High-order finite element modeling of M1-AWBS nonlocal electron transport

Milan, Vladimir, Philippe, Jean-Luc[a]

[a]*Université de Bordeaux - CNRS - CEA, CELIA, UMR 5107, F-33405 Talence, France*

Abstract

Keywords: Nonlocal transport, Kinetics, MHD, High-order methods, FEM

Contents

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

$$\boldsymbol{x} = \bar{x}^1 \boldsymbol{e}_1 + \bar{x}^2 \boldsymbol{e}_2 + \bar{x}^3 \boldsymbol{e}_3 = \bar{x}^i \boldsymbol{e}_i, \tag{1}$$

and in the case of tensor of second rank

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

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

While introducing a general curvilinear coordinates

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

where the condition on the transformation Jacobian to be nonzero

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

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.

3

The transformation represented by (4) can be used to act on *covariant* tensor as

$$A_{\alpha\beta...\mu} = \frac{\partial \bar{x}^a}{\partial q^\alpha} \frac{\partial \bar{x}^b}{\partial q^\beta} ... \frac{\partial \bar{x}^m}{\partial q^\mu} \bar{A}_{ab...m}, \tag{5}$$

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

$$A^{\alpha\beta...\mu} = \frac{\partial q^\alpha}{\partial \bar{x}^a} \frac{\partial q^\beta}{\partial \bar{x}^b} ... \frac{\partial q^\mu}{\partial \bar{x}^m} \bar{A}^{ab...m}, \tag{6}$$

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

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

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

$$\mathbf{A} = A^{\alpha\beta...\mu}_{\kappa\lambda...\nu} \boldsymbol{b}_\alpha \boldsymbol{b}_\beta ... \boldsymbol{b}_\mu \boldsymbol{b}^\kappa \boldsymbol{b}^\lambda ... \boldsymbol{b}^\nu = \bar{A}^{ab...m}_{kl...n} \boldsymbol{e}_a \boldsymbol{e}_b ... \boldsymbol{e}_m \boldsymbol{e}^k \boldsymbol{e}^l ... \boldsymbol{e}^n$$
$$= \bar{A}^{ab...m...kl...n} \boldsymbol{e}_a \boldsymbol{e}_b ... \boldsymbol{e}_m \boldsymbol{e}_k \boldsymbol{e}_l ... \boldsymbol{e}_n, \tag{8}$$

where $\boldsymbol{b}_\alpha$ and $\boldsymbol{b}^\kappa$ 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

$$\boldsymbol{b}^i = \nabla q^i, \tag{9}$$

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

$$\boldsymbol{b}_i = \frac{\partial \boldsymbol{r}}{\partial q^i}, \tag{10}$$

and the following important equality holds

$$\boldsymbol{b}_i \cdot \boldsymbol{b}^j = \delta_i^j, \tag{11}$$

4

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

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

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

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

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

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

which provides a fundamental definition of the metric tensor

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

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

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

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

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

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.

$$g_{ij} T_{..ab}^{kj} = T_{.iab}^k, \quad g^{ij} T_{.iab}^k = T_{..ab}^{kj}. \qquad (18)$$

1.2. Tensor operations

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

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

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

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

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 $\boldsymbol{c} = \boldsymbol{u} \times \boldsymbol{v}$ based on the *Levi-Civita tensor* is given by

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

and further can be written the covariant and contravariant components as

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

where 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

$$S^{ij} = \frac{1}{2}(T^{ij} + T^{ji}), \ \ A^{ij} = \frac{1}{2}(T^{ij} - T^{ji}). \quad (22)$$

1.3. Covariant differentiation

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

$$\frac{\partial^2 \bar{x}^\lambda}{\partial q^i \partial q^j} = \frac{\partial \bar{x}^\lambda}{\partial q^k} \begin{Bmatrix} k \\ ij \end{Bmatrix} - \frac{\partial \bar{x}^\alpha}{\partial q^i} \frac{\partial \bar{x}^\beta}{\partial q^j} \begin{Bmatrix} \lambda \\ \alpha\beta \end{Bmatrix}, \quad (23)$$

where $\left\{ {i \atop jk} \right\}$ 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

$$u_{i,j} = \frac{\partial u_i}{\partial q^j} = \frac{\partial \bar{x}^\alpha}{\partial q^i} \frac{\partial \bar{x}^\beta}{\partial q^j} \frac{\partial \bar{u}_\alpha}{\partial \bar{x}^\beta} + \frac{\partial^2 \bar{x}^\alpha}{\partial q^i \partial q^j} \bar{u}_\alpha = \bar{x}^\alpha_{,i} \bar{x}^\beta_{,j} \bar{u}_{\alpha,\beta} + \bar{x}^\alpha_{,ij} \bar{u}_\alpha, \qquad (24)$$

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 (23) by a vector component in bar space, we obtain

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

This can be finally rewritten as

$$u_{i;j} = \frac{\partial u_i}{\partial q^j} - \left\{ {k \atop ij} \right\} u_k = \frac{\partial \bar{x}^\alpha}{\partial q^i} \frac{\partial \bar{x}^\beta}{\partial q^j} \left(\frac{\partial \bar{u}_\alpha}{\partial \bar{x}^\beta} - \left\{ {\lambda \atop \alpha\beta} \right\} \bar{u}_\lambda \right), \qquad (25)$$

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

$$A^{ab...m}_{kl...n;j} = \frac{\partial A^{ab...m}_{kl...n}}{\partial q^j} + \left\{ {a \atop jd} \right\} A^{db...m}_{kl...n} + \left\{ {b \atop jd} \right\} A^{ad...m}_{kl...n} + ... + \left\{ {m \atop jd} \right\} A^{ab...d}_{kl...n}$$

$$- \left\{ {d \atop jk} \right\} A^{ab...m}_{dl...n} - \left\{ {d \atop jl} \right\} A^{ab...m}_{kd...n} - ... - \left\{ {d \atop jn} \right\} A^{ab...m}_{kl...d}, \qquad (26)$$

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

For the sake of applicability, some *covariant differentiation* explicit formulas

7

of tensors of various ranks are presented

$$f_{;j} = (\nabla f)_j = f_{,j}, \tag{27}$$

$$u^a_{;j} = (\nabla u^a)_j = u^a_{,j} + \begin{Bmatrix} a \\ jk \end{Bmatrix} u^k, \tag{28}$$

$$u_{a;j} = (\nabla u_a)_j = u_{a,j} - \begin{Bmatrix} k \\ ja \end{Bmatrix} u_k, \tag{29}$$

$$A^{ab}_{;j} = (\nabla A^{ab})_j = A^{ab}_{,j} + \begin{Bmatrix} a \\ jk \end{Bmatrix} A^{kb} + \begin{Bmatrix} b \\ jk \end{Bmatrix} A^{ak}, \tag{30}$$

$$A_{ab;j} = (\nabla A_{ab})_j = A_{ab,j} - \begin{Bmatrix} k \\ ja \end{Bmatrix} A_{kb} - \begin{Bmatrix} k \\ jb \end{Bmatrix} A_{ak}, \tag{31}$$

$$A^a_{b;j} = (\nabla A^a_b)_j = A_{ab,j} + \begin{Bmatrix} a \\ jk \end{Bmatrix} A^k_b - \begin{Bmatrix} k \\ jb \end{Bmatrix} A^a_k, \tag{32}$$

where f is a scalar function, $\boldsymbol{u}$ 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

$$\nabla A^{ab...m}_{kl...n} = (\nabla A^{ab...m}_{kl...n})_j \boldsymbol{b}^j = A^{ab...m}_{kl...n;j} \boldsymbol{b}^j. \tag{33}$$

Consequently, the divergence operation on a vector field reads

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

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

$$\nabla \cdot \boldsymbol{v} = v^i_{;i} = \frac{(g^{1/2} v^i)_{,i}}{g^{1/2}}, \tag{34}$$

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

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

$$T^{ij}_{;j} = \frac{(g^{1/2} S^{ij})_{,j}}{g^{1/2}} + \begin{Bmatrix} i \\ jk \end{Bmatrix} S^{jk} + \frac{(g^{1/2} A^{ij})_{,j}}{g^{1/2}}, \tag{35}$$

where the decomposition (22) has been used.

The Laplace operator in curvilinear coordinate system acts as

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

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

$$\nabla \cdot \nabla f = \frac{(g^{1/2} g^{ij} f_{,i})_{,j}}{g^{1/2}}. \tag{36}$$

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

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

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

$$(\nabla \times \boldsymbol{u})^i = g^{-1/2} (u_{k,j} - u_{j,k}). \tag{37}$$

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)

$$r = \sqrt{x^2 + y^2 + z^2}, \ \theta = \tan^{-1}\left(\frac{y}{x}\right), \ \phi = \cos^{-1}\left(\frac{z}{\sqrt{x^2 + y^2 + z^2}}\right), \tag{38}$$

and its Cartesian inverse

$$x = r\cos(\theta)\sin(\phi), \ y = r\sin(\theta)\sin(\phi), \ z = r\cos(\phi), \tag{39}$$

9

we can write the spherical curvilinear transformation

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

$$(40)$$

which is well defined (4)

$$
J = |\mathbf{T}_s| = r^2 \sin(\phi) = g_s^{1/2}. \tag{41}
$$

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

$$
\mathbf{g}_s = \begin{bmatrix} g_{rr} & 0 & 0 \\ 0 & g_{\theta\theta} & 0 \\ 0 & 0 & g_{\phi\phi} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & r^2\sin^2(\phi) & 0 \\ 0 & 0 & r^2 \end{bmatrix}. \tag{42}
$$

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 (42), which further provides the information about the basis vectors length

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

and from (11) one can directly write

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

In the case of orthogonal coordinate system it makes sense to define the scaling

$$
h_r = 1, \ h_\theta = r\sin(\phi), \ h_\phi = r, \tag{43}
$$

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

$$
\boldsymbol{u} = u^i \boldsymbol{b}_i = u_i \boldsymbol{b}^i = \sum_i u^i h_i \boldsymbol{e}_i = \sum_i \frac{u_i}{h_i} \boldsymbol{e}_i = u(i) \boldsymbol{e}_i, \tag{44}
$$

10

where a unique basis vectors $\boldsymbol{e}_i$ 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

$$
\begin{aligned}
u(r) &= u^r = u_r, \\
u(\theta) &= u^\theta r \sin(\phi) = \frac{u_\theta}{r \sin(\phi)}, \\
u(\phi) &= u^\phi r = \frac{u_\phi}{r},
\end{aligned}
\tag{45}
$$

The gradient of a scalar function f in spherical coordinates based on (33) reads

$$
\nabla f = f_{,i} \boldsymbol{b}^i = \frac{\partial f}{\partial r} \boldsymbol{e}_r + \frac{1}{r \sin(\phi)} \frac{\partial f}{\partial \theta} \boldsymbol{e}_\theta + \frac{1}{r} \frac{\partial f}{\partial \phi} \boldsymbol{e}_\phi.
\tag{46}
$$

The divergence of a vector field $\boldsymbol{v}$ in spherical coordinates based on (34)

$$
\begin{aligned}
\nabla \cdot \boldsymbol{u} = v^i_{;i} &= \frac{(r^2 \sin(\phi) v^i)_{,i}}{r^2 \sin(\phi)} = \frac{\partial v^r}{\partial r} + \frac{\partial v^\theta}{\partial \theta} + \frac{\partial v^\phi}{\partial \phi} + \frac{2v^r}{r} + \cot(\phi) v^\phi \\
&= \frac{\partial v(r)}{\partial r} + \frac{\partial v(\theta)/r \sin(\phi)}{\partial \theta} + \frac{\partial v(\phi)/r}{\partial \phi} + \frac{2v(r)}{r} + \cot(\phi) v(\phi)/r \\
&= \frac{1}{r^2} \frac{\partial v(r)}{\partial r} + \frac{1}{r \sin(\phi)} \frac{\partial v(\theta)}{\partial \theta} + \frac{1}{r \sin(\phi)} \frac{\partial \sin(\phi) v(\phi)}{\partial \phi}.
\end{aligned}
\tag{47}
$$

1.6. Cylindrical coordinates

Based on the curvilinear coordinates transformation (3)

$$
r = \sqrt{x^2 + y^2 + z^2}, \ \theta = \tan^{-1}\left(\frac{y}{x}\right), \ \phi = \cos^{-1}\left(\frac{z}{\sqrt{x^2 + y^2 + z^2}}\right),
\tag{48}
$$

and its Cartesian inverse

$$
x = r \cos(\theta) \sin(\phi), \ y = r \sin(\theta) \sin(\phi), \ z = z,
\tag{49}
$$

we can write the spherical curvilinear transformation

$$
\mathbf{T}_s = \begin{bmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial \phi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial \phi} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial \phi} \end{bmatrix} = \begin{bmatrix} \cos(\theta)\sin(\phi) & -r\sin(\theta)\sin(\phi) & r\cos(\theta)\cos(\phi) \\ \sin(\theta)\sin(\phi) & r\cos(\theta)\sin(\phi) & r\sin(\theta)\cos(\phi) \\ \cos(\phi) & 0 & -r\sin(\phi) \end{bmatrix},
\tag{50}
$$

11

which is well defined (4)

$$J = |\mathbf{T}_s| = r^2 \sin(\phi) = g_s^{1/2}. \tag{51}$$

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

$$\mathbf{g}_s = \begin{bmatrix} g_{rr} & 0 & 0 \\ 0 & g_{\theta\theta} & 0 \\ 0 & 0 & g_{\phi\phi} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & r^2 \sin^2(\phi) & 0 \\ 0 & 0 & r^2 \end{bmatrix}. \tag{52}$$

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 (52), which further provides the information about the basis vectors length

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

and from (11) one can directly write

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

In the case of orthogonal coordinate system it makes sense to define the scaling

$$h_r = 1, \ h_\theta = r\sin(\phi), \ h_\phi = r, \tag{53}$$

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

$$\boldsymbol{u} = u^i \boldsymbol{b}_i = u_i \boldsymbol{b}^i = \sum_i u^i h_i \boldsymbol{e}_i = \sum_i \frac{u_i}{h_i} \boldsymbol{e}_i = u(i)\boldsymbol{e}_i, \tag{54}$$

where a unique basis vectors $\boldsymbol{e}_i$ have been used, because they are identical for both covariant and contravariant bases, and they are also used as the basis for

55   physical components $u(i)$. The explicit relations between physical, covariant,

12

and contravariant components of vector in spherical coordinates are

$$
\begin{aligned}
u(r) &= u^r = u_r, \\
u(\theta) &= u^\theta r \sin(\phi) = \frac{u_\theta}{r \sin(\phi)}, \\
u(\phi) &= u^\phi r = \frac{u_\phi}{r},
\end{aligned}
\tag{55}
$$

The gradient of a scalar function f in spherical coordinates based on (33) reads

$$
\nabla f = f_{,i} \boldsymbol{b}^i = \frac{\partial f}{\partial r} \boldsymbol{e}_r + \frac{1}{r \sin(\phi)} \frac{\partial f}{\partial \theta} \boldsymbol{e}_\theta + \frac{1}{r} \frac{\partial f}{\partial \phi} \boldsymbol{e}_\phi.
\tag{56}
$$

The divergence of a vector field $\boldsymbol{v}$ in spherical coordinates based on (34)

$$
\begin{aligned}
\nabla \cdot \boldsymbol{u} = v^i_{;i} &= \frac{(r^2 \sin(\phi)v^i)_{,i}}{r^2 \sin(\phi)} = \frac{\partial v^r}{\partial r} + \frac{\partial v^\theta}{\partial \theta} + \frac{\partial v^\phi}{\partial \phi} + \frac{2v^r}{r} + \cot(\phi)v^\phi \\
&= \frac{\partial v(r)}{\partial r} + \frac{\partial v(\theta)/r \sin(\phi)}{\partial \theta} + \frac{\partial v(\phi)/r}{\partial \phi} + \frac{2v(r)}{r} + \cot(\phi)v(\phi)/r \\
&= \frac{1}{r^2} \frac{\partial v(r)}{\partial r} + \frac{1}{r \sin(\phi)} \frac{\partial v(\theta)}{\partial \theta} + \frac{1}{r \sin(\phi)} \frac{\partial \sin(\phi)v(\phi)}{\partial \phi}.
\end{aligned}
\tag{57}
$$

2. M1 model

2.1. AWBS Boltzmann transport equation

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

$$
v\boldsymbol{n} \cdot \nabla f + \frac{q_e}{m_e} \left(\boldsymbol{E} + \frac{v}{c} \boldsymbol{n} \times \boldsymbol{B} \right) \cdot \nabla_{\boldsymbol{v}} f = \nu_e v \frac{\partial}{\partial v} (f - f_M).
\tag{58}
$$

2.2. M1-AWBS model

In order to eliminate the dimensions of the transport problem (68) the two moment model referred to as *M1-AWBS* is introduced

$$
\begin{aligned}
\nu_e v \frac{\partial}{\partial v} (f_0 - f_M) &= v\nabla \cdot \boldsymbol{f}_1 + \frac{q_e}{m_e v^2} \boldsymbol{E} \cdot \frac{\partial}{\partial v} (v^2 \boldsymbol{f}_1), \\
\nu_e v \frac{\partial}{\partial v} \boldsymbol{f}_1 - \nu_t \boldsymbol{f}_1 &= v\nabla \cdot (\mathbf{A} f_0) + \frac{q_e}{m_e v^2} \boldsymbol{E} \cdot \frac{\partial}{\partial v} (v^2 \mathbf{A} f_0) \\
&\quad + \frac{q_e}{m_e v} \boldsymbol{E} \cdot (\mathbf{A} - \mathbf{I}) f_0 + \frac{q_e}{m_e c} \boldsymbol{B} \times \boldsymbol{f}_1,
\end{aligned}
\tag{60}
$$

13

where the anisotropy-closure matrix takes the form

$$\mathbf{A} = \frac{1}{3}\mathbf{I} + \frac{|\boldsymbol{f}_1|^2}{2f_0^2}\left(1 + \frac{|\boldsymbol{f}_1|^2}{f_0^2}\right)\left(\frac{\boldsymbol{f}_1 \otimes \boldsymbol{f}_1^T}{|\boldsymbol{f}_1|^2} - \frac{1}{3}\mathbf{I}\right), \tag{61}$$

which corresponds to the distribution function approximation

$$f = f_0 \frac{\left|\boldsymbol{M}_{(\boldsymbol{f}_1/f_0)}\right|}{4\pi \sinh\left(\boldsymbol{M}_{(\boldsymbol{f}_1/f_0)}\right)} \exp\left(\boldsymbol{n} \cdot \boldsymbol{M}_{(\boldsymbol{f}_1/f_0)}\right), \tag{62}$$

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

3. Diffusive regime

3.1. Lorentz approximation

3.1.1. BGK collision operator

3.1.2. AWBS collision operator

3.2. Physical analysis of the diffusive asymptotics

The equilibrium (maximized entropy) distribution

$$f_M = \frac{\rho}{v_{th}^3 \left(2\pi\right)^{3/2}} \exp\left(-\frac{v^2}{2v_{th}^2}\right), \tag{63}$$

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

$$\begin{aligned}
\frac{\partial f_M}{\partial v} &= -\frac{v}{v_{th}^2} f_M, \\
\frac{\partial f_M}{\partial \rho} &= \frac{1}{\rho} f_M, \\
\frac{\partial f_M}{\partial T} &= \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2}\right)\frac{1}{T} f_M.
\end{aligned} \tag{64}$$

The BGK equation, valid for highly isotropic transport, represents the simplest form of the Boltzmann transport equation

$$\boldsymbol{n} \cdot \nabla f + \boldsymbol{n} \cdot \tilde{\boldsymbol{E}}\frac{1}{v}\frac{\partial f}{\partial v} = \frac{(f_M - f)}{\lambda} + \frac{(f_0 - f)}{\tilde{\lambda}}, \tag{65}$$

where $\lambda = \frac{v}{\nu_e} = \frac{v^4}{\sigma\rho}$ is the mean free path expressed as inverse of collisional frequency multiplied by particle velocity, $\tilde{\lambda} = \frac{\lambda}{\alpha}$ is a scattering mean free path

14

expressed as α factor of λ, and f_0 is the isotropic part of the distribution function, thus making the scattering operator being conservative.

The Chapman-Enskog based small parameter (λ) approximation $f \approx f_0 + \lambda f_1 + O(\lambda^2)$ expressed as

$$\boldsymbol{n} \cdot \nabla(f_0 + \lambda f_1) + \boldsymbol{n} \cdot \tilde{\boldsymbol{E}} \frac{1}{v} \frac{\partial f_0 + \lambda f_1}{\partial v} = \frac{(f_M - (f_0 + \lambda f_1))}{\lambda} - \alpha f_1, \qquad (66)$$

tells us, that

$$
\begin{aligned}
f_0 &= f_M, \\
f_1 &= -\boldsymbol{n} \cdot \left(\nabla f_0 + \tilde{\boldsymbol{E}} \frac{1}{v} \frac{\partial f_0}{\partial v} \right) \frac{1}{1 + \alpha} = -\boldsymbol{n} \cdot \left(\nabla f_M + \tilde{\boldsymbol{E}} \frac{1}{v} \frac{\partial f_M}{\partial v} \right) \frac{1}{1 + \alpha},
\end{aligned}
$$

which means, that the localized approximation of the distribution function should behave as

$$
\begin{aligned}
f \approx f_M - \frac{\lambda}{1+\alpha} \boldsymbol{n} \cdot \left(\nabla f_M + \tilde{\boldsymbol{E}} \frac{1}{v} \frac{\partial f_M}{\partial v} \right) = \\
f_M \left(1 - \frac{\lambda}{1+\alpha} \boldsymbol{n} \cdot \left(\frac{\nabla \rho}{\rho} + \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} \right) \frac{\nabla T}{T} - \frac{\tilde{\boldsymbol{E}}}{v_{th}^2} \right) \right). \quad (67)
\end{aligned}
$$

75 *3.3. Physical analysis of the diffusive asymptotics of AWBS*

The AWBS equation, valid for fast particle transport, represents one of the simplest forms of the Boltzmann transport equation

$$v \boldsymbol{n} \cdot \nabla f + \boldsymbol{n} \cdot \tilde{\boldsymbol{E}} \frac{\partial f}{\partial v} = v \nu_e \frac{\partial}{\partial v} (f - f_M) + \nu_t (f_0 - f), \qquad (68)$$

where $\nu_e = \frac{\sigma \rho}{v^3}$ is the collisional frequency and $\nu_t = \alpha \nu_e$ is the scattering collisional frequency expressed as α factor of the collisional frequency. We can further proceed by writing the AWBS transport equation in terms of mean free path as

$$\boldsymbol{n} \cdot \nabla f + \boldsymbol{n} \cdot \tilde{\boldsymbol{E}} \frac{1}{v} \frac{\partial f}{\partial v} = \frac{v}{\lambda} \frac{\partial}{\partial v} (f - f_M) + \frac{\alpha}{\lambda} (f_0 - f), \qquad (69)$$

The Chapman-Enskog based small parameter (λ) approximation $f \approx f_0 + \lambda f_1 + O(\lambda^2)$ expressed as

$$\boldsymbol{n} \cdot \nabla(f_0 + \lambda f_1) + \boldsymbol{n} \cdot \tilde{\boldsymbol{E}} \frac{1}{v} \frac{\partial f_0 + \lambda f_1}{\partial v} = \frac{v}{\lambda} \frac{\partial}{\partial v} (((f_0 + \lambda f_1)) - f_M) - \alpha f_1, \quad (70)$$

15

tells us, that

$$\frac{\partial f_0}{\partial v} = \frac{\partial f_M}{\partial v} \to f_0 = f_M,$$

$$f_1 = -\left(\boldsymbol{n} \cdot \left(\nabla f_0 + \tilde{\boldsymbol{E}}\frac{1}{v}\frac{\partial f_0}{\partial v}\right) - v\frac{\partial f_1}{\partial v}\right)\frac{1}{\alpha},$$

which means, that the localized approximation of the distribution function should behave as

$$f \approx f_M - \frac{\lambda}{\alpha}\boldsymbol{n} \cdot \left(\nabla f_M + \tilde{\boldsymbol{E}}\frac{1}{v}\frac{\partial f_M}{\partial v}\right) + \frac{v\lambda}{\alpha}\frac{\partial f_1}{\partial v} =$$

$$f_M\left(1 - \frac{\lambda}{\alpha}\boldsymbol{n} \cdot \left(\frac{\nabla\rho}{\rho} + \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2}\right)\frac{\nabla T}{T} - \frac{\tilde{\boldsymbol{E}}}{v_{th}^2}\right)\right) + \frac{v\lambda}{\alpha}\frac{\partial f_1}{\partial v}. \quad (71)$$

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

$$\boldsymbol{j} = \int_0^\infty \int_{4\pi} q_e v \boldsymbol{n} f \, \mathrm{d}\boldsymbol{n} \; v^2 \; \mathrm{d}v = \boldsymbol{0}, \quad (72)$$

can be achieved by providing a consistent electric field in (71), i.e.

$$\tilde{\boldsymbol{E}} = \frac{v_{th}^2 \; \int_{4\pi} \boldsymbol{n} \otimes \boldsymbol{n} \cdot \int_0^\infty v f_M \frac{\lambda}{\alpha} \left(\frac{\nabla\rho}{\rho} + \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2}\right)\frac{\nabla T}{T}\right) v^2 \, \mathrm{d}v \, \mathrm{d}\boldsymbol{n}}{\int_{4\pi} \boldsymbol{n} \otimes \boldsymbol{n} \cdot \int_0^\infty v f_M \frac{\lambda}{\alpha} v^2 \, \mathrm{d}v \, \mathrm{d}\boldsymbol{n}}, \quad (73)$$

which may be further simplified as

$$\tilde{\boldsymbol{E}} = \frac{\int_0^\infty f_M \frac{1}{2}\frac{\nabla T}{T} v^9 \, \mathrm{d}v}{\int_0^\infty f_M v^7 \, \mathrm{d}v} + v_{th}^2\left(\frac{\nabla\rho}{\rho} - \frac{3}{2}\frac{\nabla T}{T}\right) = v_{th}^2\left(\frac{\nabla\rho}{\rho} + \frac{5}{2}\frac{\nabla T}{T}\right), \quad (74)$$

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

$$f \approx f_M\left(1 - \frac{\lambda}{\alpha}\boldsymbol{n} \cdot \left(\frac{v^2}{2v_{th}^2} - \frac{3}{2} - \frac{5}{2}\right)\frac{\nabla T}{T}\right) + \frac{v\lambda}{\alpha}\frac{\partial f_1}{\partial v}. \quad (75)$$

which leads to the resulting heat flux

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

Based on the Gauss integral formula

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

and Maxwell-Boltzmann distribution (63) the heat flux can be written as

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

(76)

In conclusion, equation (76) 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).

4. High-order finite element scheme

4.1. Variational principle

First, the electro-magnetic scaling

$$\tilde{\boldsymbol{E}} = \frac{q_e}{m_e}\boldsymbol{E},\ \tilde{\boldsymbol{B}} = \frac{q_e}{m_e c}\boldsymbol{B},$$

(77)

is defined in order to make the algebraic operations easier to follow. The general variational formulation of (59) and (60) constructed above the scalar (zero moment) functional space represented by test functions ϕ and the vector (first moment) functional space represented by test functions $\boldsymbol{w}$ takes the form

$$\int_\Omega \phi\nu_e\frac{\partial f_0}{\partial v} = \int_\Omega \phi\left(\mathbf{I}:\nabla\boldsymbol{f}_1 + \frac{1}{v}\tilde{\boldsymbol{E}}\cdot\frac{\partial\boldsymbol{f}_1}{\partial v} + \frac{2}{v^2}\tilde{\boldsymbol{E}}\cdot\boldsymbol{f}_1 + \nu_e\frac{\partial f_M}{\partial v}\right),$$ (78)

$$\int_\Omega \boldsymbol{w}\cdot\nu_e\frac{\partial\boldsymbol{f}_1}{\partial v} = \int_\Omega \boldsymbol{w}\cdot\left(\nabla\cdot(\mathbf{A}f_0) + \frac{1}{v^2}\tilde{\boldsymbol{E}}\cdot(3\mathbf{A}-\mathbf{I})\,f_0\right.$$

$$\left.+\frac{1}{v}\tilde{\boldsymbol{E}}\cdot\frac{\partial}{\partial v}(\mathbf{A}f_0) + \frac{1}{v}\tilde{\boldsymbol{B}}\times\boldsymbol{f}_1 + \frac{\nu_t}{v}\boldsymbol{f}_1\right).$$ (79)

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

$$\int_\Omega \boldsymbol{\phi}\otimes\boldsymbol{\phi}^T\nu_e\,\mathrm{d}\Omega\cdot\frac{\partial\boldsymbol{f}_0}{\partial v} = \int_\Omega \boldsymbol{\phi}\otimes\left(\mathbf{I}:\nabla\mathbf{w}^T + \frac{2}{v^2}\tilde{\boldsymbol{E}}^T\cdot\mathbf{w}^T\right)\mathrm{d}\Omega\cdot\boldsymbol{f}_1$$

$$+\int_\Omega \boldsymbol{\phi}\otimes\frac{1}{v}\tilde{\boldsymbol{E}}^T\cdot\mathbf{w}^T\,\mathrm{d}\Omega\cdot\frac{\partial\boldsymbol{f}_1}{\partial v} + \int_\Omega \boldsymbol{\phi}\otimes\boldsymbol{\phi}^T\nu_e\,\mathrm{d}\Omega\cdot\frac{\partial\boldsymbol{f}_M}{\partial v},$$ (80)

17

$$\int_\Omega \mathbf{w} \cdot \mathbf{w}^T \nu_e \, \mathrm{d}\Omega \cdot \frac{\partial \boldsymbol{f}_1}{\partial v} = -\int_\Omega (\mathbf{A} : \nabla \mathbf{w}) \, \boldsymbol{\phi}^T \, \mathrm{d}\Omega \cdot \boldsymbol{f}_0$$

$$+ \int_\Omega \mathbf{w} \cdot \frac{1}{v^2} \left(3\mathbf{A} - \mathbf{I}\right) \cdot \tilde{\boldsymbol{E}} \, \boldsymbol{\phi}^T \, \mathrm{d}\Omega \cdot \boldsymbol{f}_0 + \int_\Omega \mathbf{w} \cdot \frac{1}{v}\mathbf{A} \cdot \tilde{\boldsymbol{E}} \, \boldsymbol{\phi}^T \, \mathrm{d}\Omega \cdot \frac{\partial \boldsymbol{f}_0}{\partial v}$$

$$+ \int_\Omega \mathbf{w} \cdot \left(\frac{1}{v}\tilde{\boldsymbol{B}} \times \mathbf{w}^T + \frac{\nu_t}{v}\mathbf{w}^T\right) \, \mathrm{d}\Omega \cdot \boldsymbol{f}_1, \quad (81)$$

where $\boldsymbol{\phi}$ 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.

4.2. Semi-discrete formulation

In principle, only five following integrators need to be coded to provide a discrete representation (80) and (81), i.e.

$$\mathcal{M}^0_{(g)} = \int_\Omega \boldsymbol{\phi} \otimes \boldsymbol{\phi}^T g \, \mathrm{d}\Omega, \tag{82}$$

$$\mathcal{M}^1_{(g)} = \int_\Omega \mathbf{w} \cdot \mathbf{w}^T g \, \mathrm{d}\Omega, \tag{83}$$

$$\mathcal{D}_{(\mathbf{G})} = \int_\Omega \mathbf{G} : \nabla \mathbf{w} \otimes \boldsymbol{\phi}^T \, \mathrm{d}\Omega, \tag{84}$$

$$\mathcal{V}_{(\boldsymbol{g})} = \int_\Omega \mathbf{w} \cdot \boldsymbol{g} \otimes \boldsymbol{\phi}^T \, \mathrm{d}\Omega, \tag{85}$$

$$\mathcal{B}_{(\boldsymbol{g})} = \int_\Omega \mathbf{w} \cdot \boldsymbol{g} \times \mathbf{w}^T \, \mathrm{d}\Omega. \tag{86}$$

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

$$\boldsymbol{\phi} = \begin{bmatrix} \phi_1 \\ \vdots \\ \phi_{N_0} \end{bmatrix}, \ \mathbf{w} = \begin{bmatrix} w_{1,1} & \dots & w_{1,d} \\ \vdots & \ddots & \vdots \\ w_{N_1,1} & \dots & w_{N_1,d} \end{bmatrix}, \ \boldsymbol{g} = \begin{bmatrix} g_1 \\ \vdots \\ g_d \end{bmatrix}, \ \mathbf{G} = \begin{bmatrix} G_{1,1} & \dots & G_{1,d} \\ \vdots & \ddots & \vdots \\ G_{d,1} & \dots & G_{d,d} \end{bmatrix},$$
$$\tag{87}$$

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

Consequently, the discrete analog of M1-AWBS equations (59) and (60) can

18

be written based on (80), (81) as

$$\boldsymbol{\mathcal{M}}_{(\nu_e)}^0 \cdot \frac{\partial \boldsymbol{f}_0}{\partial v} - \boldsymbol{\mathcal{M}}_{(\nu_e)}^0 \cdot \frac{\partial \boldsymbol{f}_M}{\partial v} = \boldsymbol{\mathcal{D}}_{(\mathbf{I})}^T \cdot \boldsymbol{f}_1 + \frac{1}{v} \boldsymbol{\mathcal{V}}_{(\tilde{\boldsymbol{E}})}^T \cdot \frac{\partial \boldsymbol{f}_1}{\partial v} + \frac{2}{v^2} \boldsymbol{\mathcal{V}}_{(\tilde{\boldsymbol{E}})}^T \cdot \boldsymbol{f}_1, \quad (88)$$

$$\boldsymbol{\mathcal{M}}_{(\nu_e)}^1 \cdot \frac{\partial \boldsymbol{f}_1}{\partial v} - \frac{1}{v} \boldsymbol{\mathcal{M}}_{(\nu_t)}^1 \cdot \boldsymbol{f}_1 = -\boldsymbol{\mathcal{D}}_{(\mathbf{A})} \cdot \boldsymbol{f}_0$$
$$+ \frac{1}{v} \boldsymbol{\mathcal{V}}_{(\mathbf{A} \cdot \tilde{\boldsymbol{E}})} \cdot \frac{\partial \boldsymbol{f}_0}{\partial v} + \frac{1}{v^2} \boldsymbol{\mathcal{V}}_{((3\mathbf{A} - \mathbf{I}) \cdot \tilde{\boldsymbol{E}})} \cdot \boldsymbol{f}_0 + \frac{1}{v} \boldsymbol{\mathcal{B}}_{(\tilde{\boldsymbol{B}})} \cdot \boldsymbol{f}_1, \quad (89)$$

where the integrators (82), (83), (84), (85), (86) are used acting on appropriate functions ρ, ν_e, ν_t, vectors $\tilde{\boldsymbol{E}}$, $\tilde{\boldsymbol{B}}$, and matrices $\mathbf{A}$ and $\mathbf{I}$.

4.3. 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 $\boldsymbol{f}_0$ is computed as

$$\left(\boldsymbol{\mathcal{M}}_{(\nu_e)}^0 - \boldsymbol{\mathcal{M}}_{\left(\frac{1}{v \boldsymbol{f}_0^n} \tilde{\boldsymbol{E}}^T \cdot \boldsymbol{f}_1^n \right)}^0 \right) \cdot \frac{\mathrm{d} \boldsymbol{f}_0}{\mathrm{d} v}^* = \boldsymbol{\mathcal{D}}_{(\mathbf{I})}^T \cdot \boldsymbol{f}_1^n + \frac{2}{v^2} \boldsymbol{\mathcal{V}}_{(\tilde{\boldsymbol{E}})}^T \cdot \boldsymbol{f}_1^n + \boldsymbol{\mathcal{M}}_{(\nu_e)}^0 \cdot \frac{\partial \boldsymbol{f}_M}{\partial v},$$
$$(90)$$

where the actual evolution of $\boldsymbol{f}_1$ has been redefined as similar to the time evolution of $\boldsymbol{f}_0$ (compare (90) to (88)). Then, the actual computation of the time evolution of $\boldsymbol{f}_1$ follows

$$\boldsymbol{\mathcal{M}}_{(\nu_e)}^1 \cdot \frac{\mathrm{d} \boldsymbol{f}_1}{\mathrm{d} v} = -\boldsymbol{\mathcal{D}}_{(\mathbf{A})} \cdot \boldsymbol{f}_0^n + \frac{1}{v} \boldsymbol{\mathcal{V}}_{(\mathbf{A} \cdot \tilde{\boldsymbol{E}})} \cdot \frac{\mathrm{d} \boldsymbol{f}_0}{\mathrm{d} v}^*$$
$$+ \frac{1}{v^2} \boldsymbol{\mathcal{V}}_{((3\mathbf{A} - \mathbf{I}) \cdot \tilde{\boldsymbol{E}})} \cdot \boldsymbol{f}_0^n + \frac{1}{v} \boldsymbol{\mathcal{B}}_{(\tilde{\boldsymbol{B}})} \cdot \boldsymbol{f}_1^n + \frac{1}{v} \boldsymbol{\mathcal{M}}_{(\nu_t)}^1 \cdot \boldsymbol{f}_1^n. \quad (91)$$

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

As can be seen in FIG. 4.5 we get a heat flux profile corresponding to temperature and density profiles computed by Laghos [3] in 1D and we have also double checked the numerical scheme in 2D and 3D, where apparently the flux

19

profiles exhibit the same physical background. It is important to note, that the current implementation does not include neither electric or magnetic field $(\tilde{\boldsymbol{E}}, \tilde{\boldsymbol{B}})$.

¹¹⁰ It is worth mentioning, that the proposed discrete scheme (90) and (91) naturally obeys the CFL condition with respect to the mesh smallest cell size/mean-stopping-power, and consequently, we needed 8858 energy groups in 1D, 4348 energy groups in 2D, and 10030 energy groups in 3D. This would make the hydro simulation to take more than 1000x longer than classical (SH) hydro.

¹¹⁵ *4.4. AWBS diffusive asymptotic nonlinearity check*

$$\boldsymbol{q}_1 = a_1 \; T_1^{\alpha} \; \nabla T_1, \quad \boldsymbol{q}_0 = a_0 \; T_0^{\alpha} \; \nabla T_0,$$

where we keep $a_1 = a_0 = a$ and $\nabla T_1 = \nabla T_0 = \nabla T$ to be equal in every point of the computational domain. The ration of the fluxes than provides a very important information about flux nonlinearity

$$\frac{\boldsymbol{q}_1}{\boldsymbol{q}_0} = \frac{a \; T_1^{\alpha} \; \nabla T}{a \; T_0^{\alpha} \; \nabla T} = \left(\frac{T_1}{T_0}\right)^{\alpha},$$

where the nonlinearity is better expressed as

$$\alpha = \frac{\log\left(\frac{\boldsymbol{q}_1}{\boldsymbol{q}_0}\right)}{\log\left(\frac{T_1}{T_0}\right)} \tag{92}$$

Finally, based on the simulation results of two runs corresponding to temperature T_0 with the mean $T = 1000$ executed as

mpirun -np 8 nth -p 5 -m data/segment01.mesh -rs 6 -tf 0.0 -ok 4 -ot 3

-vis -fa -print -Tmax 1050 -Tmin 950 -a0 1e12,

and to temperature T_1 with the mean $T = 1100$ executed as

mpirun -np 8 nth -p 5 -m data/segment01.mesh -rs 6 -tf 0.0 -ok 4 -ot 3

-vis -fa -print -Tmax 1150 -Tmin 1050 -a0 1e12,

20

we got the following numbers

$$\boldsymbol{q}_1 = 0.0891, \ \boldsymbol{q}_0 = 0.0703, \ T_1 = 1100, \ T_0 = 1000,$$

which provide the corresponding nonlinearity
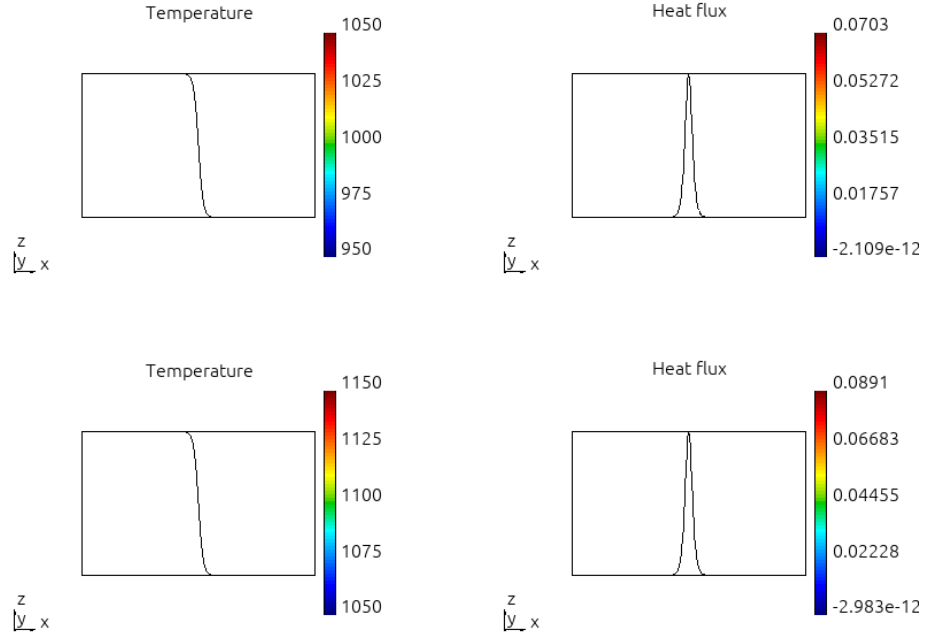
$$\alpha = 2.486487132294661. \tag{93}$$

Figure 1: Problem 5 - AWBS nonlinearity check.

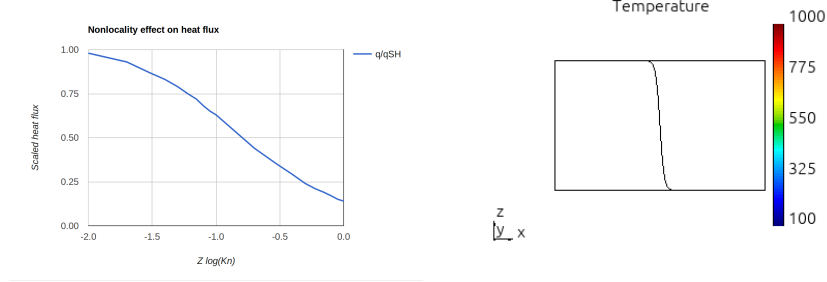### 4.5. Analysis of nonlocality

Figure 2: M1-AWBS model. Left: The maximum of computed flux normalized with respect to the value of SH flux. E field effect is not included. Right: Corresponding temperature profile. Density and ionization (scattering on Z = 100 included) have been kept constant.
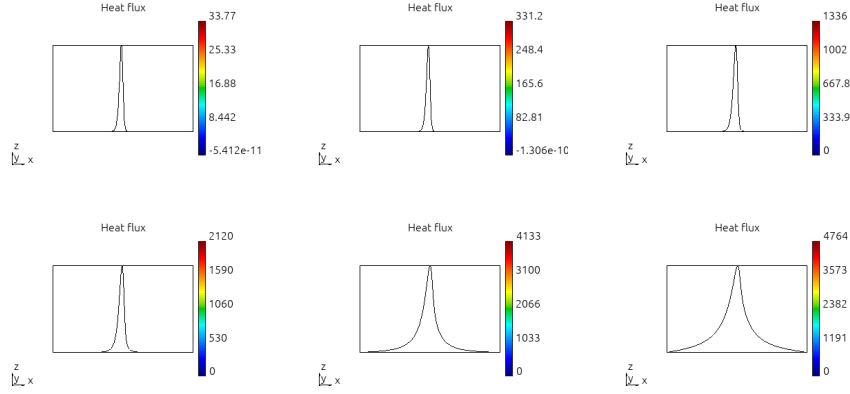

Figure 3: Heat flux calculated by M1-AWBS model. Figures in left-right top-bottom order correspond to Kn = 0.001, 0.01, 0.05, 0.1, 0.5, 1.0. E field effect is not included. Density and ionization (Z = 100) have been kept constant.

Some observations:

- Our calculated distribution function is thermalized, i.e. $f_0 = f_M$.

- With added scattering we also obtain the correct value of calculated heat flux, i.e. $q = q_{SH}$, nevertheless, this works with no E field.

- The E field effect is implemented. When tested with the analytic formula $E_{SH} = v_{th}^2(\nabla ne/ne + 5/2 nablaT/T)$ (we consider Z=100), the corresponding flux reduction due to E field is also correct (flux is reduced to 30% of its E=0 value).

125

- However, the E_{SH} does not work under any condition, i.e. it exhibits some extra dependence on temperature.
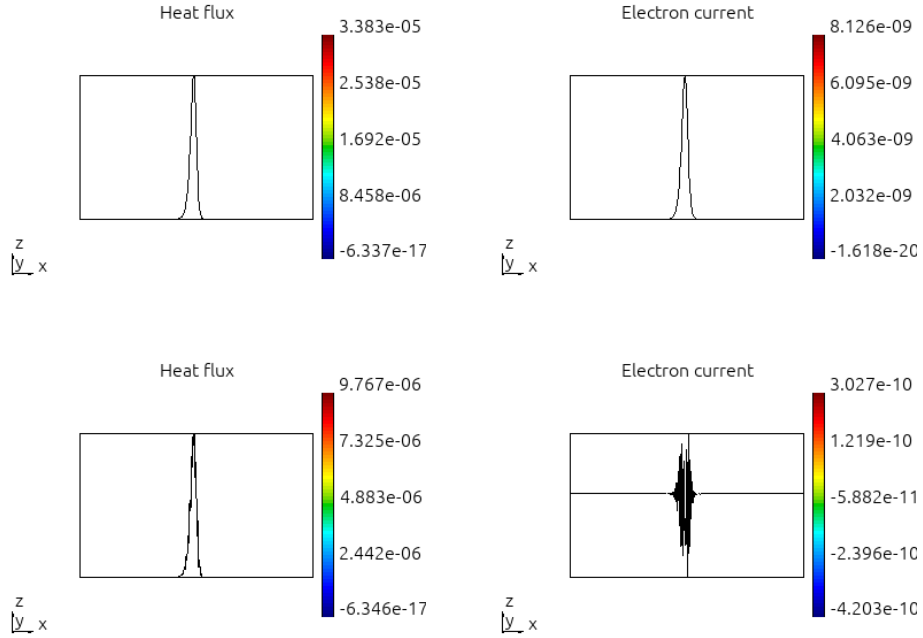

Figure 4: Preliminary results with respect to the E field effect. The SH analytic formula for E field leads to the corresponding current reduction ($j \approx 0$). The corresponding heat flux is reduced $\approx$ by 70 %, exactly as predicted. Nevertheless, the formula exhibits some dependence on temperature (not on its gradient and also not on the mean free path).
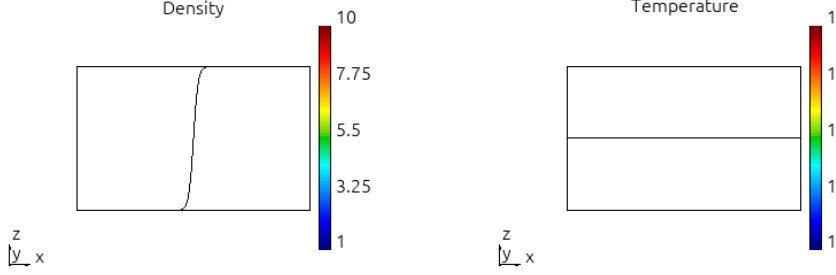
Figure 5: Problem 4 background.

4.6. Implicit fully-discrete scheme

In order to formulate a fully-discrete scheme leaning on an implicit discretiza-
tion of velocity, the equations (88) and (89) can be expressed with matrices as

$$\mathbf{M}_0 \cdot \frac{\partial \boldsymbol{f}_0}{\partial v} = \mathbf{D}_0 \cdot \boldsymbol{f}_1 + \mathbf{E}_0^1 \cdot \frac{\partial \boldsymbol{f}_1}{\partial v} + \mathbf{E}_0^2 \cdot \boldsymbol{f}_1 + \mathbf{M}_0 \cdot \frac{\partial \boldsymbol{f}_M}{\partial v},$$

$$\mathbf{M}_1 \cdot \frac{\partial \boldsymbol{f}_1}{\partial v} = -\mathbf{D}_1 \cdot \boldsymbol{f}_0 + \mathbf{E}_1^1 \cdot \frac{\partial \boldsymbol{f}_0}{\partial v} + \mathbf{E}_1^2 \cdot \boldsymbol{f}_0 + \mathbf{B} \cdot \boldsymbol{f}_1 + \mathbf{M}_1^t \cdot \boldsymbol{f}_1,$$

$$\frac{\mathrm{d}\boldsymbol{f}_0}{\mathrm{d}v} = \mathbf{M}_0^{-1} \cdot \left(\mathbf{D}_0 + \mathbf{E}_0^2 \right) \cdot \left(\boldsymbol{f}_1^n + \Delta v \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v} \right) + \mathbf{M}_0^{-1} \cdot \mathbf{E}_0^1 \cdot \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v}$$

$$+ \frac{\partial \boldsymbol{f}_M}{\partial v},$$

$$\mathbf{M}_1 \cdot \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v} = \left(\mathbf{E}_1^2 - \mathbf{D}_1 \right) \cdot \left(\boldsymbol{f}_0^n + \Delta v \frac{\mathrm{d}\boldsymbol{f}_0}{\mathrm{d}v} \right) + \mathbf{E}_1^1 \cdot \frac{\mathrm{d}\boldsymbol{f}_0}{\mathrm{d}v}$$

$$+ \left(\mathbf{B} + \mathbf{M}_1^t \right) \cdot \left(\boldsymbol{f}_1^n + \Delta v \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v} \right),$$

$$\frac{\mathrm{d}\boldsymbol{f}_0}{\mathrm{d}v} = \tilde{\mathbf{A}}_0 \cdot \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v} + \boldsymbol{b}_0 \left(\boldsymbol{f}_1^n, \frac{\partial \boldsymbol{f}_M}{\partial v} \right), \quad (94)$$

$$\left(\mathbf{M}_1 - \Delta v \left(\mathbf{B} + \mathbf{M}_1^t \right) \right) \cdot \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v} = \tilde{\mathbf{A}}_1 \cdot \frac{\mathrm{d}\boldsymbol{f}_0}{\mathrm{d}v} + \boldsymbol{b}_1 \left(\boldsymbol{f}_1^n, \boldsymbol{f}_0^n \right), \quad (95)$$

$$\left(\mathbf{M}_1 - \Delta v \left(\mathbf{B} + \mathbf{M}_1^t \right) - \tilde{\mathbf{A}}_1 \cdot \tilde{\mathbf{A}}_0 \right) \cdot \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v} = \tilde{\mathbf{A}}_1 \cdot \boldsymbol{b}_0 + \boldsymbol{b}_1, \quad (96)$$

[3]

24

References

[1] D. Mihalas, B. Mihalas, Foundations of Radiation Hydrodynamics, Oxford University Press, New York, 1985.

[2] J. R. Albritton, E. A. Williams, I. B. Bernstein, Nonlocal electron heat transport by not quite maxwell-boltzmann distributions, Phys. Rev. Lett. 57 (1986) 1887–1890.

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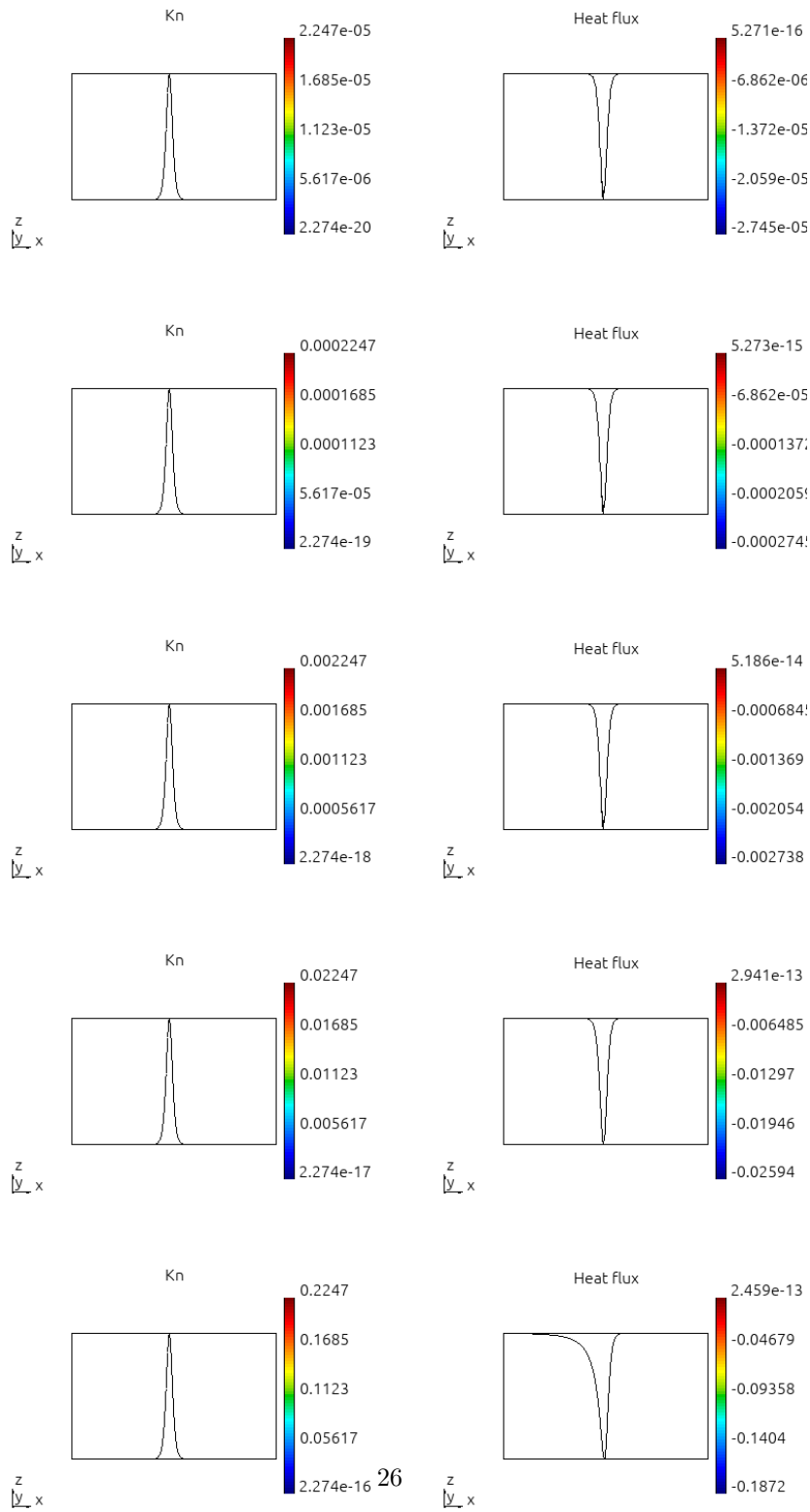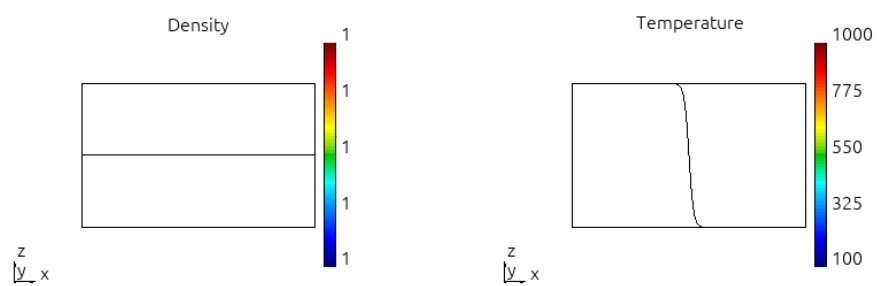
Kn

2.247e-05

1.685e-05

1.123e-05

5.617e-06

2.274e-20

z
y   x

Heat flux

5.271e-16

-6.862e-06

-1.372e-05

-2.059e-05

-2.745e-05

z
y   x

Kn

0.0002247

0.0001685

0.0001123

5.617e-05

2.274e-19

z
y   x

Heat flux

5.273e-15

-6.862e-05

-0.0001372

-0.0002059

-0.0002745

z
y   x

Kn

0.002247

0.001685

0.001123

0.0005617

2.274e-18

z
y   x

Heat flux

5.186e-14

-0.0006845

-0.001369

-0.002054

-0.002738

z
y   x

Kn

0.02247

0.01685

0.01123

0.005617

2.274e-17

z
y   x

Heat flux

2.941e-13

-0.006485

-0.01297

-0.01946

-0.02594

z
y   x

Kn

0.2247

0.1685

0.1123

0.05617

2.274e-16

z
y   x

Heat flux

2.459e-13

-0.04679

-0.09358

-0.1404

-0.1872

z
y   x

Figure 6:   Problem 4 transport.

Figure 7: VFP-paper corresponding simulations, ion background density and temperature.

Kn

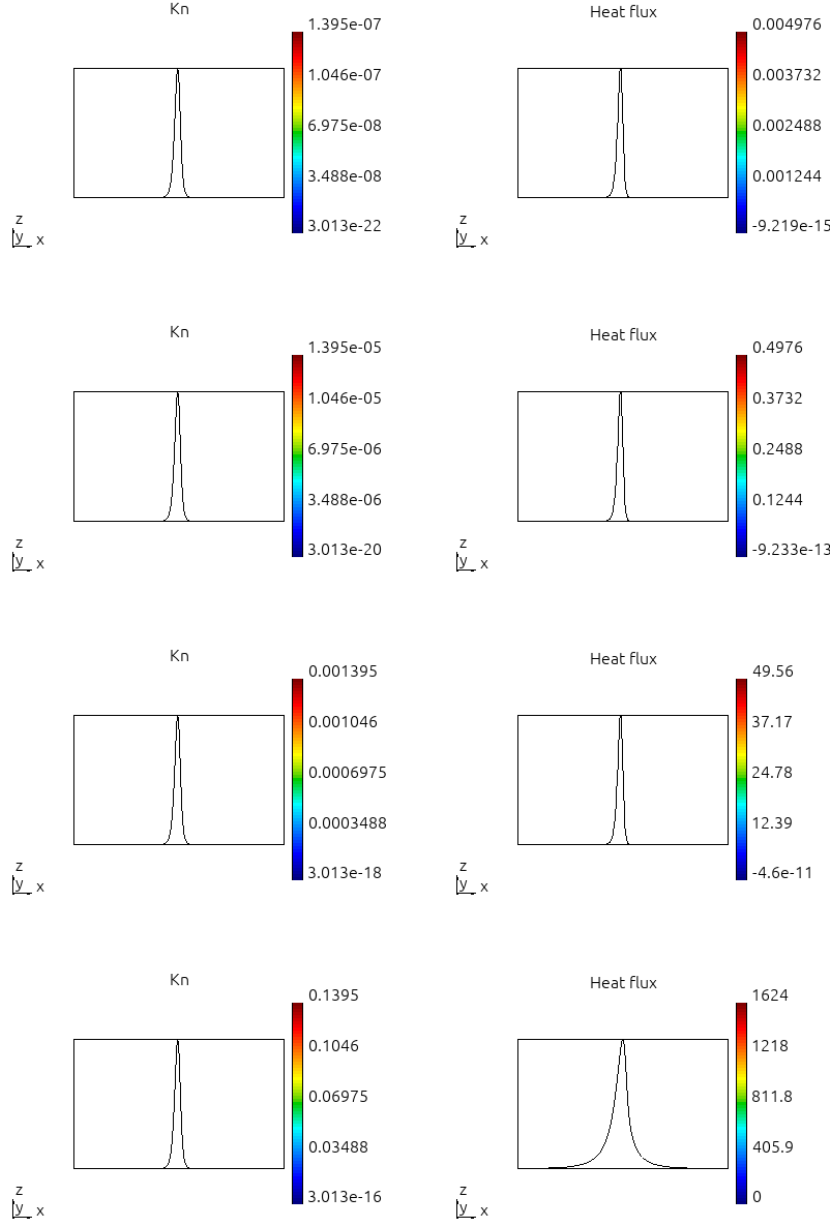1.395e-07

1.046e-07

6.975e-08

3.488e-08

3.013e-22

z
y x

Heat flux

0.004976

0.003732

0.002488

0.001244

-9.219e-15

z
y x

Kn

1.395e-05

1.046e-05

6.975e-06

3.488e-06

3.013e-20

z
y x

Heat flux

0.4976

0.3732

0.2488

0.1244

-9.233e-13

z
y x

Kn

0.001395

0.001046

0.0006975

0.0003488

3.013e-18

z
y x

Heat flux

49.56

37.17

24.78

12.39

-4.6e-11

z
y x

Kn

0.1395

0.1046

0.06975

0.03488

3.013e-16

z
y x

Heat flux

1624

1218

811.8

405.9

0

z
y x

Figure 8: VFP-paper corresponding simulations, Kn spans the interval ($\approx 10^{-7}, \approx 10^{-1}$) where flux goes from diffusive to highly nonlocal.
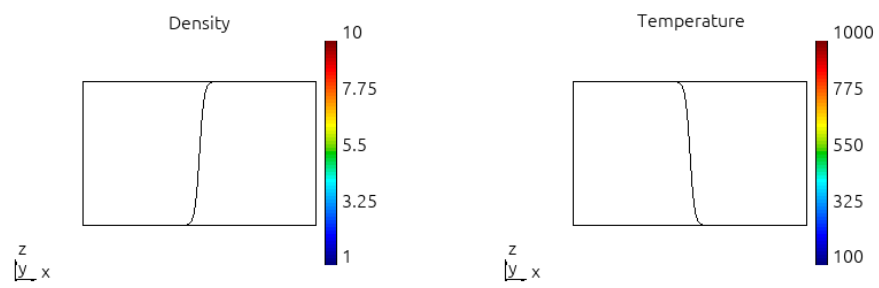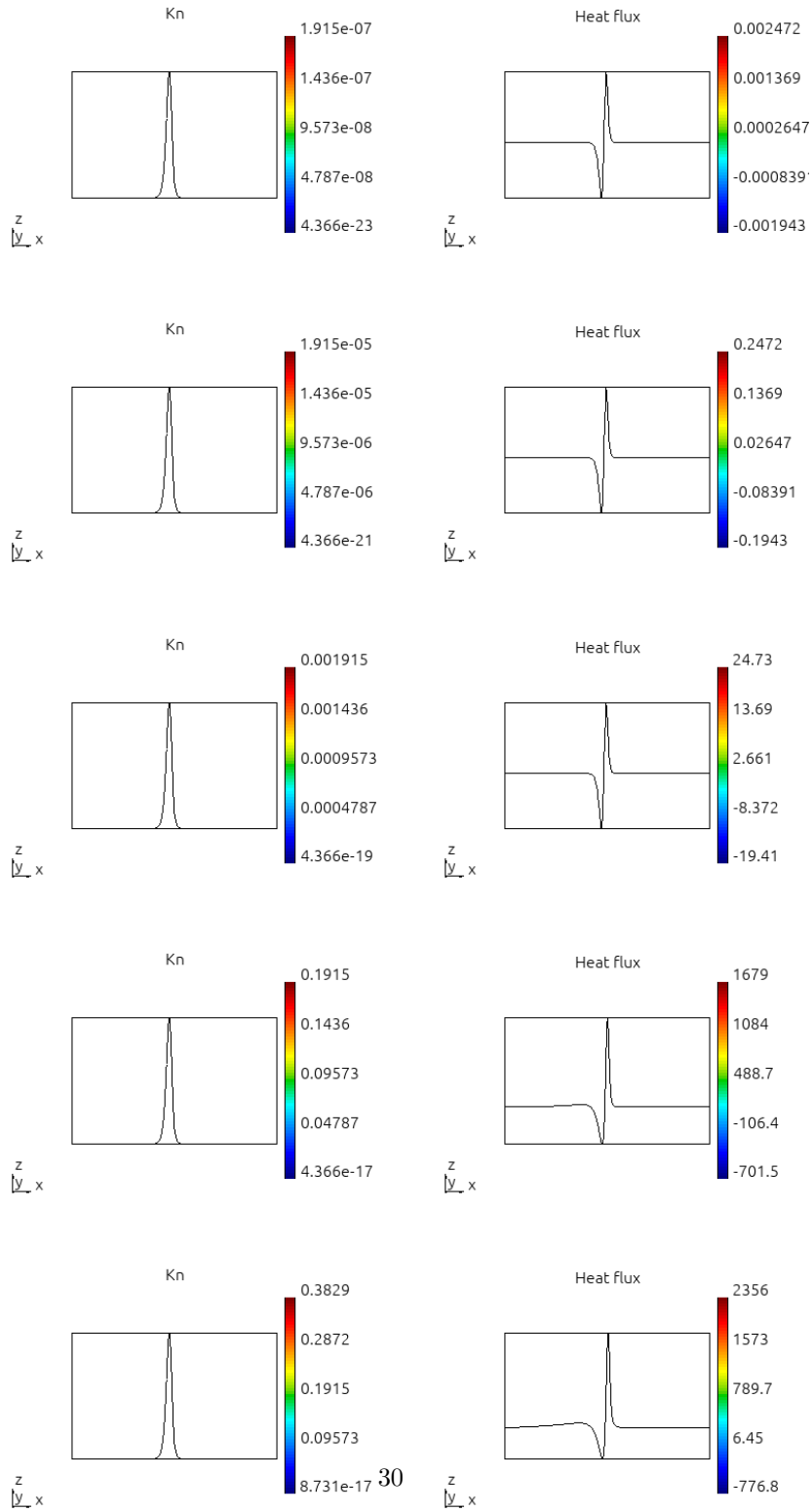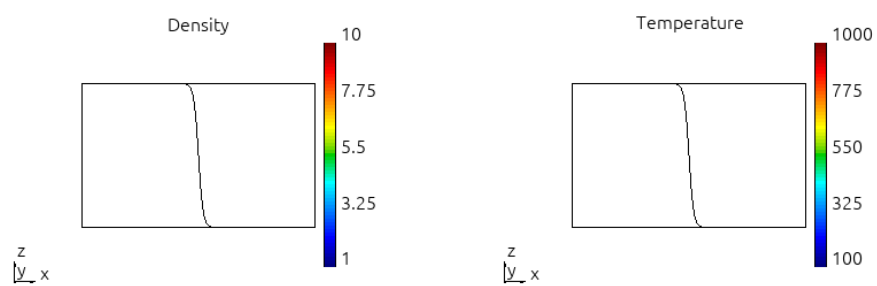
Figure 9: Problem 6 background.

Kn

1.915e-07

1.436e-07

9.573e-08

4.787e-08

4.366e-23

z
y x

Heat flux

0.002472

0.001369

0.0002647

-0.000839

-0.001943

z
y x

Kn

1.915e-05

1.436e-05

9.573e-06

4.787e-06

4.366e-21

z
y x

Heat flux

0.2472

0.1369

0.02647

-0.08391

-0.1943

z
y x

Kn

0.001915

0.001436

0.0009573

0.0004787

4.366e-19

z
y x

Heat flux

24.73

13.69

2.661

-8.372

-19.41

z
y x

Kn

0.1915

0.1436

0.09573

0.04787

4.366e-17

z
y x

Heat flux

1679

1084

488.7

-106.4

-701.5

z
y x

Kn

0.3829

0.2872

0.1915

0.09573

8.731e-17

z
y x

Heat flux

2356

1573

789.7

6.45

-776.8

z
y x

Figure 10:   Problem 6 transport.

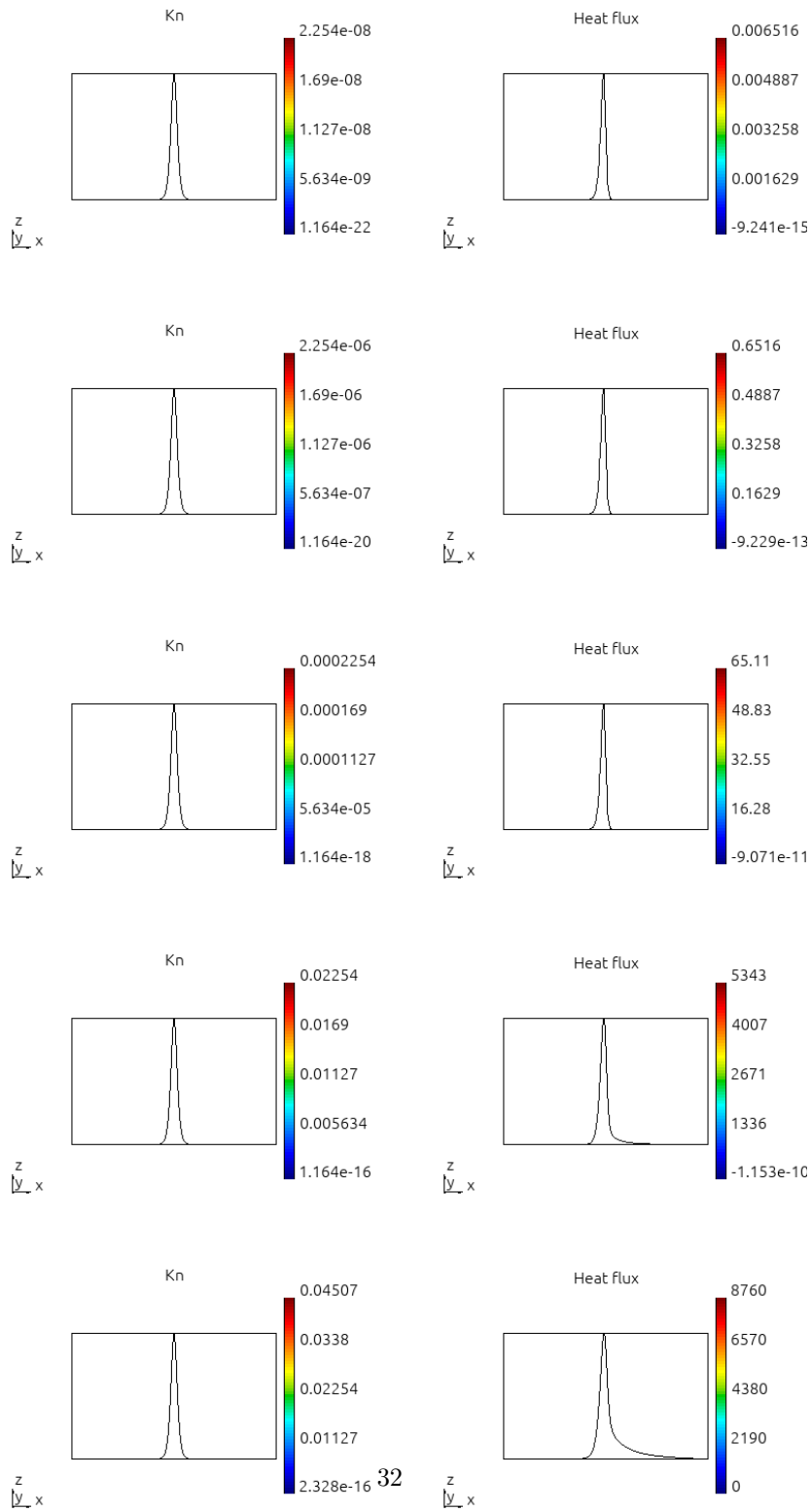Figure 11: Problem 7 background.

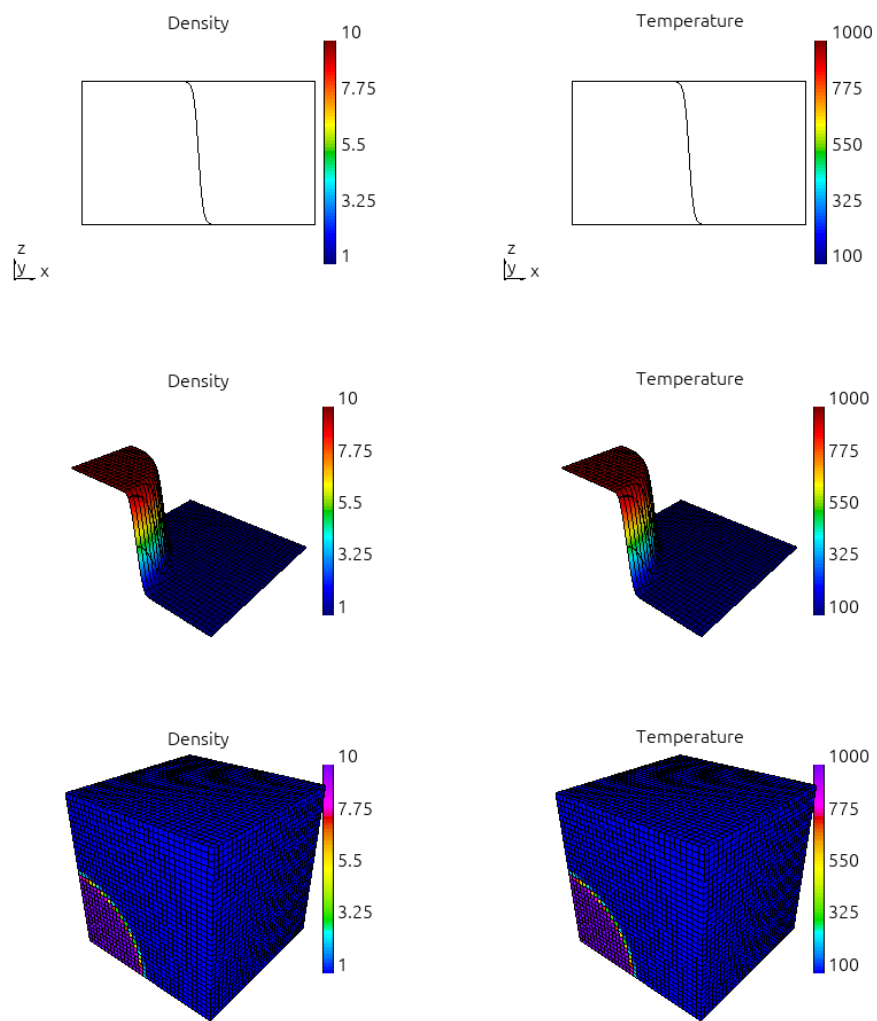Figure 12: Problem 7 transport.
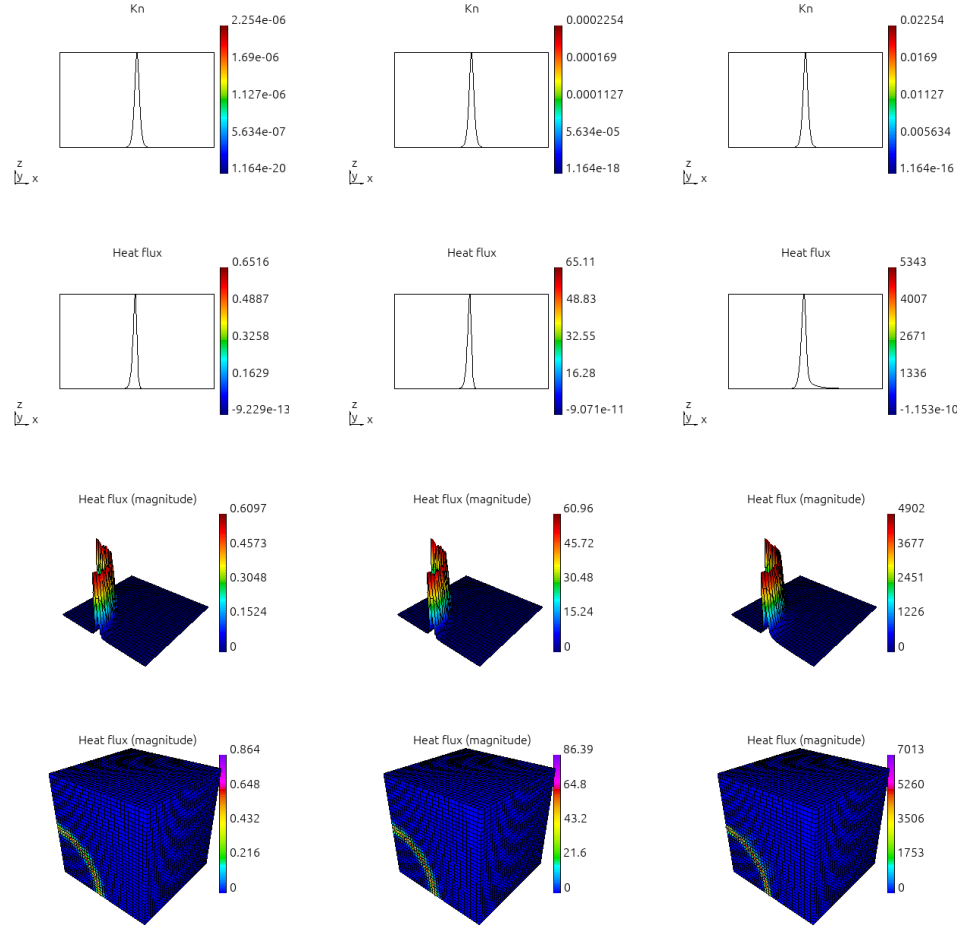
Figure 13: Problem 7 1D/2D/3D background.

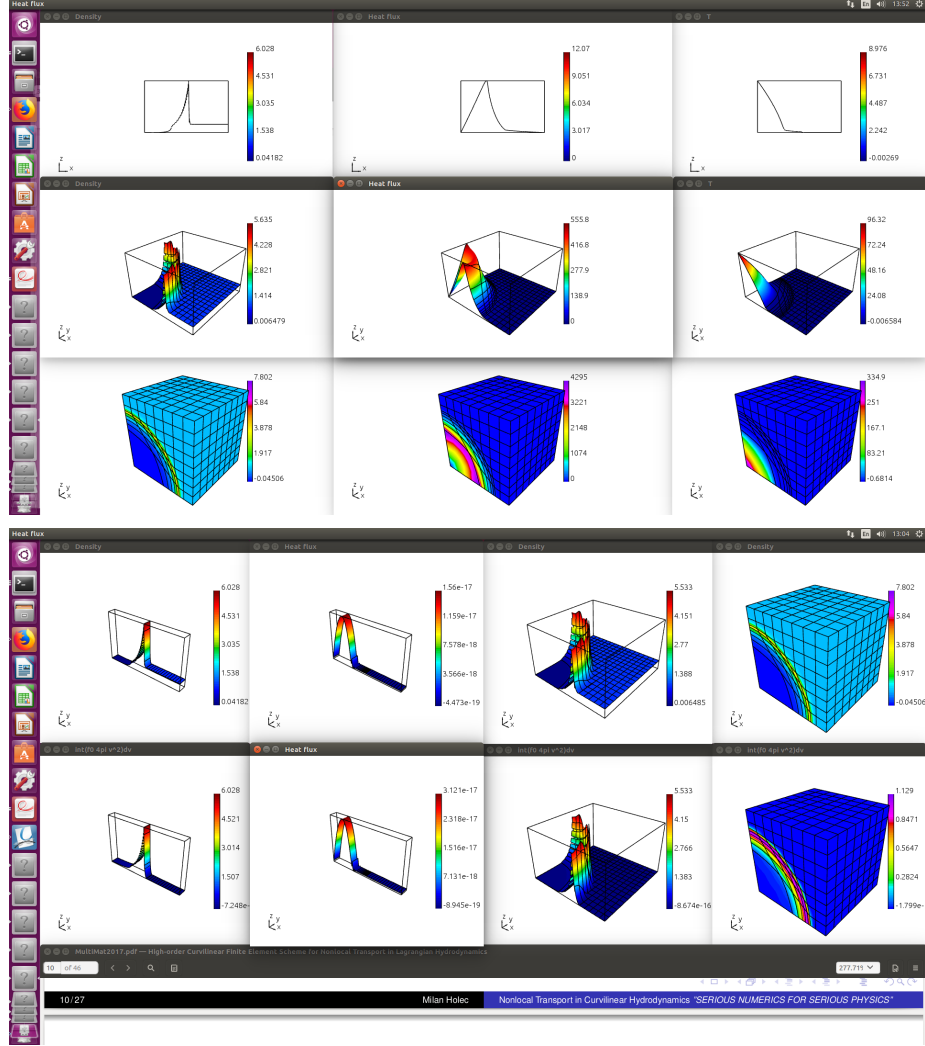Figure 14: Problem 7 1D/2D/3D transport.

34

Figure 15: Sedov blast in 1D/2D/3D from δ function hot spot. Shock propagates from left to right. Top raw corresponds to 1D (8858 energy groups) - left: density profile, right: temperature (decreasing from the original hot spot with low temperature in compressed plasma), center: heat flux with its maximum on the start of increase in density decreasing while approaching the shock (NOTICE non-zero flux ahead of the shock). Middle raw corresponds to 2D (4348 energy groups) - left: density, center: heat flux, right: temperature. Bottom raw corresponds to 3D (10030 energy groups) - left: density, center: heat flux, right: temperature.

35