

Characteristic Methods for Fokker-Planck and Fermi Pencil Beam Equations

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1 Introduction

We design an efficient and accurate numerical method for the pencil beam equations based on the principle of solving

- An *exact transport* problem on each collision free spatial segment: Let x be the beam penetration direction, $\{x_n\}$ an increasing sequence of discrete points indicating collision sites and $\{\mathcal{V}_n\}$ be a corresponding sequence of piecewise polynomial spaces on meshes $\{\mathcal{T}_n\}$ on the transversal variable x_\perp . Then given the approximate solution $J^{h,n} \in \mathcal{V}_n$ at the collision site x_n solve the pencil beam equation exactly on the collision free interval (x_n, x_{n+1}) with the data $J^{h,n}$ to give the solution $J_-^{h,n+1}$ at the next collision site x_{n+1} , before the collision.
- A *projection*: Compute $J^{h,n+1} = \mathcal{P}_{n+1} J_-^{h,n+1}$, with \mathcal{P}_{n+1} being a projection into $\{\mathcal{V}_{n+1}\}$.

There are variety of methods of this type differing in the choice of piecewise polynomial spaces $\{\mathcal{V}_n\}$ (degree of polynomials, orthogonal polynomials, continuous or discontinuous polynomials) and in the projections \mathcal{P}_n , (L_p -projections, $1 \leq p \leq \infty$, interpolation projections).

Generally the *exact transport* problem, because of the presence of the diffusion term, in the pencil beam equations, if solvable, is highly nontrivial. Besides, simple projections as L_2 -projection would create oscillatory behavior in the presence of discontinuities (e.g., on skin/tissue and tissue/bone interface, in the medical physics applications of the beam algorithms).

Our main purpose in this note is to present an approach leading to *exact transport* for model cases of pencil beam problems by characteristic methods and also containing a modified L_2 -projection raising the stability properties.

An alternative approach; the Streamline Diffusion Method (SD; a general finite element method for hyperbolic type problems), is studied by this author giving a priori error estimates for Vlasov-Poisson equations in [1], for the Fermi and Fokker-Planck equations in [2] and [3] and a posteriori error estimates for Fermi and Fokker-Planck equations in [4]. Our method is obtained through two basic modifications of a standard Galerkin method: First, the test functions are modified so that to give a weighted least square control of the residual \mathcal{R} , (measuring how well the approximate solution satisfies the considered differential equation locally), of the approximate solution, and secondly artificial viscosity is added to the diffusion coefficient of the form $Ch^2|\mathcal{R}(J^h)|$, where h is the local mesh size.

We shall consider a variant of the SD-method based on using trial functions which are discontinuous in the beams penetration direction x and continuous in the transversal variables x_\perp . Orienting the *incident-transversal* mesh approximately along the characteristics we get a particular SD-method suitable for convection dominated convection-diffusion problems referred as Characteristic Streamline Diffusion (CSD).

The domain $Q := I_x \times I_y \times I_z$ is subdivided into *slabs* $S_n = I_x^n \times I_y \times I_z$, with $I_x^n = (x_n, x_{n+1})$ corresponding to a collision-free path in the x -direction and I_y and I_z are bounded symmetric intervals representing, together, the transversal variable $x_\perp = (y, z)$. Each slab S_n has its own *incident-transversal* finite element mesh \hat{T}_n . Consequently, at each collision site x_n we have two transversal meshes $\hat{T}_n^+ = \hat{T}_n|_{x_n}$ and $\hat{T}_n^- = \hat{T}_{n-1}|_{x_n}$, respectively. In general $\hat{T}_n^+ \neq \hat{T}_n^-$ and the passage of information from one slab to the next is performed through a modified L_2 -projection. The CSD-method performs this modified projection and the *exact transport* results from satisfying, in model cases, the convection equations exactly on each slab separately.

An outline of this paper is as follows: In section 1 we derive L_2 estimates for smooth solutions. Section 2 is devoted to the amount of numerical dissipation. In section 3 we study stability in the maximum norm and finally in our concluding section 4 we give optimal error estimates for the discretized problem. Throughout the paper C will denote an absolute constant not necessarily the same at each occurrence.

A model Problem

We sketch the derivation, through the Gaussian multiple scattering theory, of the Fokker-Planck and Fermi pencil beam equations relevant in electron dose calculations. Detailed derivation strategy can be found in [?], relying on Fourier techniques, [?], using spherical harmonics and [?], based on statistical physics approaches. Below we give a general idea. For this purpose,

we start from the steady-state, monoenergetic transport equation:

$$\boldsymbol{\omega} \cdot \nabla_{\mathbf{x}} \psi(\mathbf{x}, \boldsymbol{\omega}) + \sigma_t(\mathbf{x}) \psi(\mathbf{x}, \boldsymbol{\omega}) = \int_{S^2} \sigma_s(\mathbf{x}, \boldsymbol{\omega} \cdot \boldsymbol{\omega}') \psi(\mathbf{x}, \boldsymbol{\omega}') d\boldsymbol{\omega}', \quad \text{in } Q, \quad (1)$$

associated with the boundary conditions $\psi(L, y, z, \boldsymbol{\omega}) = 0, \quad \xi < 0$, and

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

with $\mathbf{x} = (x, y, z) \in [0, L] \times R \times R$, $\boldsymbol{\omega} = (\xi, \eta, \zeta) \in S^2$, describing the spreading of a pencil beam of particles normally incident upon a purely scattering, source-free, slab of thickness L . Here ψ is the density of particles at the point \mathbf{x} moving in the direction of $\boldsymbol{\omega}$, σ_t , and σ_s are total and scattering cross-sections, respectively. Assuming a *forward peaked* scattering procedure, the transport equation 1 may, asymptotically, be approximated by the following Fokker-Planck equation

$$\boldsymbol{\omega} \cdot \nabla_{\mathbf{x}} \psi^{FP} = \sigma \left[\frac{\partial}{\partial \xi} (1 - \xi^2) \frac{\partial}{\partial \xi} + \frac{1}{1 - \xi^2} \frac{\partial^2}{\partial \vartheta^2} \right] \psi^{FP}, \quad (3)$$

where ϑ is the azimuthal angle with respect to the z -axis and

$$\sigma \equiv \frac{1}{2} \sigma_{tr}(\mathbf{x}) = \pi \int_{-1}^1 (1 - \xi) \sigma_s(\mathbf{x}, \xi) d\xi, \quad (4)$$

is the transport cross-section for a purely scattering medium. In the asymptotic expansions leading to The Fokker-Planck equation the absorption term $\sigma_t \psi$ on the left-hand side of 1 associated with a Taylor expansion of ψ on the right-hand side would give the right-hand side of 5 and a neglected remainder term of order $\mathcal{O}(\sigma^2)$,

see [4] for the details. A further approximation, assuming thin slab by letting

$$L \times \sigma \ll 1, \quad (5)$$

and simple algebraic manipulations yields to a perturbation of the Eq. 5, to the following Fermi equation;

$$\boldsymbol{\omega}_0 \cdot \nabla_{\mathbf{x}} \psi^F = \sigma \Delta_{\eta\zeta} \psi^F, \quad (6)$$

$$\psi^F(0, y, z, \eta, \zeta) = \delta(y) \delta(z) \delta(\eta) \delta(\zeta), \quad \xi > 0, \quad (7)$$

$$\psi^F(L, y, z, \eta, \zeta) = 0, \quad \xi < 0, \quad (8)$$

here $\boldsymbol{\omega}_0 = (1, \eta, \zeta)$, where $(\eta, \zeta) \in R \times R$ and $\Delta_{\eta\zeta} = \partial^2 / \partial \eta^2 + \partial^2 / \partial \zeta^2$. Geometrically, the Eq.6 corresponds to projecting $\boldsymbol{\omega} \in S^2$ in the Eq. 3, along $\boldsymbol{\omega} = (\xi, \eta, \zeta)$ onto the tangent plane to S^2 at the point $(1, 0, 0)$. In this way the Laplacian operator, on the unit sphere, in the right-hand side

of the Fokker-Planck equation 3 is transferred to the Laplacian operator on this tangent plane, as on the right-hand side of the Fermi equation 6. The equations 3-6 are formulated for the flux function ψ , while usually the measured quantity (dose) is related to the current function

$$j = \xi\psi. \quad (9)$$

Now we consider a two dimensional version of Eqs. 1- 4 leading to the following Fokker-Planck problem, see also [2]: For $0 < x < L$ and $-\infty < y < \infty$, find $\psi^{FP} \equiv \Psi^{FP}(x, y, \theta)$ such that

$$\omega \cdot \nabla_{\mathbf{x}} \psi^{FP} = \sigma \psi_{\theta\theta}^{FP}, \quad \theta \in (-\pi/2, \pi/2), \quad (10)$$

$$\psi^{FP}(0, y, \theta) = \frac{1}{2\pi} \delta(1 - \cos \theta) \delta(y), \quad \theta \in S_+^1, \quad (11)$$

$$\psi^{FP}(L, y, \theta) = 0, \quad \theta \in S_-^1, \quad (12)$$

where $\omega = (\xi, \eta) \equiv (\cos \theta, \sin \theta)$, $S_+^1 = \{\omega \in S^1 : \xi > 0\}$ and $S_-^1 = S^1 \setminus S_+^1$. We use the scaling substitution

$$z = \tan \theta, \quad \theta \in (-\pi/2, \pi/2), \quad (13)$$

and introduce the scaled current function J by

$$J(x, y, z) \equiv j(x, y, \tan^{-1} z)/(1 + z^2). \quad (14)$$

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

$$J_x + zJ_y = \sigma AJ, \quad (x, x_\perp) \in Q, \quad (15)$$

$$J_x(0, y, \pm z_0) = 0, \quad \text{for } y \in I_y, \quad (16)$$

$$J(0, \pm y_0, z) = 0, \quad \text{for } \pm z < 0, \quad (17)$$

$$J(0, x_\perp) = f(x_\perp), \quad (18)$$

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

$$A = \partial^2 / \partial z^2, \quad (\text{Fermi}), \quad (19)$$

$$A \cdot = \partial / \partial z [a(z) \partial / \partial z (b(z) \cdot)], \quad (\text{Fokker-Planck}) \quad (20)$$

where $a(z) = 1 + z^2$ and $b(z) = (1 + z^2)^{3/2}$. We shall study the Fermi equation. Fokker-Planck case is, basically, the same except some tedious

factors and therefor is omitted. Detailed Fokker-Planck studies can be found in [2]. We note that the transport cross section depends on enery and therefor on the spatial variables: $\sigma \equiv \sigma(x, y) = 1/2\sigma_{tr}(E(x, y))$.

The non-degenerate approximation of 12 would be as follows:

$$\mathcal{L}(J) := J_x + \beta \cdot \nabla_{\perp} J - \varepsilon \Delta_{\perp} J = 0, \quad (21)$$

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 16 corresponding to the Fermi equation, extensions to the Fokker-Planck case 17 are straight forward ,but lengthy (see our a priori error analysis in [2] containing such extensions), and therefore are omitted.

Note that introducing the change of coordinates $(x, \bar{x}_{\perp}) = (x, x_{\perp} - x\beta)$ and witting $\bar{J}(x, \bar{x}_{\perp}) = J(x, x_{\perp})$, we can formulate Eq. 21 as follows:

$$\bar{J}_x - \varepsilon \Delta_{\perp} \bar{J} = 0, \quad \text{in } [0, L] \times I_y \times I_z, \quad \bar{J}(0, \bar{x}_{\perp}) = f(x_{\perp}), \quad (22)$$

since $\frac{\partial \bar{J}}{\partial x} = \frac{\partial}{\partial x} J(x, \bar{x}_{\perp} + x\beta) = \frac{\partial J}{\partial x} + \beta \cdot \nabla J$. If $\varepsilon = 0$, then the solution of Eq. 22 is given by $\bar{J}(x, \bar{x}_{\perp}) = f(\bar{x}_{\perp})$ and that of Eq. 21 by

$$J(x, x_{\perp}) = f(x_{\perp} - x\beta). \quad (23)$$

Clearly the characteristics of Eq. 21 with $\varepsilon = 0$ are given by $x_{\perp} = \bar{x}_{\perp} + x\beta$, $x > 0$, and in this case ($\varepsilon = 0$) the solution $J(x, x_{\perp})$ is constant along characteristics. Let now $\{x_n\}$ be an increasing sequence of x -values with $x_0 = 0$ and let $\{\mathcal{T}_n\}$ be a corresponding sequence of triangulation \mathcal{T}_n of $I_y \times I_z$ into triangles K and let \mathcal{V}_n be the space of continuous peicewise linear functions on \mathcal{T}_n , $\mathcal{V}_n = \{v \in \mathcal{C}(I_y \times I_z) : v \text{ is linear on } K, K \in \mathcal{T}_n\}$. Here and below $\mathcal{C}(\Omega)$ denotes the continuous functions $v : \Omega \rightarrow R$ an a set Ω .

The *Characteristic Galerkin method* for Eq. 21 may be formulated as follows in the case of $\varepsilon = 0$: For $n = 1, 2, \dots, N$, find $J^{h,n} \in \mathcal{V}_n$ such that

$$\int_{I_y \times I_z} J^{h,n}(x_{\perp})v(x_{\perp}) dx_{\perp} = \int_{I_y \times I_z} J^{h,n-1}(x_{\perp} - \hbar_n\beta)v(x_{\perp}) dx_{\perp}, \quad \forall v \in \mathcal{V}_n, \quad (24)$$

where $\hbar = x_n - x_{n-1}$ and $J^{h,0} = f$. In other words

$$J^{h,n} = \mathcal{P}_n T_n J^{h,n-1}, \quad (25)$$

where $\mathcal{P}_n : L_2(I_y \times I_z) \rightarrow \mathcal{V}_n$ is the L_2 -projection defined by $(\mathcal{P}_n w, v) = (w, v)$, $\forall v \in \mathcal{V}_n$, where (\cdot, \cdot) denotes the inner product in $L_2(I_y \times I_z)$, and $T_n v(x_{\perp}) = v(x_{\perp} - \hbar_n\beta)$. Thus Eq. 25 may be expressed as *exact transport* (T_n)+ projection \mathcal{P}_n .

Next we formulate the *SD-method* for Eq. 21 and then the *CSD-method* as a special case with oriented phase-space, performed as penetrated-transversal, elements. For $n = 1, 2, \dots, N$, let $\hat{\mathcal{T}}_n = \{\hat{K}\}$ be a finite element subdivision of the slab $S_n = I_x^n \times I_\perp$, $I_x^n = (x_n, x_{n+1})$, $I_\perp = I_y \times I_z$, into finite elements \hat{K} and let $\hat{\mathcal{V}}_n$ be a space of continuous piecewise polynomials on $\hat{\mathcal{T}}_n$ of degree at most k . For $k = 1$ and small ε the SD-method may be formulated as follows: For $n = 1, 2, \dots, N$, find $\hat{J}^h \equiv \hat{J}^h|_{S_n} \in \hat{\mathcal{V}}_n$ such that

$$\begin{aligned} & \int_{S_n} (\hat{J}_x^h + \beta \cdot \nabla_\perp \hat{J}^h) (v + \delta(v_x + \beta \cdot \nabla_\perp v)) dx dx_\perp \\ & + \int_{S_n} \hat{\varepsilon} \nabla_\perp \hat{J}^h \cdot \nabla_\perp v dx dx_\perp + \int_{I_\perp} \hat{J}_+^{h,n} v_+^n dx_\perp \\ & = \int_{I_\perp} \hat{J}_-^{h,n} v_+^n dx_\perp, \quad \forall v \in \hat{\mathcal{V}}_n, \end{aligned} \quad (26)$$

where $v_\pm^n(x_\perp) = \lim_{\Delta x \rightarrow 0^+} v(x \pm \Delta x, x_\perp)$, $\hat{\varepsilon} = \max(\varepsilon, \mathcal{F}(Ch^\alpha \mathcal{R}(J^h))/M_n)$, with

$$\mathcal{R}(J^h) = |\hat{J}_x^h + \beta \cdot \nabla_\perp \hat{J}^h| + |[\hat{J}^h]|/hbar_n, \quad \text{on } S_n, \quad (27)$$

where $[v^n] = v_+^n - v_-^n$, $\mathcal{F}(v)$ is the elementwise average of v and Δ is a small parameter in general of order $\mathcal{O}(h)$ locally and $\alpha = 2 - \kappa$, κ small and positive. Here $h(x, x_\perp)$ is a continuous function measuring the local size of finite elements $\hat{K} \in \hat{\mathcal{T}}_n$. Further $M_n = \max_{x_\perp} |J_+^{h,n}(x_\perp)|$, is a normalization factor. Note that Eq. 26 is nonlinear in $\hat{J}^h|_{S_n}$ since $\hat{\varepsilon}$ depends on \hat{J}^h . By a fixed point argument using monotonicity, it is possible to show the existence of a solution to the Eq. 26. The streamline diffusion modification is given by $\delta(v_x + \beta \cdot \nabla_\perp v)$ and the degenerate-shock-capturing modification by $\hat{\varepsilon}$. Approximating β by piecewise constants on each slab, the streamline diffusion modification will disappear in the CSD-method.

We now make a special choice of the finite element subdivision $\hat{\mathcal{T}}_n = \{\hat{K}\}$ of S_n and the corresponding finite element space $\hat{\mathcal{V}}_n$ to obtain the CSD-method. Let $\hat{\mathcal{T}}_n = \{\hat{K}\}$ be a subdivision of S_n given by the prismatic elements oriented along characteristics

$$\hat{K}_n = \{(x, \bar{x}_\perp + (x - x_n)\beta) : \bar{x}_\perp \in K \in \mathcal{T}_n, x \in I_x^n\}, \quad (28)$$

where $\mathcal{T}_n = \{K\}$ is a triangulation of I_\perp given above. Further, let $\hat{\mathcal{V}}_n$ be defined by

$$\hat{\mathcal{V}}_n = \{\hat{v} \in \mathcal{C}(S_n) : \hat{v}(x, x_\perp) = v(x_\perp - (x - x_n)\beta), v \in \mathcal{V}_n\}, \quad (29)$$

with \mathcal{V}_n the space of continuous piecewise linear functions on \mathcal{T}_n as above. In other words $\hat{\mathcal{V}}_n$ consists of the continuous functions $\hat{v}(x, x_\perp)$ on S_n such that \hat{v} is constant along characteristics $x_\perp = \bar{x}_\perp + x\beta$ parallel to the sides of the prismatic elements \hat{K}_n and v_+^n is piecewise linear on \mathcal{T}_n for $x = x_n$. With this choice the SD-method 26 reduces to the following method since

$\frac{\partial \hat{v}}{\partial x} + \beta \cdot \nabla_{\perp} \hat{v} = 0$ if $\hat{v} \in \hat{\mathcal{V}}_n$: For $n = 1, 2, \dots, N$, find $\hat{J}^h \equiv \hat{J}^h|_{S_n} \in \hat{\mathcal{V}}_n$ such that

$$\int_{S_n} \hat{\varepsilon} \nabla_{\perp} \hat{J}^h \cdot \nabla_{\perp} v \, dx_{\perp} + \int_{I_{\perp}} \hat{J}_+^{h,n} v_+^n \, dx_{\perp} = \int_{I_{\perp}} \hat{J}_-^{h,n} v_+^n \, dx_{\perp}, \quad \forall v \in \hat{\mathcal{V}}_n, \quad (30)$$

where

$$\hat{\varepsilon} = \max \left(\varepsilon, \mathcal{F}(Ch^{\alpha} \frac{|\hat{J}^{h,n}|}{\hat{h}_n}) / M_n \right), \quad \text{on } S_n,$$

and $h(x, x_{\perp}) = h_n(x_{\perp} - (x - x_n)\beta)$, where $h_n(x_{\perp})$ gives the local element size of \mathcal{T}_n . If now ε is small, then Eq. 59 may be written as

$$\int_{I_{\perp}} \tilde{\varepsilon} \nabla_{\perp} \hat{J}_+^{h,n} \cdot \nabla_{\perp} v \, dx_{\perp} + \int_{I_{\perp}} \hat{J}_+^{h,n} v \, dx_{\perp} = \int_{I_{\perp}} \hat{J}_-^{h,n} v \, dx_{\perp}, \quad \forall v \in \mathcal{V}_n, \quad (31)$$

where $\tilde{\varepsilon} = \mathcal{F}(Ch^{\alpha} |\hat{J}^{h,n}|) / M_n$. Writing $\hat{J}_+^{h,n} = J^{h,n}$, we can thus state Eq.59 as follows (since $\hat{J}_-^{h,n} = T_n J^{h,n-1}$): For $n = 1, 2, \dots, N$, find $J^{h,n} \in \mathcal{V}_n$ such that

$$\int_{I_{\perp}} \tilde{\varepsilon} \nabla_{\perp} J^{h,n} \cdot \nabla_{\perp} v \, dx_{\perp} + \int_{I_{\perp}} J^{h,n} v \, dx_{\perp} = \int_{I_{\perp}} T_n J^{h,n-1} v \, dx_{\perp}, \quad \forall v \in \mathcal{V}_n, \quad (32)$$

where $J^{h,0} = f$ and $\tilde{\varepsilon} = \mathcal{F}(Ch_n^{\alpha} |J^{h,n} - T_n J^{h,n-1}|) / M_n$. Introducing the operator $\tilde{\mathcal{P}}_n : L_2(I_{\perp}) \cap L_{\infty}(I_{\perp}) \rightarrow \mathcal{V}_n$ defined by

$$(\tilde{\mathcal{P}}_n w, v) + (\tilde{\varepsilon} \nabla_{\perp} \tilde{\mathcal{P}}_n w, \nabla_{\perp} v) = (w, v), \quad \forall v \in \mathcal{V}_n, \quad (33)$$

where $\tilde{\varepsilon} = \mathcal{F}(Ch_n^{\alpha} |\tilde{\mathcal{P}}_n w - w|) / \max |\tilde{\mathcal{P}}_n w|$, and (\cdot, \cdot) denotes the $L_2(I_{\perp})^m$ inner product with $m = 1, 2$, we can write Eq. 61 as

$$J^{h,n} = \tilde{\mathcal{P}}_n T_n J^{h,n-1}. \quad (34)$$

Obviously, $\tilde{\mathcal{P}}_n$ may be viewed as a modification of the usual L_2 -projection $\mathcal{P}_n : L_2(I_{\perp}) \rightarrow \mathcal{V}_n$ defined above by $(\mathcal{P}_n w, v) = (w, v)$, $\forall v \in \mathcal{V}_n$, obtained by adding artificial viscosity with coefficient $\tilde{\varepsilon} = \mathcal{F}(Ch_n^{\alpha} |\tilde{\mathcal{P}}_n w - w|) / \max |\tilde{\mathcal{P}}_n w|$.

Note that the mesh size h_n of the triangulation \mathcal{T}_n may vary with x_{\perp} (and, evidently also, with n); it is reasonable to require that $|\nabla_{\perp} h_n(x_{\perp})| \leq c$, $x_{\perp} \in I_{\perp}$, where c is a sufficiently small constant and assume that $|K| \sim h_n(x_{\perp})$, if $x_{\perp} \in K \in \mathcal{T}_n$. For simplicity we assume in this note that \mathcal{T}_n is quasiuniform so that we may take h_n constant. The extensions to the general non-uniform mesh is straightforward.

Error estimates for smooth solutions

In this section we give the standard error estimates for the Characteristic Galerkin method (CG) 25 and the CSD-method 63, in the case of a smooth exact solution. In this case we may choose $\tilde{\varepsilon} = 0$ in 62 so that 25 and 63 indeed coincide. Our point is that using the CSD-approach we obtain sharper results than through the standard CG-approach, as we shall now see.

Starting with the standard error estimates for the CG-method we have for $J^n = J(x_n, \cdot)$ that

$$\begin{aligned} \|J^n - J^{h,n}\| &\leq \|T_n J^{n-1} - \mathcal{P}_n T_n J^{h,n-1}\| \\ &\leq \|T_n J^{n-1} - \mathcal{P}_n T_n J^{n-1}\| + \|\mathcal{P}_n T_n J^{n-1} - \mathcal{P}_n T_n J^{h,n-1}\| \\ &\leq Ch_n^2 \|J^{n-1}\|_{H^2(I_\perp)} + \|j^{n-1} - J^{h,n-1}\|, \end{aligned}$$

using a standard error estimate for \mathcal{P}_n of the form $\|w - \mathcal{P}_n w\| \leq Ch_n^2 \|w\|_{H^2(I_\perp)}$, the boundedness of $\mathcal{P}_n : L_2 \rightarrow L_2$ in the form $\|\mathcal{P}_n w\| \leq \|w\|$ and the fact that $\|T_n w\| = \|w\|$. By iteration we get

$$\|J^N - J^{h,N}\| \leq \sum_{n=1}^N Ch_n^2 \|J^{n-1}\|_{H^2(I_\perp)} = \mathcal{O}(Nh^2), \quad (35)$$

if $h_n \sim h$ for all n and J is smooth.

The standard error estimate [4] for the SD-method 26 with $\hat{\mathcal{V}}_n$ given by 58 and with $\hat{\varepsilon} = 0$ states that

$$\begin{aligned} \|J^N - J^{h,N}\| + \left(\sum_{n=1}^N \|J^{h,n} - T_n J^{h,n-1}\| \right)^{1/2} \\ \leq \left(\sum_{n=1}^N Ch_{n-1}^4 \|J^{n-1}\|_{H^2(I_\perp)} \right)^{1/2} \leq C\sqrt{N}h^2, \end{aligned} \quad (36)$$

if J is smooth, which is clearly sharper than 64. To prove the estimate 64 for 25 we note that with $e^{h,n} = J^{h,n} - J^n$, we have by 23 for $n = 1, 2, \dots, N$,

$$(e^{h,n} - T_n e^{h,n-1}, v) = 0, \quad \forall v \in \mathcal{V}_n. \quad (37)$$

Now since $\|T_n e^{h,n-1}\| = \|e^{h,n-1}\|$, we have

$$\begin{aligned} \frac{1}{2} \|e^{h,N}\|^2 + \frac{1}{2} \sum_{n=1}^N \|e^{h,n} - T_n e^{h,n-1}\|^2 \\ = \sum_{n=1}^N (e^{h,n} - T_n e^{h,n-1}, e^{h,n}) + \frac{1}{2} \|e^{h,0}\|^2 \\ = \sum_{n=1}^N (e^{h,n} - T_n e^{h,n-1}, J^n - \mathcal{P}_n J^n) \end{aligned} \quad (38)$$

$$\leq \frac{1}{4} \sum_{n=1}^N \|e^{h,n} - T_n e^{h,n-1}\|^2 + \sum_{n=1}^N \|J^n - \mathcal{P}_n J^n\|^2,$$

where we used Eq. 71 with $v = \mathcal{P}_n J^n - J^{h,n}$, the fact that $e^{h,0} = 0$, and Cauchy's inequality. Recalling now the above standard estimate for $\|\mathcal{P}_n J^n - J^{h,n}\|$, we obtain Eq. 68.

Note that the stability estimate 25 underlying 64 and 68, respectively, are as follows

$$\|J^{h,n}\| \leq \|f\|, \quad n = 1, 2, \dots, N, \quad (39)$$

$$\|J^{h,N}\| + \sum_{n=1}^N \|J^{h,n} - T_n J^{h,n-1}\|^2 = \|f\|^2, \quad (40)$$

where 73 reflects that $\|\mathcal{P}_n w\| \leq \|w\|$ and $\|T_n w\| = \|w\|$ for $w \in L_2(I_\perp)$, and Eq. 74 follows by choosing $v = J^{h,n}$ in 23 and noting as in 72 that

$$\begin{aligned} \frac{1}{2} \|J^{h,N}\|^2 &+ \frac{1}{2} \sum_{n=1}^N \|J^{h,n} - T_n J^{h,n-1}\|^2 \\ &= \sum_{n=1}^N (J^{h,n} - T_n J^{h,n-1}, J^{h,n}) + \frac{1}{2} \|f\|^2 = \frac{1}{2} \|f\|^2. \end{aligned}$$

The improvement using Eq. 74 indicates that the classical stability concept based on 73 is not fully adequate; to obtain sharp results it seems to be necessary, and also natural, to include dissipation terms in the stability estimates.

The estimate 68 is sharp as an estimate for $\|J^N - J^{h,N}\|$; for the discontinuous Galerkin method with piecewise linears, which corresponds to 25 with \mathcal{P}_n being the L_2 -projection onto the piecewise linears, in [4], we have shown that in general the error $\|J^N - J^{h,N}\|$ with $N = \mathcal{O}(h^{-1})$, $h = \mathcal{O}(h)$, is not better than $\mathcal{O}(h^{3/2})$ which corresponds to 68 with $N = \mathcal{O}(h^{-1})$.

To sum up, we get for Eq. 25 with the standard CG-approach, $\|J^N - J^{h,N}\| = \mathcal{O}(Nh^2)$, while the more careful analysis in the SD-approach gives $\|J^N - J^{h,N}\| = \mathcal{O}(\sqrt{N}h^2)$. With $N = \mathcal{O}(h^{-1})$, we thus have $\|J^N - J^{h,N}\| = \mathcal{O}(h)$ with the CG-approach and $\|J^N - J^{h,N}\| = \mathcal{O}(h^{3/2})$ with the SD-approach if the exact solution J is smooth.

Numerical Diffusion

We shall now seek quantitative estimates for the dissipation in 25, i.e., the CG-method or equivalently the CSD-method without the shock-capturing perturbation, and in the CSD-method 63 with shock-capturing.

For Eq. 25 using 74

$$\|J^{h,N}\|^2 + D_N = \|f\|^2, \quad (41)$$

where

$$D_N = \sum_{n=1}^N \|J^{h,n} - T_n J^{h,n-1}\|^2, \quad (42)$$

may be taken as a quantitative measure for the dissipation. Introducing $T_n \mathcal{V}_{n-1} = \{T_n v : v \in \mathcal{V}_{n-1}\}$, we have $T_n J^{h,n-1} \in T_n \mathcal{V}_{n-1}$ and to estimate D_N we are led to estimate $\|J^{h,n} - T_n J^{h,n-1}\| = \|(\mathcal{P}_n - I)w\|$ with $w = T_n J^{h,n-1} \in T_n \mathcal{V}_{n-1}$, i.e., the L_2 -error in the L_2 -projection of a piecewise linear function $T_n J^{h,n-1}$ on one mesh $T_n \mathcal{V}_{n-1}$ onto a set of piecewise linears \mathcal{V}_n on a different mesh. Obviously, by standard estimates we have for $w \in T_n \mathcal{V}_{n-1}$ the following first order estimate:

$$\|(\mathcal{P}_n - I)w\| \leq Ch_n \|w\|_{H^1(I_\perp)}, \quad (43)$$

with no standard second order counterpart since $w \notin H^2(I_\perp)$ if $w \in T_n \mathcal{V}_{n-1}$. However, there is in fact a second order analogue of 81 available which takes the form:

$$\|(\mathcal{P}_n - I)w\| \leq C(h_n^2 + h_{n-1}^2)^2 \|\Delta_{\perp,n-1} w\|, \quad (44)$$

where $\Delta_{\perp,n-1} : H^1(I_\perp) \rightarrow T_n \mathcal{V}_{n-1}$ is a discrete Laplacian defined by $-(\Delta_{\perp,n-1} \varphi, v) = (\nabla_\perp \varphi, \nabla_\perp v)$, $\forall v \in T_n \mathcal{V}_{n-1}$, see [4].

Inserting 83 into 79 we obtain assuming $h_n \leq h$,

$$D_N \leq C \sum_{n=1}^N \frac{h^4}{\tilde{h}_n} \|\Delta_{\perp,n-1} T_n J^{h,n-1}\|^2 \tilde{h}_n. \quad (45)$$

With $\tilde{h}_n = h$ the inequality 84 suggests that the dissipation in 25 corresponds to adding a diffusion term of the form $ch^3 \Delta_\perp^2 J$ to the continuous equation. In particular for smooth solution it appears that 25 adds little diffusion as compared to a first order upwind scheme with a corresponding continuous diffusion term of the form $Ch \Delta_\perp J$ with much larger diffusion coefficient. Thus, 25 does not appear to add excessive numerical diffusion unless of course we take \tilde{h}_n small compared to h_n , so that very many L_2 -projections of different meshes will be performed. On the other hand in some sense 25 contains too little numerical diffusion since oscillations may occur at discontinuities of the exact solution.

We now turn to the CSD-method 63 which obviously adds more numerical diffusion than the CG-method due to modification on ε -term. The stability estimate corresponding to 77 in this case takes the form

$$\|J^{h,N}\|^2 + \tilde{D}_N = \|f\|^2, \quad (46)$$

where

$$\tilde{D}_N = D_N + 2 \sum_{n=1}^N \int \tilde{\varepsilon} |\nabla_{\perp} J^{h,n}|^2 dx_{\perp}, \quad (47)$$

where $\tilde{\varepsilon} = \mathcal{F}(Ch_n^{\alpha} |J^{h,n} - T_n J^{h,n-1}|) / M_n$. It follows that the shock-capturing term in the CSD-method corresponds to adding a viscous term of the form $-div(\hat{\varepsilon} \nabla_{\perp} J)$ to the continuous equation with $\hat{\varepsilon} = \tilde{\varepsilon} / \tilde{h}_n$ in S_n . If the exact solution is smooth, we expect by 83 to have $\hat{\varepsilon} = \mathcal{O}(h^3)$ if $h_n \leq h$ and $\tilde{h}_n = h$, ($\alpha = 2$), i.e. the same amount of viscosity without the perturbation. However, close to discontinuity of J (assuming f is discontinuous) we may have $|J^{h,n} - T_n J^{h,n-1}| = \mathcal{O}(1)$ at least for n small, and then $\hat{\varepsilon} = \mathcal{O}(1)$, i.e., the shock-capturing term may add significant additional numerical diffusion in regions of nonsmoothness of the exact solution.

Stability in the Maximum norm

The stability, in the maximum norm, for the CSD-method being a particular SD-method reads as follows: For a given $L > 0$ there is a constant C such that if $J^{h,n}$, $n = 1, 2, \dots, N$ satisfies 61, then if $x_n \leq L$ we have

$$\|J^{h,n}\|_{\infty} \leq C \|f\|_{\infty}, \quad (48)$$

where $\|v\|_{\infty} = \sup_{x \in I_x} |v(x)|$. The estimate 89 may alternatively be expressed as follows

$$\|J^{h,n}\|_p \leq \|J^{h,n-1}\|_p, \quad \text{if } p \leq ch^{-\kappa/4}, \quad (49)$$

where $\kappa > 0$ appears in the definition of $\hat{\varepsilon}$ in 26, c is a sufficiently small constant, and $\|\cdot\|_p$ denotes the $L_p(I_{\perp})$ -norm:

$$\|v\|_p = \left(\int_{I_{\perp}} |v(x)|^p dx_{\perp} \right)^{1/p}, \quad p \geq 1. \quad (50)$$

More precisely, 89 follows from 90 by an inverse estimate letting $p \rightarrow \infty$. To prove 90 the essential step is to choose in 61, $v = \pi_n((J^h)^{p-1})$, where p is an even natural number $\pi_n : \mathcal{C}(I_{\perp}) \rightarrow \mathcal{V}_n$ is the standard nodal interpolation operator to get

$$\int_{I_{\perp}} (J^{h,n})^p dx_{\perp} + \int_{I_{\perp}} \tilde{\varepsilon} \nabla_{perp} J^{h,n} \cdot \nabla_{perp} (\pi_n((J^{h,n})^{p-1})) dx_{\perp} \quad (51)$$

$$= \int_{I_{\perp}} T_n J^{h,n-1} (J^{h,n})^{p-1} dx_{\perp} + E_n, \quad (52)$$

where

$$E_n = \int_{I_{\perp}} (J^{h,n} - T_n J^{h,n-1}) ((J^{h,n})^{p-1} - \pi_n((J^{h,n})^{p-1})) dx_{\perp}. \quad (53)$$

Now by standard interpolation error estimates

$$|E_n| \leq Cp^2 \int_{I_\perp} |J^{h,n} - T_n J^{h,n-1}| h_n^2 |\nabla_\perp J^{h,n}|^2 \|J^{h,n}\|_{\infty,K}^{p-3} dx_\perp, \quad (54)$$

where $\|v\|_{\infty,K} = \sup_{x_\perp \in K} |v(x_\perp)|$ on K . On the other hand, see [4], we have for some constant c independent of $p = 2m$, $m = 1, 2, \dots$, $n = 1, 2, \dots, N$,

$$\int_{I_\perp} \tilde{\varepsilon} \nabla_{perp} J^{h,n} \cdot \nabla_{perp} (\pi_n((J^{h,n})^{p-1})) dx_\perp \quad (55)$$

$$\geq \frac{c}{p^2} \int_{I_\perp} \tilde{\varepsilon} |\nabla_\perp J^{h,n}|^2 \|J^{h,n}\|_{\infty,K}^{p-2} dx_\perp. \quad (56)$$

For simplicity we now assume that $\tilde{\varepsilon}$ is defined slightly differently compared to the above, assuming now that $M_n = 1 + \|J^{h,n}\|_{\infty,K}$ on $K \in \mathcal{T}_n$, in which case $|E_n|$ is dominated by the right hand side of 93 so that recalling 91:

$$\int_{I_\perp} (J^{h,n})^p dx_\perp \leq \int_{I_\perp} T_n J^{h,n-1} (J^{h,n})^{p-1} dx_\perp, \quad \text{if } p \leq ch^{-\kappa/4}, \quad (57)$$

with c sufficiently small. Finally, 90 now follows by applying Hölder inequality to 94. Note that the proof of the crucial estimate 93 is carried out element by element and uses in an essential way that \mathcal{V}_n consists of piecewise linears.

We shall use the high accuracy and good stability features of the streamline diffusion Galerkin method, studied in [2], based on

- a) A phase-space discretization based on piecewise polynomial approximation with basis functions being continuous in x_\perp and discontinuous in x . (Discontinuity in all variables, corresponding to the a priori error estimates for the discontinuous Galerkin in [2], is a seemingly challenging a posteriori problem).
- 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 an artificial transport cross-section $\hat{\sigma}_{tr}$ is obtained modifying ε as

$$\hat{\varepsilon}(x, x_\perp) = \max \left(\varepsilon(x, y), c_1 h \mathcal{R}(J^h) / |\nabla_\perp J^h|, c_2 h (x, x_\perp)^{3/2} \right), \quad (58)$$

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 ε in 23 by σ . With a simplified form of the artificial transport cross-section as

$$\hat{\varepsilon} = \max(\varepsilon, c_1 h), \quad (59)$$

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

$$\|\hat{e}_h\|_Q \leq C^s C^i \|\hat{\varepsilon}^{-1} h^2 \mathcal{R}(J^h)\|_Q, \quad (60)$$

where $\hat{e}_h = \hat{J} - J^h$, with \hat{J} being the solution of 22 with ε replaced by $\hat{\varepsilon}$ and

$$e = J - J^h = (J - \hat{J}) + (\hat{J} - J^h) := \hat{e} + \hat{e}_h. \quad (61)$$

Note that $J - \hat{J}$ is a perturbation error caused by changing ε to $\hat{\varepsilon}$ in the continuous problem 22. Further C^s is a stability constant, C^i is an interpolation constant and $\|\cdot\|_Q$ is the $\|\cdot\|_{L_2(Q)}$ -norm. In the simplified case 25 the error estimate 26 takes the form

$$\|\hat{e}_h\|_Q \leq C^s C^i \|h \mathcal{R}(J^h)\|_Q. \quad (62)$$

The adaptive algorithm is based on 26 and seeks to find a mesh with as few degrees of freedom as possible such that for a given tolerance $TOL > 0$,

$$C^s C^i \|\hat{\varepsilon}^{-1} h^2 \mathcal{R}(J^h)\|_Q \leq TOL, \quad (63)$$

which, through 26, 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 $J = \hat{J}$, 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 (x, x_\perp) satisfying 60, typically a simple iterative procedure is used where a new mesh-size is computed by equidistribution 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 60 is as follows:

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

Below we specify the steps i)-iv). Recall that \hat{J} satisfies

$$\hat{J}_x + \beta \cdot \nabla_\perp \hat{J} - \hat{\varepsilon} \Delta_\perp \hat{J} = 0, \quad \text{in } Q, \quad (64)$$

$$\hat{J}(0, x_\perp) = f(x_\perp), \quad \text{for } x_\perp \in I_y \times I_z, \quad (65)$$

$$\hat{J}_z(x, y, \pm z_0) = 0, \quad \text{for } (x, y) \in [0, L] \times I_y, \quad (66)$$

$$\hat{J}(0, \pm y_0, z) = 0, \quad \text{for } z \in \Gamma_0^-, \quad (67)$$

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 Γ^0 is defined analogously, so that $\Gamma^0 = \{(x, y, \pm z_0)\} \cup \{(x, \pm y_0, 0)\}$.

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

$$J_x^h + \beta \cdot \nabla_{\perp} J^h - \hat{\varepsilon} \Delta_{\perp} J^h = \mathcal{R}, \quad \text{in } Q, \quad (68)$$

$$J^h(0, \cdot) = f_h, \quad \text{in } I_y \times I_z, \quad (69)$$

$$J^h = 0, \quad \text{on } \Gamma_0^-, \quad \text{and } \hat{J}_z^h = 0, \quad \text{on } \Gamma^0, \quad (70)$$

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

$$\int_Q \mathcal{R} v \, dx \, dx_{\perp} = 0, \quad \forall v \in \mathcal{V}_h. \quad (71)$$

We shall also use the following *semi-consistency* assumption:

$$\int_{\Gamma_s^-} J^h |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma = \int_{\Gamma_s^-} J |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma, \quad (72)$$

where $\Gamma_s^- := \Gamma^- \setminus \{x = 0\}$, is the *side-inflow boundary*. Observe that both in our continuous and discrete model problems 61 and 62, primarily, we may assume

$$J|_{\Gamma_s^-} = J^h|_{\Gamma_s^-} = 0, \quad (73)$$

however, there is no guarantee that “after-collision” particles would obey the same boundary condition as 68. Therefore, assumption 64 is to ensure that: in the approximation procedure the total inflow of particles is preserved.

In the sequel and to avoid multiple-indices, we shall refer to all approximated functions with alternate sub or super-index h . Subtracting 62 from 61 gives the following equation for the error $\hat{e}_h = \hat{J} - J^h$:

$$\mathcal{L}\hat{e}^h \equiv \hat{e}_x^h - \beta \cdot \nabla_{\perp} \hat{e}^h - \hat{\varepsilon} \Delta_{\perp} \hat{e}^h = -\mathcal{R}, \quad \text{in } Q, \quad (74)$$

$$\hat{e}^h(0, \cdot) = f - f_h, \quad \text{in } I_y \times I_z, \quad (75)$$

$$\hat{e}^h = 0, \quad \text{on } \Gamma_0^-, \quad \text{and } \hat{e}_z^h = 0, \quad \text{on } \Gamma^0. \quad (76)$$

We now introduce a dual for the non-degenerate problems 61 or 62 and 71 as

$$\mathcal{L}^* \psi = -\psi_x - \beta \cdot \nabla_{\perp} \psi - \hat{\varepsilon} \Delta_{\perp} \psi = \hat{e}^h, \quad \text{in } Q, \quad (77)$$

$$\psi = 0, \quad \text{on } \Gamma^+, \quad \text{and } \psi_z = 0, \quad \text{on } \Gamma^0. \quad (78)$$

Let us, for simplicity, start to consider the original Fermi case by replacing, in 61-62, $\beta \cdot \nabla_{\perp}$, Δ_{\perp} , and ψ by $z\partial_y$, ∂_{zz} , and φ , respectively. Then we have

the following version of the dual problem 72:

$$\mathcal{L}^* \varphi = -\varphi_x - z\varphi_y - \hat{\varepsilon}\varphi_{zz} = \hat{e}^h, \quad \text{in } Q, \quad (79)$$

$$\varphi = 0, \quad \text{on } \Gamma^+, \quad \text{and } \varphi_z = 0, \quad \text{on } \Gamma^0. \quad (80)$$

Recall that, in 73, $\hat{\varepsilon}$ is obtained from 13 by replacing ε by σ . We shall use $\hat{\varepsilon}$ for both degenerate and non-degenerate cases, the meaning would be obvious from the context. Using, 72, we get the following error representation formula:

$$\begin{aligned} \|\hat{e}^h\|^2 &= (\hat{e}^h, \mathcal{L}^* \varphi) = \int_Q \hat{e}^h (-\varphi_x - z\varphi_y - \varepsilon\varphi_{zz}) dx dx_\perp \\ &= (\mathcal{L}\hat{e}^h, \varphi) - \int_{I_y \times I_z} \hat{e}^h \varphi \Big|_{x=0}^{x=L} dy dz - \int_{I_x \times I_z} z \hat{e}^h \varphi \Big|_{y=-y_0}^{y=y_0} dx dz \\ &\quad - \int_{I_x \times I_y} \varepsilon \hat{e}^h \varphi_z \Big|_{z=-z_0}^{z=z_0} dx dy + \int_{I_x \times I_y} \varepsilon \hat{e}_z^h \varphi \Big|_{z=-z_0}^{z=z_0} dx dy := \sum_{i=1}^5 I_i. \end{aligned}$$

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

$$I_1 = (\mathcal{L}\hat{e}^h, \varphi) = - \int_Q \mathcal{R}\varphi dx dx_\perp. \quad (81)$$

The incidental boundary conditions give

$$\begin{aligned} I_2 &= - \int_{I_y \times I_z} \hat{e}^h(L, x_\perp) \varphi(L, x_\perp) dx_\perp + \int_{I_y \times I_z} \hat{e}^h(0, x_\perp) \varphi(0, x_\perp) dx_\perp \\ &= \int_{x=0} (f - f_h) \varphi dx_\perp, \end{aligned} \quad (82)$$

while the outflow boundary conditions, i.e., $\varphi = 0$, on Γ^+ imply that

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

where, \mathbf{n} is the outward unit normal defined at the boundary and, for the sake of generality, we have not used the assumption 64, yet. Thus

$$I_2 + I_3 = \int_{\Gamma^-} \hat{e}^h \varphi |\mathbf{n} \cdot \tilde{\beta}| d\Gamma. \quad (83)$$

Further since $\varphi_z = \hat{e}_z^h = 0$, for $z = \pm z_0$, we have $I_4 = I_5 \equiv 0$. Summing up we get

$$\|\hat{e}^h\|^2 = - \int_Q \mathcal{R}\varphi dx dx_\perp + \int_{\Gamma^-} \hat{e}^h \varphi |\mathbf{n} \cdot \tilde{\beta}| d\Gamma. \quad (84)$$

We use Galerkin orthogonality relation ?? and write

$$\int_Q \mathcal{R}\varphi \, dx \, dx_\perp = \int_Q \mathcal{R}(\varphi - \mathcal{P}_h\varphi) \, dx \, dx_\perp = \int_Q (\mathcal{R} - \mathcal{P}_h\mathcal{R})(\varphi - \mathcal{P}_h\varphi) \, dx \, dx_\perp, \quad (85)$$

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 79 as

$$\int_{\Gamma^-} \hat{e}^h \varphi |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma \leq \left(\int_{\Gamma^-} |\hat{e}^h|^2 |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma \right)^{1/2} \times \left(\int_{\Gamma^-} \varphi^2 |\mathbf{n} \cdot \tilde{\beta}| \, d\Gamma \right)^{1/2}. \quad (86)$$

Now using an interpolation error, with a symmetry assumption $\varphi_{yy} = \varphi_{zz}$ inherited from 64, of the form

$$\|\hat{e}h^{-2}(\varphi - \mathcal{P}_h\varphi)\|_Q \leq C^i \|\hat{e}\Delta_\perp\varphi\|_Q \approx C^i \|\hat{e}\varphi_{zz}\|_Q, \quad (87)$$

together with a strong stability estimate for the dual problem 73 of the form

$$\|\hat{e}\varphi_{zz}\|_Q \leq C^s \|\hat{e}^h\|_Q, \quad (88)$$

we get that

$$-\int_Q \mathcal{R}\varphi \, dx \, dx_\perp \leq C^s C^i \|\hat{e}h^{-2}(\mathcal{R} - \mathcal{P}_h\mathcal{R})\|_Q \|\hat{e}^h\|_Q. \quad (89)$$

To estimate the boundary integrals we recall the L_2 trace theorem

$$\|u^2\|_{L_2(\partial\Omega)} \leq C \|u\|_{L_2(\Omega)}^2 \|u\|_{W_2^1(\Omega)}^2, \quad (90)$$

and also the inverse estimate

$$\|v\|_{W_2^1(\Omega)}^2 \leq C \|h^{-1}v\|_{L_2(\Omega)}^2, \quad (91)$$

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 Ω has a Lipschitz boundary, see [3] or [4] for the details. So that applying 87-88 to φ and Q we get

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

where C depends on the trace theorem and inverse inequality constants. Recalling 13 we have that $\hat{e} > h^{3/2}$ and therefore $\hat{e}^{-1}h^3 \leq h^{3/2} \leq \hat{e}$. Hence

$$\|\hat{e}^{-1}h^3\varphi_{zz}\|_Q \leq \|\hat{e}^{-1}h^3\Delta_\perp\varphi\|_Q \approx \|\hat{e}\varphi_{zz}\|_Q \leq C^s \|\hat{e}^h\|_Q. \quad (92)$$

Thus

$$\int_{\Gamma^-} |\varphi|^2 |\mathbf{n} \cdot \beta| d\Gamma \leq C_T (C^s C^i)^2 \|e^h\|_Q^2. \quad (93)$$

At this moment we need to invoke 64, (note that if there is a feasible information on behavior of the secondary particles at the inflow boundary we would be able to continue without using ??), identifying 77 as

$$\int_{\Gamma^-} |e^h|^2 |\mathbf{n} \cdot \tilde{\beta}| d\Gamma = \int_{\{x=0\}} |f - f_h|^2 |\mathbf{n} \cdot \tilde{\beta}| d\Gamma. \quad (94)$$

Inserting 84, 89 and 90 in 79 we obtain

$$\|e^h\|_Q \leq C^s C^i \left[\|h^2 \varepsilon^{-1} (\mathcal{R} - \mathcal{P}_h \mathcal{R})\|_Q + \left(C_T \int_{\{x=0\}} |f - f_h|^2 |\mathbf{n} \cdot \tilde{\beta}| d\Gamma \right)^{1/2} \right]. \quad (95)$$

Thus we have estimated the error in terms of the residual and the incident boundary error and we have a complete control over all the involved constants (note that C_T being a theoretical constant is not effected by our approximation procedure). The estimate 91, which is an analogue of 26, is appropriate in the present contest with \mathcal{R} satisfying the Galerkin orthogonality relation 63 and f being a sufficiently smooth approximation for the product of incident δ functions at the boundary.

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2 Conclusion

- Remember that other instructions for paper preparation are given on the RGD21 *WEB* or *FTP* sites.
- The Scientific Organizing Committee (`rgd@cnrs-bellevue.fr`) will do its best to help you in case of difficulty.

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