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

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Abstract

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1. M1 model

1.1. AWBS Boltzmann transport equation

Simplified Boltzmann transport equation of electrons relying on the use of AWBS collision-thermalization operator [1] reads

$$v\boldsymbol{n}\cdot\nabla f+\frac{q_e}{m_e}\left(\boldsymbol{E}+\frac{v}{c}\boldsymbol{n}\times\boldsymbol{B}\right)\cdot\nabla_{\boldsymbol{v}}f=\nu_e v\frac{\partial}{\partial v}\left(f-f_M\right). \tag{1}$$

1.2. M1-AWBS model

In order to eliminate the dimensions of the transport problem (1) the two moment model referred to as *M1-AWBS* is introduced

$$\begin{aligned}\nu_e v\frac{\partial}{\partial v}\left(f_0-f_M\right) &= v\nabla\cdot\boldsymbol{f}_1+\frac{q_e}{m_e v^2}\boldsymbol{E}\cdot\frac{\partial}{\partial v}\left(v^2\boldsymbol{f}_1\right), &(2)\\ \nu_e v\frac{\partial}{\partial v}\boldsymbol{f}_1-\nu_t\boldsymbol{f}_1 &= v\nabla\cdot\left(\mathbf{A}f_0\right)+\frac{q_e}{m_e v^2}\boldsymbol{E}\cdot\frac{\partial}{\partial v}\left(v^2\mathbf{A}f_0\right)\\ &\quad+\frac{q_e}{m_e v}\boldsymbol{E}\cdot\left(\mathbf{A}-\mathbf{I}\right)f_0+\frac{q_e}{m_e c}\boldsymbol{B}\times\boldsymbol{f}_1, &(3)\end{aligned}$$

where the anisotropy-closure matrix takes the form

$$\mathbf{A}=\frac{1}{3}\mathbf{I}+\frac{|\boldsymbol{f}_1|^2}{2f_0^2}\left(1+\frac{|\boldsymbol{f}_1|^2}{f_0^2}\right)\left(\frac{\boldsymbol{f}_1\otimes\boldsymbol{f}_1^T}{|\boldsymbol{f}_1|^2}-\frac{1}{3}\mathbf{I}\right). \tag{4}$$

2. High-order finite element scheme

2.1. Variational principle

First, the electro-magnetic scaling

$$\tilde{\boldsymbol{E}}=\frac{q_e}{m_e}\boldsymbol{E},\ \tilde{\boldsymbol{B}}=\frac{q_e}{m_e c}\boldsymbol{B}, \tag{5}$$

is defined in order to make the algebraic operations easier to follow. The general variational formulation of (2) and (3) 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

$$\begin{aligned}\int_\Omega\phi\rho\frac{\partial f_0}{\partial v} &= \int_\Omega\phi\left(\frac{\rho}{\nu_e}\mathbf{I}:\nabla\boldsymbol{f}_1+\frac{\rho}{\nu_e v}\tilde{\boldsymbol{E}}\cdot\frac{\partial\boldsymbol{f}_1}{\partial v}+\frac{2\rho}{\nu_e v^2}\tilde{\boldsymbol{E}}\cdot\boldsymbol{f}_1+\rho\frac{\partial f_M}{\partial v}\right), &(6)\\ \int_\Omega\boldsymbol{w}\cdot\rho\frac{\partial\boldsymbol{f}_1}{\partial v} &= \int_\Omega\boldsymbol{w}\cdot\left(\nabla\cdot\left(\frac{\rho\mathbf{A}}{\nu_e}f_0\right)-\nabla\left(\frac{\rho}{\nu_e}\right)\cdot\mathbf{A}f_0+\frac{\rho}{\nu_e v^2}\tilde{\boldsymbol{E}}\cdot\left(3\mathbf{A}-\mathbf{I}\right)f_0\right.\\ &\quad\left.+\frac{\rho}{\nu_e v}\tilde{\boldsymbol{E}}\cdot\frac{\partial}{\partial v}\left(\mathbf{A}f_0\right)+\frac{\rho}{\nu_e v}\tilde{\boldsymbol{B}}\times\boldsymbol{f}_1+\frac{\rho\nu_t}{\nu_e v}\boldsymbol{f}_1\right). &(7)\end{aligned}$$

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

$$\int_\Omega \boldsymbol{\phi} \otimes \boldsymbol{\phi}^T \rho \,\mathrm{d}\Omega \cdot \frac{\partial \boldsymbol{f}_0}{\partial v} = \int_\Omega \boldsymbol{\phi} \otimes \left(\frac{\rho}{\nu_e} \mathbf{I} : \nabla \mathbf{w}^T + \frac{2\rho}{\nu_e v^2} \tilde{\boldsymbol{E}}^T \cdot \mathbf{w}^T \right) \mathrm{d}\Omega \cdot \boldsymbol{f}_1 + \int_\Omega \boldsymbol{\phi} \otimes \frac{\rho}{\nu_e v} \tilde{\boldsymbol{E}}^T \cdot \mathbf{w}^T \,\mathrm{d}\Omega \cdot \frac{\partial \boldsymbol{f}_1}{\partial v} + \int_\Omega \boldsymbol{\phi} \otimes \boldsymbol{\phi}^T \rho \,\mathrm{d}\Omega \cdot \frac{\partial \boldsymbol{f}_{\boldsymbol{M}}}{\partial v}, \quad (8)$$

$$\int_\Omega \mathbf{w} \cdot \mathbf{w}^T \rho \,\mathrm{d}\Omega \cdot \frac{\partial \boldsymbol{f}_1}{\partial v} = -\int_\Omega \left(\frac{\rho}{\nu_e} \mathbf{A} : \nabla \mathbf{w} + \mathbf{w} \cdot \mathbf{A} \cdot \nabla \left(\frac{\rho}{\nu_e} \right) \right) \boldsymbol{\phi}^T \,\mathrm{d}\Omega \cdot \boldsymbol{f}_0 + \int_\Omega \mathbf{w} \cdot \frac{\rho}{\nu_e v^2} (3\mathbf{A} - \mathbf{I}) \cdot \tilde{\boldsymbol{E}} \, \boldsymbol{\phi}^T \,\mathrm{d}\Omega \cdot \boldsymbol{f}_0 + \int_\Omega \mathbf{w} \cdot \frac{\rho}{\nu_e v} \mathbf{A} \cdot \tilde{\boldsymbol{E}} \, \boldsymbol{\phi}^T \,\mathrm{d}\Omega \cdot \frac{\partial \boldsymbol{f}_0}{\partial v} + \int_\Omega \mathbf{w} \cdot \left(\frac{\rho}{\nu_e v} \tilde{\boldsymbol{B}} \times \mathbf{w}^T + \frac{\rho \nu_t}{\nu_e v} \mathbf{w}^T \right) \mathrm{d}\Omega \cdot \boldsymbol{f}_1, \quad (9)$$

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.

2.2. Semi-discrete formulation

In principle, only five following integrators need to be coded to provide a discrete representation (8) and (9), i.e.

$$\boldsymbol{\mathcal{M}}^0_{(g)} = \int_\Omega \boldsymbol{\phi} \otimes \boldsymbol{\phi}^T g \,\mathrm{d}\Omega, \quad (10)$$

$$\boldsymbol{\mathcal{M}}^1_{(g)} = \int_\Omega \mathbf{w} \cdot \mathbf{w}^T g \,\mathrm{d}\Omega, \quad (11)$$

$$\boldsymbol{\mathcal{D}}_{(\mathbf{G})} = \int_\Omega \mathbf{G} : \nabla \mathbf{w} \otimes \boldsymbol{\phi}^T \,\mathrm{d}\Omega, \quad (12)$$

$$\boldsymbol{\mathcal{V}}_{(\boldsymbol{g})} = \int_\Omega \mathbf{w} \cdot \boldsymbol{g} \otimes \boldsymbol{\phi}^T \,\mathrm{d}\Omega, \quad (13)$$

$$\boldsymbol{\mathcal{B}}_{(\boldsymbol{g})} = \int_\Omega \mathbf{w} \cdot \boldsymbol{g} \times \mathbf{w}^T \,\mathrm{d}\Omega. \quad (14)$$

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

$$\boldsymbol{\phi} = \begin{bmatrix} \phi_1 \\ \vdots \\ \phi_{N_0} \end{bmatrix}, \ \mathbf{w} = \begin{bmatrix} w_{1,1} & \dots & w_{1,d} \\ \vdots & \ddots & \vdots \\ w_{N_1,1} & \dots & w_{N_1,d} \end{bmatrix}, \ \boldsymbol{g} = \begin{bmatrix} g_1 \\ \vdots \\ g_d \end{bmatrix}, \ \mathbf{G} = \begin{bmatrix} G_{1,1} & \dots & G_{1,d} \\ \vdots & \ddots & \vdots \\ G_{d,1} & \dots & G_{d,d} \end{bmatrix}, \quad (15)$$

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 (2) and (3) can be written based on (8), (9) as

$$\boldsymbol{\mathcal{M}}^0_{(\rho)} \cdot \frac{\partial \boldsymbol{f}_0}{\partial v} - \boldsymbol{\mathcal{M}}^0_{(\rho)} \cdot \frac{\partial \boldsymbol{f}_{\boldsymbol{M}}}{\partial v} = \boldsymbol{\mathcal{D}}^T_{\left(\frac{\rho}{\nu_e}\mathbf{I}\right)} \cdot \boldsymbol{f}_1 + \frac{1}{v}\boldsymbol{\mathcal{V}}^T_{\left(\frac{\rho}{\nu_e}\tilde{\boldsymbol{E}}\right)} \cdot \frac{\partial \boldsymbol{f}_1}{\partial v} + \frac{2}{v^2}\boldsymbol{\mathcal{V}}^T_{\left(\frac{\rho}{\nu_e}\tilde{\boldsymbol{E}}\right)} \cdot \boldsymbol{f}_1, \tag{16}$$

$$\begin{aligned}\boldsymbol{\mathcal{M}}^1_{(\rho)} \cdot \frac{\partial \boldsymbol{f}_1}{\partial v} - \frac{1}{v}\boldsymbol{\mathcal{M}}^1_{\left(\frac{\rho\nu_t}{\nu_e}\right)} \cdot \boldsymbol{f}_1 = &- \left(\boldsymbol{\mathcal{D}}_{\left(\frac{\rho}{\nu_e}\mathbf{A}\right)} + \boldsymbol{\mathcal{V}}_{\left(\mathbf{A}\cdot\nabla\left(\frac{\rho}{\nu_e}\right)\right)}\right) \cdot \boldsymbol{f}_0 \\ &+ \frac{1}{v}\boldsymbol{\mathcal{V}}_{\left(\frac{\rho}{\nu_e}\mathbf{A}\cdot\tilde{\boldsymbol{E}}\right)} \cdot \frac{\partial \boldsymbol{f}_0}{\partial v} + \frac{1}{v^2}\boldsymbol{\mathcal{V}}_{\left(\frac{\rho}{\nu_e}(3\mathbf{A}-\mathbf{I})\cdot\tilde{\boldsymbol{E}}\right)} \cdot \boldsymbol{f}_0 + \frac{1}{v}\boldsymbol{\mathcal{B}}_{\left(\frac{\rho}{\nu_e}\tilde{\boldsymbol{B}}\right)} \cdot \boldsymbol{f}_1,\end{aligned} \tag{17}$$

where the integrators (10), (11), (12), (13), (14) are used acting on appropriate functions ρ, ν_e, ν_t, vectors $\tilde{\boldsymbol{E}}$, $\tilde{\boldsymbol{B}}$, and matrices $\mathbf{A}$ and $\mathbf{I}$.

Also, it proves to be useful to define mass matrices

$$\mathbf{M}^c_0 = \boldsymbol{\mathcal{M}}^0_{(\rho)}, \ \mathbf{M}^c_1 = \boldsymbol{\mathcal{M}}^1_{(\rho)}, \tag{18}$$

since these are constant during the time evolution of the Lagrangian mesh, thus making the overall matrix evaluation more efficient.

2.3. 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

$$\left(\mathbf{M}^c_0 - \boldsymbol{\mathcal{M}}^0_{\left(\frac{\rho}{v\nu_e \boldsymbol{f}^n_0}\tilde{\boldsymbol{E}}^T\cdot\boldsymbol{f}^n_1\right)}\right)\cdot\frac{\mathrm{d}\boldsymbol{f}_0}{\mathrm{d}v}^* = \boldsymbol{\mathcal{D}}^T_{\left(\frac{\rho}{\nu_e}\mathbf{I}\right)}\cdot\boldsymbol{f}^n_1 + \frac{2}{v^2}\boldsymbol{\mathcal{V}}^T_{\left(\frac{\rho}{\nu_e}\tilde{\boldsymbol{E}}\right)}\cdot\boldsymbol{f}^n_1 + \mathbf{M}^c_0\cdot\frac{\partial \boldsymbol{f}_{\boldsymbol{M}}}{\partial v}, \tag{19}$$

where the actual evolution of $\boldsymbol{f}_1$ has been redefined as similar to the time evolution of $\boldsymbol{f}_0$ (compare (19) to (16)). Then, the actual computation of the time evolution of $\boldsymbol{f}_1$ follows

$$\mathbf{M}_1^c \cdot \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v} = -\left(\boldsymbol{\mathcal{D}}_{\left(\frac{\rho}{\nu_e}\mathbf{A}\right)} + \boldsymbol{\mathcal{V}}_{\left(\mathbf{A}\cdot\nabla\left(\frac{\rho}{\nu_e}\right)\right)}\right) \cdot \boldsymbol{f}_0^n + \frac{1}{v}\boldsymbol{\mathcal{V}}_{\left(\frac{\rho}{\nu_e}\mathbf{A}\cdot\tilde{\boldsymbol{E}}\right)} \cdot \frac{\mathrm{d}\boldsymbol{f}_0}{\mathrm{d}v}^* + \frac{1}{v^2}\boldsymbol{\mathcal{V}}_{\left(\frac{\rho}{\nu_e}(3\mathbf{A}-\mathbf{I})\cdot\tilde{\boldsymbol{E}}\right)} \cdot \boldsymbol{f}_0^n + \frac{1}{v}\boldsymbol{\mathcal{B}}_{\left(\frac{\rho}{\nu_e}\tilde{\boldsymbol{B}}\right)} \cdot \boldsymbol{f}_1^n + \frac{1}{v}\boldsymbol{\mathcal{M}}^1_{\left(\frac{\rho\nu_t}{\nu_e}\right)} \cdot \boldsymbol{f}_1^n. \quad (20)$$

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

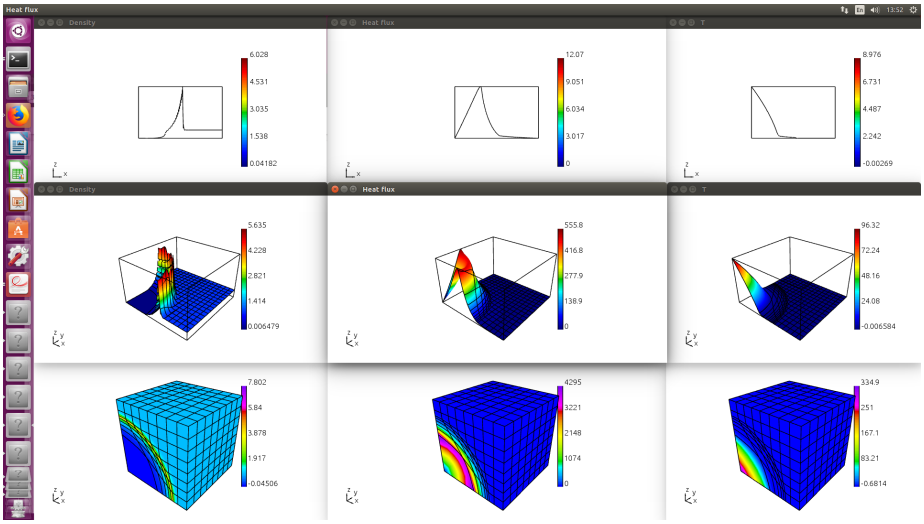

Figure 1: Sedov blast in 1D/2D/3D from δ function hot spot. Shock propagates from left to right. Top raw corresponds to 1D (8858 energy groups) - left: density profile, right: temperature (decreasing from the original hot spot with low temperature in compressed plasma), center: heat flux with its maximum 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. temperature

As can be seen in FIG. 2.3 we get a heat flux profile corresponding to temperature and density profiles computed by Laghos [2] in 1D and we have also double checked the numerical scheme in 2D and 3D, where apparently the flux profiles exhibit the same physical background. It is important to note, that

the current implementation does not include neither electric or magnetic field ($\tilde{\boldsymbol{E}}$, $\tilde{\boldsymbol{B}}$).

It is worth mentioning, that the proposed discrete scheme (19) and (20) 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.

2.4. Implicit fully-discrete scheme

In order to formulate a fully-discrete scheme leaning on an implicit discretization of velocity, the equations (16) and (17) can be expressed with matrices as

$$\begin{aligned}
\mathbf{M}_0^c \cdot \frac{\partial \boldsymbol{f}_0}{\partial v} &= \mathbf{D}_0 \cdot \boldsymbol{f}_1 + \mathbf{E}_0^1 \cdot \frac{\partial \boldsymbol{f}_1}{\partial v} + \mathbf{E}_0^2 \cdot \boldsymbol{f}_1 + \mathbf{M}_0^c \cdot \frac{\partial \boldsymbol{f}_{\boldsymbol{M}}}{\partial v}, \\
\mathbf{M}_1^c \cdot \frac{\partial \boldsymbol{f}_1}{\partial v} &= -\mathbf{D}_1 \cdot \boldsymbol{f}_0 + \mathbf{E}_1^1 \cdot \frac{\partial \boldsymbol{f}_0}{\partial v} + \mathbf{E}_1^2 \cdot \boldsymbol{f}_0 + \mathbf{B} \cdot \boldsymbol{f}_1 + \mathbf{M}_1 \cdot \boldsymbol{f}_1,
\end{aligned}$$

$$\begin{aligned}
\frac{\mathrm{d}\boldsymbol{f}_0}{\mathrm{d}v} &= \mathbf{M}_0^{c\,-1} \cdot \left(\mathbf{D}_0 + \mathbf{E}_0^2\right) \cdot \left(\boldsymbol{f}_1^n + \Delta v \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v}\right) + \mathbf{M}_0^{c\,-1} \cdot \mathbf{E}_0^1 \cdot \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v} \\
&\quad + \frac{\partial \boldsymbol{f}_{\boldsymbol{M}}}{\partial v}, \\
\mathbf{M}_1^c \cdot \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v} &= \left(\mathbf{E}_1^2 - \mathbf{D}_1\right) \cdot \left(\boldsymbol{f}_0^n + \Delta v \frac{\mathrm{d}\boldsymbol{f}_0}{\mathrm{d}v}\right) + \mathbf{E}_1^1 \cdot \frac{\mathrm{d}\boldsymbol{f}_0}{\mathrm{d}v} \\
&\quad + \left(\mathbf{B} + \mathbf{M}_1\right) \cdot \left(\boldsymbol{f}_1^n + \Delta v \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v}\right),
\end{aligned}$$

$$\frac{\mathrm{d}\boldsymbol{f}_0}{\mathrm{d}v} = \tilde{\mathbf{A}}_0 \cdot \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v} + \boldsymbol{b}_0 \left(\boldsymbol{f}_1^n, \frac{\partial \boldsymbol{f}_{\boldsymbol{M}}}{\partial v}\right), \tag{21}$$

$$\left(\mathbf{M}_1^c - \Delta v \left(\mathbf{B} + \mathbf{M}_1\right)\right) \cdot \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v} = \tilde{\mathbf{A}}_1 \cdot \frac{\mathrm{d}\boldsymbol{f}_0}{\mathrm{d}v} + \boldsymbol{b}_1 \left(\boldsymbol{f}_1^n, \boldsymbol{f}_0^n\right), \tag{22}$$

$$\left(\mathbf{M}_1^c - \Delta v \left(\mathbf{B} + \mathbf{M}_1\right) - \tilde{\mathbf{A}}_1 \cdot \tilde{\mathbf{A}}_0\right) \cdot \frac{\mathrm{d}\boldsymbol{f}_1}{\mathrm{d}v} = \tilde{\mathbf{A}}_1 \cdot \boldsymbol{b}_0 + \boldsymbol{b}_1, \tag{23}$$

[2]

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