

# Discretization Methods for the Diffusion Equation

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## Abstract

The diffusion equation arising from neutronics is an elliptic partial differential equation of the form  $-div(p \mathbf{grad} u) + cu = f$ . Continuous second order, second order hybrid, mixed and mixed-hybrid formulations are investigated theoretically, each of them in a primal and dual version. A nodal finite element scheme is applied to the mixed-hybrid formulations. Well-posedness is investigated each time. A linear system is obtained, and early numerical results are provided.

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## 1 Introduction

The time-independent mono-energetic diffusion equation (with isotropic scattering and sources) considered here arises in nuclear engineering reactor core

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calculations. This elliptic equation is the lowest-order angular approximation of the linear Boltzmann transport equation, where the flux is supposed to be linearly anisotropic. Even though the neutronic application context clearly affects the notations in the sequel, its generality makes it relevant to other applications.

Various formulations were developed to discretize second order partial differential equations ([1], [2], [3], [4], [5]) and in particular the diffusion equation in the neutronic community ([6], [7], [8]). This work wants to first classify different solution methods for the diffusion equation, namely the second order, second order hybrid, mixed and mixed-hybrid methods, each time in both primal and dual versions. (In the taxonomy of Lindahl and Weiss [9], the primal formulation corresponds to a Neumann or  $T^{-1}$  formulation, while the dual one corresponds to a Dirichlet or  $T$  formulation.) Second order methods have been extensively investigated in the literature ([10] for instance). Second order hybrid and mixed methods have been frequently studied as well (see [1] and [2] for example), but mostly for the Poisson problem or its generalized version  $\text{div}(p\mathbf{grad}u) = f$ , which does not cover the diffusion equation (actually it covers only the pure scattering case). Mixed-hybrid methods are less studied in the literature than the others. Nevertheless, Arnold and Brezzi [11] studied the dual mixed-hybrid finite element method for the generalized Poisson problem, and Babuska, Oden and Lee [12] developed a primal mixed-hybrid finite element method for the equation  $-\Delta u + u = f$  with Dirichlet boundary conditions.

For the problem discretization itself, we use a nodal finite element approximation in order to ensure particle conservation over each element. Two well-known finite element discretizations of the dual mixed formulation for second order elliptic problems have been carried out: the first by Raviart and Thomas [13], and the second by Brezzi, Douglas and Marini [14]. The first was originally developed for the Poisson equation in 2D, then extended by Nedelec to 3D [15], and extended to the elliptic problem  $-\text{div}(p\mathbf{grad}u) + \mathbf{q}\cdot\mathbf{grad}u + cu = f$  by Douglas and Roberts [16], [17]. Thus it includes the diffusion problem in the mixed dual form. As for the second, it applies to general elliptic problems and includes the mixed dual diffusion problem as well. Both these element types are included in our analysis for the general case.

The well-posedness of the different formulations will be systematically investigated. While second order methods lead to coercive problems (and therefore can be dealt with through the Lax-Milgram theorem), it is not the case for second order hybrid, mixed and mixed-hybrid methods, which in turn need to verify the LBB condition.

Our paper is organized as follows. Section 2 surveys notations and theorems used throughout the paper. In section 3, the diffusion equation is introduced.

Different continuous formulations are investigated in section 4. Each time, well-posedness results are provided. Some can be found in the literature, other ones need some adaptation. In section 5, the nodal finite element discretization is presented, and applied to the mixed-hybrid methods. The well-posedness of these discrete problems is investigated as well. Appendix A gives the well-posedness proofs for the dual diffusion problems. It is inspired by the primal proofs in [12] (for a case similar but slightly different from ours). We show that their proofs remain valid for our primal case with little changes, and we adapt them to the dual case. Finally, some numerical experiments have been carried out for the mixed-hybrid primal and dual formulations in the two-dimensional case. These early results can be found in appendix B.

## 2 Preliminaries

General references for the notions introduced below are [10], [18], and [19]. The number of space dimensions will be denoted by “ $n$ ”. We will use neutronic standard notation by denoting the considered domain as  $V$  (an open set of the Euclidean space  $\mathbf{R}^n$ ), its boundary as  $\partial V$ , the infinitesimal volume element as  $dV$  and the infinitesimal hyper-surface element as  $d\Gamma$ .  $\partial V$  denotes the boundary of  $V$ . (In neutronics, the letter  $\Omega$  is reserved to refer to the angular variable in the general transport theory.)

$L^2(V) = H^0(V)$  and  $H^1(V)$  will denote respectively the usual Lebesgue and Sobolev spaces, with their elements understood in the sense of distributions. Their associated norms are respectively  $\|v\| = \|v\|_{L^2(V)} = (\int_V |v|^2 dV)^{1/2}$  and  $\|v\|_{1,V}^2 = \|v\|_{H^1(V)}^2 = \|v\|^2 + \|\nabla v\|^2$ , with  $\|\mathbf{p}\| = \sum_{i=1}^n \|p_i\|$  for any vector  $\mathbf{p}$ . Note that for a piecewise polynomial to be in  $H^1(V)$ , it has to be continuous. Distributions in  $L^2(V)$  may correspond to discontinuous functions.

On boundaries or interfaces, our unknowns will be defined through the theorems 2.1 and 2.2 that follow. [13, pp.529-530]:

**Theorem 2.1 (Trace mapping theorem)** *Let  $V$  be an open subset of  $\mathbf{R}^n$  with Lipschitzian boundary <sup>1</sup>. 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

<sup>1</sup> that is, every point  $x \in \partial V$  has a neighborhood  $U_x$  such that  $\partial V \cap U_x$  be the graph of a Lipschitzian function, and  $V$  lies on only one side of  $\partial V$ .

a Hilbert space <sup>2</sup>, subset of  $L^2(\partial V)$ , equipped with the norm

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

The dual space of  $H^{1/2}(\partial V)$  is  $H^{-1/2}(\partial V)$ , a Hilbert space with norm

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

where  $\langle \psi, \chi \rangle = \int_{\partial V} \psi \chi \, d\Gamma$ .

Moreover we define

$$H(\operatorname{div}, V) = \{\mathbf{q} \in (L^2(V))^n : \nabla \cdot \mathbf{q} \in L^2(V)\},$$

that we endow with the norm

$$\|\mathbf{q}\|_{\operatorname{div}} = (\|\nabla \cdot \mathbf{q}\|^2 + \|\mathbf{q}\|^2)^{1/2}.$$

In the following,  $\mathbf{n}$  will always denote the unit outward normal vector to the considered (sub)domain.

**Theorem 2.2 (Normal trace mapping theorem)** *Let  $V$  be as before and with piecewise  $C^1$  boundary. 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  $H(\operatorname{div}, V)$  onto  $H^{-1/2}(\partial V)$ , called the normal trace mapping.*

The kernel of the normal trace mapping is denoted  $H_0(\operatorname{div}, V)$ , and its range is  $H^{-1/2}(\partial V)$ , which contains all the functions of  $L^2(\partial V)$ . In the sequel, we assume that all the considered (sub)domains have piecewise  $C^1$  (whence Lipschitzian) boundaries.

In hybrid methods, the domain  $V$  will be subdivided into a finite family of elements  $V_l$  (again 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  $L$  positive integer. Let  $P$  denote this family. In practice, for two-dimensional problems, the  $V_l$  will be polygons. The refinement of the mesh induced by  $P$  is represented by  $h$ , the maximal diameter <sup>3</sup> of all the  $V_l$ . We also define

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

<sup>2</sup> In fact  $H^{1/2}(\partial V)$  (as well as  $H^{-1/2}(\partial V)$  introduced later) is a Sobolev space of fractional order, defined through Fourier transforms. The proof that it coincides with the range of the trace mapping can be found in [20].

<sup>3</sup> maximal distance between two points in a domain

We will need the following trace operators:

$$\gamma_0^v = H_0^1(V) \rightarrow L^2(\Gamma) : v \rightarrow \psi = \gamma_0^v(v) = v|_\Gamma, \text{ and} \quad (3)$$

$$\gamma_0^{\mathbf{q}} = H_0(\operatorname{div}, V) \rightarrow L^2(\Gamma) : \mathbf{q} \rightarrow \chi = \gamma_0^{\mathbf{q}}(\mathbf{q}) = \mathbf{n} \cdot \mathbf{q}|_\Gamma. \quad (4)$$

The range of these two operators, respectively equipped with the norms

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

will be denoted (again respectively)  $H_0^{1/2}(\Gamma)$  and  $H_0^{-1/2}(\Gamma)$ <sup>4</sup>.

Now, let  $V$  be a Hilbert space with norm  $\|\cdot\|_V$ ,  $V'$  its dual, and let  $\langle \cdot, \cdot \rangle$  denote the duality pairing between  $V$  and  $V'$ . Let  $U$  be another Hilbert space. We recall the following generalization of the Lax-Milgram theorem for the non-coercive operators [5, sect. I.4.1, I.4.2]:

**Theorem 2.3** *Let  $U$  and  $V$  be two Hilbert spaces,  $a(u, v)$  a continuous bilinear form on  $U \times V$ , and  $A$  the bounded linear operator from  $U$  to  $V'$  defined by*

$$\forall (u, v) \in U \times V, \quad a(u, v) = \langle Au, v \rangle$$

*Then if it exists  $\alpha > 0$  such that*

$$\inf_{u \in U, u \neq 0} \sup_{v \in V, v \neq 0} \frac{|a(u, v)|}{\|u\|_U \|v\|_V} \geq \alpha, \quad (5)$$

*then the problem: find  $u \in U$  such that*

$$\forall v \in V : a(u, v) = \langle f, v \rangle$$

*with  $f \in \mathbf{R}(A)$  (range of  $A$ ), is well-posed.*

The condition (5) is called the ‘‘inf-sup’’ or ‘‘Ladyshenskaya-Babuška-Brezzi’’ (LBB) condition. The same theorem remains of course valid in the discrete case, that is if  $U$  and  $V$  are replaced by finite-dimensional subspaces  $U_h$  and  $V_h$  [5, sect. II.1.1]. In this case, the LBB condition to satisfy is thus

$$\inf_{u_h \in U_h, u_h \neq 0} \sup_{v_h \in V_h, v_h \neq 0} \frac{|a(u_h, v_h)|}{\|u_h\|_{U_h} \|v_h\|_{V_h}} \geq \alpha. \quad (6)$$

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<sup>4</sup> This notation assumes that these spaces are equivalent to the corresponding fractional order Sobolev spaces. I do not have a general proof of this fact, but then we can take this simply as a notation.

### 3 The diffusion equation

Our starting point is the within-group diffusion equation written as a coupled pair of first order differential equations, with isotropic scattering and sources [21]:

$$\nabla \cdot \mathbf{J}(\mathbf{r}) + \sigma_r \phi(\mathbf{r}) = s(\mathbf{r}) \quad (7)$$

and

$$\nabla \phi(\mathbf{r}) + 3\sigma \mathbf{J}(\mathbf{r}) = 0. \quad (8)$$

Unknowns are the scalar flux  $\phi(\mathbf{r})$  and current vector  $\mathbf{J}(\mathbf{r})$ . While (7) enforces the neutron conservation, (8) is Fick's law and relates the two unknowns. The coefficients  $\sigma$  and  $\sigma_r$  are respectively the total and removal (macroscopic) cross sections, for media with isotropic scattering. The cross section of a collision is its probability of occurrence per unit length. We have that  $\sigma = \sigma_r + \sigma_s$ , with  $\sigma_s$  being the scattering cross section. In case of a void  $\sigma = \sigma_r = \sigma_s = 0$ . There are also media where  $\sigma = \sigma_s \neq 0$  and  $\sigma_r = 0$ . These are said to be pure scattering media. In this case, the diffusion equation is just the (generalized) Poisson's equation, which has been extensively studied in the literature ([1], [11], [14]). We will therefore concentrate here on cases where both  $\sigma$  and  $\sigma_r$  are nonzero. Note that (opposite to [12]), the source  $s(\mathbf{r})$  is not supposed to belong to  $L^2(V)$  in general. At this point, it is just a general distribution in  $\mathcal{D}'(\Omega)$ , i.e. a linear functional on  $C_0^\infty(V)$ . Besides, we suppose  $\sigma_{(r)}$  and  $\frac{1}{\sigma_{(r)}}$  in  $C^\infty(V)$  for non-hybrid methods, and in  $C^\infty(V_i)$  for hybrid methods.

The methods will be characterized in two different ways. On one hand, "second order", "second order hybrid", "mixed" and "mixed-hybrid" methods can be considered. These terms will be defined in the sequel. On the other hand, all these methods exist in a "primal" and in a "dual" formulation, following the role played by  $\phi(\mathbf{r})$  and  $\mathbf{J}(\mathbf{r})$ . Note that all the weak forms that we will derive in the sequel are summarized in tables 1 and 2.

About boundary conditions, note that in diffusion theory, the in- and outgoing partial currents, respectively denoted  $j^-$  and  $j^+$ , can be shown to be [22]

$$j^\pm(\mathbf{r}) = \frac{1}{4}\phi(\mathbf{r}) \pm \frac{1}{2} \frac{1}{3\sigma} \mathbf{n} \cdot \nabla \phi(\mathbf{r}) \quad \forall \mathbf{r} \in \partial V,$$

that is, introducing  $\psi(\mathbf{r})$  and  $\chi(\mathbf{r})$  for boundary flux and current respectively,

$$j^\pm(\mathbf{r}) = \frac{1}{4}\psi(\mathbf{r}) \pm \frac{1}{2} \chi(\mathbf{r}) \quad \forall \mathbf{r} \in \partial V. \quad (9)$$

We consider vacuum and reflected boundary conditions. There is no incoming current from a vacuum, thus  $j^-(\mathbf{r}) = 0$ , and  $\psi(\mathbf{r}) = 2\chi(\mathbf{r})$ . On reflected boundaries,  $j^+(\mathbf{r}) = j^-(\mathbf{r})$ , that is  $\chi(\mathbf{r}) = 0$ .

Finally, note that second order and second order hybrid methods will be given variational formulations: second order methods lead to extremum problems, while second order hybrid methods lead to saddle point problems. Note that such analyses are not necessary as soon as we have a well-posedness result for the corresponding weak formulations. It is given here for information, and to relate to other works. As for mixed and mixed-hybrid methods, a theoretical analysis of the variational formulations gets too involved, and we will therefore not carry it out since it is not needed.

## 4 Continuous formulations

### 4.1 Second order methods

Second order methods are based on the usual weak form of second order differential equations. Nevertheless, we derive them here without using any second order equation, and show that the introduction of second order derivatives creates in fact an artificial problem.

About well-posedness, we will see that second order methods lead to bilinear forms that are continuous, symmetric and coercive. Thus existence, uniqueness and stability of the second order weak solutions and methods follow from the Lax-Milgram theorem. The primal problem is for instance treated in chapter 7 of [4]. Coercivity of  $a(u, v)$  follows from the Friedrichs inequalities. Also, these methods have variational interpretations in terms of extremum problems.

#### 4.1.1 Second order primal method

To derive the weak form, we start from (7), that we multiply by an arbitrary test function  $\tilde{\phi} \in H^1(V)$ , and integrate over the considered domain  $V$ . (This is a language abuse that we will go on using: in fact, we apply the distributions, thus functionals, to the test function  $\tilde{\phi}$ .) We get, for all  $\tilde{\phi} \in H^1(V)$ ,<sup>5</sup>

$$\int_V \nabla \cdot \mathbf{J} \tilde{\phi} dV + \int_V \sigma_r \phi \tilde{\phi} dV = \int_V s \tilde{\phi} dV,$$

that is, using the divergence theorem,

$$\int_{\partial V} \mathbf{n} \cdot \mathbf{J} \tilde{\phi} d\Gamma - \int_V \mathbf{J} \cdot \nabla \tilde{\phi} dV + \int_V \sigma_r \phi \tilde{\phi} dV = \int_V s \tilde{\phi} dV.$$

<sup>5</sup> From now on, the spatial dependence will not be explicitly written anymore.

For the last two equations to make sense, we require the source  $s$  to be in  $H^1(V)$ , the dual of  $H^1(V)$ . We now introduce a Neumann type non-homogeneous boundary condition on all the boundary of the domain :  $\mathbf{n} \cdot \mathbf{J} = \chi$  for  $\mathbf{r} \in \partial V$  ( $\chi$  is here a known boundary condition). Note that this is a convenience choice. Using (8), we obtain, for  $\sigma \neq 0$ ,

$$\int_V \left( \frac{1}{3\sigma} \nabla \phi \nabla \tilde{\phi} + \tilde{\phi} (\sigma_r \phi - s) \right) dV + \int_{\partial V} \tilde{\phi} \chi d\Gamma = 0 \quad \forall \tilde{\phi} \in H^1(V). \quad (10)$$

In this weak form, the presence of  $\nabla \phi$  forces to look for  $\phi$  in  $H^1(V)$ . Since later  $\phi$  will be approximated by piecewise polynomial functions, we have to know that, for such a function to be in  $H^1(V)$ , it has to be continuous. Also, we require  $\chi \in H^{-1/2}(\partial V)$ , and notice that taking  $\tilde{\phi}$  in  $H^1(V)$  gives a sense, through theorem 2.1, to the restriction of  $\tilde{\phi}$  to  $\partial V$  used in the surface integral, and belonging to  $H^{1/2}(\partial V)$ .

Finally we can write the primal weak form: find  $\phi$  in  $H^1(V)$  such that

$$a(\phi, \tilde{\phi}) = \langle s, \tilde{\phi} \rangle_V - \langle \chi, \tilde{\phi} \rangle_{\partial V} \quad \forall \tilde{\phi} \in H^1(V),$$

where  $a(u, v) = \int_V \left( \frac{1}{3\sigma} \nabla u \nabla v + \sigma_r u v \right) dV$  is continuous, symmetric and coercive, while  $\langle \cdot, \cdot \rangle_V$  and  $\langle \cdot, \cdot \rangle_{\partial V}$  are the duality pairings between  $H^1(V)$  and  $H^1(V)$ , and  $H^{-1/2}(\partial V)$  and  $H^{1/2}(\partial V)$ , respectively.

**4.1.1.1 Origin of the denomination** The denomination “second order method” is motivated by the fact that the weak form just derived is the usual one for the second order differential equation ( $\sigma \neq 0$ )

$$-\nabla \cdot \frac{1}{3\sigma} \nabla \phi + \sigma_r \phi - s = 0. \quad (11)$$

This equation (“strong form”) can be obtained by extracting the current out of (8), and substituting it into (7). To obtain the weak form (10) from here, we multiply (11) by an arbitrary test function  $\tilde{\phi} \in H^1(V)$ , and apply the divergence theorem, expressing a Neumann type non-homogeneous boundary condition  $-\mathbf{n} \cdot \frac{1}{3\sigma} \nabla \phi = \chi$  for  $\mathbf{r} \in \partial V$ , in the surface integral. Nevertheless, equation (11) implies that the derivatives in  $\nabla \phi$  be themselves derivable <sup>6</sup>. This “derivable derivatives” hypothesis disappears in the weak form formulation. The introduction of such a problem is in fact artificial since our first derivation of (10) shows that it can be obtained without the use of second order derivatives.

<sup>6</sup> This is less of a problem with distributions, since every distribution is infinitely derivable. A function nevertheless need to be locally integrable to be interpretable in the distribution sense.

**4.1.1.2 Variational interpretation** Since  $a(u, v)$  is symmetric, the Lax-Milgram theorem also shows that the primal weak form can be derived by looking for the minimum of the following functional :

$$F^{sp}[\phi] = \int_V \left( \frac{1}{3\sigma} (\nabla\phi)^2 + \sigma_r \phi^2 - 2\phi s \right) dV + 2 \int_{\partial V} \chi \phi d\Gamma. \quad (12)$$

We can also notice that, if we require this functional to be stationary at  $\phi$ , that is if we compute  $\nabla F^{sp}$  and require it to be zero, we obtain (10).

#### 4.1.2 Second order dual method

We start again from (7), but here multiply by an arbitrary test function  $\nabla \cdot \tilde{\mathbf{J}}$ , with  $\tilde{\mathbf{J}} \in H(\text{div}, V)$ , before integrating on  $V$ . We obtain, for all  $\tilde{\mathbf{J}} \in H(\text{div}, V)$  (and  $\sigma_r \neq 0$ ),

$$\int_V \frac{1}{\sigma_r} \nabla \cdot \mathbf{J} \nabla \cdot \tilde{\mathbf{J}} dV + \int_V \phi \nabla \cdot \tilde{\mathbf{J}} dV = \int_V \frac{1}{\sigma_r} s \nabla \cdot \tilde{\mathbf{J}} dV,$$

and the divergence theorem gives

$$\int_V \frac{1}{\sigma_r} \nabla \cdot \mathbf{J} \nabla \cdot \tilde{\mathbf{J}} dV + \int_{\partial V} \phi \mathbf{n} \cdot \tilde{\mathbf{J}} d\Gamma - \int_V \nabla\phi \cdot \tilde{\mathbf{J}} dV = \int_V \frac{1}{\sigma_r} s \nabla \cdot \tilde{\mathbf{J}} dV.$$

We require the source  $s$  to be in  $L^2(V)$ , which is its own dual. We introduce the inhomogeneous Dirichlet boundary condition  $\phi = \psi$  on  $\partial V$ , and use (8) to obtain the weak form equation

$$\int_V \left( \frac{(\nabla \cdot \mathbf{J} - s)}{\sigma_r} \nabla \cdot \tilde{\mathbf{J}} + 3\sigma \mathbf{J} \cdot \tilde{\mathbf{J}} \right) dV + \int_{\partial V} \mathbf{n} \cdot \tilde{\mathbf{J}} \psi d\Gamma = 0 \quad \forall \tilde{\mathbf{J}} \in H(\text{div}, V). \quad (13)$$

The presence of  $\nabla \cdot \mathbf{J}$  in the weak form leads us to look for  $\mathbf{J}$  in  $H(\text{div}, V)$ , which for piecewise polynomials implies continuity. We require  $\psi \in H^{1/2}(\partial V)$ , and theorem 2.2 implies that  $\mathbf{n} \cdot \tilde{\mathbf{J}} \in H^{-1/2}(\partial V)$  in the surface integral.

We finally obtain the dual weak form: find  $\mathbf{J}$  in  $H(\text{div}, V)$  such that

$$a(\mathbf{J}, \tilde{\mathbf{J}}) = \frac{1}{\sigma_r} \langle s, \nabla \cdot \tilde{\mathbf{J}} \rangle_V - \langle \mathbf{n} \cdot \tilde{\mathbf{J}}, \psi \rangle_{\partial V},$$

where  $a(\mathbf{p}, \mathbf{q}) = \int_V \left( \frac{1}{\sigma_r} \nabla \cdot \mathbf{p} \nabla \cdot \mathbf{q} + 3\sigma \mathbf{p} \cdot \mathbf{q} \right) dV$ , while  $\langle \cdot, \cdot \rangle_V$  is the duality pairing between  $L^2(V)$  and itself, and  $\langle \cdot, \cdot \rangle_{\partial V}$  is as before.

**4.1.2.1 Origin of the denomination** Here again, the weak form is the usual one for the second order differential equation ( $\sigma_r \neq 0$ ):

$$\nabla \frac{(s - \nabla \cdot \mathbf{J})}{\sigma_r} + 3\sigma \mathbf{J} = 0. \quad (14)$$

This can be obtained by extracting the flux out of (7) and substituting it into (8) to obtain (14). To obtain (13) from there, we multiply (14) by an arbitrary test function  $\tilde{\mathbf{J}} \in H(\text{div}, V)$ , apply the divergence theorem expressing in the surface integral an inhomogeneous boundary condition  $\phi = \psi$  on  $\partial V$ , that is, using (7),  $\frac{(s - \nabla \cdot \mathbf{J})}{\sigma_r} = \psi$  ( $\psi$  is known here). The same comments as in the primal case can be made here.

**4.1.2.2 Variational interpretation** Here also, symmetry implies that the dual weak form can be derived by looking for the minimum of the following functional :

$$F^{sd}[\mathbf{J}] = \int_V (3\sigma \mathbf{J} \cdot \mathbf{J} + \frac{1}{\sigma_r} (\nabla \cdot \mathbf{J} \nabla \cdot \mathbf{J} - 2s \nabla \cdot \mathbf{J})) dV - 2 \int_{\partial V} \mathbf{n} \cdot \mathbf{J} \psi d\Gamma. \quad (15)$$

Again, we can also notice that, if we require this functional to be stationary at  $\mathbf{J}$ , we obtain (13).

**4.1.2.3 Note** We see that the above expressions for the primal method are not valid in case of a void. From this point of view, the dual method is even worse since pure scattering media cannot be modeled. Also, the dual method is more restrictive on the source  $s$ , since  $L^2(V) \subset H^1(V)$ .

## 4.2 Second order hybrid methods

Hybrid methods require the discretization of the studied domain  $V$  in a finite number of elements  $V_i$  that constitute a family  $P$  as in section 2. Following [1], hybrid methods are methods which involve the simultaneous approximation of a vector field on the union of the elements of the discretization, and another defined on the union of the boundaries of the elements. Here, the internal flux  $\phi$  and the interface current  $\chi$  (not a known boundary condition anymore) will be approximated in the primal case, while the internal current  $\mathbf{J}$  and the interface flux  $\psi$  (same remark) will be approximated in the dual case. The interface variables are sometimes called Lagrange multipliers in the literature (see variational interpretations). The hybrid methods enable us to relax the regularity requirement at element interfaces, as we will see.



polynomials. This is at the price of introducing another variable  $\chi$ .

The (natural) boundary condition of the non-hybrid form  $\mathbf{n} \cdot \mathbf{J} = \chi$  is here a relationship between two unknowns. In fact, using  $H_0^{-1/2}(\Gamma)$  instead of  $H^{-1/2}(\Gamma)$  for the trial function  $\tilde{\chi}$  cancels the Dirichlet boundary condition on the flux  $\phi$  used in [12] to make the problem well-posed. This is the main difference between this method and the one presented in [12]. We motivate this way of handling boundary conditions by the particular form of the boundary condition we consider (vacuum and reflected), that are not usual Dirichlet or Neumann boundary conditions.

Finally, we can write the hybrid primal weak form: find  $(\phi, \chi) \in X \times H^{-1/2}(\Gamma)$  such that

$$\begin{cases} a(\phi, \tilde{\phi}) + c(\chi, \tilde{\phi}) &= \langle s, \tilde{\phi} \rangle & \forall \tilde{\phi} \in X \\ c(\tilde{\chi}, \phi) &= 0 & \forall \tilde{\chi} \in H_0^{-1/2}(\Gamma), \end{cases} \quad (17)$$

where

$$\begin{aligned} a(u, v) &= \sum_l \int_{V_l} \left( \frac{1}{3\sigma} \nabla u \nabla v + \sigma_r u v \right) dV, \\ c(\chi, v) &= \sum_l \langle \chi, v \rangle_{\partial V_l}, \quad \text{and} \quad \langle s, v \rangle = \sum_l \langle s, v \rangle_{V_l}, \end{aligned}$$

with the same duality pairings as in the non-hybrid (primal) case, but taken now on  $(\partial)V_l$ .

**4.2.1.1 Variational interpretation** Since  $a(u, v)$  is symmetric and positive definite, the problem (17) has a variational interpretation in terms of a saddle-point problem ([5], p.62): it is equivalent to find  $(\phi, \chi)$  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

$$F^{hp}[\phi, \chi] = \frac{1}{2} a(\phi, \phi) + b(\phi, \chi) - \langle s, \phi \rangle,$$

that is

$$F^{hp}[\phi, \chi] = \sum_l F_l^{sp}[\phi, \chi] \quad (18)$$

with

$$F_l^{hp}[\phi, \chi] = \int_{V_l} \left( \frac{1}{3\sigma} (\nabla \phi)^2 + \sigma_r \phi^2 - 2\phi s \right) dV + 2 \int_{\partial V_l} \chi \phi d\Gamma.$$

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 ((12) and (15)), but where volume and surface integrals are now taken only on the considered element, and where the interface function ( $\chi$  here) is now a distinct variable, in fact considered a Lagrange multiplier (and not as a known boundary condition).

#### 4.2.2 Second order hybrid dual method

We proceed in a way similar to the primal case. We introduce

$$Y = \{ \mathbf{v} \in (L^2(V))^n : \forall V_l, \mathbf{v}|_{V_l} \in H(\text{div}, V_l) \}$$

and note that any piecewise polynomials in  $Y$  can be discontinuous across interfaces.

We use the following result [2, proposition 1.2, p.95]:

#### Theorem 4.2

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

The weak form is then: find  $(\mathbf{J} \times \psi)$  in  $Y \times H^{1/2}(\Gamma)$  such that ( $\sigma_r \neq 0$ )

$$\begin{cases} \sum_l \int_{V_l} \sigma_r^{-1} \nabla \cdot \mathbf{J} \nabla \cdot \tilde{\mathbf{J}} + 3\sigma \mathbf{J} \cdot \tilde{\mathbf{J}} dV + \sum_l \int_{\partial V_l} \mathbf{n} \cdot \tilde{\mathbf{J}} \psi d\Gamma \\ \quad = \sum_l \int_{V_l} \sigma_r^{-1} s \nabla \cdot \tilde{\mathbf{J}} dV & \forall \tilde{\mathbf{J}} \in Y \quad (19) \\ \sum_l \int_{\partial V_l} \mathbf{n} \cdot \mathbf{J} \tilde{\psi} d\Gamma = 0 & \forall \tilde{\psi} \in H_0^{1/2}. \end{cases}$$

We impose  $s \in L^2(V_l)$ , for all  $l$ . Note again that, even if we impose only  $\mathbf{J} \in Y$ , the theorem (4.2) shows that it is in fact in  $H^1(\text{div}, V)$  thanks to the second equation.

Thus, the regularity requirement on  $\mathbf{J}$  has been relaxed, at the price of introducing another variable  $\psi$ .

We have now the following hybrid dual weak form: find  $(\mathbf{J}, \psi)$  in  $Y \times H^{1/2}(\Gamma)$  such that

$$\begin{cases} a(\mathbf{J}, \tilde{\mathbf{J}}) + c(\mathbf{n} \cdot \tilde{\mathbf{J}}, \psi) &= \frac{1}{\sigma_r} \langle s, \nabla \cdot \tilde{\mathbf{J}} \rangle & \forall \tilde{\mathbf{J}} \in Y \\ c(\mathbf{n} \cdot \mathbf{J}, \tilde{\psi}) &= 0 & \forall \tilde{\psi} \in H_0^{1/2}(\Gamma), \end{cases} \quad (20)$$

where  $c$  is as in the primal case,

$$a(\mathbf{p}, \mathbf{q}) = \sum_l \int_{V_l} (\sigma_r^{-1} \nabla \cdot \mathbf{p} \nabla \cdot \mathbf{q} + 3\sigma \mathbf{p} \mathbf{q}) dV, \quad \text{and} \quad \langle s, v \rangle = \sum_l \langle s, v \rangle_{V_l},$$

with  $\langle s, v \rangle_{V_l}$  the duality pairing between  $L^2(V_l)$  and itself.

**4.2.2.1 Variational interpretation** Since again  $a(u, v)$  is symmetric and positive definite, the problem is equivalent to a saddle-point problem: find  $(\mathbf{J}, \psi)$  in  $Y \times H^{1/2}(\Gamma)$  such that

$$F^{hd}[\mathbf{J}, \tilde{\psi}] \leq F^{hd}[\mathbf{J}, \psi] \leq F^{hd}[\tilde{\mathbf{J}}, \psi]$$

where

$$F^{hd}[\mathbf{q}, \psi] = \frac{1}{2} a(\mathbf{q}, \mathbf{q}) + b(\mathbf{q}, \psi) - \langle s, \mathbf{q} \rangle,$$

that is (except for a harmless constant term)

$$F^{hd}[\mathbf{J}, \psi] = \sum_l F_l^{sd}[\mathbf{J}, \psi], \quad (21)$$

with

$$F_l^{hd}[\mathbf{J}, \psi] = \int_{V_l} (3\sigma \mathbf{J} \cdot \mathbf{J} + \frac{1}{\sigma_r} (\nabla \cdot \mathbf{J} - s) \cdot (\nabla \cdot \mathbf{J} - s)) dV - 2 \int_{\partial V_l} \mathbf{J} \cdot \mathbf{n} \psi d\Gamma$$

Again, the sum of all the elementary contributions gives the functional for the whole domain, and on each element we find back the non-hybrid case, where the interface function ( $\psi$  here) is considered a Lagrange multiplier.

### 4.3 Mixed methods

We do not need the decomposition  $P$  of the domain  $V$  for these methods. Again following [1], the mixed methods are defined as methods involving the simultaneous approximation of two or more vector fields on the physical domain. In our case, this means that flux and current will be approximated simultaneously. In the second order methods, only one of the two unknowns

( $\phi$  or  $\mathbf{J}$ ) is approximated, thus the other one has to be computed from the first one. This process involves a loss of accuracy that is avoided in mixed methods. This is important when both flux and current are given equal interest.

For the well-posedness proofs, see appendix A. (The primal proof is similar to the one provided for the dual case.) The primal case is also treated succinctly in [12].

#### 4.3.1 Mixed primal method

In the primal case, we multiply (7) by an arbitrary test function  $\tilde{\phi} \in H^1(V)$ , and integrate over  $V$ . Then we apply the divergence theorem, and express in the surface term a Neumann-type non-homogeneous boundary condition  $\mathbf{n} \cdot \mathbf{J} = \chi$  on  $\partial V$ . Note that  $\chi$  is here a known boundary condition. We thus assume that  $\mathbf{J}$  has a normal trace on  $\partial V$ . This is the case if  $\mathbf{J} \in H(\text{div}, V)$  (by theorem 2.2), but this is not a necessary condition. Besides, we introduce a second equation, namely (8) multiplied by an arbitrary test function  $\tilde{\mathbf{J}} \in [L^2(V)]^n$ , and integrated over  $V$ . We obtain the following weak form equations:

$$\begin{cases} \int_V (-\mathbf{J} \cdot \nabla \tilde{\phi} + \sigma_r \phi \tilde{\phi} - s \tilde{\phi}) dV + \int_{\partial V} \chi \tilde{\phi} d\Gamma = 0 & \forall \tilde{\phi} \in H^1(V) \\ \int_V \tilde{\mathbf{J}} \cdot (3\sigma \mathbf{J} + \nabla \phi) dV = 0 & \forall \tilde{\mathbf{J}} \in [L^2(V)]^n. \end{cases} \quad (22)$$

In this case,  $\phi$  is to be found in  $H^1(V)$ , and  $\mathbf{J}$  in  $[L^2(V)]^n$  (where  $n$  is the number of space dimensions). We require  $\chi \in H^{-1/2}(\partial V)$  and  $s \in H^{-1}(V)$ .

**4.3.1.1 Variational interpretation** As announced earlier, a theoretical investigation of the variational interpretation gets too involved from now on, and will therefore not be carried out since it is not necessary.

#### 4.3.2 Mixed dual method

In the dual case, we multiply (8) by an arbitrary test function  $\tilde{\mathbf{J}} \in H(\text{div}, V)$ , and integrate over  $V$ . Then we apply the divergence theorem, and express this time a Dirichlet non-homogeneous boundary condition  $\phi = \psi$  on  $\partial V$ . Thus we assume that  $\phi$  has a trace on  $\partial V$ . It is true if  $\phi \in H^1(V)$  by theorem (2.1), but this is again not a necessary condition. Introducing as second equation (7) multiplied by an arbitrary  $\tilde{\phi} \in L^2(V)$  and integrated over  $V$ , we obtain the following weak form equations :

$$\begin{cases} \int_V \tilde{\phi} (\nabla \cdot \mathbf{J} + \sigma_r \phi - s) dV = 0 & \forall \tilde{\phi} \in L^2(V) \\ \int_V (3\sigma \tilde{\mathbf{J}} \mathbf{J} - \phi \nabla \cdot \tilde{\mathbf{J}}) dV + \int_{\partial V} \mathbf{n} \cdot \tilde{\mathbf{J}} \psi d\Gamma = 0 & \forall \tilde{\mathbf{J}} \in H(\text{div}, V). \end{cases} \quad (23)$$

We have now that  $(\phi, \mathbf{J})$  is to be found in  $L^2(V) \times H(\text{div}, V)$ . We require  $\psi \in H^{1/2}(\partial V)$  and  $s \in L^2(V)$ .

### 4.3.3 Note

Note that in mixed methods, there is no  $\sigma_{(r)}$  appearing in the denominator, which encourages to pursue analyzing these methods in the void case. Nevertheless, other problems arise then (several terms vanish, and there is not much left). In fact, other approaches, like ray-tracing, should be investigated to treat void streaming.

## 4.4 Mixed-hybrid Methods

Mixed-hybrid methods feature the characteristics of both mixed and hybrid methods: simultaneous approximation of the flux and current inside each element  $V_l$  of the family  $P$  (introduced in section 2 through subdividing  $V$ ), and relaxation of interface conditions through the use of an unknown interface function (or Lagrange multiplier)  $\psi$  or  $\chi$ .

Similarly to what we did to go from second order methods to second order hybrid methods, the idea is to apply the mixed primal weak form to each element  $V_l$  separately, and to sum up the equations obtained in this way. Also, the inter-element continuity is restored by introducing a constraint as an additional equation in the weak form.

As for well-posedness, see [12] and appendix A.

### 4.4.1 Mixed-hybrid primal method

Proceeding as we just said, we get as weak form equations

$$\begin{cases} \sum_l \int_{V_l} (-\mathbf{J} \nabla \tilde{\phi} + \sigma_r \tilde{\phi} \phi) dV + \sum_l \int_{\partial V_l} \chi \tilde{\phi} d\Gamma = \sum_l \int_{V_l} s \tilde{\phi} dV & \forall \tilde{\phi} \in X \\ \sum_l \int_{V_l} \tilde{\mathbf{J}} \cdot (3\sigma \mathbf{J} + \nabla \phi) dV = 0 & \forall \tilde{\mathbf{J}} \in [L^2(V)]^n \\ \sum_l \int_{\partial V_l} \phi \tilde{\chi} d\Gamma = 0 & \forall \tilde{\chi} \in H_0^{-1/2}(\Gamma). \end{cases} \quad (24)$$

Here, we look for  $\phi$  in  $X$ ,  $\mathbf{J}$  in  $[L^2(V)]^n$ , and  $\chi$  in  $H^{-1/2}(\Gamma)$ , and require  $s \in H^{-1}(V_l)$ , for all  $l$ . The regularity requirement on  $\phi$  has been relaxed: the third equation makes  $\phi \in H^1(V)$  when taken for all  $\tilde{\chi} \in H_0^{-1/2}(\Gamma)$  (theorem 4.1).

We can now write 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

$$\begin{cases} a(\phi, \tilde{\phi}) - b^p(\tilde{\phi}, \mathbf{J}) + c(\chi, \tilde{\phi}) &= \langle s, \tilde{\phi} \rangle & \forall \tilde{\phi} \in X \\ b^p(\tilde{\mathbf{J}}, \phi) + d(\mathbf{J}, \tilde{\mathbf{J}}) &= 0 & \forall \tilde{\mathbf{J}} \in [L^2(V)]^n, \\ c(\tilde{\chi}, \phi) &= 0 & \forall \tilde{\chi} \in H_0^{-1/2}(\Gamma), \end{cases} \quad (25)$$

where

$$\begin{aligned} a(u, v) &= \sum_l \int_{V_l} \sigma_r u v \, dV, & b^p(v, \mathbf{q}) &= \sum_l \int_{V_l} \mathbf{q} \cdot \nabla v \, dV, \\ \text{and} & & d(\mathbf{p}, \mathbf{q}) &= \sum_l \int_{V_l} 3\sigma \mathbf{p} \mathbf{q} \, dV, \end{aligned}$$

with  $c$  and  $\langle s, v \rangle$  defined as in the second order hybrid primal case.

#### 4.4.2 Mixed-hybrid dual method

The weak form equations become

$$\begin{cases} \sum_l \int_{V_l} \tilde{\phi} (\nabla \cdot \mathbf{J} + \sigma_r \phi) \, dV = \sum_l \int_{V_l} \tilde{\phi} s \, dV & \forall \tilde{\phi} \in L^2(V) \\ \sum_l \int_{V_l} (3\sigma \tilde{\mathbf{J}} \cdot \mathbf{J} - \phi \nabla \cdot \tilde{\mathbf{J}}) \, dV + \sum_l \int_{\partial V_l} \mathbf{n} \cdot \tilde{\mathbf{J}} \psi \, d\Gamma = 0 & \forall \tilde{\mathbf{J}} \in Y \\ \sum_l \int_{\partial V_l} \mathbf{n} \cdot \mathbf{J} \tilde{\psi} \, d\Gamma = 0. & \forall \tilde{\mathbf{J}} \in H_0^{1/2}(\Gamma) \end{cases}$$

We have now that  $(\mathbf{J}, \phi, \psi)$  is to be found in  $Y \times L^2(V) \times H^{1/2}(\Gamma)$ . We require  $s \in L^2(V_l)$ , for all  $l$ . Again,  $\mathbf{J}$  is in fact in  $H(\text{div}, V)$  by theorem 4.2.

We can write the mixed-hybrid dual weak form: find  $(\mathbf{J}, \phi, \psi)$  in  $Y \times L^2(V) \times H^{1/2}(\Gamma)$  such that

$$\begin{cases} a(\phi, \tilde{\phi}) + b^d(\tilde{\phi}, \mathbf{J}) &= \langle s, \tilde{\phi} \rangle & \forall \tilde{\phi} \in L^2(V) \\ -b^d(\tilde{\mathbf{J}}, \phi) + d(\mathbf{J}, \tilde{\mathbf{J}}) + c(\mathbf{n} \cdot \tilde{\mathbf{J}}, \psi) &= 0 & \forall \tilde{\mathbf{J}} \in Y, \\ c(\mathbf{n} \cdot \mathbf{J}, \tilde{\psi}) &= 0 & \forall \tilde{\psi} \in H_0^{1/2}(\Gamma) \end{cases} \quad (26)$$

where  $a$ ,  $d$ , and  $c$  are as in the primal case,

$$b^d(u, \mathbf{q}) = \sum_l \int_{V_l} u \nabla \cdot \mathbf{q} \, dV,$$

and  $\langle s, v \rangle$  is defined as in the second order hybrid dual case.

Table 1  
Diffusion Primal Weak Forms

---

### Second order Primal

Find  $\phi \in H^1(V)$  such that ( $\sigma \neq 0$ ,  $s \in H^{-1}(V)$ )

$$\int_V \left( \frac{1}{3\sigma} \nabla \phi \nabla \tilde{\phi} + \sigma_r \phi \tilde{\phi} \right) dV + \int_{\partial V} \tilde{\phi} \chi d\Gamma = \int_V \tilde{\phi} s dV$$

for all  $\tilde{\phi} \in H^1(V)$ .

### Second order Hybrid Primal

Find  $\phi \in X$  and  $\chi \in H^{-1/2}(\Gamma)$  such that ( $\sigma \neq 0$ ,  $s \in H^{-1}(V_l)$ )

$$\begin{cases} \sum_l \int_{V_l} \left( \frac{1}{3\sigma} \nabla \phi \nabla \tilde{\phi} + \sigma_r \phi \tilde{\phi} \right) dV + \sum_l \int_{\partial V_l} \tilde{\phi} \chi d\Gamma = \sum_l \int_{V_l} \tilde{\phi} s dV \\ \sum_l \int_{\partial V_l} \tilde{\chi} \phi d\Gamma = 0 \end{cases}$$

for all  $\tilde{\phi} \in X$  and  $\tilde{\chi} \in H_0^{-1/2}(\Gamma)$ .

### Mixed Primal

Find  $\phi \in H^1(V)$  and  $\mathbf{J} \in [L^2(V)]^n$  such that ( $s \in H^{-1}(V)$ )

$$\begin{cases} \int_V (-\mathbf{J} \nabla \tilde{\phi} + \sigma_r \phi \tilde{\phi} - s \tilde{\phi}) dV + \int_{\partial V} \chi \tilde{\phi} d\Gamma = 0 \\ \int_V \tilde{\mathbf{J}} \cdot (3\sigma \mathbf{J} + \nabla \phi) dV = 0 \end{cases}$$

for all  $\tilde{\phi} \in H^1(V)$  and  $\tilde{\mathbf{J}} \in [L^2(V)]^n$ .

### Mixed-Hybrid Primal

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

$$\begin{cases} \sum_l \int_{V_l} (-\mathbf{J} \nabla \tilde{\phi} + \sigma_r \tilde{\phi} \phi) dV + \sum_l \int_{\partial V_l} \chi \tilde{\phi} d\Gamma = \sum_l \int_{V_l} s \tilde{\phi} dV \\ \sum_l \int_{V_l} \tilde{\mathbf{J}} \cdot (3\sigma \mathbf{J} + \nabla \phi) dV = 0 \\ \sum_l \int_{\partial V_l} \phi \tilde{\chi} d\Gamma = 0, \end{cases}$$

for all  $\tilde{\phi} \in X$ ,  $\tilde{\mathbf{J}} \in [L^2(V)]^n$  and  $\tilde{\chi} \in H_0^{-1/2}(\Gamma)$ .

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## 5 Discretization

### 5.1 Nodal finite elements

In classical finite element methods, the unknowns are point values of the variable (and possibly of its derivatives) at the “nodes” of the element, which usually include the vertices. (The term “node”, used in nodal jargon instead

Table 2  
Diffusion Dual Weak Forms

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### Second order Dual

Find  $\mathbf{J} \in H(\text{div}, V)$  such that  $(\sigma_r \neq 0, s \in L^2(V))$

$$\int_V \left( \frac{(\nabla \cdot \mathbf{J} - s)}{\sigma_r} \nabla \cdot \tilde{\mathbf{J}} + 3\sigma \mathbf{J} \cdot \tilde{\mathbf{J}} \right) dV + \int_{\partial V} \mathbf{n} \cdot \tilde{\mathbf{J}} \psi d\Gamma = 0,$$

for all  $\tilde{\mathbf{J}} \in H(\text{div}, V)$ .

### Second order Hybrid Dual

Find  $\mathbf{J} \in Y$  and  $\psi \in H^{1/2}(\Gamma)$  such that  $(\sigma_r \neq 0, s \in L^2(V_l))$

$$\begin{cases} \sum_l \int_{V_l} \sigma_r^{-1} \nabla \cdot \mathbf{J} \nabla \cdot \tilde{\mathbf{J}} + 3\sigma \mathbf{J} \cdot \tilde{\mathbf{J}} dV + \sum_l \int_{\partial V_l} \mathbf{n} \cdot \tilde{\mathbf{J}} \psi d\Gamma \\ \qquad \qquad \qquad = \sum_l \int_{V_l} \sigma_r^{-1} s \nabla \cdot \tilde{\mathbf{J}} dV \\ \sum_l \int_{\partial V_l} \mathbf{n} \cdot \mathbf{J} \tilde{\psi} d\Gamma = 0. \end{cases}$$

for all  $\tilde{\mathbf{J}} \in Y$  and  $\tilde{\psi} \in H_0^{1/2}(\Gamma)$ .

### Mixed Dual

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

$$\begin{cases} \int_V \tilde{\phi} (\nabla \cdot \mathbf{J} + \sigma_r \phi - s) dV = 0 \\ \int_V (3\sigma \tilde{\mathbf{J}} \mathbf{J} - \phi \nabla \cdot \tilde{\mathbf{J}}) dV + \int_{\partial V} \mathbf{n} \cdot \tilde{\mathbf{J}} \psi d\Gamma = 0 \end{cases}$$

for all  $\tilde{\mathbf{J}} \in H(\text{div}, V)$  and  $\tilde{\phi} \in L^2(V)$ .

### Mixed-Hybrid Dual

Find  $\mathbf{J} \in Y$ ,  $\phi \in L^2(V)$  and  $\psi \in H^{1/2}(\Gamma)$  such that  $(s \in L^2(V_l))$

$$\begin{cases} \sum_l \int_{V_l} \tilde{\phi} (\nabla \cdot \mathbf{J} + \sigma_r \phi) dV = \sum_l \int_{V_l} \tilde{\phi} s dV \\ \sum_l \int_{V_l} (3\sigma \tilde{\mathbf{J}} \mathbf{J} - \phi \nabla \cdot \tilde{\mathbf{J}}) dV + \sum_l \int_{\partial V_l} \mathbf{n} \cdot \tilde{\mathbf{J}} \psi d\Gamma = 0 \\ \sum_l \int_{\partial V_l} \mathbf{n} \cdot \mathbf{J} \tilde{\psi} d\Gamma = 0, \end{cases}$$

for all  $\tilde{\mathbf{J}} \in Y$ ,  $\tilde{\phi} \in L^2(V)$  and  $\tilde{\psi} \in H_0^{1/2}(\Gamma)$ .

---

of “element” in finite element methods, will be used here always in its finite element interpretation, that is as particular points of the considered domain.) On the contrary, nodal finite elements methods (or simply nodal methods) use as unknowns moments of the variable(s), usually expanded through polynomials. With classical finite elements, the boundary conditions can thus be enforced only at points, which means that particle conservation for instance can be enforced only at these points. Nodal methods however enable a better

handling of particle conservation. According to Hennart [23], nodal finite elements lead to less couplings between neighboring elements and by the way to better structured algebraic systems.

While hybrid methods are well handled with nodal finite elements, classical finite elements are better suited for non-hybrid methods. From now, we chose to focus on mixed-hybrid methods, since they are the most advanced formulations that we investigated theoretically. Also, they have received relatively little attention in the past. We will therefore use conforming nodal finite elements. By ‘conforming’, we mean that the finite dimensional spaces are subspaces of the infinite dimensional spaces that they approximate <sup>7</sup>. Also, we consider only the two-dimensional case.

First we introduce general notations for the expansions, without looking at the choice of polynomials. The approximate functions will be denoted as the original ones, but with a subscript  $h$  representing the mesh refinement. Also, we go on using boldface for “physical” vectors only, and we use the subscript  $l$  to denote restrictions to  $V_l$ .

Inside each element  $V_l$ , we take, in the two-dimensional case :

$$\phi_{h,l}(\mathbf{r}) = f_l^T(\mathbf{r})\varphi_l \quad (27)$$

$$\mathbf{J}_{h,l}(\mathbf{r}) = g_{x,l}^T(\mathbf{r})j_{x,l}\mathbf{1}_x + g_{y,l}^T(\mathbf{r})j_{y,l}\mathbf{1}_y, \quad (28)$$

where  $f_l^T(\mathbf{r})$ ,  $g_{x,l}^T(\mathbf{r})$  and  $g_{y,l}^T(\mathbf{r})$  are row vectors of polynomial expansion functions defined everywhere on  $V$ , but non-zero only on the considered element, and  $\varphi_l$ ,  $j_{x,l}$  and  $j_{y,l}$  are coefficient column vectors to be determined. Since for both the internal flux and current, the expansion and test functions belong to the same spaces, we will take test functions equal to the (transposed) expansion functions. Thus, we write

$$\tilde{\phi}_l = f_l, \quad \tilde{\mathbf{J}}_{x,l} = g_{x,l}\mathbf{1}_x, \quad \tilde{\mathbf{J}}_{y,l} = g_{y,l}\mathbf{1}_y, \quad \text{and} \quad \tilde{\mathbf{J}}_l = \tilde{\mathbf{J}}_{x,l} + \tilde{\mathbf{J}}_{y,l}. \quad (29)$$

At element interfaces and external boundaries (that is on  $\Gamma$ ), we take :

$$\psi_{h,i} = h_i^T(\mathbf{r})\psi_i, \quad \text{and} \quad \chi_{h,i} = h_i^T(\mathbf{r})\chi_i. \quad (30)$$

$\psi_{h,i}$  and  $\chi_{h,i}$  represent respectively the flux and normal current along the edge “i” of the element  $V_l$ . (This edge lies in fact between two elements, or on the

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<sup>7</sup> Note that several authors denote by nonconforming a method where the variable(s) (and/or some of its derivatives) may suffer discontinuities across inter-element boundaries. We will not follow this convention here.

external boundary  $\partial V$ .) If we consider rectangular elements for instance, we have four edges per element, thus  $i$  ranges from 1 to 4.  $h^T(\mathbf{r})$  is a row vector of polynomial expansion functions defined on  $\Gamma$ , but having a non-zero value only on the considered edge  $i$  of  $V_l$ . They are required to be orthonormal over each side of an element :  $\int_i h_i(\mathbf{r})h_i^T(\mathbf{r}) = I$  . Note that both the interface flux and normal current are given the same expansion function here, but we could have introduced  $h_{\psi,i}$  and  $h_{\chi,i}$  to distinguish between them.  $\psi_i$  and  $\chi_i$  are coefficient column vectors to be determined. Since the expansion functions  $\psi$  and  $\chi$  belong to  $H^{\pm 1/2}(\Gamma)$ , while the test functions  $\tilde{\psi}$  and  $\tilde{\chi}$  belong to  $H_0^{\pm 1/2}(\Gamma)$ , we take test functions equal to the (transposed) expansion functions except on the external boundary  $\partial V$ , where they must vanish. Thus, we write

$$\tilde{\chi}_i = h_{0,i}, \quad \tilde{\psi}_i = h_{0,i}, \quad (31)$$

where the subscript 0 means that  $h_0$  vanishes for any edge  $i$  on  $\partial V$ . Thus  $h_{0,i}$  is identically zero on  $\Gamma$  if  $i$  is on  $\partial V$ .

## 5.2 Discrete mixed-hybrid methods

### 5.2.1 Primal case

First re-write the weak form of this problem, for approximate solutions: find  $(\phi_h, \mathbf{J}_h, \chi_h)$  in  $S_h \times V_h \times B_h$  such that

$$\begin{cases} a(\phi_h, \tilde{\phi}) - b^p(\tilde{\phi}, \mathbf{J}_h) + c^p(\tilde{\phi}, \chi_h) & = \langle s, \tilde{\phi} \rangle & \forall \tilde{\phi} \in \tilde{S}_h \\ b^p(\tilde{\mathbf{J}}, \phi_h) + d(\mathbf{J}_h, \tilde{\mathbf{J}}) & = 0 & \forall \tilde{\mathbf{J}} \in \tilde{V}_h \\ c^p(\tilde{\chi}, \phi_h) & = 0 & \forall \tilde{\chi} \in \tilde{B}_h, \end{cases} \quad (32)$$

where the different expressions were defined in section 4.4.1, and

$$(S_h \times V_h \times B_h) \subset (X \times [L^2(V)]^n \times H^{-1/2}(\Gamma))$$

since we want to make a conforming approximation. We take  $\tilde{S}_h = S_h$  and  $\tilde{V}_h = V_h$ . For  $\tilde{B}_h$ , we take it to be the subset  $B_{0,h}$  of  $B_h$ , where all the functions vanish if located on the external boundary  $\partial V$ . The approximation space for the unknowns is thus  $S_h \times V_h \times B_h$ , and the one for the test functions is  $S_h \times V_h \times B_{0,h}$ . This way, we have a finite-dimensional approximation of the spaces introduced above, made out of their subsets.

Because we consider the two-dimensional case, the second equation gives here two different equations, one for each direction. Using test functions  $\tilde{\phi}_l$  and  $\tilde{\mathbf{J}}_l$

that are zero outside of the considered element  $V_l$ , and  $\tilde{\chi}$  nonzero only on one edge “ $i$ ” between two elements  $V_l$  and  $V_{l'}$ , we get, for all  $l$ ,

$$\begin{cases} \int_{V_l} (\sigma_r \tilde{\phi}_l \phi_{h,l} - \nabla \tilde{\phi}_l \cdot \mathbf{J}_{h,l}) dV + \int_{\partial V_l} \tilde{\phi}_l \chi_{h,l} d\Gamma = \int_{V_{h,l}} s \tilde{\phi}_l dV \\ \int_{V_l} \tilde{\mathbf{J}}_{x,l} \cdot (3\sigma \mathbf{J}_{h,l} + \nabla \phi_{h,l}) dV = 0 \\ \int_{V_l} \tilde{\mathbf{J}}_{y,l} \cdot (3\sigma \mathbf{J}_{h,l} + \nabla \phi_{h,l}) dV = 0 \\ \int_i \tilde{\chi}_i \phi_{h,l} d\Gamma + \int_{i'} \tilde{\chi}_i \phi_{h,l'} d\Gamma = 0. \end{cases} \quad (33)$$

Using expansions (27) to (29), we get from the first 3 equations:

$$\begin{cases} -K_{x,l}^p j_{x,l} - K_{y,l}^p j_{y,l} + N_{r,l} \varphi_l = S_l - \int_{\partial V_l} f_l \chi_{h,l} d\Gamma \\ N_{d,x,l} j_{x,l} + K_{x,l}^{pT} \varphi_l = 0 \\ N_{d,y,l} j_{y,l} + K_{y,l}^{pT} \varphi_l = 0, \end{cases} \quad (34)$$

where the introduced matrices are defined in the following way ( $q = x, y$ ) :

$$\begin{aligned} K_{q,l}^p &= \int_{V_l} \partial_q f_l g_{q,l}^T dV & N_{d,q,l} &= \int_{V_l} 3\sigma g_{q,l} g_{q,l}^T dV \\ N_{r,l} &= \int_{V_l} \sigma_r f_l f_l^T dV & S_l &= \int_{V_l} f_l s dV. \end{aligned}$$

We now use the expansions (30) to (31) on the boundaries. Introducing

$$M_i^p = \int_i f_l h_i^T d\Gamma, \quad (35)$$

the contribution from each edge “ $i$ ” of  $V_l$  to the surface integral remaining in (34) becomes

$$\int_i f_l \chi_{h,i} d\Gamma = M_i^p \chi_i.$$

Considering a rectangular element,  $i = 1, 2, 3, 4$ , and therefore we define  $M_l^p = [M_1^p, M_2^p, M_3^p, M_4^p]$  and  $\chi_{(h),l} = [\chi_{(h),1}^T, \chi_{(h),2}^T, \chi_{(h),3}^T, \chi_{(h),4}^T]^T$ . We then can write

$$\int_{\partial V_l} f_l \chi_{h,l} d\Gamma = M_l^p \chi_l.$$

Also, the last equation in the weak form (33) becomes

$$M_{0,i}^{p,T} \varphi_l + M_{0,i'}^{p',T} \varphi_{l'} = 0,$$

where  $M_{0,i}^p$  is defined as  $M_i^p$ , but with  $h_0$  instead of  $h$  in (35). This takes into account the fact that the test functions vanish on the external boundary  $\partial V$ . We can thus write the matricial weak form:

$$\begin{cases} N_{r,l} \varphi_l - K_{x,l}^p j_{x_l} - K_{y,l}^p j_{y_l} + M_l \chi_l & = S_l \\ -K_{x,l}^{p,T} \varphi_l - N_{d,x,l} j_{x,l} & = 0 \\ -K_{y,l}^{p,T} \varphi_l - N_{d,y,l} j_{y,l} & = 0 \\ M_{0,i}^{p,T} \varphi_l + M_{0,i}^{p',T} \varphi_{l'} & = 0. \end{cases}$$

Note that

$$\begin{aligned} M_i^{p,T} \varphi_l &= \int_i h_i f_l^T \varphi_l d\Gamma = \int_i h_i \phi_h d\Gamma = \int_i h_i \psi_{h,i} d\Gamma = \int_i h_i h_i^T \psi_i d\Gamma \\ &= \psi_i, \end{aligned} \tag{36}$$

and thus

$$M_l^{p,T} \varphi_l = \psi_l.$$

We can conclude that the last equation of the matricial weak form, which was introduced earlier to enforce the continuity of the flux at inter-element boundaries, enforces here that the (absolute value of the) interface flux be the same <sup>8</sup> on each side of any inter-element boundary, but not on the external boundary  $\partial V$ . As for the interface current  $\chi$ , it is a variable in this formulation, and is thus uniquely defined at inter-element boundaries.

Eliminating the variables  $\varphi_l$ ,  $j_{x,l}$  and  $j_{y,l}$  from the matricial weak form (using (36) to replace  $\varphi_l$  by  $\psi_i$  in the last equation), and applying the change of variable (9), leads to the response matrix formalism used in the VARIANT code [24], developed by Lewis and al. at Northwestern University. In this case, one can then apply boundary conditions directly on  $j^\pm$ . A response matrix formulation makes sense if one is interested only in the interface variables. In this case, mixed (-hybrid) methods are pointless. But if, as we did in the numerical experiments of appendix B, we reconstruct the internal flux and current of each element, a response matrix formulation is a detour. A better way to proceed then, is to use directly the matricial weak form to generate a linear system  $Ax = b$ , where

$$x = (\varphi^T, j_x^T, j_y^T, \chi^T)^T, \quad b = (S^T, 0, 0, 0)^T,$$

<sup>8</sup> The sign difference is due to the opposition between the (closed) integration path orientations of  $\int_{V_l}$  and  $\int_{V_{l'}}$ .

and the matrix  $A$  contains symmetric blocks of the type (for elements with no edge on  $\partial V$ )

$$A_l = \begin{pmatrix} N_{r,l} & -K_{x,l}^p & -K_{y,l}^p & M_l^p \\ -K_{x,l}^{p,T} & -N_{d,x,l} & 0 & 0 \\ -K_{y,l}^{p,T} & 0 & -N_{d,y,l} & 0 \\ M_l^{p,T} & 0 & 0 & 0 \end{pmatrix}. \quad (37)$$

In order to solve the  $Ax = b$  system, a preconditioned conjugate gradient iterative technique can be used. The point is then to find efficient preconditioning. Different options are available. Noticing that  $A_l$  has a zero block in its lower-left corner, we can build a matrix  $A$  of the saddle-point type, i.e. consider the splitting

$$A_l = \begin{pmatrix} \tilde{A}_l & \tilde{B}_l \\ \tilde{B}_l^T & 0 \end{pmatrix}.$$

Nevertheless, with the choice of a symmetric  $A_l$  as in (37), the upper left block  $\tilde{A}_l$  is symmetric but not definite. Changing the signs of the second and third rows in (37), makes  $A_l$  a positive stable block according to our numerical tests (i.e., all its eigenvalues have positive real parts), but unsymmetric. Another approach is to consider the splitting  $A_l$  into four blocks according to:

$$A_l = \begin{pmatrix} A & B \\ B^T & -C \end{pmatrix}.$$

where  $A = N_r$ ,  $B = \begin{pmatrix} -K_{x,l}^p & -K_{y,l}^p & M_l^p \end{pmatrix}$ , and

$$C = \begin{pmatrix} N_{d,x,l} & 0 & 0 \\ 0 & N_{d,y,l} & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

This way,  $A$  is symmetric positive definite and  $C$  symmetric positive semidefinite. Preconditioning of our system matrix will be the subject of further research.

As for boundary conditions (on  $\partial V$ ), reflected boundary conditions ( $\chi_i = 0$ ) are easy to implement, while for vacuum boundaries ( $\psi_i = 2\chi_i$ ), we can use (36) to say that  $M_i^{p,T} \varphi_l = 2\chi_i$  on  $\partial V$ .

**5.2.1.1 Well-posedness of the approximation problem** That this problem is well-posed has been proved in [12] for a primal problem similar to ours. Their proof remains valid for us provided it is adapted to the presence of cross-sectional constants, and vacuum or reflected essential boundary conditions (see appendix A for details). The spaces used here are

$$\begin{aligned}
S_h^s &= \{u : u \in X, u_l \in \mathcal{P}_s(V_l), \forall l\} \\
V_h^v &= \{\mathbf{p} : \mathbf{p} \in [L^2(V)]^n, p_{i,l} \in \mathcal{P}_v(V_l), \forall l, \forall i = 1, \dots, n\} \\
B_h^b &= \{\chi : \chi \in H^{-1/2}(\Gamma), \chi_j \in \mathcal{P}_b(\text{edge } j \text{ of } \partial V_l), \forall l, \\
&\quad \forall j = 1, \dots, \# \text{ of edges of } V_l\} \\
B_{0,h}^b &= \{\chi : \chi \in B_h^b(\Gamma), \chi_j = 0 \text{ if the edge } j \text{ of } V_l \text{ lies on } \partial V\},
\end{aligned} \tag{38}$$

where  $\mathcal{P}_z(V)$  denotes a space of polynomials of order  $\leq z$  on  $V$ . The approximation space is thus defined by a triple  $(s, v, b)$ . Note that the expansion order does not have to be the same in every subdomain  $V_l$  ( $s, v$ , and  $b$  being maximum orders). Using the LBB condition, it is proved that, in case  $\nabla S_h \subset V_h$  (which occurs if  $v \geq s - 1$ ), a sufficient condition for existence and uniqueness of a solution is  $\forall \chi \in B_h$ ,

$$\int_{\partial V_l} \chi u \, d\Gamma = 0 \text{ implies that } \chi = 0, \forall u \in S_h$$

which, translated into matrices, is equivalent to require the  $M_l^p$  matrix to have a rank equal to its number of columns, that is, in case of a rectangular element  $V_l$ , four times the number of terms in the boundary expansion. This same rank condition was found empirically by Lewis et al. for their VARIANT code ([24], [25]), a well-known neutronic code. Note that this same rank condition is also obtained in case of the second order hybrid primal case (not mixed), which corresponds to the method used in VARIANT.

### 5.2.2 Dual case

We proceed in a way similar to the primal case. The mixed-hybrid dual weak form is: find  $(\mathbf{J}_h, \phi_h, \psi_h)$  in  $V_h \times S_h \times B_h$  such that

$$\begin{cases} a(\phi_h, \tilde{\phi}) + b^d(\tilde{\phi}, \mathbf{J}_h) & = \langle s, \tilde{\phi} \rangle & \forall \tilde{\phi} \in S_h^s, \\ -b^d(\tilde{\mathbf{J}}, \phi_h) + d(\mathbf{J}_h, \tilde{\mathbf{J}}) + c^d(\tilde{\mathbf{J}}, \psi_h) & = 0 & \forall \tilde{\mathbf{J}} \in V_h^v, \\ c^d(\mathbf{J}_h, \tilde{\psi}) & = 0 & \forall \tilde{\psi} \in B_{0,h}^b, \end{cases} \quad (39)$$

where the different expressions were defined in sections 4.4.1 and 4.4.2, and

$$(V_h \times S_h \times B_h) \subset (Y \times L^2(V) \times H^{1/2}(\Gamma)).$$

Then, similarly to what we got in the primal case,

$$\begin{cases} \int_{V_l} \tilde{\phi}_l (\nabla \cdot \mathbf{J}_{h,l} + \sigma_r \phi_{h,l}) dV = \int_{V_l} \tilde{\phi}_l s dV \\ \int_{V_l} (3\sigma \tilde{\mathbf{J}}_{x,l} \cdot \mathbf{J}_{h,l} - \nabla \cdot \tilde{\mathbf{J}}_{x,l} \phi_{h,l}) dV + \int_{\partial V_l} \mathbf{n} \cdot \tilde{\mathbf{J}}_{x,l} \psi_{h,l} d\Gamma = 0 \\ \int_{V_l} (3\sigma \tilde{\mathbf{J}}_{y,l} \cdot \mathbf{J}_{h,l} - \nabla \cdot \tilde{\mathbf{J}}_{y,l} \phi_{h,l}) dV + \int_{\partial V_l} \mathbf{n} \cdot \tilde{\mathbf{J}}_{y,l} \psi_{h,l} d\Gamma = 0 \\ \int_i \mathbf{n} \cdot \mathbf{J}_{h,l} \tilde{\psi}_i d\Gamma + \int_i \mathbf{n}' \cdot \mathbf{J}_{h,l'} \tilde{\psi}_i d\Gamma = 0. \end{cases} \quad (40)$$

Using expansions inside each  $V_l$  as before, we get for the first 3 equations

$$\begin{cases} K_{x,l}^{dT} j_{x,l} + K_{y,l}^{dT} j_{y,l} + N_{r,l} \varphi_l = S_l \\ N_{d,x,l} j_{x,l} - K_{x,l}^d \varphi_l + \int_{\partial V_l} \mathbf{n} \cdot g_{x,l} \mathbf{1}_x \psi_{h,l} d\Gamma = 0 \\ N_{d,y,l} j_{y,l} - K_{y,l}^d \varphi_l + \int_{\partial V_l} \mathbf{n} \cdot g_{y,l} \mathbf{1}_y \psi_{h,l} d\Gamma = 0, \end{cases} \quad (41)$$

where the  $K_q^d$  ( $q = x, y$ ) matrices are defined in the following way:

$$K_{x,l}^d = \int_{V_l} \partial_x g_{x,l} f_l^T dV, \quad K_{y,l}^d = \int_{V_l} \partial_y g_{y,l} f_l^T dV.$$

Introducing ( $q = x, y$ )

$$M_{q,i}^d = \int_i \mathbf{n} \cdot \mathbf{1}_q g_{q,l} h_i^T d\Gamma, \quad (42)$$

the contribution from the side “i” of  $V_l$  to the surface integral remaining in (41) then becomes:

$$\int_i \mathbf{n} \cdot \mathbf{1}_q g_{q,l} \psi_{h,i} d\Gamma = M_{q,i}^d \psi_i \quad q = x, y.$$

For a rectangular element, we have  $M_{q,l}^d = [M_{q,1}^d, M_{q,2}^d, M_{q,3}^d, M_{q,4}^d]$ , ( $q = x, y$ ), and  $\psi_{(h),l} = [\psi_{(h),1}, \psi_{(h),2}, \psi_{(h),3}, \psi_{(h),4}]^T$ . In practice, we use rectangular elements  $V_l$  whose edges are parallel to the axes  $x$  or  $y$ . If the edges 1 and 3 are parallel to the  $x$ -axis, and the edges 2 and 4 to the  $y$ -axis, we write

$$M_l^d = M_{x,l}^d + M_{y,l}^d = [M_{x,1}^d, M_{y,2}^d, M_{x,3}^d, M_{y,4}^d].$$

We again define  $M_{q,0}^d$  as  $M_q^d$  in (42), but where  $h$  is replaced by  $h_0$ . This since  $\tilde{\psi} \in H_0^{1/2}(\Gamma)$ , is thus zero on  $\partial V$ , and we must therefore zero the corresponding columns in the  $M_q^d$  matrix. We can write the matricial weak form (here, the elements  $V_l$  and  $V_{l'}$  are supposed to share an edge “ $i$ ” parallel to the y-axis):

$$\begin{cases} K_{x,l}^{dT} j_{x,l} + K_{y,l}^{dT} j_{y,l} + N_{r,l} \varphi_l & = S \\ N_{d,x,l} j_{x,l} - K_{x,l}^d \varphi_l + M_{x,l} \psi & = 0 \\ N_{d,y,l} j_{y,l} - K_{y,l}^d \varphi_l + M_{y,l} \psi & = 0 \\ M_{x,0,i}^{dT} j_{x,l} + M_{x,0,i}^{d',T} j_{x,l'} & = 0. \end{cases}$$

Note that, with  $\mathbf{n} \cdot \mathbf{1}_q = 1$ ,

$$\begin{aligned} M_{q,i}^{dT} j_q &= \int_i h_i g_{q,l}^T j_{q,l} d\Gamma = \int_i h_i J_{q,h,l} d\Gamma = \int_i h_i \chi_{h,i} d\Gamma = \int_i h_i h_i^T \chi_i d\Gamma \\ &= \chi_i, \end{aligned} \tag{43}$$

and thus,

$$M_{q,l}^{dT} j_q = \chi_l.$$

We can conclude that the last equation of the matricial weak form, that was introduced earlier to enforce the continuity of the current at inter-element boundaries, enforces now that the (absolute value of the) interface current be the same on both sides of any inter-element boundary, but not on the external boundary  $\partial V$ .

Eliminating the variables  $\varphi_l$ ,  $j_{x,l}$  and  $j_{y,l}$  from the matricial weak form, and applying the change of variable (9), leads again to a response matrix formalism.

We can also here build a linear system of the type  $Ax = b$ . As for boundary conditions in this case, we can use (43) to say that  $M_{q,i}^{dT} j_{q,l} = 0$  on reflected boundaries, and  $M_{q,i}^{dT} j_{q,l} = \frac{\psi_i}{2}$  on vacuum boundaries.

**5.2.2.1 Well-posedness of the approximation problem** We prove the well-posedness in appendix A for the approximation space  $V_h^v \times S_h^s \times B_h^b$ , with the same notation as in the primal case. Again, vacuum or reflected (essential) boundary conditions are assumed. The approximation space is thus defined by a triple  $(v, s, b)$ . Using the LBB condition, it is proved that, if  $\nabla \cdot V_h \subset S_h$  (which is true if  $s \geq v - 1$ ), a sufficient condition for well-posedness is  $\forall \chi \in B_h$ ,

		Boundary expansion order b		
		0(4)	1(8)	2(12)
Internal expansion order s (primal) or v (dual)	1(3)	3	3	3
	2(6)	4	5	6
	3(10)	4	7	10
	4(15)	4	8	12

Fig. 1. Computed  $M^{p \text{ or } d}$ -matrix rank for rectangular elements in x-y geometry

$$\int_{\partial V_l} \chi \mathbf{u} \, d\Gamma = 0 \text{ implies that } \chi = 0, \forall \mathbf{u} \in V_h$$

which, translated into matrices, is equivalent to require the  $M_l^d$  matrix to have a rank equal to its number of columns. This is the same rank condition as in the primal case. This rank condition is also obtained in case of the second order hybrid dual method (see appendix A).

### 5.3 Rank condition

Let us assume x-y geometry, and that  $B_h^b$  is made out of  $b+1$  polynomials of the type  $x^i, 0 < i \leq b$ , in the variable that varies along the considered edge. (For instance, we have  $\{1, x, x^2\}$  if  $b = 2$ .) Thus, the boundary expansion function (row) vector  $h^T$  has size  $b+1$ . Assume similarly that in the primal case  $S_h^s$  ( $V_h^v$  in the dual case) is made out of all the  $\sum_{i=0}^{s \text{ or } v} (i+1)$  polynomials of the type  $x^i y^j, 0 < i+j \leq s$  or  $v$ , in the primal or dual case, respectively. (For instance, if  $s$  or  $v = 2$ , we have  $\{1, x, y, x^2, xy, y^2\}$ .) Thus, the internal expansion function (column) vector  $f_l$  or  $g_{q,l}$  has size  $s+1$  or  $v+1$ , respectively. Thus, in case of a rectangular element  $V_l$ , the matrix  $M_l^{p \text{ or } d}$  has size  $\sum_{i=0}^{s \text{ or } v} (i+1) \times (4 \times (b+1))$ .

The rank condition derived above says that, if  $\nabla S_h \subset V_h$  (primal case) or  $\nabla \cdot V_h \subset S_h$  (dual case), a sufficient well-posedness condition is that the matrix  $M_l^{p \text{ or } d}$  must have a rank equal to its number of columns. A matrix not satisfying this condition is said to be rank deficient [25].

The figure 1 (from [25])<sup>9</sup> shows the computed  $M_l^{p \text{ or } d}$  matrix rank for rectan-

<sup>9</sup> Note that the polynomials used in VARIANT [24] are slightly different from the ones assumed here, but figure 1 remains valid, also in the dual case.

gular elements in x-y geometry, given its internal expansion order  $s$  (or  $v$ ), and its boundary expansion order  $b$ . The number of lines and columns of  $M_l^{p \text{ or } d}$  are mentioned in brackets next to  $s$  (or  $v$ ) and  $b$ , respectively. The lightly shaded combinations are thus disallowed even before computing the actual rank, since the rank of a matrix cannot be larger than its smallest dimension. The darkly shaded region represent a rank deficient combination, but here not for a dimensional reason.

In the numerical results of appendix B, we will concentrate on fourth order internal approximations ( $s$  or  $v = 4$ ), and on boundary expansion orders  $b$  ranging from 0 to 2. This way, the rank condition is satisfied.

## 6 Conclusions and perspectives

We gave a classification of different formulations for the diffusion equation, providing well-posedness results for the different continuous problems, as well as for the discrete hybrid problems. In this view, we adapted the primal proofs of [12] to vacuum and reflected boundary conditions, and developed them for the dual case. We showed that a sufficient condition for the well-posedness of the discrete hybrid problems <sup>10</sup> is, in the primal (dual) case, if the gradient (divergence) of any flux (current) expansion function belongs to the set of the current (flux) expansion functions, that the matrix  $M$  <sup>11</sup> defined in section 5.2, have a rank equal to its number of columns. Since we are basically dealing here with an elliptic problem, such well-posedness results could be expected. Giving more mathematical insight than the typical engineering texts on the subject, this work clarifies the theory behind the VARIANT code [24] (ex: well-posedness proofs, rank condition).

We chosed to concentrate on the mixed-hybrid formulations. They have two theoretical advantages, namely the simultaneous approximation of both the flux and current in diffusion, (avoiding errors going from one to the other), and the relaxation of their inter-element continuity requirements (at the price of introducing an interface variable).

Further research will be conducted to investigate the preconditioning of the linear systems obtained by discretizing the mixed-hybrid problems. Different options can be considered, as introduced in section 5.2.1. Also, we plan to explore further the mixed-hybrid methods, going beyond the diffusion approximation to the transport equation. In this case, both spatial and angular

<sup>10</sup> using the approximation spaces defined in section 5.2.1.1 and 5.2.2.1

<sup>11</sup> coupling the interface ( $\chi$  (primal) or  $\psi$  (dual)) and the “internal” ( $\phi$  (primal) or  $\mathbf{J}$  (dual)) expansion functions, for each element  $V_l$ .

expansion of the flux and current have to be considered.

## A Well-posedness of the dual diffusion problems

We mainly give here a proof of well-posedness of the mixed-hybrid dual problem similar to the one in [12] for the primal case, but adapted to the dual case. We also adapt the proofs to the presence of constants such as  $\sigma$  and  $\sigma_r$ , as well as to the absence of natural boundary condition. The proof for the second order hybrid method is simpler, and therefore treated more succinctly. Finally, the continuous mixed dual problem is also proved to be well-posed.

We assume that  $\sigma_{(l)}$  and  $\sigma_{r(l)}$  are strictly positive, and constant on each subdomain  $V_l$  in hybrid methods. Also, we assume (essential) vacuum or reflected boundary conditions on the external boundary  $\partial V$  of the considered domain  $V$ . The changes between the primal proofs of [12] and the proofs for our primal methods can be derived straightforwardly from the dual proofs that we provide.

### A.1 Mixed-hybrid dual method

#### A.1.1 Continuous case

Define  $\Lambda = Y \times L^2(V) \times H^{1/2}(\Gamma)$ ,  $\Lambda_0 = Y \times L^2(V) \times H_0^{1/2}(\Gamma)$ ,  $\lambda = (\mathbf{J}, \phi, \psi) \in \Lambda$ , and  $\tilde{\lambda} = (\mathbf{J}, \phi, \psi) \in \Lambda_0$ . Also,  $\|\lambda\|_\Lambda^2 = \|\mathbf{J}\|_Y^2 + \|\phi\|^2 + \|\psi\|_{1/2,\Gamma}^2$ , where  $\|\mathbf{J}\|_Y^2 = \sum_l \|\mathbf{J}\|_{div,l}^2$ . The subscript  $l$  refers to the restriction to  $V_l$  throughout this section. It will not be systematically added to unknowns to avoid too cumbersome notations. Define then

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

where

$$K_l(\lambda_l, \tilde{\lambda}_l) = a_l(\phi, \tilde{\phi}) + b_l^d(\tilde{\phi}, \mathbf{J}) - b_l^d(\tilde{\mathbf{J}}, \phi) + d_l(\mathbf{J}, \tilde{\mathbf{J}}) + c_l(\tilde{\mathbf{J}}, \psi),$$

and

$$\langle s, \tilde{\lambda} \rangle = \langle s, \tilde{\phi} \rangle.$$

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

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

We have to check that  $K(\lambda, \tilde{\lambda})$  is continuous and verifies the LBB condition ( $\langle s, \tilde{\lambda} \rangle$  being continuous by direct application of Schwartz inequality). To check the continuity of  $K(\lambda, \tilde{\lambda})$ , we write, using again Schwartz inequality,

$$\begin{aligned} K_l(\lambda_l, \tilde{\lambda}_l) &\leq \|\nabla \cdot \mathbf{J}\|_l \|\tilde{\phi}\|_l + \sigma_{r,l} \|\phi\|_l \|\tilde{\phi}\|_l + 3\sigma_l \|\mathbf{J}\|_{1,l} \|\tilde{\mathbf{J}}\|_{1,l} \\ &\quad + \|\phi\|_l \|\nabla \cdot \tilde{\mathbf{J}}\|_l + \|\psi\|_{1/2, V_l} \|\tilde{\mathbf{J}}\|_{div,l} + \|\mathbf{J}\|_{div,l} \|\tilde{\psi}\|_{1/2, V_l} \\ &\leq (\|\nabla \cdot \mathbf{J}\|_l^2 + (1 + \sigma_{r,l}) \|\phi\|_l^2 + 3\sigma_{r,l} \|\mathbf{J}\|_{1,l}^2 + \|\psi\|_{1/2, V_l}^2 + \|\mathbf{J}\|_{div,l}^2)^{1/2} \\ &\quad ((1 + \sigma_{r,l}) \|\tilde{\phi}\|_l^2 + 3\sigma_{r,l} \|\tilde{\mathbf{J}}\|_{1,l}^2 + \|\nabla \cdot \tilde{\mathbf{J}}\|_l^2 + \|\tilde{\mathbf{J}}\|_{div,l}^2 + \|\tilde{\psi}\|_{1/2, V_l}^2)^{1/2} \\ &\leq (1 + 3\sigma_{r,l}) \|\lambda_l\|_{\Lambda_l} \|\tilde{\lambda}_l\|_{\Lambda_{0,l}}. \end{aligned}$$

For the LBB condition, we introduce  $\hat{\lambda}_l = (\hat{\mathbf{J}}_l, \hat{\phi}_l, \hat{\psi}_l) \in \Lambda_0$  with <sup>12</sup>, <sup>13</sup>

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

where  $\mathbf{z}_l$  is the weak solution of  $(\Delta \mathbf{z} = \nabla(\nabla \cdot \mathbf{z}))$

$$\begin{aligned} -\Delta \mathbf{z}_l + 3\sigma_l \sigma_{r,l} \mathbf{z}_l &= 0 \quad \text{in } V_l \\ \nabla \cdot \mathbf{z}_l &= \sigma_{r,l} \psi_l \quad \text{on } \partial V_l. \end{aligned} \tag{A.1}$$

We then have

$$\begin{aligned} K_l(\lambda_l, \hat{\lambda}_l) &= \|\nabla \cdot \mathbf{J}_l\|_l^2 + 3\sigma_l(1 + \sigma_{r_l}) \|\mathbf{J}_l\|_l^2 + \sigma_{r_l} \|\phi_l\|_l^2 \\ &\quad + \int_{\partial V_l \cap \partial V} (1 + 2\sigma_{r_l}) \mathbf{n} \cdot \mathbf{J}_l \psi_l d\Gamma + \int_{\partial V_l} \sigma_{r_l} \mathbf{n} \cdot \mathbf{z}_l \psi_l d\Gamma \end{aligned}$$

First, use the hypothesis that either vacuum or reflected (essential) boundary conditions are imposed on  $\partial V$ . In the first case, it means that  $\psi = 2\chi$ , and since  $\chi = \mathbf{n} \cdot \mathbf{J}$  on  $\partial V$  (by definition in this formulation), the first integral is positive. In the second case, we have  $\chi = 0$ , and the first integral vanishes.

Then, let  $v_l = \nabla \cdot \mathbf{z}_l$ . From (A.1), we get

$$\begin{aligned} -\nabla v_l + 3\sigma_l \sigma_{r,l} \mathbf{z}_l &= 0 \quad \text{in } V_l \\ v_l &= \sigma_{r,l} \psi_l \quad \text{on } \partial V_l, \end{aligned} \tag{A.2}$$

<sup>12</sup> The presence of dimensional factors is understood, and  $0 \leq \sigma_{r,l} \leq 1$ .

<sup>13</sup>  $\psi_l|_{\partial V_l, 0}$  is the restriction of  $\psi_l$  to  $\partial V_l - \partial V$ ; it equals zero on  $\partial V \cap \partial V_l$ .

or, taking the divergence of the first equation,

$$\begin{aligned} -\Delta v_l + 3\sigma_l \sigma_{r,l} v_l &= 0 \text{ in } V_l \\ v_l &= \sigma_{r,l} \psi_l \text{ on } \partial V_l. \end{aligned}$$

In fact,  $\mathbf{z}_l = \frac{1}{3\sigma_l \sigma_{r,l}} \nabla v_l$  from the first equation of (A.2). We define the norms  $\|v\|_{1,l,*}^2 = \|\nabla v\|_l^2 + 3\sigma_l \sigma_{r,l} \|v\|_l^2$  and  $\|\mathbf{z}\|_{div,l,*}^2 = \|\nabla \cdot \mathbf{z}\|_l^2 + 3\sigma_l \sigma_{r,l} \|\mathbf{z}\|_l^2$ , that are 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 (1), but with  $\|v\|_{1,V,*}$  instead of  $\|v\|_{1,V}$ . Then,  $\|\psi\|_{1/2,\partial V_l,*} \equiv \|\psi\|_{1/2,\partial V_l}$  in general, and  $\sigma_{r,l} \|\psi_l\|_{1/2,\partial V_l,*} = \|v_l\|_{1,l,*}$ . Thus we have (with  $\tilde{C}$  a constant)

$$\begin{aligned} \|\psi_l\|_{1/2,\partial V_l} &= \tilde{C} \|v_l\|_{1,l,*} \\ &= \tilde{C} \left( \int_{\partial V_l} \sigma_{r,l} \mathbf{n} \cdot \mathbf{z}_l \psi_l d\Gamma \right)^{1/2} \\ &= \tilde{C} \|\mathbf{z}_l\|_{div,l,*} \equiv \|\mathbf{z}_l\|_{div,l}. \end{aligned}$$

Finally we can say that, for any  $l$ , there exists a constant  $C > 0$  such that  $K_l(\lambda_l, \hat{\lambda}_l) \geq C \|\lambda_l\|_{\Lambda_l}^2$ , and

$$K(\lambda, \hat{\lambda}) \geq C \sum_l \|\lambda_l\|_{\Lambda_l}^2 = C \|\lambda\|_{\Lambda}^2.$$

Since we also have (using  $ab \leq \frac{1}{2}(a^2 + b^2)$ )

$$\begin{aligned} \|\hat{\lambda}_l\|_{\Lambda_{0,l}}^2 &\leq (4 + 2\sigma_{r,l}) (\|\mathbf{J}\|_{div,l}^2 + \|\mathbf{z}_l\|_{div,l}^2) + 3\|\phi_l\|_l^2 + (1 + 2\sigma_{r,l})^2 \|\psi_l\|_{1/2,l}^2 \\ &\leq C' \|\lambda_l\|_{\Lambda_l}^2, \end{aligned}$$

where  $C'$  is another constant, we obtain

$$K(\lambda, \hat{\lambda}) \geq \frac{C}{\sqrt{C'}} \|\lambda\|_{\Lambda} \|\hat{\lambda}\|_{\Lambda_0}$$

and thus

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

and the LBB condition is verified.

Given how the mixed-hybrid weak form (and thus  $K(\lambda, \tilde{\lambda})$ ) was built, it is straightforward that, if

$$\begin{aligned}\nabla \cdot \mathbf{J}^* + \sigma_r \phi^* - s &= 0, \text{ and} \\ 3\sigma \mathbf{J}^* + \nabla \phi^* &= 0,\end{aligned}$$

then  $\lambda^* = (\mathbf{J}^*, \phi^*, \phi^*|_\Gamma)$  is such that  $K(\lambda^*, \tilde{\lambda}) = \langle s, \tilde{\lambda} \rangle$  for all  $\tilde{\lambda} \in \Lambda_0$ . Moreover, the verification of the LBB condition implies that this problem has a unique solution.

### A.1.2 Discrete case

We thus have to prove the discrete LBB condition (6), that is here the existence of an  $\alpha > 0$  such that

$$\inf_{\lambda_h \in \Lambda_h, \lambda_h \neq 0} \sup_{\tilde{\lambda}_h \in \Lambda_{0,h}, \tilde{\lambda}_h \neq 0} \frac{|a(\lambda_h, \tilde{\lambda}_h)|}{\|\lambda_h\|_{\Lambda_h} \|\tilde{\lambda}_h\|_{\Lambda_{0,h}}} \geq \alpha,$$

with  $\Lambda_h = S_h^s(V) \times V_h^v(V) \times B_h^b(\Gamma)$  and  $\Lambda_{0,h} = S_h^s(V) \times V_h^v(V) \times B_{0,h}^b(\Gamma)$ , where the different spaces were defined in (38). We introduce  $\Pi_l^s$  and  $\Pi_l^v$  the orthogonal projections of  $H^1(V_l)$  and  $[L^2(V_l)]^n$  respectively onto  $S_h^s(V_l)$  and  $V_h^v(V_l)$ , as well as  $\hat{\lambda}_h = (\hat{\mathbf{J}}_h, \hat{\phi}_h, \hat{\psi}_h)$  with

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

where

$$\begin{cases} -\Delta \Pi_l^v(\mathbf{z}_{h,l}) + 3\sigma \sigma_r \Pi_l^v(\mathbf{z}_h) = 0 & \text{in } V_l \\ \nabla \cdot \Pi_l^v(\mathbf{z}_h) = \sigma_{r,l} \psi_{h,l} & \text{on } \partial V_l \end{cases}$$

Orthogonal projections properties provide

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

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

$$\begin{aligned}
K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) &= 3\sigma_l(1 + \sigma_{r,l}) \|\mathbf{J}_{h,l}\|_l^2 + \sigma_{r,l} \|\phi_{h,l}\|_l^2 \\
&\quad + \sigma_{r,l} \|\Pi_l^v(\mathbf{z}_{h,l})\|_{div,*,l}^2 + \|\Pi_{h,l}^s(\nabla \cdot \mathbf{J}_{h,l})\|_l^2 \\
&\quad - \int_{V_l} (\nabla \cdot \mathbf{J}_{h,l})(\nabla \cdot \Pi_l^v(\mathbf{z}_{h,l}) - \Pi_{h,l}^s(\nabla \cdot \Pi_l^v(\mathbf{z}_{h,l}))) d\Gamma \\
&\quad + \int_{\partial V_l \cap \partial V} \psi_{h,l} \mathbf{n} \cdot \mathbf{J}_{h,l} (1 + 2\sigma_r).
\end{aligned}$$

The last term is positive thanks to the essential vacuum or reflected boundary conditions. Now introduce the parameters:

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

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

$$\begin{aligned}
K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) &\geq 3\sigma_l(1 + \sigma_{r,l}) \|\mathbf{J}_{h,l}\|_l^2 + \sigma_{r,l} \|\phi_{h,l}\|_l^2 + \sigma_{r,l} \mu_l \|\psi_{h,l}\|_{1/2,\partial V_l}^2 \\
&\quad + \nu_l \|\nabla \cdot \mathbf{J}_{h,l}\|_l^2 - \gamma_l \|\nabla \cdot \mathbf{J}_{h,l}\|_l \|\nabla \cdot \Pi_l^v(\mathbf{z}_{h,l})\|_l,
\end{aligned}$$

and, since  $ab \leq \frac{1}{2}(a^2 + b^2)$ ,

$$\begin{aligned}
K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) &\geq \min(3\sigma_l(1 + \sigma_{r,l}), \nu_l) \|\mathbf{J}_{h,l}\|_{1,l}^2 + \sigma_{r,l} \|\phi_{h,l}\|_l^2 \\
&\quad + \sigma_{r,l} \mu_l \|\psi_{h,l}\|_{1/2,\partial V_l}^2 - \frac{1}{2} \gamma_l \|\nabla \cdot \mathbf{J}_{h,l}\|_l^2 \\
&\quad - \frac{1}{2} \gamma_l \|\nabla \cdot \Pi_l^v(\mathbf{z}_{h,l})\|_l^2
\end{aligned}$$

Since  $\|\nabla \cdot \Pi_l^v(\mathbf{z}_{h,l})\|_l \leq \|\Pi_l^v(\mathbf{z}_{h,l})\|_{1,l} = \|\psi\|_{1/2,\partial V_l}$ ,

$$\begin{aligned}
K_l(\lambda_{h,l}, \hat{\lambda}_{h,l}) &\geq (\min(3\sigma_l(1 + \sigma_{r,l}), \nu_l) - \frac{1}{2} \gamma_l) \|\mathbf{J}_{h,l}\|_{1,l}^2 + \sigma_{r,l} \|\phi_{h,l}\|_l^2 + \\
&\quad (\sigma_{r,l} \mu_l - \frac{1}{2} \gamma_l) \|\psi_{h,l}\|_{1/2,\partial V_l}^2.
\end{aligned}$$

Thus,

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

where

$$C_l = \min((\min(3\sigma_l(1 + \sigma_{r,l}), \nu_l) - \frac{1}{2}\gamma_l), \sigma_{r,l}\mu_l - \frac{1}{2}\gamma_l)$$

Again using the properties of orthogonal projections and proceeding as in the continuous case, we get

$$\begin{aligned} \|\hat{\lambda}_{h,l}\|_{\Lambda_0}^2 &\leq (4 + 2\sigma_r) \|\mathbf{J}_{h,l}\|_{div,l}^2 + 3\|\phi_{h,l}\|_l^2 + (5 + 6\sigma_r + 4\sigma_r^2)\|\psi_{h,l}\|_{1/2,l}^2 \\ &\leq C' \|\lambda_{h,l}\|_{\Lambda}^2 \end{aligned}$$

with  $C' = (5 + 6\sigma_r + 4\sigma_r^2)$ . Finally, we can conclude as in the continuous case, and we see 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  $\nabla \cdot V_h^v(V) \subset S_h^s$ , which occurs whenever  $v - 1 \leq s$ , 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 [12], we have:

**Theorem A.1** *The parameter  $\mu_l > 0$  if and only if, for any  $\psi \in B_h^b(V_l)$ ,*

$$\int_{\partial V_l} \psi V d\Gamma = 0 \quad \forall V \in V_h^v(V_l) \text{ implies that } \psi = 0 \quad (\text{A.3})$$

This can be translated into

$$M_l^d \psi = 0 \text{ implies that } \psi = 0$$

where  $M_l^d$  is defined in section 5.2.2. But this is equivalent to require that the rank of  $M_l^d$  be equal to its number of columns. The well-posedness condition is thus equivalent to a rank condition.

### A.1.3 Note

In the primal case, the ‘final’ result in the discrete case is in fact  $C = \min_l C_l$  with  $C_l = \min((\min \sigma_r(1 + 3\sigma), \nu_l) - \gamma/2, 3\sigma\mu_l - \gamma/2)$ . The roles of  $3\sigma$  and  $\sigma_r$  are thus inverted going from primal to dual. The conclusion of [12] ( $M_l^p$  has to be full rank in the special case  $\nabla S_h^s(V) \subset V_h^v$ ), is not affected.

## A.2 Second-order hybrid dual method

In this case,  $\lambda = (\mathbf{J}, \psi) \in \Lambda = Y \times H^{1/2}$ , and  $\tilde{\lambda} \in \Lambda_0 = Y \times H_0^{1/2}$  (defined with corresponding norms). Also,

$$K_l(\lambda, \tilde{\lambda}) = \int_{V_i} (\sigma_r^{-1} \nabla \cdot \mathbf{J} \nabla \cdot \tilde{\mathbf{J}} + 3\sigma \mathbf{J} \tilde{\mathbf{J}}) dV - \int_{\partial V_i} (\psi \mathbf{n} \cdot \tilde{\mathbf{J}} + \mathbf{n} \cdot \mathbf{J} \tilde{\psi}) d\Gamma.$$

A similar (but simpler) analysis can be carried out here. The well-posedness condition for the discrete problem is again the same rank condition.

### A.3 Mixed dual method

In the mixed dual method, no partition of the domain  $V$  is needed. We introduce  $\lambda = (\mathbf{J}, \phi) \in \Lambda = H(\text{div}, V) \times L^2(V)$ , as well as the corresponding norm  $\|\cdot\|_\Lambda$ . The problem to deal with is

$$K(\lambda, \tilde{\lambda}) = \int_V s\tilde{\phi} + \int_{\partial V} \mathbf{n} \cdot \mathbf{J}_\lambda \tilde{\phi} d\Gamma,$$

where the bilinear form is

$$K(\lambda, \tilde{\lambda}) = \int_V ((\nabla \cdot \mathbf{J} + \sigma_r)\tilde{\phi} + 3\sigma \mathbf{J} \tilde{\mathbf{J}} - \phi \nabla \cdot \tilde{\mathbf{J}}) dV.$$

Arguments quite similar to those we used previously can be used again here to prove that  $K(\lambda, \tilde{\lambda})$  satisfies the LBB condition. About the right-hand side, the first term is continuous by direct application of Schwartz inequality, while for the second, it equals  $(z, \phi)_1$  where

$$\begin{cases} -\Delta z + z = 0 & \text{in } V \\ \nabla z = \mathbf{J}_\lambda & \text{on } \partial V \end{cases}$$

Applying again the Schwartz inequality shows the boundedness of the right-hand side. Therefore, the continuous mixed-dual problem is well-posed.

## B Numerical results for diffusion

Numerical experiments were carried out in the diffusion approximation, using nodal finite elements with the mixed-hybrid primal and dual formulations. Similar results were obtained solving the linear system  $Ax = b$ , and using the response matrix formulation [24], based on the change of variables (9). The response matrix results are shown here.

A very simple problem was considered in these early numerical tests, namely the diffusion problem on a square  $V$ , the left-hand side ( $0 < x < 10$ ,  $0 < y <$

20) having a unitary source, and the right-hand side ( $10 < x < 20, 0 < y < 20$ ) being source-free. The boundary conditions are reflective at  $x = 0, y = 0$  and  $y = 20$ , and vacuum at  $x = 20$ . This problem does not depend on  $y$ . The domain  $V$  is divided into  $20 \times 20$  square subdomains  $V_l$ , and for each of them (as well as for their interfaces), the same expansion functions are used. The internal and interface expansion orders used here form a combination satisfying the rank condition derived above.

Figure B.1 shows dual flux and current (in the x-direction) when (the same) fourth order polynomials are used as  $g_{x,l}, g_{y,l}$  and  $f_l$  (expansion and trial) functions inside each element  $V_l$ , and when flux and current are considered constant on the interfaces ( $b = 0$ ). The dashed line represents the exact solution. As expected, the flux and current do not depend on  $y$ , and are therefore plotted for fixed  $y$ . Since the same trial and expansion functions are used for the flux and current, we have  $s = v = 4$  and  $s \geq v - 1$ , thus the rank condition on  $M^d$  applies. Results show that the flux ends up being of the third order, and the current of the fourth order: fourth order coefficients of the flux vanish automatically. Thus, in practice,  $s = 3 = v - 1$ . We see that the numerical results are quite bad here.

Figure B.2 and B.3, also for the dual case, present better results. They are obtained by increasing the interface expansion order  $b$  to 1 and 2 respectively. The results get increasingly better. Again here, the flux is of order 3, and the current of order 4.

Figures B.4 and B.5 show the results in the primal case, as indicated. The results are good even when constant functions are used on the interfaces ( $b = 0$ ). Here again, the same polynomials are used,  $s = v = 4$ , and the condition  $v \geq s - 1$  is verified. Practically however, the fourth order current coefficients vanish automatically, thus  $v = 3 = s - 1$ . From this point of view, there is thus a “duality” between the results in the primal and dual cases.

To explain the discrepancies between the primal and dual results in the constant interface expansion case, I do not have any satisfactory explanation. Maybe this has to do with the boundary conditions of our problem, that are perhaps better suited for the primal case.

Finally, figure B.6 shows the result for a “square in a square” problem. The bottom left quarter has now a unitary source, while the three other quarters are source-free. The boundary conditions are reflected on the bottom and left edges, and vacuum on the top and right edges. The results showed here were obtained with the primal method, using fourth order expansions inside and constant expansions on interfaces. The flux and current (in the x-direction) at the bottom ( $y = 0$ ) of  $V$  are plotted, and, as expected, equal the ones presented before. Furthermore, flux at the middle ( $y = 10$ ) and at  $y = 14$  are

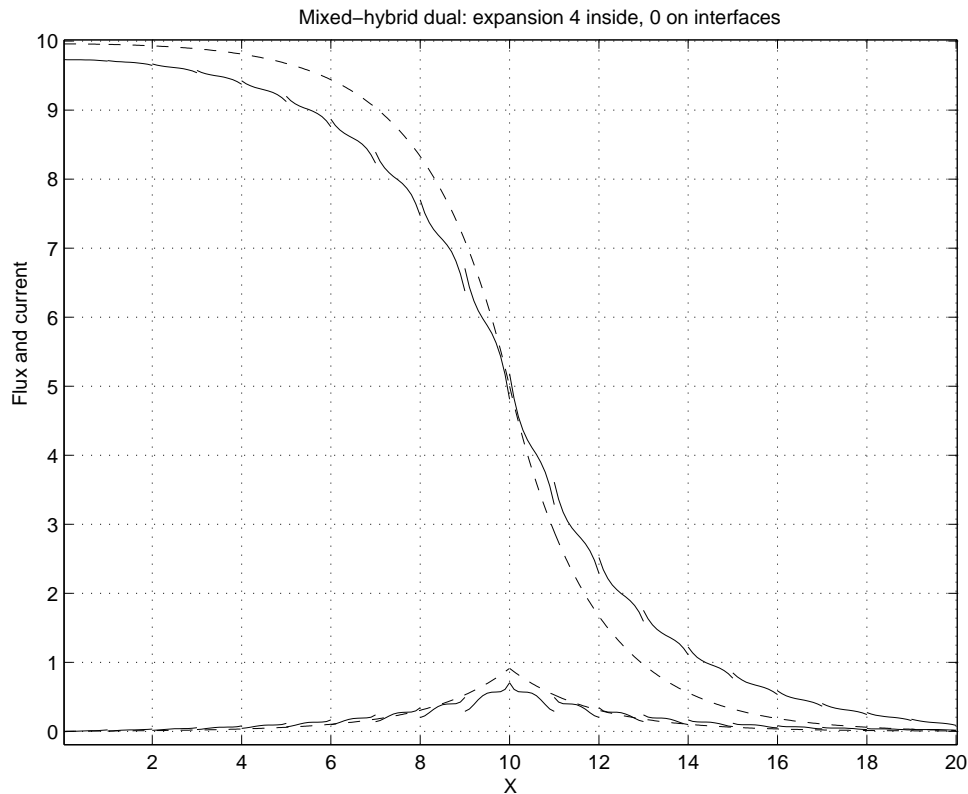


Fig. B.1. Flux and current along  $x$  for fixed  $y$  plotted, showing that the  $y$ -dependence gets treated in a satisfactory manner.

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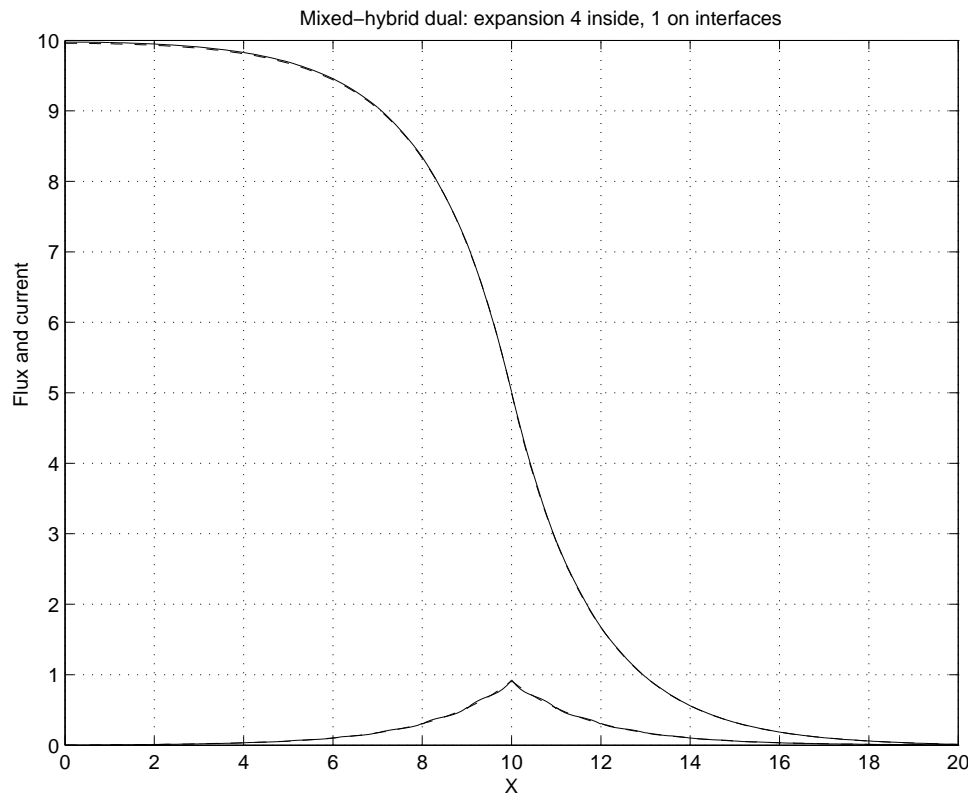


Fig. B.2. Flux and current along  $x$  for fixed  $y$

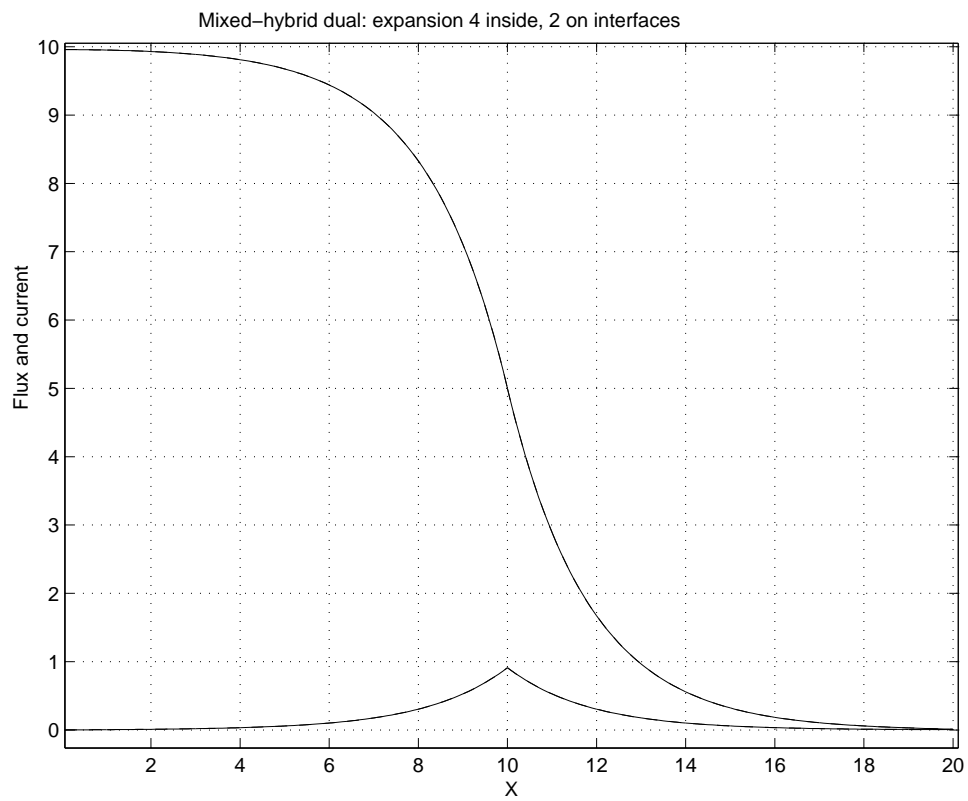


Fig. B.3. Flux and current along  $x$  for fixed  $y$

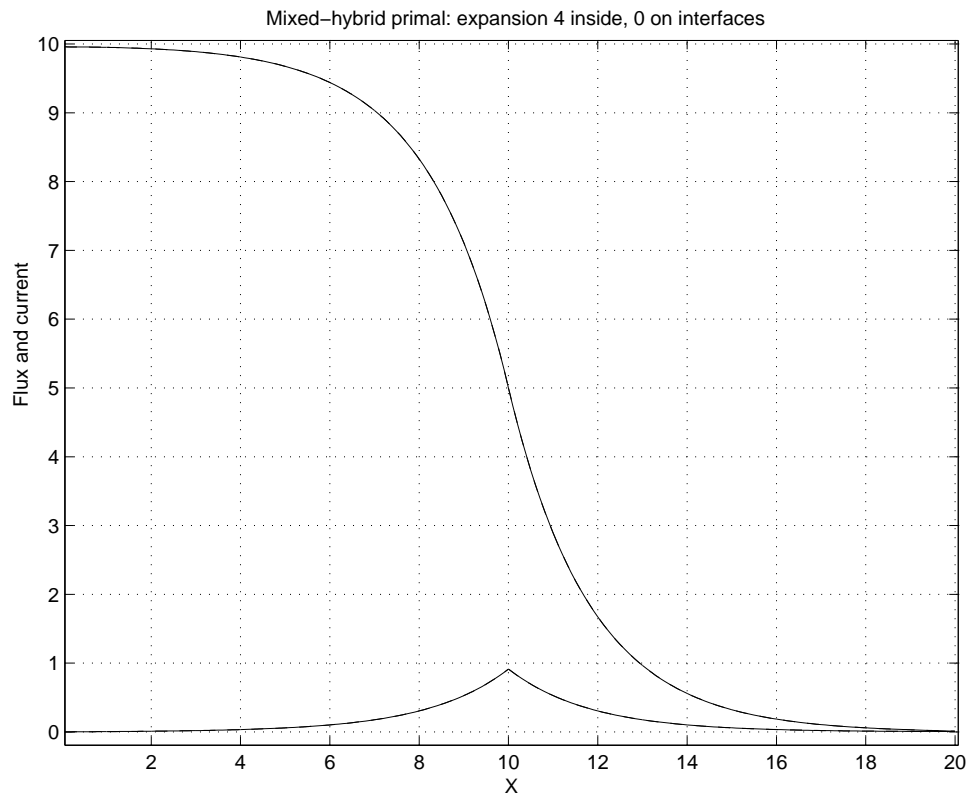


Fig. B.4. Flux and current along  $x$  for fixed  $y$

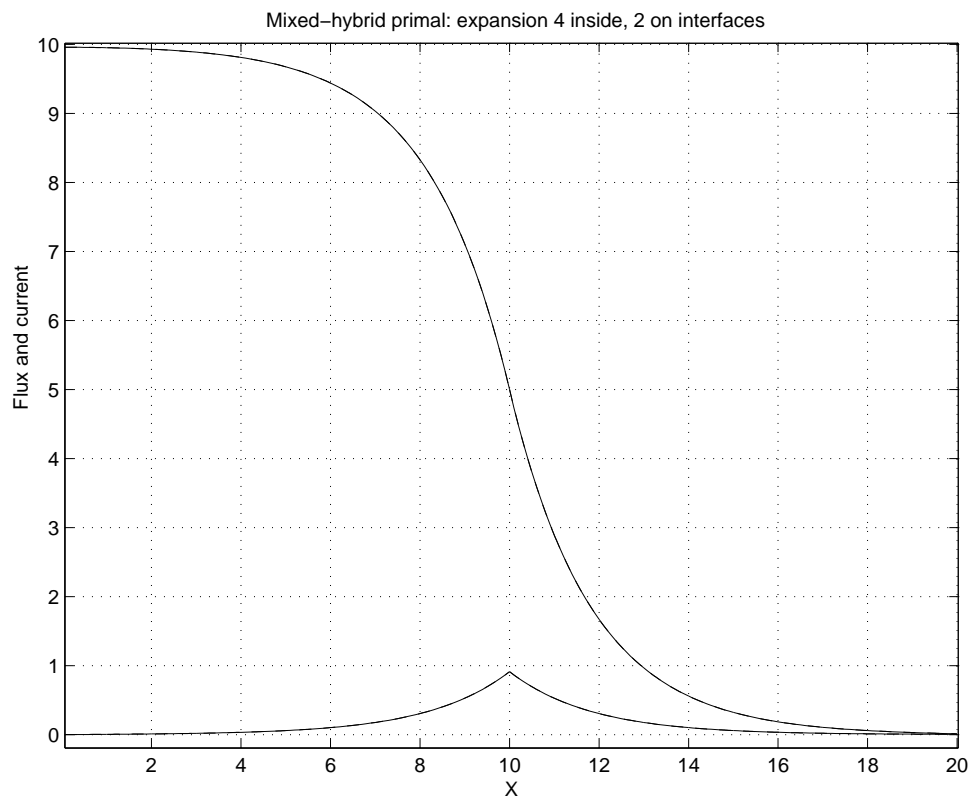


Fig. B.5. Flux and current along  $x$  for fixed  $y$

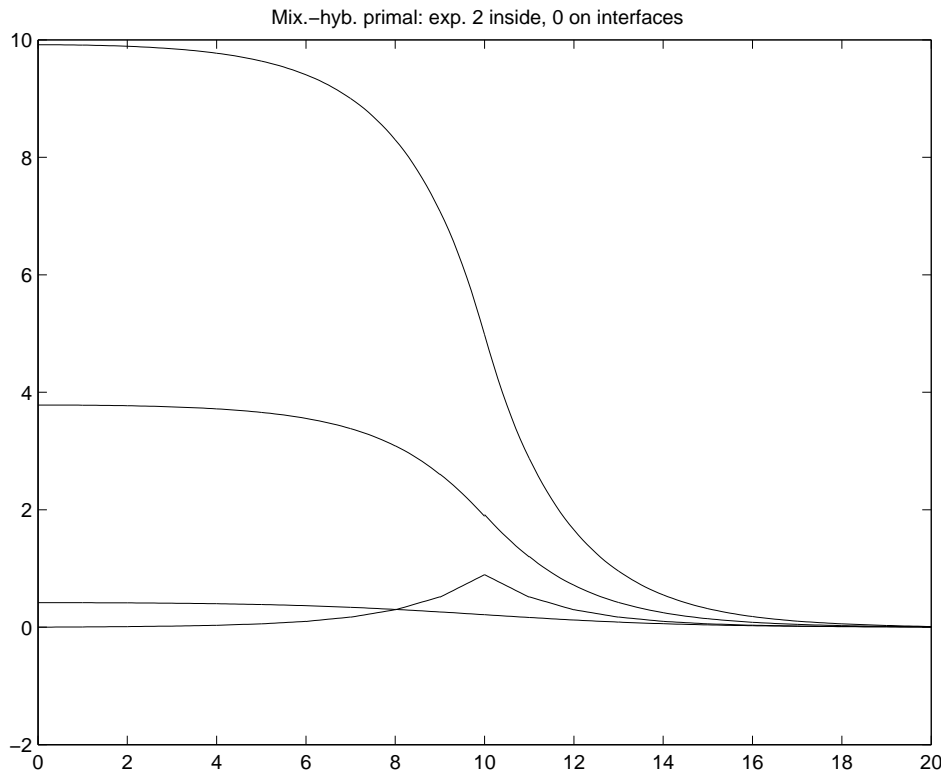


Fig. B.6. Flux for  $y = 0, 10$  and  $14$ ; current along  $x$  at  $y = 0$

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