

## A *POSTERIORI* ERROR ESTIMATES FOR THE FOKKER–PLANCK AND FERMI PENCIL BEAM EQUATIONS

MOHAMMAD ASADZADEH\*

*Department of Mathematics, Chalmers University of Technology  
and Göteborg University, SE-41296 Göteborg, Sweden*

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We prove *a posteriori* error estimates for a finite element method for steady-state, energy dependent, Fokker–Planck and Fermi pencil beam equations in two space dimensions and with a *forward-peaked scattering* (i.e. with velocities varying within the right unit semi-circle). Our estimates are based on a *transversal symmetry assumption*, together with a strong stability estimate for an associated dual problem combined with the Galerkin orthogonality of the finite element method.

### 1. Introduction

This paper is the second part in a series of two papers concerning approximate solutions for the pencil beam equations. In the first part,<sup>3</sup> we derived, for smooth solutions in the Sobolev space  $H^{k+1}$  of functions with their partial derivatives up to order  $k + 1$  in  $L_2$ , *optimal a priori* error estimates for the streamline diffusion and discontinuous Galerkin finite element methods of order  $\mathcal{O}(h^{k+1/2})$ . In this part we extend our studies to *a posteriori* error estimates dealing with the following basic problem: To construct an algorithm for the numerical solution of the pencil beam equations such that the error between the exact and approximate solutions, measured in some appropriate norm, is guaranteed to be below a given tolerance and such that the computational cost is almost minimal. These two properties are referred to as the reliability and efficiency of the algorithm, respectively. The *a posteriori* error analyses are required for the reliability in the sense that the error is controlled by a certain norm of the residual term (measuring the extent to which the computed solution fails to satisfy the actual differential equation), whereas the *a priori* error estimates are based on controlling the size of the error by some norm of the unknown solution itself. As for the efficiency the adaptivity may be invoked

\*E-mail: mohammad@math.chalmers.se

to avoid unnecessary mesh-refinements on the regions where the contribution to the error is already small.

Below, to be concise, we focus on the reliability issue, the efficiency studies are similar to the adaptive error analyses in Refs. 4 and 13. In our studies we shall assume symmetry properties, compensating for the degenerate character of the pencil beam equations, and also put a *switch* which slightly, raising the diffusion coefficient in the critical cases, modifies the continuous problem. The effect of all these manipulations would correspond to adding artificial viscosity in the case of fluid problems, see, e.g. Ref. 18. The error may be split into the perturbation error caused by the modifications and the discretization error for the modified problem. We shall combine the advantages of both Eulerian and Lagrangian approaches to derive finite element error estimates for the modified problem. Compared to the adding of artificial viscosity in the fluid problems our symmetry assumptions, being part of the nature of the particle beams, are less restrictive. Consequently the perturbation errors are less significant and therefore not included in our studies. For a similar problem with significant perturbation error, e.g. a convection dominated convection-diffusion problem, detailed perturbation error analysis is given in Ref. 13.

Pencil beam equations, considered below, are modelling, e.g. problems of collimated electron and photon particles penetrating piecewise homogeneous regions. The collisions between the beam particles and particles from beams with different directions cause deposit of some part of the energy carried by the beams at the collision sites. To obtain a desired "amount of energy deposited at certain parts of the target region" (dose) is of crucial interest in the radiative cancer therapy. To this approach radiation oncologists employ beam configurations obeying the Fermi equation, which is a certain asymptotic limit of the Fokker-Planck equation, see, e.g. Refs. 10, 17 and 21. A physical study of the Fokker-Planck equation, which itself is an asymptotic limit of the linear Boltzmann equation, is given by Risken in Ref. 22. Fermi and Fokker-Planck equations are in the class of diffusion transport equations. For a mathematical derivation of the diffusion transport equations, through asymptotic expansions, see Dautray and Lions,<sup>12</sup> (Vol. 6).

An outline of this paper is as follows: In the remaining of this section we formulate the general three-dimensional problem as an asymptotic limit of the linear transport equation and also extract our two-dimensional continuous model problem for the current function. Section 2 is devoted to notations, preliminaries and a general outline of the *a posteriori* approach. In Sec. 3 we introduce the elements of characteristic streamline diffusion method (CSD) for the pencil beam equations. Section 4 contains error representation formula, interpolation and strong stability estimates for a dual problem. In our concluding Sec. 5 we prove the main result: The *a posteriori* error estimate both in an abstract form and also in a concrete setting.

Below  $C$  will denote different constants in different occurrence independent of all the parameters involved, unless otherwise it is obvious or explicitly stated.

Furthermore,  $(\cdot, \cdot)_Q$  and  $\|\cdot\| \equiv \|\cdot\|_Q$  will denote the  $L_2(Q)$ -inner product and  $L_2(Q)$ -norm, respectively. Other measuring quantities and appropriate, discrete and continuous, function spaces are introduced upon their appearance in the relevant sections.

### 1.1. The continuous problems

The derivation strategies, through the Gaussian multiple scattering theory, for the Fokker-Planck and Fermi pencil beam equations relevant in electron and photon dose calculations can be found in Ref. 17 relying on Fourier techniques, in Ref. 21 using spherical harmonics (see also Holland<sup>15</sup>), and in Ref. 22 based on statistical physics approaches. Below we shall sketch the general idea. For this purpose we start from the steady-state neutron transport equation:

$$\omega \cdot \nabla_{\mathbf{x}} \psi(\mathbf{x}, \omega) + \sigma_t(\mathbf{x}) \psi(\mathbf{x}, \omega) = \int_{S^2} \sigma_s(\mathbf{x}, \omega \cdot \omega') \psi(\mathbf{x}, \omega') d\omega', \quad (1.1)$$

$$\psi(0, y, z, \omega) = \frac{1}{2\pi} \delta(1 - \xi) \delta(y) \delta(z), \quad \xi > 0, \quad (1.2)$$

$$\psi(L, y, z, \omega) = 0, \quad \xi < 0, \quad (1.3)$$

with  $\mathbf{x} = (x, y, z) \in [0, L] \times \mathbb{R} \times \mathbb{R}$ , and  $\omega = (\xi, \eta, \zeta) \in S^2$ , describing the spreading of a pencil beam of particles normally incident upon a purely scattering, source-free, slab of thickness  $L$ . Here  $\psi$  is the density of particles at the point  $\mathbf{x}$  moving in the direction of  $\omega$ ,  $\sigma_t$  and  $\sigma_s$  are total and scattering cross-sections, respectively. Assuming *forward-peaked* scattering, the transport equation (1.1) may, asymptotically, be approximated by the following Fokker-Planck equation

$$\omega \cdot \nabla_{\mathbf{x}} \psi^{\text{FP}} = \sigma \left[ \frac{\partial}{\partial \xi} (1 - \xi^2) \frac{\partial}{\partial \xi} + \frac{1}{1 - \xi^2} \frac{\partial^2}{\partial \vartheta^2} \right] \psi^{\text{FP}}, \quad (1.4)$$

where  $\vartheta$  is the azimuthal angle with respect to the  $x$ -axis and

$$\sigma \equiv \frac{1}{2} \sigma_{\text{tr}}(\mathbf{x}) = \pi \int_{-1}^1 (1 - \xi) \sigma_s(\mathbf{x}, \xi) d\xi, \quad (1.5)$$

is the transport cross-section for a purely scattering medium. In the expansions leading to Eq. (1.4), the absorption term  $\sigma_t \psi$  on the left-hand side of (1.1) associated with a Taylor expansion of  $\psi$  on the right-hand side gives the right-hand side of (1.4) and a neglected remainder term of order  $\mathcal{O}(\sigma^2)$ , see Refs. 3 and 10. A further approximation, assuming thin slab by letting  $L \times \sigma \ll 1$ , and a simple algebraic manipulation yields to a perturbation of Eq. (1.4), and the boundary conditions (1.2) and (1.3), to the following Fermi equation;

$$\begin{cases} \omega_0 \cdot \nabla_{\mathbf{x}} \psi^F = \sigma \Delta_{\eta\zeta} \psi^F, \\ \psi^F(0, y, z, \eta, \zeta) = \delta(y) \delta(z) \delta(\eta) \delta(\zeta), & \xi > 0, \\ \psi^F(L, y, z, \eta, \zeta) = 0, & \xi < 0, \end{cases} \quad (1.6)$$

here  $\omega_0 = (1, \eta, \zeta)$ , where  $(\eta, \zeta) \in \mathbb{R} \times \mathbb{R}$  and  $\Delta_{\eta\zeta} = \partial^2/\partial\eta^2 + \partial^2/\partial\zeta^2$ . Geometrically, Eq. (1.6) corresponds to projecting  $\omega \in S^2$ , in Eq. (1.4), along  $\omega = (\xi, \eta, \zeta)$  onto the tangent plane to  $S^2$  at the point  $(1, 0, 0)$ . In this way the Laplacian operator, on the unit sphere, on the right-hand side of the Fokker–Planck equation (1.4) is transferred to the Laplacian operator on this tangent plane, as on the right-hand side of the Fermi equation in (1.6).

Detailed mathematical analyses for variants of Fermi and Fokker–Planck equations, either as a backward Kolmogorov or some forward–backward degenerate type equations, can be found in Refs. 6–8 and 20. Asymptotic derivations and qualitative approximate behavior of these types of equations have, recently, been studied in Refs. 9, 14 and 19. Similar asymptotic approaches in the case of a modified Chapman–Enskog procedure leads to a free molecular flow, for some hydrodynamic quantity, rather than the diffusion, see Ref. 5. Asymptotic approximation is also considered for a global solution to a reaction–diffusion system with exponential convergence as in Ref. 16.

The CSD-method, used in this paper, was first analyzed by Johnson and Szepessy in Ref. 18 for the conservation laws. A *posteriori* error estimates for a more related problem has recently been carried out by Verfürth in Ref. 23.

Except in a few special cases Fokker–Planck and Fermi equations, with energy dependent scattering and having degenerate nature, are not analytically solvable. Therefore numerical approaches are the only realistic solution alternatives. However, in the numerical algorithms, so far, the priority has been given to the construction of operational codes, with no or some heuristic mathematical justifications, consequently basic approximation theory concepts such as stability and convergence are not appropriately studied. Our intension in this paper is to bridge parts of this gap and also construct numerical schemes accessible for practical purposes. In the analyses below, for simplicity, we concentrate on approximate solutions of problems (1.4) and (1.6) in two dimensions. Extensions of these studies to the real three-dimensional case, although would benefit a great deal from the present studies, would still be a real challenge.

The two-dimensional version of (1.1)–(1.3) leads to the following Fokker–Planck problem, see also Ref. 3: For  $0 < x < L$  and  $-\infty < y < \infty$ , find  $\psi^{\text{FP}} \equiv \Psi^{\text{FP}}(x, y, \theta)$  such that

$$\begin{cases} \omega \cdot \nabla_{\mathbf{x}} \psi^{\text{FP}} = \sigma \psi_{\theta\theta}^{\text{FP}}, & \theta \in (-\pi/2, \pi/2), \\ \psi^{\text{FP}}(0, y, \theta) = \frac{1}{2\pi} \delta(1 - \cos \theta) \delta(y), & \theta \in S^1_+, \\ \psi^{\text{FP}}(L, y, \theta) = 0, & \theta \in S^1_-, \end{cases} \quad (1.7)$$

where  $\omega = (\xi, \eta) \equiv (\cos \theta, \sin \theta)$ ,  $S^1_{+(-)} = \{\omega \in S^1 : \xi > 0 (< 0)\}$ .

Through Eqs. (1.1)–(1.7)  $\psi$  denotes the flux while usually the measured quantity (dose) is related to the current function

$$j = \xi \psi. \quad (1.8)$$



We use the scaling substitution  $z = \tan \theta$ , for  $\theta \in (-\pi/2, \pi/2)$ , and introduce the scaled current function  $J$  by

$$J(x, y, z) \equiv \frac{j(x, y, \tan^{-1} z)}{(1 + z^2)}. \quad (1.9)$$

Note that, now  $z$  corresponds to the angular variable  $\theta$ . Below we shall keep  $\theta$  away from the poles  $\pm\pi/2$ , and correspondingly formulate a problem for the current function  $J$ , in the bounded domain  $Q \equiv I_x \times I_y \times I_z = [0, L] \times [-y_0, y_0] \times [-z_0, z_0]$ :

$$\begin{cases} J_x + zJ_y = \sigma AJ, & (x, x_\perp) \in Q, \\ J_z(x, y, \pm z_0) = 0, & \text{for } (x, y) \in I_x \times I_y, \\ J(0, y_0, z) = 0, & \text{for } z < 0, \\ J(0, -y_0, z) = 0, & \text{for } z > 0, \\ J(0, x_\perp) = f(x_\perp), \end{cases} \quad (1.10)$$

where  $x_\perp \equiv (y, z)$  is the transversal variable and we have replaced the product of  $\delta$ -functions (the source term) at the boundary by a smoother  $L_2$ -function  $f$ . Further

$$A = \partial^2 / \partial z^2, \quad (\text{Fermi}) \quad (1.11)$$

$$A = \partial / \partial z [a(z) \partial / \partial z (b(z) \cdot)], \quad (\text{Fokker-Planck}) \quad (1.12)$$

where  $a(z) = 1 + z^2$  and  $b(z) = (1 + z^2)^{3/2}$  are indicating the diffusive behavior of the Fokker-Planck equation compared to the Fermi equation. We recall that the transport cross-section depends on the energy and therefore on the spatial variables:  $\sigma \equiv \sigma(x, y) = \sigma_{\text{tr}}(E(x, y))/2$ .

### 1.2. Approximations in the case of small angular scattering

As we indicated above Eq. (1.7) is obtained from a two-dimensional version of the linear transport equation (1.1) through a certain asymptotic expansion neglecting  $\mathcal{O}(\sigma^2)$ -terms. In other words, the absorption and scattering terms involving  $\sigma_t$  and  $\sigma_s$ , respectively, in (1.1) are combined to give the,  $\mathcal{O}(\sigma)$ , diffusion term on the right-hand side of (1.7) as well as (1.10) and also higher order terms which are neglected. Then a natural question would be: How much of the original absorption, which is a regularizing term, is kept in the Fokker-Planck diffusion term  $\sigma AJ$  with  $A$  as in (1.12)? Below, expanding  $AJ$ , we simply see that not only the whole absorption term in (1.1) is now in the neglected or cancelled part but we also have a  $\alpha\sigma J$  term hidden in  $\sigma AJ$ . Loosely speaking, in the asymptotic expansions of deriving the Fokker-Planck equation from the neutron transport equation, mathematically, a regularizing absorption term of order  $\mathcal{O}(\sigma_t + \sigma)$  is gone. More precisely:

$$AJ \equiv (a(bJ)_z)_z = a'(bJ)_z + a(bJ)_{zz} = (a'b' + ab'')J + (a'b + 2ab')J_z + abJ_{zz},$$

where  $A$ ,  $a = a(z)$  and  $b = b(z)$  are as in the Fokker-Planck case (1.12). Consequently, with this modelling, the Fokker-Planck equation can be written as

$$J_x + \beta \cdot \nabla_{\perp} J - \sigma \alpha J = \sigma ab J_{zz} \equiv \sigma(1+z^2)^{5/2} J_{zz}, \quad (1.13)$$

where  $\nabla_{\perp} = (\partial/\partial y, \partial/\partial z)$  is the transversal gradient and, for the moment

$$\alpha = (a'b' + ab'') \equiv 3(1+z^2)^{1/2}(4z^2+1), \quad \beta = (z, -8\sigma z(1+z^2)^{3/2}).$$

Thus trying to, deterministically, derive the Fermi equation in two dimensions, i.e.

$$J_x + zJ_y = \sigma J_{zz}, \quad (1.14)$$

from its Fokker-Planck counterpart, would lead to considering additional, annihilating, approximations as  $\alpha\sigma \approx 0$ , and

$$\{\beta \approx (z, 0) \quad \text{and} \quad \gamma \equiv (1+z^2)^{5/2} \approx 1\} \iff (z\sigma, z^2) \approx (0, 0).$$

This means that because of the forward-peakedness of the scattering associated with the *small angle approximations*, loosely speaking, we may interpret the Fermi equation as a consequence of yet another asymptotic behavior of the Fokker-Planck equation as  $(\sigma, z) \rightarrow (0, 0)$ , so that one can take  $(z\sigma, z^2) \approx (0, 0)$ . This is a nearly rarefied model describing, e.g. a photon path with negligible collision effects which may be simplified to  $J_x \approx 0$ , i.e. free particles flowing in the  $x$ -direction.

In a forward-peaked scattering for the *Flatland* (2-D problem) version a particle at the position  $(x_0, 0)$ , moving in the  $x$ -direction, after undergoing a collision would move in the direction of the straight line  $y = \tan(\theta)(x - x_0)$ . For small  $\theta$ -values, because of the forward-peakedness, we may use approximations:  $\sin \theta \approx \theta - \theta^3/6$ , and  $\tan \theta \approx \theta + \theta^3/3$ . Then one possible study of the Fermi equation (1.14) would be through Fourier techniques which is also considered by Jette in Ref. 17.

For a partial remove of the degeneracy we may assume that,  $J_{yy} \approx J_{zz}$ . We shall use a somewhat more involved assumption: That there are constants  $C_1$  and  $C_2$  such that

$$C_1 \frac{\partial^k J}{\partial z^k} \leq \frac{\partial^k J}{\partial y^k} \leq C_2 \frac{\partial^k J}{\partial z^k}, \quad k = 1, 2. \quad (1.15)$$

Then a nondegenerate approximation for Eq. (1.7) would be as follows:

$$\mathcal{L}(J) := J_x + \beta \cdot \nabla_{\perp} J - \varepsilon \Delta_{\perp} J = 0, \quad (1.16)$$

where  $\varepsilon \approx C\sigma/2 = C\sigma_{tr}/4$ ,  $C \approx (C_1 + C_2)/2$ ,  $\Delta_{\perp} := \partial^2/\partial y^2 + \partial^2/\partial z^2$ , is the transversal Laplacian operator, and from now on  $\beta \equiv (z, 0)$ . In our studies below  $A$  is given by (1.11) corresponding to the Fermi equation, extensions to the Fokker-Planck case (1.12) are straightforward, but lengthy (see our *a priori* error analysis in Ref. 3 involving such extensions), and therefore are omitted.

## 2. Outline and Preliminaries

We shall use high accuracy and good stability properties of the *streamline diffusion*, (SD), Galerkin finite element method, also studied in Refs. 2 and 3, based on:

- (a) A space-velocity discretization based on piecewise polynomial approximation with basis functions being continuous in  $x_{\perp} = (y, z)$  and discontinuous in  $x$ .
- (b) A streamline diffusion modification of the test function giving a weighted least square control of the residual  $\mathcal{R}(J^h) = \mathcal{L}(J^h)$  of the finite element solution  $J^h$ .
- (c) Modification of the transport cross-section  $\sigma_{tr} = 2\sigma$  so that, in the critical regions, a more diffusive equation is obtained through modifying  $\varepsilon$  as

$$\hat{\varepsilon}(x, x_{\perp}) = \max(\varepsilon(x, y), c_1 h \mathcal{R}(J^h) / |\nabla_{\perp} J^h|, c_2 h(x, x_{\perp})^{3/2}), \quad (2.1)$$

where  $h$  is a total mesh-size and  $c_i, i = 1, 2$  are sufficiently small constants. For the original degenerate problem  $\hat{\varepsilon}$  is defined by replacing  $\varepsilon$  by  $\sigma$  in (2.1). With a simplified form of the modified/artificial transport cross-section given by

$$\hat{\varepsilon} = \max(\varepsilon, c_1 h), \quad (2.2)$$

the SD-modification (b) may be omitted. The *a posteriori* error estimate (also underlying the adaptive algorithm) is, in the case of discretizing in the transversal variable  $(y, z) = x_{\perp}$  only, basically as follows:

$$\|\hat{e}_h\|_Q \leq C^s C^i \|\hat{\varepsilon}^{-1} h^2 \mathcal{R}(J^h)\|_Q, \quad (2.3)$$

where  $\hat{e}_h = \hat{J} - J^h$ , with  $\hat{J}$  being the solution of (1.16) with  $\varepsilon$  replaced by  $\hat{\varepsilon}$  and

$$e = J - J^h = (J - \hat{J}) + (\hat{J} - J^h) := \hat{e} + \hat{e}_h. \quad (2.4)$$

Note that  $J - \hat{J}$  is a perturbation error caused by changing  $\varepsilon$  to  $\hat{\varepsilon}$  in the continuous problem (1.16). Further  $C^s$  is a stability constant and  $C^i$  is an interpolation constant. In the simplified case (2.2), the error estimate (2.3) takes the form

$$\|\hat{e}_h\|_Q \leq C^s C^i \|h \mathcal{R}(J^h)\|_Q. \quad (2.5)$$

The adaptive algorithm is based on (2.3) and seeks to find a mesh with as few degrees of freedom as possible such that for a given tolerance  $\text{TOL} > 0$ ,

$$C^s C^i \|\hat{\varepsilon}^{-1} h^2 \mathcal{R}(J^h)\|_Q \leq \text{TOL}, \quad (2.6)$$

which, through (2.3), would  $L_2$ -bound  $\hat{e}_h$ . To control the remaining part of the error, i.e.  $\hat{e} = J - \hat{J}$ , we may adaptively refine the mesh until  $\hat{\varepsilon} = \varepsilon$ , giving  $\hat{J} = J$ , or alternatively approximate  $\hat{e}$  in terms of  $\hat{\varepsilon} - \varepsilon$ . To approximately minimize the total number of degrees of freedom of a mesh with mesh-size  $h(x, x_{\perp})$  satisfying (2.6), typically a simple iterative procedure is used where a new mesh-size is computed by equi-distribution of element contributions in the quantity  $C^s C^i \|\hat{\varepsilon}^{-1} h^2 \mathcal{R}(J^h)\|_Q$  with the values of  $\hat{\varepsilon}$  and  $\mathcal{R}(J^h)$  taken from the previous mesh.

The structure of the proof of the *a posteriori* error estimate (2.6) is as follows:

- (i) Representation of the error  $\hat{e}_h$  in terms of the residual  $\mathcal{R}(J^h)$  and the solution  $\psi$  of a dual problem with  $\hat{e}_h$  as the right-hand side.
- (ii) Use of the Galerkin orthogonality to replace  $\psi$  by  $\psi - \Psi$ , where  $\Psi$  is a finite element interpolant of  $\psi$ .
- (iii) Interpolation error estimates for  $\psi - \Psi$  in terms of certain derivative  $\mathcal{D}^\alpha \psi$  of  $\psi$  (in our case  $\hat{e}\psi_{zz}$  or  $\hat{e}\Delta_\perp \psi$ ) and the mesh-size  $h$ .
- (iv) Strong stability estimate for the dual solution  $\psi$  estimating  $\mathcal{D}^\alpha \psi$  in terms of the data  $\hat{e}_h$  of the dual problem.

Below we specify the steps (i)–(iv). We let  $I_\perp := I_y \times I_z$ , and recall that  $\hat{J}$  satisfies

$$\begin{cases} \hat{J}_x + \beta \cdot \nabla_\perp \hat{J} - \hat{e}\Delta_\perp \hat{J} = 0, & \text{in } Q, \\ \hat{J}(0, x_\perp) = f(x_\perp), & \text{for } x_\perp \in I_\perp, \\ \hat{J}_z(x, y, \pm z_0) = 0, & \text{for } (x, y) \in [0, L] \times I_y, \\ \hat{J}(0, \pm y_0, z) = 0, & \text{for } z \in \Gamma_0^-, \end{cases} \quad (2.7)$$

with  $\Gamma_0^- = \Gamma^- \cap \{x = 0\}$ , where  $\Gamma^{-(+)} = \{\mathbf{x} \in \Gamma = \partial Q : \tilde{\beta} \cdot \mathbf{n}(\mathbf{x}) < 0 (> 0)\}$ ,  $\tilde{\beta} = (1, \beta)$ , and similarly,  $\Gamma^0 = \{(x, y, \pm z_0)\} \cup \{(x, \pm y_0, 0)\}$ . Observe that problem (2.7) is nonlinear because  $\hat{e}$  depends on  $J^h$ . Hence, in particular,  $\hat{e}$  depends on  $z$  leading to control of some crucial terms, in the stability Lemma 4.3 below, which otherwise are not estimated in a natural way. To deal with  $\hat{e}_z$ -contributions we shall consider below some additional angular symmetry assumptions, e.g. (2.15).

Suppose now that  $J^h \in \mathcal{V}_h$ , where  $\mathcal{V}_h \subset L_2(Q)$  is a finite element space, is a Galerkin type approximate solution satisfying

$$\begin{cases} J_x^h + \beta \cdot \nabla_\perp J^h - \hat{e}\Delta_\perp J^h = \mathcal{R}, & \text{in } Q, \\ J^h(0, \cdot) = f_h, & \text{in } I_\perp, \\ J^h = 0, \text{ on } \Gamma_0^-, \text{ and } \hat{J}_z^h = 0, & \text{on } \Gamma^0, \end{cases} \quad (2.8)$$

where  $f_h$  is a finite element approximation of  $f$  and the residual  $\mathcal{R}$  satisfies Galerkin orthogonality relation

$$\int_Q \mathcal{R}v \, dx \, dx_\perp = 0, \quad \forall v \in \mathcal{V}_h. \quad (2.9)$$

Let us also assume that in the approximation procedure the total inflow of particles is preserved, i.e.

$$\int_{\Gamma_s^-} J^h |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma = \int_{\Gamma_s^-} J |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma, \quad (2.10)$$

where  $\Gamma_s^- := \Gamma^- \setminus \{x = 0\}$ , is the *side-inflow boundary* and (2.10) is referred as *side-inflow consistency*. Observe that in both our continuous and discrete model

problems (2.7) and (2.8), primarily, we may assume

$$J|_{\Gamma_s^-} = J^h|_{\Gamma_s^-} = 0, \tag{2.11}$$

then, there is no guarantee that “after-collision and/or reflected” particles would obey the same boundary condition as (2.11).

In the sequel and to avoid multiple-indices, we shall refer to all approximated functions with alternate sub- or super-index  $h$ . Subtracting (2.8) from (2.7) gives the following equation for the error  $\hat{e}^h = \hat{J} - J^h$ :

$$\begin{cases} \mathcal{L}\hat{e}^h \equiv \hat{e}_x^h + \beta \cdot \nabla_{\perp} \hat{e}^h - \hat{\varepsilon} \Delta_{\perp} \hat{e}^h = -\mathcal{R}, & \text{in } Q, \\ \hat{e}^h(0, \cdot) = f - f_h, & \text{in } I_{\perp}, \\ \hat{e}^h = 0, \text{ on } \Gamma_0^-, \text{ and } \hat{e}_z^h = 0, & \text{on } \Gamma^0. \end{cases} \tag{2.12}$$

We now introduce a dual for the problems (2.7), (2.8) or (2.12) as

$$\begin{cases} \mathcal{L}^* \psi = -\psi_x - \beta \cdot \nabla_{\perp} \psi - \hat{\varepsilon} \Delta_{\perp} \psi = \hat{e}^h, & \text{in } Q, \\ \psi = 0, \text{ on } \Gamma^+, \text{ and } \psi_z = 0, & \text{on } \Gamma^0. \end{cases} \tag{2.13}$$

Recall that the degenerate equation corresponds to replacing in (2.7)–(2.13),  $\beta \cdot \nabla_{\perp}$ ,  $\Delta_{\perp}$ , and  $\psi$  by  $z\partial_y$ ,  $\partial_{zz}$ , and  $\varphi$ , respectively, then we have the following version of the dual problem (2.13):

$$\begin{cases} \mathcal{L}^* \varphi = -\varphi_x - z\varphi_y - \hat{\varepsilon} \varphi_{zz} = \hat{e}^h, & \text{in } Q, \\ \varphi = 0, \text{ on } \Gamma^+, \text{ and } \varphi_z = 0, & \text{on } \Gamma^0. \end{cases} \tag{2.14}$$

Note that, in (2.14),  $\hat{\varepsilon}$  is obtained from (2.1) by replacing  $\varepsilon$  by  $\sigma$ . We shall keep using the notation  $\hat{\varepsilon}$  for both degenerate and nondegenerate cases,  $\varepsilon$  or  $\sigma$  version will be obvious from the context. Now, for simplicity, we assume the following *weighted angular symmetry*,

$$\int_{I_x \times I_y} (\varphi w)(z_0) dx dy = \int_{I_x \times I_y} (\varphi w)(-z_0) dx dy, \quad \forall w \in L_2(Q). \tag{2.15}$$

Integrating by parts and using (2.15) with  $w = (\hat{\varepsilon} \hat{e}^h)_z$  and  $w = \hat{\varepsilon}_z \hat{e}^h$ , we have

$$-(\hat{e}^h, \hat{\varepsilon} \varphi_{zz})_Q = -(\hat{\varepsilon}_z \hat{e}_z^h, \varphi)_Q + (\hat{\varepsilon}_z \hat{e}^h, \varphi_z)_Q - (\hat{\varepsilon} \hat{e}_{zz}^h, \varphi)_Q, \tag{2.16}$$

where we have also used the boundary conditions  $\varphi_z = \hat{e}_z^h = 0$ , on  $\Gamma^0$ . From (2.14)–(2.16), we get the following error representation formula:

$$\begin{aligned} \|\hat{e}^h\|^2 &= (\hat{e}^h, \mathcal{L}^* \varphi)_Q = \int_Q \hat{e}^h (-\varphi_x - z\varphi_y - \hat{\varepsilon} \varphi_{zz}) dx dx_{\perp} \\ &= (\mathcal{L} \hat{e}^h, \varphi)_Q - \int_{I_{\perp}} \hat{e}^h \varphi \Big|_{x=0}^{x=L} dy dz - \int_{I_x \times I_z} z \hat{e}^h \varphi \Big|_{y=-y_0}^{y=y_0} dx dz \\ &\quad - (\hat{\varepsilon}_z \hat{e}_z^h, \varphi)_Q + (\hat{\varepsilon}_z \hat{e}^h, \varphi_z)_Q := \sum_{i=1}^5 I_i. \end{aligned} \tag{2.17}$$

Below we identify each term  $I_i, i = 1, \dots, 5$ , more closely. We have that

$$I_1 = (\mathcal{L}\hat{e}^h, \varphi) = - \int_Q \mathcal{R}\varphi \, dx \, dx_\perp.$$

The incident boundary conditions give

$$I_2 = - \int_{I_\perp} \hat{e}^h(L, \cdot) \varphi(L, \cdot) \, dx_\perp + \int_{I_\perp} \hat{e}^h(0, \cdot) \varphi(0, \cdot) \, dx_\perp = \int_{\Gamma_0^-} (f - f_h) \varphi \, dx_\perp,$$

while the outflow boundary conditions, i.e.  $\varphi \equiv \hat{e}^h = 0$ , on  $\Gamma^+$  imply that

$$\begin{aligned} I_3 &= - \int_{I_x} \left\{ \int_0^{z_0} z \hat{e}^h \varphi \Big|_{y=-y_0}^{y=y_0} \, dz + \int_{-z_0}^0 z \hat{e}^h \varphi \Big|_{y=-y_0}^{y=y_0} \, dz \right\} dx \\ &= \int_{I_x} \int_0^{z_0} z \hat{e}^h(-y_0) \varphi(-y_0) - \int_{I_x} \int_{-z_0}^0 z \hat{e}^h(y_0) \varphi(y_0) = \int_{\Gamma_s^-} \hat{e}^h \varphi |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma, \end{aligned}$$

where  $\mathbf{n}$  is the outward unit normal defined at the boundary and, for the sake of generality, we have not used the assumption (2.10) yet. Thus summing up we get

$$\|\hat{e}^h\|^2 = - \int_Q \mathcal{R}\varphi \, dx + \int_{\Gamma^-} \hat{e}^h \varphi |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma - \int_Q \hat{\varepsilon}_z \hat{e}^h_z \varphi \, dx + \int_Q \hat{\varepsilon}_z \hat{e}^h \varphi_z \, dx. \quad (2.18)$$

We use Galerkin orthogonality (2.9) and write

$$\int_Q \mathcal{R}\varphi \, dx \, dx_\perp = \int_Q \mathcal{R}(\varphi - \mathcal{P}_h \varphi) \, dx \, dx_\perp = \int_Q (\mathcal{R} - \mathcal{P}_h \mathcal{R})(\varphi - \mathcal{P}_h \varphi) \, dx \, dx_\perp,$$

where  $\mathcal{P}_h : L_2(Q) \rightarrow \mathcal{V}_h$  is the  $L_2(Q)$ -projection. By Cauchy-Schwarz inequality we may estimate the boundary integral term in (2.18) as

$$\int_{\Gamma^-} \hat{e}^h \varphi |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma \leq \left( \int_{\Gamma^-} |\hat{e}^h|^2 |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma \right)^{1/2} \times \left( \int_{\Gamma^-} |\varphi|^2 |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma \right)^{1/2}.$$

Now using an interpolation error, with a symmetry assumption  $\varphi_{yy} \approx \varphi_{zz}$  inherited from (1.15), of the form

$$\|\hat{\varepsilon} h^{-2}(\varphi - \mathcal{P}_h \varphi)\|_Q \leq C^i \|\hat{\varepsilon} \Delta_\perp \varphi\|_Q \approx C^i \|\hat{\varepsilon} \varphi_{zz}\|_Q, \quad (2.19)$$

together with a strong stability estimate for the dual problem (2.14) of the form

$$\|\hat{\varepsilon} \varphi_{zz}\|_Q \leq C^s \|\hat{e}^h\|_Q, \quad (2.20)$$

we get that

$$- \int_Q \mathcal{R}\varphi \, dx \, dx_\perp \leq C^s C^i \|h^2 \hat{\varepsilon}^{-1} (\mathcal{R} - \mathcal{P}_h \mathcal{R})\|_Q \|\hat{e}^h\|_Q. \quad (2.21)$$

To estimate the boundary integrals we recall the  $L_2$  trace theorem

$$\|u\|_{L_2(\partial\Omega)}^2 \leq C_T \|u\|_{L_2(\Omega)} \|u\|_{W_2^1(\Omega)},$$

and also the inverse estimate

$$\|v\|_{W_2^1(\Omega)} \leq C_{\text{inv}} \|h^{-1} v\|_{L_2(\Omega)},$$

where  $W_p^r$  is the usual Sobolev space consisting of functions having their derivatives up to order  $r$  in  $L_p$ ,  $u$  and  $v$  are sufficiently smooth functions and  $\Omega \subset \mathbb{R}^d$ ,  $d = 2, 3$  is a bounded Lipschitz domain, see Refs. 1 and 11 for details. Applying the trace theorem and inverse estimate to  $\varphi$  and  $Q$  we get using (2.19) that

$$\begin{aligned} \int_{\Gamma^-} |\varphi|^2 |\mathbf{n} \cdot \beta| \, d\Gamma &\leq C \|\varphi\|_Q \|\varphi\|_{W_2^1(Q)} \leq C \|\varphi - \mathcal{P}_h \varphi\|_Q \|\varphi - \mathcal{P}_h \varphi\|_{W_2^1(Q)} \\ &\leq C \|\hat{\varepsilon} h^{-2} (\varphi - \mathcal{P}_h \varphi)\|_Q \|\hat{\varepsilon}^{-1} h^2 (\varphi - \mathcal{P}_h \varphi)\|_{W_2^1(Q)} \\ &\leq C C^s (C^i)^2 \|\hat{\varepsilon}^h\|_Q \|\hat{\varepsilon}^{-1} h^3 \Delta_{\perp} \varphi\|_Q, \end{aligned}$$

where  $C$  depends on the trace theorem and inverse inequality constants. Recalling (2.1) we have that  $\hat{\varepsilon} > h^{3/2}$  and therefore  $\hat{\varepsilon}^{-1} h^3 \leq h^{3/2} \leq \hat{\varepsilon}$ . Hence

$$\|\hat{\varepsilon}^{-1} h^3 \Delta_{\perp} \varphi\|_Q \approx \|\hat{\varepsilon}^{-1} h^3 \varphi_{zz}\|_Q \leq \|\hat{\varepsilon} \varphi_{zz}\|_Q \leq C^s \|\hat{\varepsilon}^h\|_Q.$$

Thus

$$\int_{\Gamma^-} |\varphi|^2 |\mathbf{n} \cdot \beta| \, d\Gamma \leq C (C^s C^i)^2 \|\hat{\varepsilon}^h\|_Q^2. \tag{2.22}$$

At this moment we need to invoke (2.10), (note that if there were any feasible information on behavior of the secondary particles at the inflow boundary then we would have been able to continue without using (2.10)), identifying the boundary integral

$$\int_{\Gamma^-} |\hat{\varepsilon}^h|^2 |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma = \int_{\Gamma_0^-} |f - f_h|^2 |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma. \tag{2.23}$$

It remains to estimate  $I_4$  and  $I_5$ , where there is no orthogonality relation, such as (2.9), available. Now we assume, for a sufficiently small constant  $c \ll 1$ , that

$$|\nabla_{\perp} \hat{\varepsilon}| \leq c \hat{\varepsilon} h_{\perp}^{-1}, \tag{2.24}$$

and let  $\tilde{C} = \sup(\hat{\varepsilon} h_{\perp}^{-1}) / \inf(\hat{\varepsilon} h_{\perp}^{-1})$ , (works for the case corresponding to  $\hat{\varepsilon} \approx \mathcal{O}(h)$  in (2.2), as well), then by (2.24) and the inverse estimate we have

$$|(\hat{\varepsilon}_z \hat{\varepsilon}_z^h, \varphi)_Q| \leq c \sup_{x \in Q} (\hat{\varepsilon} h_{\perp}^{-1}) \|h_{\perp}^{-1} \hat{\varepsilon}^h\| \|h_{\perp}^2 \Delta_{\perp} \varphi\| \leq c \tilde{C} \|\hat{\varepsilon}^h\| \|\hat{\varepsilon} \varphi_{zz}\| \leq c \tilde{C} C^s \|\hat{\varepsilon}^h\|^2,$$

the choice of  $\tilde{C}$  is for moving  $\hat{\varepsilon} h_{\perp}^{-1}$  in and outside the norms (see also proof of Lemma 5.2 below), and  $c$  is chosen so that  $c \tilde{C} C^s < 1/8$ . Estimating  $I_5$ , in a similar way we finally get

$$|(\hat{\varepsilon}_z \hat{\varepsilon}_z^h, \varphi)_Q| + |(\hat{\varepsilon}_z \hat{\varepsilon}^h, \varphi_z)_Q| \leq \frac{1}{4} \|\hat{\varepsilon}^h\|^2. \tag{2.25}$$

Inserting (2.21)–(2.25) in (2.18), and using a kick-back argument we obtain

$$\|\hat{\varepsilon}^h\|_Q \leq \tilde{C} \left[ \|h^2 \hat{\varepsilon}^{-1} (\mathcal{R} - \mathcal{P}_h \mathcal{R})\|_Q + \left( \int_{\Gamma_0^-} |f - f_h|^2 |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma \right)^{1/2} \right]. \tag{2.26}$$

Thus we have estimated the error in terms of the residual and the incident boundary error and have a complete control over all the involved constants (note that  $\bar{C} = \bar{C}(c, \tilde{C}, C_T, C_{\text{inv}}, C^s, C^i)$ , depends on the constants in the inverse estimate, trace theorem, stability estimates, interpolation estimate and energy variation. All these are, assumed, theoretical constants not effected by our approximation procedure). The estimate (2.26), which is an analogue of (2.3), is appropriate in the present setting with  $\mathcal{R}$  satisfying the Galerkin orthogonality relation (2.9) and  $f$  being a sufficiently smooth approximation for the product of  $\delta$  functions at the incident inflow boundary.

A general Galerkin method for (1.10) or (2.7), to be studied below, does not have exactly the form (2.9) with  $\mathcal{R} \in L_2(Q)$  and therefore below the projection  $\mathcal{P}_h$  will not enter into the error estimates in a concrete way as in (2.26), but a corresponding form to be derived would be, essentially, as follows:

$$\|\hat{e}^h\|_Q \leq C(\|\hat{\varepsilon}^{-1}h_{\perp}^2\mathcal{D}_{\perp,h}^2J^h\|_Q + \|\hbar\partial_x J^h\|_Q), \quad (2.27)$$

where  $\mathcal{D}_{\perp,h}^2$  is the second-order difference quotient operator in  $x_{\perp}$ ,  $\partial_x$  is the first-order difference quotient in  $x$  and  $h_{\perp}$  and  $\hbar$  are the transversal (in  $x_{\perp}$ ) and convective (in  $x$ ) step-size functions, respectively. The norms on the right-hand side of (2.27) are naturally corresponding to interpolation terms  $\|h_{\perp}^2\Delta_{\perp}J\|_Q$ , (if  $\hat{\varepsilon} = Ch$ ) and  $\|\hbar J_x\|_Q$  related to piecewise polynomial approximations.

We have now outlined the basic ideas in the proof of the *a posteriori* error estimate (2.3) which rely on the Galerkin orthogonality relation (2.9) and the strong stability (2.20) of the dual problems (2.13) and (2.14). Our main focus will be to derive the strong stability estimate (2.20) and interpolation error estimates for the dual problem.

**Remark 2.1.** The strong stability (2.20) should be compared with the nonvalidity of a *weak stability* estimate for (2.13) and (2.14) of the form

$$\|\rho\|_Q \leq C\|\hat{e}^h\|_Q, \quad \text{with } \rho = \psi, \text{ or } \varphi, \quad (2.28)$$

corresponding to the  $L_2$ -instability phenomenon, related to the lack of absorption, discussed above. However, since  $\varphi = 0$  on a part of the boundary ( $\Gamma^+$ ), with positive measure, we may derive a weak variant of (2.28) (with  $\rho$  replaced by  $\hat{\varepsilon}\rho$ ) using Poincaré inequality, (see Lemma 2.2 of Ref. 3). We note that in (2.20) the derivative  $\Delta_{\perp}\varphi \sim \varphi_{zz}$  of the dual solution is  $L_2$ -controlled (with the factor  $\hat{\varepsilon}$ ) in terms of  $\|\hat{e}^h\|_Q$ , whereas  $L_2$ -control of  $\varphi$  itself as in the estimate (2.28) is not possible to achieve in general. For the *a posteriori* error control, using the strong stability estimates of the type (2.20) (with derivative control only), it is necessary to use Galerkin orthogonalities.

To motivate for removing degeneracy through introducing  $\varepsilon$  and also the role played by the artificial viscosity  $\hat{\varepsilon}$  in the error estimate (2.3) we notice that the corresponding sharp *a posteriori* error estimate for elliptic problems is

$$\|\hat{e}^h\|_Q \leq C\|h^2\mathcal{R}(J^h)\|_Q. \quad (2.29)$$



The estimates (2.3) and (2.26) may be viewed as a variant of (2.29) where the ellipticity introduced, by  $\hat{\varepsilon}$ , in the hyperbolic problem is compensated by the multiplicative factor  $\hat{\varepsilon}^{-1}$  in (2.3) and (2.26).

In conclusion: *A posteriori* error estimates for numerical schemes may be viewed as special cases of a general stability theory controlling the effect on the solutions resulting from nonvanishing residuals. The perturbations in the finite element method corresponding to certain orthogonality relations make the *a posteriori* error estimates possible in cases where a general perturbation argument would fail.

### 3. The CSD-Method for the Pencil Beam Equations

We let  $0 = x_0 < x_1 < \dots < x_N < x_{N+1} = L$  be a sequence of discrete collision sites in the  $x$ -direction with the corresponding intervals  $I_x^n = (x_n, x_{n+1})$  and discrete steps  $\hbar_n = x_{n+1} - x_n$ . For each  $n$  let  $\mathcal{T}_n = \{\tau_n\}$  be a partition of  $I_\perp^n := \{x_n\} \times I_\perp$ , ( $I_\perp = I_y \times I_z$ ), into edge-to-edge triangular elements  $\tau_n$  (in the sequel we suppress  $n$  from  $\tau_n$ ), with corresponding mesh functions  $h_n^\perp \in C^1(I_\perp^n)$  such that for some positive constant  $c_1$  independent of  $n$ ,

$$(h_\tau \leq h_n^\perp(x_\perp), \quad \text{for } x_\perp \in \tau) \wedge \left( c_1 h_\tau^2 \leq \int_\tau dx_\perp, \quad \tau \in \mathcal{T}_n \right), \quad \forall n, \quad (3.1)$$

where  $h_\tau$  is the diameter of  $\tau$ . Further, we assume that there is a constant  $\lambda$  independent of  $n$  and  $h_\tau$  such that

$$\|\nabla_\perp h_n^\perp\|_{L^\infty(I_\perp^n)} \leq \lambda, \quad \forall n. \quad (3.2)$$

Now for each  $n$  we define the slab  $S_n = I_x^n \times I_\perp$ , and a *local mesh-convection velocity*  $\beta_n \in [C(S_n)]^2$  satisfying, for some sufficiently small constant  $c_2$ ,

$$|\beta_n(x, x_\perp) - \beta_n(x, x'_\perp)| \leq c_2 |z - z'| / \hbar_n, \quad x_\perp, x'_\perp \in I_\perp, \quad x \in I_x^n. \quad (3.3)$$

Note that in general  $\beta_n$  will be an approximation of  $\beta|_{S_n}$ . Let  $\alpha_n = \alpha_n(\bar{x}, \bar{x}_\perp)$  be the characteristic curve corresponding to  $\beta_n$  defined by

$$\begin{cases} \frac{d}{d\bar{x}} \alpha_n(\bar{x}, \bar{x}_\perp) = \beta_n(\bar{x}, \alpha_n(\bar{x}, \bar{x}_\perp)), & \bar{x} \in I_x^n, \\ \alpha_n(x_n, \bar{x}_\perp) = \bar{x}_\perp, & \bar{x}_\perp \in I_\perp. \end{cases} \quad (3.4)$$

Since  $\beta = (z, 1)$  is independent of  $x$ , we may assume that  $\beta_n = \beta_n(\bar{x}_\perp)$  and rewrite (3.4) as

$$\alpha_n(\bar{x}, \bar{x}_\perp) = \bar{x}_\perp + (\bar{x} - x_n)\beta_n(\bar{x}_\perp), \quad \text{for } \bar{x} \in I_x^n. \quad (3.5)$$

The approximate particle path  $(\bar{x}, \alpha_n(\bar{x}, \bar{x}_\perp))$  is a straight line-segment with slope  $\beta_n(\bar{x}_\perp)$  starting at  $(x_n, \bar{x}_\perp)$ . In this setting  $(x, x_\perp)$  and  $(\bar{x}, \bar{x}_\perp)$  are acting as local, (on  $S_n$ ), Euler and Lagrange coordinates, respectively. Since  $\beta$  is not constant, our local non-oriented  $(\bar{x}, \bar{x}_\perp)$  coordinates, although close, are different from the global Lagrange coordinates.

Now we introduce the local coordinate transformation  $\mathcal{F}_n : S_n \rightarrow S_n$  defined by

$$(x, x_\perp) = \mathcal{F}_n(\bar{x}, \bar{x}_\perp) = (\bar{x}, \alpha_n(\bar{x}, \bar{x}_\perp)), \quad \text{for } (\bar{x}, \bar{x}_\perp) \in S_n. \quad (3.6)$$

Denoting the Jacobian with respect to  $\bar{x}_\perp$  by  $\bar{\nabla}_\perp (\equiv \bar{\Lambda})$ , we have from (3.5) that

$$\bar{\nabla}_\perp \alpha_n(\bar{x}, \bar{x}_\perp) = I + (\bar{x} - x_n) \bar{\nabla}_\perp \beta_n(\bar{x}_\perp), \quad (3.7)$$

with  $I$  being the identity operator. Now by the inverse function theorem the mapping  $\mathcal{F}_n : S_n \rightarrow S_n$  is invertible if

$$\hbar_n \|\bar{\nabla}_\perp \beta_n\|_{L^\infty(I_\perp^n)} \leq c, \quad (3.8)$$

for some sufficiently small positive constant  $c$ . The condition (3.8) is guaranteed by our assumption (3.3) on  $\beta_n$ , ensuring that the approximate particle paths satisfying (3.4) do not cross in  $S_n$ .

**Remark 3.1.** The above approach, initially, is constructed to give a locally controlled approximate velocity field, therefore for our model problem, with  $|\beta| \leq (1 + z_0^2)^{1/2}$  (giving a total control of the quantity corresponding to the velocity field), the coordinate change may seem to be unnecessary. However, we need to be convinced that the approximation procedure do not introduce particle path crossings, otherwise the discrete model would allow additional collisions than those modelled by the continuous case making the model problem inadequate. A somewhat less involved  $\beta_n$  would be sufficient to carry out the analyses in here. We have chosen the above general framework in order to have an algorithm which is applicable to the related nonlinear problems, such as Vlasov–Poisson, as well.

For a given function  $v : S_n \rightarrow S_n$  we associate a function  $\bar{v} : S_n \rightarrow S_n$  by setting

$$\bar{v}(\bar{x}, \bar{x}_\perp) = v(x, x_\perp), \quad \text{where } (x, x_\perp) = \mathcal{F}_n(\bar{x}, \bar{x}_\perp), \quad (3.9)$$

and vice versa. Now let

$$\Gamma_{x_n}^- = \{x_\perp \in \partial(I_\perp^n) : \mathbf{n}(x_\perp) \cdot \beta < 0\}, \quad \text{and } \Gamma_n^- = \Gamma^- \cap S_n,$$

we now define for  $p \geq 0$  and  $q \geq 1$ , the function spaces

$$\mathcal{W}_n = \{v \in \mathcal{C}(I_\perp^n) : v|_\tau \in P_q(\tau), \forall \tau \in \mathcal{T}_n, \quad v = 0, \quad \text{on } \Gamma_{x_n}^-, \quad v_z|_{\pm z_0} = 0, \quad \forall n\},$$

$$\bar{\mathcal{V}}_n = \left\{ \bar{v} \in \mathcal{C}(S_n) : \bar{v}(\bar{x}, \bar{x}_\perp) = \sum_{j=0}^p (\bar{x} - x_n)^j w_j(\bar{x}_\perp), \quad w_j \in \mathcal{W}_n \right\},$$

$$\mathcal{V}_n = \{v \in \mathcal{C}(S_n) : v(x, x_\perp) = \bar{v}(\bar{x}, \bar{x}_\perp), \quad (x, x_\perp) = \mathcal{F}_n(\bar{x}, \bar{x}_\perp)\},$$

$$\mathcal{V} = \{v \in L_2(Q) : v|_{S_n} \in \mathcal{V}_n, \quad \text{for } n = 0, \dots, N\},$$

where  $P_q(\tau)$  denotes the set of polynomials of degree at most  $q$  on  $\tau$  and  $h$  denotes the global mesh function defined by a direct product as

$$h(x, x_\perp) = \hbar(x) \otimes h_\perp(x_\perp), \quad (x, x_\perp) \in S_n.$$

Note that the function  $v \in \mathcal{V}$  may be discontinuous across the discrete  $x$ -levels  $x_n$ , to account for this fact we use the notations

$$v_{\pm}^n = \lim_{\Delta x \rightarrow 0^{\pm}} v(x_n + \Delta x) \quad \text{and} \quad [v_n] = v_+^n - v_-^n.$$

We shall below seek an approximation  $J^h$  of the exact solution  $J$  for (1.10), in the space  $\mathcal{V}_h \equiv \mathcal{V}$ , by using the streamline diffusion (SD)-method defined as follows: Find  $J^h \in \mathcal{V}_h$  such that for  $n = 0, 1, \dots, N$ ,

$$\begin{aligned} & (J_x^h + \beta \cdot \nabla_{\perp} J^h, v + \kappa(v_x + \beta \cdot \nabla_{\perp} v))_n + (J_z^h, (\hat{\varepsilon}v)_z)_n - \int_{I_x^n \times I_y} \hat{\varepsilon} J_z^h v \Big|_{z=-z_0}^{z=z_0} \\ & - (\hat{\varepsilon} \kappa J_{zz}^h, v_{\beta})_n + \langle J_+^h, v_+ \rangle_{n-1} - \langle J_+^h, v_+ \rangle_{\Gamma_n^-} = \langle J_-^h, v_+ \rangle_{n-1}, \quad \forall v \in \mathcal{V}_n, \end{aligned}$$

where  $J^h(0, \cdot)_- = f_h$ . Further

$$\hat{\varepsilon} = \max(\varepsilon, C_1 h \tilde{\mathcal{R}}(J^h) / (|\nabla_{\perp} J^h| + C_2), C_3 h^{\nu}),$$

or

$$\hat{\varepsilon} = \max(\varepsilon, C_1 h^2 \tilde{\mathcal{R}}(J^h) / (|J^h| + C_2), C_3 h^{\nu}),$$

with

$$\tilde{\mathcal{R}}(J^h) = |J_x^h + \beta \cdot \nabla_{\perp} J^h| + |[J_n^h]|/\tilde{h}_n := |\mathcal{R}_1(J^h)| + |\mathcal{R}_2(J^h)|, \quad \text{on } S_n,$$

with  $[J_n^h]$  extended to  $S_n$  as constant along the characteristic curve  $\alpha_n(\bar{x}, \bar{x}_{\perp})$ . Moreover  $C_i, i = 1, 2, 3$  are positive constants,  $3/2 \leq \nu \leq 2$  and recall that

$$(v, w) = \int_Q v w \, dx \, dx_{\perp}, \quad (v, w)_n = \int_{S_n} v w \, dx \, dx_{\perp},$$

$$\langle v, w \rangle_n = \int_{I_{\perp}} v(x_n, \cdot) w(x_n, \cdot) \, dx_{\perp}, \quad \langle v, w \rangle_{\Gamma_n^-} = \int_{\Gamma_n^-} v w |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma.$$

Note that in general the finite element approximation for the hyperbolic type problems would substantially benefit, gain improved stability estimates and convergence rates, from the streamline modification. The studies, e.g. in Ref. 2 for the Vlasov-Poisson equation and Refs. 13 and 18 for fluid problems and conservation laws are some examples demonstrating this phenomenon. In the pencil beam problems, however, the convection velocity  $\beta_n$  of the mesh is either identical or sufficiently close to the velocity field  $\beta$ , therefore the streamline modification in the SD-method above may be omitted, i.e.  $\kappa = 0$ .

Below we shall concentrate on the study of the following simplified CSD-method: Find  $J^h \in \mathcal{V}_h$  such that for  $n = 0, 1, \dots, N$ ,

$$\begin{aligned} & (J_x^h + \beta \cdot \nabla_{\perp} J^h, v)_n + (J_z^h, (\hat{\varepsilon}v)_z)_n - \int_{I_x^n \times I_y} \hat{\varepsilon} J_z^h v \Big|_{z=-z_0}^{z=z_0} \\ & + \langle J_+^h, v_+ \rangle_{n-1} - \langle J_+^h, v_+ \rangle_{\Gamma_n^-} = \langle J_-^h, v_+ \rangle_{n-1}, \quad \forall v \in \mathcal{V}_n. \end{aligned} \quad (3.10)$$

Equation (3.10) with  $\hat{\varepsilon} = Ch$  corresponds to a first-order accurate upwind scheme, studied for the fluid problems, with classical artificial viscosity  $\hat{\varepsilon} = Ch$ . Note that in our SD-method with  $\hat{\varepsilon} = Ch$  the  $\hat{\varepsilon}$ -term dominates the  $\kappa$ -term and therefore, (even without using the, *forward-peaked*, properties of the pencil beams arised in the convection velocity  $\beta_n$  in the previous paragraph), we may take  $\kappa = 0$ , justifying (3.10).

Note further that there are two  $x_{\perp}$ -discretization meshes associated to each  $x_n$ -level  $I_{\perp}^n$ : the mesh  $\mathcal{T}_n$  associated to  $S_n$ , i.e. the "left-face mesh" on the slab  $S_n$ , and  $\mathcal{T}_n^- = \{\mathcal{F}_{n-1}(x_{n-1} \times \bar{\tau}); \bar{\tau} \in \mathcal{T}_{n-1}\}$ , i.e. the "right-face mesh" on the slab  $S_{n-1}$ , resulting from a direct transport, along the characteristics, of the previous "left-face mesh"  $\mathcal{T}_{n-1}$ . If  $\mathcal{T}_n^-$  is not too distorted, it is possible to choose  $\mathcal{T}_n \equiv \mathcal{T}_n^-$  corresponding to no remeshing at  $x_n$ , while remeshing would correspond to  $\mathcal{T}_n \neq \mathcal{T}_n^-$ .

Too many remeshings would affect the construction of an efficient numerical scheme. Actually, in the final estimates, the "*remeshing frequency*" appeared as a multiple of the convergence rate, we return to this issue in Sec. 5 (Remark 5.2). Finally, the existence of a unique solution to SD-method as well as CSD-method (3.10) is due to a contractivity assumption and the Lax–Milgram lemma; see Ref. 11 for details.

#### 4. Stability and Interpolation Estimates

In this section we shall consider the CSD-method (3.10) for (2.8) and give a corresponding error representation formula together with interpolation and strong stability estimates, in some weighted  $L_2$ -norms, for the dual problem (2.14). In energy depending problems, forward peakedness in energy would result in small energy diffusion which can also be represented by a small diffusion term in  $x$  and  $y$  (energy depends on  $x$  and  $y$ ) justifying (2.13). However, estimates for (2.13) are easier than those for (2.14), they are obtained in the same way, and therefore are omitted.

Dealing with discontinuities in  $x_{\perp}$ , from now on, we shall use the notation

$$(v, w)_Q = \sum_{n=0}^N \int_{S_n} vw \, dx \, dx_{\perp}, \quad \text{for } v|_{S_n}, w|_{S_n} \in L_2(S_n), \quad \forall n. \quad (4.1)$$

Compared to the outline in Sec. 2 the main difference, as we shall see below, will be the additional contributions from jumps on slab-to-slab edges. Because of the presence of the jump terms, there is a structural similarity between CSD and the discontinuous Galerkin method with the advantageous efficiency shown, e.g. in the *a priori* estimates in Ref. 3.

##### 4.1. Error representation: The dual problem and Galerkin orthogonality

The error representation is now obtained by multiplying the dual problem (2.14) by  $\hat{e}^h$ , integrating over each  $S_n$ , integrating by parts and finally summing over  $n$ ,

$$\begin{aligned}
 \|\hat{e}^h\|_Q^2 &= \sum_{n=0}^N (\hat{e}^h, -\varphi_x - z\varphi_y - \hat{e}\varphi_{zz})_n \\
 &= \sum_{n=0}^N \left\{ (\hat{e}_x^h + \beta \cdot \nabla_{\perp} \hat{e}^h, \varphi)_n + ((\hat{e}\hat{e}^h)_z, \varphi_z)_n + \int_{\Gamma_n^-} \hat{e}^h \varphi |n \cdot \tilde{\beta}| d\Gamma - ([J^h], \varphi_+^n)_n \right\} \\
 &= \sum_{n=0}^N \left\{ (\hat{J}_x + \beta \cdot \nabla_{\perp} \hat{J} - \hat{e}\hat{J}_{zz}, \varphi)_n - (\hat{e}_{zz}\hat{J} + 2\hat{e}_z\hat{J}_z, \varphi)_n + \int_{I_x^n \times I_y} (\hat{e}\hat{J})_z \varphi|_{-z_0}^{z_0} \right\} \\
 &\quad - \sum_{n=0}^N \left\{ (J_x^h + \beta \cdot \nabla_{\perp} J^h, \varphi)_n + ((\hat{e}J^h)_z, \varphi_z)_n \right\} \\
 &\quad + \sum_{n=0}^N \left\{ \int_{\Gamma_n^-} J^h \varphi |n \cdot \tilde{\beta}| d\Gamma + ([J^h], \varphi_+^n)_n \right\},
 \end{aligned}$$

where, in the second line, we have used the boundary condition  $\varphi_z = 0$ , on  $\Gamma^0$ , in partial integration with respect to  $z$  and, in the third line, the angular symmetry condition (2.15) with the weight function  $w = (\hat{e}\hat{J})_z$ . Now recalling (2.7) and using a suitable interpolant  $\Phi \in \mathcal{V}_h$ , of  $\varphi$ , we get

$$\begin{aligned}
 \|\hat{e}^h\|_Q^2 &= \sum_{n=0}^N \left\{ (J_x^h + \beta \cdot \nabla_{\perp} J^h, \Phi - \varphi)_n + ((\hat{e}J^h)_z, (\Phi - \varphi)_z)_n \right\} \\
 &\quad + \sum_{n=0}^N \left\{ (\hat{e}_{zz}\hat{J}, \Phi - \varphi)_n + 2(\hat{e}_z\hat{J}, \Phi - \varphi)_n \right\} \\
 &\quad + \sum_{n=0}^N \left\{ \int_{\Gamma_n^-} J^h (\Phi - \varphi) |n \cdot \tilde{\beta}| d\Gamma + ([J^h], (\Phi - \varphi)_+^n)_n \right\}.
 \end{aligned}$$

By an identical manipulation leading to (2.16), this time using (2.15) with  $w = \hat{e}_z\hat{J}$ , and letting  $\hat{J} = \hat{e}^h + J^h$ , we have

$$\begin{aligned}
 &(\hat{e}_{zz}, \hat{J}\varphi)_Q + 2(\hat{e}_z\hat{J}_z, \varphi)_Q \\
 &= -(\hat{e}_z\hat{J}, \varphi_z)_Q + (\hat{e}_z\hat{J}_z, \varphi)_Q \\
 &= (\hat{e}_z\hat{e}^h, \varphi_z)_Q - (\hat{e}_zJ^h, \varphi_z)_Q + (\hat{e}_z\hat{e}_z^h, \varphi)_Q + (\hat{e}_zJ_z^h, \varphi)_Q, \tag{4.2}
 \end{aligned}$$

recall that  $(\cdot, \cdot)_Q$  is now defined by (4.1). Inserting (4.2) in the error representation formula, (after summation over  $n$ ), and combining with  $(\hat{e}J^h)_z$ , we may write

$$\begin{aligned}
 \|\hat{e}^h\|_Q^2 &= -(\hat{e}_z\hat{e}^h, (\Phi - \varphi)_z)_Q + (\hat{e}_z\hat{e}_z^h, \Phi - \varphi)_Q + (\hat{e}_zJ_z^h, \Phi - \varphi)_Q \\
 &\quad + (J_x^h + \beta \cdot \nabla_{\perp} J^h, \Phi - \varphi)_Q + (\hat{e}J_z^h, (\Phi - \varphi)_z)_Q \\
 &\quad + \sum_{n=0}^N \langle J^h, \Phi - \varphi \rangle_{\Gamma_n^-} + \sum_{n=0}^N ([J^h]_n, (\Phi - \varphi)_+^n)_n \\
 &:= I + II + III + IV + V + VI + VII. \tag{4.3}
 \end{aligned}$$

The idea now is to estimate  $\varphi - \Phi$  in terms of  $\hat{e}^h$  using a strong stability estimate for the solution  $\varphi$  of the dual problem (2.14), (works equally well for (2.13)).

**4.2. Interpolation estimates for the dual solution**

We shall now define our interpolant  $\Phi \in \mathcal{V}_h$  of  $\varphi$ , appeared in (4.3). We start with defining the  $L_2$ -projections  $\bar{\mathcal{P}}_n : L_2(I_\perp^n) \rightarrow \mathcal{W}_n$  and  $\bar{\pi}_n : L_2(I_x^n) \rightarrow L_2(I_x^n)$ , respectively, by

$$\int_{I_\perp^n} (\bar{\mathcal{P}}_n \varphi) v \, dx_\perp = \int_{I_\perp^n} \varphi v \, dx_\perp, \quad \forall v \in \mathcal{W}_n, \quad \forall n, \tag{4.4}$$

and

$$\int_{I_x^n} (\bar{\pi}_n \varphi) v \, dx = \int_{I_x^n} \varphi v \, dx, \quad \forall v \in P_p(I_x^n) \cap L_2(I_x^n), \quad \forall n. \tag{4.5}$$

Now we define  $\bar{\Phi}|_{S_n} \in \mathcal{V}_n$  by letting

$$\bar{\Phi} = \bar{\mathcal{P}}_n \bar{\pi}_n \bar{\varphi} = \bar{\pi}_n \bar{\mathcal{P}}_n \bar{\varphi}, \tag{4.6}$$

where  $\varphi = \varphi|_{S_n}$  and the coordinate transformations (3.6) and (3.9) are used. Hence

$$\bar{\mathcal{P}}_n \bar{\varphi}(\bar{x}, \bar{x}_\perp) = (\bar{\mathcal{P}}_n \bar{\varphi}(\bar{x}, \cdot))(\bar{x}_\perp) \quad \text{and} \quad \bar{\pi}_n \bar{\varphi}(\bar{x}, \bar{x}_\perp) = (\bar{\pi}_n \bar{\varphi}(\cdot, \bar{x}_\perp))(\bar{x}),$$

with  $\bar{x}$  and  $\bar{x}_\perp$  acting as parameters in  $\bar{\mathcal{P}}_n$  and  $\bar{\pi}_n$ , respectively. Defining  $\mathcal{P}_n$  and  $\pi_n$  by

$$\overline{\mathcal{P}_n \varphi}(\bar{x}, \bar{x}_\perp) = \bar{\mathcal{P}}_n \bar{\varphi}(\bar{x}, \bar{x}_\perp), \quad \overline{\pi_n \varphi}(\bar{x}, \bar{x}_\perp) = \bar{\pi}_n \bar{\varphi}(\bar{x}, \bar{x}_\perp), \quad \text{for } (\bar{x}, \bar{x}_\perp) \in S_n,$$

and using the same parameter convention as above, we can alternatively write (4.6) as

$$\bar{\Phi} = \mathcal{P}_n \pi_n \varphi = \pi_n \mathcal{P}_n \varphi, \tag{4.7}$$

where  $\varphi = \varphi|_{S_n}$  and  $\bar{\Phi} = \bar{\Phi}|_{S_n}$ . We finally define  $\mathcal{P}$  and  $\pi$  by setting

$$(\mathcal{P}\varphi)|_{S_n} = \mathcal{P}_n(\varphi|_{S_n}), \quad (\pi\varphi)|_{S_n} = \pi_n(\varphi|_{S_n}),$$

and extend (4.7), to define  $\bar{\Phi} \in \mathcal{V}$  as follows:

$$\bar{\Phi} = \mathcal{P}\pi\varphi = \pi\mathcal{P}\varphi. \tag{4.8}$$

Below we split the interpolation error  $\varphi - \bar{\Phi}$  by writing

$$\varphi - \bar{\Phi} = (\varphi - \mathcal{P}\varphi) + \mathcal{P}(\varphi - \pi\varphi), \tag{4.9}$$

so that the errors of projections are separated, and then estimate the contribution from each projection, separately.

First let us once again recall (4.1), and some frequently used notations:

$$\|\varphi\|_{L_\infty(L_2)} = \text{ess sup}_{0 < x < L} \|\varphi(x, \cdot)\|_{L_2(I_\perp)}, \quad \|\varphi\|_{L_1(L_2)} = \|\varphi\|_{L_1(I_x, L_2(I_\perp))}.$$

Further, for  $\mathcal{R} \in L_2(Q)$  we write  $\tilde{\mathcal{R}} = \mathcal{R}\Lambda$ ,  $\hat{\mathcal{R}} = \tilde{\mathcal{R}}\bar{\Lambda}$  where  $\bar{\Lambda}(\bar{x}, \bar{x}_\perp) = \bar{\Lambda}_n(\bar{x}, \bar{x}_\perp)$ , for  $(\bar{x}, \bar{x}_\perp) \in S_n$ , with  $\bar{\Lambda}_n$ , the Jacobian of  $\bar{x}_\perp \rightarrow \alpha_n(\bar{x}, \bar{x}_\perp)$ , i.e.  $\bar{\Lambda}_n = \bar{\nabla}_\perp|_{S_n}$ . Finally, we define the discrete transversal averaging space,  $\tilde{\mathcal{V}}$ , associated to (1.15),

$$\tilde{\mathcal{V}} = \left\{ \bar{v} \in \bar{\mathcal{V}}_h : \left| \frac{\partial^k \bar{v}}{\partial \bar{y}^k} \right| \approx \left| \frac{\partial^k \bar{v}}{\partial \bar{z}^k} \right|; k = 1, 2 \right\}, \tag{4.10}$$

the transversal  $\hat{\varepsilon}$ -weighted discrete Laplacian  $\Delta_{\perp,h}^{\hat{\varepsilon}} : \tilde{\mathcal{V}} \rightarrow \tilde{\mathcal{V}}$  by

$$(\Delta_{\perp,h}^{\hat{\varepsilon}} w, v)_Q = -(\hat{\varepsilon} \nabla_\perp w, \nabla_\perp v)_Q, \quad \forall v \in \tilde{\mathcal{V}}, \tag{4.11}$$

and the following  $\hat{\varepsilon}$ -weighted discrete second derivatives,

$$\mathcal{D}_{\perp,h}^{2,\hat{\varepsilon}} w(x, x_\perp)|_\tau = \left| \text{div}_\perp(\hat{\varepsilon} \nabla_\perp w)|_\tau \right| + \max_{\partial\tau} \frac{1}{2} \left| \hat{\varepsilon} \left[ \frac{\partial w}{\partial \mathbf{n}_\tau} \right] \right| / h_\tau, \tag{4.12}$$

and  $\mathcal{D}_{\perp,h}^2 w = \mathcal{D}_{\perp,h}^{2,1} w$ , where  $[\frac{\partial w}{\partial \mathbf{n}_\tau}]$  denotes the jump across  $\partial\tau$  in the normal derivative  $\partial w / \partial \mathbf{n}_\tau = \mathbf{n}_\tau \cdot \nabla_\perp w$ , where  $\mathbf{n}_\tau$  is the exterior unit normal to  $\partial\tau$ .

In the rest of this section we shall focus on deriving the strong stability and some interpolation estimates, leaving the overall estimates for I-VII to the next section.

**Lemma 4.1.** *Suppose (2.24) is valid, further assume  $|\nabla_\perp h_\perp| \leq c$ , and  $|\hat{\varepsilon}_x| \leq c \hat{\varepsilon} \min_n h_n^{-1}$ , for some small constant  $c$ . Then, there is a constant  $C$  such that for  $\mathcal{R} \in L_2(Q)$ ,*

$$|(\mathcal{R}, \varphi - \mathcal{P}\varphi)_Q| \leq C \|\hat{\varepsilon}^{-1} h_\perp^2 (I - \mathcal{P}) \tilde{\mathcal{R}}\|_Q \|\hat{\varepsilon} \varphi_{zz}\|_Q, \tag{4.13}$$

$$|(\hat{\varepsilon} J_z^h, (\varphi - \mathcal{P}\varphi)_z)_Q| \leq C \|h_\perp^2 \mathcal{D}_{\perp,h}^2 J^h\|_Q \|\hat{\varepsilon} \varphi_{zz}\|_Q. \tag{4.14}$$

**Proof.** We change to  $(\bar{x}, \bar{x}_\perp)$ -coordinates and write using (4.1) and the Galerkin orthogonality,

$$\begin{aligned} (\mathcal{R}, \varphi - \mathcal{P}\varphi)_Q &= \sum_{n=0}^N \int_{S_n} \tilde{\mathcal{R}} \bar{\Lambda} (\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi}) d\bar{x} d\bar{x}_\perp \\ &= \sum_{n=0}^N \int_{S_n} (I - \bar{\mathcal{P}}_n) \tilde{\mathcal{R}} \bar{\Lambda} (\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi}) d\bar{x} d\bar{x}_\perp \\ &\leq \sum_{n=0}^N \|(I - \bar{\mathcal{P}}_n) \tilde{\mathcal{R}} \bar{\Lambda}\|_{S_n} \|\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi}\|_{S_n}. \end{aligned} \tag{4.15}$$

Further, with  $\bar{\varphi}_h \in \tilde{\mathcal{V}}_n \equiv \tilde{\mathcal{V}}|_{S_n}$ , being the standard nodal interpolant we have

$$\|\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi}\|_{S_n} \leq \|\bar{\varphi} - \bar{\varphi}_h\|_{S_n} \leq C \|\bar{h}_\perp^2 \bar{\mathcal{D}}_\perp^2 \bar{\varphi}\|_{S_n}^* \leq C \|\bar{h}_\perp^2 \bar{\varphi}_{zz}\|_{S_n}^*, \tag{4.16}$$

with

$$\|\bar{\varphi}_{zz}\|_{S_n}^* = \left\{ \sum_\tau \int_{I_\tau^n \times \tau} (\bar{\varphi}_{zz})^2 d\bar{x} d\bar{x}_\perp \right\}^{1/2} \leq C \|\varphi_{zz}\|_{S_n}, \tag{4.17}$$

where the lost inequality follows from the fact that  $\beta_n$  is piecewise smooth and the Jacobian  $\bar{\Lambda}_n$  satisfies  $C^{-1} \leq \bar{\Lambda}_n(\bar{x}, \bar{x}_\perp) \leq C$ ,  $n = 0, 1, \dots, N$ , for some positive constant  $C$ . The estimate (4.13) follows by combining (4.15)–(4.17).

To prove (4.14) as in the previous estimate we shall first transfer to  $(\bar{x}, \bar{x}_\perp)$  coordinates and write accordingly

$$\begin{aligned} (\hat{\varepsilon} J_z^h, (\varphi - \mathcal{P}\varphi)_z)_Q &= \sum_{n=0}^N \int_{S_n} \hat{\varepsilon} \bar{J}_z^h \bar{\Lambda}_n^{-1} (\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi})_{\bar{z}} \bar{\Lambda}_n^{-1} \bar{\Lambda}_n dx dx_\perp \\ &= \sum_{n=0}^N \int_{I_x^n} \left( \sum_{\tau_n} \int_{\tau_n} (\hat{\varepsilon} \bar{J}_z^h \bar{\Lambda}_n^{-1})(\bar{x}, \bar{x}_\perp) (\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi})_{\bar{z}}(\bar{x}, \bar{x}_\perp) d\bar{x}_\perp \right) d\bar{x}. \end{aligned} \tag{4.18}$$

Now we approximate the inner sum in (4.18) as

$$\begin{aligned} &\sum_{\tau_n} \int_{\tau_n} (\hat{\varepsilon} \bar{J}_z^h \bar{\Lambda}_n^{-1})(\bar{x}, \bar{x}_\perp) (\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi})_{\bar{z}}(\bar{x}, \bar{x}_\perp) d\bar{x}_\perp \\ &\approx \frac{1}{4} \sum_{\tau_n} \int_{\tau_n} (\hat{\varepsilon} \bar{\nabla}_\perp \bar{J}^h \bar{\Lambda}_n^{-1})(\bar{x}, \bar{x}_\perp) \bar{\nabla}_\perp (\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi})(\bar{x}, \bar{x}_\perp) d\bar{x}_\perp \\ &= \frac{1}{4} \sum_{\tau_n} \int_{\tau_n} \operatorname{div}_\perp (\hat{\varepsilon} \bar{\nabla}_\perp \bar{J}^h \bar{\Lambda}_n^{-1})(\bar{x}, \bar{x}_\perp) (\bar{\mathcal{P}}_n \bar{\varphi} - \bar{\varphi})(\bar{x}, \bar{x}_\perp) d\bar{x}_\perp \\ &\quad + \frac{1}{2} \sum_{\tau_n} \left( \hat{\varepsilon} \left[ \frac{\partial \bar{J}^h \bar{\Lambda}_n^{-1}}{\partial \mathbf{n}_{\tau_n}} \right] / h_{\tau_n} \right) h_{\tau_n} (\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi})|_{\partial \tau_n}(\bar{x}), \end{aligned} \tag{4.19}$$

where we have used the symmetry assumption (4.10) and integration by parts. Inserting (4.19) into (4.18) we get using (4.12) that

$$\begin{aligned} |(\hat{\varepsilon} J_z^h, (\varphi - \mathcal{P}\varphi)_z)_Q| &\leq \frac{1}{4} \sum_{n=0}^N \int_{I_x^n} \left( \sum_{\tau_n} \int_{\tau_n} |\bar{\mathcal{D}}_{\perp, h}^{2, \hat{\varepsilon}} \bar{J}^h|_{\tau_n} |(\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi}) d\bar{x}_\perp \right) d\bar{x} \\ &\quad + \sum_{n=0}^N \int_{I_x^n} \sum_{\tau_n} \left( \int_{\tau_n} |\bar{\mathcal{D}}_{\perp, h}^{2, \hat{\varepsilon}} \bar{J}^h|_{\tau_n} d\bar{x}_\perp \cdot |h_\tau (\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi})(\bar{x})|_{\partial \tau_n} d\bar{x}_\perp \right) d\bar{x}. \end{aligned}$$

By the well-known interpolation estimate for the  $L_2$ -projections  $\bar{\pi}_n \bar{\mathcal{P}}_n : L_2(Q) \rightarrow \bar{\mathcal{V}}_n$  and  $\mathcal{P}_n : L_2(I_\perp) \rightarrow \mathcal{W}_n$  we have

$$\begin{aligned} &\sum_{\tau_n} \int_{\tau_n} (\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi})^2 d\bar{x}_\perp + \sum_{\tau_n} (\bar{\varphi} - \bar{\mathcal{P}}_n \bar{\varphi})^2|_{\partial \tau_n} h_{\tau_n} \\ &\leq C \|h_\perp^2 \bar{\mathcal{D}}_{\perp, h}^2 \bar{\varphi}(\bar{x}, \cdot)\|_{L_2(I_\perp)}^2 \leq C \|h_\perp^2 \bar{\varphi}_{\bar{z}\bar{z}}(\bar{x}, \cdot)\|_{L_2(I_\perp)}^2, \end{aligned} \tag{4.20}$$

where we have used the trace estimate and also evaluated  $\bar{\mathcal{D}}_{\perp, h}^2 \bar{\varphi}(\bar{x}, \cdot)$  and consequently  $\bar{\varphi}_{\bar{z}\bar{z}}(\bar{x}, \cdot)$  on each triangle  $\tau_n$  separately. Note that  $\bar{\mathcal{D}}_{\perp, h}^{2, \hat{\varepsilon}} = \hat{\varepsilon} \bar{\mathcal{D}}_{\perp, h}^2$ ,



thus, using (4.18)–(4.20), with  $h_\perp$  transferred to the first terms, and transforming back to  $(x, x_\perp)$ -coordinates, we obtain the desired result.  $\square$

**Corollary 4.1.** *Let  $h_\perp$  and  $\hat{\varepsilon}$  satisfy the conditions in Lemma 4.1, then*

$$|(\hat{\varepsilon}_z J_z^h, \varphi - \mathcal{P}\varphi)_Q| \leq \hat{C} \|h_\perp^2 \mathcal{D}_{\perp, h}^2 J^h\|_Q \|\hat{\varepsilon} \varphi_{zz}\|_Q, \tag{4.21}$$

$$|(\hat{\varepsilon}_z \hat{\varepsilon}^h, (\varphi - \mathcal{P}\varphi)_z)_Q| \leq \hat{C} \|\hat{\varepsilon}^h\|_Q \|\hat{\varepsilon} \varphi_{zz}\|_Q, \tag{4.22}$$

$$|(\hat{\varepsilon}_z \hat{\varepsilon}_z^h, \varphi - \mathcal{P}\varphi)_Q| \leq \hat{C} \|\hat{\varepsilon}^h\|_Q \|\hat{\varepsilon} \varphi_{zz}\|_Q, \tag{4.23}$$

where  $\hat{C} = C(c, \tilde{C})$  and  $c$  and  $\tilde{C}$  are introduced in Sec. 2 to derive (2.25).

**Proof.** Using (2.24) and an inverse estimate, we derive the first estimate (4.21) in an identical way as (4.14). Further (4.22) and (4.23) are derived likewise (2.25), using the inverse estimate, (2.24) and the same techniques as in the proof of (4.14). The details are omitted.  $\square$

**Lemma 4.2.** *Assume that  $\hbar_n \sim \mathcal{O}(1)$ , and  $|\hat{\varepsilon}_x| \leq c \min_n \hbar_n^{-1} \hat{\varepsilon}$ , hold with  $c$  being a sufficiently small constant. Then, there is a constant  $C$  such that for  $\mathcal{R} \in L_2(Q)$ ,*

$$\begin{aligned} |(\mathcal{R}, \mathcal{P}(\varphi - \pi\varphi))_Q| &\leq C \|\hbar(I - \pi)\mathcal{P}\tilde{\mathcal{R}}\|_Q \|\varphi_x + \beta \cdot \nabla_\perp \varphi\|_Q \\ &\quad + C \min\{\|\hbar \varrho \hat{\varepsilon}^{-1/2}(I - \pi)\mathcal{P}\tilde{\mathcal{R}}\|_{L_1(L_2)} \|\hat{\varepsilon}^{1/2} \varphi_z\|_{L_\infty(L_2)}, \\ &\quad \|\hbar \varrho \hat{\varepsilon}^{-1/2}(I - \pi)\mathcal{P}\tilde{\mathcal{R}}\|_Q \|\hat{\varepsilon}^{1/2} \varphi_z\|_Q\}, \end{aligned}$$

where  $C = C(c, \tilde{C})$  and  $\varrho(\bar{x}, \bar{x}_\perp) = |(\bar{\beta} - \bar{\beta}_n)(\bar{x}_\perp)| \sim \mathcal{G}(|\bar{z} - \bar{z}_n|)$ , on  $S_n$ ,  $\forall n$ , with  $\mathcal{G}$  being a small, positive and smooth function on  $\mathbb{R}^+$ .

**Proof.** Once again, changing to characteristic coordinates  $(\bar{x}, \bar{x}_\perp)$ , and using the Galerkin orthogonality we have

$$\begin{aligned} |(\mathcal{R}, \mathcal{P}(\varphi - \pi\varphi))_Q| &= \left| \sum_{n=0}^N (\tilde{\mathcal{R}}\bar{\Lambda}, \tilde{\mathcal{P}}(\bar{\varphi} - \bar{\pi}\bar{\varphi}))_{S_n} \right| \\ &= \left| \sum_{n=0}^N \int_{S_n} \hat{\mathcal{R}}\tilde{\mathcal{P}}(\bar{\varphi} - \bar{\pi}\bar{\varphi}) d\bar{x} \right| = \left| \sum_{n=0}^N \int_{S_n} (I - \bar{\pi})\hat{\mathcal{R}}\tilde{\mathcal{P}}(\bar{\varphi} - \bar{\pi}\bar{\varphi}) d\bar{x} \right| \\ &\leq \sum_{n=0}^N \|\hbar_n(I - \bar{\pi})\tilde{\mathcal{P}}\hat{\mathcal{R}}\|_{S_n} \|\hbar_n^{-1}(\bar{\varphi} - \bar{\pi}\bar{\varphi})\|_{S_n} \\ &\leq C \sum_{n=0}^N \|\hbar_n(I - \bar{\pi})\tilde{\mathcal{P}}\hat{\mathcal{R}}\|_{S_n} \left\| \frac{d\bar{\varphi}}{d\bar{x}} \right\|_{S_n}, \end{aligned} \tag{4.24}$$

where a usual interpolation estimate was used in the last inequality. Now we have

$$\frac{d\bar{\varphi}}{d\bar{x}} = \overline{\varphi_x + \beta_n \cdot \nabla_\perp \varphi} = \overline{\varphi_x + \beta \cdot \nabla_\perp \varphi} + \overline{(\beta_n - \beta) \cdot \nabla_\perp \varphi},$$

and thus

$$\left\| \frac{d\bar{\varphi}}{dx} \right\|_{S_n} \leq \|\overline{\varphi_x + \beta \cdot \nabla_{\perp} \varphi}\|_{S_n} + \|\overline{(\beta_n - \beta) \cdot \nabla_{\perp} \varphi}\|_{S_n}.$$

Replacing in (4.24) and changing back to  $(x, x_{\perp})$ -coordinates we get

$$|(\mathcal{R}, \mathcal{P}(\varphi - \pi\varphi))_Q| \leq C \|\tilde{\mathcal{R}}(I - \pi)\mathcal{P}\tilde{\mathcal{R}}\|_Q (\|\varphi_x + \beta \cdot \nabla_{\perp} \varphi\|_Q + \|\varrho |\nabla_{\perp} \varphi|\|_Q). \quad (4.25)$$

Now since  $|\varphi_z| \sim \frac{1}{2} |\nabla_{\perp} \varphi|$ , the desired result is easily obtained from (4.25) and the proof is complete.  $\square$

Recall that, as outlined in Sec. 2, our basic tools of estimations are strong stability estimates for the continuous dual problem associated with the Galerkin orthogonality of the finite element method. So far our estimates have been, basically, relying on the Galerkin orthogonality. To continue we need to invoke the strong stability, as well. And it is in using this second tool where we are forced to assume a transversal symmetry assumption described below:

### 4.3. Strong stability of the continuous dual problem

To be able to control the remaining terms on the right-hand side of (4.3) we need stability estimates for the continuous dual problem (2.14), (stability of (2.13) is easily followed). These estimates will be the essential tools in deriving *a posteriori* error estimates. To derive stability estimates we shall use the *transversal convective-balance* condition:

$$\int_Q \hat{\varepsilon} \varphi_z^2 \approx \int_Q \hat{\varepsilon} \varphi_y^2. \quad (4.26)$$

The physical relevance of condition (4.26) for the pencil beam equations depends upon the forward-peakedness assumption used to derive the Fokker–Planck and Fermi equations in the sense that: For these equations, (the charged particles have peaked kernel about both a zero energy transfer and a zero direction change), the scattering angle  $\theta$  is assumed to be small justifying approximation of the type  $\sin \theta \approx \tan \theta$ , discussed in Sec. 1, leading to assumption (1.15). Actually (1.15), being valid for  $k = 1, 2$ , is stronger than (4.26), (see also (4.10)). And while the assumption (1.15) removes the *degenerateness* of the continuous problem, the condition (4.26) is sufficient for our purpose in the weak (variational) form. We want to emphasize that, in our estimates, the advantage of peaked kernel on the energy variable is not used nor the derivation of equations of this paper consider it. Our results are for the degenerate problem (2.14) under the assumption (4.26), they imply, automatically, the estimates for the problem (2.13) as special cases.

Considering (4.26), we have the following crucial result:

**Lemma 4.3.** Suppose (4.26) is valid and that  $(1+s)\hat{\varepsilon} + \hat{\varepsilon}_z(t + \hat{\varepsilon}_z) \leq r(\hat{\varepsilon}_x + z\hat{\varepsilon}_y)$ , for some parameters  $0 < r, s, t < 1$ . Then, e.g. for  $r = s = t = 1/4$ ,

$$\begin{aligned} & \|\varphi_x + z\varphi_y\|_Q + \|(\tilde{\beta} \cdot \nabla \hat{\varepsilon})^{1/2} \varphi_z\|_Q + \|\hat{\varepsilon}^{1/2} \varphi_z\|_Q + \|\hat{\varepsilon}_z^{1/2} \varphi_z\|_Q \\ & + \|\hat{\varepsilon} \varphi_{zz}\|_Q + \left( \int_{\Gamma^-} (\hat{\varepsilon} \varphi_z^2) |\mathbf{n} \cdot \beta| d\Gamma \right)^{1/2} \leq C(C^s) \|\hat{\varepsilon}^h\|_Q. \end{aligned}$$

**Proof.** We multiply the main equation in (2.14) by  $-(\varphi_x + \beta \cdot \nabla_{\perp} \varphi) = -\varphi_x - z\varphi_y$  and integrate over  $Q$ , to obtain

$$- \int_Q \hat{\varepsilon}^h (\varphi_x + z\varphi_y) d\mathbf{x} = \int_Q (\varphi_x + z\varphi_y)^2 d\mathbf{x} + \int_Q \hat{\varepsilon} \varphi_{zz} (\varphi_x + z\varphi_y) d\mathbf{x}. \quad (4.27)$$

Integrating by parts and using the boundary condition  $\varphi_z = 0$ , on  $\Gamma^-$ , we have

$$\begin{aligned} \int_Q \hat{\varepsilon} \varphi_{zz} (\varphi_x + z\varphi_y) d\mathbf{x} &= \int_Q \hat{\varepsilon} \varphi_{zz} \varphi_x d\mathbf{x} + \int_Q \hat{\varepsilon} z \varphi_{zz} \varphi_y d\mathbf{x} \\ &= - \int_Q \varphi_z (\hat{\varepsilon} \varphi_x)_z d\mathbf{x} + \int_{I_x \times I_y} \hat{\varepsilon} \varphi_x \varphi_z \Big|_{z=-z_0}^{z=z_0} \\ &\quad - \int_Q \varphi_z (\hat{\varepsilon} z \varphi_y)_z d\mathbf{x} + \int_{I_x \times I_y} \hat{\varepsilon} z \varphi_y \varphi_z \Big|_{z=-z_0}^{z=z_0} \\ &= - \int_Q \hat{\varepsilon}_z \varphi_x \varphi_z d\mathbf{x} - \int_Q \hat{\varepsilon} \varphi_z \varphi_{xz} d\mathbf{x} \\ &\quad - \int_Q \hat{\varepsilon}_z z \varphi_y \varphi_z d\mathbf{x} - \int_Q \hat{\varepsilon} \varphi_y \varphi_z d\mathbf{x} - \int_Q \hat{\varepsilon} z \varphi_z \varphi_{yz} d\mathbf{x} \\ &= - \int_Q \frac{\hat{\varepsilon}}{2} \frac{\partial}{\partial x} (\varphi_z^2) dx dx_{\perp} - \int_Q \frac{\hat{\varepsilon}}{2} z \frac{\partial}{\partial y} (\varphi_z^2) dx dx_{\perp} \\ &\quad - \int_Q \hat{\varepsilon}_z \varphi_z (\varphi_x + z\varphi_y) d\mathbf{x} - \int_Q \hat{\varepsilon} \varphi_y \varphi_z d\mathbf{x} \\ &= - \int_{I_{\perp}} \frac{\hat{\varepsilon}}{2} \{ \varphi_z^2(L, x_{\perp}) - \varphi_z^2(0, x_{\perp}) \} \\ &\quad - \int_{I_x \times I_z} \frac{\hat{\varepsilon}}{2} z \{ \varphi_z^2(y_0) - \varphi_z^2(-y_0) \} + \int_Q \frac{1}{2} (\hat{\varepsilon}_x + z\hat{\varepsilon}_y) \varphi_z^2 d\mathbf{x} \\ &\quad - \int_Q \hat{\varepsilon}_z \varphi_z (\varphi_x + z\varphi_y) d\mathbf{x} - \int_Q \hat{\varepsilon} \varphi_z \varphi_y d\mathbf{x} \\ &\geq - \int_{I_{\perp}} \frac{\hat{\varepsilon}}{2} \varphi_z^2(L) dx_{\perp} + \int_{\Gamma^-} \frac{\hat{\varepsilon}}{2} \varphi_z^2 |\mathbf{n} \cdot \tilde{\beta}| d\Gamma + \int_Q \frac{1}{2} (\hat{\varepsilon}_x + z\hat{\varepsilon}_y) \varphi_z^2 d\mathbf{x} \\ &\quad - \int_Q \frac{\hat{\varepsilon}}{2} \varphi_z^2 d\mathbf{x} - \int_Q \frac{\hat{\varepsilon}}{2} \varphi_y^2 d\mathbf{x} - \int_Q \hat{\varepsilon}_z^2 \varphi_z^2 d\mathbf{x} - \frac{1}{4} \int_Q (\varphi_x + z\varphi_y)^2 d\mathbf{x}. \end{aligned}$$

Inserting in (4.27) and using (4.26), we thus have

$$\begin{aligned}
-\int_Q \hat{e}^h(\varphi_x + z\varphi_y) &\geq \|\varphi_x + z\varphi_y\|^2 - \int_{I_\perp} \frac{\hat{\varepsilon}}{2} \varphi_z^2(L) dx_\perp + \int_{\Gamma^-} \frac{\hat{\varepsilon}}{2} \varphi_z^2 |\mathbf{n} \cdot \tilde{\beta}| d\Gamma \\
&\quad + \frac{1}{2} \|(\tilde{\beta} \cdot \nabla \hat{\varepsilon})^{1/2} \varphi_z\|_Q^2 - \int_Q \frac{\hat{\varepsilon}}{2} \varphi_z^2 - \int_Q \frac{\hat{\varepsilon}}{2} \varphi_y^2 - \frac{1}{4} \|\varphi_x + z\varphi_y\|^2 \\
&\quad - \|\hat{\varepsilon}_z \varphi_z\|_Q^2 \\
&= \frac{3}{4} \|\varphi_x + z\varphi_y\|^2 + \frac{1}{2} \int_{\Gamma^-} \hat{\varepsilon} \varphi_z^2 |\mathbf{n} \cdot \tilde{\beta}| d\Gamma \\
&\quad + \frac{1}{2} \|(\tilde{\beta} \cdot \nabla \hat{\varepsilon})^{1/2} \varphi_z\|_Q^2 - \frac{1}{2} \int_{I_\perp} \hat{\varepsilon} \varphi_z^2(L) dx_\perp \\
&\quad - \int_Q \hat{\varepsilon} \varphi_z^2 dx - \int_Q \hat{\varepsilon}_z^2 \varphi_z^2 dx. \tag{4.28}
\end{aligned}$$

Invoking the boundary conditions in (2.14), (i.e. the fact that in our problems  $\varphi = 0$ , on  $\Gamma^+$ , implies  $\varphi_z(L) = 0$ ), we get

$$\begin{aligned}
&\frac{3}{4} \|\varphi_x + z\varphi_y\|_Q^2 + \frac{1}{2} \int_{\Gamma^-} \hat{\varepsilon} \varphi_z^2 |\mathbf{n} \cdot \tilde{\beta}| d\Gamma + \frac{1}{4} \|(\tilde{\beta} \cdot \nabla \hat{\varepsilon})^{1/2} \varphi_z\|_Q^2 \\
&\leq \|\hat{e}^h\|_Q^2 + \frac{1}{4} \|\varphi_x + z\varphi_y\|_Q^2 + \int_Q \left( \hat{\varepsilon} + \hat{\varepsilon}_z^2 - \frac{1}{4} \tilde{\beta} \cdot \nabla \hat{\varepsilon} \right) \varphi_z^2 dx dx_\perp.
\end{aligned}$$

Now using the assumption on  $\hat{\varepsilon}$ , we may write

$$\begin{aligned}
&\|\varphi_x + z\varphi_y\|_Q^2 + \int_{\Gamma^-} (\hat{\varepsilon} \varphi_z^2) |\mathbf{n} \cdot \tilde{\beta}| d\Gamma \\
&\quad + \frac{1}{2} \|\hat{\varepsilon}^{1/2} \varphi_z\|^2 + \frac{1}{2} \|\hat{\varepsilon}_z^{1/2} \varphi_z\|^2 + \frac{1}{2} \|(\tilde{\beta} \cdot \nabla \hat{\varepsilon})^{1/2} \varphi_z\|^2 \leq 2\|\hat{e}^h\|_Q^2. \tag{4.29}
\end{aligned}$$

Finally, using the original dual equation in (2.14) we also get

$$\|\hat{\varepsilon} \varphi_{zz}\|_Q \leq \|\varphi_x + z\varphi_y\|_Q + \|\hat{e}^h\|_Q, \tag{4.30}$$

and the result follows from a combination of (4.29) and (4.30). One can easily check that  $C(C^s) = (\sqrt{30} + C^s)$ , other choices of the parameters  $0 < r, s, t < 1$ , give similar estimates.  $\square$

Observe that (4.29) together with (4.30) imply that the stability constant  $C^s$  in (2.20) may be taken as  $C^s \sim (1 + \sqrt{2})$ .

## 5. A Posteriori Error Estimates

In this section we proceed to compute the estimates of the terms I-VII in the error representation formula (4.3). To this approach below we shall combine the interpolation estimates in Lemmas 4.1 and 4.2, Corollary 4.1 and the strong stability

estimate in Lemma 4.3. First we note that the terms  $I-III$  and  $V$ , having the same structure, may be estimated in a similar way. In particular the pairs  $I$  and  $II$  as well as  $III$  and  $V$  are of the same order of magnitude. Let now  $\Phi = \mathcal{P}\pi\varphi = \pi\mathcal{P}\varphi \in \mathcal{V}$ , and split the first term in (4.3) as follows:

$$I = -(\hat{\varepsilon}_z \hat{e}^h, (\Phi - \varphi)_z)_Q = -(\hat{\varepsilon}_z \hat{e}^h, (\mathcal{P}\varphi - \varphi)_z) - (\hat{\varepsilon}_z \hat{e}^h, ((\pi - I)\mathcal{P}\varphi)_z) := I_1 + I_2,$$

where  $I_1$  is estimated in (4.22). To estimate  $I_2$ , note that the trial functions are continuous in  $x_\perp$  and therefore in  $z$ , we use (2.24) and the inverse estimate to write

$$|I_2| \leq \int_Q |\hat{\varepsilon}_z \hat{e}^h| |(\mathcal{P}(\pi - I)\varphi)_z| dx \leq \hat{C}C_{\text{inv}} \int_Q \hat{\varepsilon} h_\perp^{-2} |\hat{e}^h| |\mathcal{P}(\pi - I)\varphi| dx.$$

Now using the same argument as in the proof of Lemma 4.2, and (4.29) we may write

$$\begin{aligned} |I_2| &\leq \hat{C}C_{\text{inv}} \|\hat{\varepsilon} h_\perp^{-2} \mathfrak{h}(I - \pi)\mathcal{P}\hat{e}^h\|_Q (\|\varphi_x + \beta \cdot \nabla_\perp \varphi\|_Q + \|\varrho|\nabla_\perp \varphi\|_Q) \\ &\leq \hat{C}C_{\text{inv}} \|\hat{\varepsilon} \hat{e}^h\|_Q \|\varphi_x + \beta \cdot \nabla_\perp \varphi\|_Q + \hat{C}C_{\text{inv}} \|\hat{\varepsilon}^{1/2} \varrho \hat{e}^h\|_Q \|\hat{\varepsilon}^{1/2} \varphi_z\|_Q \\ &\leq 2\hat{C}C_{\text{inv}} \|\hat{e}^h\| (\|\hat{\varepsilon} \hat{e}^h\|_Q + \|\hat{\varepsilon}^{1/2} \varrho \hat{e}^h\|_Q), \end{aligned}$$

where  $\hat{C} = C(c, \tilde{C})$ . Similarly we write

$$II = (\hat{\varepsilon}_z \hat{e}_z^h, \mathcal{P}\varphi - \varphi)_Q + (\hat{\varepsilon}_z \hat{e}_z^h, \mathcal{P}(\pi - I)\varphi)_Q =: II_1 + II_2,$$

where, also in here,  $II_1$  is already estimated in (4.23) of Corollary 4.1. To estimate  $II_2$  we use again (2.24) and the inverse estimate, this time applied to  $\hat{e}^h$ , and write as in the estimation for  $I_2$ ,

$$\begin{aligned} |II_2| &\leq \hat{C}C_{\text{inv}} \int_Q \hat{\varepsilon} h_\perp^{-2} |\hat{e}^h| |\mathcal{P}(\pi - I)\varphi| dx \\ &\leq 2\hat{C}C_{\text{inv}} \|\hat{e}^h\| (\|\hat{\varepsilon} \hat{e}^h\|_Q + \|\hat{\varepsilon}^{1/2} \varrho \hat{e}^h\|_Q). \end{aligned}$$

Continuing with  $III$ , in the same way, we see that  $III_1$  is estimated by (4.21) in Corollary 4.1. And, as we shall see, the  $III_2$ -term and  $V_3$  below will lead to the same expression with opposite signs and therefore will be canceled. Otherwise, estimating  $V_2$  we would, simultaneously, have estimations for both  $III_2$  and  $V_3$  as well. Now we proceed by splitting the  $IV$ -term in (4.3) as follows:

$$IV = (\mathcal{R}_4, \mathcal{P}\varphi - \varphi)_Q + (\mathcal{R}_4, \mathcal{P}(\pi\varphi - \varphi))_Q := IV_1 + IV_2,$$

where

$$\mathcal{R}_4 = \mathcal{R}_4(J^h) = J_x + \beta \cdot \nabla_\perp J^h = \tilde{\beta} \cdot \nabla J^h, \quad \text{on } S_n, \quad \nabla = \nabla_x.$$

By Lemma 4.1, using orthogonality related to the  $L_2$ -projection  $\tilde{\mathcal{P}}_n$  we have

$$|IV_1| = |(\mathcal{R}_4, \mathcal{P}\varphi - \varphi)_Q| \leq C \|\hat{\varepsilon}^{-1} h_\perp^2 (I - \mathcal{P})\tilde{\mathcal{R}}_4\|_Q \|\hat{\varepsilon} \varphi_{zz}\|,$$

where  $\tilde{\mathcal{R}}_4 = \mathcal{R}_4 \Lambda$ . Further, from Lemma 4.2 we get that

$$|IV_2| \leq C \|\hbar(I - \pi) \mathcal{P} \tilde{\mathcal{R}}_4\|_Q \|\varphi_x + \beta \cdot \nabla_{\perp} \varphi\|_Q + C \min\{\|\hbar \varrho \hat{\varepsilon}^{-1/2} (I - \pi) \mathcal{P} \tilde{\mathcal{R}}_4\|_{L_1(L_2)} \|\hat{\varepsilon}^{1/2} \varphi_z\|_{L_{\infty}(L_2)}, \|\hbar \varrho \hat{\varepsilon}^{-1/2} (I - \pi) \mathcal{P} \tilde{\mathcal{R}}_4\|_Q \|\hat{\varepsilon}^{1/2} \varphi_z\|_Q\}.$$

Similarly we split  $V$  and use integration by parts, in the second term, to get

$$V = (\hat{\varepsilon} J_z^h, (\mathcal{P} \varphi - \varphi)_z)_Q + (\hat{\varepsilon} J_z^h, (\mathcal{P}(\pi \varphi - \varphi))_z)_Q = (\hat{\varepsilon} J_z^h, (\mathcal{P} \varphi - \varphi)_z)_Q - (\hat{\varepsilon} \mathcal{D}_{\hbar, z}^2 J^h, \mathcal{P}(\pi \varphi - \varphi))_Q - (\hat{\varepsilon}_z J_z^h, \mathcal{P}(\pi \varphi - \varphi))_Q + \int_{I_x \times I_y} \hat{\varepsilon} J_z^h \mathcal{P}(\pi \varphi - \varphi)|_{-z_0}^{z_0} \\ := V_1 + V_2 + V_3 + V_4,$$

where  $V_4$  vanishes, since  $J_z^h \equiv 0$  for  $z = \pm z_0$ , we also note that  $III_2 + V_3 \equiv 0$ . Now using the second estimate of Lemma 4.1, we have

$$|V_1| \leq C \|\hbar^2 \mathcal{D}_{\perp, \hbar}^2 J^h\|_Q \|\hat{\varepsilon} \varphi_{zz}\|_Q.$$

Further, by Lemma 4.2 and since  $\mathcal{P}$  is a bounded operator we may estimate  $V_2$  as follows:

$$|V_2| \leq C \|\hbar \hat{\varepsilon} (I - \pi) \mathcal{D}_{\hbar, z}^2 J^h\|_Q \|\varphi_x + \beta \cdot \nabla_{\perp} \varphi\|_Q + C \min\{\|\hbar \varrho \hat{\varepsilon}^{1/2} (I - \pi) \mathcal{D}_{\hbar, z}^2 J^h\|_{L_1(L_2)} \|\hat{\varepsilon}^{1/2} \varphi_z\|_{L_{\infty}(L_2)}, \|\hbar \varrho \hat{\varepsilon}^{1/2} (I - \pi) \mathcal{D}_{\hbar, z}^2 J^h\|_Q \|\hat{\varepsilon}^{1/2} \varphi_z\|_Q\}.$$

For the primary particles, if we assume (2.11) then obviously  $VI \equiv 0$ . However, as we discussed above, a condition as (2.10) is more motivated, due to the possible secondary collisions resulting from the reflected particles. Below we continue estimating  $VI$ -terms: we have that

$$\langle J_h, \Phi - \varphi \rangle_{\Gamma_n^-} = \langle J_h, \mathcal{P} \varphi - \varphi \rangle_{\Gamma_n^-} + \langle J_h, \mathcal{P}(\pi \varphi - \varphi) \rangle_{\Gamma_n^-} := VI_1 + VI_2.$$

Due to the fact that  $\mathcal{P}$  is the  $L_2$  projection on  $x_{\perp}$ , we have that  $VI_1 = (\mathcal{P} \varphi - \varphi)|_{\Gamma_n^-} \equiv 0$ , for  $n = 0, 1, \dots, N$ . As for  $VI_2$ , using interpolation estimate together with the trace inequality we get

$$|VI_2| = \left| \sum_{n=0}^N \langle J_h, \mathcal{P}(\pi - I) \varphi \rangle_{\Gamma_n^-} \right| = |\langle J_h, \mathcal{P}(\pi - I) \varphi \rangle_{\Gamma_s^-}| \\ = |\langle \bar{J}_h \bar{\Lambda}, \bar{\mathcal{P}}(\bar{\pi} - I) \bar{\varphi} \rangle_{\Gamma_s^-}| \leq \int_{\Gamma_s^-} |(\bar{\pi} - I) \bar{J}_h \bar{\Lambda} \bar{\mathcal{P}}(\bar{\pi} - I) \bar{\varphi}| d\Gamma \\ \leq C \|(\bar{\pi} - I) \bar{\mathcal{P}} \bar{J}_h \bar{\Lambda}\|_{L_2(\Gamma_s^-)} \|\varphi\|_{L_2(\Gamma_s^-)} \\ \leq C \|\hbar(\bar{\mathcal{P}} \bar{J}^h)_x\|_{L_2(\Gamma_s^-)} \|\varphi\|_{L_2(\Gamma_s^-)} \leq C \|\hbar(\bar{\mathcal{P}} \bar{J}^h)_x\|_{L_2(\Gamma_s^-)} \|\nabla \varphi\|_Q.$$

It remains to estimate the last term VII in (4.3), i.e. the contributions from the jumps. Here, for simplicity, we introduce the following notation:

$$\mathcal{R}_{71}(x) = (I - \mathcal{P}_n)J_-^{h,n}/\hbar_n, \quad x \in I_x^n, \tag{5.1}$$

observe that  $\mathcal{R}_{71} \equiv 0$  on  $S_n$  if  $J_{n,-}^h \in \mathcal{W}_n$ , i.e. no remeshing (or changing to finer mesh) at  $x = x_n$ . Further, let

$$\mathcal{R}_{72} = (J_+^{h,n} - J_-^{h,n})/\hbar_n, \quad \text{on } (\bar{x}, \bar{x}_\perp) \in S_n. \tag{5.2}$$

Now we give the estimate for VII in the following lemma:

**Lemma 5.1.** *Assume that  $\varrho$ ,  $\mathcal{R}_{71}$  and  $\mathcal{R}_{72}$  are defined as above. Then, there is a constant  $C$  such that*

$$\begin{aligned} & \sum_{n=0}^N ([J^h]_n, (\Phi - \varphi)_n^+)_n \\ & \leq C \left\{ \|\hat{\varepsilon}^{-1} h_\perp^2 \mathcal{R}_{71}\| \|\hat{\varepsilon} \varphi_{zz}\| + \sum_{i=1}^2 (\|\hbar \mathcal{R}_{7i}\| \|\varphi_x + \beta \cdot \nabla_\perp \varphi\| \right. \\ & \quad \left. + \min[\|\hbar \varrho \hat{\varepsilon}^{-1/2} \mathcal{R}_{7i}\|_{L_1(L_2)} \|\hat{\varepsilon}^{1/2} \varphi_z\|_{L_\infty(L_2)}, \|\hbar \varrho \hat{\varepsilon}^{-1/2} \mathcal{R}_{7i}\|_Q \|\hat{\varepsilon}^{1/2} \varphi_z\|_Q] \right\}. \end{aligned}$$

**Proof.** We split VII into two parts:

$$VII = \sum_{n=0}^N ([J^h]_n, (\mathcal{P}\varphi - \varphi)_+^n)_n + \sum_{n=0}^N ([J^h]_n, (\pi\mathcal{P}\varphi - \mathcal{P}\varphi)_+^n)_n := VII_1 + VII_2.$$

First, using  $[J^h]_n = J_+^{h,n} - J_-^{h,n} = \mathcal{P}_n J_-^{h,n} - J_-^{h,n}$ , we estimate VII<sub>1</sub> as

$$\begin{aligned} VII_1 &= \sum_{n=0}^N (J_-^{h,n} - \mathcal{P}_n J_-^{h,n}, (I - \mathcal{P}_n)\varphi_+^n)_n \\ &= \sum_{n=0}^N (\hbar_n \mathcal{R}_{71}(x_n)_+, (I - \mathcal{P}_n)\varphi_+^n)_n = \sum_{n=0}^N (\mathcal{R}_{71}(x_n)_+, (I - \mathcal{P}_n)\hbar_n \varphi_+^n)_n. \end{aligned} \tag{5.3}$$

Now to estimate  $(I - \mathcal{P}_n)\varphi_+^n$ , we note that

$$\begin{aligned} \varphi_+^n(\bar{x}_\perp) &= \varphi(\bar{x}, \alpha_n(\bar{x}, \bar{x}_\perp)) - \int_{x_n}^{\bar{x}} \frac{\partial}{\partial \bar{x}'} \varphi(\bar{x}', \alpha_n(\bar{x}', \bar{x}_\perp)) d\bar{x}' \\ &= \varphi(\bar{x}, \alpha_n(\bar{x}, \bar{x}_\perp)) - \int_{x_n}^{\bar{x}} (\varphi_x + \beta_n \cdot \nabla_\perp \varphi)(\bar{x}', \alpha_n(\bar{x}', \bar{x}_\perp)) d\bar{x}', \end{aligned}$$

so that

$$\hbar_n \varphi_+^n(\bar{x}_\perp) = \int_{I_x^n} \varphi(\bar{x}, \alpha_n(\bar{x}, \bar{x}_\perp)) d\bar{x} - \int_{I_x^n} \int_{x_n}^{\bar{x}} (\varphi_x + \beta_n \cdot \nabla_\perp \varphi)(\bar{x}', \bar{x}_\perp) d\bar{x}' d\bar{x}.$$

Inserting this representation into (5.3) and using estimates for  $(I - \mathcal{P}_n)$ , similar to (4.13), together with the piecewise smoothness of  $\beta_n$ , and Lemma 4.2 we get

$$\begin{aligned} |VII_1| &\leq C\{\|\hat{\varepsilon}^{-1}h_{\perp}^2\mathcal{R}_{71}\|_Q\|\hat{\varepsilon}\varphi_{zz}\|_Q + \|\hbar\mathcal{R}_{71}\|_Q\|\varphi_x + \beta \cdot \nabla\varphi\|_Q \\ &\quad + \min(\|\hbar\rho\hat{\varepsilon}^{-1/2}\mathcal{R}_{71}\|_{L_1(L_2)}\|\hat{\varepsilon}^{1/2}\varphi_z\|_{L_{\infty}(L_2)}, \|\hbar\rho\hat{\varepsilon}^{-1/2}\mathcal{R}_{71}\|_Q\|\hat{\varepsilon}^{1/2}\varphi_z\|_Q)\}. \end{aligned} \quad (5.4)$$

For the  $VII_2$ -term we write using Lemma 4.2 that

$$\begin{aligned} |VII_2| &\leq C\{\|\hbar\mathcal{R}_{72}\|_Q\|\varphi_x + \beta \cdot \nabla\varphi\|_Q \\ &\quad + \min(\|\hbar\rho\hat{\varepsilon}^{-1/2}\mathcal{R}_{72}\|_{L_1(L_2)}\|\hat{\varepsilon}^{1/2}\varphi_z\|_{L_{\infty}(L_2)}, \|\hbar\rho\hat{\varepsilon}^{-1/2}\mathcal{R}_{72}\|_Q\|\hat{\varepsilon}^{1/2}\varphi_z\|_Q)\}. \end{aligned} \quad (5.5)$$

Thus the assertion of Lemma 5.1 follows from (5.4) and (5.5).  $\square$

Finally using a kick-back argument in the contributions from the terms  $I$  and  $II$  we summarize the estimates of this paper in the following *main result*:

**Theorem 5.1.** (*A posteriori* error estimates) *Suppose that the assumptions in Lemmas 4.1 and 4.2 are valid. Let  $\hat{J}$  and  $J^h$  be the solutions of (2.7) and (3.10), respectively. Then, there is a constant  $C = C(\bar{C}, \hat{C})$  such that*

$$\begin{aligned} \|\hat{J} - J^h\|_Q &\leq C(\|\hat{\varepsilon}^{-1}h_{\perp}^2(|(I - \mathcal{P})\tilde{\mathcal{R}}_4| + |\mathcal{R}_{31}| + |\mathcal{R}_{51}| + |\mathcal{R}_{71}|)\|_Q \\ &\quad + \|\hbar(|(I - \pi)\mathcal{P}\tilde{\mathcal{R}}_4| + |(I - \pi)\tilde{\mathcal{R}}_{52}| + |\mathcal{R}_{62}| + |\mathcal{R}_{71}| + |\mathcal{R}_{72}|)\|_Q \\ &\quad + \min\{\|\hbar\rho\hat{\varepsilon}^{-1/2}(|(I - \pi)\mathcal{P}\tilde{\mathcal{R}}_4| + |(I - \pi)\tilde{\mathcal{R}}_{52}| + |\mathcal{R}_{71}| + |\mathcal{R}_{72}|)\|_{L_1(L_2)}, \\ &\quad \|\hbar\rho\hat{\varepsilon}^{-1/2}(|(I - \pi)\mathcal{P}\tilde{\mathcal{R}}_4| + |(I - \pi)\tilde{\mathcal{R}}_{52}| + |\mathcal{R}_{71}| + |\mathcal{R}_{72}|)\|_Q\}), \end{aligned}$$

where  $\tilde{\mathcal{R}}_{i(j)} = \mathcal{R}_{i(j)}\Lambda$ ,  $\mathcal{R}_{71}$  and  $\mathcal{R}_{72}$  are defined in (5.1) and (5.2), respectively, further

$$\mathcal{R}_{31} \equiv \mathcal{R}_{51} = \hat{\varepsilon}\mathcal{D}_{\perp,h}^2 J^h, \quad \mathcal{R}_{52} = \hat{\varepsilon}\mathcal{D}_{h,z}^2 J^h \quad \text{and} \quad \mathcal{R}_{62} = \mathcal{D}_{\perp}\mathcal{D}_x J^h, \quad \text{on } \Gamma_n^-.$$

Here we have used the fact that  $(I - \pi)\mathcal{P} = \mathcal{P}(I - \pi)$  and the boundedness of  $\mathcal{P}$ . Note again that  $VI_1 \equiv 0$  and  $\mathcal{R}_{71}$  vanishes whenever  $\mathcal{T}_n = \mathcal{T}_n^-$  so that  $J_-^{h,n} \in \mathcal{W}_n$ .

Theorem 5.1 may be stated in a more concrete form by estimating the terms,  $(I - \mathcal{P})\tilde{\mathcal{R}}_4$ ,  $(I - \pi)\mathcal{P}\tilde{\mathcal{R}}_4$ ,  $(I - \pi)\tilde{\mathcal{R}}_{52}$  and  $(I - \mathcal{P}_n)J_-^{h,n}$  explicitly. First we note that in Theorem 5.1 these terms are associated with weight functions:  $w = \hat{\varepsilon}^{-1}h_{\perp}^2$ ,  $\hbar$  or  $\hbar\rho\hat{\varepsilon}^{-1/2}$ , so that typically we need to estimate terms of the form

$$\|w(I - S)g\|_{L_p(I_x, L_2(I_{\perp}))}, \quad S = \pi, \text{ or } \mathcal{P}, \quad \text{and } p = 1, \text{ or } \infty,$$

with  $g$  replacing given relevant functions from the right-hand side of the estimate in Theorem 5.1. To derive concrete estimates we need some assumptions on the weight functions, (cf. Ref. 13),

$$|\nabla w| \leq \delta h^{-1}w, \quad \delta > 0 \text{ small}, \quad (5.6)$$



i.e. in our case for  $h_{\perp}$ ,  $|\nabla_{\perp}(\hat{\varepsilon}^{-1}h_{\perp}^2)| \leq \delta h_{\perp}^{-1}(\hat{\varepsilon}^{-1}h_{\perp}^2) = \delta \hat{\varepsilon}^{-1}h_{\perp}$ , while for  $\hbar$ ,  $|\hbar'| \leq \delta \hbar \hbar^{-1} = \delta$ , and also  $|\mathcal{D}_x(\hbar \rho \hat{\varepsilon}^{-1/2})| \leq \delta \hbar^{-1} \hbar \rho \hat{\varepsilon}^{-1/2} = \delta \rho \hat{\varepsilon}^{-1/2}$ . Thus, e.g. we have that  $|2\hat{\varepsilon}\mathcal{D}_{\perp}(h_{\perp}) - h_{\perp}(\mathcal{D}_{\perp}\hat{\varepsilon})| \leq \delta \hat{\varepsilon}$ , and hence (5.6) is guaranteed if the following two conditions hold true:

$$|\hbar'| \leq \min \left( \frac{1}{2\hat{\varepsilon}} \frac{|\hbar|}{(\hat{\varepsilon}_x)^{1/2}} + \frac{\delta}{\hat{\varepsilon}^{1/2}}, \delta \right), \tag{5.7}$$

$$|\nabla_{\perp} h_{\perp}| \leq \frac{|\nabla_{\perp} \hat{\varepsilon}|}{2\hat{\varepsilon}} h_{\perp} + \frac{\delta}{2}. \tag{5.8}$$

**Lemma 5.2.** (The weighted  $L_2$ -projection estimates) *Assume that the bounds (5.7) and (5.8) are valid, then there is a constant  $C$  such that for sufficiently smooth  $g$ , we have*

$$\|w(I - \pi)g\|_Q \leq C \|wh^l \mathcal{D}_x^l g\|_Q, \quad l \in \mathbb{Z}^+, \tag{5.9}$$

$$\|w(I - \mathcal{P})g\|_Q \leq C \|wh_{\perp}^k \mathcal{D}_{\perp}^k g\|_Q, \quad k \in \mathbb{Z}^+. \tag{5.10}$$

**Proof.** We give only the proof of (5.10), the estimate (5.9) is obtained in a similar way. Let  $\tilde{g}$  be an interpolant of  $g$ , then

$$\begin{aligned} \|w(I - \mathcal{P})g\|_Q &\leq \|w(g - \tilde{g})\|_Q + \|w\mathcal{P}(\tilde{g} - g)\|_Q \leq C \|w(g - \tilde{g})\|_Q \\ &\leq \left( \sum_{n,\tau} \|w(g - \tilde{g})\|_{L_2(I_x^n \times \tau)}^2 \right)^{1/2} \leq C \left( \sum_{n,\tau} (\hat{w}_{\tau} \|g - \tilde{g}\|_{L_2(I_x^n \times \tau)})^2 \right)^{1/2} \\ &\leq C \left( \sum_{n,\tau} (\hat{w}_{\tau} \|h_{\perp}^k \mathcal{D}_{\perp}^k g\|_{L_2(I_x^n \times \tau)})^2 \right)^{1/2} \\ &\leq C \left( \sum_{n,\tau} \left( \frac{\hat{w}_{\tau}}{\tilde{w}_{\tau}} \|wh_{\perp}^k \mathcal{D}_{\perp}^k g\|_{L_2(I_x^n \times \tau)} \right)^2 \right)^{1/2} \leq C \|wh_{\perp}^k \mathcal{D}_{\perp}^k g\|_Q, \end{aligned}$$

where we have used the fact that the assumption (5.6) applied to  $x_{\perp}$  variable gives that  $\tilde{w}_{\tau} \leq w(x_{\perp})|_{\tau} \leq \hat{w}_{\tau}$ , with  $\tilde{w}_{\tau} = \min_{x_{\perp} \in \mathcal{N}_{\tau}} w(x_{\perp})$ ,  $\hat{w}_{\tau} = \max_{x_{\perp} \in \mathcal{N}_{\tau}} w(x_{\perp})$  and

$$\mathcal{N}_{\tau} = \{\tilde{\tau} \in \mathcal{T} : \tilde{\tau} \text{ has a common edge or vertex with } \tau\}. \quad \square$$

In the rest of this section we prepare for a concrete version of Theorem 5.1. Below we shall estimate all the  $\mathcal{R}_{i(j)}$ -terms so that, finally, in Theorem 5.2, we can formulate such a concrete version. To this approach, first we note that

$$\|(I - \mathcal{P}_n)J_{\perp}^{h,n}\|_{S_n} \leq C \|(I - \mathcal{P}_n)J^{h,n}\|_{S_{n-1}}, \tag{5.11}$$

$$\|(I - \mathcal{P})\tilde{\mathcal{R}}_4\|_{S_n} = \|(I - \mathcal{P})(\tilde{\beta} \cdot \nabla J^h)\Lambda\|_{S_n}, \tag{5.12}$$

recall that  $\tilde{\beta} = (1, \beta)$  and  $\nabla = (\partial/\partial x, \nabla_\perp)$ . To estimate the right-hand side of (5.12) let  $\tilde{J}$  be a standard mollification of  $J^h$  on the length scales  $(\hbar, h_\perp, h_\perp)$ , i.e.

$$\tilde{J} = \int_Q J^h(x - x', x_\perp - x'_\perp) \chi_\hbar(x', x'_\perp) dx', \quad \mathbf{x}' = (x', x'_\perp), \quad (5.13)$$

where  $0 \leq \chi \in C_0^\infty(Q)$  and

$$\int_Q \chi(x, x_\perp) dx = 1, \quad \chi_\hbar(x, x_\perp) = \hbar^{-1} h_\perp^{-2} \chi(\hbar^{-1} x, h_\perp^{-1} x_\perp).$$

Then we have that

$$\|(I - \mathcal{P})(\tilde{\beta} \cdot \nabla \tilde{J})\|_Q \leq C \|h_\perp^2 \mathcal{D}_\perp^2 (\tilde{\beta} \cdot \nabla \tilde{J})\|_Q. \quad (5.14)$$

Below we shall use the following *discrete convective-symmetry* assumption for our approximate solution  $J^h \in \mathcal{V}_h$ , and the mollifier function  $\tilde{J}$ :

$$h_{\perp,z} \tilde{J}_y = h_{\perp,y} \tilde{J}_z, \quad \tilde{J} = J^h \quad \text{or} \quad \tilde{J} = \tilde{J}. \quad (5.15)$$

Note that given a sufficiently smooth function  $g$  we have the identity

$$(\beta \cdot \nabla_\perp)(h_\perp \mathcal{D}_\perp g) = \mathcal{D}_\perp(h_\perp(\beta \cdot \nabla_\perp g)) - zh_{\perp,z} g_y + zh_{\perp,y} g_z - h_\perp g_y. \quad (5.16)$$

Now to estimate (5.12) using (5.14) we need to control the  $L_2(Q)$ -norm of  $\tilde{\beta} \cdot \nabla(J^h - \tilde{J})$ , and to this approach we use (5.10) and split a Taylor expansion on  $x$ - and  $x_\perp$ -directions. Then using also (5.15) and (5.16) we get

$$\begin{aligned} \tilde{\beta} \cdot \nabla(J^h - \tilde{J}) &= (\hbar \tilde{J}_x)_x + (\beta \cdot \nabla_\perp)(h_\perp \mathcal{D}_\perp \tilde{J}) + \mathcal{O}(h^2) \\ &\sim (\hbar \tilde{J}_x)_x + \mathcal{D}_\perp(h_\perp(\beta \cdot \nabla_\perp \tilde{J})) - h_\perp \tilde{J}_y. \end{aligned} \quad (5.17)$$

It follows from (5.17) that

$$\begin{aligned} \|\tilde{\beta} \cdot \nabla(J^h - \tilde{J})\|_Q &\leq \|(\hbar_x)^{-1}(\hbar_x \tilde{J}_x) + (h_\perp^{-1})(h_\perp(\beta \cdot \nabla_\perp \tilde{J}))\|_Q \\ &\quad + \|h_\perp \tilde{J}_y\|_Q \leq \|\tilde{\beta} \cdot \nabla \tilde{J}\|_Q + \|h_\perp \tilde{J}_y\|_Q. \end{aligned} \quad (5.18)$$

Combining (5.14) and (5.18) and using (5.13) we have

$$\begin{aligned} \|(I - \mathcal{P})(\tilde{\beta} \cdot \nabla J^h)\|_Q &\leq C \|h_\perp^2 \mathcal{D}_\perp^2 (\tilde{\beta} \cdot \nabla \tilde{J})\|_Q + \|(I - \mathcal{P})h_\perp \tilde{J}_y\|_Q \\ &\leq C(\|h_\perp \mathcal{D}_\perp (\tilde{\beta} \cdot \nabla J^h)\|_Q + \|h_\perp J^h\|_Q). \end{aligned} \quad (5.19)$$

**Remark 5.1.** Note that using the mollifier  $\tilde{J}$  is necessary to transit  $\|\cdot\|_{S_n}$  norms to  $\|\cdot\|_Q$  norms. In the continuous case a direct application of Lemma 5.2 yields to our final weighted estimates.

Now we turn to give concrete estimates for  $(I - \pi)$ -terms: i.e.  $(I - \pi)\mathcal{P}\tilde{\mathcal{R}}_4$  and  $(I - \pi)\mathcal{P}\tilde{\mathcal{R}}_{52}$  on the right-hand side of Theorem 5.1. Using  $(I - \pi)\mathcal{P} = \mathcal{P}(I - \pi)$ , boundedness of  $\mathcal{P}$  and (5.9) in Lemma 5.2, with  $l = 0$ , we have

$$\|w(I - \pi)\mathcal{P}\tilde{\mathcal{R}}_4\|_Q \leq C \|w(I - \pi)\tilde{\mathcal{R}}_4\|_Q \leq C \|w(\tilde{\beta} \cdot \nabla J^h)\|_Q. \quad (5.20)$$

As for  $\tilde{\mathcal{R}}_{52}$ -term, since higher derivatives are involved we need to use again the regularizing effect induced by the mollifier function  $\tilde{J}$ . So that using Taylor expansion in  $x$ -direction

$$\begin{aligned} \|w(I - \pi)\mathcal{R}_{52}\|_Q &\leq \|w(I - \pi)\hat{\varepsilon}\mathcal{D}_{h,z}^2 J^h\|_Q \\ &\leq \|w(I - \pi)\hat{\varepsilon}\mathcal{D}_{h,z}^2 \tilde{J}\|_Q + \|w(I - \pi)\hat{\varepsilon}\mathcal{D}_{h,z}^2 (J^h - \tilde{J})\|_Q \\ &\leq \|w(I - \pi)\hat{\varepsilon}\mathcal{D}_{h,z}^2 \tilde{J}\|_Q + \|w(I - \pi)\hat{\varepsilon}\mathcal{D}_{h,z}^2 (\hbar\tilde{J}_x)\|_Q + \mathcal{O}(w\hat{\varepsilon}\hbar^2) \\ &\leq C\|w(I - \pi)(\hat{\varepsilon}\mathcal{D}_{h,z} J^h)\|_Q + \|w(I - \pi)\hat{\varepsilon}\mathcal{D}_{h,z}^2 (\hbar J^h)\|_Q \\ &\leq \|w\hbar\hat{\varepsilon}J_{xz}^h\|_Q + \|w\hbar\hat{\varepsilon}J_{zz}^h\|_Q. \end{aligned} \tag{5.21}$$

Recalling Theorem 5.1 the relevant weights in (5.20) and (5.21) are  $w = \hbar$  and  $w = \hbar\rho\hat{\varepsilon}^{-1/2}$ , respectively.

Summing up we have proved the following final and concrete version of a posteriori error estimates for (2.7).

**Theorem 5.2.** *Let  $\hat{J}$  and  $J^h$  be as in Theorem 5.1. Suppose further the discrete convective symmetry assumption (5.15). Then, there is a constant  $C = C(\bar{C}, \hat{C})$  such that*

$$\begin{aligned} \|\hat{e}_h\| &\leq C\{\|\hat{\varepsilon}^{-1}h_{\perp}^3\mathcal{D}_{\perp}(\tilde{\beta} \cdot \nabla J^h)\|_Q + \|\hat{\varepsilon}^{-1}h_{\perp}^3 J^h\|_Q + \|h_{\perp}^2\mathcal{D}_{\perp}^2 J^h\|_Q \\ &\quad + \|\hat{\varepsilon}^{-1}h_{\perp}^4\hbar^{-1}\mathcal{D}_{\perp}^2 J^h\|_Q + \|\hbar(\tilde{\beta} \cdot \nabla J^h)\|_Q + \|\hbar^2\hat{\varepsilon}J_{xz}^h\|_Q + \|\hbar^2\hat{\varepsilon}J_{zz}^h\|_Q \\ &\quad + \|\hbar\mathcal{D}_{\perp}(J_x^h)\|_{\Gamma^-} + \|\hbar h_{\perp}^2\hbar^{-1}\mathcal{D}_{\perp}^2 J^h\|_Q + \|\hbar(\partial_{\bar{x}} J^h)\|_Q \\ &\quad + \min(\|\hbar\rho\hat{\varepsilon}^{-1/2}(\tilde{\beta} \cdot \nabla J^h)\|_Q + \|\hbar^2\rho\hat{\varepsilon}^{1/2}J_{xz}^h\|_Q + \|\hbar^2\rho\hat{\varepsilon}^{1/2}J_{zz}^h\|_Q \\ &\quad + \|\hbar_{\perp}^2\rho\hat{\varepsilon}^{-1/2}\mathcal{D}_{\perp}^2 J^h\|_Q + \|\hbar\rho\hat{\varepsilon}^{-1/2}(\partial_{\bar{x}} J^h)\|_Q, \\ &\quad \|\hbar\rho\hat{\varepsilon}^{-1/2}(\tilde{\beta} \cdot \nabla J^h)\|_{L_1(L_2)} + \|\hbar^2\rho\hat{\varepsilon}^{1/2}J_{xz}^h\|_{L_1(L_2)} + \|\hbar^2\rho\hat{\varepsilon}^{1/2}J_{zz}^h\|_{L_1(L_2)} \\ &\quad + \|\hbar_{\perp}^2\rho\hat{\varepsilon}^{-1/2}\mathcal{D}_{\perp}^2 J^h\|_{L_1(L_2)} + \|\hbar\rho\hat{\varepsilon}^{-1/2}(\partial_{\bar{x}} J^h)\|_{L_1(L_2)}\}, \end{aligned}$$

where we have used (5.14)-(5.21) and

$$\partial_{\bar{x}} J^h = (J_+^{h,n} - J_-^{h,n})/\hbar_n \quad \text{on } S_n.$$

**Remark 5.2.** Note that in Theorem 5.2, the terms  $\|h_{\perp}^2\mathcal{D}_{\perp}(\tilde{\beta} \cdot \nabla J^h)\|_Q$  (if  $\hat{\varepsilon} = Ch_{\perp}$ ) and  $\|\hbar(\partial_{\bar{x}} J^h)\|_Q$  are naturally corresponding to the terms  $\|h_{\perp}^2\mathcal{D}_{\perp}(J_{\beta})\|_Q$  and  $\|\hbar J_{\bar{x}}\|_Q$  arising in pure interpolation with piecewise linear and constant functions respectively. Now assuming that  $\mathcal{T}_n = \mathcal{T}_n^-$ , all contributions from  $\mathcal{R}_{71} = (I - \mathcal{P}_n)J_-^{h,n}/\hbar_n$ , in particular, the critical term  $\|\hat{\varepsilon}^{-1}h_{\perp}^4\hbar^{-1}\mathcal{D}_{\perp}^2 J^h\|_Q$  will vanish. That is, if we take  $\mathcal{T}_n$  to be the convected mesh from the previous  $x$ -step with elements  $\{\alpha_{n-1}(x_n, \bar{x}_{\perp}); \bar{x}_{\perp} \in \tau\}$ ,  $\tau \in \mathcal{T}_{n-1}$ , then  $R_{71} = (I - \mathcal{P}_n)J_-^{h,n}/\hbar_n$  vanishes and therefore  $\hat{\varepsilon}^{-1}h_{\perp}^4\hbar^{-1}\mathcal{D}_{\perp}^2 J^h$ -term never comes up. More generally the parameter  $\hbar^{-1}$  in this term is related to how frequently we remesh. We may therefore replace

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the  $\hbar^{-1}$  factor by the “remeshing frequency”  $\hbar_*^{-1}$  which by (3.3) may be taken as small as  $\mathcal{O}(|\nabla_{\perp}\beta|) \sim 1$ , without getting difficulties with collapsing or too disordered grids. Consequently, we can claim that our *a posteriori* error estimates in here are of optimal order. There are other ways to control the  $\hat{\varepsilon}^{-1}h_{\perp}^4\hbar^{-1}\mathcal{D}_{\perp}^2J^h$ -term by requiring that the  $\Delta x_n$ -steps are not too small, but then it may be become cumbersome to get a reasonable balance between the velocity and space discretization errors, at least for  $p = 0$ . Finally with small  $\varrho$ , ( $\varrho \leq \hat{\varepsilon}^{1/2}$ ),  $\hbar \sim h_{\perp}^2$  and  $\hat{\varepsilon} = Ch_{\perp}$  we have the following absorbed version of our final result; Theorem 5.2

**Corollary 5.1.** *Suppose conditions in Theorem 5.2, together with  $\mathcal{T}_n = \mathcal{T}_n^-$ ,  $\varrho \leq \hat{\varepsilon}^{1/2}$ ,  $\hbar \sim h_{\perp}^2$  and  $\hat{\varepsilon} = Ch_{\perp}$ . Then there is a constant  $C$ , as in Theorem 5.2, such that*

$$\begin{aligned} \|\hat{e}_h\| \leq C\{ & \|h_{\perp}^2\mathcal{D}_{\perp}(\tilde{\beta} \cdot \nabla J^h)\|_Q + \|h_{\perp}^2J^h\|_Q + \|h_{\perp}^2\mathcal{D}_{\perp}^2J^h\|_Q + \|h_{\perp}^2(\tilde{\beta} \cdot \nabla J^h)\|_Q \\ & + \|h_{\perp}^5J_{xz}^h\|_Q + \|h_{\perp}^5J_{zz}^h\|_Q + \|h_{\perp}^2\mathcal{D}_{\perp}(J_x^h)\|_{\Gamma^-} + \|h_{\perp}^2\mathcal{D}_{\perp}^2J^h\|_Q + \|h_{\perp}^2(\partial_{\bar{x}}J^h)\|_Q \\ & + \min(\|h_{\perp}^2(\tilde{\beta} \cdot \nabla J^h)\|_Q + \|h_{\perp}^5J_{xz}^h\|_Q + \|h_{\perp}^5J_{zz}^h\|_Q + \|h_{\perp}^2\mathcal{D}_{\perp}^2J^h\|_Q \\ & + \|h_{\perp}^2(\partial_{\bar{x}}J^h)\|_Q, \|h_{\perp}^2(\tilde{\beta} \cdot \nabla J^h)\|_{L_1(L_2)} + \|h_{\perp}^5J_{xz}^h\|_{L_1(L_2)} + \|h_{\perp}^5J_{zz}^h\|_{L_1(L_2)} \\ & + \|h_{\perp}^2\mathcal{D}_{\perp}^2J^h\|_{L_1(L_2)} + \|h_{\perp}^2(\partial_{\bar{x}}J^h)\|_{L_1(L_2)})\} \sim C\|h_{\perp}^2\mathcal{E}(J^h)\|^{\#} \end{aligned}$$

with  $\|h_{\perp}^2\mathcal{E}(\cdot)\|^{\#}$  being a weighted norm equivalent to  $h_{\perp}^2(\|J^h\|_{H^2} + \|J^h\|_{W_{L_1(L_2)}^2})$ .

**Remark 5.3.** With arguments similar to those leading to the proof of Theorems 5.1 and 5.2, we can derive *a posteriori* error estimates in  $\|\cdot\|_{L^{\infty}(I_x, L_2(I_{\perp}))}$ -norm. Then we need to use a dual problem of the following form

$$\begin{cases} -\varphi_x - z\varphi_y - \hat{\varepsilon}\varphi_{zz} = 0, & \text{in } Q, \\ \varphi(L, \cdot) = \hat{e}_{N+1}^-, & \text{on } \Gamma_L^+, \\ \varphi = 0, \text{ on } \Gamma_s^+, \text{ and } \varphi_z = 0 \text{ on } \Gamma^0, \end{cases} \quad (5.22)$$

instead of (2.14).

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