.3.5) gives the solution to (4.2.5).

**Proof:** See [97, Thm. 7.15].

Although theorem 4.2.1 gives uniqueness of the solution to (4.2.5), it will be seen that this is in general not true for the boundary integral equations (4.3.3) and (4.3.4), i.e., although any solution to (4.3.4) gives the same exterior  $\varphi$  through (4.3.5), at certain frequencies, the solution to (4.3.4) is not unique. This non-uniqueness stems from the fact that the boundary data corresponding to interior solutions to the Helmholtz equation gives no exterior contribution through the representation formula (see [47, Thm. 3.1]).

Following a procedure analogous to that described in §4.2.2, one can derive the representation formula for the interior domain  $\Omega^-$ , analogous to (4.2.11):

$$\varphi(x') = \int_{\Gamma} \partial_n^+ \varphi(x) G(x, x') - \partial_{n,x}^+ G(x, x') \gamma^+ \varphi(x) \, dx, \ \forall x' \in \Omega^-.$$
(4.3.6)

Note that the sign of the right-hand side is reversed from (4.2.11) because the normal is now outward to the surface, unlike in (4.2.10).
Upon application of  $\gamma^-$ , (4.3.6) becomes

$$\left(\frac{1}{2}I + K\right)\varphi_{\Gamma} = Vg, \qquad (4.3.7)$$

while  $\partial_n^-$  yields

$$D\varphi_{\Gamma} = \left(\frac{1}{2}I - K^*\right)g. \tag{4.3.8}$$

Note that the operator on the left-hand side of (4.3.3) is (up to a minus sign) the adjoint of the operator on the right-hand side of (4.3.8). Scalars  $\mu$  such that there exists a non-zero solution  $u_{\mu}$  to

$$\Delta u_{\mu} + \mu u_{\mu} = 0 \text{ in } \Omega^{-}$$
  
 $\gamma^{-} u_{\mu} = 0 \text{ on } \Gamma$ 

are Dirichlet eigenvalues of the Laplacian in  $\Omega^-$ . Let  $\mu$  be such a scalar, with  $u_{\mu}$  a corresponding eigenfunction. Define

$$u_n = \partial_n^- u_\mu.$$

Assume that  $\kappa^2 = \mu$ . Then  $0 \neq u_n \in H^{-1/2}(\Gamma)$  solves (4.3.8)

$$0 = D\gamma^{-}u_{\mu} = \left(\frac{1}{2}I - K^{*}\right)u_{n}.$$

Thus, the operator  $(\frac{1}{2}I - K^*)$  is singular, and therefore, so is its adjoint,  $(\frac{1}{2}I - K)$ , which appears on the left-hand side of (4.3.3).

Similarly, if  $\kappa^2 = \mu$  is an interior Neumann eigenvalue, i.e., there exists a non-zero solution  $u_{\mu}$  to

$$\Delta u_{\mu} + \mu u_{\mu} = 0 \text{ in } \Omega^{-}$$
$$\partial_{n}^{-} u_{\mu} = 0 \text{ on } \Gamma.$$

The corresponding Dirichlet data given by

$$u_{\Gamma} = \gamma^- u_{\mu}$$

satisfy  $0 \neq u_{\Gamma} \in H^{1/2}(\Gamma)$  and solve

$$Du_{\Gamma} = \left(\frac{1}{2}I - K^*\right)\partial_n^- u_{\mu} = 0.$$

Thus, the operator D is singular in this case.

If  $\kappa^2$  is not an interior Neumann eigenvalue, then D is injective, and uniqueness of solutions to (4.3.4) follows from [48, Thm. 2]. [48, Thm. 4] also gives convergence of Galerkin schemes for (4.3.4) in  $H^{1/2}(\Gamma)$ .

In [35], Burton and Miller proposed a method for combining (4.3.3) and (4.3.4) in a way that always achieves a unique solution, which is to solve instead the linear combination  $(4.3.3)+i\eta(4.3.4)$ . The original formulation of Burton and Miller was posed for smoother functions, but the following Sobolev space formulation appears in [65].

With  $0 \neq \eta \in \mathbb{R}$ , the Burton-Miller problem is to solve

$$\left(-\frac{1}{2}I + K + i\eta D\right)\varphi_{\Gamma} = \left(V - i\eta\left(\frac{1}{2}I + K^{*}\right)\right)g \text{ in } H^{-1/2}(\Gamma).$$
(4.3.9)

Theorem 4.3.4 (Uniqueness for Burton-Miller) Let  $\varphi \in H^{1/2}(\Gamma)$ . If  $0 \neq \eta \in \mathbb{R}$ , then

$$\left(-\frac{1}{2}I + K + i\eta D\right)\varphi = 0 \tag{4.3.10}$$

implies that  $\varphi = 0$ .

**Proof:** This proof was first given by Burton and Miller [35].

Consider the function

$$v = DL\varphi$$

defined everywhere in  $\mathbb{R}^3 = \Omega^- \cup \Gamma \cup \Omega^+$ . Assume that (4.3.10) holds. From (4.3.2),

$$\gamma^{-}v = \left(-\frac{1}{2}I + K\right)\varphi$$
$$\partial_{n}^{-}v = -D\varphi.$$

Upon comparison with (4.3.10),

$$\gamma^- v - i\eta \partial_n^- v = 0. \tag{4.3.11}$$

Now, apply Green's formula (4.2.7) to v and  $\overline{v}$ . The required smoothness is provided by the Green's function, which is  $C^{\infty}$  away from its singularity. As both v and  $\overline{v}$ satisfy the Helmholtz equation in  $\Omega^-$ , take the difference of Green's formula (4.2.7) as applied to each in order to obtain

$$0 = \int_{\Gamma} v(\partial_n^- \overline{v}) - (\partial_n^- v)\overline{v} \, dx$$
$$= 2i\eta \int_{\Gamma} |\partial_n^- v|^2 \, dx.$$

Therefore,  $\partial_n^- v = 0$  on  $\Gamma$ . Note that the first integrand is pure imaginary, so it follows that any complex number  $\alpha$  could have been used with  $\operatorname{Im}(\alpha) \neq 0$  in place of  $i\eta$ , as is done in Burton and Miller's original paper. It follows from (4.3.11) that  $\gamma^- v = 0$ on  $\Gamma$  as well. Thus,  $v \equiv 0$  on  $\Omega^-$ . The jump relations (4.3.1) imply that  $\partial_n^+ v = 0$ . By the uniqueness of solutions to the exterior Neumann problem (theorem 4.2.1),  $v \equiv 0$ on  $\Omega^+$  as well. Thus, the jump relations imply that  $\varphi = 0$ .

Amini showed [4] that for a spherical geometry, the optimal choice of the coupling parameter  $\eta$  is the reciprocal  $1/\kappa$  of the wave number. In practice, this choice is often made for arbitrary geometries.

## 4.3.2 Boundary Integral Equations on Thin Bodies

While the boundary integral equations described in the previous sections work in principle for an object shaped as in figure 4.2 (i.e., for a shell), some practical difficulties are quickly encountered. Most importantly, discretizations can be very badly behaved when the shell is very thin: see, e.g., [96, 83, 89]. It is also natural in this case to take advantage of the geometry and to seek, as is done with shell equations, to reduce the dimension of the problem via suitable assumptions, namely in some



Figure 4.2: Shell as scatterer. Denote the 2d chart function with  $\phi$ . The middle surface is  $\phi(\Omega_0)$ , with normal  $a_3$ . The vectors  $n^+$  and  $n^-$  are normal respectively to the surfaces  $\Gamma^+ = \phi(\Omega_0) + ta_3/2$  and  $\Gamma^- = \phi(\Omega_0) - ta_3/2$ .

sense to ignore the thin dimension of the shell. In this section, an integral equation is derived, posed on the shell middle-surface, solution of which gives the jump in  $\varphi$ across the thin dimension of the shell for given middle surface velocity. In the next section, the limiting "screen" problems corresponding to this integral equation are discussed, as are existence and uniqueness of solutions.

Let the boundary of the scatterer once again be  $\Gamma$ , but here, it is assumed that it encloses a shell structure, with geometry depicted in figure 4.2. In general, the middle-surface normal  $a_3$  differs from the normals to the external surfaces  $\Gamma^+$  and  $\Gamma^-$ .

Following Martinez [96], three assumptions are made:

Neglect the contributions from the set Γ \ (Γ<sup>+</sup> ∩ Γ<sup>-</sup>), i.e., from the edges, so that the representation formula (4.2.11) becomes

$$\begin{split} \varphi(x') &\approx \int_{\Gamma^+} \partial_{n^+,x} G(x,x') \gamma \varphi(x) \, dx - \int_{\Gamma^+} \partial_{n^+} \varphi(x) G(x,x') \, dx + \\ &\int_{\Gamma^-} \partial_{n^-,x} G(x,x') \gamma \varphi(x) \, dx - \int_{\Gamma^-} \partial_{n^-} \varphi(x) G(x,x') \, dx, \; \forall x' \in \Omega^+. \end{split}$$

In the above formula, all traces and normal derivatives are exterior.

• Replace the integration point x with the corresponding point on the middle surface, i.e., if  $y \in \Omega_0$ , then replace  $x = \phi(y) + t(y)a_3(y)/2$  with  $\phi(y)$ . Likewise,

replace  $n^+$  with  $a_3$  and  $n^-$  with  $-a_3$ . The result is

$$\approx \int_{\phi(\Omega_0)} \partial_{n^+,x}^+ G(x,x') \gamma^+ \varphi(x) \, dx - \int_{\phi(\Omega_0)} \partial_{n^+}^+ \varphi(x) G(x,x') \, dx + \int_{\phi(\Omega_0)} \partial_{n^-,x}^- G(x,x') \gamma^- \varphi(x) \, dx - \int_{\phi(\Omega_0)} \partial_{n^-} \varphi(x) G(x,x') \, dx$$

$$\approx \int_{\phi(\Omega_0)} \partial_{a_3,x} G(x,x') \gamma^+ \varphi(x) \, dx - \int_{\phi(\Omega_0)} \partial_{a_3}^+ \varphi(x) G(x,x') \, dx + \int_{\phi(\Omega_0)} -\partial_{a_3,x} G(x,x') \gamma^- \varphi(x) \, dx - \int_{\phi(\Omega_0)} -\partial_{a_3} \varphi(x) G(x,x') \, dx$$

$$= \int_{\phi(\Omega_0)} \partial_{a_3,x} G(x,x') [\gamma^+ \varphi - \gamma^- \varphi](x) \, dx - \int_{\phi(\Omega_0)} G(x,x') [\partial_{a_3}^+ \varphi - \partial_{a_3}^- \varphi](x) \, dx.$$

$$(4.3.12)$$

Now, the traces are "interior" or "exterior" to  $\phi(\Omega_0)$  depending on whether they came from the  $\Gamma^+$  or  $\Gamma^-$  side. Note that (4.3.12) is just the representation formula (4.2.11) applied to the jumps across the surface.

• The normal component of the elastic displacement field has no jump across the shell. For shell models, this is true already: the normal displacement components are

$$u|_{\Gamma^+} \cdot a_3 = (z_i a^i + \frac{t}{2} \theta_\alpha a^\alpha) \cdot a_3 = z_3,$$

and

$$u|_{\Gamma^-}\cdot a_3=(z_ia^i-rac{t}{2} heta_lpha a^lpha)\cdot a_3=z_3.$$

Under the coupling assumptions, this implies that the jump

$$[\partial_{a_3}^+\varphi - \partial_{a_3}^-\varphi] = 0.$$

The representation formula thus becomes

$$\varphi(x') = \int_{\phi(\Omega_0)} \partial_{a_3,x} G(x,x') [\varphi(x)]_{\phi(\Omega_0)} dx.$$
(4.3.13)

Taking the normal derivative here (from either side) gives the hypersingular integral equation defined on the middle surface  $\Gamma_0 = \phi(\Omega_0)$ :

$$D_{\Gamma_0}[\varphi]_{\Gamma_0} = -g, \qquad (4.3.14)$$

on the middle surface, for the jump in  $\varphi$  in terms of the unknown Neumann data g. Here,  $D_{\Gamma_0}$  is the restriction of D defined in the usual way to the surface patch  $\Gamma_0$ . Application of the traces gives the equations

$$\gamma^{+}\varphi = \left(\frac{1}{2}I + K_{\Gamma_{0}}\right)[\varphi]_{\Gamma_{0}}$$
$$\gamma^{-}\varphi = \left(-\frac{1}{2}I + K_{\Gamma_{0}}\right)[\varphi]_{\Gamma_{0}}$$

Subtraction of the second from the first yields the useless identity

$$[\varphi]_{\Gamma_0} = [\varphi]_{\Gamma_0}.$$

Thus, something akin to Burton-Miller cannot be established by taking the usual linear combination of two integral equations. Krishnasamy, Rizzo, and Liu [83] present a modification of Martinez's assumptions, by which the Burton-Miller equations can be used on the middle surface, but this method requires extra field variables, and the discretization of additional integral operators. It also lacks existence and uniqueness theory.

Martinez [96] derived (4.3.14), and suggested that it be used, but did not discuss existence or uniqueness of solutions. Note that this theory would follow readily from theorem 4.3.3 if  $\Gamma_0$  were a closed surface. However, as is seen in the next section, it turns out that (4.3.14) does in fact have a unique solution, and that the theory had already been developed at the time Martinez published.

## 4.3.3 Screen Problems

Stephan [109] proved a well-posedness result based on integral equations for "screen" problems of the following form.

**Problem 3** [Neumann screen problem] Let  $\Gamma_0 \subset \mathbb{R}^3$  be an open, bounded, simplyconnected Lipschitz surface (i.e., locally the graph of a Lipschitz function), and find



Figure 4.3: Assume that  $\Gamma_0$  can be extended to enclose a bounded Lipschitz domain  $\Omega_1$ , with  $\partial \Omega_1 = \Gamma$ .  $B_R$  is a ball of radius R sufficiently large so that  $\Omega_1 \subset B_R$ , and  $\Omega_2 \equiv B_R \setminus \Omega_1$ .

 $\varphi \in H^1_{\text{loc}}(\mathbb{R}^3 \setminus \Gamma_0)$ , a weak solution to

 $\partial_n \varphi = g$ 

$$\Delta \varphi + \kappa^2 \varphi = 0 \qquad \qquad \text{in } \mathbb{R}^3 \setminus \Gamma_0 \qquad (4.3.15a)$$

on 
$$\Gamma_0$$
 (4.3.15b)

$$\left|\frac{\partial\varphi}{\partial r} - i\kappa\varphi\right| = O\left(\frac{1}{r^2}\right) \qquad \text{as } r \to \infty.$$
(4.3.15c)

For subsequent proofs, the geometric setting of figure 4.3 is used.

Stephan did not discuss in detail the assumptions leading to this problem, though he clearly knew that it arises as the limiting case of a thin scatterer. He presumably did not have the results of Costabel [48] for integral operators on Lipschitz domains, as they had not yet been published, and thus, used unnecessary smoothness assumptions. The uniqueness theory of Stephan [109] is repeated, using the results by Costabel [48] for boundary integral operators on Lipschitz domains to arrive at existence and uniqueness theorem 4.3.8.

First, it is necessary to establish uniqueness to solutions of the screen problem

(4.3.15).

## Lemma 4.3.5 (Uniqueness of solutions to the screen problem)

Let  $\varphi \in H^1_{loc}(\mathbb{R}^3 \setminus \Gamma_0)$  be a solution to (4.3.15) with g = 0. Then  $\varphi \equiv 0$  in  $\mathbb{R}^3 \setminus \Gamma_0$ .

**Proof:** The result [109, Lemma 2.1] is reproduced with greater detail.

If  $\varphi_1, \varphi_2 \in H^1_{\text{loc}}(\mathbb{R}^3 \setminus \Gamma_0)$  are weak solutions of

$$(\Delta + \kappa^2)\varphi_1 = 0 \qquad \qquad \text{in } \Omega_1,$$

$$(\Delta + \kappa^2)\varphi_2 = 0 \qquad \qquad \text{in } \mathbb{R}^3 \setminus \overline{\Omega_1},$$

$$\left|\frac{\partial \varphi_2}{\partial r} - i\kappa \varphi_2\right| = O\left(\frac{1}{r^2}\right)$$
 as  $r \to \infty$ 

subject to the transmission conditions

$$\varphi_1 = \varphi_2 \text{ on } \Gamma \setminus \Gamma_0, \ \partial_n \varphi_1 = \partial_n \varphi_2 \text{ on } \Gamma,$$

then

$$\begin{split} \varphi = \varphi_1 & \text{in } \Omega_1, \\ \varphi = \varphi_2 & \text{in } \mathbb{R}^3 \setminus \Omega_1. \end{split}$$

Application of Green's formula (4.2.7) for the Helmholtz equation over  $\Omega_1, \Omega_2$  gives

$$\int_{\Omega_1} |\nabla \varphi_1|^2 - \kappa^2 |\varphi_1|^2 + \int_{\Omega_2} |\nabla \varphi_2|^2 - \kappa^2 |\varphi_2|^2 = \int_{\Gamma_0} \overline{\varphi_1} \partial_n \varphi_1 + \int_{\Gamma \setminus \Gamma_0} \overline{\varphi_1} \partial_n \varphi_1 + (4.3.16)$$
$$\int_{\partial B_R} \overline{\varphi_2} \partial_n \varphi_2 - \int_{\Gamma_0} \overline{\varphi_2} \partial_n \varphi_2 - \int_{\Gamma \setminus \Gamma_0} \overline{\varphi_2} \partial_n \varphi_2$$
$$= \int_{\partial B_R} \overline{\varphi_2} \partial_n \varphi_2. \tag{4.3.17}$$

In the last step, application of the transmission conditions plus g = 0 reduces the right-hand side by canceling the terms on  $\Gamma_0, \Gamma \setminus \Gamma_0$ .

If  $\kappa > 0$  (Im( $\kappa$ ) = 0), the Sommerfeld condition implies that

$$\int_{\partial B_R} \overline{\varphi_2} \partial_n \varphi_2 = i\kappa \int_{\partial B_R} |\varphi_2|^2 + O(1/r)$$

Therefore, as  $Im(\cdot)$  of the left-hand side of (4.3.17) is zero,

$$\kappa \int_{\partial B_R} |\varphi_2|^2 \to 0 \text{ as } R \to \infty$$

This implies by a theorem of Rellich [113, Theorem 4.2] that  $\varphi_2 = 0$  in  $\mathbb{R}^3 \setminus \Omega_1$ . Thus,  $\varphi_1$  solves the Helmholtz equation with the homogeneous boundary data

$$\partial_n \varphi_1 = 0 \text{ on } \Gamma, \varphi_1 = 0 \text{ on } \Gamma \setminus \Gamma_0,$$

whence Green's identity implies that  $\varphi_1 = 0$  on  $\Omega_1$ .

Now, consider the case  $\kappa = 0$  or  $\text{Im}(\kappa) > 0$ . It will be shown that in this case,

$$\int_{\partial B_R} \overline{\varphi_2} \partial_n \varphi_2 \to 0 \text{ as } R \to \infty.$$
(4.3.18)

 $\varphi_2$  can be computed via the exterior representation formula (4.2.11) on  $\Gamma$ :

$$\varphi_2(x') = \int_{\Gamma} \partial_{n,x} G(x, x') \gamma^+ \varphi(x) - \partial_n^+ \varphi(x) G(x, x') \, dx.$$

The entire integrand is proportional to the Green's function  $\exp(i\kappa r)/4\pi r$  (where r = |x - x'|). If  $\operatorname{Im}(\kappa) > 0$ , then  $\varphi_2$  will decay exponentially with r, and (4.3.18) is satisfied. If  $\kappa = 0$ , the Sommerfeld condition (4.2.5c) ensures that

$$\int_{\partial B_R} \overline{\varphi_2} \partial_n \varphi_2 = O(1/R),$$

and (4.3.18) is also satisfied.

Therefore, the real and imaginary parts of the left-hand side of (4.3.17) vanish, implying that  $\varphi_2 = 0$  on  $\mathbb{R}^3 \setminus \Omega_1$ . Therefore,  $\varphi_1 = 0$  on  $\Omega_1$ , as before.

Next, the representation formula must be established for the screen problem.

**Theorem 4.3.6 (Screen representation formula)** Let  $\varphi \in H^1_{loc}(\mathbb{R}^3 \setminus \Gamma_0)$  be a solution to the screen problem (4.3.15). Then for  $x' \notin \Gamma_0$ ,

$$\varphi(x') = \int_{\Gamma_0} [\varphi]_{\Gamma_0} \partial_{n,x} G(x, x') \, dx. \tag{4.3.19}$$

Note the equivalence between (4.3.19) and (4.3.13).

**Proof:** This argument appears in [109, Lemma 2.4].

An important point in the following argument is that given boundary data from an exterior solution to the Helmholtz equation, the exterior representation formula yields zero when computed at interior points. Likewise, given boundary data from an interior solution to the Helmholtz equation, the interior representation formula yields zero when computed at exterior points. See [47, Thm. 3.1].

For points interior (to  $\Omega_1$ ),

$$\varphi(x') = \int_{\Gamma} \partial_n^- \varphi(x) G(x, x') - \partial_{n,x} G(x, x') \gamma^- \varphi(x) \, dx$$
$$0 = \int_{\Gamma} \partial_{n,x} G(x, x') \gamma^+ \varphi(x) - \partial_n^+ \varphi(x) G(x, x') \, dx$$

For points exterior (to  $\Omega_1$ ),

$$0 = \int_{\Gamma} \partial_n^- \varphi(x) G(x, x') - \partial_{n,x} G(x, x') \gamma^- \varphi(x) \, dx$$
$$\varphi(x') = \int_{\Gamma} \partial_{n,x} G(x, x') \gamma^+ \varphi(x) - \partial_n^+ \varphi(x) G(x, x') \, dx$$

In either case, the two equations add to

$$\varphi(x') = \int_{\Gamma} G(x, x') \underbrace{\left(\partial_n^- \varphi(x) - \partial_n^+ \varphi(x)\right)}_{=0 \text{ on } \Gamma} + \partial_{n,x} G(x, x') \underbrace{\left(\gamma^+ \varphi(x) - \gamma^- \varphi(x)\right)}_{=0 \text{ on } \Gamma \setminus \Gamma_0} dx,$$

which immediately yields the desired representation formula.

Recall that the integral operator  $D_{\Gamma_0}$  is defined via restriction of the usual integral operator D to the surface patch  $\Gamma_0 = \phi(\Omega_0)$ .

### Lemma 4.3.7 (Equivalence of the corresponding integral equation)

For given Neumann data  $g \in H^{-1/2}(\Gamma_0)$ , the jump  $[\varphi]_{\Gamma_0} \in H^{1/2}(\Gamma_0)$  solves the integral equation (cf. 4.3.14)

$$D_{\Gamma_0}\psi = -g \tag{4.3.20}$$

if and only if  $\varphi$  solves (4.3.15).

**Proof:** Suppose that  $\varphi \in H^1_{\text{loc}}(\mathbb{R}^3 \setminus \Gamma_0)$  solves (4.3.15). Apply  $\partial_n$  to the representation formula (4.3.19), and recall (4.3.2d) to see that  $[\varphi]_{\Gamma_0}$  solves (4.3.20).

Conversely, suppose that  $[\varphi]_{\Gamma_0} \in H^{1/2}(\Gamma)$  solves (4.3.20). Apply the representation formula (4.3.19) to  $[\varphi]_{\Gamma_0}$  and check that (4.3.15) is satisfied. Certainly, the Sommerfeld condition is satisfied. For  $x \notin \Gamma_0$ , the Helmholtz operator  $(\Delta + \kappa^2)$  may be moved inside the integral of the representation formula, as  $\varphi$  is  $C^{\infty}$  away from  $\Gamma_0$ . Application of  $\partial_n$  to the representation formula confirms that the boundary data matches. The more technical question of whether  $\varphi$  as determined from  $[\varphi]_{\Gamma_0}$  is in  $H^1_{\text{loc}}(\mathbb{R}^3 \setminus \Gamma_0)$  is addressed in [109, Theorem 2.6].

With these tools in hand, the main result can be proven.

#### Theorem 4.3.8 (Well-posedness of thin boundary integral equations)

Let  $\Gamma_0 \subset \mathbb{R}^3$  be an open, bounded, simply-connected Lipschitz surface (i.e., locally the graph of a Lipschitz function), and let  $g \in H^{-1/2}(\Gamma_0)$ . Let  $D_{\Gamma_0}$  be the hypersingular operator restricted to  $\Gamma_0$ . Then (4.3.20) has a unique solution  $\varphi \in H^{1/2}(\Gamma_0)$ .

#### **Proof:**

Extend  $\Gamma_0$  to enclose a bounded Lipschitz domain  $\Omega$ , with  $\partial \Omega = \Gamma$ . Then by [48, Theorem 2], there exists a constant c, and a compact operator T such that for every  $\varrho \in H^{1/2}(\Gamma)$ ,

$$\operatorname{Re}\langle (D+T)\varrho, \overline{\varrho} \rangle \ge c \|\varrho\|_{H^{1/2}(\Gamma)}^2$$

Extension by zero of  $\rho \in H^{1/2}(\Gamma_0)$  to the whole surface  $\Gamma$  shows that this strong ellipticity property also holds on the surface patch  $\Gamma_0$ : for every  $\rho \in H^{1/2}(\Gamma_0)$ ,

$$\operatorname{Re}\langle (D_{\Gamma_0} + T_{\Gamma_0})\varrho, \overline{\varrho} \rangle \ge c \|\varrho\|_{H^{1/2}(\Gamma_0)}^2.$$

Thus,  $D_{\Gamma_0}$  is Fredholm with index 0. Injectivity (and therefore invertibility) of D fails if and only if  $\kappa^2$  is an eigenvalue of the Laplacian on  $\Omega$ . However, by lemmas 4.3.5 and 4.3.7,  $D_{\Gamma_0}$  is injective for any  $\kappa$ , and therefore, existence of solutions to (4.3.20)



Figure 4.4: The  $L^2$ -error vs. mesh size h for an exterior Neumann problem on the unit sphere with constant data  $\partial_n \varphi = 1$ . The constant analytic solution  $\varphi = 1/(i\kappa - 1)$ comes from [49].

follows from uniqueness.

# 4.4 Numerical Examples

In this section, two numerical examples are presented to illustrate the convergence behavior of the piecewise-linear Galerkin boundary element scheme described in §C.1. In both cases, the given exterior Neumann data is smooth, and so the error estimate of [105, Thm. 2.3] gives

$$\|\varphi - \varphi_h\|_{L^2(\Gamma)} \le Ch^2 \|\varphi\|_{H^2(\Gamma)},$$



Figure 4.5: The  $L^2$ -error vs. mesh size h for an exterior Neumann problem on the unit sphere. The data is constructed using the Green's function with a source point interior to the sphere, i.e.,  $\partial_n \varphi = \partial_{n,x} \exp(i\kappa |x - x'|)/4\pi |x - x'|$ , with x' = (0, 0, 1/2). The corresponding Dirichlet data is thus  $\exp(i\kappa |x - x'|)/4\pi |x - x'|$ .

i.e., quadratic error in the  $L^2$ -norm for mesh size h. This is indeed what is observed in figures 4.4,4.5.

# 4.5 Shape Optimization with Boundary Integral Equations

Eppler and Harbrecht propose the solution of boundary shape optimization problems by means of boundary integral equations. They consider three-dimensional electromagnetic problems in [59], and compute first [58] and second [60] derivatives of the boundary integral operators for two-dimensional problems, using wavelet bases for acceleration. Some work has been done with boundary integral equations for topology optimization problems (obstacle location) in [27, 26]. Boundary shape derivatives are also developed without integral equations, e.g., in [52, 71].

While one would expect that shape differentiation increases the order of the kernel singularity of the integral, it turns out that for  $C^2$  surfaces, the singularity remains of the same order. This result is proven by Potthast [101, 102], and is the basis for the result I state in the next section about Fréchet differentiability for the weak form of the hypersingular operator. However, for implementation purposes, quite a bit more work is required to deal with the modified kernel, and it is also necessary to keep track of changes in geometric quantities such as element area factors and normal vectors. Thus, due presumably to the tedium of the implementation, there is little about shape derivatives in the engineering literature. There is a sensitivity study in [86] for a one-way coupled problem that does not appear to use adjoint equations.

# 4.5.1 Shape Differentiation of the Hypersingular Operator

Up until now, the boundary integral equations have been stated as integrals over the boundary  $\Gamma$  of a domain  $\Omega^-$  or a screen  $\Gamma_0$ . In order to compute shape derivatives, it is necessary to represent the shape of this surface as a mapping from reference

coordinates into  $\mathbb{R}^3$ . For the description of screen surfaces  $\Gamma_0$ , the language of the shell chapter is the natural choice.

Let  $\Omega_0 \subset \mathbb{R}^2$ , with the chart function  $\phi \in C^2(\Omega_0)^3$ . The weak form

$$\langle D_{\Gamma_0}\varphi,\varrho\rangle_{\Gamma_0} = \langle V(n\times\nabla\varphi), n\times\nabla\varrho\rangle_{\Gamma_0} - \kappa^2 \langle V(\varphi n),\varrho n\rangle_{\Gamma_0}$$

from theorem 4.3.2 is to be evaluated for  $\Gamma_0 = \phi(\Omega_0)$ .

In particular, recall the definitions given in §3.1.3 of the quantities  $a_3$  and  $\sqrt{a}$ :

$$a_{3} = \frac{\partial_{1}\phi \times \partial_{2}\phi}{\|\partial_{1}\phi \times \partial_{2}\phi\|},$$
  
$$\sqrt{a} = \sqrt{(\partial_{1}\phi \cdot \partial_{1}\phi)(\partial_{2}\phi \cdot \partial_{2}\phi) - (\partial_{1}\phi \cdot \partial_{2}\phi)^{2}},$$

In the double integral below, these are written using superscripts x or y to indicate the integration variable on which they depend, i.e.,

$$a_3^x \equiv a_3(x) = \frac{\partial_1 \phi(x) \times \partial_2 \phi(x)}{\|\partial_1 \phi(x) \times \partial_2 \phi(x)\|},\tag{4.5.1a}$$

$$\sqrt{a^x} \equiv \sqrt{a(x)} = \sqrt{(\partial_1 \phi(x) \cdot \partial_1 \phi(x))(\partial_2 \phi(x) \cdot \partial_2 \phi(x)) - (\partial_1 \phi(x) \cdot \partial_2 \phi(x))^2}.$$
 (4.5.1b)

Thus, the product  $\langle D_{\Gamma_0}\varphi, \varrho \rangle_{\Gamma_0}$  for  $\Gamma_0 = \phi(\Omega_0)$  becomes

$$\langle D(\phi)\varphi, \varrho \rangle_{\Omega_{0}}$$

$$= \iint_{\Omega_{0}} G(\phi(x), \phi(y)) \left( a_{3}^{y} \times \nabla \Phi^{-T}(x) \widetilde{\nabla} \varphi(y) \right) \cdot \left( a_{3}^{x} \times \nabla \Phi^{-T}(x) \widetilde{\nabla} \varrho(x) \right) \sqrt{a^{y}} \sqrt{a^{x}} \, dy dx$$

$$- \kappa^{2} \iint_{\Omega_{0}} G(\phi(x), \phi(y)) \left( a_{3}^{y} \varphi(y) \right) \cdot \left( a_{3}^{x} \varrho(x) \right) \sqrt{a^{y}} \sqrt{a^{x}} \, dy dx,$$

$$(4.5.2)$$

where

$$\Phi(x_1, x_2, x_3) = \phi(x_1, x_2) + a_3 x_3$$

and the derivative  $\widetilde{\nabla}$  is defined via

$$\widetilde{\nabla}\varphi(y) = \begin{pmatrix} \partial_{y_1}\varphi & \partial_{y_2}\varphi & 0 \end{pmatrix}^T.$$

In (4.5.2) the notation  $D(\phi)$  is used to emphasize that for the screen  $\Gamma_0 = \phi(\Omega_0)$ the hypersingular operator depends on the chart function  $\phi$ . The Fréchet differentiability of the hypersingular integral operator D in the weak form follows from the work of Potthast [101] for  $C^2$  charts, and is stated in the following theorem. In the following theorem recall that

$$G(\phi(x),\phi(y)) = \frac{\exp(i\kappa|\phi(x) - \phi(y)|)}{4\pi|\phi(x) - \phi(y)|} = \frac{\exp(i\kappa r(x,y))}{4\pi r(x,y)}$$

with  $r(x, y) = |\phi(x) - \phi(y)|$ .

**Theorem 4.5.1 (BEM Shape Derivatives)** Let  $\phi \in C^2(\Omega_0)^3$ , and let the chart function space be

$$\mathcal{C} = \left\{ \phi \in C^2(\Omega_0)^3 : \|\phi\|_{C^2(\Omega_0)^3} \le l \right\},\,$$

for some fixed l > 0. Then the mapping

$$\mathcal{C} \ni \phi \to \langle D(\phi)\varphi, \varrho \rangle_{\Omega_0} \in \mathbb{C}$$

is continuously Fréchet differentiable, and the derivative in the direction  $\delta\phi$  is

$$\begin{split} D_{\phi} \langle D(\phi)\varphi, \varrho \rangle_{\Omega_{0}} \delta\phi \\ &= \iint_{\Omega_{0}} \left( \frac{\partial G}{\partial r} (\bullet) \frac{\partial r}{\partial \phi} (\bullet) \delta\phi(a_{3}^{y} \times \nabla \Phi^{-T}(x) \widetilde{\nabla} \varphi(y)) \cdot (a_{3}^{x} \times \nabla \Phi^{-T}(x) \widetilde{\nabla} \varrho(x)) \right. \\ &\quad + G(\bullet) D_{\phi} ((a_{3}^{y} \times \nabla \Phi^{-T}(x) \widetilde{\nabla} \varphi(y)) \cdot (a_{3}^{x} \times \nabla \Phi^{-T}(x) \widetilde{\nabla} \varrho(x))) \delta\phi \right) \sqrt{a^{y}} \sqrt{a^{x}} \, dy dx \\ &\quad - \kappa^{2} \iint_{\Omega_{0}} \left( \frac{\partial G}{\partial r} (\bullet) \frac{\partial r}{\partial \phi} (\bullet) \delta\phi(a_{3}^{y} \varphi(y)) \cdot (a_{3}^{x} \varrho(x)) + G(\bullet) \varphi(y) \varrho(x) D_{\phi}(a_{3}^{y} \cdot a_{3}^{x}) \delta\phi \right) \sqrt{a^{y}} \sqrt{a^{x}} \, dy dx \\ &\quad + \iint_{\Omega_{0}} G(\bullet) (a_{3}^{y} \times \nabla \Phi^{-T}(x) \widetilde{\nabla} \varphi(y)) \cdot (a_{3}^{x} \times \nabla \Phi^{-T}(x) \widetilde{\nabla} \varrho(x)) D_{\phi}(\sqrt{a^{y}} \sqrt{a^{x}}) \delta\phi \, dy dx \\ &\quad - \kappa^{2} \iint_{\Omega_{0}} G(\bullet) (a_{3}^{y} \varphi(y)) \cdot (a_{3}^{x} \varrho(x)) D_{\phi}(\sqrt{a^{y}} \sqrt{a^{x}}) \delta\phi \, dy dx. \end{split}$$

$$(4.5.3)$$

Here, the abbreviations  $G(\bullet) = G(\phi(x), \phi(y))$ ,

$$\frac{\partial G}{\partial r}(\bullet) = \frac{\partial}{\partial r} \left( \frac{\exp(i\kappa r)}{4\pi r} \right) \Big|_{r} = |\phi(x) - \phi(y)|$$

and

$$\frac{\partial r}{\partial \phi}(\bullet)\delta\phi = \frac{\phi(x) - \phi(y)}{|\phi(x) - \phi(y)|} \cdot \left(\delta\phi(x) - \delta\phi(y)\right)$$

are used. In addition,  $a_3^x, a_3^y$  and  $\sqrt{a^x}, \sqrt{a^y}$ , depend on  $\phi$ ; see (4.5.1).

**Proof:** Potthast, shows in [101, Thm. 3] that under these assumptions, the kernel remains weakly singular after Fréchet differentiation. The integrand in (4.5.3) therefore includes weakly singular kernels multiplied against a function composed of geometric factors, the vector operations  $\cdot$  and  $\times$ , and the functions  $\varphi$ ,  $\varrho$ . It is established in the proof of theorem 3.5.1 that the geometric terms  $\sqrt{a}$ ,  $a_3$  are continuously Fréchet differentiable with respect to  $\phi$ , implying that the integrand is also. Since  $C \times \overline{\Omega_0}$  is compact, uniform continuity implies that the differentiation and integration can be interchanged.

In the implementation, I use a singular quadrature method developed in [98]. New analytic integration routines are also required: see §C.2.1. The derivatives of the geometric quantities in (4.5.3) are worked out in §C.2.2. Numerical tests show agreement between the directional derivative and finite differences.

# Chapter 5

# Coupling between Elastic and Acoustic Problems

# 5.1 Introduction

The elastic component of the coupled problem (1.2.1) is recast in a weak form:

$$\int_{\Omega^{-}} (H:e(u)): e(\overline{v}) - \omega^{2} \rho u \cdot \overline{v} \, dx = \int_{\Gamma} (f - i\omega \rho_{0} \varphi n) \cdot \overline{v} \, dx \quad \forall v \in H^{1}(\Omega^{-})^{3} \quad (5.1.1a)$$
$$\partial_{n} \varphi = -i\omega u \cdot n \qquad \qquad \text{on } \Gamma \quad (5.1.1b)$$

$$\Delta \varphi + \kappa^2 \varphi = 0 \qquad \qquad \text{in } \Omega^+ \quad (5.1.1c)$$

$$|\nabla \varphi \cdot x/|x| - i\kappa\varphi| = O\left(1/|x|^2\right) \qquad \text{as } |x| \to \infty. \quad (5.1.1d)$$

First, in §5.2, the existence and uniqueness theory for the coupled problem (5.1.1) worked out by Bielak, MacCamy, and Zeng in [22] is restated using the notation of this thesis. A significant deficiency of [22] is that it does not characterize the situations in which uniqueness can fail. This issue is cleared up in [90], but I otherwise prefer the exposition of the former. The crux of the matter is that it is possible in general for the elastic body to have a "Jones mode," a free eigenmode that exhibits no surface motion in the normal direction, and thus does not drive the acoustics. This is known to be possible for spheres and axisymmetric structures [90], but almost never happens for

general shapes, as shown by [73]: it turns out that any sufficiently smooth boundary can be approximated arbitrarily well by shapes that have no Jones modes.

This work was later extended to more general situations. In [80, 81], the problem is considered with an anisotropic inviscid fluid, and an anisotropic thermoelastic body.

Having summarized existing results for (5.1.1), in §5.3, three-dimensional elasticity is replaced with Naghdi shells (§3.2), and the boundary integral equations with the hypersingular "thin" boundary integral equation (§4.3.2). The existence and uniqueness result is then extended to cover this case. Finite element implementation is discussed in §5.3.2. Finally, in §5.4, adjoint equations are derived, and optimization results presented.

# 5.2 3d Elasticity Coupled to Boundary Integral Equations

It turns out that in general, uniqueness of solutions for the coupled problem (5.1.1) does not hold. Uniqueness can fail if there exists an eigenmode of the elastic structure that does not drive the acoustics. The elastic displacement  $0 \neq u \in H^1(\Omega^-)^3$  is called a *Jones mode* at frequency  $\omega$  if

$$\int_{\Omega^-} (H : e(u)) : e(\overline{v}) - \omega^2 \rho u \cdot \overline{v} \, dx = 0, \, \forall v \in H^1(\Omega^-)^3$$
$$u \cdot n = 0, \text{ on } \Gamma.$$

In the absence of Jones modes, the following lemma guarantees uniqueness of solutions to (5.1.1). The key physical idea is that the elastic boundary forcing (the sum of the contribution from f and  $\varphi$  in (5.1.1a)) does no net work on the structure. Therefore, if f = 0, the structure does no net work on the air, and it can then be shown that  $\varphi = 0$ , and that either u = 0, or u is a Jones mode.

**Lemma 5.2.1** If  $\Omega^-$  has no Jones modes at frequency  $\omega$ , then (5.1.1) has at most one solution

$$(u,\varphi) \in H^1(\Omega^-)^3 \times H^1_{loc}(\Omega^+).$$

**Proof:** It suffices to show that if  $(u, \varphi)$  solves (5.1.1) with f = 0, then  $\varphi \equiv 0$  in  $\Omega^+$ . Given that this is true,  $\varphi = \partial_n \varphi = 0$  on  $\Gamma$ , and therefore either u = 0, or u is a Jones mode.

So let f = 0. Combining (5.1.1a,b) and taking v = u,

$$\int_{\Omega^{-}} (H:e(u)): e(\overline{u}) - \omega^{2} \rho u \cdot \overline{u} \, dx = \rho_{0} \omega^{2} \int_{\Gamma} \varphi \partial_{n} \overline{\varphi} \, dx.$$

By symmetry of the elastic bilinear form, the imaginary part of the left-hand side equals zero. Therefore,

$$\operatorname{Im}\left(\int_{\Gamma}\varphi\partial_{n}\overline{\varphi}\,dx\right)=0.$$

Thus, as in the proof of lemma 4.3.5, one can conclude via Rellich's theorem ([113, Theorem 4.2],[97, Lemma 9.9]) that  $\varphi \equiv 0$  in  $\Omega^+$ . This completes the proof.

Upon replacement of the exterior Helmholtz equation with the Burton-Miller method of §4.3.1 (with  $0 \neq \eta \in \mathbb{R}$ ), (5.1.1) becomes

$$\int_{\Omega^{-}} (H:e(u)): e(\overline{v}) - \omega^{2} \rho u \cdot \overline{v} \, dx = \int_{\Gamma} (f - i\omega \rho_{0} \varphi n) \cdot \overline{v} \, dx \qquad \forall v \in H^{1}(\Omega^{-})^{3}$$
(5.2.1a)

$$\left(-\frac{1}{2}I + K + i\eta D\right)\varphi = \left(V - i\eta\left(\frac{1}{2}I + K^*\right)\right)\left(-i\omega u \cdot n\right) \quad \text{in } H^{-1/2}(\Gamma).$$
(5.2.1b)

Instead of Burton-Miller, MacCamy et al. [22] use the method of Brakhage and Werner [29], which by use of an indirect formulation gives unique solutions at all frequencies to integral equations for the exterior Dirichlet problem. However, the authors later formulate the coupled problem using a linear combination of Burton-Miller and Brakhage-Werner in order to achieve a symmetric finite element discretization. For the uniqueness result, all that maters is that the integral equation have a unique solution.

**Theorem 5.2.2 (Uniqueness of Solutions to (5.2.1))** Assume that  $\Omega^-$  has no Jones modes at frequency  $\omega$ . Then the coupled problem with the Burton-Miller integral equations (5.2.1) has at most one solution.

**Proof:** Let  $(u, \varphi_{\Gamma})$  be a solution to (5.2.1) with f = 0. Then  $(u, \varphi)$ , with  $\varphi \in H^1_{\text{loc}}(\Omega^+)$  determined from the surface data by the representation formula (4.2.11) via

$$\varphi = DL\varphi_{\Gamma} - SL(-i\omega u \cdot n)$$

solves (5.1.1) with f = 0. Thus, since  $\Omega^-$  is assumed to have no Jones modes, it holds by lemma 5.2.1 that  $(u, \varphi) = (0, 0)$ . Since u = 0, the right-hand side in (5.2.1b) is zero, and thus, by theorem 4.3.4,  $\varphi_{\Gamma} = 0$ .

Now, (5.2.1) is stated using operator notation: find  $(u, \varphi) \in \mathcal{U} = H^1(\Omega)^3 \times H^{1/2}(\Gamma)$ such that for all  $(v, \varrho) \in \mathcal{U}$ ,

$$A(u, v) + B(\varphi, v) = F(v)$$
(5.2.2a)

$$C(u,\varrho) + E(\varphi,\varrho) = G(\varrho), \qquad (5.2.2b)$$

with

$$\begin{split} A(u,v) &= \int_{\Omega^{-}} (H:e(u)): e(\overline{v}) - \omega^{2} \rho u \cdot \overline{v} \, dx \\ B(\varphi,v) &= \int_{\Gamma} i \omega \rho_{0} \varphi n \cdot \overline{v} \, dx \\ F(v) &= \int_{\Gamma} f \cdot \overline{v} \, dx \\ C(u,\varrho) &= \left\langle \left(V - i\eta \left(\frac{1}{2}I + K^{*}\right)\right) \left(-i\omega u \cdot n\right), \overline{\varrho}\right\rangle_{H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)} \\ E(\varphi,\varrho) &= \left\langle \left(-\frac{1}{2}I + K + i\eta D\right)\varphi, \overline{\varrho}\right\rangle_{H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)} \\ G(\varrho) = 0. \end{split}$$

The operator  $\tilde{A}: H^1(\Omega^-)^3 \to (H^1(\Omega^-)^3)'$  is defined by

$$A(u,v) = \langle \hat{A}(u), v \rangle$$

Analogous definitions are made for B, C, E. For the functionals F, G, these are, e.g.,

$$\langle \tilde{F}, v \rangle = F(v).$$

The key observation of Bielak, MacCamy, and Zeng is that the forms A, E are nearly coercive. For A, by Korn's second inequality, there exist constants  $k_1, k_0 > 0$ such that

$$A(u,u) \ge k_1 \|u\|_{H^1(\Omega^-)^3}^2 - k_0 \|u\|_{L^2(\Omega^-)}^2.$$
(5.2.3)

For E, consider a decomposition of the hypersingular operator D, suggested by the following lemma.

**Lemma 5.2.3** Let  $D_0$  be the hypersingular operator defined for the imaginary wave number  $\kappa = i$ . Then there exists a constant c such that

$$\langle D_0\varphi,\overline{\varphi}\rangle_{H^{-1/2}(\Gamma)\times H^{1/2}(\Gamma)} \ge c \|\varphi\|^2_{H^{1/2}(\Gamma)}, \ \forall \varphi \in H^{1/2}(\Gamma).$$

**Proof:** See [22, Lemma 4.1].

With  $D = D_0 + D_1$ , define  $E_0, E_1$  by

$$E_{0}(\varphi, \varrho) = \langle i\eta D_{0}\varphi, \overline{\varrho} \rangle_{H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)}$$
  
$$E_{1}(\varphi, \varrho) = \langle \left( -\frac{1}{2}I + K + i\eta D_{1} \right) \varphi, \overline{\varrho} \rangle_{H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma)},$$

and  $A_0, A_1$  by

$$A_0(u,v) = \int_{\Omega^-} (H:e(u)): e(\overline{v}) + k_0 u \cdot \overline{v} \, dx,$$
  
$$A_1(u,v) = \int_{\Omega^-} -(k_0 + \omega^2 \rho) u \cdot \overline{v} \, dx,$$

where  $k_0$  is the constant appearing in the Korn inequality (5.2.3). Equation (5.2.2) can be rewritten as

$$A_0(u, v) + A_1(u, v) + B(\varphi, v) = F(v)$$
$$C(u, \varrho) + E_0(\varphi, \varrho) + E_1(\varphi, \varrho) = G(\varrho).$$

**Lemma 5.2.4 (Compactness)** The operators  $\tilde{A}_1, \tilde{B}, \tilde{C}, \tilde{E}_1$  are compact.

**Proof:** See [22, Lemma 4.3].

The following theorem also appears as [77, Thm. 5.6]; it differs from [22, Thm. 3.1] in that different integral equations are used for the Helmholtz problem.

**Theorem 5.2.5 (Existence and Uniqueness)** For every  $f \in H^{1/2}(\Gamma)$ , provided that  $\Omega^-$  has no Jones modes, (5.2.2) has a unique solution.

**Proof:** Switching to operator form and using the invertibility of  $\tilde{A}_0, \tilde{E}_0$ , (5.2.2) becomes

$$u + \tilde{A}_0^{-1} \tilde{A}_1 u + \tilde{A}_0^{-1} \tilde{B} \varphi = \tilde{A}_0^{-1} \tilde{F}$$
$$\tilde{E}_0^{-1} \tilde{C} u + \varphi + \tilde{E}_0^{-1} \tilde{E}_1 \varphi = \tilde{E}_0^{-1} \tilde{G}.$$

This can be written

$$\left(I + \begin{pmatrix} \tilde{A_0}^{-1} \tilde{A_1} & \tilde{A_0}^{-1} \tilde{B} \\ \tilde{E_0}^{-1} \tilde{C} & \tilde{E_0}^{-1} \tilde{E_1} \end{pmatrix} \right) \begin{pmatrix} u \\ \varphi \end{pmatrix} = \begin{pmatrix} \tilde{A_0}^{-1} \tilde{F} \\ \tilde{E_0}^{-1} \tilde{G} \end{pmatrix}.$$

Due to the compactness of the operators  $\tilde{A}_1, \tilde{B}, \tilde{C}, \tilde{E}_1$  (lemma 5.2.4), the operator on the left hand side is Fredholm with index 0. Thus, in order to show existence, it suffices to show uniqueness. But if  $(u, \varphi)$  solves (5.2.2) for F = 0, G = 0, then it also solves (5.2.1), with f = 0. Thus, by theorem 5.2.2,  $(u, \varphi) = (0, 0)$ .

 $\square$ 

# Shell Equations Coupled to Boundary Integral

# Equations

5.3

The coupled problem (5.1.1) is now stated in the case that the body is a shell, using the assumed equality of normal velocity across the thickness to solve the exterior Helmholtz problem with (4.3.15). The elastic terms in (1.2.1) are replaced with (3.2.6) and (3.2.8).

One seeks  $U = (\theta, z)$  in  $\mathcal{U} = \{(\theta, z) \in H^1(\Omega_0)^3 \times H^1(\Omega_0)^3 : \theta \cdot a_3 = 0 \text{ a.e.}\}$  and  $\varphi$  in  $H^1_{\text{loc}}(\mathbb{R}^3 \setminus \phi(\Omega_0))$  such that

$$K(\theta, z; \overline{\eta}, \overline{y}) - \omega^2 M(\theta, z; \overline{\eta}, \overline{y})$$

$$= \int_{\Omega_0} (f \cdot \overline{y} - i\omega \rho_0 \varphi(\phi(x)) \overline{y} \cdot n) \sqrt{a} \, dx \quad \forall V = (\eta, y) \in \mathcal{U} \quad (5.3.1a)$$

$$\partial_{\tau} \varphi = -i\omega z \cdot n \qquad \text{on } \phi(\Omega_0) \quad (5.3.1b)$$

$$\Delta \varphi + \kappa^2 \varphi = 0 \qquad \qquad \text{in } \mathbb{R}^3 \setminus \phi(\Omega_0) \quad (5.3.1c)$$

$$|\nabla \varphi \cdot x/|x| - i\kappa \varphi| = O\left(1/|x|^2\right) \qquad \text{as } |x| \to \infty.$$
 (5.3.1d)

Analogous to lemma 5.2.1, the following lemma characterizes conditions required for uniqueness to solutions of (5.3.1).

**Lemma 5.3.1** Provided that there do not exist any Jones modes at frequency  $\omega$ , i.e., that there are no  $0 \neq U = (\theta, z) \in \mathcal{U}$  such that

$$\begin{split} K(\theta, z; \overline{\eta}, \overline{y}) - \omega^2 M(\theta, z; \overline{\eta}, \overline{y}) = 0 & \forall V = (\eta, y) \in \mathcal{U} \\ z \cdot n = 0, & on \ \Gamma, \end{split}$$

then (5.3.1) has at most one solution.

**Proof:** Once again, it suffices to show that if  $(\theta, z, \varphi)$  solves (5.3.1) with f = 0, then  $\varphi \equiv 0$  in  $\mathbb{R}^3 \setminus \phi(\Omega_0)$ . Given that this is true,  $\varphi = \partial_n \varphi = 0$  on  $\phi(\Omega_0)$ , and therefore either  $(\theta, z) = 0$ , or  $(\theta, z)$  is a Jones mode.

So let f = 0. Combining (5.3.1a,b) and taking  $(\eta, y) = (\theta, z)$ ,

$$K(\theta, z; \overline{\theta}, \overline{z}) - \omega^2 M(\theta, z; \overline{\theta}, \overline{z}) = \rho_0 \omega^2 \int_{\Omega_0} \varphi \partial_n \overline{\varphi} \sqrt{a} \, dx.$$

By symmetry of the shell bilinear form K (3.2.7), the imaginary part of the left-hand side equals zero. Therefore,

$$\operatorname{Im}\left(\int_{\Omega_0} \varphi \partial_n \overline{\varphi} \sqrt{a} \, dx\right) = 0. \tag{5.3.2}$$

However, one cannot conclude the proof just yet because  $\phi(\Omega_0)$  is not a closed surface, and so the argument of lemma 5.2.1 cannot be applied directly. However, using the construction of lemma 4.3.5, namely to extend the surface  $\Gamma = \phi(\Omega_0)$  to enclose a region  $\Omega_1$ , and work out the junction conditions at the interface, equation (4.3.16) will result from application of Green's formula. In this case, the terms on the fictitious surface  $\Gamma^c$  will still cancel, as  $\varphi$  is continuous away from  $\Gamma$ . In the proof of lemma 4.3.5, the zero Neumann data was necessary to eliminate the terms of (4.3.16) on  $\Gamma$  itself; the condition (5.3.2) now suffices to do so. The rest of the argument can thus be carried through without further modification to conclude that  $\varphi \equiv 0$  in  $\mathbb{R}^3 \setminus \phi(\Omega_0)$ . This completes the proof.

With this uniqueness result, the Helmholtz screen problem can be replaced with equivalent boundary integral equations, and consider the question of existence of solutions. The following problem is the primary focus of this work.

### **Problem 4** [Shell coupled to thin BEM]

Find  $U = (\theta, z)$  in  $\mathcal{U} = \{(\theta, z) \in H^1(\Omega_0)^3 \times H^1(\Omega_0)^3 : \theta \cdot a_3 = 0 \text{ a.e.}\}$  and  $\varphi$  in  $H^{1/2}(\phi(\Omega_0))$  such that for all  $V = (\eta, y) \in \mathcal{U}$ , and for all  $\varrho \in H^{1/2}(\phi(\Omega_0))$ ,

$$K(\theta, z; \overline{\eta}, \overline{y}) - \omega^2 M(\theta, z; \overline{\eta}, \overline{y}) = \int_{\Omega_0} \left( f \cdot \overline{y} - i\omega \rho_0 \varphi(\phi(x)) \overline{y} \cdot n \right) \sqrt{a} \, dx \tag{5.3.3a}$$

$$\langle D\varphi, \overline{\varrho} \rangle_{H^{-1/2}(\phi(\Omega_0)) \times H^{1/2}(\phi(\Omega_0)))} = \langle i\omega z(x(\phi)) \cdot n, \overline{\varrho} \rangle_{H^{-1/2}(\phi(\Omega_0)) \times H^{1/2}(\phi(\Omega_0)))}$$
(5.3.3b)

where K, M are the Naghdi stiffness and inertial forms, defined in (3.2.7), (3.2.8).

### 5.3.1 Existence and Uniqueness

For 3d elasticity coupled to the Helmholtz equation (or equivalently, to boundary integral equations), there exist geometries for which Jones modes preclude uniqueness. For shells, this can also happen. As a very simple example, if the shell is flat, then the in-plane motions decouple from the out-of-plane motions. The in-plane problem (2.2.17) is elliptic, so there will be an infinite sequence of positive increasing eigenvalues, corresponding to purely in-plane motions, which do not drive the acoustics through (5.3.3b). If the forcing excites one of these motions, then uniqueness will fail for the coupled problem (5.3.3). This situation seems exceedingly unlikely for general curved shells, or for joined shells, where the in-plane motions of one would drive out-of-plane motions of the other.

**Theorem 5.3.2 (Well-posedness of problem 4)** Let  $\phi \in W^{2,\infty}(\Omega_0)^3$ , and  $f \in L^2(\Omega_0)^3$ . Then if  $\phi$  admits no Jones modes (in the sense of lemma 5.3.1), then there exists a unique solution  $(\theta, z) \in \mathcal{U}, \varphi \in H^{1/2}(\phi(\Omega_0))$  to (5.3.3). Furthermore, the solution depends continuously on f, i.e.,

$$\|(\theta, z)\|_{\mathcal{U}}^2 + \|\varphi\|_{H^{1/2}(\phi(\Omega_0))}^2 \le C(\phi) \|f\|_{L^2(\Omega_0)^2}^2.$$

**Proof:** The basic method of [22], outlined in §5.2, is repeated.

Make the following definitions, analogous to (5.2.2),

$$\begin{aligned} A(U,V) &= K(\theta, z; \overline{\eta}, \overline{y}) - \omega^2 M(\theta, z; \overline{\eta}, \overline{y}) \\ B(\varphi, V) &= \int_{\Omega_0} i\omega \rho_0 \varphi(\phi(x)) \overline{y} \cdot n\sqrt{a} \, dx \\ F(V) &= \int_{\Omega_0} f \cdot \overline{y} \sqrt{a} \, dx \\ C(U, \varrho) &= \langle i\omega z(x(\phi)) \cdot n, \overline{\varrho} \rangle_{H^{-1/2}(\phi(\Omega_0)) \times H^{1/2}(\phi(\Omega_0)))} \\ E(\varphi, \varrho) &= \langle D\varphi, \overline{\varrho} \rangle_{H^{-1/2}(\phi(\Omega_0)) \times H^{1/2}(\phi(\Omega_0)))} \\ G(\varrho) &= 0 \end{aligned}$$

so that (5.3.3) is equivalent to

$$A(U, V) + B(\varphi, V) = F(V)$$
$$C(U, \varrho) + E(\varphi, \varrho) = G(\varrho).$$

Once again, define corresponding operators, e.g.,  $\tilde{A}$  via

$$A(u,v) = \langle \tilde{A}(u), v \rangle.$$

Here, the decomposition  $D = D_0 + D_1$  used in [22] (§5.2) is no longer necessary, as on the "screen"  $\phi(\Omega_0)$ ,  $\tilde{E}$  is invertible by theorem 4.3.8, which requires only that  $\phi(\Omega_0)$  be Lipschitz.

The necessary Korn inequalities on the strain tensors  $\gamma, \chi, \zeta$  in the shell bilinear form K (3.2.6) appear in [25, lemma 3.6] in the context of proving coercivity of the Naghdi bilinear form. Under positive definiteness assumptions on the constitutive tensors  $\tilde{C}^{\alpha\beta\lambda\mu}, \tilde{D}^{\lambda\mu}$ , and in light of (3.2.6), it is clear that for all  $(\theta, z) \in \mathcal{U}$ ,

$$K(\theta, z; \overline{\theta}, \overline{z}) \ge c \|(\theta, z)\|_s^2,$$

where

$$\|(\theta, z)\|_{s} \equiv \left(\sum_{\alpha, \beta} (\|\gamma_{\alpha\beta}(z)\|_{L^{2}(\Omega_{0})}^{2} + \|\chi_{\alpha\beta}(\theta, z)\|_{L^{2}(\Omega_{0})}^{2}) + \sum_{\alpha} \|\zeta_{\alpha}(\theta, z)\|_{L^{2}(\Omega_{0})}^{2}\right)^{1/2}.$$

The quantity  $\|\cdot\|_s$  is in fact a norm. It is equivalent to the Sobolev norm  $\|\cdot\|_{\mathcal{U}}$  if and only if rigid-body modes are prohibited by the boundary conditions. The Korn-type inequalities are

$$\begin{aligned} \|z\|_{H^{1}(\Omega_{0})^{3}}^{2} \leq C_{\gamma} \left( \|z\|_{L^{2}(\Omega_{0})^{3}}^{2} + \sum_{\alpha,\beta} \|\gamma_{\alpha\beta}(z)\|_{L^{2}(\Omega_{0})}^{2} \right) \\ \|(\theta,z)\|_{\mathcal{U}}^{2} \leq C_{\chi} \left( \|(\theta,z)\|_{L^{2}(\Omega_{0})^{2} \times L^{2}(\Omega_{0})}^{2} + \sum_{\alpha,\beta} \|\chi_{\alpha\beta}(\theta,z)\|_{L^{2}(\Omega_{0})}^{2} \right) \\ \|(\theta,z)\|_{\mathcal{U}}^{2} \leq C_{\zeta} \left( \|(\theta,z)\|_{L^{2}(\Omega_{0})^{2} \times L^{2}(\Omega_{0})}^{2} + \sum_{\alpha,\beta} \|\zeta_{\alpha}(\theta,z)\|_{L^{2}(\Omega_{0})}^{2} \right). \end{aligned}$$

These permit the decomposition of K (and thus of A) via

$$A_{0}(U,V) = K(\theta, z; \overline{\eta}, \overline{y}) + k_{0} \int_{\Omega_{0}} \theta \cdot \overline{\eta} + z \cdot \overline{y} \, dx$$
$$A_{1}(U,V) = -\omega^{2} M(\theta, z; \overline{\eta}, \overline{y}) - k_{0} \int_{\Omega_{0}} \theta \cdot \overline{\eta} + z \cdot \overline{y} \, dx,$$

and are proven via application of the two-dimensional Korn inequality to the vector fields

$$w_{\alpha} = z \cdot a_{\alpha}, w'_{\alpha} = \theta \cdot a_{\alpha}.$$

As in the previous section, it is necessary to establish compactness of the noncoercive part, i.e., that the compactness properties of lemma 5.2.4 still hold. The operators are

$$\begin{split} \tilde{A}_1 : \mathcal{U} &\to L^2(\Omega_0)^3 \times \left\{ \theta \in L^2(\Omega)^3 : u \cdot a_3 = 0 \text{ a.e.} \right\} \to \mathcal{U}' \\ \tilde{B} : H^{1/2}(\phi(\Omega_0)) \to H^{-1/2}(\phi(\Omega_0)) \to \mathcal{U}' \\ \tilde{C} : H^{1/2}(\phi(\Omega_0)) \to H^{-1/2}(\phi(\Omega_0)). \end{split}$$

The operator  $\tilde{A}_1$  is the composition of the injection

$$\mathcal{U} \to L^2(\Omega_0)^3 \times \left\{ \theta \in L^2(\Omega)^3 : u \cdot a_3 = 0 \text{ a.e.} \right\},$$

which is compact, and the embedding into  $\mathcal{U}'$ , which is continuous. The operator  $\tilde{B}$  involves the compact embedding  $H^{1/2}(\phi(\Omega_0)) \to H^{-1/2}(\phi(\Omega_0))$ , and the adjoint of the normal trace operator. The operator  $\tilde{C}$  composes the normal trace operator with the compact embedding  $H^{1/2}(\phi(\Omega_0)) \to H^{-1/2}(\phi(\Omega_0))$ .

Therefore, using the invertibility of  $\tilde{A}_0, \tilde{E}$ ,

$$(I+T)\begin{pmatrix} U\\\varphi \end{pmatrix} = \begin{pmatrix} \tilde{A}_0^{-1}\tilde{F}\\ \tilde{E}^{-1}\tilde{G} \end{pmatrix},$$

where

$$T = \begin{pmatrix} \tilde{A_0}^{-1} \tilde{A_1} & \tilde{A_0}^{-1} \tilde{B} \\ \tilde{E}^{-1} \tilde{C} & 0 \end{pmatrix}$$

is compact. The operator on the left-hand side is a compact perturbation of the identity, and thus, the Fredholm alternative applies. By lemma 4.3.7, solutions to (5.3.1) and (5.3.3) are equivalent, and so in the absence of Jones modes, lemma 5.3.1 implies uniqueness and therefore existence.

In order to show continuous dependence of the solution on the right-hand side p, it is necessary to show that the operator

$$\begin{pmatrix} A & B \\ C & E \end{pmatrix}$$

has a bounded inverse. Coercivity of  $\tilde{A}_0$ ,  $\tilde{E}$  implies that  $\tilde{A}_0^{-1}$ ,  $\tilde{E}^{-1}$  are bounded, and therefore, it remains to show that I + T has a bounded inverse. If this is not the case, then -1 is in the spectrum  $\sigma(T)$ . Since T is compact, this implies that -1is also in the point spectrum  $\sigma_p(T)$ . This is a contradiction since I+T is invertible.  $\Box$ 

In the next section, discretization of the coupled problem is discussed.

## 5.3.2 Finite Element Implementation

Finite element implementation of problem 4 is complicated by the fact that the boundary element code implemented in this thesis uses piecewise-linear elements, while the piecewise-linear MITC3 shell element (proposed in [87, Sec. 4], along with the MITC6 elements) is known to suffer from locking, and also exhibits mesh-dependent effects, as discussed in [88]. For a flat middle-surface, it reduces to the MITC3 triangular plate element, described in [38], which is known to be unstable. Following the work of [56, Ex. 4.1], who modified the MITC3 triangular plate element so as to achieve stability, the analogous modification is made to the MITC3 shell element. The utility of this element (as opposed to higher-order shell elements which generally exhibit better performance) is that its geometry is linear, and hence, it matches the boundary elements, making the implementation of the coupling simple: a one-to-one matching of flat facet elements on the boundary, with the same basis functions. In doing this, the implementation of the adjoint equations becomes simpler. The most significant drawback to the modified MITC3 element is that it still does not perform nearly as well with respect to locking as does the MITC6 element for general shell problems. Thus, I have also implemented the coupling with the quadratic MITC6a and MITC6b elements. In this case, once again in order to simplify the implementation, geometry errors are made in the coupling, but much improve the performance in the sense that far fewer boundary elements are required.

Now, consider the implementation of problem 4 in the case of two joined shells with the Galerkin boundary element method of section C.1 for the acoustic problem, and MITC6 shell elements or MITC3 shell elements with the Duran-Liberman modification (the latter described in section B.1.3) for the shell problem. The implementation of the shell coupling is as in §2.5, which describes two plates without acoustics. Let  $K_1, K_2$  be the stiffness matrices,  $M_1, M_2$  be the mass matrices, and  $\vec{F_1}, \vec{F_2}$  be the forcing vectors (corresponding to the term  $p^j v_j$  in (5.3.3a)). Once again,  $S = [S_1, S_2]$  is the matrix that imposes the kinematic constraints.

Each shell has its own mesh on local reference coordinates. These meshes are created to be compatible at the junction, and give rise to a three-dimensional mesh of the shell middle surface, for use with the boundary element code, which uses the matrix  $\widehat{D}(\omega)$  from section C.1.1.

It is also necessary to translate the forcing terms from the global (acoustic) mesh to and from the local shell meshes. For this purpose, the matrix  $N_{\alpha}$  is constructed, which is used to calculate  $\int_{\phi(\Omega_0)} z_3 \rho$  over the elements of shell  $\alpha$ .  $N_{\alpha}^T$  can then calculate  $\int_{\phi(\Omega_0)} y_3 \varphi$ . Note that each of these operations involves translation between the global and local meshes. The finite element system thus appears:

$$\begin{pmatrix} K_1 - \omega^2 M_1 & 0 & S_1^T & i\omega\rho_0 N_1^T \\ 0 & K_2 - \omega^2 M_2 & S_2^T & i\omega\rho_0 N_2^T \\ S_1 & S_2 & 0 & 0 \\ -i\omega N_1 & -i\omega N_2 & 0 & \widehat{D}(\omega) \end{pmatrix} \begin{pmatrix} \vec{U_1} \\ \vec{U_2} \\ \vec{\lambda} \\ \vec{\varphi} \end{pmatrix} = \begin{pmatrix} \vec{F_1} \\ \vec{F_2} \\ \vec{0} \\ \vec{0} \end{pmatrix}.$$
 (5.3.4)

Of all the matrices involved, only  $\widehat{D}$  is dense. Define the matrices

$$A = \begin{pmatrix} K_1 - \omega^2 M_1 & 0 & S_1^T \\ 0 & K_2 - \omega^2 M_2 & S_2^T \\ S_1 & S_2 & 0 \end{pmatrix}$$
$$B = \begin{pmatrix} i\omega\rho_0 N_1^T \\ i\omega\rho_0 N_2^T \\ 0 \end{pmatrix}$$
$$C = \begin{pmatrix} -i\omega N_1 & -i\omega N_2 & 0 \end{pmatrix}$$
$$D = \widehat{D}(\omega)$$

and the vectors

$$\vec{a} = \begin{pmatrix} \vec{F_1} \\ \vec{F_2} \\ 0 \end{pmatrix}, \ \vec{b} = \vec{0}, \ \vec{x} = \begin{pmatrix} \vec{U_1} \\ \vec{U_2} \\ \vec{\lambda} \end{pmatrix}, \ \vec{y} = \vec{\varphi},$$

so that the system (5.3.4), now written

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} \vec{x} \\ \vec{y} \end{pmatrix} = \begin{pmatrix} \vec{a} \\ \vec{b} \end{pmatrix},$$

can be solved via the Schur complement technique:

$$(A - BD^{-1}C)\vec{x} = \vec{a}.$$

The term  $-BD^{-1}\vec{b}$  does not appear on the right hand side because  $\vec{b} = \vec{0}$ . GMRES is used, with dense linear solves to apply  $D^{-1}$ . For larger problems, an accelerated

BEM code would provide matrix-vector products for D, and the application of  $D^{-1}$  would be performed by an iterative solver, as D is typically very well-conditioned.

In general, much can be said about the linear algebra associated with this problem, but with the present implementation, the costs associated with it are so small compared with those of matrix assembly, that I do not address the issue in any detail. For a discussion of solver strategies for this type of problem, see [63]. General theory on numerical solution of saddle-point linear systems can be found in [18].



Figure 5.1: The driven box encloses the region  $[-1, 1] \times [-1, 1] \times [0, 1]$  with unit-circle hole in the top face. It is driven with a spatially Gaussian pulse, centered near the red spot at 200 Hz.

Transfer functions for the box shown in figure 5.1 computed using this method with MITC3 and MITC6 elements are shown for different plate thicknesses in figures 5.2 and 5.3. Agreement is good at most frequencies. I have done some tests at the frequencies where significant discrepancies occur, and found that the linear systems are being solved accurately. I also tried local mesh refinement (and a uniform forcing profile) to rule out the possibility that the refinement of the mesh was changing the response through better resolution of the driving force profile. In general, boundary layers can be a significant issue for both shell problems [36] and thin boundary integral equations [109], but based on numerical experiments, this does not appear to be the case for this problem. I base the calculations on the number of elements required to resolve the shell discretization on the speed of bending waves in Kirchhoff plates (§2.7). Further mesh refinement should resolve these lingering questions, but is too expensive with the present implementation of the boundary element code.



Figure 5.2: Transfer functions of the driven box for t = 0.05. Blue indicates MITC3, while red is used for MITC6. The dashed lines were computed on a mesh with the characteristic length h halved to test for convergence.



Figure 5.3: Transfer functions of the driven box for t = 0.1. Blue indicates MITC3, while red is used for MITC6. The dashed lines were computed on a mesh with the characteristic length h halved to test for convergence.

# 5.4 The Coupled Optimization Problem

In this section, specifics are given to the optimization problem formally suggested in the introduction (§1.2), using the model problem of §5.3. Recall that under the Naghdi model, the shape is determined by the middle-surface chart function  $\phi$ , and the thickness function t. These parameters are denoted  $g = (\phi, t) \in \mathcal{G}$ . The choice of  $\mathcal{G}$  is as yet unspecified.

For  $\omega > 0$ , define the constraint function  $c : \mathcal{G} \times \mathcal{U} \to \mathcal{U}'$  by

$$\langle c(g,U;\omega),V\rangle_{\mathcal{U}'\times\mathcal{U}}$$

$$= K_g(\theta,z;\overline{\eta},\overline{y}) - \omega^2 M_g(\theta,z;\overline{\eta},\overline{y}) - \int_{\Omega_0} (f\cdot\overline{y} - i\omega\rho_0\varphi(\phi(x))\overline{y}\cdot n)\sqrt{a}\,dx$$

$$+ \langle D\varphi,\overline{\varrho}\rangle_{H^{-1/2}(\phi(\Omega_0)))\times H^{1/2}(\phi(\Omega_0)))} - \langle i\omega z(x(\phi)\cdot n),\overline{\varrho}\rangle_{H^{-1/2}(\phi(\Omega_0))\times H^{1/2}(\phi(\Omega_0)))},$$

$$(5.4.1)$$

and solve  $c(g, U; \omega) = 0 \in \mathcal{U}'$ . Assuming that a unique solution exists at the frequency  $\omega$ , it shall be denoted by  $U[g; \omega]$ ; this uniqueness would fail only in the presence of a Jones mode.

The objective function is a weighted least-squares over  $N_{\omega}$  discrete frequencies:

$$J(g) = \sum_{k=1}^{N_{\omega}} \frac{\alpha_k}{2} (|j(g, U[g; \omega_k]; \omega_k)| - r_k)^2,$$

with

$$j(g, U; \omega) = \underbrace{R_{x^*}[g; \omega]U}_{\text{rep. formula}},$$

where  $R_{x^*}$  represents the action of the representation formula (4.3.13) on the velocity potential  $\varphi$  for the point  $x^*$ .

The shape derivative of the objective function is

$$\langle DJ(g), \delta g \rangle_{\mathcal{G}' \times \mathcal{G}} = \sum_{k=1}^{N_{\omega}} \alpha_k (|j(g, U[g; \omega_k]; \omega_k)| - r_k) \left[ D| \cdot |D_g j(g, U[g; \omega_k]; \omega_k) \delta g + D| \cdot |D_U j(g, U[g; \omega_k]; \omega_k) D_g U[g; \omega_k] \delta g \right].$$

Assuming that the hypotheses of the implicit function theorem hold on the constraint function c (see theorem 5.4.1), the state derivative in

$$\langle D_U j(g, U[g; \omega_k]; \omega_k) D_g U[g; \omega_k], \delta g \rangle_{\mathcal{G}' \times \mathcal{G}}$$

can be replaced with

$$D_g U[g;\omega] = -D_U c(g, U[g;\omega];\omega)^{-1} D_g c(g; U[g;\omega];\omega).$$

By solving the adjoint equation

$$D_U c(g, U[g; \omega_k]; \omega_k)^* P_k = -D_U j(g, U[g; \omega_k]; \omega_k), \qquad (5.4.2)$$

the objective function derivative is then computed after  $N_{\omega}$  state and  $N_{\omega}$  adjoint solves via

$$\langle DJ(g), \delta g \rangle_{\mathcal{G}' \times \mathcal{G}} = \sum_{k=1}^{N_{\omega}} \alpha_k (|j(g, U[g; \omega_k]; \omega_k) - r_k)| \Big[ D| \cdot |(D_g j(g, U[g; \omega_k]; \omega_k) \delta g + D| \cdot |\langle D_g c(g, U[g; \omega_k]; \omega_k) \delta g, P_k \rangle_{\mathcal{U}' \times \mathcal{U}} \Big].$$

It is necessary to differentiate the representation formula (4.3.13). If  $r = |x' - \phi(x)|$ , and  $\hat{r} = (x' - \phi(x))/r$  (note that  $x \in \Omega_0$ , while  $x' \in \mathbb{R}^3 \setminus \phi(\Omega_0)$ ), then

$$R[g;\omega]U = \int_{\Omega_0} \frac{\partial G}{\partial r} \frac{\partial r}{\partial a_3} \varphi(x) \sqrt{a} \, dx.$$

The derivatives of the representation formula are

$$D_{g}R[g;\omega]U = \int_{\Omega_{0}} \frac{\partial G}{\partial r} \hat{r} \cdot a_{3}\varphi(x)D_{\phi}\sqrt{a}\,dx + \int_{\Omega_{0}} \left(\frac{\partial^{2}G}{\partial r^{2}}(D_{\phi}r)\hat{r} \cdot a_{3} + \frac{\partial G}{\partial r}D_{\phi}\hat{r} \cdot a_{3} + \frac{\partial G}{\partial r}\hat{r} \cdot D_{\phi}a_{3}\right)\varphi(x)\sqrt{a}\,dx$$

and

$$\langle D_U r[g;\omega]U, \delta U \rangle_{\mathcal{U}' \times \mathcal{U}} = \int_{\Omega_0} \frac{\partial G}{\partial r} \hat{r} \cdot a_3 \delta \varphi(x) \sqrt{a} \, dx.$$

The derivative of the modulus function

$$|\cdot|:\mathbb{C}\setminus 0\to \mathbb{R}^+$$

is given for z = x + iy by

$$|z + \delta z| - |z| = \frac{x\delta x + y\delta y}{\sqrt{x^2 + y^2}} + o(|\delta z|).$$

The forcing terms (assuming that the surface pressure loading p is independent of  $\phi$ ) require only differentiation of  $\sqrt{a}$ :

$$D_g \int_{\Omega_0} \left( f \cdot \overline{y} - i\omega\rho_0\varphi\overline{y} \cdot n \right) \sqrt{a} \, dx = \int_{\Omega_0} \left( f \cdot \overline{y} - i\omega\rho_0\varphi\overline{y} \cdot n \right) D_\phi\sqrt{a}\delta\phi \, dx$$
$$D_g \int_{\Omega_0} i\omega\overline{\varrho}z \cdot n\sqrt{a} \, dx = \int_{\Omega_0} i\omega\overline{\varrho}z \cdot nD_\phi\sqrt{a}\delta\phi \, dx.$$

In discretization, the method works: numerical tests of the objective function derivative computed using this method are shown in figures 5.4, 5.5.

# 5.4.1 Adjoint Equation Theory

In order to justify the adjoint equation (5.4.2), it is necessary to verify the hypotheses of the implicit function theorem for the constraint function (5.4.1).


Figure 5.4: Objective function derivative test, MITC3. The horizontal axis represents the size of the shape perturbation. The vertical axis is the difference between the derivative and the Newton quotient, i.e., it should be  $O(|\delta x|)$  as  $\delta x \to 0$ . This behavior is observed until  $|\delta x|$  becomes sufficiently small for floating-point errors to take over.

**Theorem 5.4.1** Let  $\omega > 0$  be a fixed frequency, l, L > 0 and  $t_{max} > t_{min} > 0$  be given constants, and  $g_0 = (\phi_0, t_0) \in \mathcal{G} = \mathcal{C} \times \mathcal{T}$ , where

$$\mathcal{C} = \left\{ \phi \in C^2(\Omega_0)^3 : \|\phi\|_{C^2(\Omega_0)^3} \le l \right\},$$
  
$$\mathcal{T} = \left\{ t : \overline{\Omega_0} \to \mathbb{R} : t_{max} \ge t(x) \ge t_{min} \text{ and } |t(x) - t(x')| \le L|x - x'|, \forall x, x' \in \overline{\Omega_0} \right\}.$$

If there are no Jones modes for the shape  $g_0$  at frequency  $\omega$ , then the hypotheses of the implicit function theorem are satisfied for the constraint function (5.4.1) at the point  $(g_0, U[g_0; \omega_0])$ .

Furthermore, the state  $U[g; \omega]$  is Fréchet differentiable with respect to g at the



Figure 5.5: Objective function derivative test, MITC6. The horizontal axis represents the size of the shape perturbation. The vertical axis is the difference between the derivative and the Newton quotient, i.e., it should be  $O(|\delta x|)$  as  $\delta x \to 0$ . This behavior is observed until  $|\delta x|$  becomes sufficiently small for floating-point errors to take over.

point  $g_0$ , and the derivative is given by

$$D_g U[g_0;\omega] = -\left(D_U c(g_0, U[g_0;\omega];\omega)\right)^{-1} D_g c(g_0; U[g_0;\omega];\omega).$$

**Proof:** The hypotheses of the implicit function theorem (see [19, Thm. 3.1.10]) are verified for the constraint functional  $c(g, U[g; \omega]; \omega)$ .

- By theorem 5.3.2, the equation  $c(g_0, U; \omega) = 0 \in \mathcal{U}'$  has a unique solution  $U = U[g_0; \omega].$
- The constraint c(g, U; ω) is affine-linear and continuous in U. Therefore, D<sub>U</sub>c(g<sub>0</sub>, U[g<sub>0</sub>; ω]; ω) exists, and furthermore, by theorem 5.3.2, (D<sub>U</sub>c(g<sub>0</sub>, U[g<sub>0</sub>; ω]; ω))<sup>-1</sup> is continuous.

• By theorems 3.5.1 and 4.5.1, the constraint  $c(g, U; \omega)$  is continuously Fréchet differentiable with respect to g.

In order to establish existence of solutions to the optimization problem

$$\min_{g\in\mathcal{G}}J(g),$$

it remains to specify the shape parameter space  $\mathcal{G}$ . For plate thickness optimization problems [75], compactness requires that the thickness t be uniformly Lipschitzcontinuous. Existence of solutions is proven for a class of mechanical shell shape optimization problems in [7] for  $C^2$  charts. The addition of a uniform bound on the second derivatives allows differentiability of the boundary integral operators (see §4.5.1), so this may be an appropriate requirement for  $\mathcal{G}$  in order to ensure existence of optimal solutions.

### 5.5 Coupled Optimization Results

Optimization results for the box example shown in figure 5.1 are given in this section. Recall that the problem is to find

$$\min_{g \in \mathcal{G}} J(g) = \sum_{k=1}^{N_{\omega}} \frac{\alpha_k}{2} (|j(g, U[g; \omega_k]; \omega_k)| - r_k)^2.$$

The shape space  $\mathcal{G}$  allows the chart and thickness to vary over all six (initially) planar surfaces of the box, but the chart function  $\phi$  is subject to the kinematic junction conditions from §3.6, and the thickness function t is subject to bound constraints. In addition,  $\phi$  and t are subject to Lipschitz-type constraints: to prove existence of solutions to optimal plate thickness design problems, Hlaváček and Lovíšek [75] required uniform Lipschitz continuity of the thickness function t. From the point of view of analysis, the constraints serve to enforce compactness of the design space, but

in discretization, they also prevent the optimization algorithm from making design changes that cannot be accurately represented by the finite element mesh. However, Lipschitz continuity constraints are non-linear, so I replace them with uniform bounds on the partial derivatives. This ensures that uniform Lipschitz continuity holds with a related constant.

For this problem, MITC3 elements are used with

$$\omega = 2\pi \{50, 100, 200\}, x^* = (5, 5, 5), \alpha = \{1, 1, 1\}.$$

The theory for the adjoint equation (theorem 5.4.1) further requires uniform bounds on the second derivatives of  $\phi$ , but this cannot be enforced for a piecewise-linear surface. Future work could involve investigation of whether the smoothness assumptions can be relaxed in the theory, and how the discrete solution behaves under limited smoothness assumptions.

Optimization is done using the interior point method provided by Matlab in the Optimization Toolbox function fmincon. Over the course of the optimization, the objective function (and derivative) are evaluated 146 times. The objective function value drops from  $5.19 \times 10^{-3}$  to  $5.00 \times 10^{-7}$ . The norm of the gradient never drops to levels that suggest satisfaction of first-order necessary optimality conditions; I just stop the optimization when it fails to make further significant progress. This sort of behavior is to be expected for a non-convex, non-linear problem with only first-derivative information, and a large number of optimization variables. Images of the initial and final shapes and transfer functions can be seen in figures 5.7, 5.6.



Figure 5.6: The initial shape is that of the box above with flat faces. In the optimized shape below, color indicates the shell thickness. In addition to the thickness variation, ripples also develop, and are particularly noticeable in the top of the box.



Figure 5.7: Box optimization: initial and final transfer functions. The red x marks indicate the desired values of the objective function.

## Chapter 6

# **Conclusion and Future Work**

In this thesis, I have developed a model of shell-structure acoustics using thin boundary integral equations and Naghdi shells, and proven its well-posedness. I have given theoretical justification, under additional smoothness assumptions, for the corresponding adjoint equations. I have set up finite element models for the state and adjoint computations associated with optimization of an acoustic transfer function, and demonstrated the utility of the method by solving design problems with the thickness and chart function as optimization variables, parametrized at the scale of the finite element mesh. With an accelerated BEM code, this method could be used to solve optimal design problems posed over a wide range of frequencies.

### 6.1 Accomplishments

I have implemented piecewise-linear Galerkin boundary elements with analytic singular integration described in [105] for solution of Helmholtz boundary integral equations in three dimensions, and computation of integral operator shape derivatives.

In order to make the coupling to the flat triangular boundary elements simple, I also created a new shell finite element based on the MITC3 shell element of [87], but with a modified rotation angle space. The modification is analogous to that made by [56] to the MITC3 plate element, so that the modified element, which I call MITC3-DL, reduces to the stable Duran-Liberman plate element in the case of flat shells. The second-order MITC6 elements of [87] exhibit better locking behavior, so I have implemented them as well, allowing geometry errors in the coupling. I have implemented shape derivatives for all of these elements.

With these finite element tools in hand, I have set up the fully-coupled problem corresponding to (1.2.1), and implemented adjoint equation-based optimization for the coupled problem. This involves a great deal of tedious differentiation of shape parameters, which must be carefully integrated with the finite element codes. Finally, I have solved some small-scale optimization problems involving multiple joined shells.

In order to justify the method, I have analyzed the coupled problem (5.3.3). Provided that all eigenmodes of the shell couple to the acoustics, the problem is well-posed at all frequencies. Under the assumption of a  $C^2$  midsurface, the adjoint equations and shape derivatives can be justified via the implicit function theorem. Numerical tests of the method show agreement between the calculated derivatives and finite differences.

### 6.2 Future Work

This work could be extended in several directions. First, in order to explore more fully the potential of this kind of optimization, the BEM code must run faster. There are many potential methods for doing this. It would be easy to exploit parallelism of the problem, and it is also possible to implement acceleration techniques such as hierarchical clustering [105].

A more physically realistic model would also include viscoelastic material damping. This would also alleviate the problem of non-uniqueness of solutions for certain special geometries. In practice, it would be easy to include damping via a complex frequency-dependent elastic constants determined by experiment. In the optimization problems I have tried, the gradient-based methods typically make significant progress, and then stagnate. Hessian information would likely accelerate convergence substantially, but it would require second shape derivatives of the shell and boundary integral operators, which would increase the complexity of the implementation.

Hlavacek and and Lovisek [75, 76] investigate various thickness optimization problems for plates, and prove convergence of the approximate optimal solutions. However, they do not prove rates, which could likely be worked out using error estimates for MITC elements. Work of this type could also be extended to shells, at least conditionally, by assuming that the necessary inf-sup condition holds for the shell elements.

It is also desirable to develop existence theory for the optimization of the coupled problem through combination and extension of existing work on plate thickness optimization [75] and shell chart optimization [7]. Uniform bounds on second derivatives of the chart function required in [101] for existence of Fréchet derivatives of the boundary integral operators might then be shown to be a sufficient requirement on the chart function space for existence of both optimal solutions, and of state derivatives.

# Appendix A

# **MITC Plate Elements**

### A.1 Implementation of the MITC7 Element

The weak form of the Reissner Mindlin plate equation (2.2.16) can also be written in matrix form: find  $(\theta, z) \in \mathcal{R} \times \mathcal{V}$  such that for all  $(\eta, y) \in \mathcal{R} \times \mathcal{V}$ ,

$$\int_{\Omega_0} \kappa(\eta)^T C_B \kappa(\theta) \, dx + \int_{\Omega_0} \gamma(\eta, y)^T C_S \gamma(\theta, z) \, dx = \int_{\Omega_0} Gy \, dx, \tag{A.1.1}$$

where

$$C_B = Dt^3 \begin{pmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & \frac{1-\nu}{2} \end{pmatrix}, \qquad C_S = \lambda t \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

and

$$\kappa(\theta) = \begin{pmatrix} \partial_{x_1} \theta_1 \\ \partial_{x_2} \theta_2 \\ \partial_{x_2} \theta_1 + \partial_{x_1} \theta_2 \end{pmatrix}, \qquad \gamma(\theta, z) = \begin{pmatrix} \partial_{x_1} z - \theta_1 \\ \partial_{x_2} z - \theta_2 \end{pmatrix}.$$

### A.1.1 MITC Discretization of the Reissner–Mindlin Plate Equation

For the MITC discretization of A.1.1 appropriate subspaces  $\mathcal{R}_h \subset \mathcal{R}, \mathcal{V}_h \subset \mathcal{V}$ , and a reduction operator  $R_h : \mathcal{R}_h \to \mathcal{S}_h$  must be selected. The MITC approximation  $(\theta_h, z_h) \in \mathcal{R}_h \times \mathcal{V}_h$  of the solution of A.1.1 is computed as the solution of

$$\int_{\Omega_0} \kappa(\eta_h)^T C_B \kappa(\theta_h) \, dx + \int_{\Omega_0} \gamma(R_h \eta_h, y_h)^T C_S \gamma(R_h \theta_h, z_h) \, dx = \int_{\Omega_0} Gy_h \, dx \quad (A.1.2)$$

for all  $(\eta_h, y_h) \in \mathcal{R}_h \times \mathcal{V}_h$ . Aside from taking the discrete subspaces  $\mathcal{R}_h, \mathcal{V}_h$ , the only change from (A.1.1) is the presence of the reduction operator  $R_h : \mathcal{R}_h \to \mathcal{S}_h$  in the shear term.

I describe the MITC7 discretization of the Reissner Mindlin plate equation. The MITC7 elements were introduced in [30]. Error analysis was completed in [33].

Let  $\Delta_h$  be a triangulation of  $\Omega_0$ . For a triangle T, denote by  $P_j(T)$  the space of all degree j polynomials on T and for an edge e, denote by  $P_j(e)$  the space of all degree j polynomials on e. Furthermore, for each triangle T, define the spaces

$$S_{7}(T) = \{ p \in P_{3}(T) : p|_{e} \in P_{2}(e) \text{ for all edges } e \text{ of } T \},\$$
$$RT_{1}(T) = \left\{ \begin{pmatrix} a_{1} + b_{1}x_{1} + c_{1}x_{2} + x_{2}(dx_{1} + ex_{2}) \\ a_{2} + b_{2}x_{1} + c_{2}x_{2} - x_{1}(dx_{1} + ex_{2}) \end{pmatrix} : a_{i}, b_{i}, c_{i}, d, e \in \mathbb{R}, i = 1, 2 \right\}.$$

Let  $P_j(\Omega_0)$  be the space of all degree j polynomials on  $\Omega_0$ , and let T be any triangle in the discretization. For MITC7, the spaces are given by

$$\mathcal{R}_h = \left\{ p \in \mathcal{R} : p|_T \in S_7(T)^2, \ \forall T \in \Delta_h \right\}$$
(A.1.3a)

$$\mathcal{V}_h = \{ p \in \mathcal{V} : p|_T \in P_2(T), \ \forall T \in \Delta_h \}$$
(A.1.3b)

$$S_h = \{ \gamma : \gamma |_T \in RT_1(T), \ \gamma \cdot \tau \text{ continuous at inter-element boundaries} \},$$
 (A.1.3c)

where  $\tau$  is the tangential unit vector to each each edge in T. The reduction operator  $R_h$  is defined on each triangle  $T \in \triangle_h$  via

$$\int_{e} (\theta_h - R_h \theta_h)(s) \cdot \tau(s) \ p_1(s) ds = 0, \quad \forall e \text{ edge of } T, \quad \forall p_1 \in P_1(e), \quad \forall \theta_h \in \mathcal{R}_h,$$
(A.1.4a)

$$\int_{T} \theta_{h}(x) - (R_{h}\theta_{h})(x)dx = 0, \qquad \qquad \forall \theta_{h} \in \mathcal{R}_{h}.$$
(A.1.4b)

Again,  $\tau$  is the tangential unit vector to each each edge in T. Since  $(\theta_h - R_h \theta_h)|_e \in P_2(e)$  and  $p_1 \in P_1(e)$ , it holds that  $(\theta_h - R_h \theta_h)|_e \cdot \tau p_1 \in P_3(e)$ . Since 2-point Gaussian quadrature is exact for polynomials of degree 3, see, e.g., [110, p. 154], (A.1.4a) can be enforced by requiring that

$$(\theta_h - R_h \theta_h)(x_i^e) \cdot \tau(x_i^e) = 0, \quad i = 1, 2$$

for all edges e of triangle T, where  $x_i^e$ , i = 1, 2 are the Gauss quadrature points on edge e, which for an edge with vertices  $v_1, v_2$  are given by

$$x_1^e = \frac{v_1 + v_2}{2} + \frac{v_2 - v_1}{2\sqrt{3}}, \quad x_2^e = \frac{v_1 + v_2}{2} - \frac{v_2 - v_1}{2\sqrt{3}},$$

The points  $x_i^e$  are also referred to as tying points . Thus, replace (A.1.4) by

$$(\theta_h - R_h \theta_h)(x_i^e) \cdot \tau(x_i^e) = 0, \quad i = 1, 2 \quad \forall e \text{ edge of } T, \quad \forall \theta_h \in \mathcal{R}_h, \quad (A.1.5a)$$
$$\int_T \theta_h(x) - (R_h \theta_h)(x) dx = 0, \quad \forall \theta_h \in \mathcal{R}_h. \quad (A.1.5b)$$

#### A.1.2 Ordering of Local and Global Degrees of Freedom

Each triangle  $T_k \in \Delta_h$  has seven degrees of freedom for each component of the rotation  $\theta_h$ , and six degrees of freedom for the vertical displacement z. Let  $\theta_k$  be the vector of the components of  $\theta_h$  corresponding to the kth Lagrange basis function. The vectors of finite element degrees of freedom are then written

$$\vec{\theta} = \begin{pmatrix} \theta_{k_1} \\ \vdots \\ \theta_{k_7} \end{pmatrix} \in \mathbb{R}^{14}, \ \vec{z} = \begin{pmatrix} z_{k_1} \\ \vdots \\ z_{k_6} \end{pmatrix} \in \mathbb{R}^6.$$

The local displacement vector is then

$$\vec{u} = \begin{pmatrix} \vec{ heta} \\ \vec{z} \end{pmatrix} \in \mathbb{R}^{20}.$$

The degrees of freedom are arranged globally according to vertex and triangle number:

$$\vec{U}^{T} = \begin{pmatrix} \theta_{1,1} & \theta_{1,2} & z_1 | \theta_{2,1} & \theta_{2,2} & z_2 | \cdots | \theta_{n,1} & \theta_{n,2} & z_n | \theta_{n+1,1} & \theta_{n+1,2} | \cdots | \theta_{m,1} & \theta_{m,2} \end{pmatrix}^{T}.$$
(A.1.6)

The local matrix assembly routines, including construction of the reduction operator  $R_h$  are described in A.1.5. The linear equation (A.1.11) is then written as

$$K\vec{U} = \vec{G}.$$

1

#### A.1.3 Boundary Conditions

In order to enforce the boundary conditions (2.3.5), it must be required that  $\mathcal{R}_h \subset \mathcal{R}$ , and  $\mathcal{V}_h \subset \mathcal{V}$ , with  $\mathcal{V}, \mathcal{R}$  as in (2.3.6). This is done by constructing a matrix S such that if  $\vec{U}$  is the vector of global finite element degrees of freedom, as before, then with  $\boldsymbol{\theta}_h, z_h$  defined in (A.1.10)

$$S\vec{U} = 0 \Leftrightarrow \boldsymbol{\theta}_h \in \mathcal{R}_h, z_h \in \mathcal{V}_h.$$

These are then enforced by using a standard saddle point approach, i.e., by solving

$$\begin{pmatrix} K & S^T \\ S & 0 \end{pmatrix} \begin{pmatrix} \vec{U} \\ \vec{\lambda} \end{pmatrix} = \begin{pmatrix} \vec{G} \\ 0 \end{pmatrix}.$$
(A.1.7)

#### A.1.4 Basis Polynomials

The basis for  $\mathcal{V}_h$  are the piecewise Lagrange polynomials corresponding to the triangle vertices and the edge midpoints. The basis for  $\mathcal{R}_h$  are the piecewise Lagrange polynomials corresponding to the triangle vertices, the edge midpoints and the triangle centroid. The finite element functions are then

$$z_h(x) = \sum_{i=1}^n z_i N_i^6(x),$$
$$\boldsymbol{\theta}_h(x) = \sum_{i=1}^m \boldsymbol{\theta}_i N_i^7(x).$$

m

As usual, the basis functions  $N_i^6$ ,  $N_i^7$  are constructed by mapping the Lagrange polynomials on the reference triangle

$$\widehat{T} = \left\{ \xi \in \mathbb{R}^2 : \xi_1 \ge 0, \xi_2 \ge 0, \xi_1 + \xi_2 \le 1 \right\}$$

to the triangles  $T \in \Delta_h$ .

The Lagrange basis polynomials for  $P_2(\widehat{T})$  and  $S_7(\widehat{T})$  are given by

$$\widehat{N}_{1}^{6}(\xi_{1},\xi_{2}) = (1-\xi_{1}-\xi_{2})(1-2\xi_{1}-2\xi_{2}),$$

$$\widehat{N}_{2}^{6}(\xi_{1},\xi_{2}) = \xi_{1}(2\xi_{1}-1),$$

$$\widehat{N}_{3}^{6}(\xi_{1},\xi_{2}) = \xi_{2}(2\xi_{2}-1),$$

$$\widehat{N}_{4}^{6}(\xi_{1},\xi_{2}) = 4\xi_{1}\xi_{2},$$

$$\widehat{N}_{5}^{6}(\xi_{1},\xi_{2}) = 4\xi_{2}(1-\xi_{1}-\xi_{2}),$$

$$\widehat{N}_{6}^{6}(\xi_{1},\xi_{2}) = 4\xi_{1}(1-\xi_{1}-\xi_{2}).$$
(A.1.8)

and

$$\begin{split} \widehat{N}_{1}^{7}(\xi_{1},\xi_{2}) &= (1-\xi_{1}-\xi_{2})(1-2\xi_{1}-2\xi_{2})+3\xi_{1}\xi_{2}(1-\xi_{1}-\xi_{2}), \\ \widehat{N}_{2}^{7}(\xi_{1},\xi_{2}) &= \xi_{1}(2\xi_{1}-1)+3\xi_{1}\xi_{2}(1-\xi_{1}-\xi_{2}), \\ \widehat{N}_{3}^{7}(\xi_{1},\xi_{2}) &= \xi_{2}(2\xi_{2}-1)+3\xi_{1}\xi_{2}(1-\xi_{1}-\xi_{2}), \\ \widehat{N}_{4}^{7}(\xi_{1},\xi_{2}) &= 4\xi_{1}\xi_{2}-12\xi_{1}\xi_{2}(1-\xi_{1}-\xi_{2}), \\ \widehat{N}_{5}^{7}(\xi_{1},\xi_{2}) &= 4\xi_{2}(1-\xi_{1}-\xi_{2})-12\xi_{1}\xi_{2}(1-\xi_{1}-\xi_{2}), \\ \widehat{N}_{6}^{7}(\xi_{1},\xi_{2}) &= 4\xi_{1}(1-\xi_{1}-\xi_{2})-12\xi_{1}\xi_{2}(1-\xi_{1}-\xi_{2}), \\ \widehat{N}_{7}^{7}(\xi_{1},\xi_{2}) &= 27\xi_{1}\xi_{2}(1-\xi_{1}-\xi_{2}). \end{split}$$
(A.1.9)

respectively (see also Figure A.1).

Let  $T_k$  be the triangle with vertices  $v_{k_1}, v_{k_2}, v_{k_3}$ . The map

$$\xi \mapsto v_{k_1} + J_k \xi,$$

where

$$J_k = (v_{k_2} - v_{k_1}, v_{k_3} - v_{k_1}) \in \mathbb{R}^{2 \times 2}$$

maps the unit triangle onto  ${\cal T}_k$  (see Figure A.2).



Figure A.1: Degrees of freedom for the Lagrange basis for  $P_2(\widehat{T})$  (left) and for  $S_7(\widehat{T})$  (right).

If  $N_1^6, \ldots, N_n^6$  are the basis functions for  $\mathcal{V}_h$ , then the basis functions  $N_{k_1}^6, \ldots, N_{k_6}^6$ which have support that intersects with  $T_k$  satisfy

$$N_{k_i}^6(x) = \widehat{N}_i^6(J_k^{-1}(x - v_{k_1})), \quad i = 1, \dots, 6.$$

Similarly, if  $N_1^7, \ldots, N_m^7$  are the basis functions for  $\mathcal{R}_h$ , then the basis functions  $N_{k_1}^7, \ldots, N_{k_7}^7$  which have support that intersects with  $T_k$  satisfy

$$N_{k_i}^7(x) = \widehat{N}_i^7(J_k^{-1}(x - v_{k_1})), \quad i = 1, \dots, 7.$$

#### A.1.5 Matrix Assembly

Using the basis functions, (A.1.2) can be reformulated as follows. Find

$$z_h(x) = \sum_{i=1}^n z_i N_i^6(x), \quad \boldsymbol{\theta}_h(x) = \sum_{i=1}^m \boldsymbol{\theta}_i N_i^7(x)$$
(A.1.10)

such that

$$\int_{\omega} \kappa(\mathbf{N}_{j}^{7})^{T} C_{B} \kappa(\boldsymbol{\theta}_{h}) \, dx + \int_{\omega} \gamma(R_{h} \mathbf{N}_{j}^{7}, N_{i}^{6})^{T} C_{S} \gamma(R_{h} \boldsymbol{\theta}_{h}, z_{h}) \, dx = \int_{\omega} G N_{i}^{6} \, dx \quad (A.1.11)$$



Figure A.2: Transformation between reference and physical coordinates.

for all i = 1, ..., n and all j = 1, ..., 2m, where

$$\mathbf{N}_{2j-1}^{7} = \begin{pmatrix} N_{j}^{7} \\ 0 \end{pmatrix}, \quad \mathbf{N}_{2j}^{7} = \begin{pmatrix} 0 \\ N_{j}^{7} \end{pmatrix}, \quad j = 1, \dots, m.$$

Equation (A.1.11) is a linear system of equations in the unknowns  $z_1, \ldots, z_n$  and  $\theta_1, \ldots, \theta_m$ . Since

$$\int_{\omega} \ldots = \sum_{T_k \in \Delta_h} \int_{T_k} \ldots$$

the linear system is assembled element-wise. Let  $T_k$  be the triangle with vertices  $v_{k_1}, v_{k_2}, v_{k_3}$  and nodes with indices  $k_1, \ldots, k_7$ , where  $k_1, \ldots, k_3$  are the indices of the vertices,  $k_4, \ldots, k_6$  are the indices of the edge midpoints, and  $k_7$  is the index of the centroid. For  $x \in T_k$ ,

$$z_h(x) = \sum_{i=1}^6 z_{k_i} N_{k_i}^6(x), \quad \boldsymbol{\theta}_h(x) = \sum_{i=1}^7 \boldsymbol{\theta}_{k_i} N_{k_i}^7(x), \quad x \in T_k$$

Define

$$\nabla \boldsymbol{\theta}_{h} = \begin{pmatrix} \nabla \theta_{h,1} \\ \nabla \theta_{h,2} \end{pmatrix}$$

and

$$\nabla \mathbf{N}_{2j-1}^7 = \begin{pmatrix} \nabla N_j^7 \\ 0 \end{pmatrix}, \quad \nabla \mathbf{N}_{2j}^7 = \begin{pmatrix} 0 \\ \nabla N_j^7 \end{pmatrix}, \quad j = 1, \dots, m.$$

Recall that

$$\kappa(\boldsymbol{\theta}_h) = \begin{pmatrix} \partial_{x_1} \theta_{h,1} \\ \partial_{x_2} \theta_{h,2} \\ \partial_{x_2} \theta_{h,1} + \partial_{x_1} \theta_{h,2} \end{pmatrix} = \underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}}_{=E} \begin{pmatrix} \nabla \theta_{h,1} \\ \nabla \theta_{h,2} \end{pmatrix} = E \nabla \boldsymbol{\theta}_h$$

Hence,

$$\int_{T_k} \kappa (\nabla \mathbf{N}_i^7)^T C_B \kappa(\boldsymbol{\theta}_h) \, dx$$
  
=  $\int_{T_k} (\nabla \mathbf{N}_i^7)^T E^T C_B E \nabla \boldsymbol{\theta}_h \, dx,$   
=  $\sum_j \int_{T_k} (\nabla \mathbf{N}_i^7)^T E^T C_B E \nabla \mathbf{N}_j^7 \, dx \, \boldsymbol{\theta}_j,$  (A.1.12)

where the summation is over  $j = 2k_1 - 1, 2k_1, \ldots, 2k_7 - 1, 2k_7$  and  $i \in \{2k_1 - 1, 2k_1, \ldots, 2k_7 - 1, 2k_7\}$ . The integrals in (A.1.12) are computed by transformation onto the reference triangle. If

$$\widehat{\mathbf{N}}_{2j-1}^{7} = \begin{pmatrix} \widehat{N}_{j}^{7} \\ 0 \end{pmatrix}, \quad \widehat{\mathbf{N}}_{2j}^{7} = \begin{pmatrix} 0 \\ \widehat{N}_{j}^{7} \end{pmatrix}, \quad j = 1, \dots, 7,$$

then transformation of the integrals in (A.1.12) onto the reference triangle gives

$$\int_{T_{k}} (\nabla \mathbf{N}_{2k_{i}-1}^{7})^{T} E^{T} C_{B} E \nabla \mathbf{N}_{2k_{j}-1}^{7} dx \qquad (A.1.13a)$$

$$= |J_{k}| \int_{\widehat{T}} (\nabla \widehat{\mathbf{N}}_{2i-1}^{7})^{T} \begin{pmatrix} J_{k}^{-1} & 0 \\ 0 & J_{k}^{-1} \end{pmatrix} E^{T} C_{B} E \begin{pmatrix} J_{k}^{-T} & 0 \\ 0 & J_{k}^{-T} \end{pmatrix} \nabla \widehat{\mathbf{N}}_{2j-1}^{7} d\xi.$$

and

$$\int_{T_{k}} (\nabla \mathbf{N}_{2k_{i}}^{7})^{T} E^{T} C_{B} E \nabla \mathbf{N}_{2k_{j}}^{7} dx \qquad (A.1.13b)$$

$$= |J_{k}| \int_{\widehat{T}} (\nabla \widehat{\mathbf{N}}_{2i}^{7})^{T} \begin{pmatrix} J_{k}^{-1} & 0 \\ 0 & J_{k}^{-1} \end{pmatrix} E^{T} C_{B} E \begin{pmatrix} J_{k}^{-T} & 0 \\ 0 & J_{k}^{-T} \end{pmatrix} \nabla \widehat{\mathbf{N}}_{2j}^{7} d\xi.$$

for i, j = 1, ..., 7.

For the computation of the second integral in (A.1.2) recall that

$$\gamma(R_h\boldsymbol{\theta}_h, z_h) = \nabla z_h - R_h\boldsymbol{\theta}_h,$$

where  $R_h \boldsymbol{\theta}_h |_{T_k} \in RT_1(T_k)$ . If

$$(\widehat{R_h \eta_h})(\xi) = (R_h \eta_h)(v_{k_1} + J_k \xi), \quad \xi \in \widehat{T},$$

then the transformation onto the reference triangle can again be used to obtain

$$\int_{T_k}^{T_k} \gamma(R_h \boldsymbol{\eta}_h, y_h)^T C_S \gamma(R_h \boldsymbol{\theta}_h, z_h) dx$$
  
=  $|J_k| \int_{\widehat{T}} (J_k^{-T} \nabla \widehat{y}_h - \widehat{R_h \boldsymbol{\eta}_h})^T C_S (J_k^{-T} \nabla \widehat{z}_h - \widehat{R_h \boldsymbol{\theta}_h})^T d\xi.$  (A.1.14)

Next, the computation of  $R_h \eta_h$  and  $\widehat{R_h \eta_h}$  is given in detail.

#### A.1.6 Calculation of the reduction operator $R_h$

For each triangle  $T_k$  the reduction operator  $R_h$  satisfies

$$(\boldsymbol{\theta}_h - R_h \boldsymbol{\theta}_h)(x_i^e) \cdot \boldsymbol{\tau}(x_i^e) = 0, \quad i = 1, 2 \quad \forall e \text{ edge of } T_k, \quad \forall \boldsymbol{\theta}_h \in S_7(T_k)^2, \text{ (A.1.15a)}$$
$$\int_{T_k} \boldsymbol{\theta}_h(x) - (R_h \boldsymbol{\theta}_h)(x) dx = 0, \qquad \qquad \forall \boldsymbol{\theta}_h \in S_7(T_k)^2. \text{ (A.1.15b)}$$

Since for each triangle  $T_k$ , it holds that

$$R_h: S_7(T_k)^2 \to RT_1(T_k),$$

the operator can be represented by a matrix  $\mathsf{R}_k \in \mathbb{R}^{8 \times 14}.$ 

Let  $T_k$  be the triangle with vertices  $v_{k_1}, v_{k_2}, v_{k_2}$  and nodes with indices  $k_1, \ldots, k_7$ . Define

$$M_k^R(x) = \begin{pmatrix} 1 & x_1 & x_2 & 0 & 0 & 0 & x_1x_2 & x_2^2 \\ 0 & 0 & 0 & 1 & x_1 & x_2 & -x_1^2 & -x_1x_2 \end{pmatrix}, \quad x \in T_k.$$

The columns of  $M_k^R$  are a basis for  $RT_1(T_k)$ . Furthermore, define

$$\widehat{N}(\xi) = \begin{pmatrix} \widehat{N}_1(\xi) & 0 & \dots & \widehat{N}_7(\xi) & 0 \\ 0 & \widehat{N}_1(\xi) & \dots & 0 & \widehat{N}_7(\xi) \end{pmatrix}, \quad \xi \in \widehat{T}$$

With this notation, the finite element functions are written

$$\theta_{h}(x) = \sum_{i=1}^{7} \theta_{k_{i}} N_{k_{i}}^{7}(x)$$

$$= \sum_{i=1}^{7} \theta_{k_{i},1} \mathbf{N}_{2k_{i}-1}^{7}(x) + \theta_{k_{i},2} \mathbf{N}_{2k_{i}}^{7}(x)$$

$$= \widehat{N} (J_{k}^{-1}(x - v_{k_{1}})) \widehat{\theta}, \qquad x \in T_{k}. \quad (A.1.16)$$

where

$$\widehat{\boldsymbol{\theta}} = \begin{pmatrix} \boldsymbol{\theta}_{k_1} \\ \vdots \\ \boldsymbol{\theta}_{k_7} \end{pmatrix} = \begin{pmatrix} \theta_{k_1,1} \\ \theta_{k_1,2} \\ \vdots \\ \theta_{k_7,1} \\ \theta_{k_7,2} \end{pmatrix} \in \mathbb{R}^{14}$$

is the sub-vector of  $\boldsymbol{\theta}$  corresponding to node indices in triangle  $T_k$ .

The reduction operator can now be written as

$$(R_h \boldsymbol{\theta}_h)(x) = M_k^R(x) \mathsf{R}_k \widehat{\boldsymbol{\theta}}, \quad x \in T_k.$$
(A.1.17)

Using (A.1.16) and (A.1.17), (A.1.15) can be written

$$\boldsymbol{\tau}(x_i^e) \cdot M_k^R(x_i^e) \mathsf{R}_k = \boldsymbol{\tau}(x_i^e) \cdot \widehat{N}(J_k^{-1}(x_i^e - v_{k_1})), \quad i = 1, 2 \quad \forall e \text{ edge of } T_k,$$
(A.1.18a)

$$|J_k| \int_{\widehat{T}} M_k^R(v_{k_1} + J_k\xi) d\xi \ \mathsf{R}_k = |J_k| \int_{\widehat{T}} \widehat{N}(\xi) d\xi.$$
(A.1.18b)

Note that the quantities on the right hand sides in (A.1.18) are independent of the triangle  $T_k$ .

Finally, the function  $\widehat{R_h \eta_h}$  in (A.1.14) is computed as

$$(\widehat{R_h \eta_h})(\xi) = (R_h \eta_h)(v_{k_1} + J_k \xi) = M_k^R(v_{k_1} + J_k \xi) \mathsf{R}_k \widehat{\boldsymbol{\theta}} \qquad \xi \in \widehat{T}.$$

# Appendix B

# **MITC Shell Elements**

### **B.1** General Shell Elements

Finite element discretization of (3.2.6) is usually based on what are called general shell elements; see [39, 6.3] for a detailed discussion. Recall the geometric definition of the shell (3.2.1), given by the chart function

$$\Phi(x^1, x^2, x^3) \equiv \phi(x^1, x^2) + x^3 a_3.$$

In general, the exact surface chart function  $\phi$  is not available, so it is necessary to use some sort of interpolation. Suppose that  $\phi$  is assumed to be piecewise polynomial. Then

$$a_{\alpha} = \partial_{\alpha}\phi_{\beta}$$

and

$$a_3 = \frac{a_1 \times a_2}{\|a_1 \times a_2\|}$$

in general will be discontinuous across element boundaries. This is clearly suitable neither for the definition of the shell geometry nor as a basis for the expansion of vector and tensor fields.

The general shell element approach begins once again with the mechanical assumption  $\sigma_{33} = 0$ , allowing the derivation by the procedure in section 3.2.1 of the equation (3.2.4), repeated here:

$$\frac{1}{2} \int_{\Omega} \left( C^{\alpha\beta\lambda\mu} e_{\alpha\beta}(u) e_{\lambda\mu}(u) + D^{\alpha\lambda} e_{\alpha3}(u) e_{\lambda3}(u) \right) \sqrt{g} \, dx. \tag{B.1.1}$$

Rather than continuing to the Naghdi weak form (3.2.6) by expanding the strain tensors based on the kinematic assumption (3.2.3), the general shell method approach uses a direct discretization of (B.1.1), with a polynomial-interpolated chart function. The vectors  $a_j$  are stored at the nodes, and interpolated in between, rather than being calculated as derivatives of the chart function. The result is that the Naghdi kinematic assumption is satisfied at the nodes, and nearly so elsewhere. In [39, Prop. 6.3.1], it is shown that solutions to the general shell problem still converge to those of the Naghdi model. The next section discusses the calculation of the strain terms in (B.1.1), while the following two sections discuss the interpolation schemes used for the MITC3 and MITC6b elements.

#### **B.1.1** General Shell Element Strain Calculation

This section goes through the general details, which except for the choice of the polynomial space, are common to general shell models. Let  $\Delta_h$  be a triangulation of  $\Omega_0$ , with  $N_T$  triangles  $T_1, \dots, T_{N_T}$ , and vertices labeled  $1, 2, \dots, N_V$ . The polynomials  $\Psi_j(\xi), j \in \{1, 2, \dots, N_V\}$  form a Lagrange basis for the space of piecewise linear or quadratic polynomials on  $\Delta_h$ . In the quadratic case, the vertices are assumed to include those at the edge midpoints.

The chart function  $\Phi: \Omega \to \mathbb{R}^3$  is approximated by

$$\Phi_h(\xi_1,\xi_2,\xi_3) = \phi_h(\xi_1,\xi_2) + \xi_3 \sum_{j=1}^{N_V} \Psi_j(\xi_1,\xi_2) a_3^j.$$

Here,  $\phi_h$  is the approximate middle surface chart, given by

$$\phi_h(\xi_1,\xi_2) = \sum_{j=1}^{N_V} \Psi_j(\xi_1,\xi_2) \phi^j.$$

The 3-vectors

$$\{\phi^1, \phi^2, \cdots, \phi^{N_V}\}, \{a_3^1, a_3^2, \cdots, a_3^{N_V}\}$$

determine respectively the middle-surface and its unit normals.

The displacement  $u = u_h^3$  is assumed to satisfy

$$u_h^3(\xi_1,\xi_2,\xi_3) = u_h^2(\xi_1,\xi_2) + \xi_3\theta_h(\xi_1,\xi_2).$$

where

$$u_h^2 = \sum_{j=1}^{N_V} \Psi_j(\xi_1, \xi_2) u^j$$
$$\theta_h = \sum_{j=1}^{N_V} \Psi_j(\xi_1, \xi_2) \theta^j.$$

The 3-vectors

$$\{u^1, u^2, \cdots, u^{N_V}\}, \{\theta^1, \theta^2, \cdots, \theta^{N_V}\}$$

determine respectively the middle-surface displacement and its rotation angles. While  $u^{j}$  is arbitrary, it is required that

$$\theta^j \cdot a_3^j = 0,$$

i.e., that Naghdi kinematics holds at the nodes.

The mass matrix comes from discretization of

$$\begin{split} \int_{\Omega} u_h^3(\xi) \cdot v_h^3(\xi) \sqrt{g} \, d\xi &= \int_{\Omega} (u_h^2(\xi_1, \xi_2) + \xi_3 \theta_h(\xi_1, \xi_2)) \cdot (v_h^2(\xi_1, \xi_2) + \xi_3 \eta_h(\xi_1, \xi_2)) \sqrt{g} \, d\xi \\ &= \int_{\Omega} (u_h^2 \cdot v_h^2 + \xi_3 (\theta_h \cdot v_h^2 + \eta_h \cdot u_h^2) + \xi_3^2 \theta_h \cdot \eta_h) \sqrt{g} \, d\xi \\ &\approx \int_{\Omega_0} \left( t u_h^2 \cdot v_h^2 + \frac{t^3}{12} \theta_h \cdot \eta_h \right) \sqrt{a} \, d\xi. \end{split}$$

The forcing vector comes from

$$\int_{\Omega} v_h^3 \cdot f \, d\xi = \int_{\Omega} (v_h^2(\xi_1, \xi_2) + \xi_3 \eta_h(\xi_1, \xi_2)) \cdot f \, d\xi.$$

If it is further assumed that the forcing f is independent of  $\xi_3$ , then this simplifies to

$$\int_{\Omega_0} t v_h^2(\xi_1,\xi_2) \cdot f(\xi_1,\xi_2) \, d\xi.$$

The stiffness matrix is constructed via discretization of (B.1.1) using the assumed form  $u_h^3$ . First, calculate the strain components via

$$\begin{split} e_{\alpha\beta}(u_h^3) &= \frac{1}{2} \left( \partial_\beta u_h^3 \cdot g_\alpha + \partial_\alpha u_h^3 \cdot g_\beta \right) \\ &= \frac{1}{2} \left( (\partial_\beta u_h^2 + \xi_3 \partial_\beta \theta_h) \cdot (\partial_\alpha \phi_h + \xi_3 \sum_{j=1}^{N_V} \partial_\alpha \Psi_j a_3^j) \right) \\ &+ (\partial_\alpha u_h^2 + \xi_3 \partial_\alpha \theta_h) \cdot (\partial_\beta \phi_h + \xi_3 \sum_{j=1}^{N_V} \partial_\beta \Psi_j a_3^j) \right) \\ &\approx e_{\alpha\beta}^0(u_h^3) + \xi_3 e_{\alpha\beta}^1(u_h^3), \end{split}$$

where

$$\begin{aligned} e^{0}_{\alpha\beta}(u^{3}_{h}) &= \frac{1}{2} \left( \partial_{\beta} u^{2}_{h} \cdot \partial_{\alpha} \phi_{h} + \partial_{\beta} \phi_{h} \cdot \partial_{\alpha} u^{2}_{h} \right) \\ e^{1}_{\alpha\beta}(u^{3}_{h}) &= \frac{1}{2} \left( \partial_{\beta} u^{2}_{h} \sum_{j=1}^{N_{V}} \partial_{\alpha} \Psi_{j} a^{j}_{3} + \partial_{\beta} \theta_{h} \cdot \partial_{\alpha} \phi_{h} + \partial_{\alpha} u^{2}_{h} \sum_{j=1}^{N_{V}} \partial_{\beta} \Psi_{j} a^{j}_{3} + \partial_{\alpha} \theta_{h} \cdot \partial_{\beta} \phi_{h} \right). \end{aligned}$$

The transverse shear strains are given by

$$\begin{split} e_{\alpha3}(u_h^3) = &\frac{1}{2} \left( \partial_\alpha u_h^3 \cdot g_3 + \partial_3 u_h^3 \cdot g_\alpha \right) \\ = &\frac{1}{2} \left( \left( \partial_\alpha u_h^2 + \xi_3 \partial_\alpha \theta_h \right) \cdot \sum_{j=1}^{N_V} \Psi_j a_3^j + \theta_h \cdot \left( \partial_\alpha \phi_h + \xi_3 \sum_{j=1}^{N_V} \partial_\alpha \Psi_j a_3^j \right) \right) \\ = &e_{\alpha3}^0(u_h^3) + \xi_3 e_{\alpha3}^1(u_h^3) \end{split}$$

where

$$e^{0}_{\alpha3}(u_{h}^{3}) = \frac{1}{2} \left( \partial_{\alpha}u_{h}^{2} \cdot \sum_{j=1}^{N_{V}} \Psi_{j}a_{3}^{j} + \theta_{h} \cdot \partial_{\alpha}\phi_{h} \right)$$
$$e^{1}_{\alpha3}(u_{h}^{3}) = \frac{1}{2} \left( \partial_{\alpha}\theta_{h} \cdot \sum_{j=1}^{N_{V}} \Psi_{j}a_{3}^{j} + \theta_{h} \cdot \sum_{j=1}^{N_{V}} \partial_{\alpha}\Psi_{j}a_{3}^{j} \right).$$

Neglecting the term  $e_{\alpha 3}^1$ , (B.1.1) leads to the weak form

$$\int_{\Omega} \left( C^{\alpha\beta\lambda\mu} e_{\alpha\beta}(u_h^3) e_{\lambda\mu}(v_h^3) + D^{\alpha\lambda} e_{\alpha3}(u_h) e_{\lambda3}(v_h) \right) \sqrt{g} \, d\xi \\ = \int_{\Omega_0} \left[ C^{\alpha\beta\lambda\mu} \left( t e_{\alpha\beta}^0(u_h^3) e_{\alpha\beta}^0(v_h^3) + \frac{t^3}{12} e_{\alpha\beta}^1(u_h^3) e_{\alpha\beta}^1(v_h^3) \right) + D^{\alpha\lambda} (t e_{\alpha3}^0(u_h^3) e_{\lambda3}^0(v_h^3)) \right] \sqrt{a} \, d\xi$$
(B.1.2)

#### **B.1.2** Framework for Strain Interpolation

The MITC3 and MITC6 shell elements are described in [87]. In the subsequent two sections, I discuss respectively a modified version of the MITC3 element, and the unmodified MITC6b element. In both cases, the next step in the formulation of the MITC shell elements is to replace the strain terms in (B.1.2) with carefullychosen interpolants, denoted by, e.g.,  $\tilde{e}_{\alpha\beta}$ , the interpolant of  $e_{\alpha\beta}$ . The choice of these interpolants is inspired by the MITC technique for plate models: one can think of the interpolant  $\tilde{e}$  as the image of the strain e under action of the reduction operator  $R_h$ , as in section 2.4.4.

The interpolation and the tying points are described using coordinates (r, s) for the unit reference triangle

$$\{(r,s) : r+s \le 1; 0 \le r, s \le 1\}.$$

In order to employ the interpolation, it is necessary to transform the strains  $e_{\alpha\beta}$  and  $e_{\alpha3}$  to tensors on this reference triangle. This task is discussed in section B.1.6.

#### B.1.3 MITC3 with the Duran-Liberman Modification

The MITC3 triangular shell element was proposed in [87, §4]. It is known to suffer from locking, and also exhibits mesh-dependent effects, as discussed in [88]. For a flat middle-surface, it reduces to the MITC3 triangular plate element, described in [38], and known to be unstable. Following the work of [56, Ex. 4.1], the MITC3



Figure B.1: Tying points for the MITC3 element. In the above, xx can be replaced with either rt or st, i.e., only transverse strains are interpolated.

triangular plate element can be modified so as to be stable. In this section, I make the analogous modification to the MITC3 shell element.

In the following, let  $\tau_1, \tau_2, \tau_3$  be the unit tangent vectors to the triangle  $T \in \Delta_h$ , and  $\lambda_1, \lambda_2, \lambda_3$  be its barycentric coordinates.  $\tau_i$  corresponds to the vertex opposite the side with  $\lambda_i = 0$ . Consider the Duran-Liberman plate element, which uses the spaces

$$\mathcal{R}_{h} = \{ p \in \mathcal{R} : p|_{T} \in P_{1}(T) \oplus \operatorname{span}(\tau_{1}\lambda_{2}\lambda_{3}, \tau_{2}\lambda_{1}\lambda_{3}, \tau_{3}\lambda_{1}\lambda_{2}), \forall T \in \Delta_{h} \}$$
$$\mathcal{V}_{h} = \{ p \in \mathcal{V} : p|_{T} \in P_{1}(T), \forall T \in \Delta_{h} \}$$

 $\mathcal{S}_h = \{ \gamma \in \mathcal{S} : \gamma \in RT_0(T) \, \forall T \in \Delta_h, \gamma \cdot \tau \text{ continuous at inter-element boundaries} \}.$ 

 $RT_0(T)$  is the lowest-order Raviart-Thomas space, given by

$$RT_0(T) = \left\{ \gamma \in H_0(\operatorname{rot}, \Omega_0) : \gamma|_T = \begin{pmatrix} a + cx_2 \\ b - cx_1 \end{pmatrix} \ \forall T \in \Delta_h \right\}.$$

The reduction operator  $R_h: H_0(rot, \Omega_0) \to \mathcal{S}_h$  satisfies

$$\int_{e} (R_h \gamma - \gamma) \cdot \tau_e \, ds = 0, \; \forall e \text{ edge of } T.$$

Using the notation of the shell elements described in the previous section, define (see figure B.1)

$$T = \text{blkdiag}(\tau_1^T, \tau_2^T, \tau_3^T)$$
  

$$\Upsilon = \begin{pmatrix} e_{rt}^1 & e_{st}^1 & e_{rt}^2 & e_{st}^2 & e_{st}^3 & e_{st}^3 & e_{rt}^4 & e_{st}^4 & e_{st}^5 & e_{st}^5 & e_{rt}^6 & e_{st}^6 \end{pmatrix}^T$$

The vectors  $\tau_i$  here are the tangents to the reference triangle. The coefficients a, b, con each T may then be determined by solving the  $3 \times 3$  linear system

$$T\begin{pmatrix} 1 & 0 & 0\\ 0 & 1 & -\frac{1}{2}\\ 1 & 0 & \frac{1}{2}\\ 0 & 1 & 0\\ 1 & 0 & \frac{1}{2}\\ 0 & 1 & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} a\\ b\\ c \end{pmatrix} = T\begin{pmatrix} 0 & 0 & \frac{1}{6} & 0 & \frac{1}{6} & 0\\ 0 & 0 & 0 & \frac{1}{6} & 0 & \frac{1}{6} & 0\\ \frac{1}{6} & 0 & 0 & 0 & \frac{1}{6} & 0\\ 0 & \frac{1}{6} & 0 & 0 & 0 & \frac{1}{6} & 0\\ 0 & \frac{1}{6} & 0 & 0 & 0 & \frac{1}{6} & 0\\ 0 & 0 & 0 & 0 & \frac{2}{3} & 0 & 0\\ \frac{1}{6} & 0 & \frac{1}{6} & 0 & 0 & 0 & 0\\ 0 & \frac{1}{6} & 0 & \frac{1}{6} & 0 & 0 & 0 & 0\\ 0 & \frac{1}{6} & 0 & \frac{1}{6} & 0 & 0 & 0 & 0\\ 0 & \frac{1}{6} & 0 & \frac{1}{6} & 0 & 0 & 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{2}{3} \end{pmatrix} \Upsilon.$$

The interpolated strain tensors on the reference triangle must then be transformed back into physical coordinates, as in section B.1.6.

As with the MITC3 shell element, described in [87], the in-plane strain terms are unaltered. Thus, the weak form for the stiffness matrix is

$$\int_{\Omega_0} \left[ C^{\alpha\beta\lambda\mu} \left( t e^0_{\alpha\beta}(u_h^3) e^0_{\alpha\beta}(v_h^3) + \frac{t^3}{12} e^1_{\alpha\beta}(u_h^3) e^1_{\alpha\beta}(v_h^3) \right) + D^{\alpha\lambda} (t \tilde{e}^0_{\alpha3}(u_h^3) \tilde{e}^0_{\lambda3}(v_h^3)) \right] \sqrt{a} \, d\xi.$$

#### B.1.4 MITC6b

Here, I outline implementation of the MITC6b shell element, described in [87, §4].

The MITC6b element uses interpolation for both the in and out-of plane strain components. The weak form for the stiffness matrix then becomes

$$\int_{\Omega_0} \left[ C^{\alpha\beta\lambda\mu} \left( t \tilde{e}^0_{\alpha\beta}(u_h^3) \tilde{e}^0_{\alpha\beta}(v_h^3) + \frac{t^3}{12} \tilde{e}^1_{\alpha\beta}(u_h^3) \tilde{e}^1_{\alpha\beta}(v_h^3) \right) + D^{\alpha\lambda} (t \tilde{e}^0_{\alpha3}(u_h^3) \tilde{e}^0_{\lambda3}(v_h^3)) \right] \sqrt{a} \, d\xi.$$

The in-plane strains on the reference triangle are written

$$e_{rr}, e_{ss}, e_{qq}.$$



Figure B.2: Tying points for the MITC6b element. In the above, xx can be replaced with any of rr, ss, qq, rt, st, qt. Not all of these are used.

The strain  $e_{qq}$  along the hypotenuse is used directly in the interpolation so as to enforce isotropy, and is defined via

$$e_{qq} = \frac{1}{2}(e_{rr} + e_{ss}) - e_{rs}.$$

The tying points are shown in figure B.2. They are defined via combinations of the coordinates

$$r_1 = s_1 = \frac{1}{2} - \frac{1}{2\sqrt{3}}, r_2 = s_2 = \frac{1}{2} + \frac{1}{2\sqrt{3}}.$$

Note that these are the Gauss quadrature points used to enforce (A.1.4a) for the MITC7 plate element.

However, unlike the flat MITC3 shell element, the MITC6 shell elements use interpolation for both the in-plane and transverse strains.

The in-plane strains are given by

$$\begin{pmatrix} \tilde{e}_{rr} \\ \tilde{e}_{ss} \\ \tilde{e}_{qq} \end{pmatrix} = \begin{pmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 + c_3 & b_3 - c_3 & -c_3 \end{pmatrix} \begin{pmatrix} 1 \\ r \\ s \end{pmatrix}.$$

With the definitions

the coefficients are computed via

								_
$m_{rr}^{(1)}$	$m_{ss}^{\left(2\right)}$	$m_{qq}^{\left(3 ight)}$	$l_{rr}^{\left( 1\right) }$	$l_{ss}^{(2)}$	$l_{qq}^{\left( 3\right) }$	$e_{crr}^{(1)}$	$e_{css}^{\left(2\right)}$	$e_{cqq}^{(3)}$
$\geq$								$\leq$
0	0	0	0	0	0	0	0	$\sqrt{3}$
0	0	0	0	$\sqrt{3}$	0	0	0	0
0	0	0	0	0	0	$\sqrt{3}$	0	0
0	0	1	0	0	-2	0	0	$-\sqrt{3}(1-2r_1)$
0	-1	0	0	$\sqrt{3}(1-2s_1)$	0	0	2	0
-1	0	0	2	0	0	$\sqrt{3}(1-2r_1)$	0	0
0	0	<del>, 1</del>	0	0	0	0	0	$-\sqrt{3}$
0	<b>i</b>	0	0	$-\sqrt{3}$	0	0	0	0
$^{1}$	0	0	0	0	0	$-\sqrt{3}$	0	0
$\begin{pmatrix} a_1 \end{pmatrix}$	$a_2$	$a_3$	$b_1$	$b_2$	$b_3$	C1	$c_2$	$\left( c_{3} \right)$

The transverse strains are given by

$$\begin{pmatrix} \tilde{e}_{rt} \\ \tilde{e}_{st} \end{pmatrix} = \begin{pmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \end{pmatrix} \begin{pmatrix} 1 \\ r \\ s \end{pmatrix}.$$

The coefficients are computed via

$$\begin{pmatrix} m_{rt}^{(1)} \\ m_{st}^{(2)} \\ m_{rt}^{(3)} \\ m_{st}^{(3)} \\ l_{rt}^{(3)} \\ l_{rt}^{(3)} \\ l_{rt}^{(3)} \\ l_{st}^{(3)} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \end{pmatrix} \begin{pmatrix} e_{1rt}^{(1)} \\ e_{2rt}^{(2)} \\ e_{2st}^{(3)} \\ e_{2st}^{(3)} \end{pmatrix} \\ \\ \begin{pmatrix} a_1 \\ b_1 \\ c_1 \\ a_2 \\ b_2 \\ c_2 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \\ 1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{2} & \frac{\sqrt{3}}{2} \end{pmatrix} \begin{pmatrix} m_{rt}^{(1)} \\ m_{st}^{(3)} \\ m_{rt}^{(3)} \\ m_{rt}^{(3)} \\ l_{rt}^{(1)} \\ l_{st}^{(3)} \\ l_{rt}^{(3)} \\ l_{st}^{(3)} \\ l_{st}^{(3)} \end{pmatrix} .$$

#### B.1.5 MITC6a

The MITC6a element is identical to the MITC6b element, except that it uses an additional tying point  $(r_3, s_3)$ , with  $r_3 = s_3 = 1/3$ , and a different assumed transverse shear strains. It is more closely related to MITC7 plate elements, and seems to perform better in practice [5].

The transverse strains are given by

$$\begin{pmatrix} \tilde{e}_{rt} \\ \tilde{e}_{st} \end{pmatrix} = \begin{pmatrix} a_1 & b_1 & c_1 & d_1 & e_1 & f_1 \\ a_2 & b_2 & c_2 & d_2 & e_2 & f_2 \end{pmatrix} \begin{pmatrix} 1 \\ r \\ s \\ rs \\ r^2 \\ s^2 \end{pmatrix}$$

The quantities  $m_{rt}^{(1)}, m_{st}^{(2)}, m_{rt}^{(3)}, \cdots$  are the same as for the MITC6b element. The coefficients are computed via

where  $e_{crt}, e_{cst}$  are the displacement-based strains evaluated at the new tying point  $(r_3, s_3)$ .

### **B.1.6** Tensor Transformations

As previously mentioned, the interpolation in the previous section assumes that the tensors are given with components on the unit triangle. Consider figure B.3. The



Figure B.3: The reference triangle at left with coordinates x maps to the triangle  $T_k \subset \Omega_0$  with coordinates y via y(x). The mapping  $\phi(T_k)$  then yields the patch of the middle surface corresponding to  $T_k$ .

reference coordinates on the unit triangle here are denoted x, while y is the variable corresponding to the triangle  $T_k$  in the finite element mesh of  $\Omega_0$ . The chart function  $\phi$  then takes  $T_k$  to its image on the middle surface.

The covariant basis vectors can be defined by either of the mappings  $\phi(y), \phi(y(x))$ . Let them be written

$$a_{\alpha} = \partial_{\alpha}\phi(x), \ b_{\alpha} = \partial_{\alpha}\phi(y(x)),$$

and as usual, define the contravariant basis vectors via

$$a^{\alpha} \cdot a_{\beta} = \delta^{\alpha}_{\beta}, \ b^{\alpha} \cdot b_{\beta} = \delta^{\alpha}_{\beta}.$$

Let **e** be a rank-two tensor in  $\mathcal{E}^3$ , i.e.,

$$\mathbf{e} = e^{y}_{\alpha\beta} a^{\alpha} a^{\beta} = e^{x}_{\alpha\beta} b^{\alpha} b^{\beta}. \tag{B.1.3}$$

The chain rule gives

$$\begin{pmatrix} b_1 & b_2 \end{pmatrix} = \nabla_x \phi = \nabla_y \phi(y(x)) \cdot (\nabla_x y)(x) = \begin{pmatrix} a_1 & a_2 \end{pmatrix} J_k,$$

with  $J_k$  as in figure A.2.

Dotting both sides of (B.1.3) with the covariant b vectors yields the formula for the tensor transformation:

$$e^x_{\lambda\mu} = e^y_{\alpha\beta} (a^\alpha \cdot b_\lambda) (a^\beta \cdot b_\mu).$$

These relations can be expressed in the form

$$\begin{pmatrix} e_{1t}^{x} \\ e_{2t}^{x} \end{pmatrix} = R_{1} \begin{pmatrix} e_{1t}^{y} \\ e_{2t}^{y} \end{pmatrix}$$

$$\begin{pmatrix} e_{11}^{x} \\ e_{12}^{x} \\ e_{21}^{x} \\ e_{22}^{x} \end{pmatrix} = R_{2} \begin{pmatrix} e_{11}^{y} \\ e_{12}^{y} \\ e_{21}^{y} \\ e_{22}^{y} \end{pmatrix} ,$$

with the matrices  $R_1, R_2$  given by

$$(R_1)_{\alpha\beta} = a^{\beta} \cdot b_{\alpha}$$

$$R_2 = \begin{pmatrix} (a^1 \cdot b_1)^2 & (a^1 \cdot b_1)(a^2 \cdot b_1) & (a^2 \cdot b_1)(a^1 \cdot b_1) & (a^2 \cdot b_1)^2 \\ (a^1 \cdot b_1)(a^1 \cdot b_2) & (a^1 \cdot b_1)(a^2 \cdot b_2) & (a^2 \cdot b_1)(a^1 \cdot b_2) & (a^2 \cdot b_1)(a^2 \cdot b_2) \\ (a^1 \cdot b_2)(a^1 \cdot b_1) & (a^1 \cdot b_2)(a^2 \cdot b_1) & (a^2 \cdot b_2)(a^1 \cdot b_1) & (a^2 \cdot b_2)(a^2 \cdot b_1) \\ (a^1 \cdot b_2)^2 & (a^1 \cdot b_2)(a^2 \cdot b_2) & (a^2 \cdot b_2)(a^1 \cdot b_2) & (a^2 \cdot b_2)^2 \end{pmatrix}$$

# B.2 Differentiation of Geometric Terms in Shell Equations

Listed here are the geometric terms needed for the shape differentiation of the shell equations under the MITC3 discretization.

- The triangle normal vectors  $n_j, j \in \{1, \cdots, N_T\}$ .
- The change of area factor  $\sqrt{a_j}, j \in \{1, \cdots, N_T\}$ .
- The vectors  $a_1^j, a_2^j, a_3^j, j \in \{1, \cdots, N_V\}.$
- The contravariant components  $a^{11}, a^{12}, a^{22}$  of the metric tensor on each triangle.

MITC6 is somewhat more complicated, since the normal vector (as computed from derivatives of the chart),  $\sqrt{a}$ , and  $a^{\alpha\beta}$  are not constant over each element. In this section, only the MITC3 case is discussed.

The calculation of the derivative of the normal vectors is worked out in the section on shape differentiation for boundary integral equations, §C.2.2.

The most troublesome part is the vector  $a_3$ . Recall that for MITC3 (also MITC6) elements, it does not make sense to define  $a_3$  in terms of derivatives of the chart function, because they are discontinuous at element boundaries, c.f. §B.1, and that the solution to this problem is to define  $a_3$  at each vertex, and interpolate in between. When the middle surface is something like a parabaloid, the exact formula for  $a_3$  can be used at the vertices, but in order to do optimization, explicit explicit dependence of these quantities on the chart function  $\phi$  must be established: it does not make sense to include the choice of the vectors  $a_3$  as optimization variables. Let nb(j)denote the set of all triangles that include vertex j (its neighbors). Define  $a_3$  by the area-weighted average

$$a_3^j = \frac{\sum_{i \in \operatorname{nb}(j)} \Delta_i n_i}{\|\sum_{i \in \operatorname{nb}(j)} \Delta_i n_i\|}$$

Recall that  $a_1^j, a_2^j$  need only be in the plane orthogonal to  $a_3^j$ . Let  $\{e_1, e_2, e_3\}$  be the three Cartesian coordinate vectors. Remove from this set the vector  $e_k$ , where

$$k = \operatorname{argmax}_{j \in \{1,2,3\}} |e_j \cdot a_3|,$$

leaving the set  $\{d_1, d_2\}$  (the Cartesian coordinate vectors less in the direction  $a_3^j$ ). Define  $a_1^j, a_2^j$  via the projection

$$a_1^j = (I - a_3^j (a_3^j)^T) d_1$$
$$a_2^j = (I - a_3^j (a_3^j)^T) d_2.$$

The derivative of  $a_3^j$  is

$$D_{\phi}a_3^j = \frac{1}{\|\sum_{i \in \operatorname{nb}(j)} \Delta_i n_i\|} \left(I - a_3^j (a_3^j)^T\right) \sum_{i \in \operatorname{nb}(j)} \left(n_j D_{\phi} \Delta_i + \Delta_i D_{\phi} n_i\right).$$

The derivatives of  $a_1^j, a_2^j$  are

$$D_{\phi}a_{1}^{j} = -\left((a_{3}^{j})^{T}d_{1}I + a_{3}^{j}d_{1}^{T}\right)D_{\phi}a_{3}^{j}$$
$$D_{\phi}a_{2}^{j} = -\left((a_{3}^{j})^{T}d_{2}I + a_{3}^{j}d_{2}^{T}\right)D_{\phi}a_{3}^{j}.$$

In the rest of this section, note that if, e.g.,  $a_1$  appears without the superscript j, it means the derivative  $\partial_1 \phi$ , not the nodal basis vector. The change of area factor and its derivative are given by

$$\sqrt{a} = \sqrt{a_{11}a_{22} - a_{12}^2}$$
$$D_{\phi}\sqrt{a} = \frac{1}{2\sqrt{a}} \begin{pmatrix} a_{22} & -2a_{12} & a_{11} \end{pmatrix} \cdot D_{\phi} \begin{pmatrix} a_{11} \\ a_{12} \\ a_{22} \end{pmatrix} .$$

It is also necessary to differentiate the contravariant components of the metric tensor, viz.

$$\begin{pmatrix} a^{11} & a^{12} \\ a^{21} & a^{22} \end{pmatrix} = \frac{1}{\sqrt{a^2}} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix}$$
$$D_{\phi} \begin{pmatrix} a^{11} \\ a^{12} \\ a^{22} \end{pmatrix} = \begin{bmatrix} \frac{1}{\sqrt{a^2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix} - \frac{1}{\sqrt{a^4}} \begin{pmatrix} a_{22} \\ -a_{12} \\ a_{11} \end{pmatrix} \begin{pmatrix} a_{22} & -2a_{12} & a_{11} \end{pmatrix} \end{bmatrix} D_{\phi} \begin{pmatrix} a_{11} \\ a_{12} \\ a_{22} \end{pmatrix} .$$

For both of these, the derivative

$$D_{\phi} \begin{pmatrix} a_{11} \\ a_{12} \\ a_{22} \end{pmatrix} = \begin{pmatrix} 2a_1^T & 0 \\ a_2^T & a_1^T \\ 0 & 2a_2^T \end{pmatrix} D_{\phi} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$$

is needed. Recall figure B.3, in which x is used for the reference element, and y is used for the coordinates in the mesh of the reference domain. Then

$$\begin{pmatrix} a_1 & a_2 \end{pmatrix} = \nabla_y \phi = \nabla_x \phi J_x,$$
 (B.2.1)

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where

$$J_x = \begin{pmatrix} y_2 - y_1 & y_3 - y_1 \end{pmatrix}^{-1} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

is the Jacobian of the transformation x(y). From (B.2.1), it holds that

$$D_{\phi} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \delta \phi = \begin{pmatrix} -(\alpha + \gamma)I_3 & \alpha I_3 & \gamma I_3 \\ -(\beta + \delta)I_3 & \beta I_3 & \delta I_3 \end{pmatrix} \begin{pmatrix} \delta \phi_1 \\ \delta \phi_2 \\ \delta \phi_3 \end{pmatrix}.$$
## Appendix C

# **Boundary Elements**

## C.1 Galerkin Boundary Element Methods

In this section, Galerkin discretizations of (4.3.4) and (4.3.9) are worked out. In both instances, it is assumed that the boundary  $\Gamma$  is composed of  $N_T$  triangular patches  $\{T_1, \dots, T_{N_T}\}$  with  $N_v$  vertices. The area of  $T_k$  is  $\Delta_k$ . The piecewise-linear and piecewise-constant finite element subspaces are

$$\Phi_h^+ = \left\{ \psi \in H^{1/2}(\Gamma) : \psi|_{T_j} \in P_1(T_j), \forall j \in \{1, \cdots, N_T\} \right\},$$
  
$$\Phi_h^- = \left\{ \psi \in H^{-1/2}(\Gamma) : \psi|_{T_j} \in P_0(T_j), \forall j \in \{1, \cdots, N_T\} \right\}.$$

Let  $T_k$  be the triangle with vertices  $v_{k_1}, v_{k_2}, v_{k_3}$ . The map

$$\xi \mapsto v_{k_1} + J_k \xi, \tag{C.1.1}$$

where

$$J_k = (v_{k_2} - v_{k_1}, v_{k_3} - v_{k_1}) \in \mathbb{R}^{3 \times 2}$$

maps the unit triangle  $\widehat{T}$  onto  $T_k$  (see Figure C.1).

If  $N_1^3, \ldots, N_{N_v}^3$  are Lagrange basis functions for  $\Phi_h^+$ , then the basis functions  $N_{k_1}^3, N_{k_2}^3, N_{k_3}^3$  which have support that intersects with  $T_k$  satisfy

$$N_{k_i}^3(v_{k_1}+J_k\xi) = \widehat{N}_i^3(\xi), \quad i = 1, 2, 3.$$



Figure C.1: Transformation between reference and physical coordinates.

Due to the representation formulae of theorem 4.3.2, if  $\rho_h, \varsigma_h \in \Phi_h^+$ , and  $\psi_h, \chi_h \in \Phi_h^-$ , then

$$\langle V\psi_{h}, \chi_{h} \rangle_{H^{1/2}(\Gamma) \times H^{-1/2}(\Gamma)}$$
(C.1.2a)  

$$= \frac{1}{4\pi} \int_{\Gamma} \chi_{h}(x) \int_{\Gamma} \frac{\exp(i\kappa |x-y|)}{|x-y|} \psi_{h}(y) \, dy \, dx$$
(C.1.2b)  

$$= \frac{1}{4\pi} \int_{\Gamma} \psi_{h}(x) \int_{\Gamma} (-1+i\kappa |x-y|) \exp(i\kappa |x-y|) \frac{(y-x,n(y))}{|x-y|^{3}} \varrho_{h}(y) \, dy \, dx$$
(C.1.2c)  

$$= \frac{1}{4\pi} \int_{\Gamma} \varrho_{h}(x) \int_{\Gamma} (-1+i\kappa |x-y|) \exp(i\kappa |x-y|) \frac{(x-y,n(x))}{|x-y|^{3}} \psi_{h}(y) \, dy \, dx$$
(C.1.2c)  

$$= \frac{1}{4\pi} \int_{\Gamma} \varrho_{h}(x) \int_{\Gamma} (-1+i\kappa |x-y|) \exp(i\kappa |x-y|) \frac{(x-y,n(x))}{|x-y|^{3}} \psi_{h}(y) \, dy \, dx$$
(C.1.2d)  

$$= \frac{1}{4\pi} \int_{\Gamma} \frac{\exp(i\kappa |x-y|)}{|x-y|} (n(y) \times \nabla \varrho_{h}(y)) \cdot (n(x) \times \nabla \varsigma_{h}(x)) \, dy \, dx$$
(C.1.2d)

In the formula for D, the gradient  $\nabla \varrho_h$ , is the gradient of a function  $\varrho : \mathbb{R}^3 \to \mathbb{C}$ , satisfying  $\varrho|_{\Gamma} = \varrho_h$ , and  $\partial_n \varrho = 0$  on  $\Gamma$ .

#### C.1.1 Finite Element Matrices

Galerkin discretization of (4.3.3) and (4.3.4) using respectively the spaces  $\Phi^+$  and  $\Phi^$ leads to the finite element matrices

$$\mathbb{C}^{N_T \times N_v} \ni \widehat{M}_{lm} = \int_{T_l} N_m^3(x) \, dx \tag{C.1.3a}$$

$$\mathbb{C}^{N_T \times N_T} \ni \widehat{V}_{lm} = \frac{1}{4\pi} \int_{T_l} \int_{T_m} \frac{\exp(i\kappa |x-y|)}{|x-y|} \, dy \, dx \tag{C.1.3b}$$

$$\mathbb{C}^{N_T \times N_v} \ni \widehat{K}_{lm} = \frac{1}{4\pi} \int_{T_l} \int_{\Gamma} (-1 + i\kappa |x - y|) \exp(i\kappa |x - y|) \frac{(y - x, n(y))}{|x - y|^3} N_m^3(y) \, dy \, dx$$
(C.1.3c)

$$\mathbb{C}^{N_v \times N_v} \ni \widehat{D}_{lm} = \frac{1}{4\pi} \iint_{\Gamma} \frac{\exp(i\kappa|x-y|)}{|x-y|} (n(y) \times \nabla N_m^3(y), n(x) \times \nabla N_l^3(x)) \, dy \, dx$$
$$- \frac{\kappa^2}{4\pi} \iint_{\Gamma} \frac{\exp(i\kappa|x-y|)}{|x-y|} n(y) N_m^3(y) \cdot n(x) N_l^3(x) \, dy \, dx. \quad (C.1.3d)$$

Since  $\kappa = \omega/c$ , the matrices  $\widehat{K}$ ,  $\widehat{V}$ , and  $\widehat{D}$  depend on the frequency, i.e.,

$$\widehat{K} = \widehat{K}(\omega), \quad \widehat{V} = \widehat{V}(\omega), \quad \widehat{D} = \widehat{D}(\omega).$$

The discrete forms of (4.3.3) and (4.3.4) are then

$$(-\frac{1}{2}\widehat{M} + \widehat{K})\vec{\varphi}_{\Gamma} = \widehat{V}\vec{g} \tag{C.1.4}$$

$$\widehat{D}\vec{\varphi}_{\Gamma} = -\left(\frac{1}{2}\widehat{M}^T + \widehat{K}^T\right)\vec{g}$$
(C.1.5)

Of course, (C.1.4) does not make sense for solving the Neumann problem, though it could be used to solve the Dirichlet problem.

For a discretization of the Burton-Miller formulation (4.3.9), additional matrices are required, since Burton-Miller treats the terms of (4.3.3) as elements of  $H^{-1/2}(\Gamma)$ . The new matrices are:

$$\begin{split} \mathbb{C}^{N_{v} \times N_{v}} &\ni \check{M}_{lm} = \int_{\Gamma} N_{l}^{3}(x) N_{m}^{3}(x) \, dx \\ \mathbb{C}^{N_{v} \times N_{v}} &\ni \check{K}_{lm} = \frac{1}{4\pi} \int_{\Gamma} N_{l}^{3}(x) \int_{\Gamma} (-1 + i\kappa |x - y|) \exp(i\kappa |x - y|) \frac{(y - x, n(y))}{|x - y|^{3}} N_{m}^{3}(y) \, dy \, dx \\ \mathbb{C}^{N_{v} \times N_{T}} &\ni \check{V}_{lm} = \frac{1}{4\pi} \int_{\Gamma} N_{l}^{3}(x) \int_{T_{m}} \frac{\exp(i\kappa |x - y|)}{|x - y|} \, dy \, dx. \end{split}$$

Since  $\kappa = \omega/c$ , the matrices  $\check{K}$  and  $\check{V}$  depend on the frequency, i.e.,

$$\check{K} = \check{K}(\omega), \quad \check{V} = \check{V}(\omega).$$

The discrete form of (4.3.9) is then

$$(-\frac{1}{2}\check{M}+\check{K})\vec{\varphi}_{\Gamma}+i\eta\widehat{D}\vec{\varphi}_{\Gamma}=\check{V}\vec{g}-i\eta(\frac{1}{2}\widehat{M}^{T}+\widehat{K}^{T})\vec{g}.$$
(C.1.6)

In the next two sections, the numerical procedures required to evaluate the entries of these matrices are discussed.

#### C.1.2 Singularity Subtraction

The integrals

$$\int_{T_k} N_{k_i}^3 \, dx = 2 \triangle_k \int_{\widehat{T}} \widehat{N}_i^3(\xi) \, d\xi = 2 \triangle_k \frac{1}{6} = \triangle_k/3$$
$$\int_{T_k} N_{k_i}^3 N_{k_j}^3 \, dx = 2 \triangle_k \int_{\widehat{T}} \widehat{N}_i^3(\xi) \widehat{N}_j^3(\xi) \, d\xi = 2 \triangle_k \begin{cases} \frac{1}{12} & i = j\\ \frac{1}{24} & i \neq j \end{cases}$$

allow evaluation of the mass matrix entries, yielding

$$\widehat{M}_{lm} = \begin{cases} \Delta_l/3 & \text{if } N_m^3 \text{ supported in } T_l \\\\ 0 & \text{otherwise} \end{cases}$$
$$\check{M}_{lm} = \sum_{\substack{\varphi_l,\varphi_m \\ \text{supported in } T_j}} \begin{cases} \Delta_j/6 & l = m \\ \Delta_j/12 & l \neq m. \end{cases}$$



Figure C.2: Parameterization of the triangle  $T_k = \{x = x_1 + sr_1 + tr_2 : 0 < s < s_T, \alpha_1 s < t < \alpha_2 s\}$ .  $\alpha_1 = -t_*/s_T, \alpha_2 = (t_T - t_*)/s_T$  are the tangents of the angles between  $r_1$  and  $\overline{x_1 x_2}, \overline{x_1 x_3}$ , respectively.

In the formulae for the finite element matrices, it is necessary to evaluate the following integrals, which are broken up as

$$\begin{split} \int_{T_{k}} \frac{\exp(i\kappa|x-y|)}{|x-y|} \, dy &= \underbrace{\int_{T_{k}} \frac{1}{|x-y|} \, dy}_{\text{integrate analytically}} + \underbrace{\int_{T_{k}} \frac{\exp(i\kappa|x-y|) - 1}{|x-y|} \, dy}_{\text{use quadrature}} \\ \int_{T_{k}} \frac{\exp(i\kappa|x-y|)}{|x-y|} N_{k_{j}}^{3}(y) \, dy &= \underbrace{\int_{T_{k}} \frac{1}{|x-y|} N_{k_{j}}^{3}(y) \, dy}_{\text{integrate analytically}} + \underbrace{\int_{T_{k}} \frac{\exp(i\kappa|x-y|) - 1}{|x-y|} N_{k_{j}}^{3}(y) \, dy}_{\text{use quadrature}} \\ \int_{T_{k}} (1 - i\kappa|x-y|) \exp(i\kappa|x-y|) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy = \underbrace{\int_{T_{k}} \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy}_{\text{integrate analytically}} \\ &+ \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy}_{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1) \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1 \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1 \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp(i\kappa|x-y|) - 1 \frac{(x-y,n(y))}{|x-y|^{3}} N_{k_{j}}^{3}(y) \, dy, \\ & \underbrace{\int_{T_{k}} ((1 - i\kappa|x-y|) \exp($$

In this decomposition, the analytically integrated terms are exactly those potentials that appear for the Laplace operator, while the quadrature terms are non-singular. A 5th-order quadrature scheme is used, with parameterization for analytic integration following [105, Appendix C.2]. The analytic integration is used for the singular inner integrals in (C.1.3), while quadrature is used for the non-singular parts, and for evaluation of all outer integrals.

#### C.1.3 The Parameterization

The parameterization is shown in figure C.2. The vertices of triangle  $T_k$  are  $x_1, x_2, x_3$ . The local coordinate system uses the in-plane vectors  $r_1, r_2$ , and the triangle normal n. These are computed via

$$r_{2} = \frac{x_{3} - x_{2}}{t_{T}}$$

$$t_{T} = |x_{3} - x_{2}|$$

$$x_{*} = x_{1} + s_{T}r_{1} = x_{2} + t_{*}r_{2}$$

$$t_{*} = (x_{1} - x_{2}) \cdot r_{2}$$

$$r_{1} = \frac{x_{*} - x_{1}}{s_{T}}$$

$$s_{T} = |x_{*} - x_{1}|.$$

The normal is then  $n = r_1 \times r_2$ . The source point x is then represented

$$x = x_1 + s_x r_1 + t_x r_2 + u_x n,$$

while the integration point y is written

$$y = x_1 + sr_1 + tr_2.$$

#### C.1.4 Single Layer Potential

Using the parameters

$$p = \frac{\alpha t_x + s_x}{1 + \alpha^2}, \ q^2 = u_x^2 + \frac{(t_x - \alpha s_x)^2}{1 + \alpha^2},$$

the first of these integrals can be computed as

$$\int_{T_k} \frac{1}{|x-y|} \, dy = \int_0^{s_T} \int_{\alpha_1 s}^{\alpha_2 s} \frac{1}{\sqrt{(s-s_x)^2 + (t-t_x)^2 + u_x^2}} \, dt \, ds$$
$$= (F(s_T, \alpha_2) - F(0, \alpha_2) - F(s_T, \alpha_1) + F(0, \alpha_1)) \, dt$$

where (from  $[105, \S C.2.1]$ )

$$F(s,\alpha) = (s - s_x) \log \left( \alpha s - t_x + \sqrt{(s - s_x)^2 + (\alpha s - t_x)^2 + u_x^2} \right) - s + \frac{\alpha s_x - t_x}{\sqrt{1 + \alpha^2}} \log \left( \sqrt{1 + \alpha^2} (s - p) + \sqrt{(1 + \alpha^2)(s - p)^2 + q^2} \right) + 2u_x \arctan \frac{\left(q - \frac{\alpha s_x - t_x}{1 + \alpha^2}\right) \sqrt{(1 + \alpha^2)(s - p)^2 + q^2} + (\alpha s - t_x - q)q}{(s - p)u_x}$$

There is numerical trouble with the arctan term in  $F(s, \alpha)$  when  $s \to p$ . In this case, the argument of arctan approaches a limit, but will be inaccurately computed in floating point. The term can be written

$$2u_x \arctan \frac{2A_2v + A_1}{2\sqrt{1+\alpha^2}u_x},$$

where

$$A_{1} = 2\alpha\sqrt{1+\alpha^{2}}q$$

$$A_{2} = (1+\alpha)^{2}q - (\alpha s_{x} - t_{x})$$

$$v = \frac{\sqrt{(1+\alpha^{2})(s-p)^{2} + q^{2}} - q}{\sqrt{1+\alpha^{2}}(s-p)}.$$

Then,

$$\lim_{s \to p} v = 0,$$

and thus,

$$\lim_{s \to p} \frac{2A_2v + A_1}{2\sqrt{1 + \alpha^2}u_x} = \frac{\alpha q}{u_x}.$$

If  $u_x = 0$ , the arctan term vanishes, and if  $s \to s_x$ , it is necessary to use

$$\lim_{s \to s_x} (s - s_x) \log \left( \alpha s - t_x + \sqrt{(s - s_x)^2 + (\alpha s - t_x)^2 + u_x^2} \right) = 0.$$

Likewise,

$$\lim_{\alpha \to s_x/t_x} \frac{\alpha s_x - t_x}{\sqrt{1 + \alpha^2}} \log \left( \sqrt{1 + \alpha^2} (s - p) + \sqrt{(1 + \alpha^2)(s - p)^2 + q^2} \right) = 0.$$

#### C.1.5 Single-Layer Potential With Basis Function

Recall that calculation of the integral

$$\int_{T_k} \frac{1}{|x-y|} N_{k_j}^3(y) \, dy \tag{C.1.7}$$

is also needed. Following a personal communication from O. Steinbach [108] in which the procedure from [105, C.2.1] is modified for the basis function, the integral can be written as

$$\int_{T_k} \frac{1}{|x-y|} N_{k_j}^3(y) \, dy = \frac{1}{s_T} \left( F(s_T, \alpha_2) - F(0, \alpha_2) - \left( F(s_T, \alpha_1) - F(0, \alpha_1) \right) \right),$$

where the function F is now given by

$$\begin{split} F(s,\alpha) &= \frac{1}{2} \left( s_x^2 + 2s_T (s - s_x) - s^2 \right) \log \left( \alpha s - t_x + \sqrt{(1 + \alpha^2)(s - p)^2 + q^2} \right) + \\ &= \frac{s^2}{4} + \frac{1}{2} s(s_x - 2s_T) + \frac{1}{2} u_x^2 \left( \log(2q) - \log \left( q + \sqrt{\beta^2(s - p)^2 + q^2} \right) \right) + \\ &= \frac{1}{2\beta} \left( \alpha q^2 + 2(t_x - \alpha s_x)(s_x - s_T) \right) \left( \log \left( \beta(s - p) + \sqrt{\beta^2(s - p)^2 + q^2} \right) - \log q \right) + \\ &= \frac{1}{2\beta^2} (t_x - \alpha s_x) \left( \sqrt{\beta^2(s - p)^2 + q^2} + q \right) - \frac{1}{2} u_x^2 \log \left( A_2 v^2 + A_1 v + A_0 \right) - \\ &= 2u_x (s_x - s_T) \arctan \frac{1}{u_x} \left( \frac{(\beta^2 q - (\alpha s_x - t_x))(s - p)}{\sqrt{\beta^2(s - p)^2 + q^2} + q} + \alpha q \right), \end{split}$$

where  $\beta = \sqrt{1 + \alpha^2}$ . If  $u_x = 0$ , then this becomes

$$F(s,\alpha) = \frac{1}{2} \left( s_x^2 + 2s_T(s - s_x) - s^2 \right) \log \left( \alpha s - t_x + \sqrt{(1 + \alpha^2)(s - p)^2 + q^2} \right) + \frac{s^2}{4} + \frac{1}{2} s(s_x - 2s_T) + \frac{1}{2\beta^2} (t_x - \alpha s_x) \left( \sqrt{\beta^2(s - p)^2 + q^2} + q \right) + \frac{1}{2\beta} \left( \alpha q^2 + 2(t_x - \alpha s_x)(s_x - s_T) \right) \left( \log \left( \beta(s - p) + \sqrt{\beta^2(s - p)^2 + q^2} \right) - \log q \right).$$

Once again, if  $u_x = 0$ , the limit

$$\lim_{s \to s_x} \frac{1}{2} \left( s_x^2 + 2s_T (s - s_x) - s^2 \right) \log \left( \alpha s - t_x + \sqrt{(1 + \alpha^2)(s - p)^2 + q^2} \right) = 0$$

must be used. Likewise,

$$\lim_{s \to s_x/t_x} \frac{1}{2\beta} \left( \alpha q^2 + 2(t_x - \alpha s_x)(s_x - s_T) \right) \left( \log \left( \beta(s-p) + \sqrt{\beta^2(s-p)^2 + q^2} \right) - \log q \right) = 0.$$

### C.1.6 Double-Layer Potential

The integral of the double-layer potential against the basis function  ${\cal N}^3_{k_1}$  can be computed as

$$\int_{T_k} \frac{(x-y,n(y))}{|x-y|^3} N_{k_1}^3(y) \, dy = \int_0^{s_T} \frac{s_T-s}{s_T} \int_{\alpha_1 s}^{\alpha_2 s} \frac{u_x}{((t-t_x)^2 + (s-s_x)^2 + u_x^2)^{3/2}} \, dt \, ds$$
(C.1.8)
$$= \frac{1}{s_T} \left( F(s_T,\alpha_2) - F(0,\alpha_2) - F(s_T,\alpha_1) + F(0,\alpha_1) \right).$$

Once again, the vertex order can be permuted to get the integrals against the other basis functions. Here, F (see [105, §C.2.2]) is given by

$$F(s,\alpha) = -\frac{1}{2}u_x \log \left(v^2 + A_1v + B_1\right) + (s_T - s_x)\frac{u_x}{|u_x|} \arctan \left(\frac{2v + A_1}{2G_1}\right) + \frac{1}{2}u_x \log \left(v^2 + A_2v + B_2\right) - (s_T - s_x)\frac{u_x}{|u_x|} \arctan \left(\frac{2v + A_2}{2G_2}\right) - u_x \frac{\alpha}{\sqrt{1 + \alpha^2}} \log \left(\sqrt{1 + \alpha^2}(s - p) + \sqrt{(1 + \alpha^2)(s - p)^2 + q^2}\right),$$

where

$$\begin{aligned} A_1 &= -\frac{2\alpha\sqrt{1+\alpha^2}q}{u_x^2 + \alpha^2 q^2} \left(\frac{t_x - \alpha s_x}{1+\alpha^2} + q\right), \quad A_2 &= -\frac{2\alpha\sqrt{1+\alpha^2}q}{u_x^2 + \alpha^2 q^2} \left(\frac{t_x - \alpha s_x}{1+\alpha^2} - q\right) \\ B_1 &= \frac{1+\alpha^2}{u_x^2 + \alpha^2 q^2} \left(\frac{t_x - \alpha s_x}{1+\alpha^2} + q\right)^2, \qquad B_2 &= \frac{1+\alpha^2}{u_x^2 + \alpha^2 q^2} \left(\frac{t_x - \alpha s_x}{1+\alpha^2} - q\right)^2 \\ G_1 &= \frac{\sqrt{1+\alpha^2}|u_x|}{u_x^2 + \alpha^2 q^2} \left(q + \frac{t_x - \alpha s_x}{1+\alpha^2}\right), \qquad G_2 &= \frac{\sqrt{1+\alpha^2}|u_x|}{u_x^2 + \alpha^2 q^2} \left(q - \frac{t_x - \alpha s_x}{1+\alpha^2}\right). \end{aligned}$$

Once again, as  $s \to p, v \to 0$ . When  $u_x \to 0$ , the integral just becomes zero.

#### C.1.7 Numerical Evaluation of the Representation Formula

Evaluation of  $\varphi$  in the exterior domain relies on (4.2.11), repeated here:

$$\varphi = DL\gamma^+\varphi - SL\partial_n^+\varphi.$$

The evaluation of the SL and DL operators is done using the machinery developed respectively for V and K; there is no singularity since the source point is now in the exterior domain.

### C.2 Differentiation of Boundary Integral Equations

#### C.2.1 Double-Layer Potential for Shape Differentiation

This section deals with the discretization of the derivatives of the hypersingular operator, appearing in (4.5.3). The term

$$-\kappa^2 \iint_{\Omega_0} \left( \frac{\partial G}{\partial r} \frac{\partial r}{\partial \phi} (a_3^y \varphi(y)) \cdot (a_3^x \varrho(x)) + G\varphi(y) \varrho(x) D_\phi(a_3^y \cdot a_3^x) \right) \sqrt{a_y} \sqrt{a_x} \delta \phi \, dy dx$$

provides the worst of the added complication: upon singularity subtraction, it is necessary to evaluate an integral that is like the double-layer potential (C.1.8), but with the piecewise constant term n(y) replaced by the differential shape change z, which is piecewise-linear. Moreover, z can have non-zero components in the plane of integration. This means that unlike the case of the double-layer potential (C.1.8), the integral does not vanish in-plane, and so it is necessary to compute the finitepart integrals arising when the source quadrature point is in the integration triangle. These are evaluated using the finite part quadrature method of [98].

When the source point is not inside the triangle (but is near enough that quadrature is expensive), the parameterizated integral

$$\frac{1}{4\pi} \int_{T} \frac{(x-y,z)}{|x-y|^3} N_{k_j}^3(y) \, dy = \frac{1}{4\pi} \int_{0}^{s_T} \frac{s_T-s}{s_T} \int_{\alpha_1 s}^{\alpha_2 s} \frac{(s_x-s)z_1 + (t_x-t)z_2 + u_x z_n}{((t-t_x)^2 + (s-s_x)^2 + u_x^2)^{3/2}} \, dt ds$$

is used, where

$$z = z_1 r_1 + z_2 r_2 + z_n n$$

In order to deal with the piecewise-linear nature of z, introduce another copy of either the first or second Lagrange basis functions on the triangle, respectively

$$\frac{s_T-s}{s_T}, \ \frac{\alpha_2 s-t}{s_T(\alpha_2-\alpha_1)},$$

and thus must compute the integrals

$$-\frac{1}{4\pi} \int_0^{s_T} \left(\frac{s_T - s}{s_T}\right)^2 \int_{\alpha_1 s}^{\alpha_2 s} \frac{(s_x - s)z_1 + (t_x - t)z_2 + u_x z_n}{((t - t_x)^2 + (s - s_x)^2 + u_x^2)^{3/2}} dt ds, \qquad (C.2.1)$$

$$\frac{1}{4\pi} \int_0^{s_T} \frac{s_T - s}{s_T} \int_{\alpha_1 s}^{\alpha_2 s} \frac{\alpha_2 s - t}{s_T (\alpha_2 - \alpha_1)} \frac{(s_x - s)z_1 + (t_x - t)z_2 + u_x z_n}{((t - t_x)^2 + (s - s_x)^2 + u_x^2)^{3/2}} dt ds.$$
(C.2.2)

To compute these integrals, one must modify the procedure for the double-layer potential found in [105, §C.2.2]. In both cases, one does the inner integration over tfirst, obtaining

$$F(s,\alpha) = \frac{1}{4\pi s_T^2} \int (s_T - s)^2 \left[ \frac{(\alpha s - t_x)((s_x - s)r_1 + u_x n)}{(s - s_x)^2 + u_x^2} + r_2 \right] \frac{ds}{\sqrt{(\alpha s - t_x)^2 + (s - s_x)^2 + u_x^2}}$$

for (C.2.1), and

$$F(s,\alpha) = \frac{1}{4\pi s_T^2(\alpha_2 - \alpha_1)} \int (s_T - s) \left[ r_2 \log(\alpha s - t_x + \sqrt{(1 + \alpha^2)(s - p)^2 + q^2}) + \frac{(\alpha_2 - \alpha)sr_2}{\sqrt{(1 + \alpha^2)(s - p)^2 + q^2}} + \frac{((s_x - s)r_1 + u_xn)((s - s_x)^2 + t_x(t_x - \alpha s) + u_x^2 + \alpha_2s(\alpha s - t_x))}{((s - s_x)^2 + u_x^2)\sqrt{(1 + \alpha^2)(s - p)^2 + q^2}} \right] ds$$

for (C.2.2). These integrals can be computed using essentially the same technique involved in the calculation of the integral (C.1.8). The trick is to factor the term  $((s-s_x)^2+u_x^2)$  out of the numerator. This reduces the integral to the sum of a simpler integral, and the same integral as before, but with a lower-degree polynomial in the numerator. See [105, §C.2.2] for details. Unlike that case, in order to evaluate (C.2.1) and (C.2.2), it is necessary to repeat this step several times until the numerator is reduced to first order in s. Then, unless  $a_1 = u_x^2 + \alpha^2 q^2 = 0$ , the rest of the procedure beginning on page 250 works with only slight modification: if  $u_x = 0$ ,  $G_{1/2} = 0$ , and the integral  $\int (v^2 + A_{1/2}v + B_{1/2})^{-1} dv$  must be evaluated differently. If  $a_1 = 0$ , the integral at the top of p. 250 (but with different coefficients in the numerator) must be treated differently. In particular, the relevant cases are q = 0, and  $q \neq 0$ , but  $\alpha = 0$ . In the latter of these two, it is necessary to take ratios between log terms arising for s = 0 and  $s = s_{\tau}$ , as these may not make sense for  $F(s_{\tau}, 0)$  and F(0, 0) separately.

It is also important to note that when the source point is in-plane  $(u_x = 0)$ , and when  $s = s_x$ , it does not make sense to divide by  $((s - s_x)^2 + u_x^2)$  as in [105, §C.2.2], even if the source point is outside the triangle. If in addition to the basis function combinations (1, 1) and (1, 2), corresponding respectively to (C.2.1) and (C.2.2), one has the above integral evaluated for the combinations

$$\frac{s_{\tau} - s}{s_{\tau}} \frac{\alpha_1 s - t}{s_{\tau}(\alpha_1 - \alpha_2)} \tag{1,3}$$

$$\left(\frac{\alpha_2 s - t}{s_\tau(\alpha_2 - \alpha_1)}\right)^2 \tag{2,2}$$

$$\frac{\alpha_2 s - t}{s_\tau (\alpha_2 - \alpha_1)} \frac{\alpha_1 s - t}{s_\tau (\alpha_1 - \alpha_2)}$$

$$(2,3)$$

$$(\alpha_1 s - t)^2$$

$$(2,3)$$

$$\left(\frac{\alpha_1 s - t}{s_\tau(\alpha_1 - \alpha_2)}\right) \quad , \tag{3,3}$$

it is always possible to choose an ordering of the triangle vertices so that at least one will work, as a point cannot lie between all three pairs of parallel lines generated by the triangle's edges without being in the triangle.

#### C.2.2 Differentiation of Geometric Factors

The metric factor  $\sqrt{a}$  associated with the mapping (C.1.1) is given by

$$\sqrt{a} = |(x_2 - x_1) \times (x_3 - x_1)| = \sqrt{\det(J_k^T J_k)}.$$

The unit normal vector is

$$n = \frac{(x_2 - x_1) \times (x_3 - x_1)}{\sqrt{a}}$$

Let a differential change  $(\delta x_1, \delta x_2, \delta x_3)$  be made to  $(x_1, x_2, x_3)$ , and use the fact that

$$|x+\delta| - |x| = \frac{x}{|x|} \cdot \delta + o(|\delta|).$$

The corresponding change in  $\sqrt{a}$  is

$$\delta\sqrt{a} = |(x_2 + \delta x_2 - x_1 - \delta x_1) \times (x_3 + \delta x_3 - x_1 - \delta x_1)| - \sqrt{a}$$
$$= n \cdot ((\delta x_2 - \delta x_1) \times (x_3 - x_1) + (x_2 - x_1) \times (\delta x_3 - \delta x_1)) + o(|\delta|).$$

The change in the normal vector is

$$\delta n = \frac{(x_2 + \delta x_2 - x_1 - \delta x_1) \times (x_3 + \delta x_3 - x_1 - \delta x_1)}{|(x_2 + \delta x_2 - x_1 - \delta x_1) \times (x_3 + \delta x_3 - x_1 - \delta x_1)|} - n$$
  
=  $\frac{1}{\sqrt{a}} \left( I - nn^T \right) \left( (\delta x_2 - \delta x_1) \times (x_3 - x_1) + (x_2 - x_1) \times (\delta x_3 - \delta x_1) \right) + o(|\delta|).$ 

The differential change in the coordinates x is just the derivative of the mapping (C.1.1):

$$\delta x(\xi) = \left(\delta x_2 - \delta x_1 \quad \delta x_3 - \delta x_1\right) \xi + \delta x_1.$$

The change in the distance r = |x - y| is

$$\delta r = \delta |x - y| = \frac{x - y}{|x - y|} \cdot (\delta x - \delta y).$$

For calculation of the term

$$(n(y) \times \nabla N_m^3(y), n(x) \times \nabla N_l^3(x))$$

appearing in (C.1.3d), it is necessary to be able to differentiate the gradient terms with respect to shape. These functions are defined on the reference element shown in figure (C.1) via

$$\hat{N}_1(\xi) = 1 - \xi_1 - \xi_2$$
  
 $\hat{N}_2(\xi) = \xi_1$   
 $\hat{N}_e(\xi) = \xi_2,$ 

with gradients

$$\nabla \hat{N}_1 = \begin{pmatrix} -1 \\ -1 \\ 0 \end{pmatrix}, \ \nabla \hat{N}_2 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \ \nabla \hat{N}_3 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

The meaning of these gradients, as explained in theorem 4.3.2 is as derivatives with respect to the mapping

$$N_{k_j}(x) = \hat{N}_j(\xi(x)),$$

where

$$x(\xi) = \begin{pmatrix} x_2 - x_1 & x_3 - x_1 & n \end{pmatrix} \xi + x_1.$$

Thus by the chain rule,

$$\begin{pmatrix} x_2 - x_1 & x_3 - x_1 & n \end{pmatrix}^T \nabla N_{k_j}(x) = \nabla \hat{N}_j(\xi).$$

Differentiation of the shape coordinates yields the equation

$$\begin{pmatrix} x_2 - x_1 & x_3 - x_1 & n \end{pmatrix}^T \begin{pmatrix} \delta \nabla N_{k_j}(x) \end{pmatrix} = -\begin{pmatrix} \delta x_2 - \delta x_1 & \delta x_3 - \delta x_1 & \delta n \end{pmatrix}^T \nabla N_{k_j}(x).$$

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