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The positivity-preserving finite volume scheme with fixed stencils for radiation diffusion problems on general polyhedral meshes

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Outline

1. Motivation
2. PPFV scheme for steady diffusion problem
3. PPFV scheme for three temperature model
4. Numerical examples

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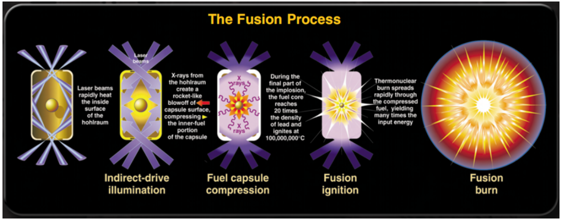
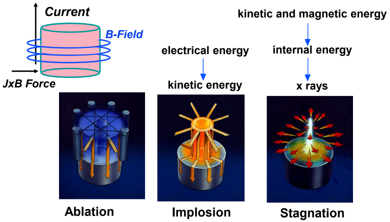
1. Motivation
2. PPFV scheme for steady diffusion problem
3. PPFV scheme for three temperature model
4. Numerical examples

A three temperature plasma model in ICF

Development of new methods is mainly driven by needs of large scale multiphysics simulation, for instance a three temperature plasma model in the fields of inertial confinement fusion

$$
\begin{aligned}
\frac{\partial E_e}{\partial t} - \nabla \cdot (\lambda_e' \nabla T_e) &= c\sigma_P \left(E_r - aT_e^4\right) + c\kappa \left(T_i - T_e\right) + Q_e, \\
\frac{\partial E_i}{\partial t} - \nabla \cdot (\lambda_i' \nabla T_i) &= c\kappa \left(T_e - T_i\right) + Q_i, \\
\frac{\partial E_r}{\partial t} - \nabla \cdot (\lambda_r \nabla E_r) &= c\sigma_P \left(aT_e^4 - E_r\right) + Q_r.
\end{aligned}
$$





A three temperature plasma model in ICF

The three energies E_e, E_i and E_r can not be negative, and a conservative postprocessing is not a best choice. It adds additional complexity that can be used to build a better discretization method.

$$
\begin{aligned}
\frac{\partial E_e}{\partial t} - \nabla \cdot \left(\lambda_e' \nabla T_e\right) &= c\sigma_P \left(E_r - aT_e^4\right) + c\kappa \left(T_i - T_e\right) + Q_e, \\
\frac{\partial E_i}{\partial t} - \nabla \cdot \left(\lambda_i' \nabla T_i\right) &= c\kappa \left(T_e - T_i\right) + Q_i, \\
\frac{\partial E_r}{\partial t} - \nabla \cdot \left(\lambda_r \nabla E_r\right) &= c\sigma_P \left(aT_e^4 - E_r\right) + Q_r.
\end{aligned}
$$

The goal of this talk: construct a positivity-preserving finite volume scheme (PPFV) for the three temperature model !

Positivity-preserving property

$$\frac{\partial E_e}{\partial t} - \nabla \cdot (\lambda_e' \nabla T_e) = S_e(T) + Q_e$$
$$\frac{\partial E_i}{\partial t} - \nabla \cdot (\lambda_i' \nabla T_i) = S_i(T) + Q_i$$
$$\frac{\partial E_r}{\partial t} - \nabla \cdot (\lambda_r \nabla E_r) = S_r(T) + Q_r$$

For simplicity $\longrightarrow$

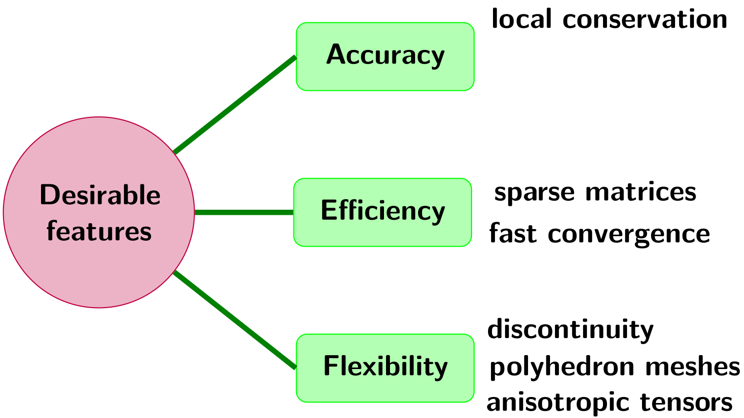
$$-\nabla \cdot (\Lambda \nabla u) = f$$

Positivity-preserving property

Let $u \in C^2(\Omega) \cap C^0(\bar{\Omega})$ satisfy that $f \geq 0$ in Ω and $u \geq 0$ on $\partial\Omega$ under the assumption that Λ should be locally uniformly positive definite in Ω. Then $u \geq 0$ in Ω.

From the weak maximum principle,this property is immediate to derive.

Why nonlinear finite volume scheme?



Linear schemes

- FEM VEM
- MFD MFV
- MPFA HFV
- LPFV NPS

Positivity-preserving property: impose some restrictions on mesh topology and anisotropy of diffusion tensor Λ !

Why nonlinear finite volume scheme?

Desirable features

- **Accuracy**
  - local conservation
  - positivity-preserving
  - extremum-preserving
- **Efficiency**
  - sparse matrices
  - fast convergence
- **Flexibility**
  - discontinuity
  - polyhedron meshes
  - anisotropic tensors

Linear schemes

- FEM VEM
- MFD MFV
- MPFA HFV
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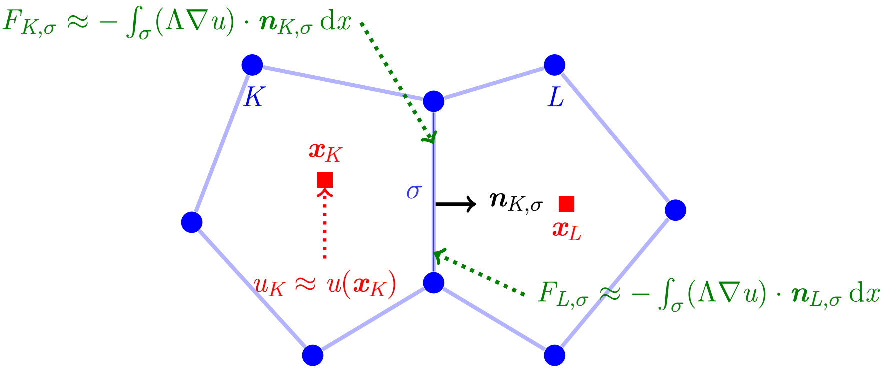
Nonlinear schemes

- NLTPFA
- NMPFA
- Postprocessing

Expensive to solve the nonlinear system $A(U)U = F(U)$ but may be very nice for Newton type methods in a multiphysics simulations such as a 3T plasma model !

Principle of finite volume methods

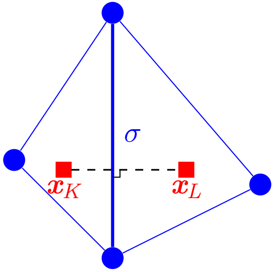


Finite volume equation

$$\text{(Flux balance)} \quad \forall K: \sum_{\sigma \in \mathcal{E}_K} F_{K,\sigma} = |K| f_K.$$

$$\text{(Flux conservativity)} \quad \forall \sigma = K|L: \; F_{K,\sigma} + F_{L,\sigma} = 0.$$

PPFV scheme with a nonlinear TPFA



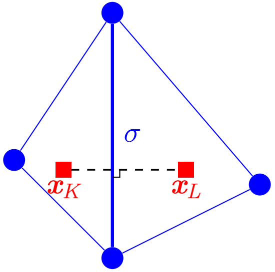
$\forall \sigma = K|L,\ (\boldsymbol{x}_K \boldsymbol{x}_L) \perp \sigma$

Two-Point Flux Approximation

- Assume that $(\boldsymbol{x}_K \boldsymbol{x}_L) \perp \sigma$ and $\Lambda = \mathrm{Id}$, the classical TPFA is

$$F_{K,\sigma} = \int_\sigma -\Lambda \nabla u \cdot \boldsymbol{n}_{K,\sigma} = |\sigma| \frac{u(\boldsymbol{x}_K) - u(\boldsymbol{x}_L)}{\mathrm{d}(\boldsymbol{x}_K, \boldsymbol{x}_L)}$$

PPFV scheme with a nonlinear TPFA



$\forall \sigma = K|L,\ (\boldsymbol{x}_K \boldsymbol{x}_L) \perp \sigma$

Two-Point Flux Approximation

- Assume that $(\boldsymbol{x}_K \boldsymbol{x}_L) \perp \sigma$ and $\Lambda = \mathrm{Id}$, the classical TPFA is

$$F_{K,\sigma} = \int_\sigma -\Lambda \nabla u \cdot \boldsymbol{n}_{K,\sigma} = |\sigma| \frac{u(\boldsymbol{x}_K) - u(\boldsymbol{x}_L)}{\mathrm{d}(\boldsymbol{x}_K, \boldsymbol{x}_L)}$$

- TPFA is linear and monotone, but inaccurate for arbitrary meshes.
- **Pioneer work (C Le Potier, 2005)**: a nonlinear TPFA on triangle grids

$$F_{K,\sigma} = \alpha_{K,\sigma}(u) u_K - \alpha_{L,\sigma}(u) u_L \text{ with } \alpha_{K,\sigma} > 0 \text{ and } \alpha_{L,\sigma} > 0.$$

- We need interpolation method for auxiliary cell-vertex unknowns.

PPFV scheme with a nonlinear TPFA

Interpolation-based PPFV scheme

- general meshes or general diffusion tensors:(Lipnikov et.al. 07)(Kapyrin, 07)(Yuan & Sheng, 08,12)(Wang,Hang,Yuan, 2018)(Xie,et.al,2018)(Peng, Yang, Gao, 2021,2022)
- Interpolation method for auxiliary unknowns affects the accuracy.

Interpolation-free PPFV schemes

- Refs. (Lipnikov et.al., 09) (Danilov & Vassilevski, 09) (Lipnikov et.al., 12)
- need to know the location of discontinuity beforehand

VEM-based PPFV schemes

- use VEM for auxiliary unknowns (Sheng, Yang, Gao,2022)

Our goal in this talk

Design the interpolation-based PPFV scheme with approximately 2nd-order accuracy for three temperature radiation diffusion problems on general polyhedral meshes.

Outline

The framework for the cell-centered FVM

1 Construct the one-sided flux

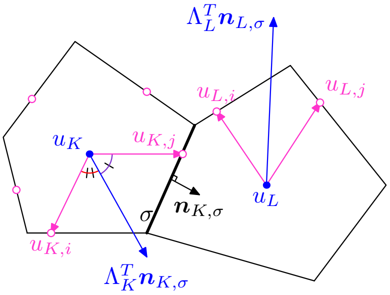
$$F_{K,\sigma} = \sum_{i=1}^{n_K} \alpha_{K,\sigma,i}(u_K - u_{K,i})$$

2 Define the unique flux

$$\tilde{F}_{K,\sigma} = \mu_{K,\sigma} F_{K,\sigma} - \mu_{L,\sigma} F_{L,\sigma}, \quad \mu_{K,\sigma} + \mu_{L,\sigma} = 1$$

3 The interpolation method for auxiliary unknowns

$$u_{K,i} = \sum_{L \in \mathcal{T}_{K,i}} \omega_{K,i}^L u_L$$



4 The final FV equation

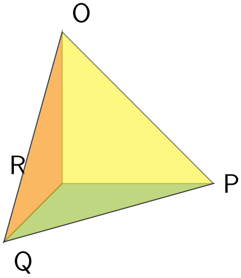
Solve $\{u_K, K \in \mathcal{T}\}$ s.t. $\sum_{\sigma \in \mathcal{E}_K} \tilde{F}_{K,\sigma} = |K| f_K, \ \forall\, K \in \mathcal{T}.$

Step 1: construction of one-sided flux

- **Discretization of the flux**

$$F_{K,\sigma} = -\int_\sigma (\Lambda_K \nabla u)\cdot n_{K,\sigma} \mathrm{d}s \simeq -|\sigma|\left(\Lambda_K \nabla u\right)\cdot \boldsymbol{n}_{K,\sigma} = -|\sigma| \Lambda_K^\top \boldsymbol{n}_{K,\sigma}\cdot \nabla u.$$

- **Discretization of gradient**



Let T_{OPQR} be a tetrahedron composed of vertex O, P, Q, R, and $\det(\mathbb{X}) > 0$:

$$\mathbb{X} = \begin{pmatrix} \overrightarrow{OP}^\top \\ \overrightarrow{OQ}^\top \\ \overrightarrow{OR}^\top \end{pmatrix} = \begin{pmatrix} x_P - x_O & y_P - y_O & z_P - z_O \\ x_Q - x_O & y_Q - y_O & z_Q - z_O \\ x_R - x_O & y_R - y_O & z_R - z_O \end{pmatrix}.$$

Hence for the function u defined on the tetrahedron T_{OPQR}, we have

$$\nabla u \simeq \frac{1}{6 V_{\mathrm{T}_{OPQR}}}\left[(u_P - u_O)(\overrightarrow{OQ}\times\overrightarrow{OR}) + (u_Q - u_O)(\overrightarrow{OR}\times\overrightarrow{OP}) + (u_R - u_O)(\overrightarrow{OP}\times\overrightarrow{OQ})\right].$$

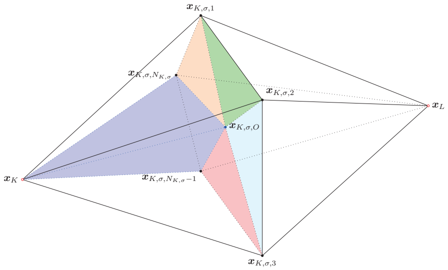
Step 1: construction of one-sided flux

- **The linearity-preserving one-sided flux**

$$F_{K,\sigma} = \sum_{i=1}^{N_{K,\sigma}} a_{K,\sigma,i} \left(u_K - u_{K,\sigma,i} \right), \ K \in \mathcal{T}.$$

If K is a star-shaped polyhedron w.r.t. $\boldsymbol{x}_K$, then it can be proved that

$$\sum_{i=1}^{N_{K,\sigma}} a_{K,\sigma,i} > 0, \ \ \sigma \in \mathcal{E}_K.$$



Gradient on tetrahedron $\boldsymbol{x}_K \boldsymbol{x}_{K,\sigma,O} \boldsymbol{x}_{K,\sigma,i} \boldsymbol{x}_{K,\sigma,i+1}$

$$(\nabla u)|_{K,\sigma,i} \simeq \boldsymbol{\alpha}^1_{K,\sigma,i}(u_{K,\sigma,O} - u_K) + \boldsymbol{\alpha}^2_{K,\sigma,i}(u_{K,\sigma,i} - u_K) + \boldsymbol{\alpha}^3_{K,\sigma,i}(u_{K,\sigma,i+1} - u_K).$$

Step 2: construction of the final flux

$$(\mu_{L,\sigma} a_{L,\sigma} - \mu_{K,\sigma} a_{K,\sigma})$$

$$\tilde{F}_{K,\sigma} = \left(\mu_{K,\sigma} \sum_{i=1}^{n_K} \alpha_{K,\sigma,i} \right) u_K - \left(\mu_{L,\sigma} \sum_{i=1}^{n_L} \alpha_{L,\sigma,i} \right) u_L + B_\sigma$$

Step 2: construction of the final flux

$$\frac{a_{K,\sigma}}{a_{K,\sigma}+a_{L,\sigma}} \qquad (\mu_{L,\sigma} a_{L,\sigma} - \mu_{K,\sigma} a_{K,\sigma})$$

$$\tilde{F}_{K,\sigma} = \left(\mu_{K,\sigma} \sum_{i=1}^{n_K} \alpha_{K,\sigma,i} \right) u_K - \left(\mu_{L,\sigma} \sum_{i=1}^{n_L} \alpha_{L,\sigma,i} \right) u_L + B_\sigma$$

Classical NLTPFA [C. Le Potier, CRAS'05]

$$\tilde{F}_{K,\sigma} = A_{K,\sigma}(u)\ u_K - A_{L,\sigma}(u)\ u_L$$

$$\mu_{K,\sigma} \sum_{i=1}^{n_K} \alpha_{K,\sigma,i}$$

Step 2: construction of the final flux

$$\frac{|a_{K,\sigma}|}{|a_{K,\sigma}|+|a_{L,\sigma}|}$$

$$(\mu_{L,\sigma} a_{L,\sigma} - \mu_{K,\sigma} a_{K,\sigma})$$

$$\tilde{F}_{K,\sigma} = \left(\mu_{K,\sigma} \sum_{i=1}^{n_K} \alpha_{K,\sigma,i} \right) u_K - \left(\mu_{L,\sigma} \sum_{i=1}^{n_L} \alpha_{L,\sigma,i} \right) u_L + B_\sigma$$

new NLTPFA[Gao & Wu, SISC'15]

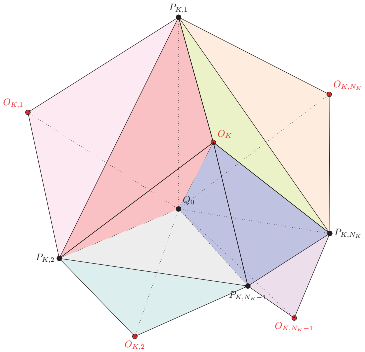
$$\tilde{F}_{K,\sigma} = A_{K,\sigma}(u)\, u_K - A_{L,\sigma}(u)\, u_L + B_\sigma^\epsilon$$

$$\mu_{K,\sigma} \sum_{i=1}^{n_K} \alpha_{K,\sigma,i} + \frac{B_\sigma^+}{u_K+\epsilon}$$

$$\frac{B_\sigma^+ \epsilon}{u_K+\epsilon} - \frac{B_\sigma^- \epsilon}{u_L+\epsilon} \le Ch^2$$

Step 3: vertex interpolation algorithm[1]

(1) The contour integrations of the normal component of flux along the boundaries of polyhedron $Q_0 O_k P_{k,1}, \ldots, P_{k,N_k}$ is zero under lineariity-preserving criterion.



We have the contour integration relation as follows

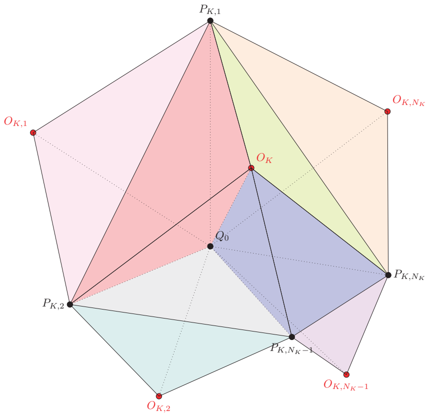
$$\sum_{k=1}^{N(Q_0)} \sum_{j=1}^{N_k} \boldsymbol{F}_k \cdot \boldsymbol{n}_0^{k,j} = 0.$$

It can be known from the above discrete gradient that

$$\boldsymbol{F}_k \cdot \boldsymbol{n}_0^{k,j} = \zeta_{k,j,1}(u_{P_{k,j}} - u_0) + \zeta_{k,j,2}(u_{P_{k,j+1}} - u_0) + \zeta_{k,j,3}(u_k - u_0)$$

[1]D. Yang, Z. Gao, G. Ni. IJNMF, 2022, 94(12): 2137-2171.

(2) We employ the flux continuity condition across the common face of the tetrahedron $O_k Q_0 P_{k,j} P_{k,j+1}$ and tetrahedron $O_{k,j} Q_0 P_{k,j} P_{k,j+1}$, i.e.



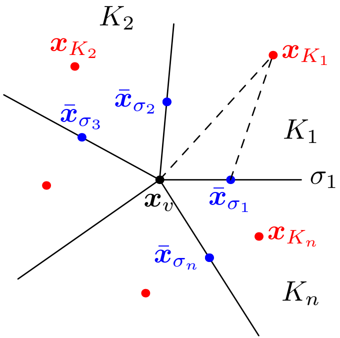
$$\boldsymbol{F}_k \cdot \boldsymbol{n}_f^{k,j} + \boldsymbol{F}_{k,j} \cdot \left(-\boldsymbol{n}_f^{k,j}\right) = 0.$$

Thus, the explicit weight expression can be obtained

$$\omega_k = \frac{\psi_{k,1} + \sum_{m=1}^{\mathcal{N}(Q_0)} \sum_{i=2}^{N_m+1} \psi_{m,i} \cdot \delta(m,i,k)}{\sum_{k=1}^{\mathcal{N}(Q_0)} \left(\psi_{k,1} + \sum_{j=2}^{N_k+1} \psi_{k,j}\right)}.$$

[2] D. Yang, Z. Gao, G. Ni. IJNMF, 2022, 94(12): 2137-2171.

2D version of vertex interpolation method can be found in [Gao, Wu, 2011][3]



$$u_v = \sum_{i=1}^{n} w_i u_{K_i} \text{ with } w_i = \frac{\bar{w}_i}{\sum_{k=1}^{n} \bar{w}_k}$$

$$\begin{aligned}
\bar{w}_k &= \frac{\eta_{k-1,1} - \eta_{k,2}}{\bar{\xi}_{k-1,2} + \bar{\xi}_{k,1}} \xi_{k,1} + \frac{\eta_{k,1} - \eta_{k+1,2}}{\bar{\xi}_{k,2} + \bar{\xi}_{k+1,1}} \xi_{k,2} \\
\xi_{i,j} &= \frac{1}{2S_{i,j}} \left(\mathcal{R}\boldsymbol{x}_v \bar{\boldsymbol{x}}_{\sigma_{i+j-1}}\right)^T \Lambda_{K_i} \mathcal{R}\left(\boldsymbol{x}_v \bar{\boldsymbol{x}}_{\sigma_{i+j-1}}\right) \\
\bar{\xi}_{i,j} &= \frac{1}{2S_{i,j}} \left(\mathcal{R}\left(\boldsymbol{x}_v \bar{\boldsymbol{x}}_{\sigma_{i+j-1}}\right)\right)^T \Lambda_{K_i} \mathcal{R}\left(\boldsymbol{x}_{K_i} \boldsymbol{x}_v\right) \\
\eta_{i,j} &= \frac{\left(\mathcal{R}\left(\bar{\boldsymbol{x}}_{\sigma_i} \bar{\boldsymbol{x}}_{\sigma_{i+1}}\right)\right)^T \Lambda_{K_i} \mathcal{R}\left(\boldsymbol{x}_v \bar{\boldsymbol{x}}_{\sigma_{i+j-1}}\right)}{2S_{\triangle \boldsymbol{x}_v \bar{\boldsymbol{x}}_{\sigma_i} \bar{\boldsymbol{x}}_{\sigma_{i+1}}}}
\end{aligned}$$

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[3] Z. Gao, J. Wu. IJNMF, 67(12)(2011)2157-2183.

Step 4: the final finite volume equation

Finite volume equation

The PPFV scheme: find $\{u_K, K \in \mathcal{T}\}$ such that

$$\sum_{\sigma \in \mathcal{E}_K} \tilde{F}_{K,\sigma} = |K| f_K, \quad \forall\, K \in \mathcal{T}.$$

Now we get a nonlinear algebraic system $\mathbb{M}(\mathbf{U})\mathbf{U} = \mathbf{F}(\mathbf{U})$, which can be solved by Picard iterations.

Positivity of the discrete solution

Let $f \geq 0$, $g_D \geq 0$ and $g_N \leq 0$. Assume that $\sum_{i=1}^{n_K} \alpha_{K,\sigma,i} > 0,\ \forall \sigma \in \mathcal{T}$ holds. If the initial solution vector $\mathbf{U}^0 \geq 0$ and linear systems in the Picard iterations are solved exactly, then $\mathbf{U}^k \geq 0$ for $k \geq 1$.

Outline

Three temperature radiation diffusion problems

The energy evolution of radiation, electrons and ions can be respectively described by

$$
\begin{aligned}
\frac{\partial E_e}{\partial t} - \nabla \cdot \left(\lambda_e' \nabla T_e\right) &= c\sigma_P \left(E_r - aT_e^4\right) + c\kappa \left(T_i - T_e\right) + Q_e, \\
\frac{\partial E_i}{\partial t} - \nabla \cdot \left(\lambda_i' \nabla T_i\right) &= c\kappa \left(T_e - T_i\right) + Q_i, \\
\frac{\partial E_r}{\partial t} - \nabla \cdot \left(\lambda_r \nabla E_r\right) &= c\sigma_P \left(aT_e^4 - E_r\right) + Q_r.
\end{aligned}
$$

- E_e, E_i and E_r are respectively the radiative, electronic and ionic energy densities.
- c denotes the speed of light, a denotes the Stefan constant;
- Planck opacity σ_P is a given nonlinear function of T_e and T_r;
- κ is a positive relaxation coefficient which depends on T_e and T_i;
- The electronic, ionic and radiative thermal conductivities are given by

$$\lambda_\alpha' = K_\alpha T_\alpha^{5/2},\ \alpha = e, i \quad \text{(Spitzer-Harm)} \quad \lambda_r = \frac{c}{3\sigma_R(T_e)} \quad \text{(Rosseland diffusion)}.$$

Model recasting with $\phi_\alpha = aT_\alpha^4$

Following the idea in [Enaux, et.al., JSC2020][4], three temperature model is recast in the following form by setting $\phi_\alpha = aT_\alpha^4$:

$$\begin{aligned}
\frac{\partial \phi_e}{\partial t} - \beta_e \nabla \cdot (\lambda_e \nabla \phi_e) &= \beta_e c \sigma_P (\phi_r - \phi_e) + \beta_e c \kappa \delta_{ie} (\phi_i - \phi_e) + \beta_e Q_e \\
\frac{\partial \phi_i}{\partial t} - \beta_i \nabla \cdot (\lambda_i \nabla \phi_i) &= \beta_i c \kappa \delta_{ie} (\phi_e - \phi_i) + \beta_i Q_i \\
\frac{\partial \phi_r}{\partial t} - \beta_r \nabla \cdot (\lambda_r \nabla \phi_r) &= \beta_r c \sigma_P (\phi_e - \phi_r) + \beta_r Q_r
\end{aligned}$$

where

$$\lambda_e = \frac{\lambda_e'}{\rho c_{ve} \beta_e}, \quad \lambda_i = \frac{\lambda_i'}{\rho c_{vi} \beta_i}, \quad \lambda_r = \frac{c}{3\sigma_R}, \quad \beta_\alpha = \frac{d\phi_\alpha}{dE_\alpha} = \frac{\mathrm{d}\phi_\alpha}{\mathrm{d}T_\alpha}\frac{\mathrm{d}T_\alpha}{\mathrm{d}E_\alpha} = \frac{4aT_\alpha^3}{\rho c_{v,\alpha}}, \ \alpha = e, i, r.$$

[4] C. Enaux, S.Guisset, C.Lasuen, Q.Ragueneau, J. Sci. Comput. (2020)82:51.

Spatial and temporal discretization of 3T model

The temporal discretization chosen consist in the backward-Euler scheme, and the spatial-temporal discretization of 3T model reads:

$$\phi_{e,K}^{n+1} - \phi_{e,K}^{n} + \frac{\tau}{|K|}\beta_{e,K}^{n+1} \sum_{\sigma\in\mathcal{E}_K} F_{e,K,\sigma}^{n+1} = \tau c\sigma_P \beta_{e,K}^{n+1}\left(\phi_{r,K}^{n+1} - \phi_{e,K}^{n+1}\right) + \tau\beta_{e,K}^{n+1} Q_{e,K}^{n+1}$$

$$+ \tau c\kappa\beta_{e,K}^{n+1}\delta_{ie,K}^{n+1}\left(\phi_{i,K}^{n+1} - \phi_{e,K}^{n+1}\right),$$

$$\phi_{i,K}^{n+1} - \phi_{i,K}^{n} + \frac{\tau}{|K|}\beta_{i,K}^{n+1} \sum_{\sigma\in\mathcal{E}_K} F_{i,K,\sigma}^{n+1} = \tau c\kappa\beta_{i}^{n+1}\delta_{ie,K}^{n+1}\left(\phi_{e,K}^{n+1} - \phi_{i,K}^{n+1}\right) + \tau\beta_{i,K}^{n+1} Q_{i,K}^{n+1},$$

$$\phi_{r,K}^{n+1} - \phi_{r,K}^{n} + \frac{\tau}{|K|}\beta_{r,K}^{n+1} \sum_{\sigma\in\mathcal{E}_K} F_{r,K,\sigma}^{n+1} = \tau c\sigma_P\left(\phi_{e,K}^{n+1} - \phi_{r,K}^{n+1}\right) + \tau\beta_{r,K}^{n+1} Q_{r,K}^{n+1},$$

where the derivation of face flux $F_{\alpha,K,\sigma}^{n+1}, \alpha = e, i, r$ is given in the previous section.

The final finite volume equation

The PPFV scheme for 3T model: find $\{u_K, K \in \mathcal{T}\}$ such that

$$\phi_{\alpha,K}^{n+1} + \sum_{\gamma\in\{e,i,r\}} w_{\alpha,\gamma,K}^{n+1} G_{\gamma,K}^{n+1} = \sum_{\gamma\in\{e,i,r\}} w_{\alpha,\gamma,K}^{n+1} \left(\phi_{\gamma,K}^{n} + q_{\gamma,K}^{n+1}\right), \quad \alpha = e, i, r, \forall K \in \mathcal{T}.$$

where

$$G_{\alpha,K}^{n+1} = \frac{\tau}{|K|}\beta_{\alpha,K}^{n+1} \sum_{\sigma\in\mathcal{E}_K} \tilde{F}_{\alpha,K,\sigma}^{n+1}, \; q_{\alpha,K}^{n+1} = \tau\beta_{\alpha,K}^{n+1} Q_{\alpha,K}^{n+1},$$

and the definition of the flux

- For $\sigma \in \mathcal{E}_K \cap \mathcal{E}_L$: $\tilde{F}_{\alpha,K,\sigma}^{n} = A_{\alpha,K,\sigma}^{n}(\phi_\alpha^n)\phi_{\alpha,K}^n - A_{\alpha,L,\sigma}^{n}(\phi_\alpha^n)\phi_{\alpha,L}^n$
- For $\sigma \in \mathcal{E}_K \cap \Gamma_D$: $\tilde{F}_{\alpha,K,\sigma}^{n} = \lambda_{\alpha,K,\sigma}^{n} \sum_{i=1}^{N_{K,\sigma}} a_{K,\sigma,i} \left(\phi_{\alpha,K}^n - g_\alpha^D\left(\boldsymbol{x}_{K,\sigma,i}, t^n\right)\right), \; \boldsymbol{x}_{K,\sigma,i} \in \sigma$
- For $\sigma \in \mathcal{E}_K \cap \Gamma_N$: $\tilde{F}_{\alpha,K,\sigma}^{n} = \int_\sigma g_\alpha^N\left(\boldsymbol{x}, t^n\right) \mathrm{d}s$

The nonlinear algebraic system

We get a nonlinear algebraic system

$$\mathbb{M}\left(\boldsymbol{\phi}^n\right)\boldsymbol{\phi}^n = \boldsymbol{b}\left(\boldsymbol{\phi}^n\right).$$

where

$$\mathbb{M}\left(\boldsymbol{\phi}^n\right) = \tilde{\mathbb{M}}\left(\boldsymbol{\phi}^n\right) + \mathbb{I},$$

and

$$\tilde{\mathbb{M}}\left(\boldsymbol{\phi}^n\right) = \left[\begin{array}{c|c|c} \mathbb{W}^n_{e,e}\mathbb{A}^n_e & \mathbb{W}^n_{e,i}\mathbb{A}^n_i & \mathbb{W}^n_{e,r}\mathbb{A}^n_r \\ \hline \mathbb{W}^n_{i,e}\mathbb{A}^n_e & \mathbb{W}^n_{i,i}\mathbb{A}^n_i & \mathbb{W}^n_{i,r}\mathbb{A}^n_r \\ \hline \mathbb{W}^n_{r,e}\mathbb{A}^n_e & \mathbb{W}^n_{r,i}\mathbb{A}^n_i & \mathbb{W}^n_{r,r}\mathbb{A}^n_r \end{array}\right], \ \boldsymbol{\phi}^n = \left[\begin{array}{c} \boldsymbol{\phi}^n_e \\ \hline \boldsymbol{\phi}^n_i \\ \hline \boldsymbol{\phi}^n_r \end{array}\right], \boldsymbol{b}\left(\boldsymbol{\phi}^n\right) = \left[\begin{array}{c} \tilde{\boldsymbol{b}}^n_e \\ \hline \tilde{\boldsymbol{b}}^n_i \\ \hline \tilde{\boldsymbol{b}}^n_r \end{array}\right],$$

Some theoretical results

Positivity of the discrete solution

Let $\phi_\alpha^0 \geq 0,\ Q_\alpha \geq 0, g_\alpha^D \geq 0, g_\alpha^N \leq 0,\ \alpha \in \{e, i, r\}$, and assume that each mesh cell K is a star-shaped polyhedron w.r.t. $\boldsymbol{x}_K$. If the initial solution vector $\boldsymbol{\phi}^{n,0} \geq 0$ and linear systems in the Picard iterations are solved exactly, then $\boldsymbol{\phi}^{n+1,k} \geq 0$ for $k \geq 1$.

Stability

Let $\phi_\alpha^0 \geq 0,\ Q_\alpha \geq 0,\ \alpha \in \{e, i, r\}$, assume that ($\Gamma = \partial\Omega,\ g_\alpha^D = 0$) and $\rho c_{v,\alpha} = 4aT_\alpha^3$, $\alpha = e, i$, then for $\phi_{\alpha,\mathcal{T}}^n = \{\phi_{\alpha,K}^n, K \in \mathcal{T}\} \in \mathbb{X}(\mathcal{T})$ we have

$$\left\| \phi_{\alpha,\mathcal{T}}^{N^t} \right\|_{L^1,\mathcal{T}} \leq \left(\left\| \phi_{m,\mathcal{T}}^0 \right\|_{L^1,\mathcal{T}} + \tau \sum_{k=1}^{N^t} \left\| Q_{m,\mathcal{T}}^k \right\|_{L^1,\mathcal{T}} \right),\ \alpha = e, i, r.$$

where $\phi_{m,K}^n = \max\limits_{\gamma \in \{e,i,r\}} \phi_{\gamma,K}^n,\ Q_{m,K}^n = \max\limits_{\gamma \in \{e,i,r\}} Q_{\gamma,K}^n,\ t_{\max} = N^t \tau.$

Outline

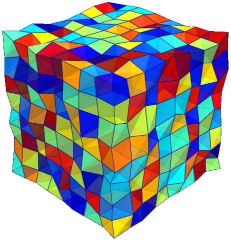
(P1) The continuous problem on nonplanar meshes

The computational domain $\Omega = [0,1]^3$, and the diffusion tensor:

$$\Lambda = \begin{pmatrix} 1 & 0.5 & 0 \\ 0.5 & 1 & 0.5 \\ 0 & 0.5 & 1 \end{pmatrix}.$$

The exact solution:

$$u = 3 - (x^2 + y^2 + z^2), \quad (x, y, z) \in \Omega.$$

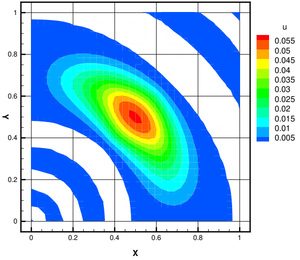


nunkw	E_u	R_u	E_q	R_q	umin	umax
64	1.05E-02	-	6.18E-02	-	3.870E-01	2.888
512	2.45E-03	2.095	2.33E-02	1.405	2.447E-01	2.972
4096	5.83E-04	2.069	9.24E-03	1.336	1.061E-01	2.993
32768	1.43E-04	2.027	4.05E-03	1.190	5.602E-02	2.998

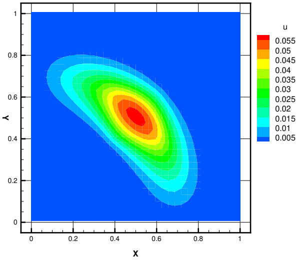
(P2) Positivity of the solution

The anisotropic diffusion tensor and the source term:

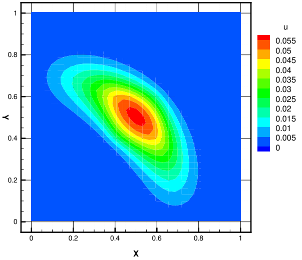
$$\Lambda = \begin{pmatrix} y^2 + cx^2 & -(1-c)xy & 0 \\ -(1-c)xy & x^2 + cy^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad f = \begin{cases} 1, & (x, y) \in \left[\frac{3}{8}, \frac{5}{8}\right]^2, \quad z \in [0, 1], \\ 0, & \text{otherwise}, \end{cases}$$



Linear LPFV



PPFV_LPDI



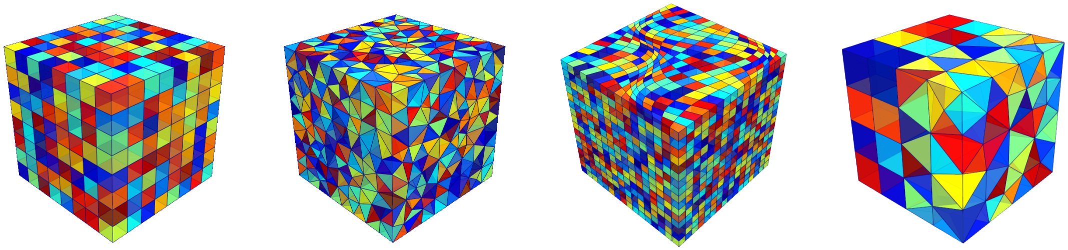
PPFV_LPDII

(P3) Convergence test for a continuous 3T model

We set the computational domain $\Omega = [0,1]^3$, and the following exact solution

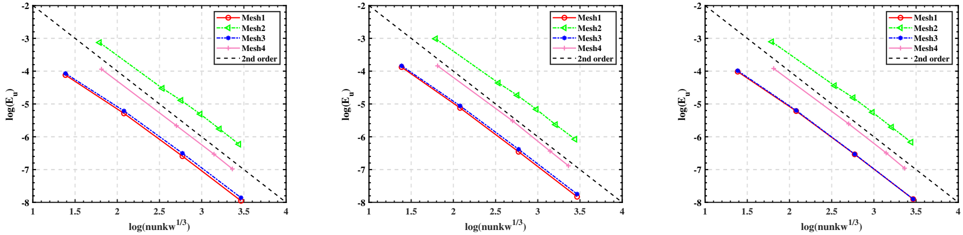
$$\phi_e = 1 - 2\,(x-0.5)^2 - (y-0.5)^2 - (z-0.5)^2\,,$$
$$\phi_i = 1 - (x-0.5)^2 - 2\,(y-0.5)^2 - (z-0.5)^2\,,$$
$$\phi_r = 1 - (x-0.5)^2 - (y-0.5)^2 - 2\,(z-0.5)^2\,,$$

The associated parameter: $\rho c_{v,\alpha} = 4aT_\alpha^3$, $a = c = \sigma_P = \sigma_R = 1$, $\lambda_e = 1$, $\lambda_i = 0.5$.

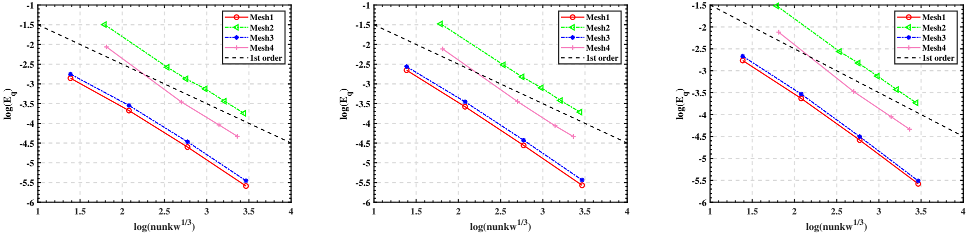


(a) Mesh1 (b) Mesh2 (c) Mesh3 (d) Mesh4

(P3) Convergence test for a continuous 3T model



L^2 error of electronic (left), ionic (middle) and radiative (right) energy densities.



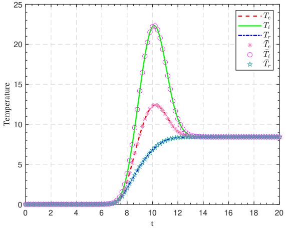
H^1 error of electronic (left), ionic (middle) and radiative (right) energy densities.

(P4) 0D test (no spatial variation)

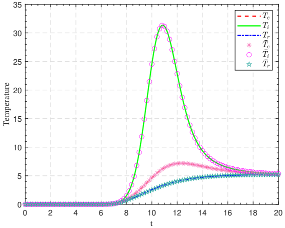
- **Problem 1–Problem 2**: At initial time the three temperaturss are equal.
- A decoupling of the three temperatures are observed when source terms Q are applied:

$$Q_i(t) = \frac{A}{\sqrt{2\pi}t_w} \exp\left(-\left(\frac{t-tc}{\sqrt{2}t_w}\right)^2\right), \qquad Q_e = Q_r = 0.$$

	Problem 1	Problem 2
c	29.979	29.979
a	0.01372	0.01372
σ_P	$0.5\,T_e^{-2}$	$0.1\,T_e^{-2}$
κ	0.1	$0.01379\,T_e^{-0.5}$
$\rho c_{v,i}$	0.15	0.15
$\rho c_{v,e}$	0.3	$0.3\,T_e$
T_α	$2.52487 \cdot 10^{-5}$	$2.52487 \cdot 10^{-5}$
A	75.19884	15.03978



Problem 1



Problem 2

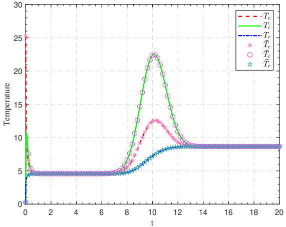
The numerical results in [1][1] are recovered. The ionic temperature is higher than others.

[1] [1]C. Enaux, et.al., J. Sci. Comput. (2020)82:51.

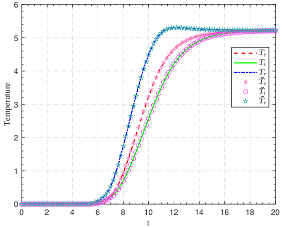
(P4) 0D test (no spatial variation)

- **Problem 3**: source term is applied on ions, and the initial temperatures are different.
- **Problem 4**: source term is applied on photons.

	Problem 3	Problem 4
c	29.979	29.979
a	0.01372	0.01372
σ_P	$0.5\,T_e^{-2}$	$0.1\,T_e^{-2}$
κ	0.1	$0.01379\,T_e^{-0.5}$
$\rho c_{v,i}$	0.15	0.15
$\rho c_{v,e}$	0.3	$0.3\,T_e$
T_e	$2.52487 \cdot 10^{-1}$	$2.52487 \cdot 10^{-5}$
T_i	$2.52487 \cdot 10^{1}$	$2.52487 \cdot 10^{-5}$
T_r	$2.52487 \cdot 10^{-1}$	$2.52487 \cdot 10^{-5}$
A	75.19884	15.03978



Problem 3



Problem 4

The time evolution of temperatures are graphically shown, and the numerical results in [1][1] are exactly recovered.

[1] [1]C. Enaux, et.al., J. Sci. Comput. (2020)82:51.

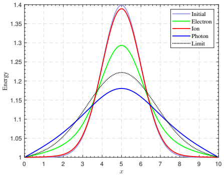
(P5) Asymptotic behavior

The asymptotic-preserving property is studied: $T_e = T_i = T_r$ when $c\sigma_P \to \infty$ and $c\kappa \to \infty$.

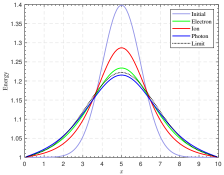
- Choose an initial energy profile for different values of $c\sigma_P$ and $c\kappa$ of the form

$$\phi_e = \phi_i = \phi_r = 1 + \frac{1}{\sqrt{2\pi}} \exp\left(-0.5(x-5)^2\right).$$

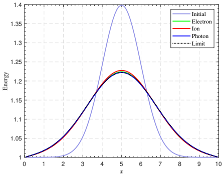
- For small values of $c\sigma_P$, the three temperature profiles are very different while they become closer as $c\sigma_P$ and $c\kappa$ increases.
- For large values $c\sigma_P = c\kappa$, it is expected that **the three temperatures to be equal**.



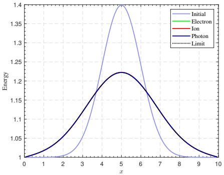
$c\sigma_P = c\kappa = 10^{-1}$



$c\sigma_P = c\kappa = 10^{0}$



$c\sigma_P = c\kappa = 10^{1}$

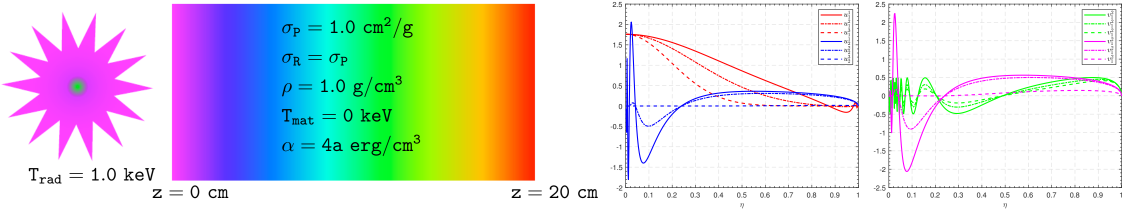


$c\sigma_P = c\kappa = 10^{2}$

(P6) The Su–Olson problem

- The Su-Olson problem[5] consists of a half-space, non-equilibrium Marshak wave.
- As the energy density of the radiation field increases, energy is transfered to the material.
- The dimensionless solution for the radiation energy density:

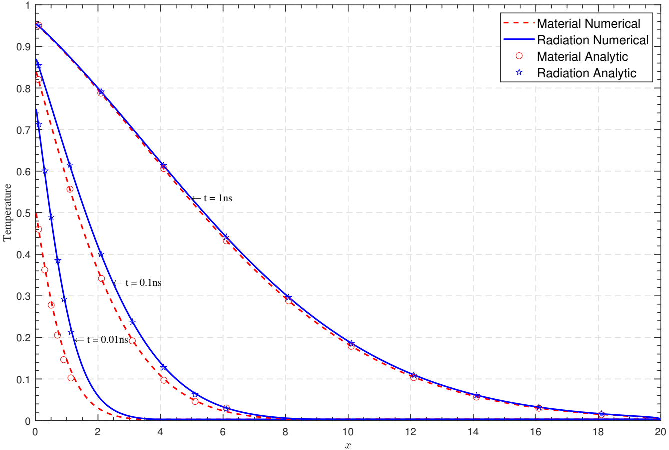
$$u(x,\tau,\epsilon)=1-\frac{2\sqrt{3}}{\pi}\int_0^1\left[\frac{\sin[x\gamma_1(\eta,\epsilon)+\theta_1(\eta)]}{\eta\sqrt{3+4\gamma_1^2(\eta,\epsilon)}}\right]e^{-\tau\eta^2}\,d\eta-\frac{\sqrt{3}e^{-\tau}}{\pi}\int_0^1\left[\frac{\sin[x\gamma_2(\eta,\epsilon)+\theta_2(\eta)]}{\eta(1+\epsilon\eta)\sqrt{3+4\gamma_2^2(\eta,\epsilon)}}\right]e^{\frac{-\tau}{\epsilon}\eta}\,d\eta.$$



Setup and parameters for the Su-Olson problem, and key components of the solution.

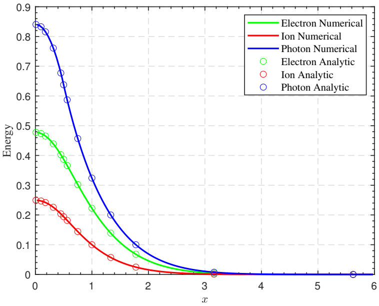
[5] B.Su,G.L.Olson, JQSRT, 1996, 56 (3): 337–351

(P6) The Su–Olson problem

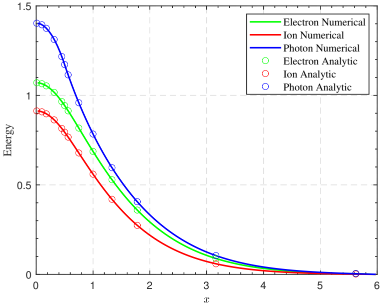


- Initially, the radiation streams into the slab and T_m lags behind T_r;
- As the radiation energy density builds up, the material temperature catches up;
- At $t = 1$ns, the radiation and material temperatures are essentially identical.

(P7) A 3T version of the Su–Olson problem [7]



(e) $t_m = 3.16228$



(f) $t_m = 10$

- A 3T version of the fixed-source problem solved by Su-Olson [6] which is useful for verifying computer code such as xRage code.
- An excellent agreement between the numerical and semi-analytical solutions can be seen.

[6] B.Su, G.L.Olson, Ann.Nucl.Energy,1997;24(13):1035–55

[7] R.G.McClarren, J.G.Wohlbier. JQSRT, 2011;112(1):119–130.

Summary

- Presented nonlinear two-point flux discretization for three temperature model
- Local mass conservation
- Positivity-preserving property
- Arbitrary polyhedral meshes
- SPD diffusion matrix for three temperature model
- Second-order convergence rate for temperature
- First-order convergence rate for flux
- Stability result for the discrete FV equations
- Coupling with Lagrangian hydrodynamics is easy

Key References

- D. Yang, Z. Gao, G. Ni. The positivity-preserving finite volume scheme with fixed stencils for anisotropic diffusion problems on general polyhedral meshes. International Journal for Numerical Methods in Fluids, 2022, 94(12): 2137-2171.
- G. Peng, Z. Gao, W. Yan, X. Feng. A positivity-preserving finite volume scheme for three-temperature radiation diffusion equations. Applied Numerical Mathematics,2020, 152:125-140.
- Z. Gao, J. Wu. A second-order positivity-preserving finite volume scheme for diffusion equations on general meshes. SIAM J. Sci. Comput., 37(1)(2015)A420-A438
- J. Wu, Z. Gao. Interpolation-based second-order monotone finite volume schemes for anisotropic diffusion equations on general grids. Journal of Computational Physics 275 (2014) 569-588.
- Z. Gao, J. Wu. A linearity preserving cell-centered scheme for the heterogeneous and anisotropic diffusion equations on general meshes. Int. J. Numer. Meth. Fluids, 67(12)(2011)2157-2183.

铸国防基石，
做民族脊梁！

Thank you!