

C7: An efficient 7D plasma kinetic code born to be coupled with multi-material ALE hydrodynamics

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Abstract

A submitted program is expected to be of benefit to other physicists or physical chemists, or be an exemplar of good programming practice, or illustrate new or novel programming techniques which are of importance to some branch of computational physics or physical chemistry.

Acceptable program descriptions can take different forms. The following Long Write-Up structure is a suggested structure but it is not obligatory. Actual structure will depend on the length of the program, the extent to which the algorithms or software have already been described in literature, and the detail provided in the user manual.

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Keywords: keyword1; keyword2; keyword3; etc.

PROGRAM SUMMARY

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Program Title:

*Licensing provisions(please choose one): CC0 1.0/CC By 4.0/MIT/Apache-2.0/BSD
3-clause/BSD 2-clause/GPLv3/GPLv2/LGPL/CC BY NC 3.0/MPL-2.0*

Programming language:

Supplementary material:

Journal reference of previous version:

Does the new version supersede the previous version?:

Reasons for the new version:

*Summary of revisions:**

Nature of problem(approx. 50-250 words):

Solution method(approx. 50-250 words):

Additional comments including Restrictions and Unusual features (approx. 50-250 words):

* Items marked with an asterisk are only required for new versions of programs previously published in the CPC Program Library.

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1. Introduction to Tensor Calculus

1.1. Transformation properties

The representation of a tensor in the Cartesian (reference) coordinate system is in the case of tensor of first rank

$$\mathbf{x} = \bar{x}^1 \mathbf{e}_1 + \bar{x}^2 \mathbf{e}_2 + \bar{x}^3 \mathbf{e}_3 = \bar{x}^i \mathbf{e}_i, \quad (1)$$

and in the case of tensor of second rank

$$\begin{aligned} \mathbf{uv} = \mathbf{A} &= \bar{A}^{11} \mathbf{e}_1 \mathbf{e}_1 + \bar{A}^{12} \mathbf{e}_1 \mathbf{e}_2 + \bar{A}^{13} \mathbf{e}_1 \mathbf{e}_3 \\ &\quad \bar{A}^{21} \mathbf{e}_2 \mathbf{e}_1 + \bar{A}^{22} \mathbf{e}_2 \mathbf{e}_2 + \bar{A}^{23} \mathbf{e}_2 \mathbf{e}_3 \\ &\quad \bar{A}^{31} \mathbf{e}_3 \mathbf{e}_1 + \bar{A}^{32} \mathbf{e}_3 \mathbf{e}_2 + \bar{A}^{33} \mathbf{e}_3 \mathbf{e}_3 = \bar{A}^{ij} \mathbf{e}_i \mathbf{e}_j = \bar{u}^i \mathbf{e}_i \bar{v}^j \mathbf{e}_j, \end{aligned} \quad (2)$$

where (1) defines the Cartesian coordinates (vector) \bar{x}^i of \mathbf{x} in orthonormal global basis $\mathbf{e}_1 = [1, 0, 0]$, $\mathbf{e}_2 = [0, 1, 0]$, $\mathbf{e}_3 = [0, 0, 1]$, and (2) shows the creation of second rank tensor \mathbf{A} as a outer (tensor) product of first rank tensors \mathbf{u} and \mathbf{v} , and consequently, its coordinates (matrix) $\bar{A}^{ij} = \bar{u}^i \bar{v}^j$.

While introducing a general curvilinear coordinates

$$\begin{aligned} q^i &= f^i(\bar{x}^1, \bar{x}^2, \bar{x}^3), \\ \bar{x}^i &= g^i(q^1, q^2, q^3), \\ q_i &= f_i(\bar{x}_1, \bar{x}_2, \bar{x}_3), \\ \bar{x}_i &= g_i(q_1, q_2, q_3), \end{aligned} \quad (3)$$

where the condition on the transformation Jacobian to be nonzero

$$J = \left| \frac{\partial \bar{x}^i}{\partial q^j} \right| \neq 0 \quad (4)$$

is sufficient to have a well defined curvilinear coordinate system. It is worth mentioning that two types of coordinates are used in definition (3), i.e. *covariant* q_i and *contravariant* q^i in the case of curvilinear coordinates, and also in the case of the Cartesian coordinates, where the equality $\bar{x}^i = \bar{x}_i$ holds. The transformation represented by (4) can be used to act on *covariant* tensor as

$$A_{\alpha\beta\dots\mu} = \frac{\partial \bar{x}^a}{\partial q^\alpha} \frac{\partial \bar{x}^b}{\partial q^\beta} \dots \frac{\partial \bar{x}^m}{\partial q^\mu} \bar{A}_{ab\dots m}, \quad (5)$$

and the corresponding inverse transformation can be used to act on *contravariant* tensor as

$$A^{\alpha\beta\dots\mu} = \frac{\partial q^\alpha}{\partial \bar{x}^a} \frac{\partial q^\beta}{\partial \bar{x}^b} \dots \frac{\partial q^\mu}{\partial \bar{x}^m} \bar{A}^{ab\dots m}, \quad (6)$$

and finally, in the case of a mixed tensor the transformation acts as

$$A_{\kappa\lambda\dots\nu}^{\alpha\beta\dots\mu} = \frac{\partial q^\alpha}{\partial \bar{x}^a} \frac{\partial q^\beta}{\partial \bar{x}^b} \dots \frac{\partial q^\mu}{\partial \bar{x}^m} \frac{\partial \bar{x}^k}{\partial q^\kappa} \frac{\partial \bar{x}^l}{\partial q^\lambda} \dots \frac{\partial \bar{x}^n}{\partial q^\nu} \bar{A}_{kl\dots n}^{ab\dots m}. \quad (7)$$

Equation (7) represents a general rule of transformation of tensor components $\bar{A}_{kl\dots n}^{ab\dots m}$ defined in the Cartesian coordinates to the tensor components $A_{\kappa\lambda\dots\nu}^{\alpha\beta\dots\mu}$ applying in curvilinear coordinates. Then, tensor \mathbf{A} treated in (7) can be expressed as

$$\begin{aligned} \mathbf{A} &= A_{\kappa\lambda\dots\nu}^{\alpha\beta\dots\mu} \mathbf{b}_\alpha \mathbf{b}_\beta \dots \mathbf{b}_\mu \mathbf{b}^\kappa \mathbf{b}^\lambda \dots \mathbf{b}^\nu = \bar{A}_{kl\dots n}^{ab\dots m} \mathbf{e}_a \mathbf{e}_b \dots \mathbf{e}_m \mathbf{e}^k \mathbf{e}^l \dots \mathbf{e}^n \\ &= \bar{A}^{ab\dots m\dots kl\dots n} \mathbf{e}_a \mathbf{e}_b \dots \mathbf{e}_m \mathbf{e}_k \mathbf{e}_l \dots \mathbf{e}_n, \end{aligned} \quad (8)$$

where \mathbf{b}_α and \mathbf{b}^κ are *covariant* and *contravariant* bases in curvilinear coordinates. The last equality in (8) applies only to the global Cartesian basis, because the *covariant* and *contravariant* tensor components and also the bases vectors are identical. The *contravariant* basis vectors are defined as locally normal to the isosurface created by other coordinates as

$$\mathbf{b}^i = \nabla q^i, \quad (9)$$

and the *covariant* basis vectors are defined as locally tangent to their associated coordinate path-line given by radius vector \mathbf{r} as

$$\mathbf{b}_i = \frac{\partial \mathbf{r}}{\partial q^i}, \quad (10)$$

and the following important equality holds

$$\mathbf{b}_i \cdot \mathbf{b}^j = \delta_i^j, \quad (11)$$

which stresses the property, that covariant and contravariant bases vectors are always aligned in direction.

The line element can be described in the Cartesian coordinates as

$$ds^2 = d\mathbf{r} \cdot d\mathbf{r} = (d\bar{x}^i \mathbf{e}_i) \cdot (d\bar{x}^j \mathbf{e}_j) = \mathbf{e}_i \cdot \mathbf{e}_j d\bar{x}^i d\bar{x}^j = d\bar{x}^i d\bar{x}^i, \quad (12)$$

where the last equality is due to the orthonormal Cartesian basis. The same line element can be described in the curvilinear coordinates as

$$ds^2 = d\mathbf{r} \cdot d\mathbf{r} = (dq^i \mathbf{b}_i) \cdot (dq^j \mathbf{b}_j) = \mathbf{b}_i \cdot \mathbf{b}_j dq^i dq^j, \quad (13)$$

More importantly, one can use (12), (6), and (12) to write

$$ds^2 = d\bar{x}^k d\bar{x}^k = \frac{\partial \bar{x}^k}{\partial q^i} dq^i \frac{\partial \bar{x}^k}{\partial q^j} dq^j = \mathbf{b}_i \cdot \mathbf{b}_j dq^i dq^j = g_{ij} dq^i dq^j, \quad (14)$$

which provides a fundamental definition of the metric tensor

$$g_{ij} = \frac{\partial \bar{x}^k}{\partial q^i} \frac{\partial \bar{x}^k}{\partial q^j} = \mathbf{b}_i \cdot \mathbf{b}_j. \quad (15)$$

Similarly to (13) one can find the definition of contravariant metric tensor

$$ds^2 = d\mathbf{r} \cdot d\mathbf{r} = (dq_i \mathbf{b}^i) \cdot (dq_j \mathbf{b}^j) = \mathbf{b}^i \cdot \mathbf{b}^j dq_i dq_j = g^{ij} dq_i dq_j, \quad (16)$$

It is quite easy to show based on (11), (15) and (16) that

$$g_{ij} g^{jk} = \delta_i^k, \quad (17)$$

which represents a practical way to express the contravariant metric tensor explicitly.

One of the most useful operations with the metric tensors is converting *contravariant* to *covariant* components and vice versa, i.e.

$$g_{ij} T^{kj}_{..ab} = T^k_{.iab}, \quad g^{ij} T^k_{.iab} = T^{kj}_{..ab}. \quad (18)$$

1.2. Tensor operations

General tensors obey simple algebraic rules. Thus if $\mathbf{B} = \alpha\mathbf{A}$ then $B_{kl\dots n}^{ab\dots m} = \alpha A_{kl\dots n}^{ab\dots m}$ and also if $\mathbf{C} = \mathbf{A} \pm \mathbf{B}$, $C_{kl\dots n}^{ab\dots m} = A_{kl\dots n}^{ab\dots m} \pm B_{kl\dots n}^{ab\dots m}$. Similarly $\mathbf{A} + \mathbf{B} = \mathbf{B} + \mathbf{A}$ and $\mathbf{A} + (\mathbf{B} + \mathbf{C}) = (\mathbf{A} + \mathbf{B}) + \mathbf{C}$.

The meaning of the *null tensor* $\mathbf{0}$, i.e. a tensor whose components are all zero in some coordinate system, is of a particular importance, because it represents a physical quantity, which is zero in every coordinate system, as can be seen from (7). Consequently, any tensor equation $\mathbf{A} = \mathbf{B}$, or component-wise $A_{kl\dots n}^{ab\dots m} = B_{kl\dots n}^{ab\dots m}$, is valid in any coordinate system, because $\mathbf{A} - \mathbf{B} = \mathbf{0}$, and for any two coordinate systems \bar{x}^i and q^i holds

$$\frac{\partial q^\alpha}{\partial \bar{x}^a} \frac{\partial q^\beta}{\partial \bar{x}^b} \cdots \frac{\partial q^\mu}{\partial \bar{x}^m} \frac{\partial \bar{x}^k}{\partial q^\kappa} \frac{\partial \bar{x}^l}{\partial q^\lambda} \cdots \frac{\partial \bar{x}^n}{\partial q^\nu} (\bar{A}_{kl\dots n}^{ab\dots m} - \bar{B}_{kl\dots n}^{ab\dots m}) = A_{\kappa\lambda\dots\nu}^{\alpha\beta\dots\mu} - B_{\kappa\lambda\dots\nu}^{\alpha\beta\dots\mu} = 0. \quad (19)$$

A special case of a tensor operation is the general formula of the scalar product of two vectors, which can be written based on (11) and (18) as

$$\mathbf{u} \cdot \mathbf{v} = (u^i \mathbf{b}_i) \cdot (v_j \mathbf{b}^j) = \mathbf{b}_i \cdot \mathbf{b}^j u^i v_j = u^j v_j = g^{ij} u_i v_j = g_{ij} u^i v^j = u_j v^j. \quad (20)$$

It is worth noting, that even though neither *contravariant* nor *covariant* components are in general real physical representation (have different units), the product of contra- with co-variant components provides physically correct units.

The general form of the cross product based on the *Levi-Civita tensor* is given by

$$\mathbf{u} \times \mathbf{v} = \mathbf{c} = c^i \mathbf{b}_i = \varepsilon^{ijk} \mathbf{b}_i \mathbf{b}_j \mathbf{b}_k \cdot u_n \mathbf{b}^n \cdot v_m \mathbf{b}^m = \varepsilon^{ijk} \mathbf{b}_i u_j v_k,$$

and further can be written the covariant and contravariant components as

$$c_i = g^{1/2} e_{ijk} u^j v^k = g^{1/2} (u_j v_k - u_k v_j), \quad (21)$$

$$c^i = g^{-1/2} e^{ijk} u_j v_k = \frac{u_j v_k - u_k v_j}{g^{1/2}}, \quad (22)$$

where the *cyclic permutation* (i.e. $i \rightarrow j \rightarrow k \rightarrow i$) is applied and the scaling $\varepsilon^{ijk} = g^{-1/2} e^{ijk}$ and $\varepsilon_{ijk} = g^{1/2} e_{ijk}$ with respect to curvilinear coordinates has been used.

Any tensor of rank two T^{ij} can be uniquely decomposed into a symmetric part and an antisymmetric part as $\mathbf{T} = \mathbf{S} + \mathbf{A}$, which are defined as

$$S^{ij} = \frac{1}{2} (T^{ij} + T^{ji}), \quad A^{ij} = \frac{1}{2} (T^{ij} - T^{ji}). \quad (23)$$

1.3. Covariant differentiation

In [1] a very important result (A3.70) is obtained

$$\frac{\partial^2 \bar{x}^\lambda}{\partial q^i \partial q^j} = \frac{\partial \bar{x}^\lambda}{\partial q^k} \left\{ \begin{matrix} k \\ ij \end{matrix} \right\} - \frac{\partial \bar{x}^\alpha}{\partial q^i} \frac{\partial \bar{x}^\beta}{\partial q^j} \left\{ \begin{matrix} \lambda \\ \alpha\beta \end{matrix} \right\}, \quad (24)$$

where $\left\{ \begin{matrix} i \\ jk \end{matrix} \right\}$ is the Christoffel symbol of second kind.

If we differentiate the *covariant* vector

$$u_i = \frac{\partial \bar{x}^\alpha}{\partial q^i} \bar{u}_\alpha,$$

we obtain

$$u_{i,j} = \frac{\partial u_i}{\partial q^j} = \frac{\partial \bar{x}^\alpha}{\partial q^i} \frac{\partial \bar{x}^\beta}{\partial q^j} \frac{\partial \bar{u}_\alpha}{\partial \bar{x}^\beta} + \frac{\partial^2 \bar{x}^\alpha}{\partial q^i \partial q^j} \bar{u}_\alpha = \bar{x}_{,i}^\alpha \bar{x}_{,j}^\beta \bar{u}_{\alpha,\beta} + \bar{x}_{,ij}^\alpha \bar{u}_\alpha, \quad (25)$$

which does not represent a tensor equation, because the differentiation in bar coordinate system $\bar{u}_{\alpha,\beta}$ does not transform properly to $u_{i,j}$ in curvilinear coordinate system. However, when multiplying (24) by a vector component in bar space, we obtain

$$\frac{\partial u_i}{\partial q^j} = \frac{\partial \bar{x}^\alpha}{\partial q^i} \frac{\partial \bar{x}^\beta}{\partial q^j} \frac{\partial \bar{u}_\alpha}{\partial \bar{x}^\beta} + \frac{\partial \bar{x}^\lambda}{\partial q^k} \left\{ \begin{matrix} k \\ ij \end{matrix} \right\} \bar{u}_\lambda - \frac{\partial \bar{x}^\alpha}{\partial q^i} \frac{\partial \bar{x}^\beta}{\partial q^j} \left\{ \begin{matrix} \lambda \\ \alpha\beta \end{matrix} \right\} \bar{u}_\lambda.$$

This can be finally rewritten as

$$u_{i;j} = \frac{\partial u_i}{\partial q^j} - \left\{ \begin{matrix} k \\ ij \end{matrix} \right\} u_k = \frac{\partial \bar{x}^\alpha}{\partial q^i} \frac{\partial \bar{x}^\beta}{\partial q^j} \left(\frac{\partial \bar{u}_\alpha}{\partial \bar{x}^\beta} - \left\{ \begin{matrix} \lambda \\ \alpha\beta \end{matrix} \right\} \bar{u}_\lambda \right), \quad (26)$$

which represents definition of *covariant differentiation* of vector $u_{i;j}$, which apparently obeys the tensor transformation.

The *covariant differentiation* of a general tensor reads

$$\begin{aligned} A_{kl\dots n;j}^{ab\dots m} &= \frac{\partial A_{kl\dots n}^{ab\dots m}}{\partial q^j} + \left\{ \begin{matrix} a \\ jd \end{matrix} \right\} A_{kl\dots n}^{db\dots m} + \left\{ \begin{matrix} b \\ jd \end{matrix} \right\} A_{kl\dots n}^{ad\dots m} + \dots + \left\{ \begin{matrix} m \\ jd \end{matrix} \right\} A_{kl\dots n}^{ab\dots d} \\ &\quad - \left\{ \begin{matrix} d \\ jk \end{matrix} \right\} A_{dl\dots n}^{ab\dots m} - \left\{ \begin{matrix} d \\ jl \end{matrix} \right\} A_{kd\dots n}^{ab\dots m} - \dots - \left\{ \begin{matrix} d \\ jn \end{matrix} \right\} A_{kl\dots d}^{ab\dots m}, \end{aligned} \quad (27)$$

where the notation above means the $\frac{ab\dots m}{kl\dots n}$ component of the differentiation of tensor \mathbf{A} along the covariant basis vector \mathbf{b}_j .

For the sake of applicability, some *covariant differentiation* explicit formulas of tensors of various ranks are presented

$$f_{;j} = (\nabla f)_j = f_{,j}, \quad (28)$$

$$u^a_{;j} = (\nabla u^a)_j = u^a_{,j} + \left\{ \begin{matrix} a \\ jk \end{matrix} \right\} u^k, \quad (29)$$

$$u_{a;j} = (\nabla u_a)_j = u_{a,j} - \left\{ \begin{matrix} k \\ ja \end{matrix} \right\} u_k, \quad (30)$$

$$A^{ab}_{;j} = (\nabla A^{ab})_j = A^{ab}_{,j} + \left\{ \begin{matrix} a \\ jk \end{matrix} \right\} A^{kb} + \left\{ \begin{matrix} b \\ jk \end{matrix} \right\} A^{ak}, \quad (31)$$

$$A_{ab;j} = (\nabla A_{ab})_j = A_{ab,j} - \left\{ \begin{matrix} k \\ ja \end{matrix} \right\} A_{kb} - \left\{ \begin{matrix} k \\ jb \end{matrix} \right\} A_{ak}, \quad (32)$$

$$A^a_{b;j} = (\nabla A^a_b)_j = A^a_{b,j} + \left\{ \begin{matrix} a \\ jk \end{matrix} \right\} A^k_b - \left\{ \begin{matrix} k \\ jb \end{matrix} \right\} A^a_k, \quad (33)$$

where f is a scalar function, \mathbf{u} is a vector field, and \mathbf{A} is a second rank tensor field.

1.4. General form of Gradient, Divergence, Laplace, and Curl

Covariant generalization of operations with the *del operator* ∇ can in most instances be obtained simply by replacing the partial derivatives in the Cartesian coordinate system with covariant derivatives.

Then, the gradient operator acting on a general tensor $\nabla \mathbf{A}$ can be expressed component-wise as

$$\nabla A^{ab\dots m}_{kl\dots n} = (\nabla A^{ab\dots m}_{kl\dots n})_j \mathbf{b}^j = A^{ab\dots m}_{kl\dots n;j} \mathbf{b}^j. \quad (34)$$

Consequently, the divergence operation on a vector field reads

$$\nabla \cdot \mathbf{v} = \nabla_i \mathbf{b}^i \cdot v^j \mathbf{b}_j = (\mathbf{b}^i \cdot \mathbf{b}_j) \nabla_i v^j = \delta^i_j \nabla_i v^j = \nabla_i v^i = v^i_{;i} = v^i_{,i} + \left\{ \begin{matrix} i \\ ij \end{matrix} \right\} v^j,$$

where the right hand side can be further simplified and the general form of divergence reads

$$\nabla \cdot \mathbf{v} = v^i_{;i} = \frac{(g^{1/2} v^i)_{,i}}{g^{1/2}}, \quad (35)$$

where g is the determinant of the metric tensor \mathbf{g} .

The tensor contraction due to the divergence operation on its second component reads

$$T_{ij}^{ij} = \frac{(g^{1/2} S^{ij})_{,j}}{g^{1/2}} + \left\{ \begin{matrix} i \\ jk \end{matrix} \right\} S^{jk} + \frac{(g^{1/2} A^{ij})_{,j}}{g^{1/2}}, \quad (36)$$

where the decomposition (23) has been used.

The Laplace operator in curvilinear coordinate system acts as

$$\nabla \cdot \nabla f = \nabla_j \mathbf{b}^j \cdot g^{ik} f_{,i} \mathbf{b}_k = \delta_k^j \nabla_j (g^{ik} f_{,i}) = \nabla_j (g^{ij} f_{,i}) = (g^{ij} f_{,i})_{,j},$$

where the contravariant representation $f^{,k} = g^{ik} f_{,i}$ of gradient of scalar function has been used. Then the general form of Laplace operator can be written as

$$\nabla \cdot \nabla f = \frac{(g^{1/2} g^{ij} f_{,i})_{,j}}{g^{1/2}}. \quad (37)$$

The contravariant generalization of the curl of vector can be obtained while using the Levi-Civita tensor and covariant derivative

$$(\nabla \times \mathbf{u})^i = g^{-1/2} e^{ijk} u_{k;j} = g^{-1/2} (u_{k;j} - u_{j;k}),$$

however, since the Christoffel symbols of second kind are symmetric in lower indices, the general form of curl can be written as

$$(\nabla \times \mathbf{u})^i = g^{-1/2} (u_{k,j} - u_{j,k}), \quad (38)$$

where (i, j, k) are distinct and are a cyclic permutation of $(1, 2, 3)$.

1.5. Spherical coordinates

Spherical coordinates, also called spherical polar coordinates (Walton 1967, Arfken 1985), are a system of curvilinear coordinates with local orthogonal basis that are natural for describing positions on a sphere or spheroid. Define θ to be the azimuthal angle in the xy -plane from the x -axis with $0 < \theta < 2\pi$, ϕ to be the polar angle from the positive z -axis with $0 < \phi < \pi$, and r to be distance (radius) from a point to the origin. This is the convention commonly used in mathematics.

Based on the curvilinear coordinates transformation (3)

$$r = \sqrt{x^2 + y^2 + z^2}, \quad \phi = \cos^{-1} \left(\frac{z}{\sqrt{x^2 + y^2 + z^2}} \right), \quad \theta = \tan^{-1} \left(\frac{y}{x} \right), \quad (39)$$

and its Cartesian inverse

$$x = r \cos(\theta) \sin(\phi), \quad y = r \sin(\theta) \sin(\phi), \quad z = r \cos(\phi), \quad (40)$$

we can write the spherical curvilinear transformation

$$\mathbf{T}_s = \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \phi} & \frac{\partial x}{\partial \theta} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \phi} & \frac{\partial y}{\partial \theta} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \phi} & \frac{\partial z}{\partial \theta} \end{bmatrix} = \begin{bmatrix} \cos(\theta) \sin(\phi) & r \cos(\theta) \cos(\phi) & -r \sin(\theta) \sin(\phi) \\ \sin(\theta) \sin(\phi) & r \sin(\theta) \cos(\phi) & r \cos(\theta) \sin(\phi) \\ \cos(\phi) & -r \sin(\phi) & 0 \end{bmatrix}, \quad (41)$$

which is well defined (4)

$$J = |\mathbf{T}_s| = r^2 \sin(\phi) = g_s^{1/2}. \quad (42)$$

Then according to (15) we can express the metric tensor (diagonal for orthogonal basis) as

$$\mathbf{g}_s = \begin{bmatrix} g_{rr} & 0 & 0 \\ 0 & g_{\phi\phi} & 0 \\ 0 & 0 & g_{\theta\theta} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2 \sin^2(\phi) \end{bmatrix}. \quad (43)$$

From (11) it is obvious, that in general contravariant basis vectors are aligned with covariant basis vectors, and are inverse in magnitude. It can be directly observed, that the covariant basis vectors are orthogonal from (15) and explicit formulation of the metric tensor (43), which further provides the information about the basis vectors length

$$|\mathbf{b}_r| = 1, \quad |\mathbf{b}_\phi| = r, \quad |\mathbf{b}_\theta| = r \sin(\phi),$$

and from (11) one can directly write

$$|\mathbf{b}^r| = 1, \quad |\mathbf{b}^\phi| = \frac{1}{r}, \quad |\mathbf{b}^\theta| = \frac{1}{r \sin(\phi)}.$$

It makes sense to define the scaling

$$h_r = 1, \quad h_\phi = r, \quad h_\theta = r \sin(\phi), \quad (44)$$

which comes to be handy when defining the relation between *physical*, *covariant*, and *contravariant* components as

$$\mathbf{u} = u^i \mathbf{b}_i = u_i \mathbf{b}^i = \sum_i u^i h_i \mathbf{e}_i = \sum_i \frac{u_i}{h_i} \mathbf{e}_i = u(i) \mathbf{e}_i, \quad (45)$$

where a unique basis vectors \mathbf{e}_i have been used, because they are identical for both covariant and contravariant bases, and they are also used as the basis for physical components $u(i)$. The explicit relations between physical, covariant, and contravariant components of vector in spherical coordinates are

$$\begin{aligned} u(r) &= u^r = u_r, \\ u(\phi) &= u^\phi r = \frac{u_\phi}{r}, \\ u(\theta) &= u^\theta r \sin(\phi) = \frac{u_\theta}{r \sin(\phi)}, \end{aligned} \quad (46)$$

The scalar product of two vectors \mathbf{u} and \mathbf{v} expressed in physical components $u(i), v(j)$ in spherical coordinates can be expressed based on (20) as

$$\mathbf{u} \cdot \mathbf{v} = u_i v^i = u(r)v(r) + u(\phi)v(\phi) + u(\theta)v(\theta). \quad (47)$$

The cross product of two vectors \mathbf{u} and \mathbf{v} expressed in physical components $u(i), v(j)$ in spherical coordinates can be expressed based on (22) and (45) as

$$\begin{aligned} \mathbf{u} \times \mathbf{v} &= \mathbf{c} = c^i \mathbf{b}_i = c^r \mathbf{b}_r + c^\phi \mathbf{b}_\phi + c^\theta \mathbf{b}_\theta \\ &= \frac{1}{r^2 \sin(\phi)} [(u_\phi v_\theta - u_\theta v_\phi) \mathbf{b}_r + (u_\theta v_r - u_r v_\theta) \mathbf{b}_\phi + (u_r v_\phi - u_\phi v_r) \mathbf{b}_\theta] \\ &= \frac{1}{r^2 \sin(\phi)} [(u_\phi v_\theta - u_\theta v_\phi) \mathbf{e}_r + (u_\theta v_r - u_r v_\theta) r \mathbf{e}_\phi + (u_r v_\phi - u_\phi v_r) r \sin(\phi) \mathbf{e}_\theta] \\ &= [u(\phi)v(\theta) - u(\theta)v(\phi)] \mathbf{e}_r + [u(\theta)v(r) - u(r)v(\theta)] \mathbf{e}_\phi + [u(r)v(\phi) - u(\phi)v(r)] \mathbf{e}_\theta. \end{aligned} \quad (48)$$

The gradient of a scalar function f in spherical coordinates based on (34) reads

$$\nabla f = f_{,i} \mathbf{b}^i = \frac{\partial f}{\partial r} \mathbf{e}_r + \frac{1}{r} \frac{\partial f}{\partial \phi} \mathbf{e}_\phi + \frac{1}{r \sin(\phi)} \frac{\partial f}{\partial \theta} \mathbf{e}_\theta. \quad (49)$$

The divergence of a vector field \mathbf{v} in spherical coordinates based on (35) reads

$$\begin{aligned} \nabla \cdot \mathbf{u} &= v^i_{;i} = \frac{(r^2 \sin(\phi) v^i)_{,i}}{r^2 \sin(\phi)} = \frac{\partial v^r}{\partial r} + \frac{\partial v^\phi}{\partial \phi} + \frac{\partial v^\theta}{\partial \theta} + \frac{2v^r}{r} + \cot(\phi) v^\phi \\ &= \frac{\partial v(r)}{\partial r} + \frac{\partial(v(\phi)/r)}{\partial \phi} + \frac{\partial(v(\theta)/r \sin(\phi))}{\partial \theta} + \frac{2v(r)}{r} + \cot(\phi) v(\phi)/r \\ &= \frac{1}{r^2} \frac{\partial(r^2 v(r))}{\partial r} + \frac{1}{r \sin(\phi)} \frac{\partial(\sin(\phi) v(\phi))}{\partial \phi} + \frac{1}{r \sin(\phi)} \frac{\partial v(\theta)}{\partial \theta}. \end{aligned} \quad (50)$$

In the case of Laplacian operator, we first need to find the contravariant representation of gradient, i.e.

$$\nabla f = f^{,j} \mathbf{b}_j = g^{ij} f_{,i} \mathbf{b}_j = \frac{\partial f}{\partial r} \mathbf{b}_r + \frac{1}{r^2} \frac{\partial f}{\partial \phi} \mathbf{b}_\phi + \frac{1}{r^2 \sin^2(\phi)} \frac{\partial f}{\partial \theta} \mathbf{b}_\theta,$$

then, the Laplace of a scalar f in spherical coordinates based on (37) reads

$$\begin{aligned} \nabla \cdot \nabla f &= (f^{,i})_{;i} = \frac{(r^2 \sin(\phi) f^{,i})_{,i}}{r^2 \sin(\phi)} \\ &= \frac{1}{r^2 \sin(\phi)} \left(\frac{\partial}{\partial r} (r^2 \sin(\phi) f_{,r}) + \frac{\partial}{\partial \phi} (\sin(\phi) f_{,\phi}) + \frac{\partial}{\partial \theta} \left(\frac{f_{,\theta}}{\sin(\phi)} \right) \right) \\ &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial f}{\partial r} \right) + \frac{1}{r^2 \sin(\phi)} \frac{\partial}{\partial \phi} \left(\sin(\phi) \frac{\partial f}{\partial \phi} \right) + \frac{1}{r^2 \sin^2(\phi)} \frac{\partial^2 f}{\partial \theta^2}. \quad (51) \end{aligned}$$

The physical components of curl applied on a vector field \mathbf{v} in spherical coordinates based on (38), i.e. $(\nabla \times \mathbf{u})^i = g^{-1/2} (u_{k,j} - u_{j,k})$, are

$$\begin{aligned} (\nabla \times \mathbf{v})(r) &= (\nabla \times \mathbf{v})^r = \frac{v_{\theta,\phi} - v_{\phi,\theta}}{r^2 \sin(\phi)} = \frac{1}{r \sin(\phi)} \left[\frac{\partial(\sin(\phi) v(\theta))}{\partial \phi} - \frac{\partial v(\phi)}{\partial \theta} \right], \\ (\nabla \times \mathbf{v})(\phi) &= (\nabla \times \mathbf{v})^\phi r = \frac{v_{r,\theta} - v_{\theta,r}}{r^2 \sin(\phi)} r = \frac{1}{r} \left[\frac{1}{\sin(\phi)} \frac{\partial v(r)}{\partial \theta} - \frac{\partial(rv(\theta))}{\partial r} \right], \\ (\nabla \times \mathbf{v})(\theta) &= (\nabla \times \mathbf{v})^\theta r \sin(\phi) = \frac{v_{\phi,r} - v_{r,\phi}}{r^2 \sin(\phi)} r \sin(\phi) = \frac{1}{r} \left[\frac{\partial(rv(\phi))}{\partial r} - \frac{\partial v(r)}{\partial \phi} \right], \end{aligned}$$

where one should be aware, that the coordinates follow the order (r, ϕ, θ) . Then, the curl applied on a vector field \mathbf{v} in spherical coordinates based on (38) reads

$$\begin{aligned} \nabla \times \mathbf{v} &= \frac{1}{r \sin(\phi)} \left[\frac{\partial(\sin(\phi) v(\theta))}{\partial \phi} - \frac{\partial v(\phi)}{\partial \theta} \right] \mathbf{e}_r \\ &+ \frac{1}{r} \left[\frac{1}{\sin(\phi)} \frac{\partial v(r)}{\partial \theta} - \frac{\partial(rv(\theta))}{\partial r} \right] \mathbf{e}_\phi + \frac{1}{r} \left[\frac{\partial(rv(\phi))}{\partial r} - \frac{\partial v(r)}{\partial \phi} \right] \mathbf{e}_\theta. \quad (52) \end{aligned}$$

1.6. Cylindrical coordinates

Cylindrical coordinates are a generalization of two-dimensional polar coordinates to three dimensions by superposing a height (z) axis. Unfortunately, there are a number of different notations used for the other two coordinates. Either r or ρ is used to refer to the radial coordinate and either ϕ

or θ to the azimuthal coordinates. Arfken (1985), for instance, uses (ρ, ϕ, z) , while Beyer (1987) uses (r, θ, z) . In this work, the notation (r, θ, z) is used.

Based on the curvilinear coordinates transformation (3)

$$r = \sqrt{x^2 + z^2}, \quad \theta = \tan^{-1} \left(\frac{y}{x} \right), \quad z = z, \quad (53)$$

and its Cartesian inverse

$$x = r \cos(\theta), \quad y = r \sin(\theta), \quad z = z, \quad (54)$$

we can write the cylindrical curvilinear transformation

$$\mathbf{T}_s = \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial z} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial z} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial z} \end{bmatrix} = \begin{bmatrix} \cos(\theta) & -r \sin(\theta) & 0 \\ \sin(\theta) & r \cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad (55)$$

which is well defined (4)

$$J = |\mathbf{T}_s| = r = g_c^{1/2}. \quad (56)$$

Then according to (15) we can express the metric tensor (diagonal for orthogonal basis) as

$$\mathbf{g}_s = \begin{bmatrix} g_{rr} & 0 & 0 \\ 0 & g_{\theta\theta} & 0 \\ 0 & 0 & g_{zz} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (57)$$

From (11) it is obvious, that in general contravariant basis vectors are aligned with covariant basis vectors, and are inverse in magnitude. It can be directly observed, that the covariant basis vectors are orthogonal from (15) and explicit formulation of the metric tensor (57), which further provides the information about the basis vectors length

$$|\mathbf{b}_r| = 1, \quad |\mathbf{b}_\theta| = r, \quad |\mathbf{b}_z| = 1,$$

and from (11) one can directly write

$$|\mathbf{b}^r| = 1, \quad |\mathbf{b}^\theta| = \frac{1}{r}, \quad |\mathbf{b}^z| = 1.$$

It makes sense to define the scaling

$$h_r = 1, \quad h_\theta = r, \quad h_z = 1, \quad (58)$$

which comes to be handy when defining the relation between *physical*, *covariant*, and *contravariant* components as

$$\mathbf{u} = u^i \mathbf{b}_i = u_i \mathbf{b}^i = \sum_i u^i h_i \mathbf{e}_i = \sum_i \frac{u_i}{h_i} \mathbf{e}_i = u(i) \mathbf{e}_i, \quad (59)$$

where a unique basis vectors \mathbf{e}_i have been used, because they are identical for both covariant and contravariant bases, and they are also used as the basis for physical components $u(i)$. The explicit relations between physical, covariant, and contravariant components of vector in cylindrical coordinates are

$$\begin{aligned} u(r) &= u^r = u_r, \\ u(\theta) &= u^\theta r = \frac{u_\theta}{r}, \\ u(z) &= u^z = u_z, \end{aligned} \quad (60)$$

The scalar product of two vectors \mathbf{u} and \mathbf{v} expressed in physical components $u(i), v(j)$ in cylindrical coordinates can be expressed based on (20) as

$$\mathbf{u} \cdot \mathbf{v} = u_i v^i = u(r)v(r) + u(\theta)v(\theta) + u(z)v(z). \quad (61)$$

The cross product of two vectors \mathbf{u} and \mathbf{v} expressed in physical components $u(i), v(j)$ in cylindrical coordinates can be expressed based on (22) and (59) as

$$\begin{aligned} \mathbf{u} \times \mathbf{v} &= \mathbf{c} = c^r \mathbf{b}_r + c^\theta \mathbf{b}_\theta + c^z \mathbf{b}_z \\ &= \frac{1}{r} [(u_\theta v_z - u_z v_\theta) \mathbf{b}_r + (u_z v_r - u_r v_z) \mathbf{b}_\theta + (u_r v_\theta - u_\theta v_r) \mathbf{b}_z] \\ &= \frac{1}{r} [(u_\theta v_z - u_z v_\theta) \mathbf{e}_r + (u_z v_r - u_r v_z) r \mathbf{e}_\theta + (u_r v_\theta - u_\theta v_r) \mathbf{e}_z] \\ &= [u(\theta)v(z) - u(z)v(\theta)] \mathbf{e}_r + [u(z)v(r) - u(r)v(z)] \mathbf{e}_\theta + [u(r)v(\theta) - u(\theta)v(r)] \mathbf{e}_z. \end{aligned} \quad (62)$$

The gradient of a scalar function f in cylindrical coordinates based on (34) reads

$$\nabla f = f_{,i} \mathbf{b}^i = \frac{\partial f}{\partial r} \mathbf{e}_r + \frac{1}{r} \frac{\partial f}{\partial \theta} \mathbf{e}_\theta + \frac{\partial f}{\partial z} \mathbf{e}_z. \quad (63)$$

The divergence of a vector field \mathbf{v} in cylindrical coordinates based on (35)

$$\begin{aligned} \nabla \cdot \mathbf{u} &= v^i_{;i} = \frac{(rv^i)_{,i}}{r} = \frac{\partial v^r}{\partial r} + \frac{\partial v^\theta}{\partial \theta} + \frac{\partial v^z}{\partial z} + \frac{v^r}{r} \\ &= \frac{1}{r} \frac{\partial(rv(r))}{\partial r} + \frac{1}{r} \frac{\partial v(\theta)}{\partial \theta} + \frac{\partial v(z)}{\partial z}. \end{aligned} \quad (64)$$

In the case of Laplacian operator, we first need to find the contravariant representation of gradient, i.e.

$$\nabla f = f^i \mathbf{b}_i = g^{ij} f_{,j} \mathbf{b}_i = \frac{\partial f}{\partial r} \mathbf{b}_r + \frac{1}{r^2} \frac{\partial f}{\partial \theta} \mathbf{b}_\theta + \frac{\partial f}{\partial z} \mathbf{b}_z,$$

then, the Laplace of a scalar f in cylindrical coordinates based on (37) reads

$$\begin{aligned} \nabla \cdot \nabla f &= (f^i)_{,i} = \frac{(rf^i)_{,i}}{r} = \frac{1}{r} \left(\frac{\partial}{\partial r} (rf_{,r}) + \frac{\partial}{\partial \theta} \left(\frac{f_{,\theta}}{r} \right) + \frac{\partial}{\partial z} f_{,z} \right) \\ &= \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial f}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\partial^2 f}{\partial z^2} = \frac{\partial^2 f}{\partial r^2} + \frac{1}{r^2} \frac{\partial^2 f}{\partial \theta^2} + \frac{\partial^2 f}{\partial z^2} + \frac{1}{r} \frac{\partial f}{\partial r}. \end{aligned} \quad (65)$$

The physical components of curl applied on a vector field \mathbf{v} in cylindrical coordinates based on (38), i.e. $(\nabla \times \mathbf{u})^i = g^{-1/2}(u_{k,j} - u_{j,k})$, are

$$\begin{aligned} (\nabla \times \mathbf{v})(r) &= (\nabla \times \mathbf{v})^r = \frac{v_{z,\theta} - v_{\theta,z}}{r} = \frac{1}{r} \frac{\partial v(z)}{\partial \theta} - \frac{\partial v(\theta)}{\partial z}, \\ (\nabla \times \mathbf{v})(\theta) &= (\nabla \times \mathbf{v})^\theta r = \frac{v_{r,z} - v_{z,r}}{r} r = \frac{\partial v(r)}{\partial z} - \frac{\partial v(z)}{\partial r}, \\ (\nabla \times \mathbf{v})(z) &= (\nabla \times \mathbf{v})^z = \frac{v_{\theta,r} - v_{r,\theta}}{r} = \frac{1}{r} \left[\frac{\partial(rv(\theta))}{\partial r} - \frac{\partial v(r)}{\partial \theta} \right], \end{aligned}$$

where one should be aware, that the coordinates follow the order (r, θ, z) . Then, the curl applied on a vector field \mathbf{v} in cylindrical coordinates based on (38) reads

$$\nabla \times \mathbf{v} = \left[\frac{1}{r} \frac{\partial v(z)}{\partial \theta} - \frac{\partial v(\theta)}{\partial z} \right] \mathbf{e}_r + \left[\frac{\partial v(r)}{\partial z} - \frac{\partial v(z)}{\partial r} \right] \mathbf{e}_\theta + \frac{1}{r} \left[\frac{\partial(rv(\theta))}{\partial r} - \frac{\partial v(r)}{\partial \theta} \right] \mathbf{e}_z. \quad (66)$$

2. Diffusive regime

The equilibrium (maximized entropy) distribution

$$f_M = \frac{\rho}{v_{th}^3 (2\pi)^{3/2}} \exp \left(-\frac{v^2}{2v_{th}^2} \right), \quad (67)$$

where $v_{th} = \sqrt{k_B T / m_e}$.

$$\begin{aligned}\frac{\partial f_M}{\partial v} &= -\frac{v}{v_{th}^2} f_M, \\ \frac{\partial f_M}{\partial \rho} &= \frac{1}{\rho} f_M, \\ \frac{\partial f_M}{\partial T} &= \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} \right) \frac{1}{T} f_M.\end{aligned}$$

2.1. Lorentz approximation

$$\mathbf{v} \cdot \nabla_{\mathbf{x}} f + \frac{q_e}{m_e} \left(\mathbf{E} + \frac{1}{c} \mathbf{v} \times \mathbf{B} \right) \cdot \nabla_{\mathbf{v}} f = C_e(f) + \frac{\rho \sigma_{ei}}{2} \nabla_{\mathbf{v}} \cdot \left[\frac{1}{v} \left(\delta - \frac{\mathbf{v} \mathbf{v}}{v^2} \right) \cdot \nabla_{\mathbf{v}} f \right], \quad (68)$$

$$C_{ei}(f, f_i) = \frac{\rho \sigma}{2} \nabla_{\mathbf{v}} \cdot \left[\frac{1}{v} \left(\delta - \frac{\mathbf{v} \mathbf{v}}{v^2} \right) \cdot \nabla_{\mathbf{v}} f \right], \quad (69)$$

$$\mathbf{v} = v \mathbf{n} = v \mathbf{b}^v = v \mathbf{b}_v, \quad (70)$$

$$\delta = \delta_j^i \mathbf{b}_i \mathbf{b}^j, \quad (71)$$

$$\nabla_{\mathbf{v}} f = f^{,j} \mathbf{b}_j = g^{ij} f_{,i} \mathbf{b}_j = \frac{\partial f}{\partial v} \mathbf{b}_v + \frac{1}{v^2} \frac{\partial f}{\partial \phi} \mathbf{b}_\phi + \frac{1}{v^2 \sin^2(\phi)} \frac{\partial f}{\partial \theta} \mathbf{b}_\theta = u^j \mathbf{b}_j = \mathbf{u},$$

$$\delta \cdot \mathbf{u} = \delta_j^i \mathbf{b}_i \mathbf{b}^j \cdot u^k \mathbf{b}_k = \delta_j^i \mathbf{b}_i \delta_k^j u^k = \delta_k^i \mathbf{b}_i u^k = u^k \mathbf{b}_k = \mathbf{u},$$

$$\begin{aligned}\left(\delta - \frac{\mathbf{v} \mathbf{v}}{v^2} \right) \cdot \nabla_{\mathbf{v}} f &= \frac{\partial f}{\partial v} \mathbf{b}_v + \frac{1}{v^2} \frac{\partial f}{\partial \phi} \mathbf{b}_\phi + \frac{1}{v^2 \sin^2(\phi)} \frac{\partial f}{\partial \theta} \mathbf{b}_\theta \\ &\quad - \mathbf{b}_v \mathbf{b}^v \cdot \left[\frac{\partial f}{\partial v} \mathbf{b}_v + \frac{1}{v^2} \frac{\partial f}{\partial \phi} \mathbf{b}_\phi + \frac{1}{v^2 \sin^2(\phi)} \frac{\partial f}{\partial \theta} \mathbf{b}_\theta \right] \\ &= \frac{\partial f}{\partial v} \mathbf{b}_v + \frac{1}{v^2} \frac{\partial f}{\partial \phi} \mathbf{b}_\phi + \frac{1}{v^2 \sin^2(\phi)} \frac{\partial f}{\partial \theta} \mathbf{b}_\theta - \frac{\partial f}{\partial v} \mathbf{b}_v \\ &= \frac{1}{v^2} \frac{\partial f}{\partial \phi} \mathbf{b}_\phi + \frac{1}{v^2 \sin^2(\phi)} \frac{\partial f}{\partial \theta} \mathbf{b}_\theta = u^i \mathbf{b}_i, \quad (72)\end{aligned}$$

$$\begin{aligned}
C_{ei}(f, f_i) &= \frac{\sigma\rho}{2} \left(\frac{1}{v} u^i \right)_{,i} = \frac{\sigma\rho}{2} \frac{(g^{1/2} \frac{1}{v} u^i)_{,i}}{g^{1/2}} = \frac{\sigma\rho}{2} \frac{(v \sin(\phi) u^i)_{,i}}{v^2 \sin(\phi)} \\
&= \frac{\sigma\rho}{2} \frac{1}{v^2 \sin(\phi)} \left[\frac{\partial}{\partial\phi} \left(\frac{\sin(\phi)}{v} \frac{\partial f}{\partial\phi} \right) + \frac{\partial}{\partial\theta} \left(\frac{1}{v \sin(\phi)} \frac{\partial f}{\partial\theta} \right) \right] \\
&= \frac{\sigma\rho}{2v^3} \frac{1}{\sin(\phi)} \left[\frac{\partial}{\partial\phi} \left(\sin(\phi) \frac{\partial f}{\partial\phi} \right) + \frac{1}{\sin(\phi)} \frac{\partial^2 f}{\partial\theta^2} \right] \tag{73}
\end{aligned}$$

$$\frac{df}{d\phi} = \frac{\partial f}{\partial \cos(\phi)} \frac{\partial \cos \phi}{\partial \phi} = -\frac{\partial f}{\partial \cos(\phi)} \sin(\phi) \tag{74}$$

$$C_{ei}(f, f_i) = \frac{\sigma\rho}{2v^3} \left(\frac{\partial}{\partial\mu} \left((1 - \mu^2) \frac{\partial f}{\partial\mu} \right) + \frac{1}{\sin^2(\phi)} \frac{\partial^2 f}{\partial\theta^2} \right) \tag{75}$$

where $\mu = \cos(\phi)$

First, the electro-magnetic scaling

$$\tilde{\mathbf{E}} = \frac{q_e}{m_e} \mathbf{E}, \quad \tilde{\mathbf{B}} = \frac{q_e}{m_e c} \mathbf{B}, \tag{76}$$

is defined in order to make the algebraic operations easier to follow.

$$\begin{aligned}
v\mathbf{n} \cdot \nabla f &= -\left(\tilde{\mathbf{E}} + v\mathbf{n} \times \tilde{\mathbf{B}}\right) \cdot \left[\frac{\partial f}{\partial v}\mathbf{n} + \frac{1}{v}\frac{\partial f}{\partial \phi}\mathbf{e}_\phi + \frac{1}{v\sin(\phi)}\frac{\partial f}{\partial \theta}\mathbf{e}_\theta\right] \\
&+ C_e(f) + \frac{\nu_{ei}}{2} \left(\frac{\partial}{\partial \mu} \left((1-\mu^2)\frac{\partial f}{\partial \mu}\right) + \frac{1}{\sin^2(\phi)}\frac{\partial^2 f}{\partial \theta^2}\right) \\
&= -\left(\left[\left(\tilde{\mathbf{E}} \cdot \mathbf{n}\right)\mathbf{n} + \left(\tilde{\mathbf{E}} \cdot \mathbf{e}_\phi\right)\mathbf{e}_\phi + \left(\tilde{\mathbf{E}} \cdot \mathbf{e}_\theta\right)\mathbf{e}_\theta\right]\right. \\
&+ v\mathbf{n} \times \left[\left(\tilde{\mathbf{B}} \cdot \mathbf{n}\right)\mathbf{n} + \left(\tilde{\mathbf{B}} \cdot \mathbf{e}_\phi\right)\mathbf{e}_\phi + \left(\tilde{\mathbf{B}} \cdot \mathbf{e}_\theta\right)\mathbf{e}_\theta\right] \cdot \\
&\quad \left[\frac{\partial f}{\partial v}\mathbf{n} + \frac{1}{v}\frac{\partial f}{\partial \phi}\mathbf{e}_\phi + \frac{1}{v\sin(\phi)}\frac{\partial f}{\partial \theta}\mathbf{e}_\theta\right] \\
&+ C_e(f) + \frac{\nu_{ei}}{2} \left(\frac{\partial}{\partial \mu} \left((1-\mu^2)\frac{\partial f}{\partial \mu}\right) + \frac{1}{\sin^2(\phi)}\frac{\partial^2 f}{\partial \theta^2}\right) \\
&= -\left(\left[\tilde{E}(v)\mathbf{n} + \tilde{E}(\phi)\mathbf{e}_\phi + \tilde{E}(\theta)\mathbf{e}_\theta\right] + v\left[\tilde{B}(\phi)\mathbf{e}_\theta - \tilde{B}(\theta)\mathbf{e}_\phi\right]\right) \cdot \\
&\quad \left[\frac{\partial f}{\partial v}\mathbf{n} + \frac{1}{v}\frac{\partial f}{\partial \phi}\mathbf{e}_\phi + \frac{1}{v\sin(\phi)}\frac{\partial f}{\partial \theta}\mathbf{e}_\theta\right] \\
&+ C_e(f) + \frac{\nu_{ei}}{2} \left(\frac{\partial}{\partial \mu} \left((1-\mu^2)\frac{\partial f}{\partial \mu}\right) + \frac{1}{\sin^2(\phi)}\frac{\partial^2 f}{\partial \theta^2}\right) \\
&= -\left(\left[\tilde{E}(v)\frac{\partial f}{\partial v} + \frac{\tilde{E}(\phi)}{v}\frac{\partial f}{\partial \phi} + \frac{\tilde{E}(\theta)}{v\sin(\phi)}\frac{\partial f}{\partial \theta}\right]\right. \\
&+ v\left[\frac{\tilde{B}(\phi)}{v\sin(\phi)}\frac{\partial f}{\partial \theta} - \frac{\tilde{B}(\theta)}{v}\frac{\partial f}{\partial \phi}\right] \Bigg) \\
&+ C_e(f) + \frac{\nu_{ei}}{2} \left(\frac{\partial}{\partial \mu} \left((1-\mu^2)\frac{\partial f}{\partial \mu}\right) + \frac{1}{\sin^2(\phi)}\frac{\partial^2 f}{\partial \theta^2}\right) \tag{77}
\end{aligned}$$

$$\begin{aligned}
v \cdot \nabla f + \tilde{\mathbf{E}} \cdot \mathbf{n} \frac{\partial f}{\partial v} + \frac{\tilde{\mathbf{E}} \cdot \mathbf{e}_\phi - v\tilde{\mathbf{B}} \cdot \mathbf{e}_\theta}{v} \frac{\partial f}{\partial \phi} + \frac{\tilde{\mathbf{E}} \cdot \mathbf{e}_\theta + v\tilde{\mathbf{B}} \cdot \mathbf{e}_\phi}{v\sin(\phi)} \frac{\partial f}{\partial \theta} = \\
C_e(f) + \frac{\nu_{ei}}{2} \left(\frac{\partial}{\partial \mu} \left((1-\mu^2)\frac{\partial f}{\partial \mu}\right) + \frac{1}{\sin^2(\phi)}\frac{\partial^2 f}{\partial \theta^2}\right), \tag{78}
\end{aligned}$$

2.1.1. BGK collision operator

The BGK electron transport equation in 6D reads

$$\mathbf{n} \cdot \nabla f + \frac{1}{v} \left[\tilde{\mathbf{E}} \cdot \mathbf{n} \frac{\partial f}{\partial v} + \frac{\tilde{\mathbf{E}} \cdot \mathbf{e}_\phi - v \tilde{\mathbf{B}} \cdot \mathbf{e}_\theta}{v} \frac{\partial f}{\partial \phi} + \frac{\tilde{\mathbf{E}} \cdot \mathbf{e}_\theta + v \tilde{\mathbf{B}} \cdot \mathbf{e}_\phi}{v \sin(\phi)} \frac{\partial f}{\partial \theta} \right] = \frac{(f_M - f)}{\lambda_e} + \frac{1}{2\lambda_{ei}} \left(\frac{\partial}{\partial \mu} \left((1 - \mu^2) \frac{\partial f}{\partial \mu} \right) + \frac{1}{\sin^2(\phi)} \frac{\partial^2 f}{\partial \theta^2} \right), \quad (79)$$

where $\mu = \cos(\phi)$, λ_e is the electron-electron mean free path, and λ_{ei} is the electron-ion mean free path. We also approximate $\lambda_e = \bar{Z}\lambda_{ei}$.

We can try to find an approximate solution while using the first term of expansion in λ_e and $muas$

$$\tilde{f}(z, v, \mu) = f^0(z, v) + f^1(z, v)\lambda_{ei}\mu. \quad (80)$$

Clearly, $\frac{\partial \tilde{f}}{\partial \theta} = 0$, and if $\tilde{\mathbf{B}} = \tilde{B}_z \mathbf{e}_z$, there is no effect of magnetic field. We also assume, that $\nabla f = \frac{\partial f}{\partial z} \mathbf{e}_z$ and appropriately $\tilde{\mathbf{E}} = \tilde{E}_z \mathbf{e}_z$. From the orientation of the Cartesian basis vectors and spherical basis vectors, one can find $\tilde{\mathbf{E}} \cdot \mathbf{n} = \tilde{E}_z \cos(\phi) = \mu$ and $\tilde{\mathbf{E}} \cdot \mathbf{e}_\phi = -\tilde{E}_z \sin(\phi)$. As a result, the analyzed BGK equation reads

$$\mu \frac{\partial}{\partial z} (f^0 + f^1 \lambda_{ei} \mu) + \frac{1}{v} \left[\tilde{E}_z \mu \frac{\partial}{\partial v} (f^0 + f^1 \lambda_{ei} \mu) - \frac{\tilde{E}_z \sin(\phi)}{v} \frac{\partial}{\partial \phi} (f^0 + f^1 \lambda_{ei} \mu) \right] = \frac{(f_M - (f^0 + f^1 \lambda_{ei} \mu))}{\lambda_e} + \frac{1}{2\lambda_{ei}} \frac{\partial}{\partial \mu} \left((1 - \mu^2) \frac{\partial}{\partial \mu} (f^0 + f^1 \lambda_{ei} \mu) \right), \quad (81)$$

$$\mu \frac{\partial f^0}{\partial z} + \mu^2 \frac{\partial}{\partial z} (f^1 \lambda_{ei}) + \frac{\tilde{E}_z}{v} \left[\mu \frac{\partial f^0}{\partial v} + \mu^2 \frac{\partial}{\partial v} (f^1 \lambda_{ei}) + \frac{1 - \mu^2}{v} f^1 \lambda_{ei} \right] = \frac{f_M - f^0}{\bar{Z}\lambda_{ei}} - \mu \frac{1}{\bar{Z}} f^1 - \mu f^1, \quad (82)$$

consequently, we have the following anisotropy expansion $\mu^0, \mu^1, \mu^2, \dots$ equa-

tions

$$\begin{aligned}\frac{f_M - f^0}{\bar{Z}\lambda_{ei}} &= \frac{1}{v}f^1\lambda_{ei}, \\ \frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v}\frac{\partial f^0}{\partial v} &= -\frac{1}{\bar{Z}}f^1 - f^1, \\ \frac{\partial}{\partial z}(f^1\lambda_{ei}) + \frac{\tilde{E}_z}{v}\left[\frac{\partial}{\partial v}(f^1\lambda_{ei}) - \frac{1}{v}f^1\lambda_{ei}\right] &= 0,\end{aligned}$$

which lead to the definitions

$$f^0 = f_M + \frac{1}{v}f^1\bar{Z}\lambda_{ei}^2, \quad (83)$$

$$\begin{aligned}f^1 &= -\frac{\bar{Z}}{\bar{Z}+1}\left[\frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v}\frac{\partial f^0}{\partial v}\right] \\ &= -\frac{\bar{Z}}{\bar{Z}+1}\left[\frac{1}{\rho}\frac{\partial \rho}{\partial z} + \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2}\right)\frac{1}{T}\frac{\partial T}{\partial z} - \frac{\tilde{E}_z}{v_{th}^2}\right]f_M\end{aligned} \quad (84)$$

In order to ensure the plasma to be quasi-neutral, the zero-current condition

$$\mathbf{j} = \int_0^\infty \int_{4\pi} q_e v \mathbf{n} f d\mathbf{n} v^2 dv = \mathbf{0}, \quad (85)$$

can be achieved by providing a consistent electric field in (92), i.e.

$$\tilde{\mathbf{E}} = \frac{v_{th}^2 \int_{4\pi} \mathbf{n} \otimes \mathbf{n} \cdot \int_0^\infty v f_M \frac{\lambda}{\alpha} \left(\frac{\nabla \rho}{\rho} + \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} \right) \frac{\nabla T}{T} \right) v^2 dv d\mathbf{n}}{\int_{4\pi} \mathbf{n} \otimes \mathbf{n} \cdot \int_0^\infty v f_M \frac{\lambda}{\alpha} v^2 dv d\mathbf{n}}, \quad (86)$$

which may be further simplified as

$$\tilde{\mathbf{E}} = \frac{\int_0^\infty f_M \frac{1}{2} \frac{\nabla T}{T} v^9 dv}{\int_0^\infty f_M v^7 dv} + v_{th}^2 \left(\frac{\nabla \rho}{\rho} - \frac{3}{2} \frac{\nabla T}{T} \right) = v_{th}^2 \left(\frac{\nabla \rho}{\rho} + \frac{5}{2} \frac{\nabla T}{T} \right), \quad (87)$$

where it is worth mentioning, that the part $f_M + \frac{v\lambda}{\alpha} \frac{\partial f_1}{\partial v}$ of the distribution does not contribute to the current since it is isotropic. One can write the quasi-neutral distribution function explicitly distinguishing between original part (blue color) and E field correction (red color) as

$$f \approx f_M \left(1 - \frac{\lambda}{\alpha} \mathbf{n} \cdot \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} - \frac{5}{2} \right) \frac{\nabla T}{T} \right) + \frac{v\lambda}{\alpha} \frac{\partial f_1}{\partial v}. \quad (88)$$

which leads to the resulting heat flux

$$\mathbf{q}_H = \int_{4\pi} \int_0^\infty \frac{m_e v^2}{2} v \mathbf{n} f v^2 dv d\mathbf{n} = \frac{4\pi}{3} \frac{m_e}{2} \frac{1}{\alpha \sigma \rho} \int_0^\infty \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} - \frac{5}{2} \right) v^9 f_M dv \frac{\nabla T}{T}.$$

Based on the Gauss integral formula

$$\int v^{2s+1} \exp\left(-\frac{v^2}{2v_{th}^2}\right) dv = \frac{s! (2v_{th}^2)^{s+1}}{2}$$

and Maxwell-Boltzmann distribution (67) the heat flux can be written as

$$\mathbf{q}_H = \frac{4\pi}{3} \frac{m_e}{2} \frac{1}{\alpha \sigma \rho} \frac{\rho}{v_{th}^3} \frac{1}{(2\pi)^{3/2}} \frac{4!}{T} \frac{2^4 v_{th}^{10}}{T} \left(5 - \frac{3}{2} - \frac{5}{2} \right) \nabla T = \frac{m_e}{\alpha \sigma} \frac{128}{\sqrt{2\pi}} \left(\frac{k_B}{m_e} \right)^{\frac{7}{2}} T^{\frac{5}{2}} \nabla T. \quad (89)$$

In conclusion, equation (89) provides nothing else than the well known Lorentz approximation heat flux and its nonlinearity 2.5 in temperature. What is worth mentioning is the effect of E field (quasi-neutrality), which reduces the flux of about 71.4% (also assuming constant density).

Finally, one can find the approximate solution

$$\tilde{f} = f_M - \lambda_{ei} \frac{\bar{Z}}{\bar{Z} + 1} \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} - \alpha \right) \frac{\mathbf{n} \cdot \nabla T}{T} f_M. \quad (90)$$

2.1.2. AWBS collision operator

The AWBS electron transport equation in 6D reads

$$\mathbf{n} \cdot \nabla f + \frac{1}{v} \left[\tilde{\mathbf{E}} \cdot \mathbf{n} \frac{\partial f}{\partial v} + \frac{\tilde{\mathbf{E}} \cdot \mathbf{e}_\phi - v \tilde{\mathbf{B}} \cdot \mathbf{e}_\theta}{v} \frac{\partial f}{\partial \phi} + \frac{\tilde{\mathbf{E}} \cdot \mathbf{e}_\theta + v \tilde{\mathbf{B}} \cdot \mathbf{e}_\phi}{v \sin(\phi)} \frac{\partial f}{\partial \theta} \right] = \frac{v}{\lambda_e} \frac{\partial}{\partial v} (f - f_M) + \frac{1}{2\lambda_{ei}} \left(\frac{\partial}{\partial \mu} \left((1 - \mu^2) \frac{\partial f}{\partial \mu} \right) + \frac{1}{\sin^2(\phi)} \frac{\partial^2 f}{\partial \theta^2} \right), \quad (91)$$

where $\mu = \cos(\phi)$, λ_e is the electron-electron mean free path, and λ_{ei} is the electron-ion mean free path.

We can try to find an approximate solution while using the first term of expansion in λ_e and μ as

$$\tilde{f}(z, v, \mu) = f^0(z, v) + f^1(z, v) \lambda_{ei} \mu. \quad (92)$$

Clearly, $\frac{\partial \tilde{f}}{\partial \theta} = 0$, and if $\tilde{\mathbf{B}} = \tilde{B}_z \mathbf{e}_z$, there is no effect of magnetic field. We also assume, that $\nabla f = \frac{\partial f}{\partial z} \mathbf{e}_z$ and appropriately $\tilde{\mathbf{E}} = \tilde{E}_z \mathbf{e}_z$. From the orientation of the Cartesian basis vectors and spherical basis vectors, one can find $\tilde{\mathbf{E}} \cdot \mathbf{n} = \tilde{E}_z \cos(\phi) = \mu$ and $\tilde{\mathbf{E}} \cdot \mathbf{e}_\phi = -\tilde{E}_z \sin(\phi)$. As a result, the analyzed AWBS equation reads

$$\mu \frac{\partial}{\partial z} (f^0 + f^1 \lambda_{ei} \mu) + \frac{1}{v} \left[\tilde{E}_z \mu \frac{\partial}{\partial v} (f^0 + f^1 \lambda_{ei} \mu) - \frac{\tilde{E}_z \sin(\phi)}{v} \frac{\partial}{\partial \phi} (f^0 + f^1 \lambda_{ei} \mu) \right] = \frac{v}{\lambda_e} \frac{\partial}{\partial v} ((f^0 + f^1 \lambda_{ei} \mu) - f_M) + \frac{1}{2\lambda_{ei}} \frac{\partial}{\partial \mu} \left((1 - \mu^2) \frac{\partial}{\partial \mu} (f^0 + f^1 \lambda_{ei} \mu) \right), \quad (93)$$

$$\mu \frac{\partial f^0}{\partial z} + \mu^2 \frac{\partial}{\partial z} (f^1 \lambda_{ei}) + \frac{\tilde{E}_z}{v} \left[\mu \frac{\partial f^0}{\partial v} + \mu^2 \frac{\partial}{\partial v} (f^1 \lambda_{ei}) + \frac{1 - \mu^2}{v} f^1 \lambda_{ei} \right] = \frac{v}{\bar{Z} \lambda_{ei}} \frac{\partial}{\partial v} (f^0 - f_M) + \mu \frac{v}{\bar{Z} \lambda_{ei}} \frac{\partial (f^1 \lambda_{ei})}{\partial v} - \mu f^1, \quad (94)$$

consequently, we have the following anisotropy expansion $\mu^0, \mu^1, \mu^2, \dots$ equations

$$\begin{aligned} \frac{v}{\bar{Z} \lambda_{ei}} \frac{\partial}{\partial v} (f^0 - f_M) &= \frac{1}{v} f^1 \lambda_{ei}, \\ \frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v} \frac{\partial f^0}{\partial v} &= \frac{v}{\bar{Z} \lambda_{ei}} \frac{\partial (f^1 \lambda_{ei})}{\partial v} - f^1, \\ \frac{\partial}{\partial z} (f^1 \lambda_{ei}) + \frac{\tilde{E}_z}{v} \left[\frac{\partial}{\partial v} (f^1 \lambda_{ei}) - \frac{1}{v} f^1 \lambda_{ei} \right] &= 0, \end{aligned}$$

which lead to the definitions

$$\begin{aligned} \frac{\partial}{\partial v} (f^0 - f_M) &= \frac{1}{v^2} f^1 \bar{Z} \lambda_{ei}^2, \\ \frac{v}{\bar{Z} \lambda_{ei}} \frac{\partial (f^1 \lambda_{ei})}{\partial v} - f^1 &= \frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v} \frac{\partial f^0}{\partial v} \\ \frac{v}{\bar{Z}} \frac{\partial f^1}{\partial v} + \frac{4}{\bar{Z}} f^1 - f^1 &= \frac{\partial f^0}{\partial z} + \frac{\tilde{E}_z}{v} \frac{\partial f^0}{\partial v} \\ \frac{\partial f^1}{\partial v} + \frac{1}{v} (4 - \bar{Z}) f^1 &= \frac{\bar{Z}}{v} \left(\frac{1}{\rho} \frac{\partial \rho}{\partial z} + \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} \right) \frac{1}{T} \frac{\partial T}{\partial z} - \frac{\tilde{E}_z}{v_{th}^2} \right) f_M. \end{aligned} \quad (95)$$

3. M1 model

3.1. AWBS Boltzmann transport equation

Simplified Boltzmann transport equation of electrons relying on the use of AWBS collision-thermalization operator [2] reads

$$v\mathbf{n} \cdot \nabla f + \frac{q_e}{m_e} \left(\mathbf{E} + \frac{v}{c} \mathbf{n} \times \mathbf{B} \right) \cdot \nabla_{\mathbf{v}} f = \nu_e v \frac{\partial}{\partial v} (f - f_M). \quad (97)$$

3.2. M1-AWBS model

In order to eliminate the dimensions of the transport problem (97) the two moment model referred to as *M1-AWBS* is introduced

$$\nu_e v \frac{\partial}{\partial v} (f_0 - f_M) = v \nabla \cdot \mathbf{f}_1 + \frac{q_e}{m_e v^2} \mathbf{E} \cdot \frac{\partial}{\partial v} (v^2 \mathbf{f}_1), \quad (98)$$

$$\begin{aligned} \nu_e v \frac{\partial}{\partial v} \mathbf{f}_1 - \nu_t \mathbf{f}_1 &= v \nabla \cdot (\mathbf{A} f_0) + \frac{q_e}{m_e v^2} \mathbf{E} \cdot \frac{\partial}{\partial v} (v^2 \mathbf{A} f_0) \\ &\quad + \frac{q_e}{m_e v} \mathbf{E} \cdot (\mathbf{A} - \mathbf{I}) f_0 + \frac{q_e}{m_e c} \mathbf{B} \times \mathbf{f}_1, \end{aligned} \quad (99)$$

where the anisotropy-closure matrix takes the form

$$\mathbf{A} = \frac{1}{3} \mathbf{I} + \frac{|\mathbf{f}_1|^2}{2f_0^2} \left(1 + \frac{|\mathbf{f}_1|^2}{f_0^2} \right) \left(\frac{\mathbf{f}_1 \otimes \mathbf{f}_1^T}{|\mathbf{f}_1|^2} - \frac{1}{3} \mathbf{I} \right), \quad (100)$$

which corresponds to the distribution function approximation

$$f = f_0 \frac{|\mathbf{M}_{(\mathbf{f}_1/f_0)}|}{4\pi \sinh(\mathbf{M}_{(\mathbf{f}_1/f_0)})} \exp(\mathbf{n} \cdot \mathbf{M}_{(\mathbf{f}_1/f_0)}), \quad (101)$$

where $\mathbf{M}_{(\mathbf{f}_1/f_0)} \rightarrow 0$ when $\mathbf{f}_1/f_0 \rightarrow \mathbf{0}$.

4. Maxwell equations

$$\frac{\partial \mathbf{E}}{\partial t} + 4\pi \mathbf{j} = c \nabla \times \mathbf{B}, \quad (102)$$

$$\frac{\partial \mathbf{B}}{\partial t} = -c \nabla \times \mathbf{E}, \quad (103)$$

$$v \mathbf{f}_1 = \frac{\nu_e v^2}{\nu_t} \frac{\partial \mathbf{f}_1}{\partial v} - \frac{v^2}{\nu_t} \mathbf{A} \cdot \nabla f_0 - \frac{q_e v}{m_e \nu_t} \frac{\partial f_0}{\partial v} \mathbf{A} \cdot \mathbf{E} - \frac{q_e v}{m_e c \nu_t} \mathbf{B} \times \mathbf{f}_1, \quad (104)$$

$$\begin{aligned} \frac{\partial \mathbf{E}}{\partial t} - \frac{4\pi q_e^2}{m_e} \int \frac{v}{\nu_t} \frac{\partial f_0}{\partial v} v^2 dv \mathbf{A} \cdot \mathbf{E} = & -4\pi q_e \int \left(\frac{\nu_e v^2}{\nu_t} \frac{\partial \mathbf{f}_1}{\partial v} - \frac{v^2}{\nu_t} \mathbf{A} \cdot \nabla f_0 \right) v^2 dv \\ & - \int \frac{4\pi q_e^2 v}{m_e c \nu_t} \mathbf{f}_1 \times \mathbf{B} v^2 dv + c \nabla \times \mathbf{B}, \end{aligned} \quad (105)$$

MFEM Joule app: "This is the main computational code that computes dX/dt implicitly where X is the state vector containing P, E, B, F, T, and W

$$S0(\sigma)P = 0 \quad (106)$$

$$(M1 + dtS1(\sigma))E = WeakCurl^T B + GradP \quad (107)$$

$$dB = -CurlE \quad (108)$$

$$(M2 + dtS2)F = WeakDiv^T T \quad (109)$$

$$M3dT = WeakDivF + W \quad (110)$$

where W is the Joule heating." This means the Maxwell equations look like this

$$\begin{aligned} \frac{\partial \mathbf{E}}{\partial t} + 4\pi \mathbf{j} &= c \nabla \times \mathbf{B}, \\ \mathbf{j} &= \sigma (\mathbf{E} - \nabla \Phi), \end{aligned}$$

where current originates from the Ohm's law and electric field has induced \mathbf{E} and electrostatic (potential Φ) contributions.

- Write the above equations as variational principle in H(curl).
- Try to build Nedelec for Efield on 1D mesh. Project Efield coeff and plot to see how it works ;).
- Prepare integrators on H(curl) in (??).

5. High-order finite element scheme

5.1. Variational principle in Electromagnetics

We multiply Amperes law (105) by a 1-form test function $\mathbf{W}_c \in H(Curl)$ and integrate over the three dimensional problem domain Ω to obtain the variational form

$$\begin{aligned} \int_{\Omega} \mathbf{W}_c \cdot \left[\mathbf{W}_c^T \cdot \frac{\partial \mathbf{E}}{\partial t} - \frac{4\pi q_e^2}{m_e} \int \frac{v}{\nu_t} \frac{\partial f_0}{\partial v} v^2 dv \mathbf{A} \cdot \mathbf{W}_c^T \cdot \mathbf{E} \right] d\Omega = \\ 4\pi q_e \int_{\Omega} \mathbf{W}_c \cdot \int \left(\frac{v^2}{\nu_t} \mathbf{A} \cdot \nabla f_0 - \frac{\nu_e v^2}{\nu_t} \frac{\partial \mathbf{f}_1}{\partial v} - \frac{q_e v}{m_e c \nu_t} \mathbf{f}_1 \times \mathbf{B} \right) v^2 dv d\Omega \\ + c \int_{\Omega} \mathbf{W}_c \cdot \nabla \times \mathbf{B} d\Omega \quad (111) \end{aligned}$$

Now we perform integration by parts on (111), apply the Gauss divergence theorem and move the resulting surface integral term to the right hand side to obtain

$$\begin{aligned} \int_{\Omega} \mathbf{W}_c \cdot \left[\mathbf{W}_c^T \cdot \frac{\partial \mathbf{E}}{\partial t} - \frac{4\pi q_e^2}{m_e} \int \frac{v}{\nu_t} \frac{\partial f_0}{\partial v} v^2 dv \mathbf{A} \cdot \mathbf{W}_c^T \cdot \mathbf{E} \right] d\Omega = \\ 4\pi q_e \int_{\Omega} \mathbf{W}_c \cdot \int \left(\frac{v^2}{\nu_t} \mathbf{A} \cdot \nabla f_0 - \frac{\nu_e v^2}{\nu_t} \frac{\partial \mathbf{f}_1}{\partial v} - \frac{q_e v}{m_e c \nu_t} \mathbf{f}_1 \times \mathbf{B} \right) v^2 dv d\Omega \\ + c \int_{\Omega} \nabla \times \mathbf{W}_c \cdot \mathbf{B} d\Omega + c \int_{\Gamma} (\mathbf{W}_c \times \mathbf{B}) \cdot \mathbf{n}_{\Gamma} d\Gamma, \quad (112) \end{aligned}$$

5.2. Variational principle in Kinetics

The general variational formulation of (98) and (99) constructed above the scalar (zero moment) functional space represented by test functions ψ and the vector (first moment) functional space represented by test functions \mathbf{w} takes the form

$$\begin{aligned} \int_{\Omega} \psi \nu_e \frac{\partial f_0}{\partial v} &= \int_{\Omega} \psi \left(\mathbf{I} : \nabla \mathbf{f}_1 + \frac{1}{v} \tilde{\mathbf{E}} \cdot \frac{\partial \mathbf{f}_1}{\partial v} + \frac{2}{v^2} \tilde{\mathbf{E}} \cdot \mathbf{f}_1 + \nu_e \frac{\partial f_M}{\partial v} \right) \quad (113) \\ \int_{\Omega} \mathbf{w} \cdot \nu_e \frac{\partial \mathbf{f}_1}{\partial v} &= \int_{\Omega} \mathbf{w} \cdot \left(\nabla \cdot (\mathbf{A} f_0) + \frac{1}{v^2} \tilde{\mathbf{E}} \cdot (3\mathbf{A} - \mathbf{I}) f_0 \right. \\ &\quad \left. + \frac{1}{v} \tilde{\mathbf{E}} \cdot \frac{\partial}{\partial v} (\mathbf{A} f_0) + \frac{1}{v} \tilde{\mathbf{B}} \times \mathbf{f}_1 + \frac{\nu_t}{v} \mathbf{f}_1 \right). \quad (114) \end{aligned}$$

The corresponding discrete variational principal based on the method of finite elements then reads

$$\begin{aligned} \int_{\Omega} \boldsymbol{\psi} \otimes \boldsymbol{\psi}^T \nu_e \, d\Omega \cdot \frac{\partial \mathbf{f}_0}{\partial v} &= \int_{\Omega} \boldsymbol{\psi} \otimes \left(\mathbf{I} : \nabla \mathbf{w}^T + \frac{2}{v^2} \tilde{\mathbf{E}}^T \cdot \mathbf{w}^T \right) d\Omega \cdot \mathbf{f}_1 \\ &+ \int_{\Omega} \boldsymbol{\psi} \otimes \frac{1}{v} \tilde{\mathbf{E}}^T \cdot \mathbf{w}^T \, d\Omega \cdot \frac{\partial \mathbf{f}_1}{\partial v} + \int_{\Omega} \boldsymbol{\psi} \otimes \boldsymbol{\psi}^T \nu_e \, d\Omega \cdot \frac{\partial \mathbf{f}_M}{\partial v}, \end{aligned} \quad (115)$$

$$\begin{aligned} \int_{\Omega} \mathbf{w} \cdot \mathbf{w}^T \nu_e \, d\Omega \cdot \frac{\partial \mathbf{f}_1}{\partial v} &= - \int_{\Omega} (\mathbf{A} : \nabla \mathbf{w}) \boldsymbol{\psi}^T \, d\Omega \cdot \mathbf{f}_0 \\ &+ \int_{\Omega} \mathbf{w} \cdot \frac{1}{v^2} (3\mathbf{A} - \mathbf{I}) \cdot \tilde{\mathbf{E}} \boldsymbol{\psi}^T \, d\Omega \cdot \mathbf{f}_0 + \int_{\Omega} \mathbf{w} \cdot \frac{1}{v} \mathbf{A} \cdot \tilde{\mathbf{E}} \boldsymbol{\psi}^T \, d\Omega \cdot \frac{\partial \mathbf{f}_0}{\partial v} \\ &+ \int_{\Omega} \mathbf{w} \cdot \left(\frac{1}{v} \tilde{\mathbf{B}} \times \mathbf{w}^T + \frac{\nu_t}{v} \mathbf{w}^T \right) d\Omega \cdot \mathbf{f}_1, \end{aligned} \quad (116)$$

where $\boldsymbol{\psi}$ is the finite vector of scalar bases functions, \mathbf{w} is the finite vector of vector bases functions, Ω represents the computational domain, in principle 1D/2D/3D spatial mesh.

5.3. Semi-discrete formulation

In principle, only five following integrators need to be coded to provide a discrete representation (115) and (116), i.e.

$$\mathcal{M}_{(g)}^0 = \int_{\Omega} \boldsymbol{\psi} \otimes \boldsymbol{\psi}^T g \, d\Omega, \quad (117)$$

$$\mathcal{M}_{(g)}^1 = \int_{\Omega} \mathbf{w} \cdot \mathbf{w}^T g \, d\Omega, \quad (118)$$

$$\mathcal{D}_{(\mathbf{G})} = \int_{\Omega} \mathbf{G} : \nabla \mathbf{w} \otimes \boldsymbol{\psi}^T \, d\Omega, \quad (119)$$

$$\mathcal{V}_{(g)} = \int_{\Omega} \mathbf{w} \cdot \mathbf{g} \otimes \boldsymbol{\psi}^T \, d\Omega, \quad (120)$$

$$\mathcal{B}_{(g)} = \int_{\Omega} \mathbf{w} \cdot \mathbf{g} \times \mathbf{w}^T \, d\Omega. \quad (121)$$

The algebraic representation of the above mathematical objects, which form the basis for numerical discretization, reads

$$\boldsymbol{\psi} = \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_{N_0} \end{bmatrix}, \quad \mathbf{w} = \begin{bmatrix} w_{1,1} & \dots & w_{1,d} \\ \vdots & \ddots & \vdots \\ w_{N_1,1} & \dots & w_{N_1,d} \end{bmatrix}, \quad \mathbf{g} = \begin{bmatrix} g_1 \\ \vdots \\ g_d \end{bmatrix}, \quad \mathbf{G} = \begin{bmatrix} G_{1,1} & \dots & G_{1,d} \\ \vdots & \ddots & \vdots \\ G_{d,1} & \dots & G_{d,d} \end{bmatrix}, \quad (122)$$

where d is the number of spatial dimensions, N_0 the number of degrees of freedom of scalar unknown \mathbf{f}_0 , and N_1 is the number of degrees of freedom of vector unknown \mathbf{f}_1 .

Consequently, the discrete analog of M1-AWBS equations (98) and (99) can be written based on (115), (116) as

$$\mathcal{M}_{(\nu_e)}^0 \cdot \frac{\partial \mathbf{f}_0}{\partial v} - \mathcal{M}_{(\nu_e)}^0 \cdot \frac{\partial \mathbf{f}_M}{\partial v} = \mathcal{D}_{(\mathbf{I})}^T \cdot \mathbf{f}_1 + \frac{1}{v} \boldsymbol{\nu}_{(\tilde{\mathbf{E}})}^T \cdot \frac{\partial \mathbf{f}_1}{\partial v} + \frac{2}{v^2} \boldsymbol{\nu}_{(\tilde{\mathbf{E}})}^T \cdot \mathbf{f}_1, \quad (123)$$

$$\begin{aligned} \mathcal{M}_{(\nu_e)}^1 \cdot \frac{\partial \mathbf{f}_1}{\partial v} - \frac{1}{v} \mathcal{M}_{(\nu_t)}^1 \cdot \mathbf{f}_1 &= -\mathcal{D}_{(\mathbf{A})} \cdot \mathbf{f}_0 \\ &+ \frac{1}{v} \boldsymbol{\nu}_{(\mathbf{A} \cdot \tilde{\mathbf{E}})} \cdot \frac{\partial \mathbf{f}_0}{\partial v} + \frac{1}{v^2} \boldsymbol{\nu}_{((3\mathbf{A}-\mathbf{I}) \cdot \tilde{\mathbf{E}})} \cdot \mathbf{f}_0 + \frac{1}{v} \mathcal{B}_{(\tilde{\mathbf{B}})} \cdot \mathbf{f}_1, \end{aligned} \quad (124)$$

where the integrators (117), (118), (119), (120), (121) are used acting on appropriate functions ρ , ν_e , ν_t , vectors $\tilde{\mathbf{E}}$, $\tilde{\mathbf{B}}$, and matrices \mathbf{A} and \mathbf{I} .

5.4. Explicit fully-discrete scheme

The easiest way to define a fully discrete scheme is to apply the explicit integration in time, e.g. RK4. Because of the use of different finite element spaces for zero and first moment, and a consequent difficulties of "mass" inversion, a modified two-step explicit scheme is used.

In the first step the time evolution of zero moment quantity \mathbf{f}_0 is computed as

$$\left(\mathcal{M}_{(\nu_e)}^0 - \mathcal{M}_{\left(\frac{1}{v \mathbf{f}_0^n} \tilde{\mathbf{E}}^T \cdot \mathbf{f}_1^n\right)}^0 \right) \cdot \frac{d \mathbf{f}_0^*}{dv} = \mathcal{D}_{(\mathbf{I})}^T \cdot \mathbf{f}_1^n + \frac{2}{v^2} \boldsymbol{\nu}_{(\tilde{\mathbf{E}})}^T \cdot \mathbf{f}_1^n + \mathcal{M}_{(\nu_e)}^0 \cdot \frac{\partial \mathbf{f}_M}{\partial v}, \quad (125)$$

where the actual evolution of \mathbf{f}_1 has been redefined as similar to the time evolution of \mathbf{f}_0 (compare (125) to (129)). Then, the actual computation of the time evolution of \mathbf{f}_1 follows

$$\begin{aligned} \mathcal{M}_{(\nu_e)}^1 \cdot \frac{d\mathbf{f}_1}{dv} = & -\mathcal{D}_{(\mathbf{A})} \cdot \mathbf{f}_0^n + \frac{1}{v} \mathcal{V}_{(\mathbf{A} \cdot \tilde{\mathbf{E}})} \cdot \frac{d\mathbf{f}_0^*}{dv} \\ & + \frac{1}{v^2} \mathcal{V}_{((3\mathbf{A}-\mathbf{I}) \cdot \tilde{\mathbf{E}})} \cdot \mathbf{f}_0^n + \frac{1}{v} \mathcal{B}_{(\tilde{\mathbf{B}})} \cdot \mathbf{f}_1^n + \frac{1}{v} \mathcal{M}_{(\nu_t)}^1 \cdot \mathbf{f}_1^n. \end{aligned} \quad (126)$$

The superscript n stands for quantities from the previous level of velocity.

5.5. Implicit fully-discrete scheme

$$\mathcal{M}_{(\nu_e)}^0 \cdot \frac{\partial \mathbf{f}_0}{\partial v} = \mathcal{D}_{(\mathbf{I})}^T \cdot \mathbf{f}_1 + \frac{1}{v} \mathcal{V}_{(\tilde{\mathbf{E}})}^T \cdot \frac{\partial \mathbf{f}_1}{\partial v} + \mathcal{M}_{(\nu_e)}^0 \cdot \frac{\partial \mathbf{f}_M}{\partial v}, \quad (127)$$

$$\mathcal{M}_{(\nu_e)}^1 \cdot \frac{\partial \mathbf{f}_1}{\partial v} = -\mathcal{D}_{(\mathbf{A})} \cdot \mathbf{f}_0 + \frac{1}{v} \mathcal{V}_{(\mathbf{A} \cdot \tilde{\mathbf{E}})} \cdot \frac{\partial \mathbf{f}_0}{\partial v} + \frac{1}{v} \left(\mathcal{M}_{(\nu_t)}^1 + \mathcal{B}_{(\tilde{\mathbf{B}})} \right) \cdot \mathbf{f}_1, \quad (128)$$

$$\frac{\partial \mathbf{f}_0}{\partial v} = \frac{1}{v} \mathcal{M}_{(\nu_e)}^{0^{-1}} \cdot \mathcal{V}_{(\tilde{\mathbf{E}})}^T \cdot \frac{\partial \mathbf{f}_1}{\partial v} + \mathcal{M}_{(\nu_e)}^{0^{-1}} \cdot \mathcal{D}_{(\mathbf{I})}^T \cdot \left(\mathbf{f}_1^n + \Delta v \frac{\partial \mathbf{f}_1}{\partial v} \right) + \frac{\partial \mathbf{f}_M}{\partial v}, \quad (129)$$

$$\begin{aligned} \mathcal{M}_{(\nu_e)}^1 \cdot \frac{\partial \mathbf{f}_1}{\partial v} = & \frac{1}{v} \mathcal{V}_{(\mathbf{A} \cdot \tilde{\mathbf{E}})} \cdot \frac{\partial \mathbf{f}_0}{\partial v} - \mathcal{D}_{(\mathbf{A})} \cdot \left(\mathbf{f}_0^n + \Delta v \frac{\partial \mathbf{f}_0}{\partial v} \right) \\ & + \frac{1}{v} \left(\mathcal{B}_{(\tilde{\mathbf{B}})} + \mathcal{M}_{(\nu_t)}^1 \right) \cdot \left(\mathbf{f}_1^n + \Delta v \frac{\partial \mathbf{f}_1}{\partial v} \right), \end{aligned} \quad (130)$$

$$\begin{aligned} \mathcal{M}_{(\nu_e)}^1 \cdot \frac{\partial \mathbf{f}_1}{\partial v} = & \left(\frac{1}{v} \mathcal{V}_{(\mathbf{A} \cdot \tilde{\mathbf{E}})} - \Delta v \mathcal{D}_{(\mathbf{A})} \right) \cdot \mathcal{M}_{(\nu_e)}^{0^{-1}} \cdot \left(\frac{1}{v} \mathcal{V}_{(\tilde{\mathbf{E}})}^T + \Delta v \mathcal{D}_{(\mathbf{I})}^T \right) \cdot \frac{\partial \mathbf{f}_1}{\partial v} \\ & + \frac{\Delta v}{v} \left(\mathcal{B}_{(\tilde{\mathbf{B}})} + \mathcal{M}_{(\nu_t)}^1 \right) \cdot \frac{\partial \mathbf{f}_1}{\partial v} + \frac{1}{v} \left(\mathcal{B}_{(\tilde{\mathbf{B}})} + \mathcal{M}_{(\nu_t)}^1 \right) \cdot \mathbf{f}_1^n \\ & + \left(\frac{1}{v} \mathcal{V}_{(\mathbf{A} \cdot \tilde{\mathbf{E}})} - \Delta v \mathcal{D}_{(\mathbf{A})} \right) \cdot \left[\mathcal{M}_{(\nu_e)}^{0^{-1}} \cdot \mathcal{D}_{(\mathbf{I})}^T \cdot \mathbf{f}_1^n + \frac{\partial \mathbf{f}_M}{\partial v} \right] - \mathcal{D}_{(\mathbf{A})} \cdot \mathbf{f}_0^n \end{aligned} \quad (131)$$

[3]

6. Simulation results

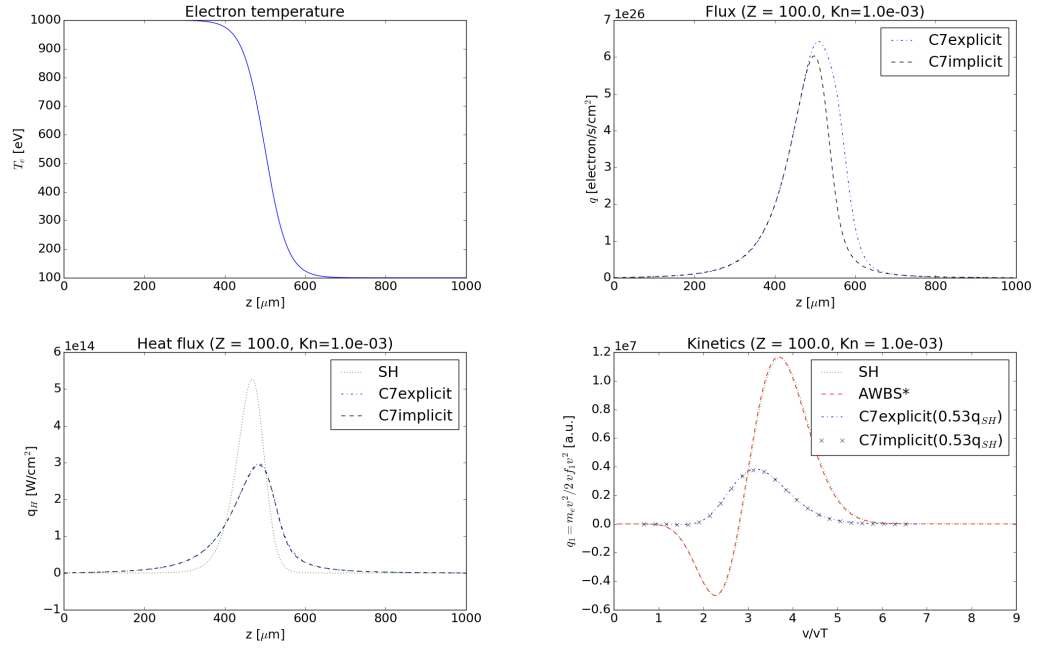


Figure 1: C7 explicit (63140 groups) vs implicit (25 groups) for $\text{Kn} = 0.001$ nonlocality. $t_{\text{expl}} \approx 4000 \times t_{\text{impl}}$.

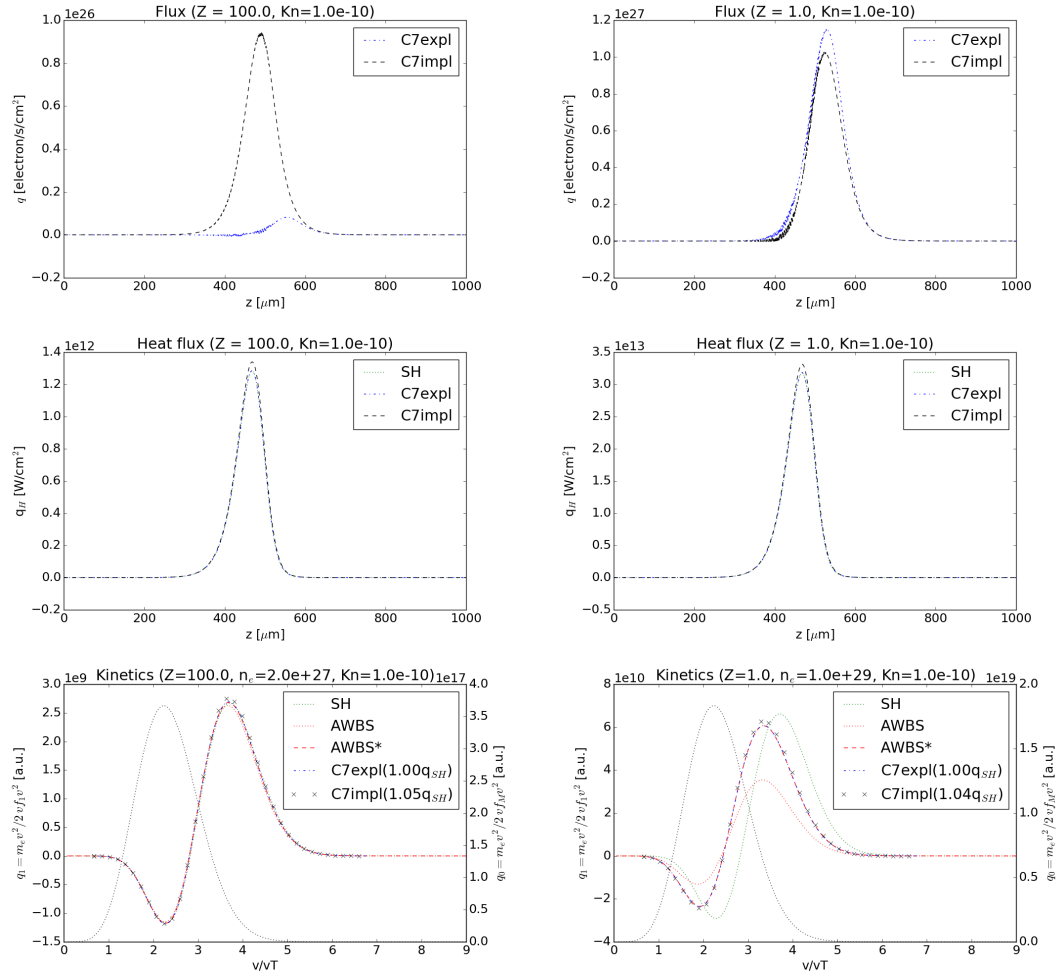


Figure 2: C7 explicit vs implicit for diffusive regime ($\text{Kn} = 10^{-10}$) including the SH Efield.

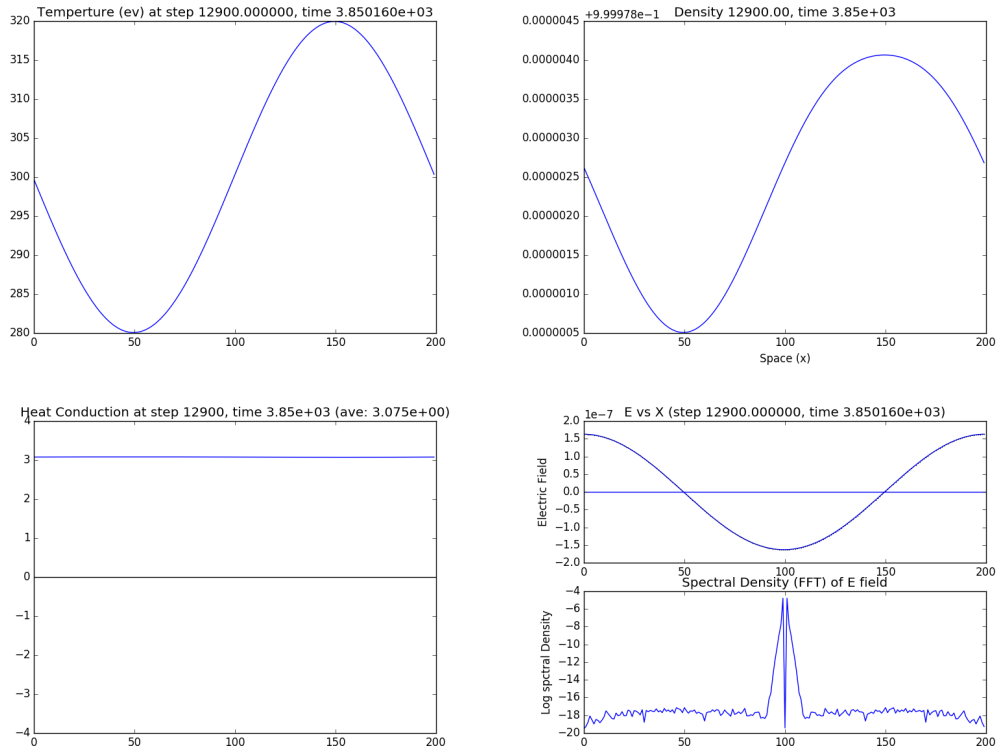


Figure 3: OSHUN simulation of Spitzer-Harm conductivity.

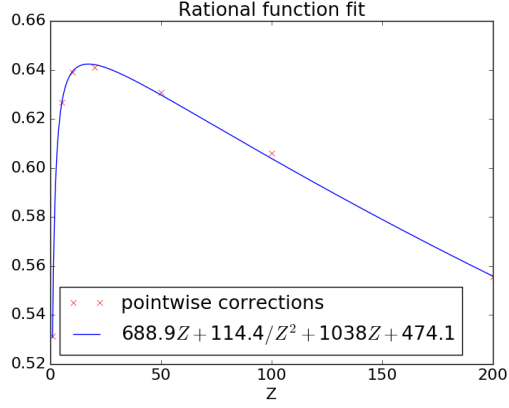


Figure 4: Analytic fit to the Z correction ($\nu_e^* = \frac{688.9\bar{Z}+114.4}{\bar{Z}^2+1038\bar{Z}+474.1}\nu_e$, where $\nu_e = \nu_{ei}/\bar{Z}$) of the diffusion asymptotic of AWBS with respect to SH.

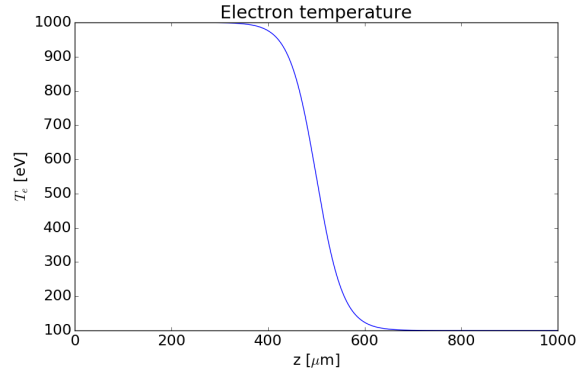


Figure 5: Temperature used in simulations. Ion density constant $n_i = 10^{20}$ [1/cm³].

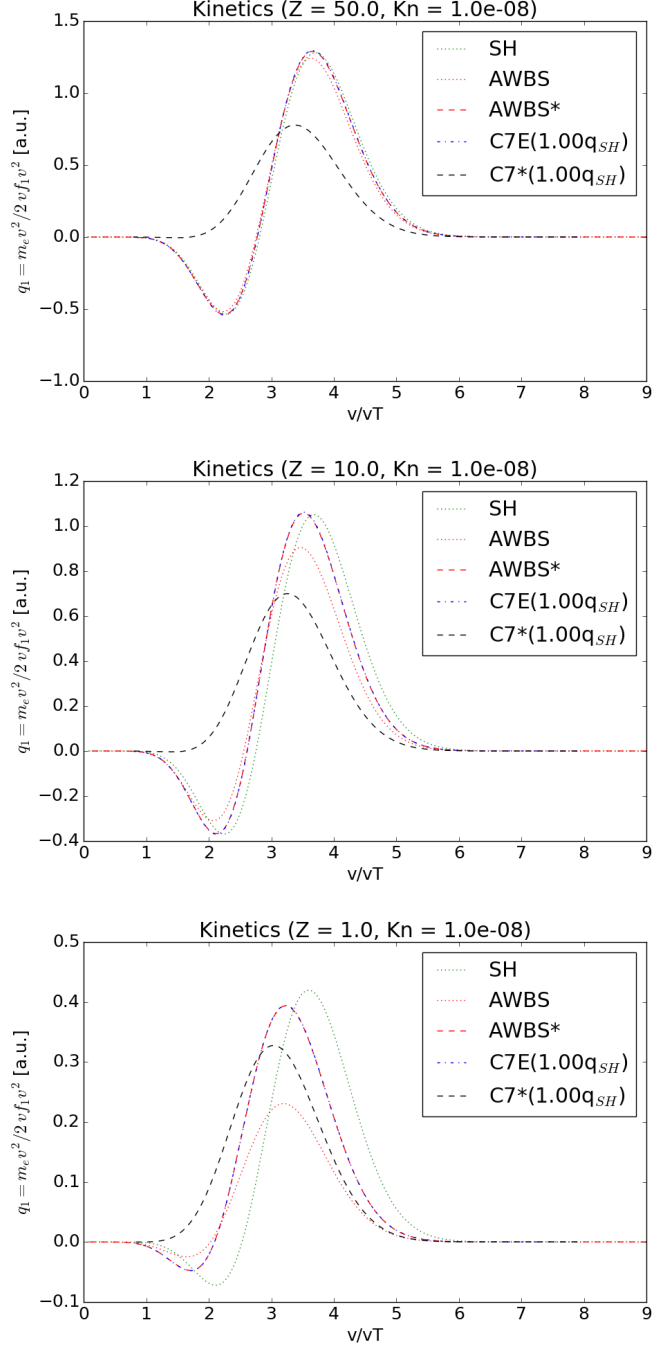


Figure 6: The diffusion asymptotic of C7 and analytic AWBS with respect to SH using Z-correction formula of mean free path and Spitzer electric field.

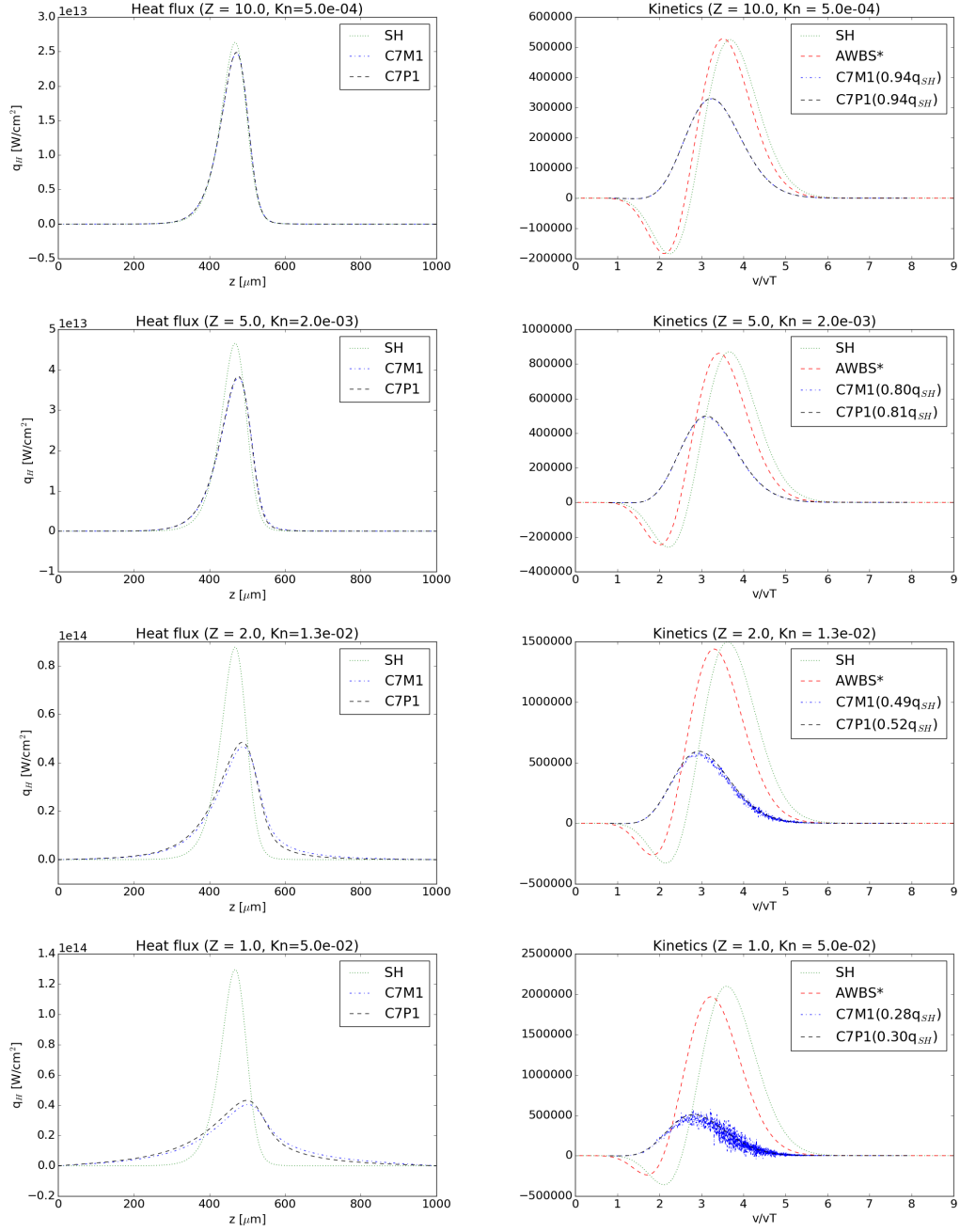


Figure 7: The nonlocal transport computations of electron heat flux with varying ionization. $Kn \approx \frac{\lambda_{ei}}{L} = \frac{v_{th}^4}{\sigma Z n_e} \frac{|\nabla T|}{T}$.

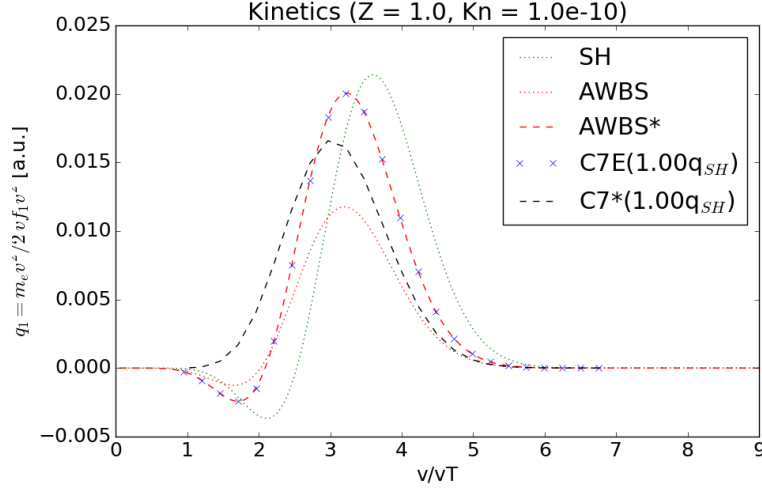


Figure 8: Efficiency of C7 (24 groups). Definition of Efield free C7* calculation based on reduction of the density of fast electrons.

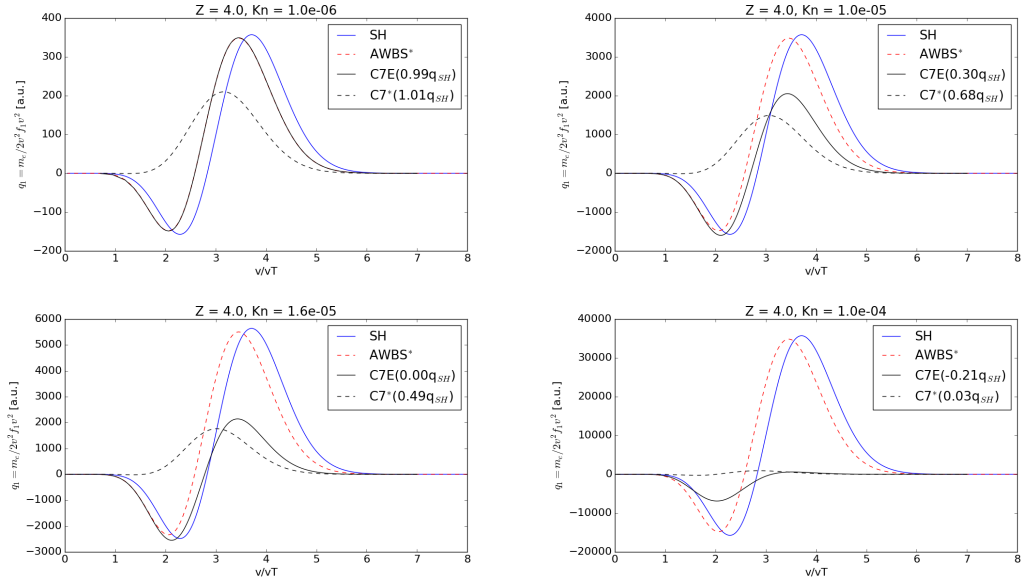


Figure 9: The effect of the diffusive electric field $\mathbf{E} = v_{th}^2 \left(1 + \frac{3}{2} \frac{\bar{Z} + 0.477}{\bar{Z} + 2.15}\right) \frac{\nabla T}{T}$ in AWBS model.

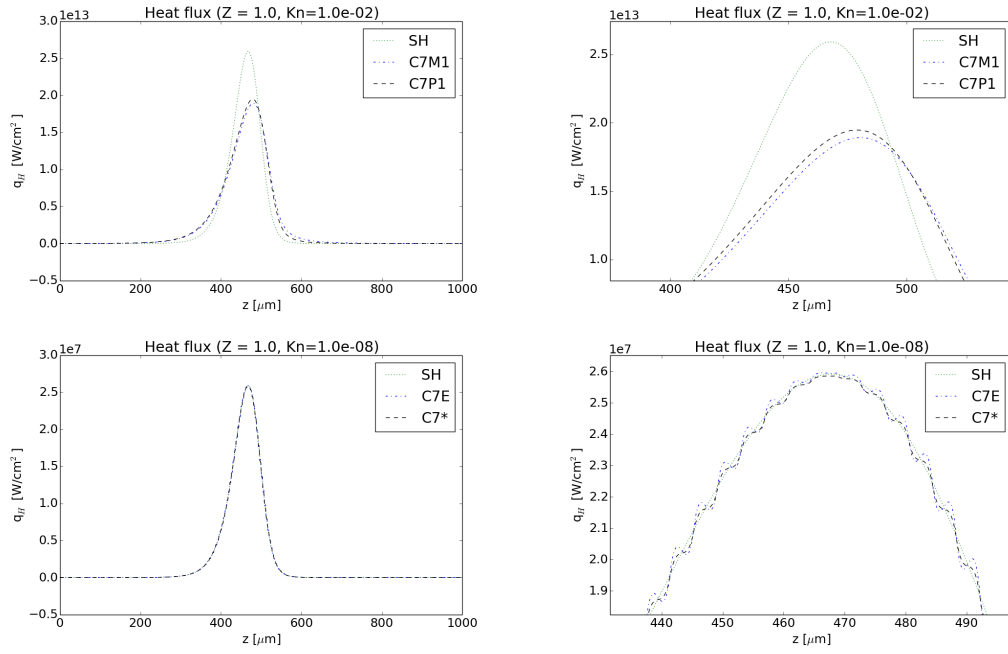


Figure 10: A spurious behavior of "strictly positive" Bernstein basis of f_0 .

7. Hydrodynamic diffusive electron collision operator HDECO

In order to improve the electron collision operator AWBS analyzed in Sec. 2.1.2, one can add the effect of diffusion in velocity space as

$$\left. \frac{\partial f}{\partial t} \right|_{coll} = \nu_e v \frac{\partial}{\partial v} \left(f + \frac{v_{th}^2}{v} \frac{\partial f}{\partial v} \right). \quad (132)$$

Nevertheless, the *diffusive electron collision operator* (132) does not provide a good bridge to hydrodynamics because of

$$\left. \frac{\partial f_M - f}{\partial t} \right|_{coll} = \left. \frac{\partial f}{\partial t} \right|_{coll}, \quad (133)$$

i.e. there is no relation to hydrodynamics via temperature. The reason for (133) is actually perfectly correct since

$$\left. \frac{\partial f_M}{\partial t} \right|_{coll} = 0, \quad \implies \quad \left. \frac{\partial f}{\partial t} \right|_{coll} \xrightarrow{f \rightarrow f_M} 0, \quad (134)$$

which directly demonstrates that (133) obeys the Boltzmann's H-theorem. The left side of (134) holds due to the form of Maxwell-Boltzmann distribution (67).

A non-trivial remedy of the absence of bridge of the electron distribution function f and the background fluid modeled by hydrodynamics can be found by introducing a source of electrons, i.e. we propose a "collision operator"

$$\begin{aligned} \left. \frac{\partial f}{\partial t} \right|_{coll} = & n_i \frac{d\bar{Z}}{dt} \frac{f_M(T)}{n_e} + \nu_e v \frac{\partial}{\partial v} \left(f + \frac{v_{th}^2}{v} \frac{\partial f}{\partial v} \right) + \\ & \frac{\nu_{ei}}{2} \left(\frac{\partial}{\partial \mu} \left((1 - \mu^2) \frac{\partial f}{\partial \mu} \right) + \frac{1}{\sin^2(\phi)} \frac{\partial^2 f}{\partial \theta^2} \right), \end{aligned} \quad (135)$$

where $\mu = \cos(\phi)$ and $n_i \frac{d\bar{Z}}{dt} \frac{f_M(T)}{n_e}$ is a source of electrons, where the distribution of ionized electrons is $f_M(T)$ (T corresponding to bounded "hydrodynamic" electrons).

Consequently, one can write the simplified (linear) Boltzmann transport equation of electrons as

$$\begin{aligned} \frac{\partial f}{\partial t} + v \mathbf{n} \cdot \nabla f + \tilde{\mathbf{E}} \cdot \mathbf{n} \frac{\partial f}{\partial v} + \frac{\tilde{\mathbf{E}} \cdot \mathbf{e}_\phi - v \tilde{\mathbf{B}} \cdot \mathbf{e}_\theta}{v} \frac{\partial f}{\partial \phi} + \frac{\tilde{\mathbf{E}} \cdot \mathbf{e}_\theta + v \tilde{\mathbf{B}} \cdot \mathbf{e}_\phi}{v \sin(\phi)} \frac{\partial f}{\partial \theta} = \\ n_i \frac{\partial \bar{Z}}{\partial t} \frac{f_M(T)}{n_e} + \nu_e v \frac{\partial}{\partial v} \left(f + \frac{v_{th}^2}{v} \frac{\partial f}{\partial v} \right) + \nu_{ei} (f_0 - f), \end{aligned} \quad (136)$$

where λ_e is the electron-electron mean free path, and λ_{ei} is the electron-ion mean free path. We also approximate $\lambda_e = \bar{Z}\lambda_{ei}$. The form of the electron-ion scattering operator arises from a low anisotropy approximation ($f \approx f_0 + \mathbf{n} \cdot \mathbf{f}_1$).

We can match the time derivatives together $\left(n_i \frac{\partial \bar{Z}}{\partial t} \frac{f_M(T)}{n_e} - \frac{\partial f}{\partial t}\right)$, and consequently, provide a steady model

$$\mathbf{n} \cdot \nabla f + \frac{1}{v} \left[\tilde{\mathbf{E}} \cdot \mathbf{n} \frac{\partial f}{\partial v} + \frac{\tilde{\mathbf{E}} \cdot \mathbf{e}_\phi - v \tilde{\mathbf{B}} \cdot \mathbf{e}_\theta}{v} \frac{\partial f}{\partial \phi} + \frac{\tilde{\mathbf{E}} \cdot \mathbf{e}_\theta + v \tilde{\mathbf{B}} \cdot \mathbf{e}_\phi}{v \sin(\phi)} \frac{\partial f}{\partial \theta} \right] = \frac{1}{v} \frac{\Delta(f_M(T) - f)}{\Delta t_{hydro}} + \frac{v}{\lambda_e} \frac{\partial}{\partial v} \left(f + \frac{v_{th}^2}{v} \frac{\partial f}{\partial v} \right) + \frac{f_0 - f}{\lambda_{ei}}. \quad (137)$$

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- [3] V. Dobrev, T. Kolev, R. Rieben, High-order curvilinear finite element methods for Lagrangian hydrodynamics, SIAM J. Sci. Comput. 34 (2012) B606–B641.