

Mixed-Hybrid Discretization Methods for the Linear Transport Equation

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van Criekingen Serge. Mixed-Hybrid Discretization Methods for the Linear Transport Equation. Mathematics [math]. Northwestern University, 2004. English. tel-00570084

HAL Id: tel-00570084

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NORTHWESTERN UNIVERSITY

Mixed-Hybrid Discretization Methods for the Linear Transport Equation

A DISSERTATION

SUBMITTED TO THE GRADUATE SCHOOL
IN PARTIAL FULFILLMENT OF THE REQUIREMENTS

for the degree

DOCTOR OF PHILOSOPHY

Field of MECHANICAL ENGINEERING

By

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EVANSTON, ILLINOIS

June 2004

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ABSTRACT

Mixed-Hybrid Discretization Methods for the Linear Transport Equation

Serge Van Criekingen

The linear Boltzmann equation describes neutron transport in nuclear systems. We consider discretization methods for the time-independent mono-energetic transport equation, and focus on mixed-hybrid primal and dual formulations obtained through an even- and odd-parity flux decomposition. A finite element technique discretizes the spatial variable, and a P_N spherical harmonic technique discretizes the angular variable.

Mixed-hybrid methods combine attractive features of both mixed and hybrid methods, namely the simultaneous approximation of even- and odd-parity fluxes (thus of flux and current) and the use of Lagrange multipliers to enforce interface regularity constraints. While their study provides insight into purely mixed and purely hybrid

methods, mixed-hybrid methods can also be used as such. Mixed and mixed-hybrid methods, so far restricted to diffusion theory, are here generalized to higher order angular approximations.

We first adapt existing second-order elliptic mixed-hybrid theory to the lowest-order spherical harmonic approximation, i.e., the P_1 approximation. Then, we introduce a mathematical setting and provide well-posedness proofs for the general P_N spherical harmonic approximation. Well-posedness theory in the transport case has thus far been restricted to the first-order (integro-differential) form of the transport equation.

Proceeding from P_1 to P_N , the primal/dual distinction related to the spatial variable is supplemented by an even-/odd-order P_N distinction in the expansion of the angular variable. The spatial rank condition is supplemented by an angular rank condition satisfied using interface angular expansions corresponding to the Rumyantsev conditions, for which we establish a new derivation using the Wigner coefficients.

Demonstration of the practical use of even-order P_N approximations is in itself a significant achievement. Our numerical results exhibit an interesting enclosing property when both even- and odd-order P_N approximations are employed.

Acknowledgments - Remerciements

I thank Professor Lewis for giving me the opportunity to do my thesis at the Northwestern University. Thanks for your continuous support and open-minded attitude towards my research interests not always matching yours. Thanks also for suggesting and implementing the cooperation agreement with Professor Beauwens, so that I could pursue my thesis collaborating with him in Brussels.

Merci à Robert Beauwens de m'avoir encouragé sur la voie d'un doctorat, et mis en contact avec Elmer Lewis. Merci pour m'avoir ensuite accueilli dans le service de métrologie nucléaire, et pour les nombreux conseils qui m'ont permis de mener à bien ma thèse.

I thank Professor Jerome for the support in the Mathematics Department. I very much appreciate your confidence and your interest in my research.

I also thank Professor Chen in the Mathematics Department, even if we did not work together eventually.

I thank Professor Volpert and Dr. Yang for joining my thesis committee. Special thanks to Professor Volpert for organizing a soccer game at the end of the class.

I thank Mike Smith for the Variant numerical results included in this thesis.

Merci à Yvan Notay pour m'avoir conseillé dans la résolution de systèmes.

Merci à tous les membres du service de métrologie nucléaire pour votre accueil, et l'ambiance agréable du service.

I thank the friends in Chicago who helped me through hard times and shared with me the good times. Best wishes for your future, wherever it is in the world.

Merci à tous ceux qui en Belgique m'ont soutenu et encouragé, et qui se reconnaîtront dans ces lignes.

Enfin, merci à mes parents, à Mathieu et Olga, ainsi qu'aux membres de ma famille, pour m'avoir soutenu dans mon parcours parfois chaotique, et permis de mener à bien cette thèse.

This work was supported in part by Los Alamos National Laboratory Award #1152 – 001 – 004*T/W* – 7405 – *E* and Department of Energy contract 541 – 0080 – 11021*DE* – *FG07* – 01*ID141*.

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Chapter 1

Introduction

1.1 Background

1.1.1 The linear Boltzmann transport equation

Ludwig Boltzmann introduced the equation bearing his name in 1872 to study classical gases. Properly generalized, it has been proved fruitful to study various transport phenomena, such as electron transport in solids and plasmas, radiative transfer in planetary and stellar atmospheres, and neutron transport in nuclear reactors (Cercignani 1988). This last application constitutes the subject of this work, and our notations are those traditionally used for nuclear reactor core calculations. Nevertheless, the Boltzmann equation as studied here can in some cases be applied to other

neutral particles. Therefore the methods developed in this thesis could possibly be found useful outside the nuclear engineering field.

Two general references for the derivation of the linear Boltzmann transport equation used in reactor physics are Lewis and Miller, Jr. (1984) and Bell and Glasstone (1970). The particle flux $\Psi(\mathbf{r}, \boldsymbol{\Omega}, E, t)$ depends on the position \mathbf{r} , the particle direction of travel $\boldsymbol{\Omega}$ (unit vector), the particle energy E , and the time t . We consider only stationary problems in this work, while a multigroup energy discretization (lumping the particles into groups, each characterized by a single energy) eliminates the energy dependence. The time-independent mono-energetic equation is therefore often called “within-group” equation. It reads

$$\boldsymbol{\Omega} \cdot \nabla \Psi(\mathbf{r}, \boldsymbol{\Omega}) + \sigma(\mathbf{r})\Psi(\mathbf{r}, \boldsymbol{\Omega}) = \int_S d\Omega' \sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')\Psi(\mathbf{r}, \boldsymbol{\Omega}') + s(\mathbf{r}, \boldsymbol{\Omega}), \quad (1.1)$$

where the nabla operator ∇ acts on the spatial variable \mathbf{r} only, the positive coefficients $\sigma(\mathbf{r})$ and $\sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')$ ¹ are respectively the macroscopic total and differential scattering cross sections (i.e. reaction probabilities per unit length), $s(\mathbf{r}, \boldsymbol{\Omega})$ is the external source term, and S represents the unit sphere. A common assumption made when studying discretization methods for (1.1) is the isotropy of the source and of the scattering

¹ $\boldsymbol{\Omega}'$ and $\boldsymbol{\Omega}$ respectively correspond to the neutron direction before and after a scattering collision.

cross-section, leading to

$$\boldsymbol{\Omega} \cdot \nabla \Psi(\mathbf{r}, \boldsymbol{\Omega}) + \sigma(\mathbf{r})\Psi(\mathbf{r}, \boldsymbol{\Omega}) = \sigma_s(\mathbf{r}) \int_S d\Omega \Psi(\mathbf{r}, \boldsymbol{\Omega}) + s(\mathbf{r}). \quad (1.2)$$

One necessarily has $\sigma(\mathbf{r}) \geq \sigma_s(\mathbf{r})$ for all \mathbf{r} . A void region is characterized by $\sigma = \sigma_s = 0$, while pure scattering media are those where $\sigma = \sigma_s > 0$. For boundary conditions, we consider vacuum and reflected boundaries, which cover most practical applications. Vacuum boundary conditions correspond to a zero incoming flux in the domain, while reflected boundary conditions correspond to an incoming flux equal to the spectrally reflected outgoing flux. To avoid re-entrant neutrons, we consider convex domains.

A widely used angular discretization technique for (1.1) or (1.2) is based on spherical harmonics, which form an orthogonal basis for square integrable functions on the unit sphere. Angular dependences are then expanded in truncated spherical harmonic series. For historical reasons, this technique is known as a P_N approximation (Gelbard 1968), with N referring to the order at which the spherical harmonic series is truncated. In the lowest-order ($N = 1$) of these angular discretizations, that is the P_1 approximation, the unknowns are the first two angular moments of $\Psi(\mathbf{r}, \boldsymbol{\Omega})$, namely the scalar flux $\phi = \int_S d\Omega \Psi(\mathbf{r}, \boldsymbol{\Omega})$ and the vector current $\mathbf{J} = \int_S d\Omega \boldsymbol{\Omega} \Psi(\mathbf{r}, \boldsymbol{\Omega})$. In the

anisotropic case, $\sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')$ is expanded in Legendre polynomials, and we denote by $\sigma_{s,0}$ and $\sigma_{s,1}$ the zero and first order moments of this expansion. Introducing $\sigma_0(\mathbf{r}) = \sigma(\mathbf{r}) - \sigma_{s,0}(\mathbf{r})$ and $\sigma_1(\mathbf{r}) = 3(\sigma(\mathbf{r}) - \sigma_{s,1}(\mathbf{r}))$, the within-group P_1 equations for $\phi(\mathbf{r})$ and $\mathbf{J}(\mathbf{r})$ can be written as the coupled pair of first order differential equations (Bell and Glasstone 1970, pp.149–150):

$$\begin{cases} \nabla \cdot \mathbf{J}(\mathbf{r}) + \sigma_0(\mathbf{r}) \phi(\mathbf{r}) = s_0(\mathbf{r}) \\ \nabla \phi(\mathbf{r}) + \sigma_1(\mathbf{r}) \mathbf{J}(\mathbf{r}) = \mathbf{s}_1(\mathbf{r}) \end{cases} \quad (1.3)$$

where $s_0(\mathbf{r}) = \int_S d\Omega s(\mathbf{r}, \boldsymbol{\Omega})$ and $\mathbf{s}_1(\mathbf{r}) = 3 \int_S d\Omega \boldsymbol{\Omega} s(\mathbf{r}, \boldsymbol{\Omega})$. Note that no explicit angular dependence remains in these equations. The coefficients $\sigma_0(\mathbf{r})$, $\sigma_1(\mathbf{r})$ and $s_0(\mathbf{r})$ are necessarily positive.

Assuming scattering and source to be isotropic in the P_1 approximation yields the diffusion approximation, whose within-group equations read

$$\begin{cases} \nabla \cdot \mathbf{J}(\mathbf{r}) + \sigma_r(\mathbf{r}) \phi(\mathbf{r}) = s(\mathbf{r}) \\ \nabla \phi(\mathbf{r}) + 3\sigma(\mathbf{r}) \mathbf{J}(\mathbf{r}) = 0 \end{cases} \quad (1.4)$$

where $\sigma_r(\mathbf{r}) = \sigma(\mathbf{r}) - \sigma_s(\mathbf{r})$ is the removal cross-section. While the first equation of (1.4) enforces neutron conservation, the second equation is Fick's law.

1.1.2 Discretization of the diffusion equation

Eliminating either the flux or the current from (1.4) yields a second-order elliptic partial differential equation. Finite-element discretizations for such equations are studied at large in the literature. See for instance Ciarlet (1978) or Quarteroni and Valli (1994). Keeping only the flux in (1.4) yields the primal formulation of the second order (or standard) method, while keeping only the current yields its dual formulation. Various non-standard finite element methods for second-order elliptic problems have been developed as well. We consider here mixed, hybrid and mixed-hybrid methods. Depending on the role played by the flux and current, these methods can also be cast into a primal or a dual formulation.

Note that what is traditionally known as a “second order” method in the nuclear engineering literature, is known as a “standard” method in the finite element literature, where in turn mixed, hybrid, and mixed-hybrid methods are known as “non-standard” methods. Since these two traditions seem irreconcilable, both terminology are used in this text. Another terminology point is that non-standard methods are often characterized as “nonconforming”. A discretization scheme is said to be nonconforming (or external) when the finite dimensional space where the unknown is searched is not a subspace of the infinite dimensional space containing the unknown in the corresponding continuous standard method. In practice, a nonconforming method

allows inter-element discontinuities.

Mixed formulations are characterized by their leading to simultaneous approximations of two unknowns, namely the flux and current in the diffusion case. The discretization scheme is then nonconforming with respect to one of the two unknowns. Raviart and Thomas (1977a) developed their well-known mixed (dual) finite elements for the Poisson equation in two dimensions. The Raviart-Thomas elements were extended to three dimensions by Nedelec (1980), and to the general elliptic problem $-\nabla \cdot (p \nabla u) + \mathbf{q} \cdot \nabla u + cu = f$ by Douglas, Jr and Roberts (1982). Brezzi, Douglas, and Marini developed in 1985 another widespread type of mixed (dual) finite elements. In nuclear applications, the non-conforming (thus discontinuous) flux approximation provided by the mixed dual formulation allows taking into account discontinuity factors, i.e., describing strong flux variations at interfaces (Lautard and Moreau 1993). Although the flux is the most interesting data in reactor physics, the current is often useful in homogenization procedures, and in computing outgoing radiations in shielding problems.

Hybrids formulations use Lagrange multipliers to enforce interface regularity constraints. While Lagrange multipliers can be used on the external boundary “to avoid difficulty in fulfilling essential boundary conditions” (Babüska 1973), they can also be used on the interfaces of a spatially decomposed domain, then yielding a hybrid

method (Raviart and Thomas 1977b).

Hybrid and mixed methods have been frequently studied in the literature. See for instance Roberts and Thomas (1991) and Brezzi and Fortin (1991) for an integrated presentation. See also the introduction of Babūška, Oden, and Lee (1977) for historical references on mixed and hybrid methods.

Mixed-hybrid methods are simultaneously mixed and hybrid. They were introduced by Babūška, Oden, and Lee (1977) who developed a primal mixed-hybrid finite element method for the equation $-\Delta u + u = f$ with Dirichlet boundary conditions. Mixed-hybrid methods received comparatively less attention in the literature than purely mixed or purely hybrid methods. Nevertheless Brezzi, Douglas, and Marini (1985) also presented a hybrid form of their mixed (dual) formulation, thus a mixed-hybrid formulation, which they argue simplifies the solution of the linear system associated to their mixed formulation.

In the nuclear engineering community, mixed and mixed-hybrid methods were applied to the diffusion equation by Coulomb and Fedon-Magnaud (1988) and Hennart et al. (1992, 1996, 1999). For historical reasons, the term “node” in the nuclear community refers to one cell of the decomposed spatial domain (reactor core), that is to what would be termed “element” in a finite element context. In addition, the most common finite element techniques seek to determine point values of the unknown (and

possibly of its derivatives) at the “nodes” (here in the finite element sense) of a grid, which most often includes the vertices of the elements. Several non-standard finite element techniques (such as the hybrid and mixed-hybrid), rather seek to determine moments of the unknown(s) expanded in polynomial series. The nuclear engineering community often uses the term “nodal finite elements” or “nodal methods” to denote such techniques (Hennart and Del Valle 1993), which in fact are *not* based on what is known as “nodes” in the finite element context. We therefore avoid using such terminology in this work.

1.1.3 Discretization of the transport equation

In the transport equation, the complexity of the second-order elliptic spatial problem is supplemented with the presence of the angular variable. Two methods find most use in the nuclear engineering community to treat the angular variable, namely the spherical harmonic (or P_N) method and the discrete ordinate (or S_N) method. The already introduced P_N method is the one used in this work. This method can be seen as a Galerkin method with respect to the angular variable (Dautray and Lions 1993, XX, 6.7.1). The S_N method on the other hand consists of evaluating the transport equation in discrete angular directions. Although this approach is simpler than the P_N approach, it has the drawback of yielding unphysical oscillations in the solution,

a phenomenon known as ray effects (Lewis and Miller, Jr. 1984, 4-6).

The transport equation in its integro-differential first-order form (1.1) or (1.2) was investigated mathematically in Dautray and Lions (1993, Ch.XXI). A second-order (with respect to the spatial variable) form can be obtained using the even- and odd- (angular) parity decomposition for the angular flux $\Psi(\mathbf{r}, \boldsymbol{\Omega})$ introduced by Vladimirov (1963)². This decomposition reads

$$\Psi^\pm(\mathbf{r}, \boldsymbol{\Omega}) = \frac{1}{2} (\Psi(\mathbf{r}, \boldsymbol{\Omega}) \pm \Psi(\mathbf{r}, -\boldsymbol{\Omega})) \quad (1.5)$$

$$s^\pm(\mathbf{r}, \boldsymbol{\Omega}) = \frac{1}{2} (s(\mathbf{r}, \boldsymbol{\Omega}) \pm s(\mathbf{r}, -\boldsymbol{\Omega})). \quad (1.6)$$

In the isotropic case (1.2), $s(\mathbf{r}) = s^+(\mathbf{r})$ and the decomposition leads to the coupled pair of first order equations

$$\begin{cases} \boldsymbol{\Omega} \cdot \nabla \Psi^-(\mathbf{r}, \boldsymbol{\Omega}) + \sigma \Psi^+(\mathbf{r}, \boldsymbol{\Omega}) = \sigma_s \phi(\mathbf{r}) + s(\mathbf{r}) \\ \boldsymbol{\Omega} \cdot \nabla \Psi^+(\mathbf{r}, \boldsymbol{\Omega}) + \sigma \Psi^-(\mathbf{r}, \boldsymbol{\Omega}) = 0. \end{cases} \quad (1.7)$$

Then eliminating the odd-parity flux Ψ^- yields a second-order equation in the even-parity flux Ψ^+ known as the primal (or even-parity) second-order formulation. Similarly eliminating Ψ^+ yields the dual (or odd-parity) second-order formulation. Fur-

²who also gives credit for it to Kuznetsov (Kuznetsov 1951)

thermore, this treatment was shown to give rise to self-adjoint second-order problems (Pomraning and Clark, Jr 1963; Toivanen 1966; Kaplan and Davis 1967), and thus symmetric matrix systems to solve, while the first-order form typically yields more cumbersome nonsymmetric equations (Lewis and Miller, Jr. 1984, 6-1).

Non-standard methods, i.e. mixed, hybrid, and mixed-hybrid methods, can be derived from equations (1.7), with Ψ^+ and Ψ^- playing the roles of ϕ and \mathbf{J} in the diffusion case. Depending on the role played by the even- and odd-parity fluxes, these methods can again be cast into a primal or a dual formulation. Here, mixed methods provide simultaneous approximations of Ψ^+ and Ψ^- , thus of flux and current since $\phi = \int_S d\Omega \Psi^+(\mathbf{r}, \boldsymbol{\Omega})$ and $\mathbf{J} = \int_S d\Omega \boldsymbol{\Omega} \Psi^-(\mathbf{r}, \boldsymbol{\Omega})$.

Table 1.1 displays a non-exhaustive list of well-known neutron transport production codes. As several others, the EVENT code (de Oliveira 1986) is based on the second-order primal formulation. In contrast, the VARIANT code (Palmiotti, Lewis, and Carrico 1995) is based on a hybrid primal formulation. Both these codes use only odd-order P_N ³ spherical harmonic approximations to discretize the angular variable. Mixed methods have been so far developed only in the diffusion approximation⁴, in the CRONOS/MINOS code (Lautard, Schneider, and Baudron 1999). This code uses

³i.e., where N is odd

⁴or simplified spherical harmonics (SP_N) approximation, obtained by coupling several diffusion equations.

Table 1.1: Some existing production codes.

Some existing production codes
 Transport
 Diffusion only

Primal Formulations

| | |
|-------------------------------------|---|
| Second order Primal EVENT | Mixed Primal |
| Hybrid Primal VARIANT | Mixed-Hybrid Primal This work |

Dual Formulations

| | |
|-------------------|---------------------------------------|
| Second order Dual | Mixed Dual CRONOS/MINOS |
| Hybrid Dual | Mixed-Hybrid Dual This work |

the Raviart-Thomas (1977a) elements, developed to simultaneously approximate a scalar unknown (the flux) and a vectorial unknown (the current). These elements are not directly applicable to the transport case where both the odd- and even-parity fluxes are scalar unknowns including higher-order angular moments.

Historically, hybrid methods have been developed to perform coarse mesh whole-core reactor calculations ensuring particle conservation within each homogenized element (or node) subdividing the core. Presently, increased computer capabilities allow the use of finer mesh refinements, as well as sub-element refinements (Lewis et al. 1999; Smith et al. 2003). Also, hybrid methods are known in the neutron transport community to ensure the positivity of the flux (even though never formally proved) while standard methods sometimes yield (slightly) negative flux in low flux regions.

1.2 Motivation, objectives and outline

This thesis deals with discretization methods for the within-group transport equation. The focus is primarily on mixed-hybrid primal and dual formulations that use a finite element technique in space and a P_N spherical harmonic technique in angle. We consider the P_1 approximation in chapter 2 and the general P_N approximation in chapter 3.

As far as we know, mixed-hybrid methods have not been investigated in the transport case. They combine attractive features of both mixed and hybrid methods, namely the simultaneous approximation of even- and odd-parity fluxes (thus of flux and current) and the relaxation of interface continuity requirement using Lagrange multipliers. An important motivation for examining these methods is therefore the possibility of particularizing the theoretical results to purely mixed or purely hybrid methods.

Moreover, mixed-hybrid methods can also be used as such. In fact, referring to pioneering work by Fraeijs de Veubeke for elasticity problems, Arnold and Brezzi (1985) and Brezzi, Douglas, and Marini (1985) argued (for the Poisson equation) that the mixed-hybrid method can be seen as an improved mixed method when used with a condensation approach, in that it results in symmetric positive definite matrix systems of reduced size. We show in section 3.5.3 that these favorable mixed-hybrid features apply to the transport case as well. As a result, the mixed-hybrid methods appear to be an efficient generalization to transport of the mixed methods that were so far restricted to diffusion (Lautard, Schneider, and Baudron 1999). Moreover, they also generalize the hybrid methods of Palmiotti, Lewis, and Carrico (1995) to a mixed formulation, which includes both even- and odd-parity internal unknowns as well as the interface unknown.

Although we have alluded to some exceptions, a great deal of the literature on second-order elliptic equations treats only the Poisson-like equation $-\nabla \cdot (p\nabla u) = f$. In mixed(-hybrid) methods, a vector unknown directly proportional to ∇u is then introduced in addition to the scalar unknown u . Such a Fick's diffusion law is not valid in the P_1 approximation (1.3) if $\mathbf{s}_1(\mathbf{r}) \neq 0$. In section 2.2, we therefore adapt the second-order (or standard), mixed, hybrid and mixed-hybrid continuous formulations to the P_1 approximation. A discretization scheme is provided in section 2.3 for the mixed-hybrid primal and dual formulations, and well-posedness is investigated in section 2.4. Babuška, Oden, and Lee (1977) provided complete well-posedness proofs for the mixed-hybrid method applied to $-\Delta u + u = f$, but only in the primal diffusion case. We generalize this study to our P_1 case and provide a complete proof for the dual case. This is a necessary step toward the establishment in chapter 3 of a mathematical setting and well-posedness theory for the transport equation with a general P_N expansion.

“Computations were done (with success!) using theoretically dubious elements or at best, using elements on which theory remained silent.” This quote of Fortin cited in Brezzi and Fortin (1991, p.78) applies to our domain as well, and sheds a very down-to-earth light on well-posedness investigations such as the ones in sections 2.4 and 3.4 (with the proofs put in appendix for ease of readability). Nevertheless,

these investigations lead to substantial accomplishments, the first being the proof of existence and uniqueness for the mixed-hybrid methods. To the best of our knowledge, no well-posedness theory had been established to date for the non-standard methods in the transport case. Although the analysis in Dautray and Lions (1993, chap.XXI) includes time-dependence, it is restricted to the first order form (1.1).

These investigations moreover show how, going from P_1 to P_N , the introduction of the angular variable interacts with the spatial variable. The spatial rank condition appearing in the P_1 approximation is well-known in the finite element community (Raviart and Thomas 1977b) and was discovered empirically in Carrico, Lewis, and Palmiotti (1994) for the VARIANT code. This condition is typical of hybrid methods, and establishes a dependence between internal and interface spatial expansions. In the P_N approximation, the spatial rank condition is supplemented by an angular rank condition, that establishes a dependence between internal and interface angular expansions. This condition can be satisfied using interface expansions corresponding to the so-called Rumyantsev conditions (Rumyantsev 1962), recently re-investigated by Yang, Smith, Palmiotti, and Lewis (2004). Our derivation of these conditions from the angular rank condition is new, and we use Wigner coefficients (in appendix A) to perform this derivation. In turn, we establish in §3.5.2 interface continuity properties for the flux and current, that we verify in our numerical experiments.

Another challenge in proceeding from P_1 to P_N concerns the dependence between the approximation spaces for the internal unknowns, typical of mixed methods. This is also well-known in the finite element community for second order elliptic problems. In the diffusion or P_1 case, this leads to inclusion conditions between internal unknown approximation spaces written in short-hand notation ⁵ as “ $\nabla\phi \subset \mathbf{J}$ ” and “ $\nabla \cdot \mathbf{J} \subset \phi$ ”. In the P_N approximation, we show that these become “ $\boldsymbol{\Omega} \cdot \nabla\Psi^\pm \subset \Psi^\mp$ ” and “ $\nabla\Psi^\pm \subset \boldsymbol{\Omega}\Psi^\mp$ ”. In turn, this shows that the primal/dual distinction, related to the spatial variable and therefore already present in the P_1 (or diffusion) approximation, is supplemented by a even-/odd-order P_N distinction due to the angular variable.

While odd-order P_N approximations have been widely used in neutron transport codes, even-order ones have been so far neglected. Historically, the preference for odd-order P_N approximations was motivated in Davison (1957, §10.3.2) for the first order (integro-differential) form of the transport equation. With the even- and odd-parity flux decomposition, both even- and odd-order P_N approximations can be considered. This was done as early as 1966 by Davis to derive vacuum boundary conditions by variational methods. Nevertheless, the use of even-order P_N approximations for angular expansions has until now not been implemented in practice. We demonstrate in section 3.5 the practical use of even-order P_N approximations as well as the odd-

⁵In these relations, an unknown stands for the finite-dimensional subspace where they are searched. See sections 2.4 and 3.4 for more rigorous notations.

order ones. It appears repeatedly in our numerical experiments that, when odd-order approximations approximate from below, even-order approximations tend to approximate from above, and vice-versa. Although no strict rule is derived, this is a very interesting enclosing property.

While sections 3.2 to 3.5 (including the well-posedness investigation) consider the isotropic case (1.2), section 3.6 provides a generalization to the anisotropic case (1.1) in a multi-group context.

Some restrictions apply to this work. First, even though our well-posedness proofs are more general, in our numerical tests we consider only regular convex domains of the “union-of-rectangles” type. Another restriction is that our well-posedness proofs are only valid for the case $\sigma > \sigma_s > 0$, thus excluding void and pure scattering regions. In our numerical tests, the resulting system can become singular in case of a void region, as detailed in §3.5.3.

Finally, we follow in this text the traditional neutronic notation using V for the (convex) spatial domain, while Ω is used for the angular variable.

Chapter 2

*P*₁ approximation

Recall that the P_1 approximation yields the coupled pair of first-order equations

$$\nabla \cdot \mathbf{J}(\mathbf{r}) + \sigma_0(\mathbf{r}) \phi(\mathbf{r}) = s_0(\mathbf{r}) \quad (2.1)$$

$$\nabla \phi(\mathbf{r}) + \sigma_1(\mathbf{r}) \mathbf{J}(\mathbf{r}) = \mathbf{s}_1(\mathbf{r}) \quad (2.2)$$

where $\sigma_0(\mathbf{r}) = \sigma(\mathbf{r}) - \sigma_{s,0}(\mathbf{r})$ and $\sigma_1(\mathbf{r}) = 3(\sigma(\mathbf{r}) - \sigma_{s,1}(\mathbf{r}))$. Note that no explicit angular dependence remains in (2.1) and (2.2). After some preliminaries in §2.1, we classify in §2.2 different solution methods for the P_1 system, namely the second order (or standard), hybrid, mixed and mixed-hybrid methods, with each in both primal and dual versions. The classification is presented first for the continuous formulations, that

is the abstract problems posed in infinite-dimensional spaces. Then in §2.3 we apply a finite element approximation to the mixed-hybrid methods. We do not proceed to the discretized weak form in a matrix setting since the P_1 matrix system can be retrieved as a particular case of the P_N matrix system derived in section 3.5. Thus numerical results for the P_1 approximation are provided in §3.5.4 along with those for the P_N approximation, $N > 1$. Well-posedness is investigated in §2.4, with proofs in appendix B.

2.1 Preliminaries

We first introduce some notations. General references for the notions introduced below are Ciarlet (1978) and Richtmyer (1978, Vol.1).

With n the number of space dimensions, let V be a convex open Lipschitzian domain of the Euclidean space \mathbf{R}^n with piecewise smooth boundary ∂V . We denote by $L^2(V) = H^0(V)$, $H^1(V)$ and $H(\text{div}, V)$ the usual Lebesgue and Sobolev spaces on V with their elements understood in the sense of distributions. Their associated

norms are respectively

$$\begin{aligned}\|v\| &= \|v\|_{L^2(V)} = \left(\int_V |v|^2 dV \right)^{1/2}, \\ \|v\|_1 &= \|v\|_{H^1(V)} = (\|\nabla v\|^2 + \|v\|^2)^{1/2}, \text{ and} \\ \|\mathbf{q}\|_{div} &= \|\mathbf{q}\|_{H(div,V)} = (\|\nabla \cdot \mathbf{q}\|^2 + \|\mathbf{q}\|^2)^{1/2},\end{aligned}$$

with $\|\mathbf{p}\|^2 = \sum_{i=1}^n \|p_i\|^2$ for any vector \mathbf{p} . Throughout this chapter we assume $s_0(\mathbf{r})$ in $L^2(V)$ and $\mathbf{s}_1(\mathbf{r})$ in $[L^2(V)]^n$.

The following theorems (Roberts and Thomas (1991, pp.529-530), Temam (1979, Th.1.2, p.9)), define the spaces $H^{1/2}(\partial V)$ and $H^{-1/2}(\partial V)$ that respectively contain the trace (i.e., value on the boundary) of functions in $H^1(V)$ and $H(div, V)$. Their correspondence with Sobolev spaces of fractional order is proved in Lions and Magenes (1968). Also, \bar{V} denotes the closure of V , and \mathbf{n} denotes the unit outward normal vector to the considered (sub)domain.

Theorem 2.1.1 (Trace mapping theorem) *The map $v \rightarrow v|_{\partial V}$ defined a priori for functions v continuous on \bar{V} , can be extended to a continuous linear mapping called the trace map of $H^1(V)$ into $L^2(\partial V)$. The kernel of the trace mapping is denoted $H_0^1(V)$, and its range $H^{1/2}(\partial V)$ is a Hilbert space, subset of $L^2(\partial V)$, equipped with*

the norm

$$\|\psi\|_{1/2,\partial V} = \inf_{\{\nu \in H^1(V): \nu|_{\partial V} = \psi\}} \|\nu\|_{1,V}. \quad (2.3)$$

Theorem 2.1.2 (Normal trace mapping theorem) *The map $\mathbf{q} \rightarrow \mathbf{n} \cdot \mathbf{q}$ defined a priori for vector functions \mathbf{q} from $(H^1(V))^n$ into $L^2(\partial V)$ can be extended to a continuous linear mapping from $H(\text{div}, V)$ onto $H^{-1/2}(\partial V)$, the dual space of $H^{1/2}(\partial V)$, called the normal trace mapping. $H^{-1/2}(\partial V)$ is a Hilbert space with norm*

$$\|\chi\|_{-1/2,\partial V} = \sup_{\{\psi \in H^{1/2}(\partial V): \|\psi\|_{1/2,\partial V} = 1\}} \langle \psi, \chi \rangle$$

where $\langle \psi, \chi \rangle = \int_{\partial V} \psi \chi \, d\Gamma$. We also have the characterization

$$\|\chi\|_{-1/2,\partial V} = \inf_{\{\mathbf{q} \in H(\text{div}, V): \mathbf{n} \cdot \mathbf{q}|_{\partial V} = \chi\}} \|\mathbf{q}\|_{\text{div}, V}. \quad (2.4)$$

The kernel of the normal trace mapping is denoted $H_0(\text{div}, V)$.

We have $H^{1/2}(\partial V) \subset L^2(\partial V) \subset H^{-1/2}(\partial V)$.

In hybrid and mixed-hybrid methods, the domain V is subdivided into a finite family of elements V_l (open sets) such that $V_l \cap V_k = \emptyset$ if $l \neq k$, and $\bar{V} = \bigcup_{l=1}^L \bar{V}_l$, with L a positive integer. We assume in the sequel that all the V_l have piecewise

smooth boundaries. We also define

$$\Gamma = \bigcup_l \partial V_l.$$

Note that Γ includes the external boundary ∂V . The spaces $H_0^{1/2}(\Gamma)$ and $H_0^{-1/2}(\Gamma)$ are respectively the subspaces of $H^{1/2}(\Gamma)$ and $H^{-1/2}(\Gamma)$ whose members vanish on the external boundary ∂V . With the subdivision just described, norms in $H_{(0)}^{1/2}(\Gamma)$ and $H_{(0)}^{-1/2}(\Gamma)$ are respectively

$$\|\psi\|_{H_{(0)}^{1/2}(\Gamma)}^2 = \sum_l \|\psi\|_{1/2, \partial V_l}^2 \quad \text{and} \quad \|\chi\|_{H_{(0)}^{-1/2}(\Gamma)}^2 = \sum_l \|\chi\|_{-1/2, \partial V_l}^2.$$

Furthermore, we introduce

$$\begin{aligned} X &= \{v \in L^2(V) : \forall l, v|_{V_l} \in H^1(V_l)\}, \text{ and} \\ Y &= \{\mathbf{v} \in [L^2(V)]^n : \forall l, \mathbf{v}|_{V_l} \in H(\text{div}, V_l)\}, \end{aligned}$$

with corresponding norms $\|v\|_X^2 = \sum_l \|v\|_{1, V_l}^2$ and $\|v\|_Y^2 = \sum_l \|v\|_{\text{div}, V_l}^2$. The following two theorems (propositions 1.1 and 1.2 of Brezzi and Fortin (1991, p.95)) tell us how to enforce the interface regularity of members of X and Y .

Theorem 2.1.3

$$H^1(V) = \left\{ v \in X : \sum_l \int_{\partial V_l} \tilde{\chi} v \, d\Gamma = 0, \quad \forall \tilde{\chi} \in H_0^{-1/2}(\Gamma) \right\}.$$

Theorem 2.1.4

$$H(\text{div}, V) = \left\{ \mathbf{q} \in Y : \sum_l \int_{\partial V_l} \mathbf{n} \cdot \mathbf{q} \tilde{\psi} \, d\Gamma = 0 \quad \forall \tilde{\psi} \in H_0^{1/2}(\Gamma) \right\}.$$

2.2 Continuous formulations**2.2.1 Second order (or standard) methods****Primal case**

Multiplying (2.1) by a test function $\tilde{\phi}$ (i.e. applying distributions in equations (2.1) to a test function $\tilde{\phi}$) and integrating by parts yields

$$\int_V \left(-\mathbf{J} \cdot \nabla \tilde{\phi} + \sigma_0 \phi \tilde{\phi} \right) dV + \int_{\partial V} \tilde{\phi} \mathbf{n} \cdot \mathbf{J} \, d\Gamma = \int_V s_0 \tilde{\phi} \, dV.$$

Introducing the boundary condition $\mathbf{n} \cdot \mathbf{J} = \chi$ on ∂V , and extracting the current out of (2.2) yields the following weak form:

find $\phi \in H^1(V)$ such that (with $\sigma_1 \neq 0$)

$$\int_V \left(\frac{1}{\sigma_1} \nabla \phi \nabla \tilde{\phi} + \sigma_0 \phi \tilde{\phi} \right) dV + \int_{\partial V} \tilde{\phi} \chi d\Gamma = \int_V \left(s_0 \tilde{\phi} + \frac{1}{\sigma_1} \mathbf{s}_1 \cdot \nabla \tilde{\phi} \right) dV \quad (2.5)$$

for all $\tilde{\phi} \in H^1(V)$. In (2.5), we furthermore assume $\sigma_0(\mathbf{r})$ and $\sigma_1(\mathbf{r})$ in $C^\infty(V)$ (i.e. infinitely continuously differentiable on V), and $\chi \in H^{-1/2}(\partial V)$.

Dual case

Applying (2.2) to a test function $\tilde{\mathbf{J}}$ and integrating by parts leads to

$$\int_V \left(-\phi \nabla \cdot \tilde{\mathbf{J}} + \sigma_1 \mathbf{J} \cdot \tilde{\mathbf{J}} \right) dV + \int_{\partial V} \phi \mathbf{n} \cdot \tilde{\mathbf{J}} d\Gamma = \int_V \mathbf{s}_1 \cdot \tilde{\mathbf{J}} dV.$$

Introducing the boundary condition $\phi = \psi$ on ∂V , and extracting the flux out of (2.1) yields the weak form:

find $\mathbf{J} \in H(\text{div}, V)$ such that (with $\sigma_0 \neq 0$)

$$\begin{aligned} \int_V \left(\frac{1}{\sigma_0} \nabla \cdot \mathbf{J} \nabla \cdot \tilde{\mathbf{J}} + \sigma_1 \mathbf{J} \cdot \tilde{\mathbf{J}} \right) dV + \int_{\partial V} \psi \mathbf{n} \cdot \tilde{\mathbf{J}} d\Gamma \\ = \int_V \left(\mathbf{s}_1 \cdot \tilde{\mathbf{J}} + \frac{1}{\sigma_0} s_0 \nabla \cdot \tilde{\mathbf{J}} \right) dV \quad (2.6) \end{aligned}$$

for all $\tilde{\mathbf{J}} \in H(\text{div}, V)$. In (2.6), we assume $\sigma_0(\mathbf{r})$ and $\sigma_1(\mathbf{r})$ as in the primal case, and $\psi \in H^{1/2}(\partial V)$.

Note

We point out that both (2.5) and (2.6) were obtained without using any second order derivatives. In fact, the denomination “second order method” can be understood by the fact that, for instance in the primal case, (2.5) is the usual weak form for the second order differential equation (with $\sigma_1 \neq 0$)

$$-\nabla \cdot \frac{1}{\sigma_1} \nabla \phi + \sigma_0 \phi = s_0 - \nabla \cdot \frac{1}{\sigma_1} \mathbf{s}_1 \quad (2.7)$$

This equation (“strong form”) can be obtained by extracting the current out of (2.2), and substituting it into (2.1). To obtain the weak form (2.5) from here, we multiply (2.7) by an arbitrary test function $\tilde{\phi} \in H^1(V)$, integrate by parts, and express a non-homogeneous boundary condition $\mathbf{n} \cdot \frac{1}{\sigma_1} (\mathbf{s}_1 - \nabla \phi) = \chi$ for $\mathbf{r} \in \partial V$ in the surface integral. Nevertheless, equation (2.7) implies that the derivatives in $\nabla \phi$ be themselves differentiable, and $\mathbf{s}_1 \in H(\text{div}, \Omega)$. These additional hypotheses disappear in the weak form (2.5), and are thus artificial since our first derivation of (2.5) shows that it can be obtained without them.

2.2.2 Hybrid methods

Hybrid methods necessitate a subdivision of the domain V into elements V_l as described in section 2.1. The idea of hybrid methods is to apply the non-hybrid (here standard) method to each element V_l separately, keeping only weak (but natural) regularity conditions at the interfaces of the spatially decomposed domain. In this view, an interface unknown χ (primal case) or ψ (dual case) is introduced (ψ and χ are not right-hand sides of boundary conditions anymore), representing respectively the interface normal current and the interface flux. Also, an additional equation given by theorems 2.1.3 (primal case) or 2.1.4 (dual case) enforces the interface regularity of the internal unknown ϕ or \mathbf{J} respectively.

Primal case

Thus, applying (2.5) in each V_l , summing over the resulting equations, and introducing the additional regularity constraint, we obtain the mixed-hybrid primal weak form:

find $(\phi, \chi) \in X \times H^{-1/2}(\Gamma)$ such that (with $\sigma_1 \neq 0$)

$$\left\{ \begin{array}{l} \sum_l \int_{V_l} \left(\frac{1}{\sigma_1} \nabla \phi \nabla \tilde{\phi} + \sigma_0 \phi \tilde{\phi} \right) dV + \sum_l \int_{\partial V_l} \tilde{\phi} \chi d\Gamma \\ \qquad \qquad \qquad = \sum_l \int_{V_l} \left(s_0 \tilde{\phi} + \frac{1}{\sigma_1} \mathbf{s}_1 \cdot \nabla \tilde{\phi} \right) dV \\ \sum_l \int_{\partial V_l} \phi \tilde{\chi} d\Gamma = 0. \end{array} \right. \quad (2.8)$$

for all $(\tilde{\phi}, \tilde{\chi}) \in X \times H_0^{-1/2}(\Gamma)$. Note that $\tilde{\chi}$ in the second equation can be interpreted as a Lagrange multiplier enforcing the interface regularity of ϕ . We assume $\sigma_0(\mathbf{r})$ and $\sigma_1(\mathbf{r})$ in $C^\infty(V_l)$ for all l .

Dual case

In the dual case, we obtain:

find $(\mathbf{J}, \psi) \in Y \times H^{1/2}(\Gamma)$ such that (with $\sigma_0 \neq 0$)

$$\left\{ \begin{array}{l} \sum_l \int_{V_l} \left(\frac{1}{\sigma_0} \nabla \cdot \mathbf{J} \nabla \cdot \tilde{\mathbf{J}} + \sigma_1 \mathbf{J} \tilde{\mathbf{J}} \right) dV + \sum_l \int_{\partial V_l} \psi \mathbf{n} \cdot \tilde{\mathbf{J}} d\Gamma \\ \qquad \qquad \qquad = \sum_l \int_{V_l} \left(\mathbf{s}_1 \tilde{\mathbf{J}} + \frac{1}{\sigma_0} s_0 \nabla \cdot \tilde{\mathbf{J}} \right) dV \\ \sum_l \int_{\partial V_l} \tilde{\psi} \mathbf{n} \cdot \mathbf{J} d\Gamma = 0. \end{array} \right. \quad (2.9)$$

for all $(\tilde{\mathbf{J}}, \tilde{\psi}) \in Y \times H_0^{1/2}(\Gamma)$. Here, $\tilde{\psi}$ can be interpreted as a Lagrange multiplier in the second equation. We assume $\sigma_0(\mathbf{r})$ and $\sigma_1(\mathbf{r})$ as in hybrid the primal case.

2.2.3 Mixed methods

Mixed methods consist in the simultaneous approximation of both flux and current, therefore avoiding errors propagating from one to the other. To obtain the mixed weak forms, we apply (2.1) and (2.2) to test functions $\tilde{\phi}$ and $\tilde{\mathbf{J}}$ respectively. Then, using

integration by parts in the first or second equation leads respectively to the primal or dual mixed formulation. A non-homogeneous boundary condition is introduced on ∂V , namely $\mathbf{n} \cdot \mathbf{J} = \chi$ in the primal case, and $\phi = \psi$ in the dual case, with χ and ψ given as in the standard method.

Primal case

The mixed primal weak form reads:

find $(\phi, \mathbf{J}) \in H^1(V) \times [L^2(V)]^n$ such that

$$\begin{cases} \int_V (-\mathbf{J} \cdot \nabla \tilde{\phi} + \sigma_0 \phi \tilde{\phi}) dV + \int_{\partial V} \chi \tilde{\phi} d\Gamma = \int_V s_0 \tilde{\phi} dV \\ \int_V (\nabla \phi \cdot \tilde{\mathbf{J}} + \sigma_1 \mathbf{J} \cdot \tilde{\mathbf{J}}) dV = \int_V \mathbf{s}_1 \cdot \tilde{\mathbf{J}} dV. \end{cases} \quad (2.10)$$

for all $(\tilde{\phi}, \tilde{\mathbf{J}}) \in H^1(V) \times [L^2(V)]^n$, where we assume $\sigma_0(\mathbf{r})$ and $\sigma_1(\mathbf{r})$ in $C^\infty(V)$.

Dual case

As for the mixed dual weak form, it reads:

find $(\mathbf{J}, \phi) \in H(\text{div}, V) \times L^2(V)$ such that

$$\begin{cases} \int_V (\nabla \cdot \mathbf{J} \tilde{\phi} + \sigma_0 \phi \tilde{\phi}) dV = \int_V s_0 \tilde{\phi} dV \\ \int_V (-\phi \nabla \cdot \tilde{\mathbf{J}} + \sigma_1 \mathbf{J} \cdot \tilde{\mathbf{J}}) dV + \int_{\partial V} \psi \mathbf{n} \cdot \tilde{\mathbf{J}} d\Gamma = \int_V \mathbf{s}_1 \cdot \tilde{\mathbf{J}} dV. \end{cases} \quad (2.11)$$

for all $(\tilde{\mathbf{J}}, \tilde{\phi}) \in H(\text{div}, V) \times L^2(V)$, with $\sigma_0(\mathbf{r})$ and $\sigma_1(\mathbf{r})$ as in the mixed primal case.

2.2.4 Mixed-hybrid methods

Similarly to what we did to go from the standard to the hybrid method, we introduce a subdivision of the domain V into elements V_l , and apply the mixed method to each element V_l separately, keeping only weak (but natural) regularity conditions at interfaces. Again, χ (primal case) and ψ (dual case) are now interface variables representing respectively the interface normal current and the interface flux. An additional equation enforces the interface regularity of ϕ in the primal case, and \mathbf{J} in the dual case.

Primal case

Applying (2.10) in each V_l , summing up the resulting equations, and introducing the additional regularity constraint, we obtain the mixed-hybrid primal weak form:

find $(\phi, \mathbf{J}, \chi) \in X \times [L^2(V)]^n \times H^{-1/2}(\Gamma)$ such that

$$\begin{cases} \sum_l \int_{V_l} (-\mathbf{J} \cdot \nabla \tilde{\phi} + \sigma_0 \phi \tilde{\phi}) dV + \sum_l \int_{\partial V_l} \chi \tilde{\phi} d\Gamma = \sum_l \int_{V_l} s_0 \tilde{\phi} dV \\ \sum_l \int_{V_l} (\nabla \phi \cdot \tilde{\mathbf{J}} + \sigma_1 \mathbf{J} \cdot \tilde{\mathbf{J}}) dV = \sum_l \int_{V_l} \mathbf{s}_1 \cdot \tilde{\mathbf{J}} dV \\ \sum_l \int_{\partial V_l} \phi \tilde{\chi} d\Gamma = 0. \end{cases} \quad (2.12)$$

for all $(\tilde{\phi}, \tilde{\mathbf{J}}, \tilde{\chi}) \in X \times [L^2(V)]^n \times H_0^{-1/2}(\Gamma)$. We assume $\sigma_0(\mathbf{r})$ and $\sigma_1(\mathbf{r})$ in $C^\infty(V_l)$ for all l .

Dual case

Similarly, from (2.11), the mixed-hybrid dual weak form is:

find $(\mathbf{J}, \phi, \psi) \in Y \times L^2(V) \times H^{1/2}(\Gamma)$ such that

$$\begin{cases} \sum_l \int_{V_l} (\nabla \cdot \mathbf{J} \tilde{\phi} + \sigma_0 \phi \tilde{\phi}) dV = \sum_l \int_{V_l} s_0 \tilde{\phi} dV \\ \sum_l \int_{V_l} (-\phi \nabla \cdot \tilde{\mathbf{J}} + \sigma_1 \mathbf{J} \cdot \tilde{\mathbf{J}}) dV + \sum_l \int_{\partial V_l} \psi \mathbf{n} \cdot \tilde{\mathbf{J}} d\Gamma = \sum_l \int_{V_l} \mathbf{s}_1 \cdot \tilde{\mathbf{J}} dV \\ \sum_l \int_{\partial V_l} \mathbf{n} \cdot \mathbf{J} \tilde{\psi} d\Gamma = 0. \end{cases} \quad (2.13)$$

for all $(\tilde{\mathbf{J}}, \tilde{\phi}, \tilde{\psi}) \in Y \times L^2(V) \times H_0^{1/2}(\Gamma)$. We assume $\sigma_0(\mathbf{r})$ and $\sigma_1(\mathbf{r})$ as in the mixed-hybrid primal case.

Notes

In (2.12) and (2.13), we could introduce discontinuities with a non-zero right-hand side in the last equation of both hybrid weak forms. This could also be done in (2.8) and (2.9) for the purely hybrid case. Nevertheless, we will not investigate this option here.

Because their roles are similar, we refer to ϕ in the primal case and to \mathbf{J} in the dual

case as the “principal” unknowns, and to \mathbf{J} in the primal case and to ϕ in the dual case as the “secondary” unknowns. Also, $\tilde{\chi}$ and $\tilde{\psi}$ can be interpreted as Lagrange multipliers in the third equation of the primal and dual weak forms respectively, enforcing in each case the regularity of the principal unknown.

2.3 Discrete mixed-hybrid formulations

The subscript h will be used to distinguish discretized unknowns from continuous ones. We denote by S_h , \mathbf{V}_h and B_h (respectively for Scalar, Vector, and Boundary) the finite-dimensional approximation spaces. In the primal case, we look for a triple $(\phi_h, \mathbf{J}_h, \chi_h)$ in $S_h \times \mathbf{V}_h \times B_h$ that satisfies the primal weak form equations (2.12) for any $(\tilde{\phi}_h, \tilde{\mathbf{J}}_h, \tilde{\chi}_h)$ in $S_h \times \mathbf{V}_h \times B_{h,0}$ ¹ with

$$S_h \subset X, \quad \mathbf{V}_h \subset [L^2(V)]^n, \quad \text{and} \quad B_{h,(0)} \subset H_{(0)}^{-1/2}(\Gamma).$$

Similarly in the dual case, we look for a triple $(\mathbf{J}_h, \phi_h, \psi_h)$ in $\mathbf{V}_h \times S_h \times B_h$ satisfying the dual weak form equations (2.13) for any $(\tilde{\mathbf{J}}_h, \tilde{\phi}_h, \tilde{\psi}_h)$ in $\mathbf{V}_h \times S_h \times B_{h,0}$ with

$$\mathbf{V}_h \subset Y, \quad S_h \subset L^2(V), \quad \text{and} \quad B_{h,(0)} \subset H_{(0)}^{1/2}(\Gamma).$$

¹ $B_{h,0}$ is the subset of B_h whose functions vanish on the external boundary ∂V .

For the choice of S_h , \mathbf{V}_h and B_h , with interface regularity requirements made natural in our mixed-hybrid formulations, we use limited polynomial expansions whose moments become the coefficients to be determined. We denote by $\mathcal{P}_z(U)$ the space of polynomials of (total) order less than or equal to z on a domain U . Then the internal unknown approximation spaces are defined as

$$S_h = S_h^s(V) = \{u : u_l \in \mathcal{P}_s(V_l), \forall l\}$$

$$\mathbf{V}_h = \mathbf{V}_h^v(V) = \{\mathbf{p} : p_{i,l} \in \mathcal{P}_v(V_l), \forall l, \forall i = 1, \dots, n\}.$$

For the interface unknowns, we first write $\Gamma = \bigcup_g \Gamma_g$ where Γ_g is any smooth closed arc on the interface between two elements or on an element side that is part of the external boundary. We then define in the primal case

$$B_h = B_h^b(\Gamma) = \{\chi : \chi \in \mathcal{P}_b(\Gamma_g), \forall g\}$$

$$B_{h,0} = B_{h,0}^b(\Gamma) = \{\chi : \chi \in B_h^b(\Gamma), \chi = 0 \text{ on } \partial V\}.$$

and in the dual case

$$B_h = B_h^b(\Gamma) = \{\psi : \psi \in \mathcal{P}_b(\Gamma_g), \forall g\}$$

$$B_{h,0} = B_{h,0}^b(\Gamma) = \{\psi : \psi \in B_h^b(\Gamma), \psi = 0 \text{ on } \partial V\}.$$

The approximation space is thus defined by a triple (s, v, b) once the subdivision of V into V_l is determined. We can consider then that the subscript h represents the maximal diameter (i.e. maximal distance between two points in an element) of all the elements V_l .

Finally, inserting the above described expansions into the weak forms (2.12) and (2.13) leads to a linear system in the expansion moments. This will be detailed in the P_N case.

2.4 Well-posedness

The second order (or standard) methods are well-posed by the Lax-Milgram theorem. This theorem, however, cannot be applied to the non-standard mixed, hybrid and mixed-hybrid methods, where the problems are not coercive. In turn, the “Ladyshenskaya-Babuška-Brezzi” (or “inf-sup”) condition must be verified (Roberts and Thomas (1991), Oden and Reddy (1976, chapters 7-8)).

Mixed-hybrid continuous and discrete well-posedness proofs for the theorems below can be found in appendix B. These proofs were inspired by Babuška, Oden, and Lee (1977), who dealt with the equation $-\Delta u + u = f$ in the primal case only. Therefore, we develop our proof in the dual case. The changes between the primal proofs of Babuška, Oden, and Lee and the proofs for our primal methods (treatment

of boundary conditions, treatment of the constants σ_0 and σ_1 through equivalent norms, presence of \mathbf{s}_1) can be derived from the dual proofs that we provide. About boundary conditions, Bell and Glasstone (1970, pp.134-136) showed that on vacuum boundaries $\mathbf{n} \cdot \mathbf{J} = \frac{\phi}{2}$, and on reflected boundaries $\mathbf{n} \cdot \mathbf{J} = 0$. Finally, by following the methods of Babuška, Oden, and Lee, our proofs could be particularized to purely mixed or purely hybrid methods.

2.4.1 Continuous formulations

For the mixed-hybrid methods, we have the following theorem:

Theorem 2.4.1 *Assume vacuum or reflected boundary conditions on the external boundary ∂V of the considered domain V , as well as σ_0 and σ_1 strictly positive and constant on each element V_i subdividing V . Then the mixed-hybrid continuous primal and dual weak forms (2.12) and (2.13) constitute well-posed problems.*

The proof for the dual case can be found in appendix §B.1.

2.4.2 Discrete formulations

We have the following theorem:

Theorem 2.4.2 *Assume vacuum or reflected boundary conditions on the external boundary ∂V of the considered domain V , as well as σ_0 and σ_1 strictly positive and*

constant on each element V_l subdividing V . Assume furthermore that the primal mixed-hybrid discrete problems satisfy $\nabla S_h^s \subset \mathbf{V}_h^v$ (true if $s - 1 \leq v$), and that the dual mixed-hybrid discrete problems satisfy $\nabla \cdot \mathbf{V}_h^v \subset S_h^s$ (true if $v - 1 \leq s$). Then these discrete problems are well-posed, provided in the primal case, for any $\chi \in B_h^b(\partial V_l)$ in any V_l ,

$$\int_{\partial V_l} \chi u \, d\Gamma = 0 \quad \forall u \in S_h^s(V_l) \text{ implies that } \chi = 0, \quad (2.14)$$

while in the dual case, for any $\psi \in B_h^b(\partial V_l)$ in any V_l ,

$$\int_{\partial V_l} \psi \mathbf{n} \cdot \mathbf{p} \, d\Gamma = 0 \quad \forall \mathbf{p} \in \mathbf{V}_h^v(V_l) \text{ implies that } \psi = 0. \quad (2.15)$$

The proof for the dual case can be found in appendix §B.2.

Conditions (2.14) and (2.15), common in any hybrid method, are in fact equivalent to a rank condition: with the mixed-hybrid weak forms in a matrix system shape, they are equivalent to require that the matrix coupling internal and interface expansions in each V_l have a maximum rank. For different element shapes, it establishes a dependence between the principal unknown expansion order s (primal case) or v (dual case) and the interface expansion order b . For instance, for triangular elements (Raviart and Thomas 1977b), we have

$$\min s \text{ or } v = \begin{cases} b + 1 & \text{if } b \text{ is even} \\ b + 2 & \text{if } b \text{ is odd,} \end{cases} \quad (2.16)$$

and for rectangular elements (Carrico, Lewis, and Palmiotti 1994)

$$\min s \text{ or } v = \begin{cases} b + 2 & \text{if } b \text{ is even} \\ b + 3 & \text{if } b \text{ is odd.} \end{cases} \quad (2.17)$$

This last result was obtained empirically in Carrico, Lewis, and Palmiotti (1994). The derivation above thus shows the well-posedness motivation of this spatial rank condition. Also, conditions (2.16) and (2.17) characterize s or v once b is fixed, or equivalently characterize b once s or v are fixed.

While this (spatial) rank condition is typical of hybrid methods, the inclusion conditions between internal unknown approximation spaces $\nabla S_h \subset \mathbf{V}_h$ (primal) and $\nabla \cdot \mathbf{V}_h \subset S_h$ (dual) are typical of mixed methods. Note that both well-known mixed dual finite elements due to Raviart and Thomas (1977a) and Brezzi, Douglas, and Marini (1985), satisfy the dual inclusion condition, and are thus included in our analysis for the general case. In practice, we take the maximal spatial order allowed by the inclusion conditions in theorem 2.4.2, that is we define the discrete mixed-

hybrid primal method with $s = v + 1$ and the discrete mixed-hybrid dual method with $v = s + 1$.

2.4.3 Note on error estimates

With $\lambda = (\mathbf{J}, \phi, \psi)$ the solution of the continuous mixed-hybrid problem (where $\psi = \mathbf{n} \cdot \mathbf{J}|_\Gamma$), and $\lambda_h = (\mathbf{J}_h, \phi_h, \psi_h)$ the solution of the discrete mixed-hybrid problem, let

$$e = \lambda - \lambda_h = (\mathbf{J} - \mathbf{J}_h, \phi - \phi_h, \psi - \psi_h)$$

and thus

$$\|e\|_\Lambda^2 = \|\lambda - \lambda_h\|_\Lambda^2 = \|\mathbf{J} - \mathbf{J}_h\|_Y^2 + \|\phi - \phi_h\|^2 + \|\psi - \psi_h\|_{1/2,\Gamma}^2.$$

We then have in view of Babůska, Oden, and Lee (1977, theorem 2.2)

$$\|e\|_\Lambda \leq (1 + C_1/\beta_h) \inf_{\bar{\lambda}_h \in \Lambda_h} \|\lambda - \bar{\lambda}_h\|_\Lambda$$

where the constant $C_1 = \sum_l (2 + \sigma_{0,l} + \sigma_{1,l})$ comes from (B.4) and the constant β_h is defined in (B.11).

The order of convergence of the method, i.e., the way $e \rightarrow 0$ as $h \rightarrow 0$, depends on

further assumptions that can be made on the finite element approximations spaces V_h , S_h and B_h (see Babuška, Oden, and Lee (1977, §6) for such an analysis in the primal diffusion case).

2.5 Note on variational interpretations

The formulations introduced above can be given a variational interpretation. While standard formulations yield extremum problems, mixed and hybrid formulations yield saddle-point problems. As for mixed-hybrid formulations, they yield “generalized saddle-point” problems with 3 variables. Their analyses is thus more involved, and we will not investigate them here. Note that a variational interpretation is not necessary either to derive the weak form equations, or to prove the well-posedness of a problem. It is given here for information, and to relate to other works. We consider only the primal case. A similar analysis can be performed for the dual case.

The Lax-Milgram implies (Girault and Raviart 1986, I.1.2, corollary 1.2) that the standard primal weak form (2.5) can be derived by looking for the minimum $\phi \in H^1(V)$ of the following functional:

$$F^{sp}[\phi] = \int_V \left[\frac{1}{2} \left(\frac{1}{\sigma_1} (\nabla \phi)^2 + \sigma_0 \phi^2 \right) - s_0 \phi - \frac{1}{\sigma_1} \mathbf{s}_1 \cdot \nabla \phi \right] dV + \int_{\partial V} \phi \chi d\Gamma$$

where $\chi = \mathbf{n} \cdot \mathbf{J}$ on ∂V is a known boundary condition. One can verify that requiring this functional to be stationary at ϕ , that is making the substitution $\phi \rightarrow \phi + \delta\tilde{\phi}$ where δ is an arbitrarily small positive constant, and requiring the linear terms in δ to vanish (in other words, requiring ∇F^{sp} to vanish at ϕ), yields (2.5).

The hybrid primal problem (2.8) has a variational interpretation in terms of a saddle-point problem (Girault and Raviart (1986, theorem 4.2 p.62), Roberts and Thomas (1991, chapter 1)): it is equivalent to finding (ϕ, χ) in $X \times H^{-1/2}(\Gamma)$ such that

$$F^{hp}[\phi, \tilde{\chi}] \leq F^{hp}[\phi, \chi] \leq F^{hp}[\tilde{\phi}, \chi] \quad \forall (\tilde{\chi}, \tilde{\phi}) \in X \times H_0^{-1/2}(\Gamma),$$

where

$$F^{hp}[\phi, \chi] = \sum_l F_l^{hp}[\phi, \chi]$$

with

$$F_l^{hp}[\phi, \chi] = \int_{V_l} \left[\frac{1}{2} \left(\frac{1}{\sigma_1} (\nabla \phi)^2 + \sigma_0 \phi^2 \right) - s_0 \phi - \frac{1}{\sigma_1} \mathbf{s}_1 \cdot \nabla \phi \right] dV + \int_{\partial V_l} \phi \chi d\Gamma. \quad (2.18)$$

One can verify that making the substitutions $\phi \rightarrow \phi + \delta\tilde{\phi}$ and $\chi \rightarrow \chi + \epsilon\tilde{\chi}$ in (2.18), where δ and ϵ are arbitrarily small positive constants, and requiring the linear terms

in δ and ϵ to vanish, yields (2.8). From a variational point of view, the functional for the whole domain V is thus the sum of all the elementary contributions coming from each element V_l . For each of these, the functional is the same as the one stated in the non-hybrid case (2.5), but where volume and surface integrals are now taken only on the considered element, and where the interface function (χ here) is now a distinct variable, in fact considered a Lagrange multiplier (and not a known boundary condition).

For the mixed primal case, solving (2.10) is equivalent to finding (Roberts and Thomas 1991, chapter 1) the saddle-point $(\phi, \mathbf{J}) \in H^1(V) \times [L^2(V)]^n$ such that

$$F^{hp}[\phi, \tilde{\mathbf{J}}] \leq F^{hp}[\phi, \mathbf{J}] \leq F^{hp}[\tilde{\phi}, \mathbf{J}] \quad \forall (\tilde{\phi}, \tilde{\mathbf{J}}) \in H^1(V) \times [L^2(V)]^n,$$

with

$$F^{sp}[\phi, \mathbf{J}] = \int_V \left[\frac{1}{2} (\sigma_0 \phi^2 - \sigma_1 \mathbf{J} \cdot \mathbf{J}) - \mathbf{J} \cdot \nabla \phi - s_0 \phi + \mathbf{s}_1 \cdot \mathbf{J} \right] dV + \int_{\partial V} \phi \chi d\Gamma \quad (2.19)$$

where $\chi = \mathbf{n} \cdot \mathbf{J}$ on ∂V is a known boundary condition. One can verify as well that making the substitutions $\phi \rightarrow \phi + \delta \tilde{\phi}$ and $\mathbf{J} \rightarrow \mathbf{J} + \epsilon \tilde{\mathbf{J}}$ in (2.19) where δ and ϵ are arbitrarily small positive constants, and requiring the linear terms in δ and ϵ to vanish, yields (2.10).

Chapter 3

P_N approximation

We now consider the general spherical harmonic approximation, referred to as the P_N approximation (Gelbard 1968). Recall that the even- and odd-parity flux decomposition

$$\Psi^\pm(\mathbf{r}, \boldsymbol{\Omega}) = \frac{1}{2}(\Psi(\mathbf{r}, \boldsymbol{\Omega}) \pm \Psi(\mathbf{r}, -\boldsymbol{\Omega})) \quad (3.1)$$

yields (in the isotropic case) the coupled pair of first order equations

$$\boldsymbol{\Omega} \cdot \nabla \Psi^-(\mathbf{r}, \boldsymbol{\Omega}) + \sigma(\mathbf{r}) \Psi^+(\mathbf{r}, \boldsymbol{\Omega}) = \sigma_s(\mathbf{r}) \phi(\mathbf{r}) + s(\mathbf{r}) \quad (3.2)$$

$$\boldsymbol{\Omega} \cdot \nabla \Psi^+(\mathbf{r}, \boldsymbol{\Omega}) + \sigma(\mathbf{r}) \Psi^-(\mathbf{r}, \boldsymbol{\Omega}) = 0 \quad (3.3)$$

where $\phi(\mathbf{r}) = \int_S d\Omega \Psi(\mathbf{r}, \boldsymbol{\Omega}) = \int_S d\Omega \Psi^+(\mathbf{r}, \boldsymbol{\Omega})$ is the scalar flux, and the cross-sections satisfy $\sigma(\mathbf{r}) \geq \sigma_s(\mathbf{r})$ for all \mathbf{r} . The equations (3.2) and (3.3) will be the starting point for our analysis of the P_N case, as (2.1) and (2.2) were for the P_1 case. Both the spatial and angular variables are here explicitly present.

We first generalize in §3.1 the concepts of §2.1 with the introduction of the angular variable $\boldsymbol{\Omega}$. Then we establish the continuous mixed-hybrid primal and dual formulations (§3.2), followed by their discrete counterparts (§3.3) using a finite-element approximation in space and a P_N spherical harmonic approximation in angle. The well-posedness investigation follows (§3.4 and appendix C), performed here for both primal and dual cases. We emphasize the interface angular expansions, providing a new derivation of the Romyantsev conditions. In §3.5, we proceed from the discrete formulations to the discretized weak form in a matrix setting. We also derive the flux and currents interface continuity condition. Finally, §3.6 treats the generalization to the anisotropic case.

3.1 Preliminaries

From now on, (\cdot, \cdot) and $\|\cdot\|$ denote the scalar product and norm in $L^2(S \times V)$, where S represents the unit sphere and V the spatial domain in \mathbf{R}^n ($n \leq 3$) as in section 2.1. We often write $\|\cdot\|_V$, shorthand notation for $\|\cdot\|_{S \times V}$, to emphasize the spatial

domain where this and subsequent norms are taken. Furthermore, define

$$\begin{aligned} H(grad, S \times V) &= \{\Psi \in L^2(S \times V) \text{ such that } \nabla \Psi \in [L^2(S \times V)]^n\}, \\ H(div, S \times V) &= \{\Psi \in [L^2(S \times V)]^n \text{ such that } \nabla \cdot \Psi \in L^2(S \times V)\}, \\ L^2(\Omega, S \times V) &= \{\Psi \in L^2(S \times V) \text{ such that } \Omega \Psi \in [L^2(S \times V)]^n\}, \text{ and} \\ H(\Omega \cdot \nabla, S \times V) &= \{\Psi \in L^2(\Omega, S \times V) \text{ such that } \Omega \cdot \nabla \Psi \in L^2(S \times V)\}. \end{aligned}$$

The scalar product in $L^2(\Omega, S \times V)$ is defined as

$$(\Psi_1, \Psi_2)_\Omega = \int_S \int_V (\Omega \Psi_1) \cdot (\Omega \Psi_2) dV d\Omega = \int_S \int_V \Psi_1 \Psi_2 dV d\Omega = (\Psi_1, \Psi_2)$$

since Ω is a unit vector, and thus $L^2(\Omega, S \times V) = L^2(S \times V)$. We nevertheless continue to use both notations. The other scalar products are defined as follows: in

$H(grad, S \times V)$

$$(\Psi_1, \Psi_2)_{grad} = \int_S \int_V \nabla \Psi_1 \cdot \nabla \Psi_2 dV d\Omega + \int_S \int_V \Psi_1 \Psi_2 dV d\Omega,$$

in $H(div, S \times V)$

$$(\Psi_1, \Psi_2)_{div} = \int_S \int_V \nabla \cdot \Psi_1 \nabla \cdot \Psi_2 dV d\Omega + \int_S \int_V \Psi_1 \cdot \Psi_2 dV d\Omega,$$

and in $H(\boldsymbol{\Omega} \cdot \nabla, S \times V)$

$$(\Psi_1, \Psi_2)_{\boldsymbol{\Omega} \cdot \nabla} = \int_S \int_V (\boldsymbol{\Omega} \cdot \nabla \Psi_1)(\boldsymbol{\Omega} \cdot \nabla \Psi_2) dV d\Omega + \int_S \int_V \Psi_1 \Psi_2 dV d\Omega.$$

The corresponding norms are thus $\|\Psi\|_{grad}^2 = \|\Psi\|^2 + \sum_i \|\partial_i \Psi\|^2$ in $H(grad, S \times V)$, $\|\Psi\|_{div}^2 = \sum_i \|\Psi_i\|^2 + \|\nabla \cdot \Psi\|^2$ in $H(div, S \times V)$, and $\|\Psi\|_{\boldsymbol{\Omega} \cdot \nabla}^2 = \|\Psi\|^2 + \|\boldsymbol{\Omega} \cdot \nabla \Psi\|^2$ in $H(\boldsymbol{\Omega} \cdot \nabla, S \times V)$. Note that $H(grad, S \times V)$ could have been denoted $H^1(S \times V)$ as in Sobolev space theory, but here the first-order derivative is taken with respect to only part of the variables, and moreover the choice of $H(grad, S \times V)$ provides a more homogeneous set of notation together with $H(div, S \times V)$. These two spaces are Hilbert spaces, and we also have

Theorem 3.1.1 $H(\boldsymbol{\Omega} \cdot \nabla)$ is a Hilbert space, and $H(grad) \subset H(\boldsymbol{\Omega} \cdot \nabla) \subset L^2(S \times V)$.

Proof 3.1.1 One has to show the completeness of $H(\boldsymbol{\Omega} \cdot \nabla)$. In this view, one can proceed similarly to what is usually done to prove the completeness of the Sobolev space H^1 , that is take a Cauchy sequence $\{\Psi_n\}$ in $H(\boldsymbol{\Omega} \cdot \nabla)$, note that $\{\Psi_n\}$ and $\{\boldsymbol{\Omega} \cdot \nabla \Psi_n\}$ are Cauchy sequences in $L^2(S \times V)$, and, denoting by Ψ^0 and Ψ^1 their respective limits (in $L^2(S \times V)$), prove using integration by parts that $\boldsymbol{\Omega} \cdot \nabla \Psi^0 = \Psi^1$, that is $\Psi^0 \in H(\boldsymbol{\Omega} \cdot \nabla)$. The second part of the theorem follows from $\|\Psi\|_{\boldsymbol{\Omega} \cdot \nabla} \leq \|\Psi\|_{grad}$.

Note that an advection operator similar to $\mathbf{\Omega} \cdot \nabla$ was already introduced and studied in (Dautray and Lions 1993, XXI §2.2).

The following two trace theorems generalize the theorems 2.1.1 and 2.1.2.

Theorem 3.1.2 *There exists a continuous linear map $\Psi \rightarrow \Psi|_{\partial V}$ from $H(\text{grad}, S \times V)$ into $L^2(S \times \partial V)$. The kernel of this mapping is denoted $H_0(\text{grad}, S \times V)$, and its range, denoted $H^{1/2}(S \times \partial V)$, is endowed with the norm*

$$\|\Psi^\alpha\|_{1/2, \partial V} = \inf_{\{\Psi \in H(\text{grad}, S \times V) : \Psi|_{S \times \partial V} = \Psi^\alpha\}} \|\Psi\|_{\text{grad}, V}. \quad (3.4)$$

Proof 3.1.2 *Apply theorem 2.1.1, the angular variables playing a passive role.*

Theorem 3.1.3 *There exists a continuous linear map $\Psi \rightarrow \Psi|_{\partial V}$ from $H(\mathbf{\Omega} \cdot \nabla, S \times V)$ onto $H_\Omega^{-1/2}(S \times \partial V)$ where*

$$H_\Omega^{-1/2}(S \times \partial V) = \{\Psi \text{ defined on } S \times \partial V \text{ such that } \mathbf{n} \cdot \mathbf{\Omega} \Psi \in H^{-1/2}(S \times \partial V)\},$$

with $H^{-1/2}(S \times \partial V)$ the dual of $H^{1/2}(S \times \partial V)$. The kernel of this mapping is denoted $H_0(\mathbf{\Omega} \cdot \nabla, S \times V)$, and its range $H_\Omega^{-1/2}(S \times \partial V)$ is endowed with the norm

$$\|\Psi\|_{\Omega, -1/2, \partial V} = \|\mathbf{n} \cdot \mathbf{\Omega} \Psi\|_{-1/2, \partial V}, \quad (3.5)$$

with

$$\|\Psi^\alpha\|_{-1/2,\partial V} = \inf_{\{\Psi^q \in H(\text{div}, S \times V) : \mathbf{n} \cdot \Psi^q|_{S \times \partial V} = \Psi^\alpha\}} \|\Psi^q\|_{\text{div}, V}. \quad (3.6)$$

Proof 3.1.3 $\Psi \in H(\Omega \cdot \nabla, S \times V)$ if and only if $\Omega \Psi \in H(\text{div}, S \times V)$, and one can apply the normal trace mapping theorem 2.1.2.

Domain decomposition as described in §2.1 is needed for the hybrid and mixed-hybrid methods. The spaces $H_0^{1/2}(S \times \Gamma)$ and $H_{\Omega,0}^{-1/2}(S \times \Gamma)$ respectively designate the subsets of $H^{1/2}(S \times \Gamma)$ and $H_\Omega^{-1/2}(S \times \Gamma)$ whose elements vanish on the outer boundary ∂V . Besides, norms in $H_{(0)}^{1/2}(S \times \Gamma)$ and $H_{\Omega,(0)}^{-1/2}(S \times \Gamma)$ are respectively $\|\Psi\|_{1/2,\Gamma}^2 = \sum_l \|\Psi\|_{1/2,\partial V_l}^2$ and $\|\Psi\|_{\Omega,-1/2,\Gamma}^2 = \sum_l \|\Psi\|_{\Omega,-1/2,\partial V_l}^2$. Furthermore, we introduce

$$\begin{aligned} X &= \{\Psi \in L^2(S \times V) \text{ such that } \forall l, \Psi|_{S \times V_l} \in H(\text{grad}, S \times V_l)\} \text{ and} \\ X_\Omega &= \{\Psi \in L^2(\Omega, S \times V) \text{ such that } \forall l, \Psi|_{S \times V_l} \in H(\Omega \cdot \nabla, S \times V_l)\} \end{aligned}$$

with corresponding norms $\|\Psi\|_X^2 = \sum_l \|\Psi\|_{\text{grad}, V_l}^2$ and $\|\Psi\|_{X_\Omega}^2 = \sum_l \|\Psi\|_{\Omega \cdot \nabla, V_l}^2$. The following two theorems (generalizing propositions 2.1.3 and 2.1.4) tell us how to enforce the interface regularity (with respect to the spatial variable) of the functions in $X_{(\Omega)}$.

Theorem 3.1.4

$$H(\text{grad}, S \times V) = \left\{ \Psi^\pm \in X \ : \ \sum_l \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}^\alpha \Psi^\pm = 0 \right. \\ \left. \forall \tilde{\Psi}^\alpha \in H_{\Omega,0}^{-1/2}(S \times \Gamma) \right\}.$$

Proof 3.1.4 *Following theorem 3.1.3, there exists a Ψ in $H(\boldsymbol{\Omega} \cdot \nabla, S \times V)$ whose restrictions to each $S \times V_l$ have traces equal to the corresponding restrictions of $\tilde{\Psi}^\alpha \in H_{\Omega,0}^{-1/2}(S \times \Gamma)$. Thus $\Psi \in H_0(\boldsymbol{\Omega} \cdot \nabla, S \times V)$. Clearly, $H(\text{grad}, S \times V) \subset X$, and if $\Psi^\pm \in H(\text{grad}, S \times V)$, we obtain successively*

$$\begin{aligned} \sum_l \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}^\alpha \Psi^\pm &= \sum_l \int_S d\Omega \int_{V_l} dV \boldsymbol{\Omega} \cdot \nabla (\Psi \Psi^\pm) \\ &= \int_S d\Omega \int_V dV \boldsymbol{\Omega} \cdot \nabla (\Psi \Psi^\pm) \\ &= \int_S d\Omega \int_{\partial V} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}^\alpha \Psi^\pm, \end{aligned}$$

which vanishes for any $\tilde{\Psi}^\alpha \in H_{\Omega,0}^{-1/2}(S \times \Gamma)$. Conversely, the proposed characterization of $H(\text{grad}, S \times V)$ implies using integration by parts

$$\begin{aligned} \int_S d\Omega \int_V dV \Psi^\pm (\boldsymbol{\Omega} \cdot \nabla \Psi) &= \\ &= - \int_S d\Omega \int_V dV (\nabla \Psi^\pm) \cdot \boldsymbol{\Omega} \Psi \quad \forall \Psi \in H_0(\boldsymbol{\Omega} \cdot \nabla, S \times V), \end{aligned}$$

and thus for all Ψ in $C_0^\infty(V)$ (i.e., compactly supported infinitely continuously derivable),

$$\left| \int_S d\Omega \int_V dV \Psi^\pm (\boldsymbol{\Omega} \cdot \nabla \Psi) \right| \leq \left(\sum_l \|\Psi^\pm\|_{grad, V_l}^2 \right)^{1/2} \|\boldsymbol{\Omega} \Psi\|.$$

Since $(\nabla \Psi^\pm, \boldsymbol{\Omega} \Psi) = -(\Psi^\pm, \nabla \cdot \boldsymbol{\Omega} \Psi)$ in the distribution sense, $(\nabla \Psi^\pm, \cdot)$ is thus a bounded linear functional that can be extended to $L^2(S \times V)$. Hence $\Psi^\pm \in H(grad, S \times V)$.

Similar arguments lead to

Theorem 3.1.5

$$H(\boldsymbol{\Omega} \cdot \nabla, S \times V) = \left\{ \Psi^\pm \in X_\Omega \quad : \quad \sum_l \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}^\alpha \Psi^\pm = 0 \right. \\ \left. \forall \tilde{\Psi}^\alpha \in H_0^{1/2}(S \times \Gamma) \right\}.$$

3.2 Continuous mixed-hybrid formulations

We multiply the equations (3.2) and (3.3) by (or rather apply the distributions to) test functions depending on both space and angle, and respectively of even $(\tilde{\Psi}^+(\mathbf{r}, \boldsymbol{\Omega}))$

or odd ($\tilde{\Psi}^-(\mathbf{r}, \boldsymbol{\Omega})$) angular parity. Integrating over space and angle yields

$$\int_S d\Omega \int_V dV \left(\boldsymbol{\Omega} \cdot \nabla \Psi^- + \sigma \Psi^+ - \sigma_s \int_S d\Omega' \Psi^+ \right) \tilde{\Psi}^+ = \int_S d\Omega \int_V dV s \tilde{\Psi}^+ \quad (3.7)$$

$$\int_S d\Omega \int_V dV \left(\boldsymbol{\Omega} \cdot \nabla \Psi^+ + \sigma \Psi^- \right) \tilde{\Psi}^- = 0. \quad (3.8)$$

Integrating by parts (with respect to \mathbf{r}) these two equations, and introducing the notations $\Psi^\psi(\boldsymbol{\Omega}, \mathbf{r})$ and $\Psi^\chi(\boldsymbol{\Omega}, \mathbf{r})$ to respectively represent the traces on ∂V of Ψ^+ and Ψ^- , we obtain successively

$$\begin{aligned} & - \int_S d\Omega \int_V dV \boldsymbol{\Omega} \cdot \nabla \tilde{\Psi}^+ \Psi^- + \int_S d\Omega \int_{\partial V} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}^+ \Psi^\chi \\ & + \int_S d\Omega \int_V dV \tilde{\Psi}^+ \left(\sigma \Psi^+ - \sigma_s \int_S d\Omega' \Psi^+ \right) \\ & = \int_S d\Omega \int_V dV s \tilde{\Psi}^+ \end{aligned} \quad (3.9)$$

and

$$\begin{aligned} & - \int_S d\Omega \int_V dV \Psi^+ \boldsymbol{\Omega} \cdot \nabla \tilde{\Psi}^- + \int_S d\Omega \int_{\partial V} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}^- \Psi^\psi \\ & + \int_S d\Omega \int_V dV \sigma \tilde{\Psi}^- \Psi^- = 0. \end{aligned} \quad (3.10)$$

Equations (3.8) and (3.9) lead to the mixed primal weak form, while (3.7) and (3.10) lead to the mixed dual weak form. We now introduce hybridization as in §2.2, keep-

ing only weak (but natural) regularity conditions at the interfaces of the spatially decomposed domain. In this view, we restrict the above equations to $S \times V_l$ (that is spatial integrations are now taken on V_l and ∂V_l), and sum them up. In the choice of approximation spaces, regularity requirements can then be restricted to each $S \times V_l$ separately, and interface regularity conditions are enforced by a third equation arising from theorem 3.1.4 or 3.1.5. In the sequel, we require $\sigma_l(\mathbf{r})$ and $\sigma_{s,l}(\mathbf{r})$ to be in $C^\infty(V_l)$. Using a subscript l to denote restrictions to $S \times V_l$, the mixed-hybrid primal weak form equations are

$$\left\{ \begin{array}{l} - \sum_l \int_S d\Omega \int_{V_l} dV \Psi_l^- \boldsymbol{\Omega} \cdot \nabla \tilde{\Psi}_l^+ + \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}_l^+ \Psi_l^\chi \\ \quad + \int_S d\Omega \int_{V_l} dV \tilde{\Psi}_l^+ (\sigma_l \Psi_l^+ - \sigma_{s,l} \int_S d\Omega' \Psi_l^+) \\ \quad = \sum_l \int_S d\Omega \int_{V_l} dV s \tilde{\Psi}_l^+ \\ \sum_l \int_S d\Omega \int_{V_l} dV \tilde{\Psi}_l^- \boldsymbol{\Omega} \cdot \nabla \Psi_l^+ + \int_S d\Omega \int_{V_l} dV \sigma_l \tilde{\Psi}_l^- \Psi_l^- = 0 \\ \sum_l \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}_l^\chi \Psi_l^+ = 0, \end{array} \right. \quad (3.11)$$

and we consider two possibilities for the choice of spaces (see definitions on pages 43, 45 and 46) ¹:

¹The even- and odd- order denominations introduced here will be motivated by the angular discretization: they refer to the parity of the angular expansion order N in section 3.3.

- even-order primal choice: we look for (Ψ^+, Ψ^-, Ψ^x) in $X \times L^2(\mathbf{\Omega}, S \times V) \times H_{\Omega}^{-1/2}(S \times \Gamma)$ for all $(\tilde{\Psi}^+, \tilde{\Psi}^-, \tilde{\Psi}^x)$ in $X \times L^2(\mathbf{\Omega}, S \times V) \times H_{\Omega,0}^{-1/2}(S \times \Gamma)$ (in this case we require s to be in X'),
- odd-order primal choice: we look for (Ψ^+, Ψ^-, Ψ^x) in $X_{\Omega} \times L^2(S \times V) \times H^{1/2}(S \times \Gamma)$ for all $(\tilde{\Psi}^+, \tilde{\Psi}^-, \tilde{\Psi}^x)$ in $X_{\Omega} \times L^2(S \times V) \times H_0^{1/2}(S \times \Gamma)$ (in this case we require s to be in X'_{Ω}).

In addition, given the decomposition (3.1), we require Ψ^+ to be even in $\mathbf{\Omega}$, and Ψ^- and Ψ^x to be odd in $\mathbf{\Omega}$. These angular parity properties are assumed throughout the remaining of this study even if they are not explicitly included in the notations (to avoid making them too cumbersome).

For the mixed-hybrid dual formulation, we obtain the equations

$$\left\{ \begin{array}{l} \sum_l \int_S d\Omega \int_{V_l} dV \tilde{\Psi}_l^+ (\mathbf{\Omega} \cdot \nabla \Psi_l^- + \sigma_l \Psi_l^+ - \sigma_{s,l} \int_S d\Omega' \Psi_l^+) \\ \quad = \sum_l \int_S d\Omega \int_{V_l} dV s \tilde{\Psi}_l^+ \\ - \sum_l \int_S d\Omega \int_{V_l} dV \Psi_l^+ \mathbf{\Omega} \cdot \nabla \tilde{\Psi}_l^- + \int_S d\Omega \int_{\partial V_l} d\Gamma \mathbf{\Omega} \cdot \mathbf{n} \tilde{\Psi}_l^- \Psi_l^\psi \\ \quad + \int_S d\Omega \int_{V_l} dV \sigma_l \tilde{\Psi}_l^- \Psi_l^- = 0 \\ \sum_l \int_S d\Omega \int_{\partial V_l} d\Gamma \mathbf{\Omega} \cdot \mathbf{n} \tilde{\Psi}_l^\psi \Psi_l^- = 0, \end{array} \right. \quad (3.12)$$

and the two choices of spaces are here

- even-order dual choice: we look for $(\Psi^-, \Psi^+, \Psi^\psi)$ in $X_\Omega \times L^2(S \times V) \times H^{1/2}(S \times \Gamma)$ for all $(\tilde{\Psi}^-, \tilde{\Psi}^+, \tilde{\Psi}^\psi)$ in $X_\Omega \times L^2(S \times V) \times H_0^{1/2}(S \times \Gamma)$ (then $s \in L^2(S \times V)$),
- odd-order dual choice: we look for $(\Psi^-, \Psi^+, \Psi^\psi)$ in $X \times L^2(\Omega, S \times V) \times H_\Omega^{-1/2}(S \times \Gamma)$ for all $(\tilde{\Psi}^-, \tilde{\Psi}^+, \tilde{\Psi}^\psi)$ in $X \times L^2(\Omega, S \times V) \times H_{\Omega,0}^{-1/2}(S \times \Gamma)$ (then $s \in L^2(\Omega, S \times V)$).

Here we require Ψ^- and Ψ^ψ to be odd in Ω , and Ψ^+ and Ψ^ψ to be even in Ω .

As stated earlier for the P_1 case, we could introduce discontinuities with a non-zero right-hand side in the third equations of both weak forms. The internal unknowns can again be characterized as “principal” or “secondary”: in the primal case Ψ^+ is “principal” and Ψ^- “secondary”, while the opposite is true in the dual case. Also, $\tilde{\Psi}^\psi$ and $\tilde{\Psi}^\psi$ can be interpreted as Lagrange multipliers in the third equation of the primal and dual weak forms (respectively), enforcing in each case the regularity of the principal unknown.

3.3 Discrete mixed-hybrid formulations

The subscript h denotes here the unknowns that have been discretized in both space and angle. We denote by P_h , M_h and B_h (respectively for Plus (even-parity), Minus (odd-parity) and Boundary) the finite-dimensional approximation spaces. In the pri-

mal case, we look for a triple $(\Psi_h^+, \Psi_h^-, \Psi_h^x) \in P_h \times M_h \times B_h$ that satisfies the primal weak form equations for any $(\tilde{\Psi}_h^+, \tilde{\Psi}_h^-, \tilde{\Psi}_h^x) \in P_h \times M_h \times B_{h,0}$ ² with in the even-order formulation

$$P_h \subset X, \quad M_h \subset L^2(\Omega, S \times V), \quad \text{and} \quad B_{h,(0)} \subset H_{\Omega,(0)}^{-1/2}(S \times \Gamma),$$

and in the odd-order formulation

$$P_h \subset X_\Omega, \quad M_h \subset L^2(S \times V), \quad \text{and} \quad B_{h,(0)} \subset H_{(0)}^{1/2}(S \times \Gamma).$$

Similarly in the dual case, we look for a triple $(\Psi_h^-, \Psi_h^+, \Psi_h^\psi) \in M_h \times P_h \times B_h$ satisfying the dual weak form equations for any $(\tilde{\Psi}_h^-, \tilde{\Psi}_h^+, \tilde{\Psi}_h^\psi) \in M_h \times P_h \times B_{h,0}$, with in the even-order formulation

$$M_h \subset X_\Omega, \quad P_h \subset L^2(S \times V), \quad \text{and} \quad B_{h,(0)} \subset H_{(0)}^{1/2}(S \times \Gamma),$$

and in the odd-order formulation

$$M_h \subset X, \quad P_h \subset L^2(\Omega, S \times V), \quad \text{and} \quad B_{h,(0)} \subset H_{\Omega,(0)}^{-1/2}(S \times \Gamma).$$

² $B_{h,0}$ is the subset of B_h where all the functions vanish on the external boundary ∂V .

We must introduce both spatial and angular discrete expansions to build P_h , M_h , and B_h .

For the spatial variable, we proceed as in section 2.3 for the P_1 approximation. That is, we use the polynomial spaces $\mathcal{P}_{p \text{ or } m}(V_l)$ for Ψ^\pm and $\mathcal{P}_b(\Gamma_g)$ for Ψ^χ or ψ .

For the angular expansions, we use the spherical harmonics, well-known to form an orthogonal basis for square integrable functions on the unit sphere. As in Palmiotti, Lewis, and Carrico (1995), Y_{nm} ($|m| < n$) designates the real and imaginary parts of the spherical harmonics, with the convention that values $m \geq 0$ refer to the real (cosine) part, and values $m < 0$ refer to the imaginary (sine) part. Moreover, we take the convention that the direction $\mathbf{\Omega}$ is expressed in terms of (θ, ϕ) , with θ the colatitude ($\theta \in [0, \pi]$) and ϕ the azimuthal angle ($\phi \in [0, \pi]$). Also, $\mu = \cos(\theta)$. Thus, our angular expansion functions read

$$\begin{aligned} Y_{lm}(\mathbf{\Omega}) &= C_{lm}^{1/2} P_l^m(\mu) \cos(m\phi), & l = 0, 1, 2, \dots; m = 0, 1, 2, \dots, l, & \quad \text{and} \\ Y_{lm}(\mathbf{\Omega}) &= C_{lm}^{1/2} P_l^m(\mu) \sin(|m|\phi), & l = 0, 1, 2, \dots; m = -1, -2, \dots, -l \end{aligned}$$

where the $P_l^m(\mu)$ are the associated Legendre functions and the C_{lm} are chosen such that $\int_S d\Omega Y_{lm}(\mathbf{\Omega}) Y_{l'm'}(\mathbf{\Omega}) = \delta_{ll'} \delta_{mm'}$. A P_N approximation truncates the series at the value $n = N$ in Y_{nm} . We denote by Y_N^+ and Y_N^- the set spanned by the spherical

harmonics Y_{nm} up to order $n = N$ that are respectively even or odd in Ω , that is

$$\begin{aligned} Y_N^+ &= \text{span} \{Y_{pq}, \text{ with } p = 0, 2, 4, \dots, N^+, |q| \leq p\}, \\ Y_N^- &= \text{span} \{Y_{pq}, \text{ with } p = 1, 3, 5, \dots, N^-, |q| \leq p\} \end{aligned}$$

where if N is even $N^+ = N = N^- + 1$, and if N is odd $N^- = N = N^+ + 1$. These sets are used to expand the angular dependence of the internal unknowns Ψ^\pm . For the interface unknowns Ψ^χ or ψ , we define the sets Y_N^χ and Y_N^ψ , and for parity reasons we have $Y_N^\chi \subset Y_N^-$ and $Y_N^\psi \subset Y_N^+$.

Total expansions are obtained by tensor (or Kronecker) product of spatial and angular expansions, and we are now prepared to define our approximation spaces.

We have for internal variables

$$\begin{aligned} P_h &= P_h^{N,p}(V) = \{\Psi^+ : \Psi^+ \in Y_N^+ \otimes \mathcal{P}_p(V_l), \forall l\} \\ M_h &= M_h^{N,m}(V) = \{\Psi^- : \Psi^- \in Y_N^- \otimes \mathcal{P}_m(V_l), \forall l\}. \end{aligned}$$

For interface variables, we have in the primal case

$$\begin{aligned} B_h &= B_h^{N,b}(\Gamma) = \{\Psi^\chi : \Psi^\chi \in Y_N^\chi \otimes \mathcal{P}_b(\Gamma_g), \forall g\} \\ B_{h,0} &= B_{h,0}^{N,b}(\Gamma) = \{\Psi^\chi : \Psi^\chi \in B_h^{N,b}, \Psi^\chi = 0 \text{ on } \partial V\}, \end{aligned}$$

and in the dual case

$$\begin{aligned} B_h &= B_h^{N,b}(\Gamma) = \{\Psi^\psi : \Psi^\psi \in Y_N^\psi \otimes \mathcal{P}_b(\Gamma_g), \forall g\} \\ B_{h,0} &= B_{h,0}^{N,b}(\Gamma) = \{\Psi^\psi : \Psi^\psi \in B_h^{N,b}, \Psi^\psi = 0 \text{ on } \partial V\}. \end{aligned}$$

In section 3.5, we detail how inserting the above described expansions into the weak forms (3.11) and (3.12) leads to a linear system in the expansion coefficients.

3.4 Well-posedness

We now provide well-posedness proofs for the general P_N equations. Vacuum and reflected boundary conditions are considered. The incoming neutron flux vanishes on vacuum boundaries. Thus, for any \mathbf{r} on such a boundary, one has $\Psi(\mathbf{r}, \boldsymbol{\Omega}) = 0$ for incoming directions, that is for $\boldsymbol{\Omega} \cdot \mathbf{n} < 0$ with \mathbf{n} the outward unit normal on the vacuum boundary. In terms of even- and odd-parity fluxes, we obtain

$$\Psi^+(\mathbf{r}, \boldsymbol{\Omega}) = \begin{cases} \Psi^-(\mathbf{r}, \boldsymbol{\Omega}) & \boldsymbol{\Omega} \cdot \mathbf{n} > 0 \\ -\Psi^-(\mathbf{r}, \boldsymbol{\Omega}) & \boldsymbol{\Omega} \cdot \mathbf{n} < 0. \end{cases} \quad (3.13)$$

For reflected boundary conditions, consider the polar axis to be aligned with the

boundary normal. Then, with Ω expressed in terms of (θ, ϕ) as above, a reflection corresponds to a transformation $\theta \rightarrow \Pi - \theta$, ϕ remaining unchanged. Thus, on a reflected boundary, $\Psi^+(\theta, \phi) = \Psi^+(\Pi - \theta, \phi)$ and $\Psi^-(\theta, \phi) = \Psi^-(\Pi - \theta, \phi)$. Besides, parity properties imply $\Psi^+(\Pi - \theta, \phi) = \Psi^+(\theta, \Pi + \phi)$ and $\Psi^-(\Pi - \theta, \phi) = -\Psi^-(\theta, \Pi + \phi)$. Thus $\Psi^+(\theta, \phi) = \Psi^+(\theta, \Pi + \phi)$ and $\Psi^-(\theta, \phi) = -\Psi^-(\theta, \Pi + \phi)$ on a reflected boundary.

3.4.1 Continuous formulations

Without loss of generality, any flux $\Psi(\mathbf{r}, \Omega)$ can be expanded in spherical harmonics according to $\Psi = \sum_{n=0}^{\infty} \sum_{|m| \leq n} (\Psi, Y_{nm})_{\Omega} Y_{nm}$, where the Y_{nm} form an orthonormal basis and $(\Psi, Y_{nm})_{\Omega} = \int_S d\Omega \Psi Y_{nm}$. Clearly, the coefficients $(\Psi, Y_{nm})_{\Omega}$ must decrease for $n \rightarrow \infty$ in order to meet the square integrable requirement with respect to the angular variable. We make this behavior more precise in the next definition.

Definition 3.4.1 *A flux $\Psi(\mathbf{r}, \Omega)$ is mildly anisotropic when there exists a sequence of numbers α_n such that*

$$(1 + \alpha_n) \sum_{|m| \leq n} \|(\Psi, Y_{nm})_{\Omega}\|^2 \geq \sum_{|m| \leq n} \|(\Psi, Y_{n+1, m})_{\Omega}\|^2 \text{ for any } n \geq 1, n \text{ odd.}$$

with

$$\alpha_n \rightarrow 0 \text{ when } n \rightarrow \infty$$

and

$$\alpha_n < \alpha^* \quad \forall n \quad \text{where} \quad \alpha^* = 2 \frac{\sigma}{\sigma_s} - 1.$$

Note that an assumption of this kind is implicitly made whenever a truncated spherical harmonic series is used to expand an angular dependent function.

The following theorem is proved in appendix C.1.

Theorem 3.4.1 *Assume vacuum or reflected boundary conditions on the external boundary ∂V . Assume σ_l and $\sigma_{s,l}$ constant on each element V_l , and $\sigma_l > \sigma_{s,l} > 0$ for all l . The mixed-hybrid continuous primal and dual weak forms (3.11) and (3.12), together with the odd- or even-order choice of spaces described in section 3.2, constitute well-posed problems provided the flux $\Psi(\mathbf{r}, \boldsymbol{\Omega}) = \Psi^+(\mathbf{r}, \boldsymbol{\Omega}) + \Psi^-(\mathbf{r}, \boldsymbol{\Omega})$ is mildly anisotropic in each element.*

The hypothesis $\sigma_l > \sigma_{s,l} > 0$ excludes void (i.e. $\sigma_l = 0$), pure scattering ($\sigma_{s,l} = \sigma_l$) and pure absorbing ($\sigma_{s,l} = 0$) media.

Finally, an alternative proof is also given in appendix C.1, showing that the mild anisotropy assumption in the previous theorem can be replaced by the assumption $\sigma_{s,l} < \frac{4}{5}\sigma_l$, for all l .

3.4.2 Discrete formulations

The following theorem is proved in appendix C.2. Note that this theorem establishes the existence and uniqueness of a solution, but not its stability. See appendix C.2 for details.

Theorem 3.4.2 *Assume vacuum or reflected boundary conditions on the external boundary ∂V . Assume σ_l and $\sigma_{s,l}$ constant on each element V_l , and $\sigma_l > \sigma_{s,l} > 0$ for all l . With the notation introduced above, assume furthermore that the primal mixed-hybrid discrete problems satisfy either*

- $\nabla P_h^{N,p} \subset \Omega M_h^{N,m}$ (true if $p - 1 \leq m$ and $N^+ \leq N^- + 1$), or
- $\Omega \cdot \nabla P_h^{N,p} \subset M_h^{N,m}$ (true if $p - 1 \leq m$ and $N^+ + 1 \leq N^-$),

and assume that the dual mixed-hybrid discrete problems satisfy either

- $\Omega \cdot \nabla M_h^{N,m} \subset P_h^{N,p}$ (true if $m - 1 \leq p$ and $N^- + 1 \leq N^+$), or
- $\nabla M_h^{N,m} \subset \Omega P_h^{N,p}$ (true if $m - 1 \leq p$ and $N^- \leq N^+ + 1$),

where if N is even $N^+ = N = N^- + 1$, and if N is odd $N^- = N = N^+ + 1$.

Then, these discrete problems have a unique solution provided the flux $\Psi_h(\mathbf{r}, \Omega) = \Psi_h^+(\mathbf{r}, \Omega) + \Psi_h^-(\mathbf{r}, \Omega)$ is mildly anisotropic in each element, and in the primal case,

for any $\Psi_{h,l}^\chi \in B_h^{N,b}(V_l)$ in any V_l ,

$$\int_{\Omega} d\Omega \int_{\partial V_l} d\Gamma \mathbf{\Omega} \cdot \mathbf{n} \Psi_{h,l}^\chi \Psi_{h,l}^+ = 0 \quad \forall \Psi_{h,l}^+ \in P_h^{N,p}(V_l) \text{ implies that } \Psi_{h,l}^\chi = 0, \quad (3.14)$$

while in the dual case, for any $\Psi_{h,l}^\psi \in B_h^{N,b}(V_l)$ in any V_l ,

$$\int_{\Omega} d\Omega \int_{\partial V_l} d\Gamma \mathbf{\Omega} \cdot \mathbf{n} \Psi_{h,l}^\psi \Psi_{h,l}^- = 0 \quad \forall \Psi_{h,l}^- \in M_h^{N,m}(V_l) \text{ implies that } \Psi_{h,l}^\psi = 0. \quad (3.15)$$

As conditions (2.14) and (2.15) in §2.4.2, conditions (3.14) and (3.15) are equivalent to a rank condition. In fact, with the total expansions obtained by tensor product of spatial and angular dependences, they both lead to a spatial and an angular rank condition. The spatial rank condition is the same as the one described in §2.4.2. It establishes a dependence between the main internal spatial expansion order (namely p for Ψ^+ or m for Ψ^-) and the interface expansion order (b for Ψ^χ or ψ), leading to relations such as (2.16) and (2.17), with the roles of s and v played here by p and m respectively. Thus the spatial rank condition characterizes the interface spatial expansion once the internal spatial expansions are defined. The angular rank condition characterizes the interface angular expansions (thus Y_N^χ or ψ) once the internal angular expansions are defined. In §3.4.3, we show how this leads to the Rumyantsev conditions (Rumyantsev 1962).

While this rank condition is typical of hybrid methods, inclusion conditions of the type $\nabla P_h \subset \mathbf{\Omega}M_h$, $\mathbf{\Omega} \cdot \nabla P_h \subset M_h, \dots$ are typical of mixed methods. Compared to the equivalent relations in §2.4.2, our conditions involve not only the nabla operator ∇ , but also $\mathbf{\Omega}$.

Taking the maximal spatial and angular order allowed by theorem 3.4.2, we can define four mixed-hybrid methods, namely the

- even-order primal, with $p = m + 1$ and N even,
- odd-order primal, with $p = m + 1$ and N odd,
- even-order dual, with $m = p + 1$ and N even, and
- odd-order dual, with $m = p + 1$ and N odd.

The primal/dual distinction, related to the spatial variable and therefore already present in the diffusion case, is thus completed in the transport case with an even/odd order P_N approximation distinction, related to the angular variable.

Note that the mild anisotropy assumption is not very restrictive here in the discrete case, since such an assumption is implicitly made whenever a P_N approximation is used.

3.4.3 Rumyantsev and the angular rank condition

We first concentrate on the primal case. Consider that the angular part of $\Psi_{h,l}^+$ is expanded in spherical harmonics according to $\sum_{p,q} \alpha_{pq}^+ Y_{pq}$ with the sum taken over all the even $p \leq N^+$ and all the $|q| \leq p$ for each p . From (3.14), the angular rank condition then reads

$$\sum_{pq} \alpha_{pq}^+ \int_{\Omega} d\Omega \mathbf{\Omega} \cdot \mathbf{n} \Psi_{h,l}^{\chi} Y_{pq} = 0 \quad \text{for any set } \{\alpha_{pq}^+\}, \text{ implies that } \Psi_{h,l}^{\chi} = 0. \quad (3.16)$$

In a matrix format (see §3.5.1), this is equivalent to require that the matrix coupling internal and interface angular expansions have maximum rank. Although the choice is not unique, condition (3.16) is satisfied taking

$$Y_N^{\chi} = \text{span} \left\{ \sum_{l_j, m_j} \left(\int_S d\Omega \mathbf{\Omega} \cdot \mathbf{n} Y_{pq} Y_{l_j m_j} \right) Y_{l_j m_j} \text{ with } |m_j| \leq l_j \leq N \text{ such that} \right. \\ \left. \int_S d\Omega \mathbf{\Omega} \cdot \mathbf{n} Y_{pq} Y_{l_j m_j} \neq 0, \text{ where } Y_{pq} \in Y_N^+ \right\} \quad (3.17)$$

where the l_j are necessarily odd. The calculations detailed in appendix A show that this choice leads (for P_1 to P_5 approximations) to the expansions $Y_N^{\chi} = \text{span}\{y_{\chi}\}$

where

$$P1 : y_\chi = (Y_{10}),$$

$$P2 : y_\chi = (Y_{10}, Y_{1\pm 1}),$$

$$P3 : y_\chi = (Y_{10}, Y_{30}, Y_{1\pm 1} + \sqrt{\frac{8}{7}}Y_{3\pm 1}, Y_{3\pm 2}),$$

$$P4 : y_\chi = (Y_{10}, Y_{1\pm 1}, Y_{30}, Y_{3\pm 1}, Y_{3\pm 2}, Y_{3\pm 3}),$$

$$P5 : y_\chi = (Y_{10}, Y_{30}, Y_{1\pm 1} + \sqrt{\frac{8}{7}}Y_{3\pm 1}, Y_{3\pm 2}, Y_{50}, \sqrt{\frac{15}{7}}Y_{3\pm 1} + 2\sqrt{\frac{6}{11}}Y_{5\pm 1}, \\ Y_{5\pm 2}, Y_{3\pm 3} + \frac{4}{\sqrt{11}}Y_{5\pm 3}, Y_{5\pm 4}).$$

These expansions correspond to what is known in the literature as the Rumyantsev conditions (Rumyantsev 1962), recently re-examined by Yang et al. (2004). Our derivation of these conditions, which proceeds from the angular rank condition, differs from the one by Rumyantsev and Yang et al., but leads to the same result. Also, we use Wigner coefficients in appendix A to perform our derivation.

Other choices than (3.17) are possible. For odd-order P_N approximations, Lewis,

Carrico, and Palmiotti (1996, appendix A) proved the validity of the choice

$$P1 : y_\chi = (Y_{10}),$$

$$P3 : y_\chi = (Y_{10}, Y_{30}, Y_{3\pm 1}, Y_{3\pm 2}),$$

$$P5 : y_\chi = (Y_{10}, Y_{30}, Y_{3\pm 1}, Y_{3\pm 2}, Y_{50}, Y_{5\pm 1}, Y_{5\pm 2}, Y_{5\pm 3}, Y_{5\pm 4}),$$

where the $Y_{n\pm n}$ are excluded. One can verify that the dimension of Y_N^χ is the same with both choices.

In the remaining of the text, we use the choice (3.17). A numerical comparison between this choice and the one by Lewis, Carrico, and Palmiotti (1996) has been recently performed by Yang et al. (2004). Note that the choice of interface angular expansion affects the interface continuity properties (see §3.5.2).

In the dual case, the equivalent of (3.17) is

$$Y_N^\psi = \text{span} \left\{ \sum_{l_j, m_j} \left(\int_S d\Omega \mathbf{\Omega} \cdot \mathbf{n} Y_{pq} Y_{l_j m_j} \right) Y_{l_j m_j} \text{ with } |m_j| \leq l_j \leq N \text{ such that} \right. \\ \left. \int_S d\Omega \mathbf{\Omega} \cdot \mathbf{n} Y_{pq} Y_{l_j m_j} \neq 0, \text{ where } Y_{pq} \in Y_N^- \right\}. \quad (3.18)$$

Calculations in appendix A yield the following expansions

$$P1 : y_\psi = (Y_{00}),$$

$$P2 : y_\psi = (Y_{00} + \frac{2}{\sqrt{5}}Y_{20}, Y_{2\pm 1}),$$

$$P3 : y_\psi = (Y_{00}, Y_{20}, Y_{2\pm 1}, Y_{2\pm 2}),$$

$$P4 : y_\psi = (Y_{00} + \frac{2}{\sqrt{5}}Y_{20}, Y_{2\pm 1}, \frac{3}{\sqrt{5}}Y_{20} + \frac{4}{3}Y_{40}, Y_{4\pm 1}, Y_{2\pm 2} + \frac{2}{\sqrt{3}}Y_{4\pm 2}, Y_{4\pm 3}),$$

$$P5 : y_\psi = (Y_{00}, Y_{20}, Y_{2\pm 1}, Y_{2\pm 2}, Y_{40}, Y_{4\pm 1}, Y_{4\pm 2}, Y_{4\pm 3}, Y_{4\pm 4}).$$

3.5 Discretized mixed-hybrid weak forms

3.5.1 The linear matrix system

We derive here a linear matrix system representing the discretized version of the weak forms (3.11) and (3.12).

For the spatial variable, we introduce for the internal unknowns the (column) vectors $f_{\pm,l}(\mathbf{r})$ whose elements constitute a basis for $\mathcal{P}_{p \text{ or } m}(V_l)$. For the interface unknowns, we introduce the vector $h_i(\mathbf{r})$ whose elements constitute a basis for $\mathcal{P}_b(\Gamma_i)$. In our tests, we consider regular convex union-of-rectangle domains, such that the intersection between two rectangular elements or between a rectangular element and the external boundary corresponds to exactly one side of these elements. We can

thus consider that the subscript i refers to the edge i of the element V_l . The choice of expansion orders must satisfy the well-posedness conditions derived above. In our numerical experiments (3.5.4), we take in the primal case $p = 6$ and $m = 5$, and in the dual case $m = 6$ and $p = 5$. In both cases, we take $b = 2$. This way, conditions from theorem 3.4.2 (with particularization in (2.17) for rectangles) are satisfied. Also, the polynomials are chosen such that the obtained bases are orthonormal. In fact, they correspond to those used in Palmiotti, Lewis, and Carrico (1995).

For the angular variable, we introduce the vectors $y_{\pm,l}(\mathbf{\Omega})$ whose elements constitute a basis for Y_N^{\pm} :³

$$\begin{aligned} y_{+,l}^T(\mathbf{\Omega}) &= (Y_{00}, Y_{20}, Y_{2\pm 1}, Y_{2\pm 2}, Y_{40}, Y_{4\pm 1}, Y_{4\pm 2}, Y_{4\pm 3}, Y_{4\pm 4}, Y_{60} \dots, Y_{N+\pm N+}), \text{ and} \\ y_{-,l}^T(\mathbf{\Omega}) &= (Y_{10}, Y_{1\pm 1}, Y_{30}, Y_{3\pm 1}, Y_{3\pm 2}, Y_{3\pm 3}, Y_{50}, \dots, Y_{N-\pm N-}). \end{aligned}$$

These two vectors are used to expand the angular dependence of the internal unknowns Ψ^{\pm} . As for the interface unknowns Ψ^{χ} (primal case) and Ψ^{ψ} (dual case), we use the vectors $y_{\chi}(\mathbf{\Omega})$ and $y_{\psi}(\mathbf{\Omega})$ already introduced in §3.4.3. These vectors constitute a basis for Y_N^{χ} or Y_N^{ψ} , and satisfy the angular rank condition while corresponding to the Rumyantsev conditions.

³In these expansions, $Y_{l\pm m}$ means that both Y_{lm} and Y_{l-m} are separately present in the vector.

Note that in the P_1 approximation, Y_{00} corresponds to the flux ϕ , while Y_{10} and $Y_{1\pm 1}$ correspond (in 3D) to the three components of the current vector \mathbf{J} .

With the spatial and angular expansions coupled through the Kronecker product, we obtain the total expansions

$$\Psi_{h,l}^{\pm}(\mathbf{r}, \boldsymbol{\Omega}) = [y_{\pm,l}^T(\boldsymbol{\Omega}) \otimes f_{\pm,l}^T(\mathbf{r})] \varphi_l^{\pm} \quad (3.19)$$

for the internal variables, and

$$\Psi_{h,i}^{\psi} = [y_{\psi,i}^T(\boldsymbol{\Omega}) \otimes h_i^T(\mathbf{r})] \psi_i \quad \text{and} \quad \Psi_{h,i}^{\chi} = [y_{\chi,i}^T(\boldsymbol{\Omega}) \otimes h_i^T(\mathbf{r})] \chi_i \quad (3.20)$$

for the interface variables, where φ_l^{\pm} , ψ_i and χ_i are the coefficient column vectors to be determined. These expansions are to be inserted in the weak forms (3.11) and (3.12) to yield the discrete weak forms.

We now need to define several matrices. First note that

$$I_{y_{\pm,l}} = \int_S d\Omega y_{\pm,l} y_{\pm,l}^T \quad \text{and} \quad N_{\sigma,l}^{\pm} = \int_{V_l} dV \sigma_l f_{\pm,l} f_{\pm,l}^T$$

are respectively identity and diagonal matrices since our bases are taken orthonormal.

Then we define

$$P_l = \int_S d\Omega y_{+,l} \quad \text{and} \quad \mathbf{E}_l = \int_S d\Omega \boldsymbol{\Omega} y_{+,l} y_{-,l}^T,$$

as well as

$$\mathbf{K}_l^p = \int_{V_l} dV \nabla f_{+,l} f_{-,l}^T \quad \text{and} \quad \mathbf{K}_l^d = \int_{V_l} dV \nabla f_{-,l} f_{+,l}^T.$$

The source term is cast into $S_l = \int_{V_l} dV f_{+,l} s$. Furthermore, we introduce matrices coupling internal and interface expansions. We write for the angular variable

$$\mathbf{E}_{\chi,i} \cdot \mathbf{n} = \int_S d\Omega \boldsymbol{\Omega} \cdot \mathbf{n} y_{+,l} y_{\chi,i}^T, \quad \text{and} \quad \mathbf{E}_{\psi,i} \cdot \mathbf{n} = \int_S d\Omega \boldsymbol{\Omega} \cdot \mathbf{n} y_{-,l} y_{\psi,i}^T, \quad (3.21)$$

and for the spatial variable

$$M_i^p = \int_i d\Gamma f_{+,l} h_i^T \quad \text{and} \quad M_i^d = \int_i d\Gamma f_{-,l} h_i^T. \quad (3.22)$$

These $\mathbf{E}_{\chi \text{ or } \psi,i} \cdot \mathbf{n}$ and $M^p \text{ or } d$ matrices have full rank since our spatial and angular expansions have been chosen so as to satisfy both angular and spatial rank conditions.

For a rectangular element V_l , with sides $i = 1, 2, 3, 4$ corresponding respectively to the bottom, right, top and left edges, and with x - and y -axis parallel to the bottom

and left sides, we define

$$\begin{aligned} EM_l^p &= [\mathbf{E}_{\chi,1} \cdot \mathbf{1}_y \otimes M_1^p, \mathbf{E}_{\chi,2} \cdot \mathbf{1}_x \otimes M_2^p, \mathbf{E}_{\chi,3} \cdot \mathbf{1}_y \otimes M_3^p, \mathbf{E}_{\chi,4} \cdot \mathbf{1}_x \otimes M_4^p], \\ EM_l^d &= [\mathbf{E}_{\psi,1} \cdot \mathbf{1}_y \otimes M_1^d, \mathbf{E}_{\psi,2} \cdot \mathbf{1}_x \otimes M_2^d, \mathbf{E}_{\psi,3} \cdot \mathbf{1}_y \otimes M_3^d, \mathbf{E}_{\psi,4} \cdot \mathbf{1}_x \otimes M_4^d], \end{aligned}$$

$\psi_l = [\psi_1, \psi_2, \psi_3, \psi_4]^T$, and $\chi_l = [\chi_1, \chi_2, \chi_3, \chi_4]^T$. As a consequence, the part of EM_l^p referring to the side i of V_l is denoted by $EM_{l,i}^p$, and similarly with $EM_{l,i}^d$. Also, $EM_{0,l,i}^p$ and $EM_{0,l,i}^d$ are defined equal to $EM_{l,i}^p$ and $EM_{l,i}^d$ except that they vanish if the side i lies on the external boundary. We discuss below the treatment of the boundary conditions.

We are now prepared to use the expansions (3.19) and (3.20) to write the discretized versions of the weak forms (3.11) and (3.12). For any element V_l , and for an edge i shared by the elements V_l and $V_{l'}$, we obtain in the primal case

$$\begin{aligned} -(\mathbf{E}_l \otimes \cdot \mathbf{K}_l^p) \varphi_l^- + (I_{+,l} \otimes N_{\sigma,l}^+) \varphi_l^+ + (EM_l^p) \chi_l - (P_l P_l^T \otimes N_{\sigma,l}^+) \varphi_l^+ &= P_l \otimes S_l \\ (\mathbf{E}_l^T \otimes \cdot \mathbf{K}_l^{pT}) \varphi_l^+ + (I_{-,l} \otimes N_{\sigma,l}^-) \varphi_l^- &= 0 \quad (3.23) \\ (EM_{0,l,i}^p)^T \varphi_l^+ + (EM_{0,l',i}^p)^T \varphi_{l'}^+ &= 0, \end{aligned}$$

and in the dual case

$$\begin{aligned}
(\mathbf{E}_l \otimes \cdot \mathbf{K}_l^{dT}) \varphi_l^- + (I_{+,l} \otimes N_{\sigma,l}^+) \varphi_l^+ - (P_l P_l^T \otimes N_{\sigma_s,l}^+) \varphi_l^+ &= P_l \otimes S_l \\
-(\mathbf{E}_l^T \otimes \cdot \mathbf{K}_l^d) \varphi_l^+ + (I_{-,l} \otimes N_{\sigma,l}^-) \varphi_l^- + (EM_l^d) \psi_l &= 0 \\
(EM_{0,l,i}^d)^T \varphi_l^- + (EM_{0,l',i}^d)^T \varphi_{l'}^- &= 0.
\end{aligned} \tag{3.24}$$

In §3.5.3 we discuss the solving of this linear matrix system.

Further inspection of the third equation set of both discretized weak forms is instructive. In the primal case, we have

$$\begin{aligned}
(\mathbf{E}_{\chi,i}^T \cdot \mathbf{n} \otimes M_i^{pT}) \varphi_l^+ &= \left(\int_S d\Omega \mathbf{\Omega} \cdot \mathbf{n} y_{\chi,l} y_{+,l}^T \otimes \int_i d\Gamma h_i f_{+,l}^T \right) \varphi_l^+ \\
&= \int_S d\Omega \int_i d\Gamma \mathbf{\Omega} \cdot \mathbf{n} (y_{\chi,l} \otimes h_i) \Psi_{N,h,l}^+(\mathbf{r}, \mathbf{\Omega}).
\end{aligned}$$

Defining ⁴ $\Psi_{N,h,i}^\psi = (y_{+,l}^T \otimes h_i^T) \psi_i$ as the trace of $\Psi_{N,h,l}^+$ on the interfaces then yields

$$\begin{aligned}
(\mathbf{E}_{\chi,i}^T \cdot \mathbf{n} \otimes M_i^{pT}) \varphi_l^+ &= \int_S d\Omega \int_i d\Gamma \mathbf{\Omega} \cdot \mathbf{n} (y_{\chi,l} \otimes h_i) (y_{+,l}^T \otimes h_i^T) \psi_i \\
&= (\mathbf{E}_{\chi,i}^T \cdot \mathbf{n} \otimes I_{N_h}) \psi_i.
\end{aligned} \tag{3.25}$$

In the dual case, we define $\Psi_{N,h,i}^\chi = (y_{-,l}^T \otimes h_i^T) \chi_i$ as the trace of $\Psi_{N,h,l}^-$ on the interfaces,

⁴ Ψ^ψ was so far not defined in the primal case

and obtain similarly

$$(\mathbf{E}_{\psi,i}^T \cdot \mathbf{n} \otimes M_i^{dT}) \varphi_i^- = (\mathbf{E}_{\psi,i}^T \cdot \mathbf{n} \otimes I_{N_h}) \chi_i. \quad (3.26)$$

With ψ_i and χ_i uniquely defined on any interface between two elements, we can verify with equations (3.25) and (3.26) that the third equation set of both our discretized weak forms enforces the (spatial) continuity of the principal unknown (namely Ψ^+ for primal and Ψ^- for dual) across any (internal) interface. This continuity is however only partly achieved due to the discretization, as detailed in the next paragraph (§3.5.2).

Finally, a word on boundary conditions is in order. For reflected boundary conditions, Lewis, Carrico, and Palmiotti (1996) showed that the angular symmetry conditions are satisfied if the coefficients ψ_i of any Y_{nm} with odd m are set to zero on such a boundary, as well as the coefficients χ_i of any Y_{nm} with even m . This can be understood as follows. Given that Ψ^ψ and Ψ^χ are respectively the boundary value of Ψ^+ and Ψ^- , our discussion on boundary conditions in section 3.4 shows that $\Psi^\psi(\theta, \phi) = \Psi^\psi(\theta, \Pi + \phi)$ and $\Psi^\chi(\theta, \phi) = -\Psi^\chi(\theta, \Pi + \phi)$ on reflected boundaries. Now, since $Y_{lm}(\theta, \Pi + \phi) = Y_{lm}(\theta, \phi)$ for even m and $Y_{lm}(\theta, \Pi + \phi) = -Y_{lm}(\theta, \phi)$ for odd m , we can withdraw the Y_{lm} with odd m out of the Ψ^ψ expansion, as well as the Y_{lm}

with even m out of the Ψ^χ expansion.

For vacuum boundaries we adapt here the procedure of Palmiotti, Lewis, and Carrico (1995). Following (3.13), we can write $(\boldsymbol{\Omega} \cdot \mathbf{n})\Psi^\psi = |\boldsymbol{\Omega} \cdot \mathbf{n}|\Psi^\chi$ on a vacuum boundary. In the primal case, we obtain for an edge i on such a boundary

$$\int_S d\Omega \int_i d\Gamma y_{+,i} \otimes h_i (|\boldsymbol{\Omega} \cdot \mathbf{n}|(y_{+,i}^T \otimes h_i^T)\psi_i - (\boldsymbol{\Omega} \cdot \mathbf{n})(y_{\chi,i}^T \otimes h_i^T)\chi_i) = 0,$$

which simplifies to

$$\left(\int_S d\Omega |\boldsymbol{\Omega} \cdot \mathbf{n}| (y_{+,i} y_{+,i}^T) \otimes I_{N_h} \right) \psi_i - \left(\int_S d\Omega (\boldsymbol{\Omega} \cdot \mathbf{n}) (y_{\chi,i} y_{\chi,i}^T) \otimes I_{N_h} \right) \chi_i = 0$$

or

$$(\mathbf{E}_{\chi,i} \cdot \mathbf{n} \otimes I_{N_h}) \chi_i = (L^p \otimes I_{N_h}) \psi_i,$$

where $L^p = \int_S d\Omega |\boldsymbol{\Omega} \cdot \mathbf{n}|(y_{+,l} y_{+,l}^T)$. Then, from (3.25), the primal vacuum boundary conditions are enforced through

$$\left(\mathbf{E}_{\chi,i}^T \cdot \mathbf{n} \otimes M_i^{pT} \right) \varphi_l^\dagger = \underline{L}^p,$$

where

$$\underline{L}^p = (\mathbf{E}_{\chi,i}^T \cdot \mathbf{n} \otimes I_{N_h}) (L^p \otimes I_{N_h})^{-1} (\mathbf{E}_{\chi,i} \cdot \mathbf{n} \otimes I_{N_h}) \chi_i. \quad (3.27)$$

Similarly for the dual case,

$$\int_S d\Omega \int_i d\Gamma y_{-,i} \otimes h_i ((\boldsymbol{\Omega} \cdot \mathbf{n})(y_{\psi,i}^T \otimes h_i^T)\psi_i - |\boldsymbol{\Omega} \cdot \mathbf{n}|(y_{-,i}^T \otimes h_i^T)\chi_i) = 0$$

reduces to

$$(\mathbf{E}_{\psi,i} \cdot \mathbf{n} \otimes I_{N_h}) \psi_i = (L^d \otimes I_{N_h}) \chi_i,$$

where $L^d = \int_S d\Omega |\boldsymbol{\Omega} \cdot \mathbf{n}| (y_{-,l} y_{-,l}^T)$. Then, from (3.26), the dual vacuum boundary conditions are enforced through

$$\left(\mathbf{E}_{\psi,i}^T \cdot \mathbf{n} \otimes M_i^{dT} \right) \varphi_l^- = \underline{L}^d,$$

where

$$\underline{L}^d = (\mathbf{E}_{\psi,i}^T \cdot \mathbf{n} \otimes I_{N_h}) (L^d \otimes I_{N_h})^{-1} (\mathbf{E}_{\psi,i} \cdot \mathbf{n} \otimes I_{N_h}) \psi_i. \quad (3.28)$$

3.5.2 Interface continuity properties

The spatial continuity of the principal unknown is enforced through the third equation set of both weak forms. Nevertheless, this continuity, although guaranteed in infinite-dimensional spaces, is only partly achieved after discretization. We concentrate here mainly on the consequences of using truncated angular expansions. We will denote

by N_+ , N_- , N_χ and N_ψ respectively the lengths of y_+ , y_- , y_χ and y_ψ . We notice that $y_\psi = y_+$ and $N_\chi = N_\psi = N_+ < N_-$ for odd-order P_N approximations, while $y_\chi = y_-$ and $N_\chi = N_\psi = N_- < N_+$ for even-order P_N approximations.

Let us consider the principal unknown. In the primal case, the continuity of Ψ^+ is enforced through the equation

$$(EM_{0,i}^p)^T \varphi_l^+ + (EM_{0,i}^{p'})^T \varphi_{l'}^+ = 0 \quad (3.29)$$

Concentrating on the angular variable, we observe from the definition (3.21) of $\mathbf{E}_{\chi,i} \cdot \mathbf{n}$ that if $N_\chi < N_+$, (3.29) does not provide enough equations to enforce the continuity of all the Ψ^+ components. In fact, only N_χ combinations of φ_l^+ coefficients are selected in (3.29), and thus only the corresponding combinations of Ψ^+ components are enforced continuous. In odd-order primal methods, $N_\chi = N_+$, and the interface continuity of all the Ψ^+ components can therefore be enforced. In even-order primal methods, $N_\chi < N_+$, and we now show that the N_χ continuous Ψ^+ components are in fact the ones constituting the y_ψ basis derived for the corresponding dual method (since $N_\psi = N_\chi$, this yields the right number of components). Indeed, again from the definition (3.21) of $\mathbf{E}_{\chi,i} \cdot \mathbf{n}$, we note that the Ψ^+ components for which continuity is

enforced are the multiples of the combinations

$$\sum_{p_j, q_j} \left(\int_S d\Omega \mathbf{\Omega} \cdot \mathbf{n} Y_{lm} Y_{p_j q_j} \right) Y_{p_j q_j}$$

where $Y_{p_j q_j}$ is a y_+ basis component such that

$$\int_S d\Omega \int_{\partial V_i} d\Gamma \mathbf{\Omega} \cdot \mathbf{n} Y_{lm} Y_{p_j q_j} \neq 0$$

for any given y_χ basis components Y_{lm} . But, since in even-order primal methods $y_\chi = y_-$, this is the same as finding y_ψ for the corresponding dual method in (3.18). Thus the continuous Ψ^+ components in an even-order primal method are the ones spanned by the y_ψ set derived for the corresponding dual method. This remains true in odd-order primal method, since then $y_\psi = y_+$ and all the Ψ^+ components are continuous. Hence in any primal method, y_ψ spans all the continuous Ψ^+ components (at interfaces). Similarly in any dual method, y_χ spans all the continuous Ψ^- components.

As for secondary unknowns, in the primal case, with Ψ^χ representing the trace of Ψ^- on interfaces (and since y_χ is a subset of $\text{span}(y_-)$), only the components of Ψ^- spanned by y_χ will match on both sides of an interface edge. Thus, in any primal method, y_χ spans all the continuous Ψ^- components. Similarly in any dual method,

y_ψ spans all the continuous Ψ^+ components.

Thus, the continuity of both principal and secondary unknowns at interfaces is determined by the interface angular expansions: y_ψ for Ψ^+ and y_χ for Ψ^- .

In reactor physics applications, the most valuable quantities are the Y_{00} , Y_{10} and $Y_{1\pm 1}$ components, corresponding to the scalar flux ϕ (Y_{00}) and the current vector \mathbf{J} (with our conventions, Y_{10} corresponds to the normal current, and $Y_{1\pm 1}$ to the two components of the parallel current (in three dimensions)). Developments in §3.4.3 show that y_ψ contains Y_{00} on its own only when N is odd, y_χ contains Y_{10} on its own regardless of the parity of N , and y_χ contains $Y_{1\pm 1}$ on its own only when N is even. Consequently, we have shown the following for *both primal and dual* mixed-hybrid methods (using Romyantsev interface conditions):

- in odd-order P_N methods, the continuity of the flux and normal current, but not the continuity of the parallel current, is enforced at interfaces,
- in even-order P_N methods, the continuity of the normal and parallel currents, but not the continuity of the flux, is enforced at interfaces.

Note that the continuity of the normal current is required in order to ensure neutron conservation properties within each element V_l . Note also that other interface continuity conditions would arise using other choices of interface angular expansions $y_{\chi \text{ or } \psi}$, in particular the choice of Palmiotti, Lewis, and Carrico (1995). One could

furthermore conceive choices making the flux and all the components of the current continuous for any even- or odd-order P_N approximation.

A similar analysis concentrating on the consequences of using truncated spatial expansions may be performed. Then the various spatial Ψ^\pm components that can be enforced continuous are the ones selected by the M^p or d matrix. This, however, seems to have less practical interest: these properties can be seen only when an enlarged scale is used in numerical experiments.

3.5.3 Solving the linear matrix system

Even though the emphasis of this thesis is on the discretization methods, we give here some insight into the matrix system solution and outline some related future prospects. First, we define the global vectors $\varphi^\pm = (\varphi_1^\pm, \dots, \varphi_L^\pm)$, $\chi = (\chi_1, \dots, \chi_{N_{edges}})$ and $\psi = (\psi_1, \dots, \psi_{N_{edges}})$, where L is the total number of elements, and N_{edges} the total number of edges (either shared by two elements or on the external boundary).

In the primal case, the global matrix system is obtained by assembling the ele-

mental contributions given by (3.23). The resulting primal system takes the form

$$\begin{pmatrix} A & B & C \\ B^T & -D & 0 \\ C^T & 0 & -L_{bc} \end{pmatrix} \begin{pmatrix} \varphi^+ \\ \varphi^- \\ \chi \end{pmatrix} = \begin{pmatrix} Q \\ 0 \\ 0 \end{pmatrix} \quad (3.30)$$

where $A = \text{diag}(A_1, \dots, A_L)$, $B = \text{diag}(B_1, \dots, B_L)$ and $D = \text{diag}(D_1, \dots, D_L)$ with

$$A_l = I_{+,l} \otimes N_{\sigma,l}^+ - P_l P_l^T \otimes N_{\sigma_s,l}^+,$$

$$B_l = -\mathbf{E}_l \otimes \cdot \mathbf{K}_l^p,$$

$$D_l = I_{-,l} \otimes N_{\sigma,l}^-, \text{ and}$$

$$Q_l = P_l \otimes S_l.$$

As detailed below for rectangular elements, C is made out of the EM_l^p elements defined in §3.5.1, and L_{bc} out of the \underline{L}^p matrix defined in (3.27) for vacuum boundary conditions. For reflected boundary conditions applied to an edge i , we can remove the lines and columns corresponding to the coefficients χ_i of any Y_{nm} with even m (see §3.5.1).

More precisely, let us consider rectangular elements V_l as in §3.5.1 with

$$EM_l^p = (EM_{l,1}^p, EM_{l,2}^p, EM_{l,3}^p, EM_{l,4}^p).$$

To have a most general example, we consider an element V_l such that

- the edge 1 of V_l is also the edge i of $V_{l'}$,
- the edge 2 of V_l is also to the edge j of $V_{l''}$,
- the edge 3 of V_l lies on a vacuum boundary, and
- the edge 4 of V_l lies on a reflected boundary.

Then C and L_{bc} have the general form

$$C = \begin{pmatrix} & & & EM_{l'',j}^p & & & & & & \\ \dots & EM_{l,1}^p & \dots & EM_{l,2}^p & \dots & EM_{l,3}^p & \dots & \widehat{EM}_{l,4}^p & \dots & \\ & & & EM_{l',i}^p & & & & & & \end{pmatrix} \quad (3.31)$$

$$L_{bc} = \text{diag} \left(\dots \quad \mathbf{O} \quad \dots \quad \mathbf{O} \quad \dots \quad \underline{L}^p \quad \dots \quad \widehat{\mathbf{O}} \quad \dots \right) \quad (3.32)$$

where \mathbf{O} represents a zero block, \underline{L}^p is defined in (3.27), $\widehat{EM}_{l,4}^p$ is obtained from $EM_{l,4}^p$ removing the lines corresponding to Y_{nm} with even m , and $\widehat{\mathbf{O}}$ is obtained similarly

from O.

Assembling the elemental contributions given by (3.24), the dual counterpart to (3.30) is

$$\begin{pmatrix} A & B & C \\ B^T & -D & 0 \\ C^T & 0 & -L_{bc} \end{pmatrix} \begin{pmatrix} \varphi^- \\ \varphi^+ \\ \psi \end{pmatrix} = \begin{pmatrix} 0 \\ -Q \\ 0 \end{pmatrix} \quad (3.33)$$

where again $A = \text{diag}(A_1, \dots, A_L)$, $B = \text{diag}(B_1, \dots, B_L)$ and $D = \text{diag}(D_1, \dots, D_L)$ with

$$\begin{aligned} A_l &= I_{-,l} \otimes N_{\sigma,l}^- \\ B_l &= -\mathbf{E}_l^T \otimes \cdot \mathbf{K}_l^d, \\ D_l &= I_{+,l} \otimes N_{\sigma,l}^+ - P_l P_l^T \otimes N_{\sigma_s,l}^+, \\ Q_l &= P_l \otimes S_l. \end{aligned}$$

Similarly to the primal case, C is made out of the EM_l^d elements, and L_{bc} out of the \underline{L}^d matrix defined in (3.28). Their general form for rectangular elements is obtained as in (3.31) and (3.32) with p superscripts replaced by d . As for reflected boundary conditions applied to an edge i , we can remove the lines and columns corresponding

to the coefficient ψ_i of any Y_{nm} with odd m .

In both primal and dual cases, the A_l and D_l blocks, thus also the A and D blocks, are diagonal (since we chose orthogonal bases) and positive definite if $\sigma \neq 0$ and $\sigma \neq \sigma_s$ (i.e., $\sigma > \sigma_s$). Also, \underline{L}^p and \underline{L}^d are symmetric positive definite.

In a void element V_l , we have $\sigma_l = \sigma_{s,l} = 0$, which imply $A_l = D_l = 0$ in both primal and dual cases. Our numerical tests show that both primal (3.30) and dual (3.33) systems become singular when one or more elements are void. Thus both primal and dual methods are not suited to treat void regions. In a pure scattering element, we have $\sigma_l = \sigma_{s,l} \neq 0$, which makes some of the (diagonal) components of A_l vanish in the primal case, while some of the (diagonal) components of D_l vanish in the dual case ⁵. Then, our numerical tests show that the presence of a pure scattering element does not make the primal or dual system singular. Note that the isotropic P_1 (i.e., diffusion) approximation yields in fact the Poisson equation in the pure scattering case (see equations (2.1) and (2.1) on page 18 with $\sigma_0 = \sigma - \sigma_s = 0$ and $\sigma_1 = 3\sigma$).

The global system matrices (3.30) and (3.33) are symmetric but indefinite, and of

⁵In fact, given the definition of P_l in §3.5.1, the vanishing lines are those corresponding to the Y_{00} component, i.e., the first lines of the matrix (A_l or D_l).

the generalized saddle-point type, i.e., they can be cast into the form

$$\begin{pmatrix} \tilde{X} & \tilde{Y} \\ \tilde{Y}^T & 0 \end{pmatrix}$$

by permuting the χ or ψ elements. In our primal and dual cases, \tilde{X} is made out of A , $-D$, and the non-zero lines in L_{bc} . Such a matrix is “saddle-point” because it has a zero lower-right block, and “generalized” because the block \tilde{X} is not definite ⁶ (Little, Saad, and Smoch 2003).

The primal and dual system of equations can be approached directly as a whole, providing direct access to both internal and interface unknowns. This approach is the one taken in the numerical experiments presented in section 3.5.4. We developed a stand-alone MATLAB (Quarteroni and Saleri 2003) code, and solutions were obtained using the standard MATLAB routine “minres”, a minimum residual iterative technique. Various preconditioned iterative techniques for generalized saddle-point systems have been proposed in the literature (see for instance Little, Saad, and Smoch (2003) and Keller, Gould, and Wathen (2000)). Developing methods based on them could probably provide a faster solution algorithm.

An alternative approach for solving (3.30) and (3.33) is to eliminate selective

⁶This can be seen simply by noticing that, when $\sigma \neq \sigma_s$, A is positive definite while $-D$ is negative definite.

unknowns to obtain smaller systems. This is known as a condensation approach. We present here a condensation approach based on the elimination of the internal unknowns φ^\pm . Such an approach seems to have been first developed by Fraeijs de Veubeke for elasticity problems (see citations in Brezzi, Douglas, and Marini (1985) or in Brezzi and Fortin (1991, V.1)).

In the primal system (3.30), if $\sigma_l \neq 0$ for all l ⁷, one can eliminate φ^- to obtain $\varphi^- = D^{-1}B^T\varphi^+$ and

$$\begin{pmatrix} A + BD^{-1}B^T & C \\ C^T & -L_{bc} \end{pmatrix} \begin{pmatrix} \varphi^+ \\ \chi \end{pmatrix} = \begin{pmatrix} Q \\ 0 \end{pmatrix}.$$

If moreover $\sigma_l \neq \sigma_{s,l}$ for all l ⁸, we can further eliminate the even-parity flux by writing

$$\varphi^+ = (A + BD^{-1}B^T)^{-1}(-C\chi + Q)$$

to yield

$$H\chi = F, \tag{3.34}$$

⁷otherwise $D_l = 0$ and D is thus not invertible

⁸otherwise the first lines of A_l are zero, and since the first line of B_l is always zero (because the spatial part of B_l is given by \mathbf{K}_l^p (defined in §3.5.1), whose first line vanish since it involves taking the gradient of a constant), $A_l + B_l D_l^{-1} B_l^T$ is not invertible, which in turn makes $A + BD^{-1}B^T$ not invertible.

where

$$H = C^T(A + BD^{-1}B^T)^{-1}C + L_{bc} \quad \text{and}$$

$$F = C^T(A + BD^{-1}B^T)^{-1}Q.$$

Since we had to assume $\sigma_l \neq \sigma_{s,l}$, the condensation presented here is thus not applicable to pure scattering regions, even if the primal system matrix itself is not singular.

Similarly, in the dual system (3.33), if $\sigma_l \neq \sigma_{s,l}$ for all l ⁹, one can eliminate φ^+ to obtain $\varphi^+ = D^{-1}B^T\varphi^- + D^{-1}Q$ and

$$\begin{pmatrix} A + BD^{-1}B^T & C \\ C^T & -L_{bc} \end{pmatrix} \begin{pmatrix} \varphi^- \\ \psi \end{pmatrix} = \begin{pmatrix} -BD^{-1}Q \\ 0 \end{pmatrix}.$$

We can then further eliminate the odd-parity flux by writing

$$\varphi^- = (A + BD^{-1}B^T)^{-1}(-C\psi - BD^{-1}Q)$$

to yield

$$H\psi = F, \tag{3.35}$$

⁹otherwise D is not invertible

where

$$\begin{aligned} H &= C^T(A + BD^{-1}B^T)^{-1}C + L_{bc} \quad \text{and} \\ F &= -C^T(A + BD^{-1}B^T)^{-1}BD^{-1}Q. \end{aligned}$$

In both primal and dual cases with $\sigma_l \neq \sigma_{s,l}$ for all l , the fact that A and D are symmetric positive definite (SPD) makes $C^T(A + BD^{-1}B^T)^{-1}C$ a SPD matrix as well. Since the non-zero elements of L_{bc} come from the SPD blocks \underline{L}^p or d , both primal and dual H matrices are SPD. The condensed systems (3.34) and (3.35) are much smaller than the indefinite systems (3.30) and (3.33). Many preconditioned iterative techniques are available to solve SPD systems, and are thus applicable to our condensed systems. These yield the interface unknowns, and, from them, both odd- and even- parity fluxes can be re-constructed within each element as required.

Working with the Poisson equation, Arnold and Brezzi (1985) and Brezzi, Douglas, and Marini (1985) argued that, when used with a condensation approach, the mixed-hybrid method can be seen as an improved mixed method, in that it results in SPD matrix systems of reduced size. This idea was also developed in Brezzi and Fortin (1991, V.1), Quarteroni and Valli (1994, 7.3), Coulomb and Fedon-Magnaud (1988) and Roberts and Thomas (1991, IV, 17.5), all of them for the diffusion (or Poisson)

equation. Our discussion above thus shows that condensed mixed-hybrid methods lead to SPD matrix systems of reduced size in the transport case as well.

We did not develop a purely mixed method in the transport case, thus we cannot make a fair comparison between mixed and mixed-hybrid methods. However, one can readily notice that the size of the condensed mixed-hybrid systems is smaller than the size of the system that would arise from a purely mixed formulation (with only internal unknowns). This is true even if the purely mixed system is condensed (keeping only even- or odd-parity internal fluxes), since the rank condition imposes the polynomial expansion order to be less for the interface variable than for any internal variable.

Nevertheless, computing the H matrix in the condensation approach can be expensive. In fact, a condensation approach is not necessarily the fastest way to solve generalized saddle-point systems, and should be compared with preconditioned iterative techniques performed on the system as a whole (Little, Saad, and Smoch (2003)). Such comparisons, however, are beyond the scope of this thesis. They should be the subject of future investigations.

Since it is relevant to future investigations, let us mention that de Oliveira, Pain, and Eaton (2000) developed a hierarchical angular preconditioner for the EVENT code (de Oliveira 1986), based on multi-level cycles and using the P_1 approximation

as the coarsest level. Such an approach might also be applicable to the mixed-hybrid method, and we could additionally use the even-order P_N approximations together with the odd-order ones in the level definitions.

Note also that the knowledge of the interface unknown could possibly be used to produce a more accurate secondary unknown. Indeed, such a process has been investigated for the mixed-hybrid dual formulation of the Poisson equation in Arnold and Brezzi (1985) (see also Brezzi and Fortin (1991, V.3)).

Finally, a response matrix formalism such as the one used in the VARIANT code (Palmiotti, Lewis, and Carrico 1995) can be retrieved from (3.30). In fact, such a formalism can be given to any discretized hybrid or mixed-hybrid system. In the primal case, extracting φ^- in terms of φ^+ , and expressing φ^+ in terms of the even-parity interface unknown coefficients ψ_i using (3.25), yields a system in both interface coefficients ψ and χ . Hence, a response matrix formalism is obtained introducing the partial currents j^\pm defined in terms of the interface even- and odd-parity flux according to

$$j^\pm = \frac{1}{4}\psi \pm \frac{1}{2}\chi. \quad (3.36)$$

These currents are then interpreted as in- and out-going currents in each element (or node, or cell), and a response matrix determines for each of them the relationship between in- and out-going currents. In the response matrix taxonomy of Lindhal and

Weiss (1981), the primal formulation corresponds to a Neumann or T^{-1} formulation, while the dual one corresponds to a Dirichlet or T formulation. The response matrix formulation has been proved appropriate for parallelization (Hanebutte and Lewis 1992). Nevertheless, the j^\pm correspond to the actual in- and out-going currents only in the diffusion approximation (Duderstadt and Hamilton 1976, p 143), but not in the transport approximation. The definitions (3.36) then appear merely as a change of unknown (that can be optimized as shown in Lewis and Palmiotti (1998)). From the computed j^\pm , interface flux and currents are then reconstructed. Our approach is more direct than this formalism. The change of unknown (3.36) makes it more difficult to examine the properties of the resulting matrix system. The response matrix formalism might thus not be the best option if a new code is to be written.

3.5.4 Numerical results

We performed tests on two shielding problems, namely the Azmy (1987) and the Iron-Water (Khalil 1985) benchmark problems.

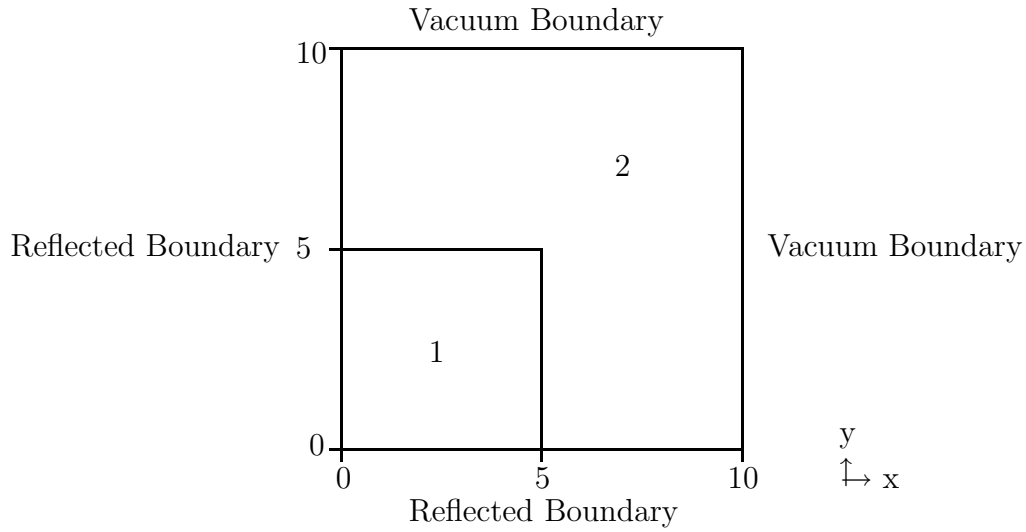
Both these tests are two-dimensional. In fact, one looks at what happens in a plane (azimuthal angle $\phi = 0$), and assumes symmetry with respect to this plane. This corresponds to considering an horizontal “slice” in a nuclear system of infinite height. We then keep only the functions even in ϕ in our angular expansions. In terms

of spherical harmonics, this implies to keep the cosine series ($m \geq 0$) and delete the sine series ($m < 0$) in the expansion vectors y_{\pm} and y_{χ} or ψ .

To highlight the effects of the different P_N approximations, results presented here were obtained with fixed spatial polynomial expansion order. As stated earlier, sixth order polynomial expansions are used inside each V_l for the principal variable, and fifth order expansions for the secondary variable. On interfaces, second order polynomial expansions are used. Since the flux is derived from Ψ^+ and the current from Ψ^- , the actual spatial expansion order is thus 6 for the primal flux and the dual current, while it is 5 for the primal current and the dual flux.

Azmy benchmark

The Azmy benchmark problem (Azmy 1987) is based on a “square in a square” geometry displayed on figure 3.1: a 10-by-10 square, whose bottom left quarter (zone 1) has a constant non-zero source and whose three other quarters (zone 2) are source-free. The boundary conditions are reflected on the bottom and left edges, and vacuum on the right and top edges. We use this benchmark to check our results comparing them with the VARIANT code (Palmiotti, Lewis, and Carrico 1995). VARIANT uses a primal (non-mixed) hybrid formulation with odd-order P_N approximations. A severe test is obtained with plots close to the vacuum boundary. Figures 3.2 and 3.3



| zone | σ | σ_s | s |
|------|----------|------------|-----|
| 1 | 1 | 0.5 | 1 |
| 2 | 2 | 0.1 | 0 |

Figure 3.1: Azmy benchmark geometry and data ($\sigma_{(s)}$ per unit length, s per unit volume).

respectively display the mixed-hybrid primal and dual flux along the line $y = 9.84375$, together with the (primal) VARIANT results. A 32×32 grid was used to minimize the effects of spatial truncation. For the odd-order P_N approximations, the match is acceptable globally between mixed-hybrid and VARIANT results, although P_5 results appear to be quite far apart. Also, P_5 primal and dual mixed-hybrid results do not match very closely. This is due to the results being highly sensitive to the vacuum boundary treatment. Indeed, we checked that the primal and dual mixed-hybrid

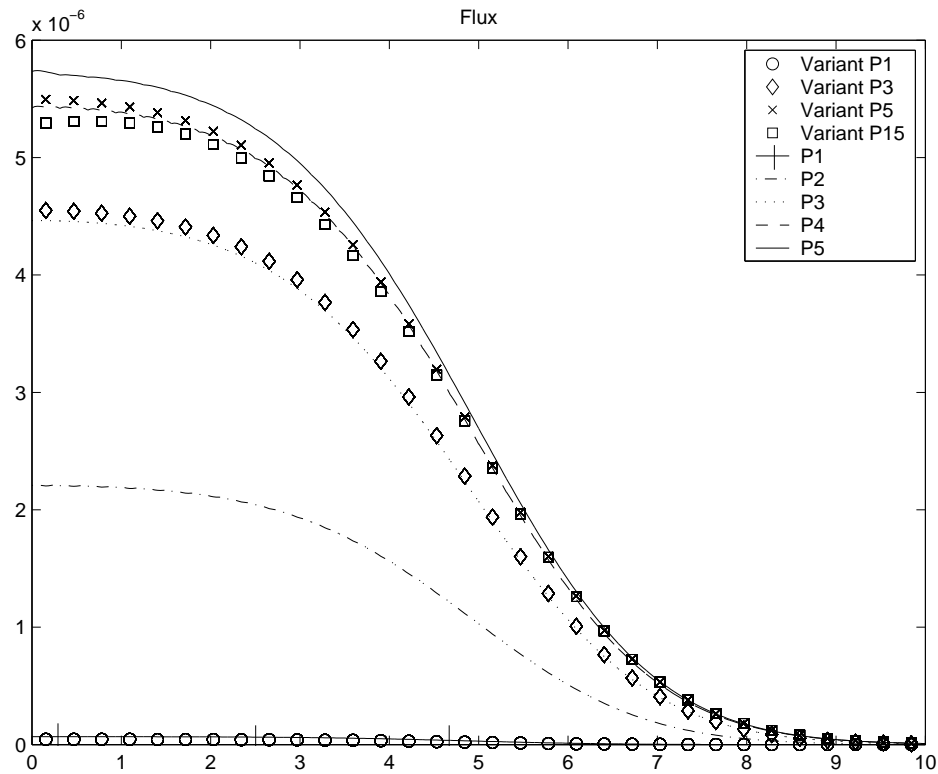


Figure 3.2: Mixed-hybrid primal and VARIANT flux along $y = 9.84375$ for the Azmy benchmark.

results come closer together further away from the vacuum boundary, i.e., they become undistinguishable for $y \approx 9$ and smaller. Moreover, we performed tests adding a layer of pure absorber around the vacuum boundary. The resulting primal and dual plots are labeled “P5+” on figures 3.4 and 3.5, respectively. We see that the P5+ primal and dual results nearly superimpose while closely matching the P15 VARIANT solution. Further research is needed to establish a more accurate vacuum boundary

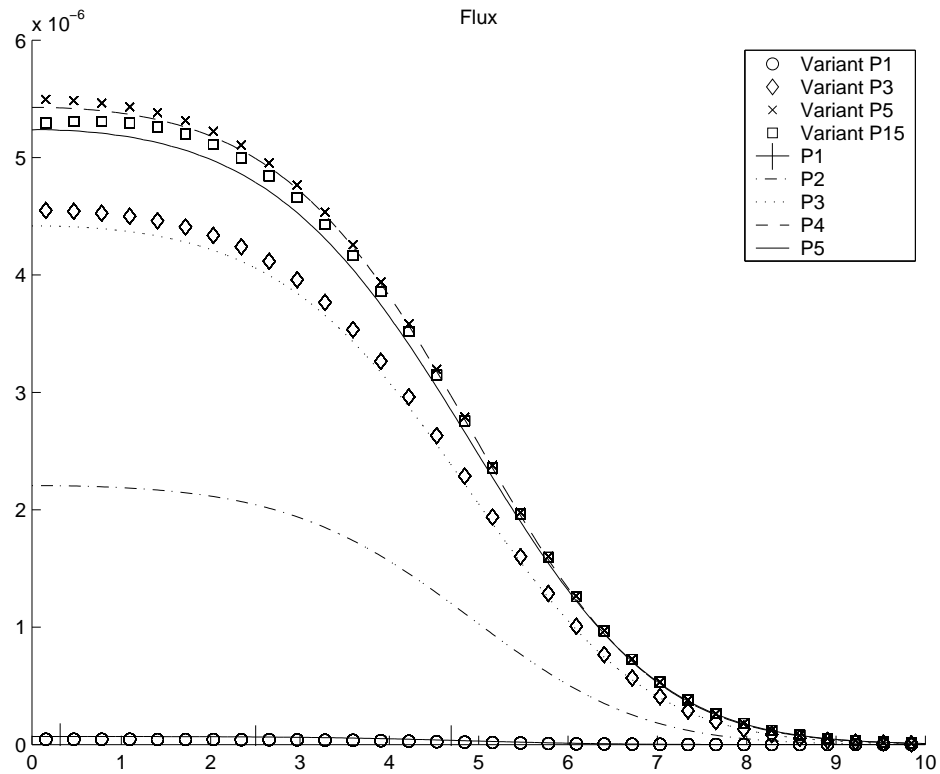


Figure 3.3: Mixed-hybrid dual and (primal) VARIANT flux along $y = 9.84375$ for the Azmy benchmark.

treatment, i.e., a treatment that matches more closely the pure absorber behavior for P_5 (and possibly higher order) approximations. Finally, obtaining a converged scalar flux value for x close to zero would require using higher order spherical harmonics approximations.

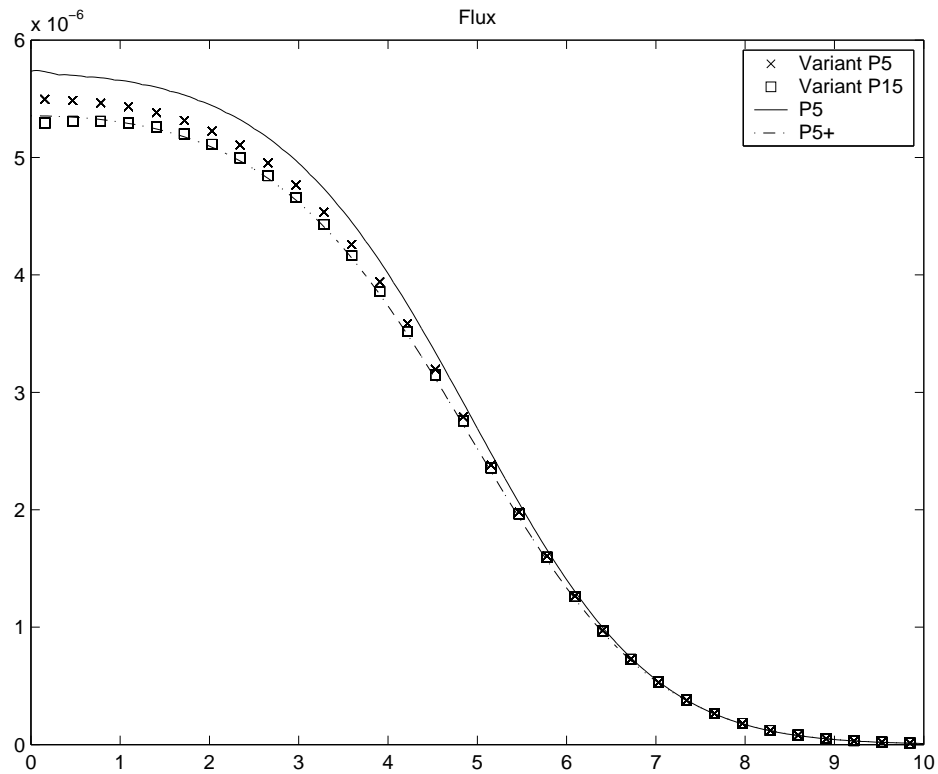


Figure 3.4: Mixed-hybrid primal P5 results along $y = 9.84375$, results obtained using a layer of pure absorber around the vacuum boundary (P5+), and VARIANT results for the Azmy benchmark.

Iron-water benchmark

The geometry of the 2D iron-water benchmark problem Khalil (1985) is displayed on figure 3.6. Zones 1, 2 and 3 respectively correspond to water with source, water alone, and iron. A 30×30 grid was used.

The mixed-hybrid flux along $y = 29.75$ is plotted on figure 3.7 for the primal case,

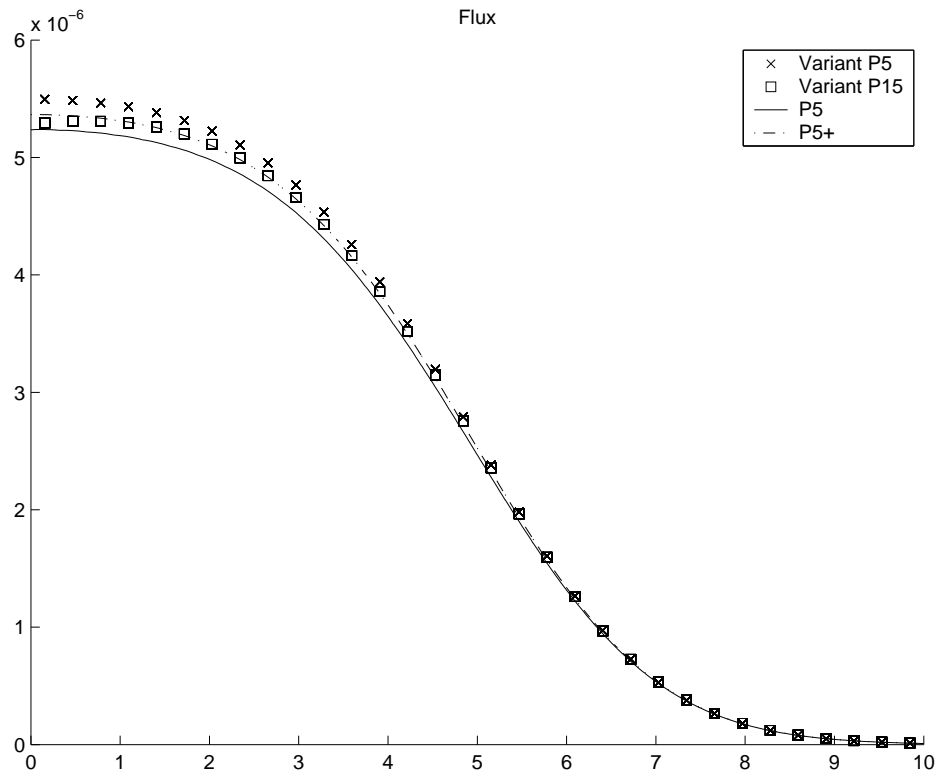
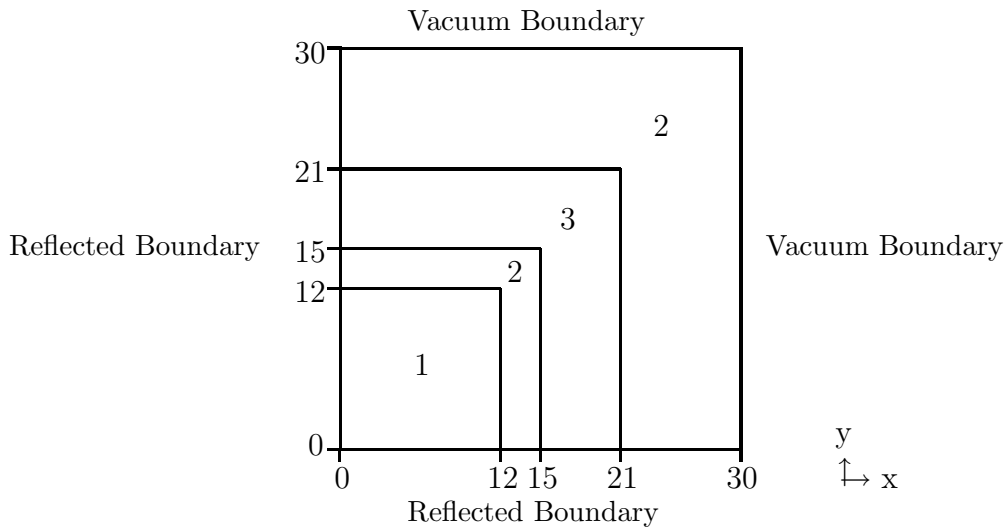


Figure 3.5: Mixed-hybrid dual P5 results along $y = 9.84375$, results obtained using a layer of pure absorber around the vacuum boundary (P5+), and VARIANT results for the Azmy benchmark.

and on figure 3.8 for the dual case. A probable cause for the wiggling visible in the dual case (zoom of figure 3.8) but not in the primal case, is the difference in actual scalar flux spatial expansion order (primal flux of the sixth order, dual flux of the fifth order). We notice in both zooms that the even-parity P_N methods approximate from above, while the odd-parity P_N methods approximate from below. Such an enclosing property appeared repeatedly in our tests, even if no strict rule could be derived. We

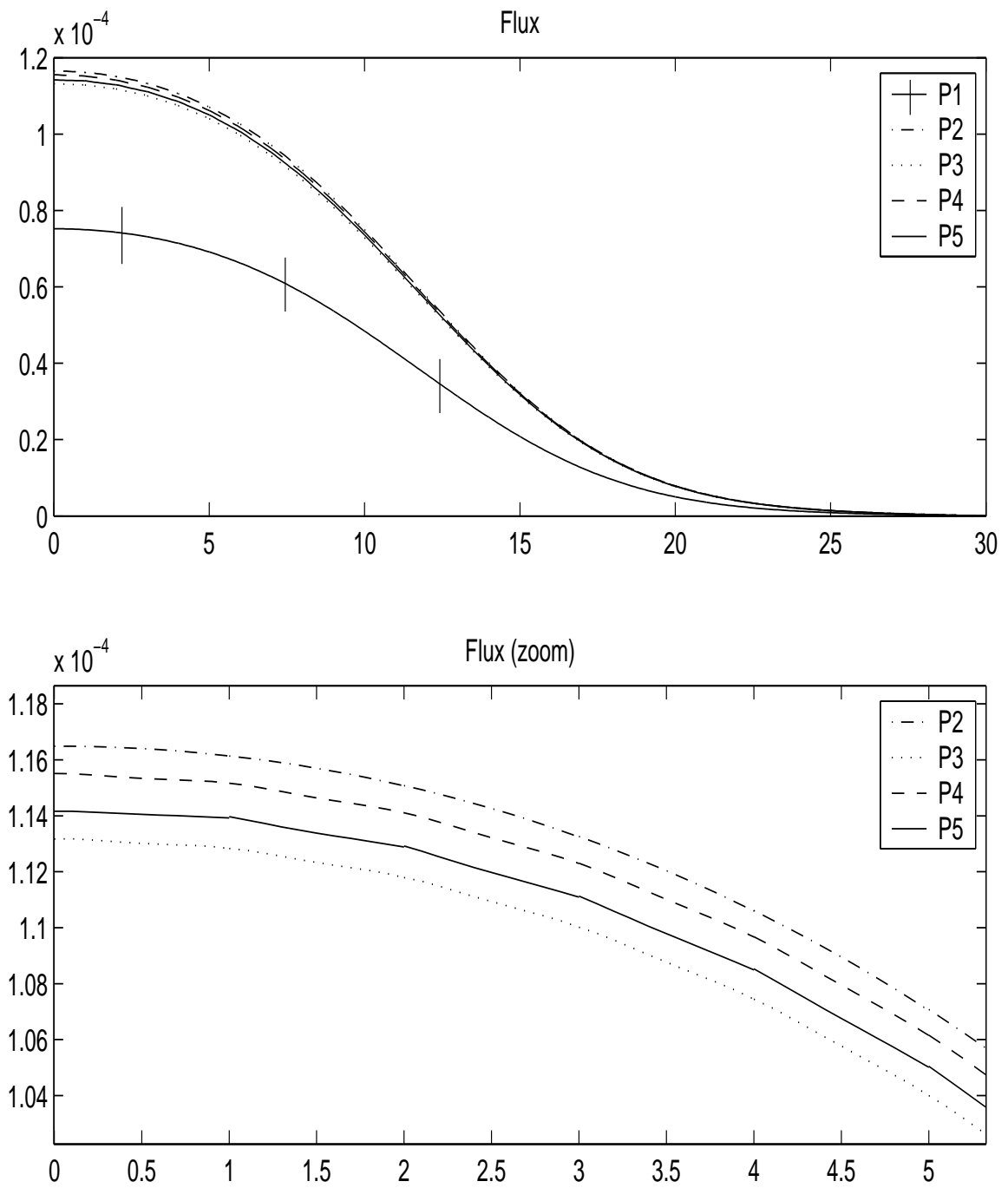


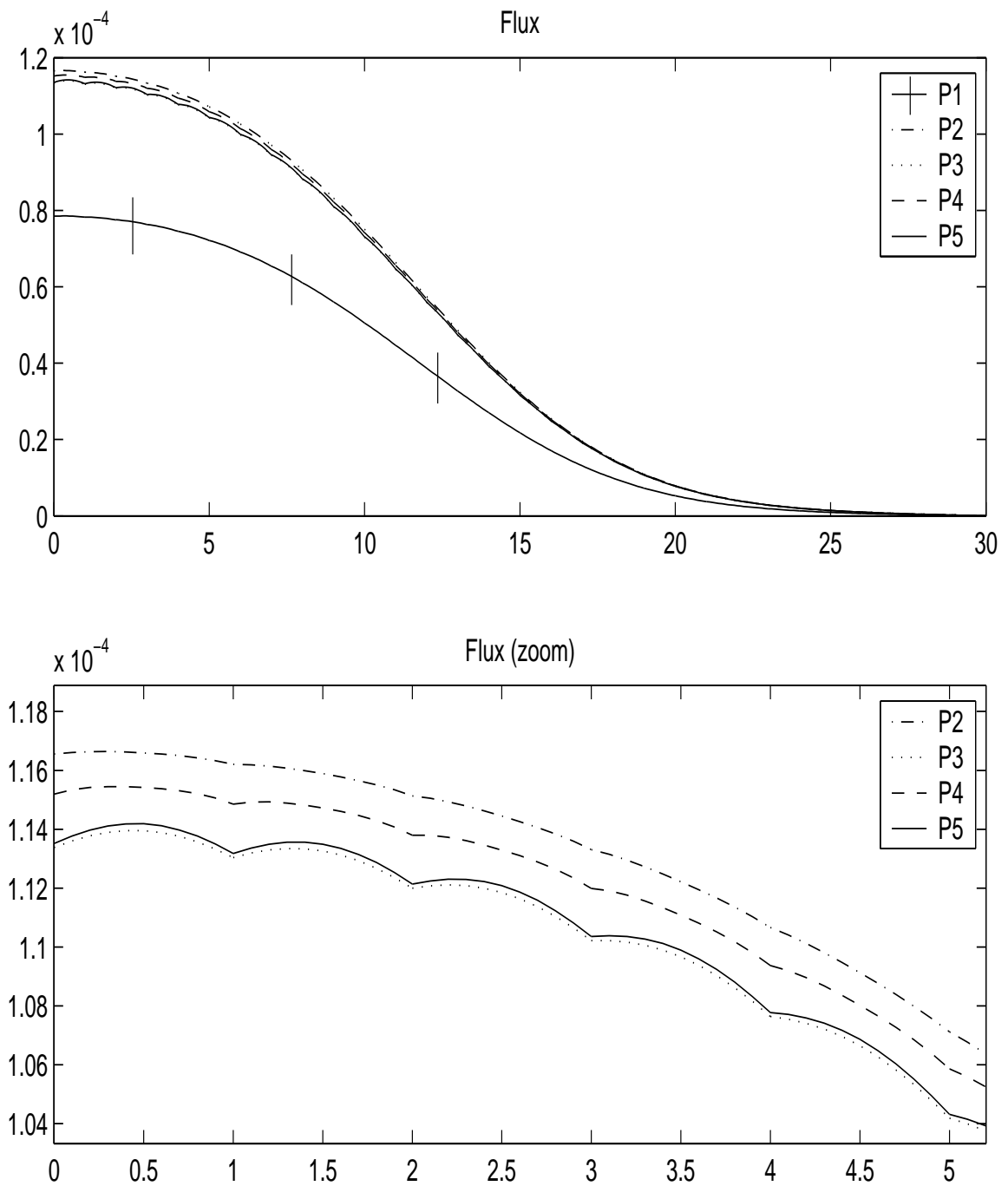
| zone | σ | σ_s | s |
|------|----------|------------|-----|
| 1 | 3.33 | 0.994 | 1 |
| 2 | 3.33 | 0.994 | 0 |
| 3 | 1.33 | 0.831 | 0 |

Figure 3.6: Iron-water benchmark geometry and data ($\sigma_{(s)}$ per unit length, s per unit volume).

verified that the Azmy benchmark also exhibits this behavior when plots for lower values of y are displayed. Other occurrences of the enclosing property follow.

To illustrate the continuity properties discussed in §3.5.2, mixed-hybrid results along $y = 7.5$ are displayed. Primal flux and currents are plotted on figure 3.9 and 3.10. We zoom on the discontinuities arising at $x = 15$ up to a scale showing the effects of limited angular expansions. Zooming in further would show the effects of limited spatial expansions. We verify on figure 3.9 that the even-order primal

Figure 3.7: Mixed-hybrid primal flux along $y = 29.75$ for the Iron-Water benchmark.

Figure 3.8: Mixed-hybrid dual flux along $y = 29.75$ for the Iron-Water benchmark.

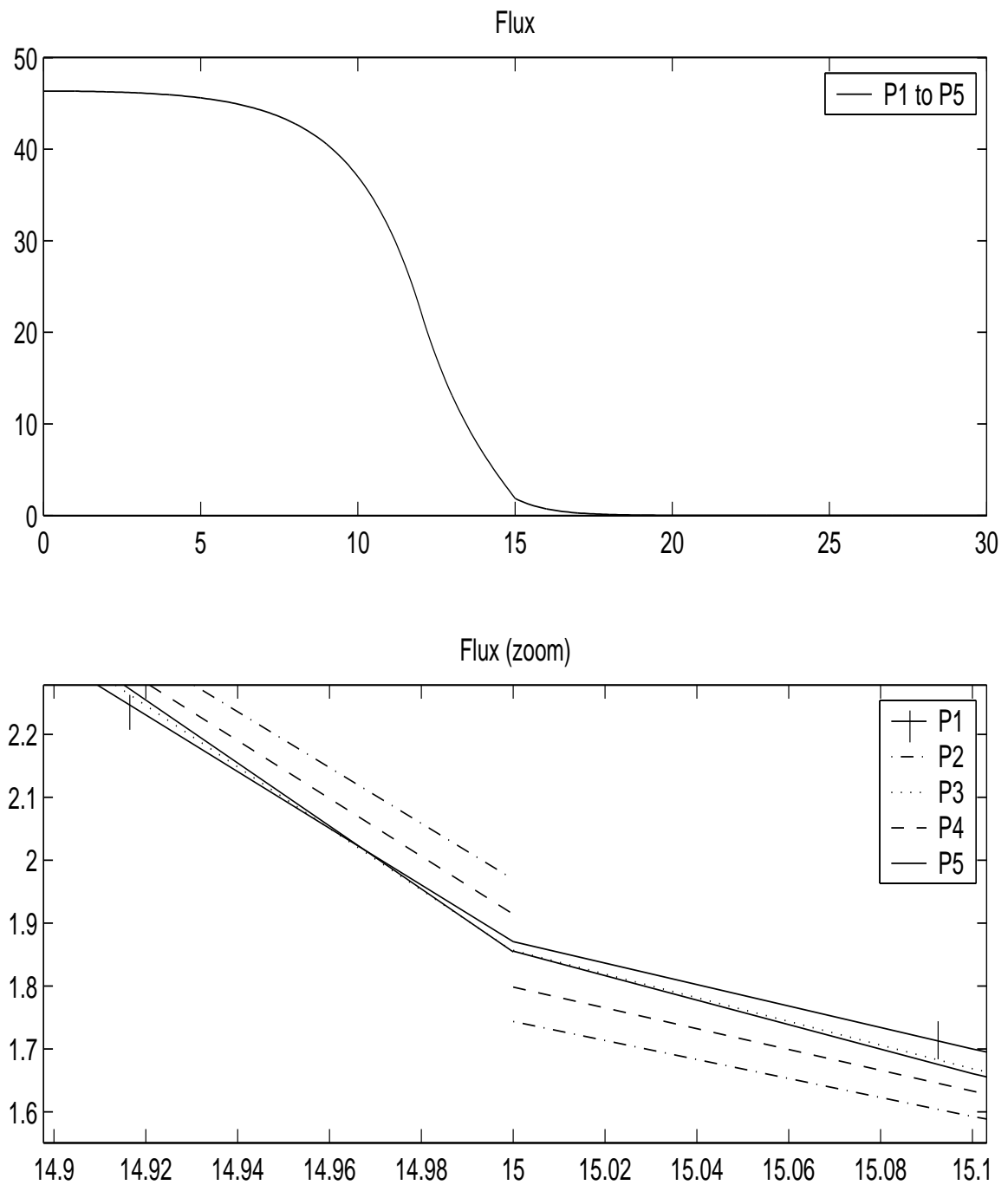


Figure 3.9: Mixed-hybrid primal flux along $y = 7.5$ for the Iron-Water benchmark. Note the discontinuity of the even-order fluxes.

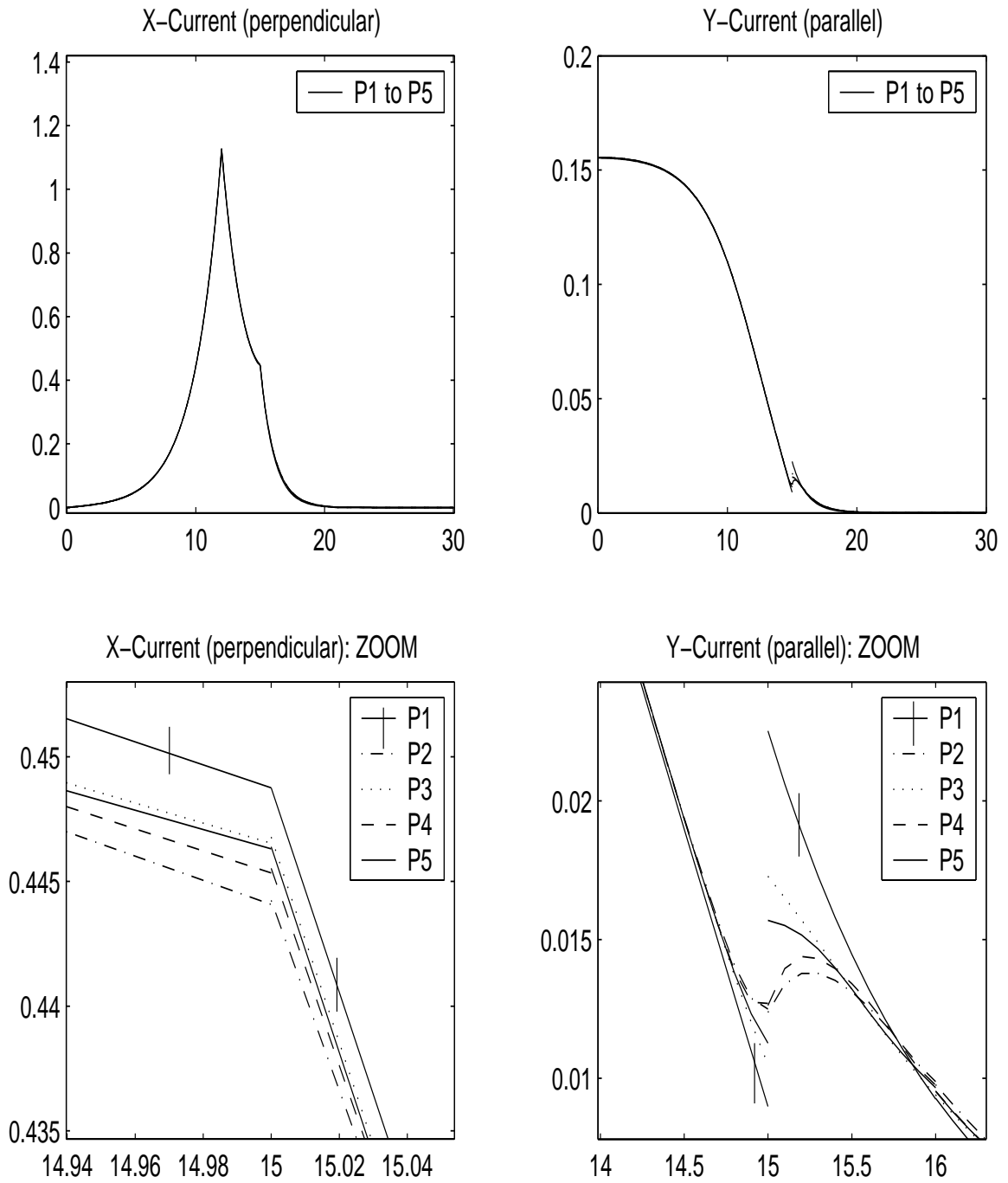


Figure 3.10: Mixed-hybrid primal X- and Y-current along $y = 7.5$ for the Iron-Water benchmark. Note the discontinuity of the odd-order Y-currents.

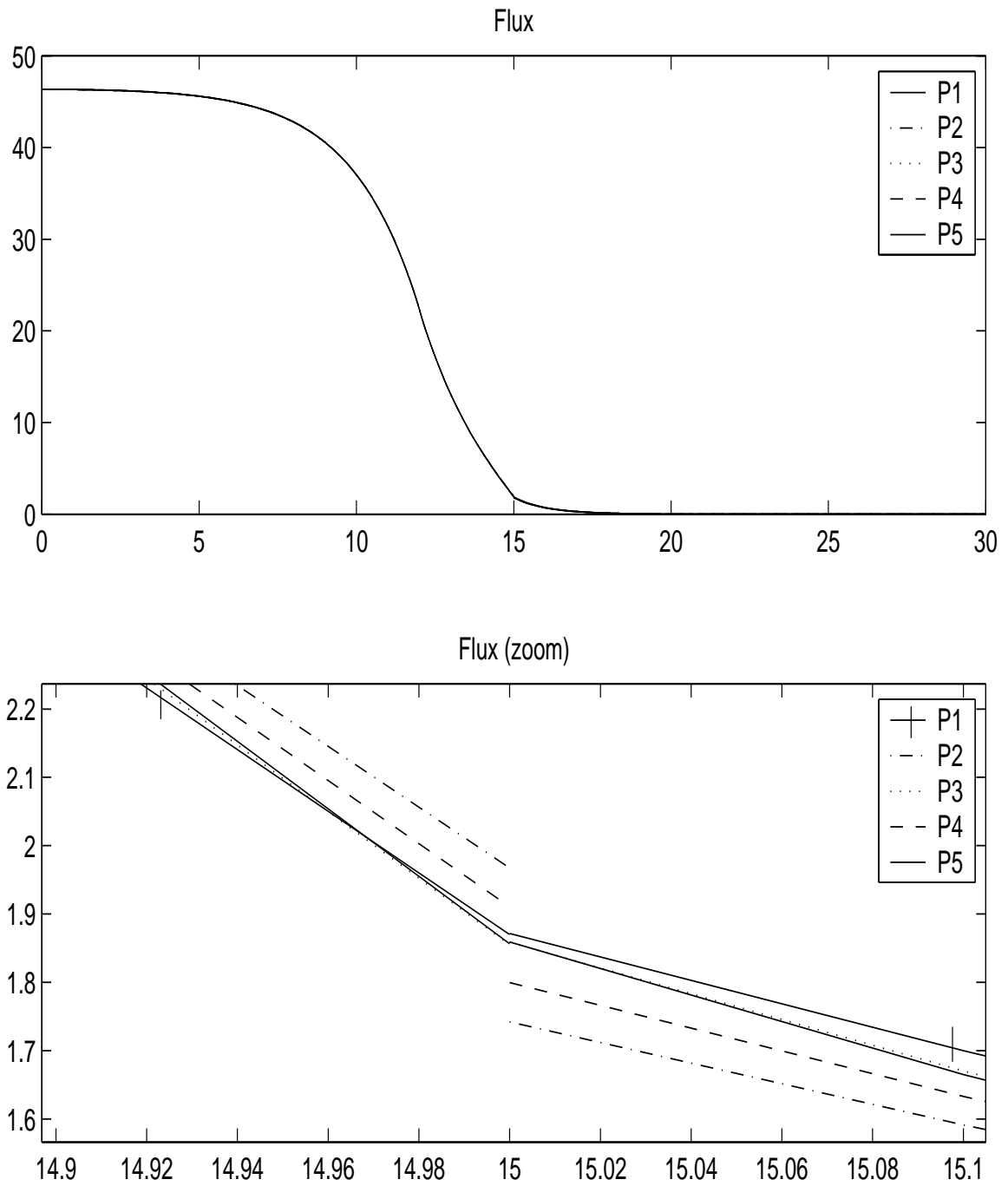


Figure 3.11: Mixed-hybrid dual flux along $y = 7.5$ for the Iron-Water benchmark. Note the discontinuity of the even-order fluxes.

methods do not ensure the continuity of the flux. Also we verify on figure 3.10 that odd-order primal methods do not ensure the continuity of the parallel current J_{\parallel} , that is here the Y-current. Note that the enclosing property is visible on these plots as well, i.e., the even-order P_N methods approximate from above when odd-order P_N methods approximate from below, and vice-versa. Dual case results exhibit the same continuity and enclosing properties. The mixed-hybrid dual flux along $y = 7.5$ is plotted on figure 3.11.

3.6 Anisotropic scattering multigroup extension

In this section, we establish the formalism necessary to extend our results to the case of anisotropic scattering and sources. Parallel treatments may be found in de Oliveira (1986) and Lewis and Miller, Jr. (1984, §2.2). We do not detail here the mathematical aspects, but provide numerical results showing the adequacy of our formalism.

3.6.1 Anisotropic multigroup P_N equations

Let us start over with the first order form of the time-independent mono-energetic transport equation (1.1)

$$\boldsymbol{\Omega} \cdot \nabla \Psi(\mathbf{r}, \boldsymbol{\Omega}) + \sigma(\mathbf{r})\Psi(\mathbf{r}, \boldsymbol{\Omega}) = \int_S \sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')\Psi(\mathbf{r}, \boldsymbol{\Omega}') d\boldsymbol{\Omega}' + s(\mathbf{r}, \boldsymbol{\Omega}) \quad (3.37)$$

where the scattering cross section $\sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')$ now depends on angle.

We expand $\sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}')$ into Legendre polynomials P_n (defined as in the appendix A of Lewis and Miller, Jr.) according to

$$\sigma_s(\mathbf{r}, \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') = \sum_{n=0}^{N^s} (2n+1) \sigma_{s,n}(\mathbf{r}) P_n(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') \quad (3.38)$$

where N^s is the maximum cross-section expansion order. Equation (3.37) then becomes

$$\begin{aligned} \boldsymbol{\Omega} \cdot \nabla \Psi(\mathbf{r}, \boldsymbol{\Omega}) + \sigma(\mathbf{r}) \Psi(\mathbf{r}, \boldsymbol{\Omega}) \\ = \sum_{n=0}^{N^s} (2n+1) \sigma_{s,n}(\mathbf{r}) \int_S \Psi(\mathbf{r}, \boldsymbol{\Omega}') P_n(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') d\boldsymbol{\Omega}' + s(\mathbf{r}, \boldsymbol{\Omega}). \end{aligned}$$

The even- and odd-parity decomposition for the angular flux (1.5) and the source

(1.6) yields the following coupled pair of first order equations

$$\begin{aligned} \boldsymbol{\Omega} \cdot \nabla \Psi^-(\mathbf{r}, \boldsymbol{\Omega}) + \sigma(\mathbf{r}) \Psi^+(\mathbf{r}, \boldsymbol{\Omega}) \\ = \sum_{n \text{ even}}^{N^s} (2n+1) \sigma_{s,n}(\mathbf{r}) \int_S \Psi^+(\mathbf{r}, \boldsymbol{\Omega}') P_n(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') d\boldsymbol{\Omega}' + s^+(\mathbf{r}, \boldsymbol{\Omega}) \end{aligned} \quad (3.39)$$

$$\begin{aligned} \boldsymbol{\Omega} \cdot \nabla \Psi^+(\mathbf{r}, \boldsymbol{\Omega}) + \sigma(\mathbf{r}) \Psi^-(\mathbf{r}, \boldsymbol{\Omega}) \\ = \sum_{n \text{ odd}}^{N^s} (2n+1) \sigma_{s,n}(\mathbf{r}) \int_S \Psi^-(\mathbf{r}, \boldsymbol{\Omega}') P_n(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') d\boldsymbol{\Omega}' + s^-(\mathbf{r}, \boldsymbol{\Omega}). \end{aligned} \quad (3.40)$$

In a multi-group context with G energy groups, we obtain for $g = 1 \dots G$

$$\begin{aligned} \boldsymbol{\Omega} \cdot \nabla \Psi_g^-(\mathbf{r}, \boldsymbol{\Omega}) + \sigma^g(\mathbf{r}) \Psi_g^+(\mathbf{r}, \boldsymbol{\Omega}) \\ = \sum_{n \text{ even}}^{N^s} (2n+1) \sigma_{s,n}^{gg}(\mathbf{r}) \int_S \Psi_g^+(\mathbf{r}, \boldsymbol{\Omega}') P_n(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') d\boldsymbol{\Omega}' + s_g^+(\mathbf{r}, \boldsymbol{\Omega}) \end{aligned}$$

$$\begin{aligned} \boldsymbol{\Omega} \cdot \nabla \Psi_g^+(\mathbf{r}, \boldsymbol{\Omega}) + \sigma^g(\mathbf{r}) \Psi_g^-(\mathbf{r}, \boldsymbol{\Omega}) \\ = \sum_{n \text{ odd}}^{N^s} (2n+1) \sigma_{s,n}^{gg}(\mathbf{r}) \int_S \Psi_g^-(\mathbf{r}, \boldsymbol{\Omega}') P_n(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') d\boldsymbol{\Omega}' + s_g^-(\mathbf{r}, \boldsymbol{\Omega}) \end{aligned}$$

where $\sigma^g(\mathbf{r})$ and $\sigma_{s,n}^{gg}(\mathbf{r})$ are the total and scattering cross-section within group g , and

where the source terms for the group g are

$$\begin{aligned}
s_g^+(\mathbf{r}, \boldsymbol{\Omega}) &= Q_g^+(\mathbf{r}, \boldsymbol{\Omega}) + \chi_g \sum_{g'=1}^G \nu \sigma_{f,g'}(\mathbf{r}) \int_S \Psi_{g'}^+(\mathbf{r}, \boldsymbol{\Omega}') d\boldsymbol{\Omega}' \\
&\quad + \sum_{\substack{g'=1 \\ g' \neq g}}^G \sum_{\substack{n \text{ even} \\ n \leq N^s}} (2n+1) \sigma_{s,n}^{g'g}(\mathbf{r}) \int_S P_n(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') \Psi_{g'}^+(\mathbf{r}, \boldsymbol{\Omega}') d\boldsymbol{\Omega}' \\
s_g^-(\mathbf{r}, \boldsymbol{\Omega}) &= Q_g^-(\mathbf{r}, \boldsymbol{\Omega}) \\
&\quad + \sum_{\substack{g'=1 \\ g' \neq g}}^G \sum_{\substack{n \text{ odd} \\ n \leq N^s}} (2n+1) \sigma_{s,n}^{g'g}(\mathbf{r}) \int_S P_n(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}') \Psi_{g'}^-(\mathbf{r}, \boldsymbol{\Omega}') d\boldsymbol{\Omega}'
\end{aligned}$$

with $\sigma_{s,n}^{g'g}(\mathbf{r})$ the scattering from group g' to group g , χ_g the fission spectrum (probability that a fission neutron be produced with an energy corresponding to group g), $\nu \sigma_{f,g'}(\mathbf{r})$ the mean number of fission neutrons produced by a neutron in group g' times the corresponding fission cross-section, and Q_g^\pm the even/odd part of a prescribed external source.

3.6.2 Continuous mixed-hybrid weak forms

We develop the mixed-hybrid methods for the within-group equation without the group indices, for simplicity. We multiply the equations (3.39) and (3.40) by test functions $\tilde{\Psi}^+(\mathbf{r}, \boldsymbol{\Omega})$ and $\tilde{\Psi}^-(\mathbf{r}, \boldsymbol{\Omega})$ respectively, integrate over space and angle, and

obtain:

$$\begin{aligned} \int_S d\Omega \int_V dV \tilde{\Psi}^+ \left(\boldsymbol{\Omega} \cdot \nabla \Psi^- + \sigma \Psi^+ - \sum_{n \text{ even}}^{N^s} (2n+1) \sigma_{s,n} \int_S \Psi^+ P_n d\Omega' \right) \\ = \int_S d\Omega \int_V dV s^+ \tilde{\Psi}^+ \end{aligned} \quad (3.41)$$

$$\begin{aligned} \int_S d\Omega \int_V dV \tilde{\Psi}^- \left(\boldsymbol{\Omega} \cdot \nabla \Psi^+ + \sigma \Psi^- - \sum_{n \text{ odd}}^{N^s} (2n+1) \sigma_{s,n} \int_S \Psi^- P_n d\Omega' \right) \\ = \int_S d\Omega \int_V dV s^- \tilde{\Psi}^-, \end{aligned} \quad (3.42)$$

where spatial and angular dependences were omitted for brevity. Integrating by parts the first and second equations yields respectively

$$\begin{aligned} - \int_S d\Omega \int_V dV \boldsymbol{\Omega} \cdot \nabla \tilde{\Psi}^+ \Psi^- + \int_S d\Omega \int_{\partial V} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}^+ \Psi^- \\ + \int_S d\Omega \int_V dV \tilde{\Psi}^+ \left(\sigma \Psi^+ - \sum_{n \text{ even}}^{N^s} (2n+1) \sigma_{s,n} \int_S \Psi^+ P_n d\Omega' \right) \\ = \int_S d\Omega \int_V dV s^+ \tilde{\Psi}^+, \quad \text{and} \end{aligned} \quad (3.43)$$

$$\begin{aligned}
& - \int_S d\Omega \int_V dV \boldsymbol{\Omega} \cdot \nabla \tilde{\Psi}^- \Psi^+ + \int_S d\Omega \int_{\partial V} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}^- \Psi^+ \\
& + \int_S d\Omega \int_V dV \tilde{\Psi}^- \left(\sigma \Psi^- - \sum_{n \text{ odd}}^{N^s} (2n+1) \sigma_{s,n} \int_S \Psi^- P_n d\Omega' \right) \\
& = \int_S d\Omega \int_V dV s^- \tilde{\Psi}^-.
\end{aligned} \tag{3.44}$$

As in the isotropic case, we now introduce the notations $\Psi_l^\psi(\boldsymbol{\Omega}, \mathbf{r})$ and $\Psi_l^\chi(\boldsymbol{\Omega}, \mathbf{r})$ to represent the traces on ∂V_l of Ψ_l^+ and Ψ_l^- , respectively. To obtain the weak form equations, we sum up the appropriate equations ((3.42) and (3.43) for primal, (3.41) and (3.44) for dual) on each element V_l and add a third equation to restore the continuity of Ψ^\pm . For the mixed-hybrid primal formulation, we obtain, using a subscript l to denote restrictions to $S \times V_l$, the following weak form equations:

$$\left\{ \begin{aligned}
& - \sum_l \left\{ \int_S d\Omega \int_{V_l} dV \boldsymbol{\Omega} \cdot \nabla \tilde{\Psi}_l^+ \Psi_l^- + \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}_l^+ \Psi_l^\chi \right. \\
& \quad \left. + \int_S d\Omega \int_{V_l} dV \tilde{\Psi}_l^+ \left(\sigma_l \Psi_l^+ - \sum_{n \text{ even}}^{n \leq N^s} (2n+1) \sigma_{s,n,l} \int_S \Psi_l^+ P_n d\Omega' \right) \right\} \\
& = \sum_l \int_S d\Omega \int_{V_l} dV s_l^+ \tilde{\Psi}_l^+ \\
& \sum_l \int_S d\Omega \int_{V_l} dV \tilde{\Psi}_l^- \left(\boldsymbol{\Omega} \cdot \nabla \Psi_l^+ + \sigma_l \Psi_l^- - \sum_{n \text{ odd}}^{n \leq N^s} (2n+1) \sigma_{s,n,l} \int_S \Psi_l^- P_n d\Omega' \right) \\
& = \sum_l \int_S d\Omega \int_{V_l} dV s_l^- \tilde{\Psi}_l^- \\
& \sum_l \int_S d\Omega \int_{\partial V_l - \partial V} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}_l^\chi \Psi_l^+ = 0.
\end{aligned} \right. \tag{3.45}$$

For the mixed-hybrid dual formulation, we get the equations

$$\left\{ \begin{aligned}
 & \sum_l \int_S d\Omega \int_{V_l} dV \tilde{\Psi}_l^+ \left(\mathbf{\Omega} \cdot \nabla \Psi_l^- + \sigma_l \Psi_l^+ - \sum_{n \text{ even}}^{n \leq N^s} (2n+1) \sigma_{s,n,l} \int_S \Psi_l^+ P_n d\Omega' \right) \\
 & \quad = \sum_l \int_S d\Omega \int_V dV s_l^+ \tilde{\Psi}_l^+ \\
 & - \sum_l \left\{ \int_S d\Omega \int_{V_l} dV \mathbf{\Omega} \cdot \nabla \tilde{\Psi}_l^- \Psi_l^+ + \int_S d\Omega \int_{\partial V_l} d\Gamma \mathbf{\Omega} \cdot \mathbf{n} \tilde{\Psi}_l^- \Psi_l^\psi \right. \\
 & \quad \left. + \int_S d\Omega \int_{V_l} dV \tilde{\Psi}_l^- (\sigma_l \Psi_l^- - \sum_{n \text{ odd}}^{n \leq N^s} (2n+1) \sigma_{s,n,l} \int_S \Psi_l^- P_n d\Omega') \right\} \\
 & \quad = \sum_l \int_S d\Omega \int_{V_l} dV s_l^- \tilde{\Psi}_l^- \\
 & \sum_l \int_S d\Omega \int_{\partial V_l - \partial V} d\Gamma \mathbf{\Omega} \cdot \mathbf{n} \tilde{\Psi}_l^\psi \Psi_l^- = 0.
 \end{aligned} \right. \tag{3.46}$$

3.6.3 Discrete mixed-hybrid weak forms

As in the isotropic case, we now insert the expansions (3.19) and (3.20) into (3.45) and (3.46). For consistency, we chose the angular P_N expansion order $N \geq N^s$, where N^s is the maximum anisotropic cross-section expansion order. Also, N must not be smaller than the maximum external source ($Q_g^\pm(\mathbf{r}, \mathbf{\Omega})$) expansion order. We need to

pay special attention to the term

$$\int_S d\Omega \tilde{\Psi}_l^\pm(\mathbf{r}, \Omega) \sum_{n \text{ even/odd}}^{N^s} (2n+1) \sigma_{s,n} \int_S d\Omega' \Psi_l^\pm(\mathbf{r}, \Omega') P_n(\Omega \cdot \Omega'). \quad (3.47)$$

With our conventions, the addition theorem for spherical harmonics states

$$P_n(\Omega \cdot \Omega') = \frac{1}{2n+1} \sum_{m=-n}^n Y_{nm}(\Omega) Y_{nm}(\Omega')$$

such that (3.47) becomes

$$\sum_{n \text{ even/odd}}^{N^s} \sigma_{s,n} \sum_{m=-n}^n \left(\int_S d\Omega \tilde{\Psi}_l^\pm(\mathbf{r}, \Omega) Y_{nm}(\Omega) \right) \left(\int_S d\Omega' \Psi_l^\pm(\mathbf{r}, \Omega') Y_{nm}(\Omega') \right).$$

On top of the matrices defined in the isotropic case (§3.5.1), we furthermore define

$$\begin{aligned} Z_{nm,l}^\pm &= \int_S d\Omega y_{\pm,l} Y_{nm}, & \text{and} \\ S_l^\pm &= \int_{V_i} dV (y_{\pm,l} \otimes f_{\pm,l}) s_l^\pm(\mathbf{r}, \Omega). \end{aligned}$$

Applying (3.45) and (3.46), and using the orthonormality of the spherical harmonics, we obtain for the discretized weak form in the primal case

$$\left\{ \begin{array}{l}
\left(I_{+,l} \otimes N_{\sigma,l}^+ - \sum_{n \text{ even}}^{n \leq N^s} \sum_{m=-n}^n Z_{nm,l}^+ Z_{nm,l}^{+T} \otimes N_{\sigma_s,n,l}^+ \right) \varphi_l^+ \\
\quad - (\mathbf{E}_l \otimes \cdot \mathbf{K}_l^p) \varphi_l^- + (EM_l^p) \chi_l = S_l^+ \\
\left(I_{-,l} \otimes N_{\sigma,l}^- - \sum_{n \text{ odd}}^{n \leq N^s} \sum_{m=-n}^n Z_{nm,l}^- Z_{nm,l}^{-T} \otimes N_{\sigma_s,n,l}^- \right) \varphi_l^- \\
\quad + (\mathbf{E}_l^T \otimes \cdot \mathbf{K}_l^{pT}) \varphi_l^+ = S_l^- \\
(EM_{0,i}^p)^T \varphi_l^+ + (EM_{0,i}^{p'})^T \varphi_{l'}^+ = 0,
\end{array} \right. \quad (3.48)$$

and in the dual case:

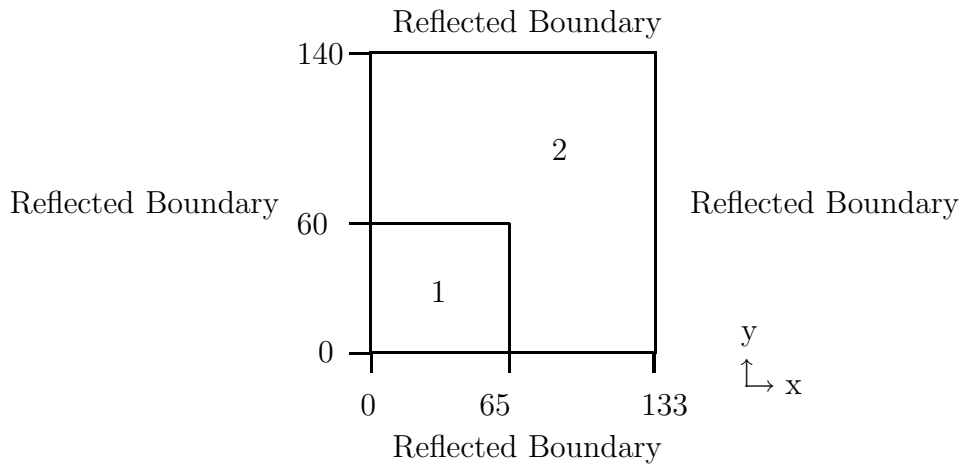
$$\left\{ \begin{array}{l}
\left(I_{+,l} \otimes N_{\sigma,l}^+ - \sum_{n \text{ even}}^{n \leq N^s} \sum_{m=-n}^n Z_{nm,l}^+ Z_{nm,l}^{+T} \otimes N_{\sigma_s,n,l}^+ \right) \varphi_l^+ \\
\quad + (\mathbf{E}_l \otimes \cdot \mathbf{K}_l^{dT}) \varphi_l^- = S_l^+ \\
\left(I_{-,l} \otimes N_{\sigma,l}^- - \sum_{n \text{ odd}}^{n \leq N^s} \sum_{m=-n}^n Z_{nm,l}^- Z_{nm,l}^{-T} \otimes N_{\sigma_s,n,l}^- \right) \varphi_l^- \\
\quad - (\mathbf{E}_l^T \otimes \cdot \mathbf{K}_l^d) \varphi_l^+ + (EM_l^d) \psi_l = S_l^- \\
(EM_{0,i}^d)^T \varphi_l^- + (EM_{0,i}^{d'})^T \varphi_{l'}^- = 0.
\end{array} \right. \quad (3.49)$$

Note that for $N^s = 0$, we re-obtain the isotropic weak forms since $Z_{00,l}^+ = P_l$.

Equations (3.48) and (3.49) are the anisotropic counterparts of isotropic equations (3.23) and (3.24). From there, the assembly parallels the treatment in §3.5.3.

3.6.4 Numerical results

We consider a shielding problem out of the Argonne Benchmark book (Argonne National Laboratory (1972, Problem 5-A2) ; also in de Oliveira (1986, 8.2)) with 2 groups, linear anisotropic scattering, and again a “square in a square” x-y geometry (see figure 3.12). We consider only the fast group here. The boundary conditions are all reflected.



| zone | σ | $\sigma_{s,0}$ | $\sigma_{s,1}$ | s |
|------|----------|----------------|----------------|----------|
| 1 | 0.10108 | 0.015923 | 0.008976 | 0.006546 |
| 2 | 0.10108 | 0.015923 | 0.008976 | 0 |

Figure 3.12: ANL benchmark geometry and data for the fast group ($\sigma_{(s)}$ per unit length, s per unit volume).

Figure 3.13 displays the primal flux for the fast group along the line $y = 80$, together with the reference solution in the Argonne Benchmark Book. The match is fine between the reference solution and the mixed-hybrid primal results. Again the enclosing property is visible.

The $P4$ results on figure 3.13 present some wiggling, that in fact get more pronounced when plotting the flux for y closer to 140. Further investigations (e.g. tests on other benchmarks) would be needed to understand this behavior. Nevertheless, results for $P1$, $P2$, $P3$, and $P5$ remain correct and properly match the reference solution along $y = 139$ and $y = 140$, just as it does along $y = 80$. The adequacy of the formalism is thus proved.

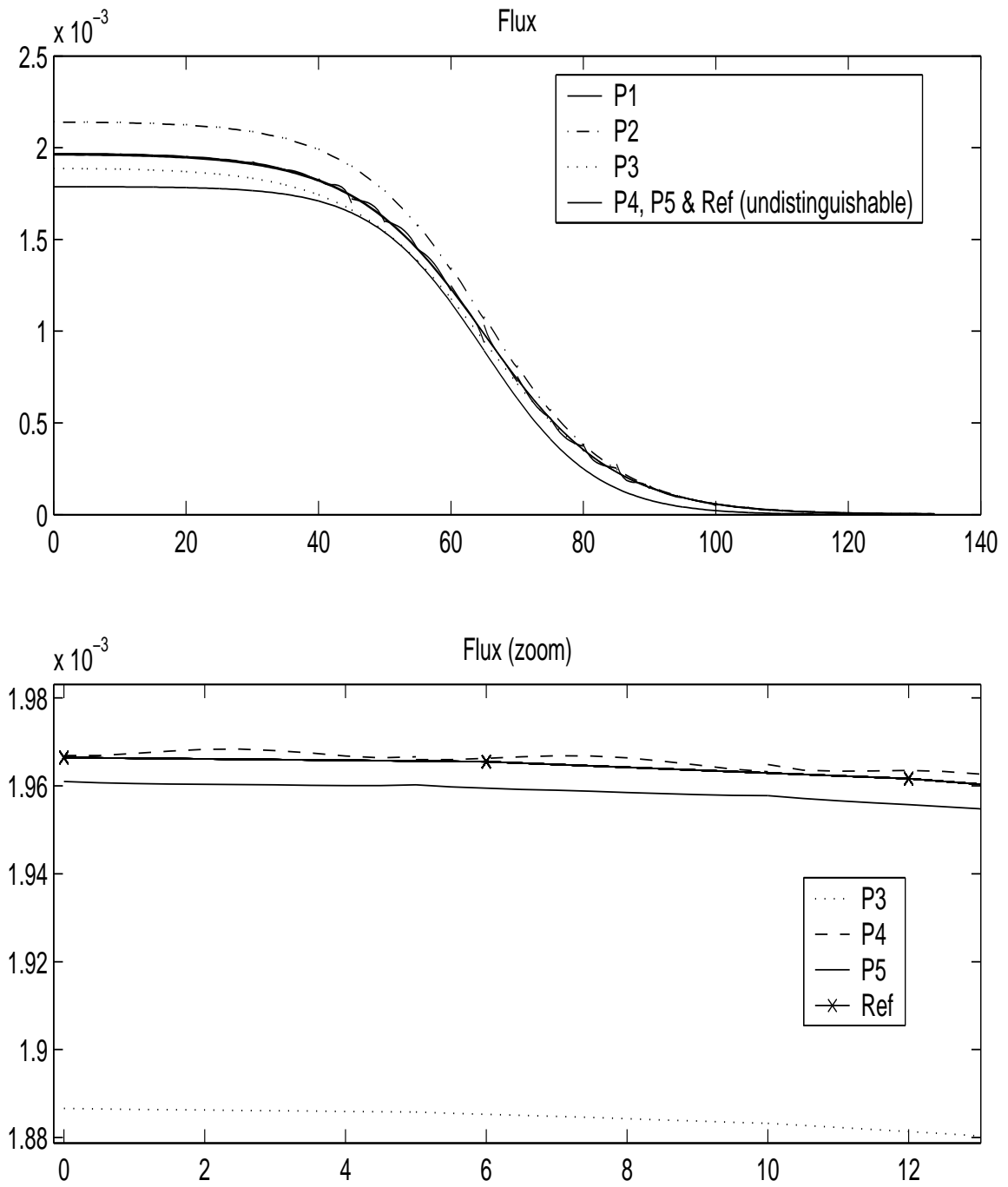


Figure 3.13: Primal flux along $y = 80$ for ANL benchmark, with reference solution.

Chapter 4

Conclusions

4.1 Achievements

Let us now review the significant achievements of our work.

- Mixed-hybrid methods were applied to the transport equation. They generalize the existing mixed and hybrid transport methods, combining their attractive features. More specifically, mixed methods were thus far restricted to diffusion, and our work provides a method for generalizing them to transport through hybridization.
- A well-posedness theory was established for the mixed-hybrid formulation of the transport equation.

- Proceeding from P_1 to P_N , the spatial rank condition is supplemented by an angular rank condition satisfied using interface angular expansions corresponding to the Rumyantsev conditions. This method for deriving these conditions, from the angular rank condition, is new, as well as the derivation itself, based on the Wigner coefficients.
- Proceeding from P_1 to P_N , the inclusion conditions between approximation spaces are modified by the introduction of $\mathbf{\Omega}$ besides the ∇ operator, as shown in theorem 3.4.2. In turn, the primal/dual distinction related to the spatial variable is complemented by an even/odd-order P_N distinction related to the angular variable. Four mixed-hybrid methods are then considered, namely the primal even, primal odd, dual even and dual odd methods.
- Flux and current plots for both even- and odd-order P_N approximations are displayed. Even-order approximations had been so far neglected in practice. Furthermore, an enclosing behavior appeared repeatedly in our numerical tests when both even- and odd-order P_N approximations were used. Even if no strict rule is derived, this is a promising property.
- The continuity properties corresponding to the Rumyantsev conditions are established and numerically verified for even- and odd-order P_N approximations.

- The solution process employed does not use a response matrix formalism, but a more direct approach (see §3.5.3).
- With the condensation approach of §3.5.3, mixed-hybrid method were shown to lead to positive definite system of reduced size. This was known in diffusion, and we extended it to the transport case.
- A multigroup anisotropic extension was developed and numerically tested.

4.2 Further work

A logical next step after this work is the investigation of numerical methods for the solution of the mixed-hybrid systems (3.30) and (3.33) that we showed to be of the generalized saddle-point type. Different approaches can be considered, as introduced in section 3.5.3. Then, performances could be compared with existing codes on the basis of k_{eff} calculations. This requires going beyond the stand-alone code used for our present results. Also, parallelization of solution algorithms should be investigated.

Another area of future research is testing spatial decompositions using triangular and hexagonal elements, frequently used in reactor physics. Generalization to more geometrically intricate domains and sub-element decompositions could make use of

the existing mortar finite element literature (e.g. Achdou and Pironneau (1995), Hoppe and Wohlmuth (1998)).

On another hand, one could envision developing purely mixed methods for the transport equation without performing hybridization. If one also investigates solution methods for the resulting systems, such developments would allow a fair comparison between mixed and mixed-hybrid methods. One can expect mixed methods to lead to negative fluxes in low flux regions, while hybrid (and thus also mixed-hybrid) methods are known to avoid such non-physical behavior (indeed avoided in our numerical tests). However, no formal proof of this positivity property exists as far as we know, and this could deserve some attention.

Even if mixed(-hybrid) methods avoid the presence of σ in the denominator, they lead to singular matrices when $\sigma = 0$ as seen in §3.5.3. Thus they do not apply to void regions. Very recently, Smith, Palmiotti, and Lewis (2003) developed a method capable of treating such regions based on the first-order (integro-differential) form of the transport equation. Further research might possibly show that this can be adapted to mixed-hybrid formulations.

Finally, on a more mathematical level, time dependence could be incorporated. Then the semi-group theory should be used to establish a well-posedness theory (Belleni-Morante 1979; Jerome 1983). A semi-group setting was provided by Dautray

and Lions (1993) for the first-order (integro-differential) form of the transport equation. Including time-dependence into our well-posedness investigations might lead to a semi-group setting for mixed-hybrid formulations.

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Appendices

Appendix A

Rumyantsev conditions

Derivation of the Rumyantsev interface conditions

The finite-dimensional space for the principal unknown angular expansion is in the primal case

$$Y_N^+ = \text{span} \{ Y_{pq}, \text{ with } p = 0, 2, 4, \dots N^+, |q| \leq p \},$$

and in the dual case

$$Y_N^- = \text{span} \{ Y_{pq}, \text{ with } p = 1, 3, 5, \dots N^-, |q| \leq p \}.$$

We now build the interface unknown angular expansions y_{χ} or $y_{\psi}(\boldsymbol{\Omega})$ such that, in the primal case

$$Y_N^\chi = \text{span}\{y_\chi\},$$

and in the dual case

$$Y_N^\psi = \text{span}\{y_\psi\}.$$

We take the convention that these Y_{lm} are defined with respect to a polar axis normal to the considered interface (or boundary). Thus they have to be “rotated” between non-parallel interfaces (i.e., in two dimensions, exchange the roles of the x - and y -axis for perpendicular interfaces). Then, we have that $\boldsymbol{\Omega} \cdot \mathbf{n} = Y_{10}/\sqrt{3}$.

From (3.17) and (3.18), we thus need to find those l, m that make

$$\int_S d\Omega Y_{10} Y_{pq} Y_{lm} \neq 0 \tag{A.1}$$

for each given couple p, q present in the principal unknown expansion. In case more than one couple l, m (denoted l_j, m_j) satisfies (A.1) for the same couple p, q , we combine them as

$$\sum_{l_j, m_j} \left(\int_S d\Omega Y_{10} Y_{pq} Y_{l_j m_j} \right) Y_{l_j m_j}$$

to generate our y_{χ} or ψ basis.

Our idea is now to use the property that the integral of three spherical harmonics is given by the Wigner “3j” coefficients (Messiah 1999, Volume 2, appendix C). We need to relate the Y_{lm} introduced in section 3.3 to the classical spherical harmonics of Messiah, denoted Y_{lm}^{cla} here. One can check that

$$\begin{aligned}\sqrt{4\pi} Y_{lm}^{cla} &= \frac{1}{\sqrt{2}} (Y_{lm} + i(-1)^{m+1} Y_{l-m}) && \text{for } m > 0 \\ \sqrt{4\pi} Y_{lm}^{cla} &= \frac{1}{\sqrt{2}} ((-1)^m Y_{l-m} + iY_{lm}) && \text{for } m < 0, \quad \text{and} \\ \sqrt{4\pi} Y_{l0}^{cla} &= \frac{1}{\sqrt{2}} Y_{l0} && \text{for } m = 0.\end{aligned}$$

Now, let us find the l, m satisfying (A.1) for fixed p, q . Note that, since Y_{10} does not depend on ϕ , the integral (A.1) contains the factor $\int_0^{2\pi} \cos(m\phi) \cos(q\phi) d\phi$ if $m \geq 0, q \geq 0$, which vanishes unless $m = q$. This conclusion remains true for any m, q , and we have thus that the integral (A.1) vanishes unless $m = q$. Besides, for $q > 0$,

$$\begin{aligned}(4\pi)^{3/2} \int_S d\Omega Y_{10}^{cla} Y_{l-q}^{cla} Y_{pq}^{cla} &= \int_S d\Omega \frac{Y_{10}}{2^{3/2}} ((-1)^q Y_{lq} + iY_{l-q}) (Y_{pq} + i(-1)^{q+1} Y_{p-q}) \\ &= \frac{(-1)^q}{2^{3/2}} \int_S d\Omega Y_{10} (Y_{lq} Y_{pq} + Y_{l-q} Y_{p-q})\end{aligned}$$

since it has to be real. Now, using the Legendre polynomial property $P_l^{-m} =$

$(-1)^m \frac{(l-m)!}{(l+m)!} P_l^m$ and the fact that $C_{l-m}^{1/2} = \frac{(l+m)!}{(l-m)!} C_{lm}^{1/2}$, we get

$$\begin{aligned} & Y_{lq} Y_{pq} + Y_{l-q} Y_{p-q} \\ &= C_{lq}^{1/2} P_l^q(\mu) \cos(q\phi) C_{pq}^{1/2} P_p^q(\mu) \cos(q\phi) + C_{l-q}^{1/2} P_l^{-q}(\mu) \sin(q\phi) C_{p-q}^{1/2} P_p^{-q}(\mu) \sin(q\phi) \\ &= P_l^q(\mu) C_{lq}^{1/2} P_p^q(\mu) C_{pq}^{1/2} \end{aligned}$$

such that

$$\int_S d\Omega Y_{10} Y_{lq} Y_{pq} = \int_S d\Omega Y_{10} (Y_{lq} Y_{pq} + Y_{l-q} Y_{p-q}) \cos^2(q\phi)$$

and therefore, since again Y_{10} does not depend on ϕ ,

$$\int_S d\Omega Y_{10} Y_{lq} Y_{pq} = \left(\int_0^{2\pi} \cos^2(q\phi) d\phi \right) \frac{(-1)^q (8\pi)^{3/2}}{2\pi} \int_S d\Omega Y_{10}^{cla} Y_{l-q}^{cla} Y_{pq}^{cla}$$

for $q > 0$, and this remains valid for $q < 0$ (swap p and l). With this relationship, we can use the classical spherical harmonic property saying that

$$\int_S d\Omega Y_{10}^{cla} Y_{l-q}^{cla} Y_{pq}^{cla} = \left(\frac{3(2l+1)(2p+1)}{4\pi} \right)^{1/2} \begin{pmatrix} 1 & l & p \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & l & p \\ 0 & -q & q \end{pmatrix},$$

where the last two factors are Wigner “3j” coefficients (Messiah 1999, Volume 2,

appendix C). These are different from zero only when $l = p - 1$ or $p + 1$ (and of course $|m| \leq l$ and $|q| \leq p$). Note that l and p have thus opposite parities, which is required since, for the primal (dual) case, $\Psi^{+(-)}$ and $\Psi^{\chi(\psi)}$ have opposite (angular) parities. Thus, the elements to put in our angular bases for each given couple p, q , are multiples of

$$Y_{p-1,q} \left(\frac{3(2p-1)(2p+1)}{4\pi} \right)^{1/2} \begin{pmatrix} 1 & p-1 & p \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & p-1 & p \\ 0 & -q & q \end{pmatrix} +$$

$$Y_{p+1,q} \left(\frac{3(2p+3)(2p+1)}{4\pi} \right)^{1/2} \begin{pmatrix} 1 & p+1 & p \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & p+1 & p \\ 0 & -q & q \end{pmatrix}$$

Computing the Wigner coefficients and canceling the common factors in both terms lead to

$$Y_{p-1,q} \sqrt{\frac{(p-q)(p+q)}{(2p-1)}} + Y_{p+1,q} \sqrt{\frac{(p-q+1)(p+q+1)}{(2p+3)}}.$$

with $p = 0, 1, 2, \dots, N$ and $|q| \leq p$. Now, $Y_{lm} = 0$ if $l > N$, $l < 0$ or $|m| > l$. Then taking $q = \pm p$ yields the elements $Y_{p+1,\pm p}$. Also, $Y_{N-1,q}$ must be in the expansions, as well as $Y_{N-3,q}, Y_{N-5,q}, \dots$. Finally, the interface angular expansions for odd-order

P_N expansions are made out of

$$\begin{aligned}
 & Y_{r,s}, \quad r = 0, 2, 4, \dots, N-1, \quad |s| \leq r, \\
 & Y_{r,s} \sqrt{\frac{(r-s+1)(r+s+1)}{(2r+1)}} + Y_{r+2,s} \sqrt{\frac{(r-s+2)(r+s+2)}{(2r+5)}} \\
 & \quad \text{with } r = 1, 3, 5, \dots, N-2, \quad |s| \leq r, \text{ and} \\
 & Y_{r,\pm(r-1)}, \quad r = 1, 3, 5, \dots, N.
 \end{aligned}$$

The expansions for even-order P_N expansions are made out of

$$\begin{aligned}
 & Y_{r,s}, \quad r = 1, 3, 5, \dots, N-1, \quad |s| \leq r, \\
 & Y_{r,s} \sqrt{\frac{(r-s+1)(r+s+1)}{(2r+1)}} + Y_{r+2,s} \sqrt{\frac{(r-s+2)(r+s+2)}{(2r+5)}} \\
 & \quad \text{with } r = 0, 2, 4, \dots, N-2, \quad |s| \leq r, \text{ and} \\
 & Y_{r,\pm(r-1)}, \quad r = 2, 4, \dots, N.
 \end{aligned}$$

These conditions lead to the expansions mentioned in §3.4.3. This form of the Rumyantsev conditions was first derived by Yang, Smith, Palmiotti, and Lewis (2004), who followed the original path of Rumyantsev (1962). The derivation presented here is different, but leads to the same result.

Appendix B

P_1 well-posedness proofs

B.1 Continuous problems (Theorem 2.4.1)

We here prove the theorem 2.4.1 in the dual case. We define

$$\Lambda = Y \times L^2(V) \times H^{1/2}(\Gamma) \text{ and } \Lambda_0 = Y \times L^2(V) \times H_0^{1/2}(\Gamma),$$

as well as $\lambda = (\mathbf{J}, \phi, \psi) \in \Lambda$ and $\tilde{\lambda} = (\tilde{\mathbf{J}}, \tilde{\phi}, \tilde{\psi}) \in \Lambda_0$. Then, $\|\lambda\|_\Lambda^2 = \|\mathbf{J}\|_Y^2 + \|\phi\|^2 + \|\psi\|_{1/2,\Gamma}^2$ where $\|\mathbf{J}\|_Y^2 = \sum_l \|\mathbf{J}\|_{div,l}^2$. In the sequel, the subscript l refers to restrictions

to V_l . We introduce the bilinear form

$$K(\lambda, \tilde{\lambda}) = \sum_l K_l(\lambda_l, \tilde{\lambda}_l)$$

where

$$\begin{aligned} K_l(\lambda_l, \tilde{\lambda}_l) = & \int_{V_l} (\nabla \cdot \mathbf{J} \tilde{\phi} + \sigma_0 \phi \tilde{\phi}) dV + \int_{V_l} (\phi \nabla \cdot \tilde{\mathbf{J}} - \sigma_1 \mathbf{J} \cdot \tilde{\mathbf{J}}) dV \\ & - \int_{\partial V_l} \psi \mathbf{n} \cdot \tilde{\mathbf{J}} d\Gamma - \int_{\partial V_l} \mathbf{n} \cdot \mathbf{J} \tilde{\psi} d\Gamma. \end{aligned}$$

Note that $K_l(\lambda_l, \tilde{\lambda}_l)$ is symmetric. With

$$\langle s, \tilde{\lambda} \rangle = \int_{V_l} s_0 \tilde{\phi} dV - \int_{V_l} \mathbf{s}_1 \cdot \tilde{\mathbf{J}} dV,$$

we thus face the problem: find $\lambda \in \Lambda$ such that

$$K(\lambda, \tilde{\lambda}) = \langle s, \tilde{\lambda} \rangle \quad \forall \tilde{\lambda} \in \Lambda_0.$$

According to the generalization of the Lax-Milgram theorem for the non-coercive operators, well-posedness is ensured provided we can demonstrate the continuity of K , as well as the ‘‘Ladyshenskaya-Babuška-Brezzi’’ (LBB, or just BB) or ‘‘inf-sup’’

condition for K . See for instance Babuška (1971, Theorem 2.1), Babuška, Oden, and Lee (1977, Theorem 2.1), Brezzi (1974), and Roberts and Thomas (1991, Theorem 9.1 p.564). We therefore prove here the existence of strictly positive constants C_1 and C_2 such that

$$K_l(\lambda_l, \tilde{\lambda}_l) \leq C_1 \|\lambda_l\|_{\Lambda_l} \|\tilde{\lambda}_l\|_{\Lambda_{0,l}} \quad (\text{B.1})$$

and

$$\inf_{\lambda \in \Lambda, \lambda \neq 0} \sup_{\tilde{\lambda} \in \Lambda_0, \tilde{\lambda} \neq 0} \frac{K(\lambda, \tilde{\lambda})}{\|\lambda\|_{\Lambda} \|\tilde{\lambda}\|_{\Lambda_0}} \geq C_2 \quad (\text{B.2})$$

as well as

$$\sup_{\lambda \in \Lambda, \|\lambda\|_{\Lambda}=1} K(\lambda, \tilde{\lambda}) > 0 \quad \forall \tilde{\lambda} \in \Lambda_0 \quad \text{with } \tilde{\lambda} > 0. \quad (\text{B.3})$$

To check (B.1), we first notice that, with t_l the trace operator from $H(\text{div}, V_l)$ to $H^{-1/2}(\partial V_l)$, we have

$$\int_{\partial V_l} \psi_l \mathbf{n} \cdot \mathbf{J}_l \, d\Gamma \leq \|\psi_l\|_{1/2, \partial V_l} \|t_l(\mathbf{J})_l\|_{-1/2, l} \leq \|\psi_l\|_{1/2, \partial V_l} \|\mathbf{J}_l\|_{\text{div}, l}$$

where we used (2.4). Using Schwarz inequality and assuming $\sigma_{0,l}$ and $\sigma_{1,l}$ constant in

each V_l , we have

$$\begin{aligned}
K_l(\lambda_l, \tilde{\lambda}_l) &\leq \|\nabla \cdot \mathbf{J}_l\|_l \|\tilde{\phi}_l\|_l + \sigma_{0,l} \|\phi_l\|_l \|\tilde{\phi}_l\|_l + \sigma_{1,l} \|\mathbf{J}_l\|_{div,l} \|\tilde{\mathbf{J}}_l\|_{div,l} \\
&\quad + \|\phi_l\|_l \|\nabla \cdot \tilde{\mathbf{J}}_l\|_l + \|\psi_l\|_{1/2,\partial V_l} \|\tilde{\mathbf{J}}_l\|_{div,l} + \|\mathbf{J}_l\|_{div,l} \|\tilde{\psi}_l\|_{1/2,\partial V_l} \\
&\leq (\|\nabla \cdot \mathbf{J}_l\|_l^2 + (1 + \sigma_{0,l}) \|\phi_l\|_l^2 + (1 + \sigma_{1,l}) \|\mathbf{J}_l\|_{div,l}^2 + \|\psi_l\|_{1/2,\partial V_l}^2)^{1/2} \\
&\quad ((1 + \sigma_{0,l}) \|\tilde{\phi}_l\|_l^2 + (1 + \sigma_{1,l}) \|\tilde{\mathbf{J}}_l\|_{div,l}^2 + \|\nabla \cdot \tilde{\mathbf{J}}_l\|_l^2 + \|\tilde{\psi}_l\|_{1/2,\partial V_l}^2)^{1/2} \\
&\leq (2 + \sigma_{0,l} + \sigma_{1,l}) \|\lambda_l\|_{\Lambda_l} \|\tilde{\lambda}_l\|_{\Lambda_{0,l}}
\end{aligned} \tag{B.4}$$

which proves the continuity of K .

For the LBB condition (B.2), we introduce $\hat{\lambda}_l = (\hat{\mathbf{J}}_l, \hat{\phi}_l, \hat{\psi}_l)$ with ¹

$$\begin{aligned}
\hat{\mathbf{J}}_l &= -(1 + \sigma_{0,l}) \mathbf{J}_l - \sigma_{0,l} \mathbf{z}_l \\
\hat{\phi}_l &= \nabla \cdot \mathbf{J}_l + \phi_l + \nabla \cdot \mathbf{z}_l \\
\hat{\psi}_l &= (1 + 2\sigma_{0,l}) \psi_l|_{\partial V_l,0}
\end{aligned}$$

where $\psi_l|_{\partial V_l,0}$ is the restriction of ψ_l to $\partial V_l \setminus \partial V$ (extended by zero on $\partial V \cap \partial V_l$), and

where $\mathbf{z}_l \in H(div, V_l)$ is the weak solution of the auxiliary problem

¹The presence of dimensional factors is understood.

$$\begin{cases} -\nabla(\nabla \cdot \mathbf{z}_l) + \sigma_{0,l} \sigma_{1,l} \mathbf{z}_l = 0 & \text{in } V_l \\ \nabla \cdot \mathbf{z}_l = \sigma_{0,l} \psi_l & \text{on } \partial V_l. \end{cases} \quad (\text{B.5})$$

After some manipulations, we obtain

$$\begin{aligned} K_l(\lambda_l, \hat{\lambda}_l) &= \|\nabla \cdot \mathbf{J}_l\|_l^2 + \sigma_{1,l}(1 + \sigma_{0,l})\|\mathbf{J}_l\|_l^2 + \sigma_{0,l}\|\phi_l\|_l^2 \\ &\quad + \int_{\partial V_l \cap \partial V} (1 + 2\sigma_{0,l}) \mathbf{n} \cdot \mathbf{J}_l \psi_l \, d\Gamma + \int_{\partial V_l} \sigma_{0,l} \mathbf{n} \cdot \mathbf{z}_l \psi_l \, d\Gamma. \end{aligned}$$

Boundary conditions make the first integral of this last expression non-negative. Indeed, in the vacuum case $\psi = 2\mathbf{n} \cdot \mathbf{J}|_{\partial V}$ and the first integral is positive, while in the reflected case $\mathbf{n} \cdot \mathbf{J}|_{\partial V} = 0$ and the first integral vanishes. Then, let $v_l = \nabla \cdot \mathbf{z}_l$. From (B.5) we obtain $\mathbf{z}_l = \frac{1}{\sigma_{0,l}\sigma_{1,l}}\nabla v_l$ and

$$\begin{cases} -\Delta v_l + \sigma_{0,l} \sigma_{1,l} v_l = 0 & \text{in } V_l \\ v_l = \sigma_{0,l} \psi_l & \text{on } \partial V_l. \end{cases}$$

We define the norms $\|v\|_{1,l,*}^2 = \|\nabla v\|_l^2 + \sigma_{0,l} \sigma_{1,l} \|v\|_l^2$ and $\|\mathbf{z}\|_{div,l,*}^2 = \|\nabla \cdot \mathbf{z}\|_l^2 + \sigma_{0,l} \sigma_{1,l} \|\mathbf{z}\|_l^2$, respectively equivalent to $\|v\|_{1,l}$ and $\|\mathbf{z}\|_{div,l}$. We also define the norm $\|\psi\|_{1/2,\partial V_l,*}$ the same way we defined $\|\psi\|_{1/2,\partial V_l}$ in (2.3), but with $\|\nu\|_{1,V,*}$ instead

of $\|\nu\|_{1,V}$, such that $\|\psi\|_{1/2,\partial V_l,*}$ is equivalent to $\|\psi\|_{1/2,\partial V_l}$. Then, $\|\sigma_{0,l}\psi_l\|_{1/2,\partial V_l,*} = \|v_l\|_{1,l,*}$, while $\|v_l\|_{1,l,*}^2 = \int_{\partial V_l} \sigma_{0,l}^2 \sigma_{1,l} \mathbf{n} \cdot \mathbf{z}_l \psi_l d\Gamma$. Thus we have

$$\int_{\partial V_l} \sigma_{0,l} \mathbf{n} \cdot \mathbf{z}_l \psi_l d\Gamma = \frac{\sigma_{0,l}}{\sigma_{1,l}} \|\psi_l\|_{1/2,\partial V_l,*}^2. \quad (\text{B.6})$$

Finally we can say that, for any l , there exists a constant $C_l > 0$ such that $K_l(\lambda_l, \hat{\lambda}_l) \geq C_l \|\lambda_l\|_{\Lambda_l}^2$. Since we also have $\|\hat{\lambda}_l\|_{\Lambda_{0,l}}^2 \leq C'_l \|\lambda_l\|_{\Lambda_l}^2$, where $C'_l > 0$ is another constant, we obtain $K_l(\lambda_l, \hat{\lambda}_l) \geq \frac{C}{\sqrt{C'}} \|\lambda_l\|_{\Lambda_l} \|\hat{\lambda}_l\|_{\Lambda_{0,l}}$. Hence there is a constant $\beta > 0$ such that

$$\sup_{\tilde{\lambda} \in \Lambda_0} \frac{K(\lambda, \tilde{\lambda})}{\|\tilde{\lambda}\|_{\Lambda_0}} \geq \beta \|\lambda\|_{\Lambda} \quad \forall \lambda \in \Lambda$$

and the LBB condition (B.2) is verified. Besides, the symmetry of $K(\lambda, \tilde{\lambda})$ leads to (B.3).

B.2 Discrete problems (Theorem 2.4.2)

We here prove the theorem 2.4.2 in the dual case. We define

$$\Lambda_h = \mathbf{V}_h^v(V) \times S_h^s(V) \times B_h^b(\Gamma) \text{ and } \Lambda_{0,h} = \mathbf{V}_h^v(V) \times S_h^s(V) \times B_{0,h}^b(\Gamma),$$

as well as $\lambda_h = (\mathbf{J}_h, \phi_h, \psi_h) \in \Lambda_h$ and $\tilde{\lambda}_h = (\tilde{\mathbf{J}}_h, \tilde{\phi}_h, \tilde{\psi}_h) \in \Lambda_{0,h}$. Furthermore, we introduce Π_l^v and Π_l^s respectively the orthogonal projections of $H(\text{div}, V_l)$ and $L^2(V_l)$ (with respect to their scalar product) onto (again respectively) $\mathbf{V}_h^v(V_l)$ and $S_h^s(V_l)$. We need to verify the LBB condition in the discrete case (Roberts and Thomas (1991, Theorem 9.2 p.564), Babüska, Oden, and Lee (1977, Theorem 2.2), and Babüska (1971, Theorem 2.2)). In this view, we define $\hat{\lambda}_{h,l} = (\hat{\mathbf{J}}_{h,l}, \hat{\phi}_{h,l}, \hat{\psi}_{h,l})$ with

$$\begin{aligned}\hat{\mathbf{J}}_{h,l} &= -(1 + \sigma_{0,l})\mathbf{J}_{h,l} - \sigma_{0,l}\Pi_l^v(\mathbf{z}_{h,l}) \\ \hat{\phi}_{h,l} &= \Pi_l^s(\nabla \cdot \mathbf{J}_{h,l}) + \phi_{h,l} + \Pi_l^s(\nabla \cdot \Pi_l^v(\mathbf{z}_{h,l})) \\ \hat{\psi}_{h,l} &= (1 + 2\sigma_{0,l})\psi_{h,l}|_{\partial V_l,0}\end{aligned}$$

where $\mathbf{z}_{h,l} \in H(\text{div}, V_l)$ is the weak solution of

$$\begin{cases} -\nabla(\nabla \cdot \mathbf{z}_{h,l}) + \sigma_{0,l}\sigma_{1,l}\mathbf{z}_{h,l} = 0 & \text{in } V_l \\ \nabla \cdot \mathbf{z}_h = \sigma_{0,l}\psi_{h,l} & \text{on } \partial V_l. \end{cases} \quad (\text{B.7})$$

Orthogonal projections properties provide

$$\begin{aligned}
(\phi_{h,l}, \nabla \cdot \mathbf{J}_{h,l} - \Pi_l^s(\nabla \cdot \mathbf{J}_{h,l})) &= 0 \quad \forall \phi_{h,l} \in S_h^s(V_l) \\
(\phi_{h,l}, \nabla \cdot \Pi_l^v(\mathbf{z}_{h,l}) - \Pi_l^s(\nabla \cdot \Pi_l^v(\mathbf{z}_{h,l}))) &= 0 \quad \forall \phi_{h,l} \in S_h^s(V_l) \\
(\nabla \cdot \mathbf{J}_{h,l}, \Pi_l^s(\nabla \cdot \mathbf{J}_{h,l})) &= \|\Pi_l^s(\nabla \cdot \mathbf{J}_{h,l})\|^2 \quad \forall \mathbf{J}_{h,l} \in \mathbf{V}_h^v(V_l).
\end{aligned}$$

Proceeding as in the continuous case and using these properties lead to

$$\begin{aligned}
K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) &= \sigma_{1,l}(1 + \sigma_{0,l}) \|\mathbf{J}_{h,l}\|_l^2 + \sigma_{0,l} \|\phi_{h,l}\|_l^2 \\
&\quad + \|\Pi_l^v(\mathbf{z}_{h,l})\|_{div,*,l}^2 + \|\Pi_l^s(\nabla \cdot \mathbf{J}_{h,l})\|_l^2 \\
&\quad - \int_{V_l} (\nabla \cdot \mathbf{J}_{h,l})(\nabla \cdot \Pi_l^v(\mathbf{z}_{h,l}) - \Pi_l^s(\nabla \cdot \Pi_l^v(\mathbf{z}_{h,l}))) \, d\Gamma \\
&\quad + \int_{\partial V_l \cap \partial V} \psi_{h,l} \mathbf{n} \cdot \mathbf{J}_{h,l} (1 + 2\sigma_{0,l})
\end{aligned}$$

where we used $\int_{\partial V} \sigma_{0,l} \mathbf{n} \cdot \mathbf{J}_{h,l} \psi_{h,l} = (\mathbf{J}_{h,l}, \mathbf{z}_{h,l})_{div,*,l} = (\mathbf{J}_{h,l}, \Pi_l^v(\mathbf{z}_{h,l}))_{div,*,l}$. The last term is non-negative thanks to the vacuum or reflected boundary conditions, as in

the continuous case. We introduce the following parameters:

$$\begin{aligned}
\mu_l &= \mu_l(\mathbf{V}_h^v(V_l), B_h^b(\partial V_l)) = \inf_{\psi_{h,l} \in B_h^b(\partial V_l)} \frac{\|\Pi_l^v(\mathbf{z}_{h,l})\|_{div,l,*}^2}{\|\psi_{h,l}\|_{1/2,\partial V_l}^2} \\
\nu_l &= \nu_l(\mathbf{V}_h^v(V_l), S_h^s(V_l)) = \inf_{\mathbf{p} \in \mathbf{V}_h^v(V_l)} \frac{\|\Pi_l^s(\nabla \cdot \mathbf{p})\|_l^2}{\|\nabla \cdot \mathbf{p}\|_l^2} \\
\gamma_l &= \gamma_l(\mathbf{V}_h^v(V_l), S_h^s(V_l)) = \sup_{\mathbf{p} \in \mathbf{V}_h^v(V_l)} \frac{\|\nabla \cdot \mathbf{p} - \Pi_l^s(\nabla \cdot \mathbf{p})\|_l}{\|\nabla \cdot \mathbf{p}\|_l}.
\end{aligned} \tag{B.8}$$

Note that they are all contained in the interval $[0, 1]$. Then,

$$\begin{aligned}
K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) &\geq \sigma_{1,l} (1 + \sigma_{0,l}) \|\mathbf{J}_{h,l}\|_l^2 + \sigma_{0,l} \|\phi_{h,l}\|_l^2 + \mu_l \|\psi_{h,l}\|_{1/2,\partial V_l}^2 \\
&\quad + \nu_l \|\nabla \cdot \mathbf{J}_{h,l}\|_l^2 - \gamma_l \|\nabla \cdot \mathbf{J}_{h,l}\|_l \|\nabla \cdot \Pi_l^v(\mathbf{z}_{h,l})\|_l
\end{aligned}$$

hence

$$\begin{aligned}
K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) &\geq \min(\sigma_{1,l} (1 + \sigma_{0,l}), \nu_l) \|\mathbf{J}_{h,l}\|_{div,l}^2 + \sigma_{0,l} \|\phi_{h,l}\|_l^2 \\
&\quad + \mu_l \|\psi_{h,l}\|_{1/2,\partial V_l}^2 - \frac{1}{2} \gamma_l \|\nabla \cdot \mathbf{J}_{h,l}\|_l^2 \\
&\quad - \frac{1}{2} \gamma_l \|\nabla \cdot \Pi_l^v(\mathbf{z}_{h,l})\|_l^2.
\end{aligned}$$

Using $\|\nabla \cdot \Pi_l^v(\mathbf{z}_{h,l})\|_l \leq \|\Pi_l^v(\mathbf{z}_{h,l})\|_{div,l} \leq \|\mathbf{z}_{h,l}\|_{div,l}$ and (as in (B.6))

$$\|\mathbf{z}_{h,l}\|_{div,*,l}^2 = \int_{\partial V_l} \sigma_{0,l} \mathbf{n} \cdot \mathbf{z}_{h,l} \psi_{h,l} dV = \frac{\sigma_{0,l}}{\sigma_{1,l}} \|\psi_{h,l}\|_{1/2,*,\partial V_l}^2, \quad (\text{B.9})$$

we can say that there is a constant $k > 0$ such that

$$\begin{aligned} K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) &\geq (\min(\sigma_{1,l}(1 + \sigma_{0,l}), \nu_l) - \frac{1}{2} \gamma_l) \|\mathbf{J}_{h,l}\|_{div,l}^2 + \sigma_{0,l} \|\phi_{h,l}\|_l^2 \\ &\quad + (\mu_l - \frac{1}{2} k \gamma_l) \|\psi_{h,l}\|_{1/2,\partial V_l}^2. \end{aligned}$$

Thus, $K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) \geq C_l \|\lambda_{h,l}\|_{\Lambda,l}^2$ where

$$C_l = \min((\min(\sigma_{1,l}(1 + \sigma_{0,l}), \nu_l) - \frac{1}{2} \gamma_l), \sigma_{0,l}, \mu_l - \frac{1}{2} k \gamma_l). \quad (\text{B.10})$$

Since we also have $\|\hat{\lambda}_{h,l}\|_{\Lambda_{0,h,l}}^2 \leq C' \|\lambda_{h,l}\|_{\Lambda_{h,l}}^2$ with C' positive, we can conclude that, for the discrete mixed-hybrid dual problem to be well-posed, the quantity $C = \min_l C_l$ has to be strictly positive.

In the special case $\nabla \cdot \mathbf{V}_h^v(V_l) \subset S_h^s(V_l)$ in any V_l (which occurs whenever $v - 1 \leq s$ in V_l) we have that for all l , $\nu_l = 1$ and $\gamma_l = 0$. The well-posedness condition is then $\min_l \mu_l > 0$. Similarly to what is proved in Babuška, Oden, and Lee (1977), we have:

Lemma B.2.1 *The parameter $\mu_l > 0$ if and only if, for any $\psi \in B_h^b(\partial V_l)$,*

$$\int_{\partial V_l} \psi \mathbf{n} \cdot \mathbf{p} \, d\Gamma = 0 \quad \forall \mathbf{p} \in \mathbf{V}_h^v(V_l) \text{ implies that } \psi = 0.$$

Then, there is thus a $\beta_h > 0$ such that

$$\inf_{\lambda_h \in \Lambda_h, \lambda_h \neq 0} \sup_{\tilde{\lambda}_h \in \Lambda_{h,0}, \tilde{\lambda}_h \neq 0} \frac{K(\lambda_h, \tilde{\lambda}_h)}{\|\lambda_h\|_{\Lambda_h} \|\tilde{\lambda}_h\|_{\Lambda_{h,0}}} \geq \beta_h \quad (\text{B.11})$$

that is the discrete LBB condition is verified, and again the symmetry of $K(\lambda, \tilde{\lambda})$ leads to

$$\sup_{\lambda_h \in \Lambda_h, \lambda_h \neq 0} K(\lambda_h, \tilde{\lambda}_h) > 0 \quad \forall \tilde{\lambda}_h \in \Lambda_{h,0} \text{ with } \|\tilde{\lambda}_h\|_{\Lambda_h} = 1.$$

The parameter μ_l in (B.10) depends on h . To ensure stability of the method, we therefore still need to show the existence of a lower bound for μ_l (and thus for β_h) as $h \rightarrow 0$.

We do it for two-dimensional V . In this view, for each V_l , we introduce a master element \hat{V}_l defined by

$$\hat{V}_l = \{\hat{\mathbf{r}} : \hat{\mathbf{r}} = \mathbf{r}/h_l, \mathbf{r} \in V_l, h_l = \text{diameter of } V_l\}.$$

and for each $\mathbf{u}(\mathbf{r})$ defined for $\mathbf{r} \in V_l$, $\hat{\mathbf{u}}(\hat{\mathbf{r}}) = \mathbf{u}(\mathbf{r})$. Also,

$$\hat{\nabla} = h_l \nabla, \quad \hat{\sigma}_{0,l} = h_l \sigma_{0,l}, \quad \hat{\sigma}_{1,l} = h_l \sigma_{1,l}, \quad d\hat{V}_l = \frac{dV_l}{h_l^2}$$

and we introduce furthermore

$$\begin{aligned} [\hat{\mathbf{u}}, \hat{\mathbf{v}}]_{div,l,*} &= \int_{\hat{V}_l} (\hat{\nabla} \cdot \hat{\mathbf{u}} \hat{\nabla} \cdot \hat{\mathbf{v}} + \hat{\sigma}_{0,l} \hat{\sigma}_{1,l} \hat{\mathbf{u}} \cdot \hat{\mathbf{v}}) d\hat{V}, \\ |\hat{\mathbf{u}}, \hat{\mathbf{v}}|_{div,l} &= \int_{\hat{V}_l} (\hat{\nabla} \cdot \hat{\mathbf{u}} \hat{\nabla} \cdot \hat{\mathbf{v}}) d\hat{V} \end{aligned}$$

and $[\hat{\mathbf{u}}]_{div,l,*} = [\hat{\mathbf{u}}, \hat{\mathbf{u}}]_{div,l,*}^{1/2}$, such that $[\hat{\mathbf{u}}]_{div,l,*} = \|\mathbf{u}\|_{div,l,*}$.

We first look at the denominator in the expression (B.8) of μ_l , i.e., $\|\psi_{h,l}\|_{1/2,\partial V_l}^2$.

We have in view of (B.9)

$$\|\psi_{h,l}\|_{1/2,\partial V_l,*}^2 = \frac{\sigma_{1,l}}{\sigma_{0,l}} \|\mathbf{z}_{h,l}\|_{div,l,*}^2$$

where $\mathbf{z}_{h,l} \in H(div, V_l)$ is the weak solution of (B.7). Then, $\|\mathbf{z}_{h,l}\|_{div,l,*} = [\hat{\mathbf{z}}_{h,l}]_{div,l,*}$

with $\hat{\mathbf{z}}_{h,l} \in H(div, \hat{V}_l)$ the weak solution of

$$\begin{cases} -\hat{\nabla}(\hat{\nabla} \cdot \hat{\mathbf{z}}_{h,l}) + \hat{\sigma}_{0,l} \hat{\sigma}_{1,l} \hat{\mathbf{z}}_{h,l} = 0 & \text{in } \hat{V}_l \\ \hat{\nabla} \cdot \hat{\mathbf{z}}_{h,l} = \hat{\sigma}_{0,l} \hat{\psi}_{h,l} & \text{on } \partial \hat{V}_l. \end{cases}$$

that is

$$[\hat{\mathbf{z}}_{h,l}, \hat{\mathbf{v}}_{h,l}]_{div,l,*} = \int_{\partial\hat{V}_l} \hat{\sigma}_{0,l} \hat{\psi}_{h,l} \hat{\mathbf{n}} \cdot \hat{\mathbf{v}}_{h,l} d\hat{\Gamma} \quad \forall \hat{\mathbf{v}}_{h,l} \in H(div, \hat{V}_l). \quad (\text{B.12})$$

There is thus a constant $D(\sigma_{0,l}, \sigma_{1,l}) > 0$ such that

$$\|\psi_{h,l}\|_{1/2,\partial V_l}^2 \leq D(\sigma_{0,l}, \sigma_{1,l}) \|[\hat{\mathbf{z}}_{h,l}]_{div,l,*}^2, \quad (\text{B.13})$$

Next, we define $\hat{\mathbf{q}}_{h,l} \in H(div, \hat{V}_l)$ as the weak solution of

$$\begin{cases} \hat{\nabla}(\hat{\nabla} \cdot \hat{\mathbf{q}}_{h,l}) = \mathbf{A} & \text{in } \hat{V}_l \\ \hat{\nabla} \cdot \hat{\mathbf{q}}_{h,l} = \hat{\sigma}_{0,l} \hat{\psi}_{h,l} & \text{on } \partial\hat{V}_l \end{cases} \quad (\text{B.14})$$

where

$$\mathbf{A} = \frac{\int_{\partial\hat{V}_l} \mathbf{n} \hat{\sigma}_{0,l} \hat{\psi}_{h,l} d\hat{\Gamma}}{\int_{\hat{V}_l} d\hat{V}}$$

is defined such that the existence of $\hat{\mathbf{q}}_{h,l}$ is guaranteed. Furthermore, assuming

$\int_{\hat{V}_l} \hat{\mathbf{q}}_{h,l} d\hat{V} = 0$ guarantees its unicity. We now show that

Lemma B.2.2

$$\|\hat{\mathbf{z}}_{h,l}\|_{div,l,*}^2 \leq |\hat{\mathbf{q}}_{h,l}|_{div,l}^2 + \mathcal{A}(h) \quad \text{where } \mathcal{A}(h) = \frac{\mathbf{A} \cdot \mathbf{A}}{\hat{\sigma}_{0,l} \hat{\sigma}_{1,l}} \int_{\hat{V}_l} d\hat{V} > 0.$$

Proof B.2.1 Introducing $\hat{\mathbf{p}}_{h,l} = \hat{\mathbf{z}}_{h,l} - \frac{\mathbf{A}}{\hat{\sigma}_{0,l} \hat{\sigma}_{1,l}}$, we have

$$\|\hat{\mathbf{p}}_{h,l}\|_{div,l,*}^2 = [\hat{\mathbf{z}}_{h,l}, \hat{\mathbf{p}}_{h,l}]_{div,l,*} - \mathbf{A} \cdot \int_{\hat{V}_l} \hat{\mathbf{p}}_{h,l} d\hat{V} \quad (\text{B.15})$$

Now, from (B.12), $[\hat{\mathbf{z}}_{h,l}, \mathbf{A}]_{div,l,*} = \mathbf{A} \cdot \mathbf{A} \int_{\hat{V}_l} d\hat{V}$, thus

$$\mathbf{A} \cdot \int_{\hat{V}_l} \hat{\sigma}_{0,l} \hat{\sigma}_{1,l} \mathbf{z}_{h,l} d\hat{V} = \mathbf{A} \cdot \mathbf{A} \int_{\hat{V}_l} d\hat{V}.$$

Since $\hat{\sigma}_{0,l} \hat{\sigma}_{1,l} \mathbf{z}_{h,l} = \hat{\sigma}_{0,l} \hat{\sigma}_{1,l} \hat{\mathbf{p}}_{h,l} + \mathbf{A}$, this implies $\mathbf{A} \cdot \int_{\hat{V}_l} \hat{\mathbf{p}}_{h,l} d\hat{V} = 0$, and (B.15) yields

$$\|\hat{\mathbf{p}}_{h,l}\|_{div,l,*}^2 = \|\hat{\mathbf{z}}_{h,l}\|_{div,l,*}^2 - \mathcal{A}(h). \quad \text{Thus,}$$

$$\|\hat{\mathbf{z}}_{h,l}\|_{div,l,*}^2 = \|\hat{\mathbf{p}}_{h,l}\|_{div,l,*}^2 + \mathcal{A}(h)$$

while (B.12), (B.14) and (B.15) enable to write $|\hat{\mathbf{q}}_{h,l}, \hat{\mathbf{p}}_{h,l}|_{div,l} = \|\hat{\mathbf{p}}_{h,l}\|_{div,l,*}^2$, that is

$$\|\hat{\mathbf{p}}_{h,l}\|_{div,l,*}^2 \leq |\hat{\mathbf{q}}_{h,l}|_{div,l} \|\hat{\mathbf{p}}_{h,l}\|_{div,l,*}.$$

The conclusion follows.

We now look at the numerator in the expression (B.8) of μ_l , i.e., $\|\Pi_l^v(\mathbf{z}_{h,l})\|_{div,l,*}$.

In this view, we introduce

$$\hat{\mathbf{V}}_{h,l}^v(\hat{V}_l) = \{\hat{\mathbf{v}} : \hat{\mathbf{v}}(\hat{\mathbf{r}}) = \mathbf{v}(\mathbf{r}) \text{ with } \mathbf{v}(\mathbf{r}) \in \mathbf{V}_{h,l}^v(V_l)\}.$$

as well as $\hat{\Pi}_{h,l}^v$ and $\hat{\Xi}_{h,l}^v$ the orthogonal projections of $H(div, \hat{V}_l)$ onto $\hat{\mathbf{V}}_{h,l}^v(\hat{V}_l)$ with respect to $[\cdot, \cdot]_{div,l,*}$ and $|\cdot, \cdot|_{div,l}$, respectively. Then $\|\Pi_l^v(\mathbf{z}_{h,l})\|_{div,l,*} = \|\hat{\Pi}_l^v(\hat{\mathbf{z}}_{h,l})\|_{div,l,*}$, and we have

Lemma B.2.3

$$\|\hat{\Pi}_l^v(\hat{\mathbf{z}}_{h,l})\|_{div,l,*}^2 \geq (1 - \hat{\sigma}_{0,l} \hat{\sigma}_{1,l} C^*) |\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l})|_{div,l}^2 + \mathcal{A}(h)$$

with $C^* > 0$ independent of h .

Proof B.2.2 With $\hat{\Pi}_l^v(\hat{\mathbf{p}}_{h,l}) = \hat{\Pi}_l^v(\hat{\mathbf{z}}_{h,l}) - \frac{\mathbf{A}}{\hat{\sigma}_{0,l} \hat{\sigma}_{1,l}}$, we can show as in the previous lemma that

$$\|\hat{\Pi}_l^v(\hat{\mathbf{z}}_{h,l})\|_{div,l,*}^2 = \|\hat{\Pi}_l^v(\hat{\mathbf{p}}_{h,l})\|_{div,l,*}^2 + \mathcal{A}(h). \quad (\text{B.16})$$

Besides,

$$\begin{aligned}
|\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l})|_{div,l}^2 &= \int_{\partial\hat{V}_l} \mathbf{n} \cdot \hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l}) \hat{\sigma}_{0,l} \hat{\psi}_{h,l} - \mathbf{A} \cdot \int_{\hat{V}_l} \hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l}) dV \\
&= [\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l}), \hat{\Pi}_l^v(\hat{\mathbf{p}})]_{div,l,*} \\
&\leq \frac{1}{2}([\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l})]_{div,l,*}^2 + [\hat{\Pi}_l^v(\hat{\mathbf{p}}_{h,l})]_{div,l,*}^2),
\end{aligned}$$

while, with $C^* > 0$ independent of h ,

$$\begin{aligned}
[\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l})]_{div,l,*}^2 &= |\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l})|_{div,l}^2 + \hat{\sigma}_{0,l} \hat{\sigma}_{1,l} \|\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l})\|_l^2 \\
&\leq (1 + \hat{\sigma}_{0,l} \hat{\sigma}_{1,l} C^*) |\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l})|_{div,l}^2
\end{aligned}$$

where we used Poincaré's inequality together with $\int_{\hat{V}_l} \hat{\mathbf{q}}_{h,l} d\hat{V} = 0$. With the last two inequalities, we get

$$[\hat{\Pi}_l^v(\hat{\mathbf{p}}_{h,l})]_{div,l,*}^2 \geq (1 - \hat{\sigma}_{0,l} \hat{\sigma}_{1,l} C^*) |\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l})|_{div,l}^2,$$

which combined with (B.16) proves our lemma.

Gathering our previous results, we obtain

Theorem B.2.1

$$\mu_l \geq \frac{(1 - h^2 \sigma_{0,l} \sigma_{1,l} C^*)}{D(\sigma_{0,l}, \sigma_{1,l})} \inf_{\psi_{h,l} \in B_h^b(\partial V_l)} \frac{|\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l})|_{div,l}^2}{|(\hat{\mathbf{q}}_{h,l})|_{div,l}^2}$$

where $\sigma_{0,l}$, $\sigma_{1,l}$, C^* and $D(\sigma_{0,l}, \sigma_{1,l})$ are strictly positive and independent of h .

Proof B.2.3 From (B.8), we get using (B.13), lemma B.2.2 and lemma B.2.3,

$$\begin{aligned} \mu_l &= \inf_{\psi_{h,l} \in B_h^b(\partial V_l)} \frac{\|\Pi_l^v(\mathbf{z}_{h,l})\|_{div,*l}^2}{\|\psi_{h,l}\|_{1/2,\partial V_l}^2} \\ &\geq \frac{1}{D(\sigma_{0,l}, \sigma_{1,l})} \inf_{\psi_{h,l} \in B_h^b(\partial V_l)} \frac{(1 - \hat{\sigma}_{0,l} \hat{\sigma}_{1,l} C^*) |\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l})|_{div,l}^2 + \mathcal{A}(h)}{|\hat{\mathbf{q}}_{h,l}|_{div,l}^2 + \mathcal{A}(h)} \\ &\geq \frac{(1 - \hat{\sigma}_{0,l} \hat{\sigma}_{1,l} C^*)}{D(\sigma_{0,l}, \sigma_{1,l})} \inf_{\psi_{h,l} \in B_h^b(\partial V_l)} \frac{|\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l})|_{div,l}^2}{|(\hat{\mathbf{q}}_{h,l})|_{div,l}^2} \end{aligned}$$

where the last step is valid since $|\hat{\mathbf{q}}_{h,l}|_{div,l}^2 > 0$, $\mathcal{A}(h) > 0$, and

$$(1 - \hat{\sigma}_{0,l} \hat{\sigma}_{1,l} C^*) |\hat{\Xi}_l^v(\hat{\mathbf{q}}_{h,l})|_{div,l}^2 \leq |\hat{\mathbf{q}}_{h,l}|_{div,l}^2.$$

Now, with $\hat{\sigma}_{0,l} = h\sigma_{0,l}$ and $\hat{\sigma}_{1,l} = h\sigma_{1,l}$, our theorem is proved.

Thus, there is a strictly positive lower bound for μ_l as $h \rightarrow 0$, which guarantees the stability of our method. This concludes the proof of theorem 2.4.2 in the dual case.

Appendix C

P_N well-posedness proofs

C.1 Continuous problems (Theorem 3.4.1)

C.1.1 Proofs for the primal case

Even-order primal method

We define

$$\Lambda = X \times L^2(\Omega, S \times V) \times H_{\Omega}^{-1/2}(S \times \Gamma),$$

$$\Lambda_0 = X \times L^2(\Omega, S \times V) \times H_{\Omega,0}^{-1/2}(S \times \Gamma),$$

$\lambda = (\Psi^+, \Psi^-, \Psi^\chi) \in \Lambda$ and $\tilde{\lambda} = (\tilde{\Psi}^+, \tilde{\Psi}^-, \tilde{\Psi}^\chi) \in \Lambda_0$ ¹. As for norms, we have $\|\lambda\|_\Lambda^2 = \|\Psi^+\|_X^2 + \|\Psi^-\|^2 + \|\Psi^\chi\|_{\Omega, -1/2, \Gamma}^2$. Then we introduce the symmetric bilinear form

$$K(\lambda, \tilde{\lambda}) = \sum_l K_l(\lambda, \tilde{\lambda}),$$

where

$$\begin{aligned} K_l(\lambda, \tilde{\lambda}) &= - \int_S d\Omega \int_{V_l} dV \Psi_l^- \boldsymbol{\Omega} \cdot \nabla \tilde{\Psi}_l^+ + \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}_l^+ \Psi_l^\chi \\ &\quad + \int_S d\Omega \int_{V_l} dV \sigma_l \tilde{\Psi}_l^+ \Psi_l^+ - \int_S d\Omega \int_{V_l} dV \left(\sigma_{s,l} \tilde{\Psi}_l^+ \int_S d\Omega' \Psi_l^+ \right) \\ &\quad - \int_S d\Omega \int_{V_l} dV \tilde{\Psi}_l^- \boldsymbol{\Omega} \cdot \nabla \Psi_l^+ - \int_S d\Omega \int_{V_l} dV \sigma_l \tilde{\Psi}_l^- \Psi_l^- \\ &\quad + \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}_l^\chi \Psi_l^+. \end{aligned}$$

With

$$\langle s, \tilde{\Psi}^+ \rangle = \sum_l \int_S d\Omega \int_{V_l} dV s \tilde{\Psi}_l^+,$$

¹We as well assume the usual parity properties.

we have to examine the problem: find $\lambda \in \Lambda$ such that

$$K(\lambda, \tilde{\lambda}) = \langle s, \tilde{\Psi}^+ \rangle, \quad \forall \tilde{\lambda} \in \Lambda_0.$$

As in the P_1 case, we verify the continuity of K as well as the LBB condition.

For the continuity issue, we first notice that, with t_l the trace operator from $H(\text{grad}, S \times V_l)$ to $H^{1/2}(S \times \partial V_l)$, we have

$$\begin{aligned} \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \Psi_l^+ \Psi_l^\chi &\leq \|t_l(\Psi_l^+)\|_{1/2, \partial V_l} \|\Psi_l^\chi\|_{\Omega, -1/2, \partial V_l} \\ &\leq \|\Psi_l^+\|_{\text{grad}, V_l} \|\Psi_l^\chi\|_{\Omega, -1/2, \partial V_l} \end{aligned}$$

where we used (3.4). Then, assuming σ_l and $\sigma_{s,l}$ constant in each V_l , the Schwartz

inequality yields

$$\begin{aligned}
K_l(\lambda, \tilde{\lambda}) &\leq \|\nabla \tilde{\Psi}_l^+\| \|\Omega \Psi_l^-\| + \|\Psi_l^\chi\|_{\Omega, -1/2, \partial V_l} \|\tilde{\Psi}_l^+\|_{grad, V_l} + (\sigma_l + \sigma_{s,l}) \|\tilde{\Psi}_l^+\| \|\Psi_l^+\| \\
&\quad + \|\Omega \tilde{\Psi}_l^-\| \|\nabla \Psi_l^+\| + \sigma_l \|\tilde{\Psi}_l^-\| \|\Psi_l^-\| + \|\tilde{\Psi}_l^\chi\|_{\Omega, -1/2, \partial V_l} \|\Psi_l^+\|_{grad, V_l} \\
&\leq \left(\|\Omega \Psi_l^-\|^2 + \|\Psi_l^\chi\|_{\Omega, -1/2, \partial V_l}^2 + (\sigma_l + \sigma_{s,l}) \|\Psi_l^+\|^2 + \|\nabla \Psi_l^+\|^2 + \sigma_l \|\Psi_l^-\|^2 \right. \\
&\quad \left. + \|\Psi_l^+\|_{grad, V_l}^2 \right)^{1/2} \\
&\quad \left(\|\nabla \tilde{\Psi}_l^+\|^2 + \|\tilde{\Psi}_l^+\|_{grad, V_l}^2 + (\sigma_l + \sigma_{s,l}) \|\tilde{\Psi}_l^+\|^2 + \|\Omega \tilde{\Psi}_l^-\|^2 + \sigma_l \|\tilde{\Psi}_l^-\|^2 \right. \\
&\quad \left. + \|\tilde{\Psi}_l^\chi\|_{\Omega, -1/2, \partial V_l}^2 \right)^{1/2} \\
&\leq (2 + \sigma_l + \sigma_{s,l}) \|\lambda_l\|_{\Lambda_l} \|\tilde{\lambda}_l\|_{\Lambda_{0,l}}
\end{aligned}$$

so that the continuity of K is proved.

For the LBB condition, assume $\sigma_l > \sigma_{s,l} > 0$ and consider $\hat{\lambda} = (\hat{\Psi}_l^+, \hat{\Psi}_l^-, \hat{\Psi}_l^\chi) \in \Lambda_0$ with

$$\begin{aligned}
\hat{\Psi}_l^+ &= 2\Psi_l^+ + \Psi_l^z \\
(\Omega \hat{\Psi}_l^-, \nabla \Psi_l^+ + \sigma_l \Omega \Psi_l^-)_n &= \left(-\frac{1}{\sigma_l} \nabla \Psi_l^+ - \Omega \Psi_l^- - \frac{1}{\sigma_l} \nabla \Psi_l^z, \nabla \Psi_l^+ + \sigma_l \Omega \Psi_l^- \right)_n \\
\hat{\Psi}_l^\chi &= \left(-3 + \frac{\sigma_s}{\sigma_l} \right) \Psi_l^\chi|_{\partial V_l, 0},
\end{aligned}$$

where $(\cdot, \cdot)_n$ denotes the scalar product in $[L^2(S \times V)_l]^n$, $\Psi_l^\chi|_{\partial V_l, 0}$ is the restriction

of Ψ_l^χ to $\partial V_l \setminus \partial V$ (extended by zero on $\partial V \cap \partial V_l$), and $\Psi_l^z \in H(\text{grad}, S \times V_l)$ is the weak solution of the auxiliary problem

$$\begin{cases} -\Delta \Psi_l^z + \sigma_l(\sigma_l - \sigma_{s,l}) \Psi_l^z = 0 & \text{in } V_l \\ \mathbf{n} \cdot \nabla \Psi_l^z = (\sigma_l - \sigma_{s,l}) \mathbf{n} \cdot \boldsymbol{\Omega} \Psi_l^\chi & \text{on } \partial V_l. \end{cases} \quad (\text{C.1})$$

Note that since $(\boldsymbol{\Omega} \hat{\Psi}_l^-, \nabla \Psi_l^+ + \sigma_l \boldsymbol{\Omega} \Psi_l^-)_n = (\hat{\Psi}_l^-, \boldsymbol{\Omega} \cdot \nabla \Psi_l^+ + \sigma_l \Psi_l^-)$, the above definition of $\hat{\Psi}_l^-$ specifies only its $L^2(S \times V_l)$ scalar product on a given $L^2(S \times V_l)$ element, namely $\boldsymbol{\Omega} \cdot \nabla \Psi_l^+ + \sigma_l \Psi_l^-$, which indeed belongs to $L^2(S \times V_l)$ since $\Psi_l^+ \in H(\text{grad}, S \times V_l) \subset H(\boldsymbol{\Omega} \cdot \nabla, S \times V_l)$ and $\Psi_l^- \in L^2(\boldsymbol{\Omega}, S \times V_l) = L^2(S \times V_l)$. Thus, this definition does not determine $\hat{\Psi}_l^-$ entirely, but only the existence of $\hat{\Psi}_l^-$ (not its uniqueness) is needed here.

Then, after some manipulations (including the addition and subtraction of the term $\int_S d\Omega \int_{V_l} dV \sigma_{s,l} \Psi_l^+ \Psi_l^z$), we obtain

$$\begin{aligned} K_l(\lambda, \hat{\lambda}) &= 2\sigma_l \|\Psi_l^+\|^2 + \frac{1}{\sigma_l} \|\nabla \Psi_l^+\|^2 + \sigma_l \|\Psi_l^-\|^2 + \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \Psi_l^\chi \Psi_l^z \\ &\quad - \int_S d\Omega \int_{V_l} dV 2\sigma_{s,l} \Psi_l^+ \int_S d\Omega' \Psi_l^+ \\ &\quad - \int_S d\Omega \int_{V_l} dV \sigma_{s,l} \Psi_l^z \left(\int_S d\Omega' \Psi_l^+ - \Psi_l^+ \right) \\ &\quad + \int_S d\Omega \int_{\partial V_l \cap \partial V} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \left(3 - \frac{\sigma_{s,l}}{\sigma_l} \right) \Psi_l^\chi \Psi_l^+. \end{aligned}$$

The last term is non-negative as soon as vacuum or reflected boundary conditions are enforced. Indeed, (3.13) shows that $\mathbf{\Omega} \cdot \mathbf{n} \Psi_l^\chi \Psi_l^+ = |\mathbf{\Omega} \cdot \mathbf{n}| (\Psi_l^\chi)^2$ on a vacuum boundary, while on a reflected boundary, the last term vanishes since

$$\begin{aligned} \int_{\partial V_l \cap \partial V} d\Gamma \int_S d\Omega \mathbf{\Omega} \cdot \mathbf{n} \Psi_l^\chi \Psi_l^+ \\ = \frac{1}{4\pi} \int_{\partial V_l \cap \partial V} d\Gamma \int_0^{2\pi} d\phi \left[\int_0^{\pi/2} d\theta \sin \theta \cos \theta \Psi_l^\chi(\theta, \phi) \Psi_l^+(\theta, \phi) \right. \\ \left. + \int_{\pi/2}^\pi d\theta \sin \theta \cos \theta \Psi_l^\chi(\theta, \phi) \Psi_l^+(\theta, \phi) \right] \end{aligned}$$

and the reflection condition $\Psi_l^{\chi(\text{resp.}+)}(\theta, \phi) = \Psi_l^{\chi(\text{resp.}+)}(\pi - \theta, \phi)$ implies

$$\int_{\pi/2}^\pi d\theta \sin \theta \cos \theta \Psi_l^\chi(\theta, \phi) \Psi_l^+(\theta, \phi) = \int_{\pi/2}^0 d\theta \sin \theta \cos \theta \Psi_l^\chi(\theta, \phi) \Psi_l^+(\theta, \phi).$$

Defining $\|\Psi_l\|_{grad, V_l, *}^2 = \|\nabla \Psi_l\|^2 + \sigma_l(\sigma_l - \sigma_{s,l}) \|\Psi_l\|^2$, $\|\Psi_l\|_{div, V_l, *}^2 = \|\nabla \cdot \Psi_l\|^2 + \sigma_l(\sigma_l - \sigma_{s,l}) \|\Psi_l\|^2$, and consequently $\|\Psi_l^\chi\|_{\Omega, -1/2, \partial V_l, *}$ as in (3.5) and (3.6), with starred norms replacing unstarred ones, we have that

$$\int_S d\Omega \int_{\partial V_l} d\Gamma \mathbf{\Omega} \cdot \mathbf{n} (\sigma_l - \sigma_{s,l}) \Psi_l^\chi \Psi_l^z = \|\Psi_l^z\|_{grad, V_l, *}^2$$

Then,

$$\begin{aligned} K_l(\lambda, \hat{\lambda}) &\geq 2(\sigma_l - \sigma_{s,l}) \|\Psi_l^+\|^2 + \frac{1}{\sigma_l} \|\nabla \Psi_l^+\|^2 + \sigma_l \|\Psi_l^-\|^2 \\ &\quad + \frac{1}{\sigma_l - \sigma_{s,l}} \|\Psi_l^z\|_{grad, V_l, *}^2 - \sigma_{s,l} \|\Psi_l^z\| \|\phi_l - \Psi_l^+\|, \end{aligned}$$

where $\phi_l = \int_S d\Omega \Psi_l^+$. Now, since for any Ψ , we can write without loss of generality

$\Psi = \sum_{n=0}^{\infty} \sum_{|m| \leq n} (\Psi, Y_{nm})_{\Omega} Y_{nm}$, we have

$$\begin{aligned} \|\Psi_l^-\|^2 &= \sum_{n=1, n \text{ odd}}^{\infty} \sum_{|m| \leq n} \|(\Psi_l^-, Y_{nm})_{\Omega}\|^2, \\ \|\phi_l - \Psi_l^+\|^2 &= \sum_{n=2, n \text{ even}}^{\infty} \sum_{|m| \leq n} \|(\Psi_l^+, Y_{nm})_{\Omega}\|^2. \end{aligned}$$

Thus if

$$(1 + \alpha_n) \sum_{|m| \leq n} \|(\Psi_l, Y_{nm})_{\Omega}\|^2 \geq \sum_{|m| \leq n} \|(\Psi_l, Y_{n+1, m})_{\Omega}\|^2 \text{ for any } n \geq 1, n \text{ odd},$$

then $(1 + \alpha_n) \|\Psi_l^-\|^2 \geq \|\phi_l - \Psi_l^+\|^2$, and we can write

$$\begin{aligned} K_l(\lambda, \hat{\lambda}) &\geq 2(\sigma_l - \sigma_{s,l}) \|\Psi_l^+\|^2 + \frac{1}{\sigma_l} \|\nabla \Psi_l^+\|^2 + \sigma_l \|\Psi_l^-\|^2 \\ &\quad + \frac{1}{\sigma_l - \sigma_{s,l}} \|\Psi_l^z\|_{grad, V_l, *}^2 - \frac{1}{2} \sigma_{s,l} (\|\Psi_l^z\|^2 + (1 + \alpha_n) \|\Psi_l^-\|^2), \end{aligned}$$

The coefficient of $\|\Psi^-\|^2$ is thus $\sigma_l - \frac{1}{2}\sigma_{s,l}(1 + \alpha_n)$ which is strictly positive for all l if the angular flux Ψ_l is assumed mildly anisotropic. With the starred norms introduced above, we have $\|\Psi_l^z\|^2 \leq \frac{1}{\sigma_l(\sigma_l - \sigma_{s,l})} \|\Psi_l^z\|_{grad, V_l, *}^2$ and the coefficient of $\|\Psi_l^z\|_{grad, V_l, *}^2$ is $\frac{1}{\sigma_l - \sigma_{s,l}}(1 - \frac{\sigma_{s,l}}{2\sigma_l})$, thus as well strictly positive. Furthermore, from (C.1), $\|\Psi_l^z\|_{grad, V_l, *}$ is directly proportional to $\|\Psi_l^x\|_{\Omega, -1/2, \partial V_l, *}$, while $\|\cdot\|_{\Omega, -1/2, \partial V_l, *}$ and $\|\cdot\|_{\Omega, -1/2, \partial V_l}$ are equivalent norms. Thus, there is a strictly positive constant C_l such that

$$K_l(\lambda, \hat{\lambda}) \geq C_l \|\lambda_l\|_{\Lambda_0, l}^2$$

provided we can assume mild anisotropy in each V_l . Since we also have $\|\hat{\lambda}_l\|_{\Lambda_0, l}^2 \leq C'_l \|\lambda_l\|_{\Lambda_l}^2$ for another strictly positive constant C'_l , we obtain

$$K_l(\lambda, \hat{\lambda}) \geq \frac{C_l}{\sqrt{C'_l}} \|\lambda_l\|_{\Lambda_l} \|\hat{\lambda}_l\|_{\Lambda_0, l}.$$

Thus there is a constant $\beta > 0$ such that

$$\sup_{\tilde{\lambda} \in \Lambda_0, \tilde{\lambda} \neq 0} \frac{K(\lambda, \tilde{\lambda})}{\|\tilde{\lambda}\|_{\Lambda_0}} \geq \beta \|\lambda\|_{\Lambda} \quad \forall \lambda \in \Lambda,$$

and the LBB condition

$$\inf_{\lambda \in \Lambda, \lambda \neq 0} \sup_{\tilde{\lambda} \in \Lambda_0, \tilde{\lambda} \neq 0} \frac{K(\lambda, \tilde{\lambda})}{\|\lambda\|_{\Lambda} \|\tilde{\lambda}\|_{\Lambda_0}} \geq \beta$$

is satisfied. Besides, the symmetry of $K(\lambda, \tilde{\lambda})$ leads to

$$\sup_{\lambda \in \Lambda, \|\lambda\|_{\Lambda}=1} K(\lambda, \tilde{\lambda}) > 0 \quad \forall \tilde{\lambda} \in \Lambda_0 \quad \text{with} \quad \tilde{\lambda} \neq 0.$$

Alternative proof in the even-order primal case In the absence of the mild anisotropy assumption, well-posedness can be proved with the assumption $0 < \sigma_{s,l} < \frac{4}{5}\sigma_l$ for all l . Indeed, consider $\hat{\lambda} = (\hat{\Psi}_l^+, \hat{\Psi}_l^-, \hat{\Psi}_l^\chi) \in \Lambda_0$ with

$$\begin{aligned} \hat{\Psi}_l^+ &= 2\Psi_l^+ + \sigma_l \Psi_l^z \\ (\Omega \hat{\Psi}_l^-, \nabla \Psi_l^+ + \sigma_l \Omega \Psi_l^-)_n &= \left(-\frac{1}{\sigma_l} \nabla \Psi_l^+ - \Omega \Psi_l^- - \frac{1}{\sigma_l} \nabla \Psi_l^z, \nabla \Psi_l^+ + \sigma_l \Omega \Psi_l^-\right)_n \\ \hat{\Psi}_l^\chi &= -3 \Psi_l^\chi|_{\partial V_l, 0}, \end{aligned}$$

where $\Psi_l^z \in H(\text{grad}, S \times V_l)$ is the weak solution of the auxiliary problem

$$\begin{cases} -\Delta \Psi_l^z + \sigma_l^2 \Psi_l^z = 0 & \text{in } V_l \\ \mathbf{n} \cdot \nabla \Psi_l^z = \sigma_l \mathbf{n} \cdot \Omega \Psi_l^\chi & \text{on } \partial V_l. \end{cases} \quad (\text{C.2})$$

Then, some manipulations yield

$$\begin{aligned}
K_l(\lambda, \hat{\lambda}) &= 2\sigma_l \|\Psi_l^+\|^2 + \frac{1}{\sigma_l} \|\nabla \Psi_l^+\|^2 + \sigma_l \|\Psi_l^-\|^2 + \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \Psi_l^x \Psi_l^z \\
&\quad - \int_S d\Omega \int_{V_l} dV \left(\sigma_{s,l} [2\Psi_l^+ + \Psi_l^z] \int_S d\Omega \Psi_l^+ \right) \\
&\quad + \int_S d\Omega \int_{\partial V_l \cap \partial V} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} (3\sigma_l) \Psi_l^x \Psi_l^+.
\end{aligned}$$

The last term is again non-negative as soon as vacuum or reflected boundary conditions are enforced. Defining this time $\|\Psi_l\|_{grad, V_l, *}^2 = \|\nabla \Psi_l\|^2 + \sigma_l^2 \|\Psi_l\|^2$, $\|\Psi_l\|_{div, V_l, *}^2 = \|\nabla \Psi_l\|^2 + \sigma_l^2 \|\Psi_l\|^2$ (and consequently $\|\Psi^x\|_{\Omega, -1/2, \partial V_l, *}$ as in (3.5) and (3.6) with starred norms replacing unstarred ones), we have

$$\int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \sigma_l \Psi_l^x \Psi_l^z = \|\Psi_l^z\|_{grad, V_l, *}^2.$$

Then,

$$\begin{aligned}
K_l(\lambda, \hat{\lambda}) &\geq 2(\sigma_l - \sigma_{s,l}) \|\Psi_l^+\|^2 + \frac{1}{\sigma_l} \|\nabla \Psi_l^+\|^2 + \sigma_l \|\Psi_l^-\|^2 \\
&\quad + \frac{1}{\sigma_l} \|\Psi_l^z\|_{grad, V_l, *}^2 - \sigma_{s,l} \int_{V_l} dV \left(\int_S d\Omega \Psi_l^+ \int_S d\Omega \Psi_l^z \right).
\end{aligned}$$

Now, with

$$\int_{V_l} dV \left(\int_S d\Omega \Psi_l^+ \int_S d\Omega \Psi_l^z \right) \leq \|\Psi_l^+\| \|\Psi_l^z\| \leq \frac{1}{2} (\|\Psi_l^+\|^2 + \|\Psi_l^z\|^2),$$

and $\|\Psi_l^z\|^2 \leq \frac{1}{\sigma_l^2} \|\Psi_l^z\|_{grad, V_l, *}^2$, we have

$$\begin{aligned} K_l(\lambda, \hat{\lambda}) &\geq (2\sigma_l - \frac{5}{2}\sigma_{s,l}) \|\Psi_l^+\|^2 + \frac{1}{\sigma_l} \|\nabla \Psi_l^+\|^2 + \sigma_l \|\Psi_l^-\|^2 \\ &\quad + \frac{1}{\sigma_l} \left(1 - \frac{1}{2} \frac{\sigma_{s,l}}{\sigma_l}\right) \|\Psi_l^z\|_{grad, V_l, *}^2. \end{aligned}$$

From (C.2), $\|\Psi_l^z\|_{grad, V_l, *}$ is directly proportional to $\|\Psi_l^x\|_{\Omega, -1/2, \partial V_l, *}$, while $\|\cdot\|_{\Omega, -1/2, \partial V_l, *}$ and $\|\cdot\|_{\Omega, -1/2, \partial V_l}$ are equivalent norms. There is thus a strictly positive constant C_l such that

$$K_l(\lambda, \hat{\lambda}) \geq C_l \|\lambda_l\|_{\Lambda_0, l}^2$$

provided $0 < \sigma_{s,l} < \frac{4}{5}\sigma_l$. We conclude as before that the LBB condition is satisfied under this condition.

Odd-order primal method

We define here

$$\Lambda = X_\Omega \times L^2(S \times V) \times H^{1/2}(S \times \Gamma),$$

$$\Lambda_0 = X_\Omega \times L^2(S \times V) \times H_0^{1/2}(S \times \Gamma),$$

$\lambda = (\Psi^+, \Psi^-, \Psi^\chi) \in \Lambda$ and $\tilde{\lambda} = (\tilde{\Psi}^+, \tilde{\Psi}^-, \tilde{\Psi}^\chi) \in \Lambda_0$. As for norms, we have $\|\lambda\|_\Lambda^2 = \|\Psi^+\|_{X_\Omega}^2 + \|\Psi^-\|^2 + \|\Psi^\chi\|_{1/2,\Gamma}^2$. The bilinear form $K(\lambda, \tilde{\lambda})$, as well as the problem to solve, are formally the same as in the even-order case, but the functional spaces are different. We thus check the continuity and the LBB condition for K within this new framework.

For continuity, with this time t_l the trace operator from $H(\mathbf{\Omega} \cdot \nabla, S \times V_l)$ to $H_\Omega^{-1/2}(S \times \partial V_l)$, we have

$$\begin{aligned} \int_S d\Omega \int_{\partial V_l} d\Gamma \mathbf{\Omega} \cdot \mathbf{n} \Psi_l^+ \Psi_l^\chi &\leq \|t_l(\Psi_l^+)\|_{\mathbf{\Omega}, -1/2, \partial V_l} \|\Psi_l^\chi\|_{1/2, \partial V_l} \\ &\leq \|\mathbf{\Omega} \Psi_l^+\|_{div, V_l} \|\Psi_l^\chi\|_{1/2, \partial V_l} \\ &\leq \|\Psi_l^+\|_{\mathbf{\Omega} \cdot \nabla, V_l} \|\Psi_l^\chi\|_{1/2, \partial V_l} \end{aligned}$$

where we used (3.5) and (3.6). Then the Schwartz inequality yields

$$\begin{aligned}
K_l(\lambda, \tilde{\lambda}) &\leq \|\mathbf{\Omega} \cdot \nabla \tilde{\Psi}_l^+\| \|\Psi_l^-\| + \|\Psi_l^x\|_{1/2, \partial V_l} \|\tilde{\Psi}_l^+\|_{\mathbf{\Omega} \cdot \nabla, l} + (\sigma_l + \sigma_{s,l}) \|\tilde{\Psi}_l^+\| \|\Psi_l^+\| \\
&\quad + \|\tilde{\Psi}_l^-\| \|\mathbf{\Omega} \cdot \nabla \Psi_l^+\| + \sigma_l \|\tilde{\Psi}_l^-\| \|\Psi_l^-\| + \|\Psi_l^x\|_{1/2, \partial V_l} \|\Psi_l^+\|_{\mathbf{\Omega} \cdot \nabla, l} \\
&\leq \text{constant} \|\lambda\|_{\Lambda_l} \|\tilde{\lambda}\|_{\Lambda_{0,l}}
\end{aligned}$$

Next, the LBB condition can be proved adapting what is done in the even-order case. The $\hat{\lambda}$ to consider here is

$$\begin{aligned}
\hat{\Psi}_l^+ &= 2\Psi_l^+ + \Psi_l^z \\
\hat{\Psi}_l^- &= -\frac{1}{\sigma_l} \mathbf{\Omega} \cdot \nabla \Psi_l^+ - \Psi_l^- - \frac{1}{\sigma_l} \mathbf{\Omega} \cdot \nabla \Psi_l^z \\
\hat{\Psi}_l^x &= \left(-3 + \frac{\sigma_l}{\sigma_{s,l}}\right) \Psi_l^x|_{\partial V_l, 0},
\end{aligned}$$

where $\Psi_l^z \in H(\mathbf{\Omega} \cdot \nabla, S \times V_l)$ is the weak solution of the auxiliary problem

$$\begin{cases} -\nabla(\mathbf{\Omega} \cdot \nabla \Psi_l^z) + \sigma_l(\sigma_{s,l} - \sigma_l) \mathbf{\Omega} \Psi_l^z = 0 & \text{in } V_l \\ \mathbf{\Omega} \cdot \nabla \Psi_l^z = (\sigma_l - \sigma_{s,l}) \Psi_l^x & \text{on } \partial V_l. \end{cases}$$

Alternative proof in the odd-order primal case Again, the mild anisotropy assumption can be replaced by the assumption $0 < \sigma_{s,l} < \frac{4}{5}\sigma_l$, using

$$\begin{aligned}\hat{\Psi}_l^+ &= 2\Psi_l^+ + \Psi_l^z \\ \hat{\Psi}_l^- &= -\frac{1}{\sigma_l}\boldsymbol{\Omega} \cdot \nabla \Psi_l^+ - \Psi_l^- - \frac{1}{\sigma_l}\boldsymbol{\Omega} \cdot \nabla \Psi_l^z \\ \hat{\Psi}_l^\chi &= -3\Psi_l^\chi|_{\partial V_l,0},\end{aligned}$$

where $\Psi_l^z \in H(\boldsymbol{\Omega} \cdot \nabla, S \times V_l)$ is the weak solution of

$$\begin{cases} -\nabla(\boldsymbol{\Omega} \cdot \nabla \Psi_l^z) + \sigma_l^2 \boldsymbol{\Omega} \Psi_l^z = 0 & \text{in } V_l \\ \boldsymbol{\Omega} \cdot \nabla \Psi_l^z = \sigma_l \Psi_l^\chi & \text{on } \partial V_l. \end{cases}$$

C.1.2 Proofs for the dual case

Even-order dual method

Here we define

$$\Lambda = X_\Omega \times L^2(S \times V_l) \times H^{1/2}(S \times \Gamma),$$

$$\Lambda_0 = X_\Omega \times L^2(S \times V_l) \times H_0^{1/2}(S \times \Gamma),$$

$\lambda = (\Psi^-, \Psi^+, \Psi^\psi) \in \Lambda$ and $\tilde{\lambda} = (\tilde{\Psi}^-, \tilde{\Psi}^+, \tilde{\Psi}^\psi) \in \Lambda_0$. As for norms, we have $\|\lambda\|_\Lambda^2 = \|\Psi^-\|_{X_\Omega}^2 + \|\Psi^+\|^2 + \|\Psi^\psi\|_{1/2,\Gamma}^2$. Define then

$$K(\lambda, \tilde{\lambda}) = \sum_l K_l(\lambda, \tilde{\lambda}),$$

where

$$\begin{aligned} K_l(\lambda, \tilde{\lambda}) &= - \int_S d\Omega \int_{V_l} dV \tilde{\Psi}_l^+ \boldsymbol{\Omega} \cdot \nabla \Psi_l^- - \int_S d\Omega \int_{V_l} dV \sigma_l \tilde{\Psi}_l^+ \Psi_l^+ \\ &\quad + \int_S d\Omega \int_{V_l} dV \sigma_{s,l} (\tilde{\Psi}_l^+ \int_S d\Omega' \Psi_l^+) - \int_S d\Omega \int_{V_l} dV \Psi_l^+ \boldsymbol{\Omega} \cdot \nabla \tilde{\Psi}_l^- \\ &\quad + \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}_l^- \Psi_l^\psi + \int_S d\Omega \int_{V_l} dV \sigma_l \tilde{\Psi}_l^- \Psi_l^- \\ &\quad + \int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \tilde{\Psi}_l^\psi \Psi_l^-. \end{aligned}$$

With

$$\langle s, \tilde{\Psi}^+ \rangle = \sum_l \int_S d\Omega \int_{V_l} dV s \tilde{\Psi}_l^+,$$

we have to examine the problem: find $\lambda \in \Lambda$ such that

$$K(\lambda, \tilde{\lambda}) = \langle s, \tilde{\Psi}^+ \rangle, \quad \forall \tilde{\lambda} \in \Lambda_0.$$

From there, we can check the continuity and the LBB condition for K in a way similar to what we did in the odd-order primal case.

Odd-order dual method

We define in this case

$$\Lambda = X \times L^2(\Omega, S \times V) \times H_{\Omega}^{-1/2}(S \times \Gamma),$$

$$\Lambda_0 = X \times L^2(\Omega, S \times V) \times H_{\Omega,0}^{-1/2}(S \times \Gamma),$$

$\lambda = (\Psi^-, \Psi^+, \Psi^x) \in \Lambda$ and $\tilde{\lambda} = (\tilde{\Psi}^-, \tilde{\Psi}^+, \tilde{\Psi}^x) \in \Lambda_0$. As for norms, we have $\|\lambda\|_{\Lambda}^2 = \|\Psi^+\|_X^2 + \|\Psi^-\|^2 + \|\Psi^x\|_{\Omega, -1/2, \Gamma}^2$. The bilinear form $K(\lambda, \tilde{\lambda})$ is formally the same as in the even-order dual case. The continuity and LBB condition for K can be proved in a way similar to what was done in the even-order primal case.

C.2 Discrete problems (Theorem 3.4.2)

C.2.1 Proofs for the primal case

Even-order primal method

We introduce

$$\Lambda_h = P_h^{N,p} \times M_h^{N,m} \times B_h^{N,b} \text{ and } \Lambda_{0,h} = P_h^{N,p} \times M_h^{N,m} \times B_{0,h}^{N,b},$$

where the different finite-dimensional spaces were defined in section 3.3. We define Π_l^+ and Π_l^- as the orthogonal projections of $H(\text{grad}, S \times V_l)$ and $[L^2(S \times V_l)]^n$ (with respect to their scalar product) respectively onto $P_h^{N,p}$ and $\Omega M_h^{N,m}$.

We define $\hat{\lambda}_h = (\hat{\Psi}_h^+, \hat{\Psi}_h^-, \hat{\Psi}_h^\chi) \in \Lambda_{0,h}$ with

$$\begin{aligned} \hat{\Psi}_{h,l}^+ &= 2\Psi_{h,l}^+ + \Pi_l^+(\Psi_{h,l}^z) \\ (\Omega \hat{\Psi}_{h,l}^-, \nabla \Psi_l^+ + \sigma_l \Omega \Psi_l^-)_n &= \left(-\frac{1}{\sigma_l} \Pi_l^-(\nabla \Psi_{h,l}^+) - \Omega \Psi_{h,l}^- - \frac{1}{\sigma_l} \Pi_l^-(\nabla \Pi_l^+(\Psi_{h,l}^z))\right), \\ &\quad \nabla \Psi_l^+ + \sigma_l \Omega \Psi_l^-)_n \\ \hat{\Psi}_{h,l}^\chi &= \left(-3 + \frac{\sigma_{s,l}}{\sigma_l}\right) \Psi_{h,l}^\chi|_{\partial V_l,0} \end{aligned}$$

where $\Psi_{h,l}^z \in H(\text{grad}, S \times V_l)$ is the weak solution of

$$\begin{cases} -\Delta \Psi_{h,l}^z + \sigma_l (\sigma_l - \sigma_{s,l}) \Psi_{h,l}^z = 0 & \text{in } S \times V_l \\ \mathbf{n} \cdot \nabla \Psi_{h,l}^z = (\sigma_l - \sigma_{s,l}) \mathbf{n} \cdot \boldsymbol{\Omega} \Psi_{h,l}^x & \text{on } S \times \partial V_l. \end{cases}$$

We define as in the primal even continuous case $\|\Psi_l\|_{grad, V_l, *}^2 = \|\nabla \Psi_l\|^2 + \sigma_l (\sigma_l - \sigma_{s,l}) \|\Psi_l\|^2$ such that

$$\|\Pi_l^+ \Psi_{h,l}^z\|_{grad, V_l, *}^2 = (\sigma_l - \sigma_{s,l}) \int_S d\Omega \int_{V_l} dV \mathbf{n} \cdot \boldsymbol{\Omega} \Psi_{h,l}^x \Pi_l^+(\Psi_{h,l}^z).$$

Orthogonal projections properties provide

$$(\nabla \Psi_{h,l}^+, \Pi_l^-(\nabla \Psi_{h,l}^+)) = \|\Pi_l^-(\nabla \Psi_{h,l}^+)\|^2 \quad \forall \Psi_{h,l}^+ \in P_h^{N,p}(V_l)$$

$$(\boldsymbol{\Omega} \Psi_{h,l}^-, \nabla \Psi_{h,l}^+ - \Pi_l^-(\nabla \Psi_{h,l}^+)) = 0 \quad \forall \Psi_{h,l}^- \in M_h^{N,m}(V_l)$$

$$(\boldsymbol{\Omega} \Psi_{h,l}^-, \nabla \Pi_l^+(\Psi_{h,l}^z) - \Pi_l^-(\nabla \Pi_l^+(\Psi_{h,l}^z))) = 0 \quad \forall \Psi_{h,l}^- \in M_h^{N,m}(V_l).$$

Then some manipulations using these properties lead to

$$\begin{aligned}
K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) &= 2\sigma_l \|\Psi_{h,l}^+\|^2 + \frac{1}{\sigma_l} \|\Pi_l^-(\nabla \Psi_{h,l}^+)\|^2 + \sigma_l \|\Psi_{h,l}^-\|^2 \\
&\quad + \frac{1}{\sigma_l - \sigma_{s,l}} \|\Pi_l^+(\Psi_{h,l}^z)\|_{grad, V_l, *}^2 \\
&\quad + \frac{1}{\sigma_l} \int_S d\Omega \int_{V_l} dV (\nabla \Psi_{h,l}^+) (\Pi_l^-(\nabla \Pi_l^+(\Psi_{h,l}^z)) - \nabla \Pi_l^+(\Psi_{h,l}^z)) \\
&\quad - \int_S d\Omega \int_{V_l} dV 2\sigma_{s,l} \Psi_{h,l}^+ \int_S d\Omega' \Psi_{h,l}^+ \\
&\quad - \int_S d\Omega \int_{V_l} dV \sigma_{s,l} \Pi_l^+(\Psi_{h,l}^z) \left(\int_S d\Omega' \Psi_{h,l}^+ - \Psi_{h,l}^+ \right) \\
&\quad + \int_S d\Omega \int_{\partial V_l \cap \partial V} d\Gamma \left(3 - \frac{\sigma_{s,l}}{\sigma_l} \right) \Psi_{h,l}^x \Psi_{h,l}^+.
\end{aligned}$$

The last term can again be proved non-negative when reflected or vacuum boundary conditions are imposed. Besides, mild anisotropy implies $(1 + \alpha_n) \|\Psi_{h,l}^-\|^2 \geq \|\phi_{h,l} - \Psi_{h,l}^+\|^2$, and since $\|\Psi_{h,l}^z\|^2 \leq \frac{1}{\sigma_l(\sigma_l - \sigma_{s,l})} \|\Psi_{h,l}^z\|_{grad, V_l, *}^2$ for any $\Psi_l \in H(grad, S \times V_l)$, we can write

$$\begin{aligned}
K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) &\geq 2(\sigma_l - \sigma_{s,l}) \|\Psi_{h,l}^+\|^2 + \frac{1}{\sigma_l} \|\Pi_l^-(\nabla \Psi_{h,l}^+)\|^2 \\
&\quad + \left(\sigma_l - \frac{1}{2}(1 + \alpha_n) \sigma_{s,l} \right) \|\Psi_{h,l}^-\|^2 \\
&\quad + \frac{1}{\sigma_l - \sigma_{s,l}} \left(1 - \frac{1}{2} \frac{\sigma_{s,l}}{\sigma_l} \right) \|\Pi_l^+(\Psi_{h,l}^z)\|_{grad, V_l, *}^2 \\
&\quad + \frac{1}{\sigma_l} \int_S d\Omega \int_{V_l} dV (\nabla \Psi_{h,l}^+) (\Pi_l^-(\nabla \Pi_l^+(\Psi_{h,l}^z)) - \nabla \Pi_l^+(\Psi_{h,l}^z)).
\end{aligned}$$

Thus there exist a constant $C_l > 0$ such that

$$\begin{aligned} K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) &\geq C_l (\|\Psi_{h,l}^+\|^2 + \|\Pi_l^-(\nabla\Psi_{h,l}^+)\|^2 + \|\Psi_{h,l}^-\|^2 + \|\Pi_l^+(\Psi_{h,l}^z)\|_{grad, V_l, *}^2) \\ &\quad + \frac{1}{\sigma_l} \int_S d\Omega \int_{V_l} dV (\nabla\Psi_{h,l}^+) (\Pi_l^-(\nabla\Pi_l^+(\Psi_{h,l}^z)) - \nabla\Pi_l^+(\Psi_{h,l}^z)). \end{aligned}$$

We now introduce the parameters

$$\begin{aligned} \mu_l &= \mu_l(P_h^{N,p}, B_h^{N,b}) = \inf_{\Psi_{h,l}^x \in B_h^{N,b}} \frac{\|\Pi_l^+(\Psi_{h,l}^z)\|_{grad, V_l, *}^2}{\|\Psi_{h,l}^x\|_{\Omega, -1/2, \partial V_l}^2}, \\ \nu_l &= \nu_l(P_h^{N,p}, M_h^{N,m}) = \inf_{\Psi_{h,l}^+ \in P_h^{N,p}} \frac{\|\Pi_l^-(\nabla\Psi_{h,l}^+)\|^2}{\|\nabla\Psi_{h,l}^+\|^2}, \\ \gamma_l &= \gamma_l(P_h^{N,p}, M_h^{N,m}) = \sup_{\Psi_{h,l}^+ \in P_h^{N,p}} \frac{\|\nabla\Psi_{h,l}^+ - \Pi_l^-(\nabla\Psi_{h,l}^+)\|}{\|\nabla\Psi_{h,l}^+\|}, \end{aligned}$$

and note that they are all contained in the interval $[0, 1]$. Then

$$\begin{aligned} K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) &\geq C_l (\|\Psi_{h,l}^+\|^2 + \nu_l \|\nabla\Psi_{h,l}^+\|^2 + \|\Psi_{h,l}^-\|^2 + \mu_l \|\Psi_{h,l}^x\|_{\Omega, -1/2, l}^2) \\ &\quad - \gamma_l \|\nabla\Psi_{h,l}^+\| \|\nabla\Pi_l^+(\Psi_{h,l}^z)\|. \end{aligned}$$

Using $\|\nabla\Pi_l^+(\Psi_{h,l}^z)\| \leq \|\Psi_{h,l}^z\|_{grad, V_l, *}$ as well as the direct proportionality between $\|\Psi_{h,l}^z\|_{grad, V_l, *}$ and $\|\Psi_{h,l}^x\|_{\Omega, -1/2, \partial V_l}^2$, we obtain that there exists a constant $k > 0$ such

that

$$K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) \geq C_l \left(\|\Psi_{h,l}^+\|^2 + (\nu_l - \frac{1}{2}\gamma_l) \|\nabla \Psi_{h,l}^+\|^2 + \|\Psi_{h,l}^-\|^2 + (\mu_l - k\gamma_l) \|\Psi_{h,l}^x\|_{\Omega, -1/2, \partial V_l}^2 \right)$$

that is

$$K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) \geq C_l \min(1, \nu_l - \frac{1}{2}\gamma_l, \mu_l - k\gamma_l) \|\lambda\|_{\Lambda}^2.$$

Also there is a constant $C'_l > 0$ such that

$$\|\hat{\lambda}_l\|_{\Lambda_{0,l}}^2 \leq C'_l \|\lambda_l\|_{\Lambda_l}^2.$$

The LBB condition is thus satisfied provided

$$\min(1, \nu_l - \frac{1}{2}\gamma_l, \mu_l - k\gamma_l) > 0. \tag{C.3}$$

In case $\nabla P_h^{N,p} \subset \mathbf{\Omega} M_h^{N,m}$ in any V_l , which occurs as soon as $p - 1 \leq m$ and $N^+ \leq N^- + 1$, we get $\nu_l = 1$ and $\gamma_l = 0$. Then, the condition becomes $\mu_l > 0$. Similarly to what is proved in Babuška, Oden, and Lee (1977), we have:

Lemma C.2.1 *The parameter $\mu_l > 0$ if and only if, for any $\Psi_{h,l}^x \in B_h^{N,b}(V_l)$,*

$$\int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \Psi_{h,l}^x \Psi_{h,l}^+ = 0 \quad \forall \Psi^+ \in P_h^{N,p}(V_l) \text{ implies that } \Psi_{h,l}^x = 0. \quad (\text{C.4})$$

Proof C.2.1 *If we suppose $\mu_l = 0$, then by the definition of μ_l there exist a non-zero*

$\Psi_{h,l}^x \in B_h^{N,b}(V_l)$ such that

$$\|\Pi_l^+(\Psi_{h,l}^z)\|_{grad, V_l, *}^2 = 0. \quad (\text{C.5})$$

*Since $\int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \Psi_{h,l}^x \Psi_{h,l}^+ = \frac{1}{\sigma_l - \sigma_{s,l}} (\Psi_{h,l}^+, \Pi^+(\Psi_{h,l}^z))_{grad, V_l, *}$, (C.4) and (C.5) imply $\Psi_{h,l}^x = 0$, a contradiction. Now take $\mu_l > 0$. Then, if $\Psi_{h,l}^x \neq 0$,*

$$\int_S d\Omega \int_{\partial V_l} d\Gamma \boldsymbol{\Omega} \cdot \mathbf{n} \Psi_{h,l}^x \Pi_l^+(\Psi_{h,l}^z) \neq 0,$$

which is the contrapositive of (C.4).

As discussed in section 3.4.2, condition (C.4) is in fact equivalent to a spatio-angular rank condition.

In (C.3), ν_l and γ_l do not depend on h , but μ_l does. To ensure stability of the method, we should therefore show the existence of a lower bound for μ_l as $h \rightarrow 0$. This can probably be done adapting what is done at the end of section B.2 in the $P1$ case.

Odd-order primal method

The spaces Λ_h and $\Lambda_{0,h}$ are formally the same as in the even-order case, but the definition of the approximation spaces $P_h^{N,p}$, $M_h^{N,m}$ and $B_h^{N,b}$ differ as explained in section 3.3. We here define Π_l^+ and Π_l^- as the orthogonal projections of $H(\mathbf{\Omega} \cdot \nabla, S \times V_l)$ and $L^2(S \times V_l)$ respectively onto $P_h^{N,p}$ and $M_h^{N,m}$.

The LBB condition can be proved here using $\hat{\lambda}_h = (\hat{\Psi}_h^+, \hat{\Psi}_h^-, \hat{\Psi}_h^\chi) \in \Lambda_{0,h}$ with

$$\begin{aligned}\hat{\Psi}_{h,l}^+ &= 2\Psi_l^+ + \Pi_l^+(\Psi_{h,l}^z) \\ \hat{\Psi}_{h,l}^- &= -\frac{1}{\sigma_l}\Pi_l^-(\mathbf{\Omega} \cdot \nabla\Psi_l^+) - \Psi_l^- - \frac{1}{\sigma_l}\Pi_l^-(\mathbf{\Omega} \cdot \nabla\Pi_l^+(\Psi_{h,l}^z)) \\ \hat{\Psi}_{h,l}^\chi &= -(3 + \frac{\sigma_{s,l}}{\sigma_l})\Psi_l^\chi|_{\partial V_l,0},\end{aligned}$$

where $\Psi^z \in H(\mathbf{\Omega} \cdot \nabla, S \times V_l)$ is the weak solution of the auxiliary problem

$$\begin{cases} -\nabla(\mathbf{\Omega} \cdot \nabla\Psi^z) + \sigma_l(\sigma_{s,l} - \sigma_l)\mathbf{\Omega}\Psi^z = 0 & \text{in } V_l \\ \mathbf{\Omega} \cdot \nabla\Psi^z = (\sigma_l - \sigma_{s,l})\Psi^\chi & \text{on } \partial V_l. \end{cases}$$

The proof follows the same lines as in C.2.1. The parameter μ_l , ν_l and γ_l involved

here become

$$\begin{aligned}\mu_l &= \mu_l(P_h^{N,p}, B_h^{N,b}) = \inf_{\Psi_{h,l}^x \in B_h^{N,b}} \frac{\|\Pi_l^+(\Psi_{h,l}^z)\|_{\Omega \cdot \nabla, V_l, *}^2}{\|\Psi_{h,l}^x\|_{1/2, \partial V_l}^2}, \\ \nu_l &= \nu_l(P_h^{N,p}, M_h^{N,m}) = \inf_{\Psi_{h,l}^+ \in P_h^{N,p}} \frac{\|\Pi_l^-(\Omega \cdot \nabla \Psi_{h,l}^+)\|^2}{\|\Omega \cdot \nabla \Psi_{h,l}^+\|^2}, \\ \gamma_l &= \gamma_l(P_h^{N,p}, M_h^{N,m}) = \sup_{\Psi_{h,l}^+ \in P_h^{N,p}} \frac{\|\Omega \cdot \nabla \Psi_{h,l}^+ - \Pi_l^-(\Omega \cdot \nabla \Psi_{h,l}^+)\|}{\|\Omega \cdot \nabla \Psi_{h,l}^+\|}.\end{aligned}$$

In case $\Omega \cdot \nabla P_h^{N,p} \subset M_h^{N,m}$, which occurs as soon as $p-1 \leq m$ and $N^+ + 1 \leq N^-$, we get $\nu_l = 1$, $\gamma_l = 0$, and one can again show that the LBB condition becomes $\mu_l > 0$.

Lemma C.2.1 remains valid in this case.

C.2.2 Proofs for the dual case

Roughly speaking, the roles of $P_h^{N,p}$ and $M_h^{N,m}$ are swapped when going from primal to dual. Working with the finite-dimensional subspaces

$$\Lambda_h = M_h^{N,m} \times P_h^{N,p} \times B_h^{N,b} \text{ and } \Lambda_{0,h} = M_h^{N,m} \times P_h^{N,p} \times B_{0,h}^{N,b},$$

we can again verify the LBB condition.