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Numerical methods for inertial confinement fusion

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Outline



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• High power laser facilities

- Experimental setting
- Modelling: hydrodynamics
- Modelling: radiative transfer
- Diffusion approximation
 - Boundary conditions
 - Frequency dependent diffusion
 - Marshak waves
 - Flux limitation
- Discretization
 - Frequency
 - Time
 - Space

Outline (continued)



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- Diffusion schemes
 - VF4 scheme
 - Other schemes
 - Lapln scheme
- P1 model
- PN model
- M1 model
- Boundary condition (continued)

High power laser facilities

- Laser MegaJoule (Bordeaux) + HiPER (PetAL) project
- National Ignition Facility (Livermore)
- LFEX (Osaka)

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LMJ project

High power laser facilities

- Laser MegaJoule (Bordeaux) + HiPER (PetAL) project
- National Ignition Facility (Livermore)
- LFEX (Osaka)

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NIF project

Inertial confinement fusion



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Principle : implode a capsule of fusion fuel by laser pulses.
Objective : Reaching conditions under which fusion reactions start.
Mainly two strategies:

- **Direct drive** : the target is directly heated by lasers
- Indirect drive : the lasers heat the inner walls of a cavity. The walls emit X-rays toward the target.



Inertial confinement fusion



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Indirect drive

Advantage: Heating is more uniform.

Drawback: Energy loss (up to 80%) in heating walls.



The X-rays rapidly (1) heat the capsule, (2) causing its surface to fly outward. This outward force causes an opposing inward force that compresses the fuel inside the capsule. When the compression reaches the center, temperatures increase to 100,000,000 °C, (3) igniting the fusion fuel and (4) producing a thermonuclear burn that yields many times the energy input (energy gain).





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Size of capsule: $\sim 1mm$



• Size of Hohlraum: $\sim 10mm$





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LMJ: 300 meters



Hohlraum: 10 mm



LMJ chamber: 10 meters



Capsule: 1 mm

Typical sizes

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Starting fusion reactions: need $T \ge 5 \times 10^7 K$ Lawson's criterion for reaching fusion (τ confinement time, n_e electronic density):

 $n_e \tau \approx 10^{14} s \ cm^{-3}.$

Typically $\rho \approx 10^3 g \ cm^{-3}$, $T \approx 5 \times 10^7 K$, $\tau \approx 10^{-9} s$. Hot spot at the center of the capsule



Modelling issues

Coupling between:



- Laser-plasma interaction
- Hydrodynamical instabilities
- Suprathermic particles
- Loss of thermodynamic equilibrium
- Dealing with uncertainties
-

Hydrodynamics

Laser plasmas: hot, dense.



Bitemperature compressible Euler equations $(\frac{d}{dt} = \frac{\partial}{\partial t} + u \cdot \nabla)$:

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$$\begin{cases} \frac{d\rho}{dt} + \rho \operatorname{div}(u) &= 0, \\ \rho \frac{du}{dt} + \nabla \left(p_e + p_i\right) &= F_r, \\ \rho \frac{dE_e}{dt} + p_e \operatorname{div}(u) - \operatorname{div} \left(\chi_e \nabla T_e\right) + \gamma_{ei} \left(T_e - T_i\right) &= Q_r + S, \\ \rho \frac{dE_i}{dt} + p_i \operatorname{div}(u) - \operatorname{div} \left(\chi_i \nabla T_i\right) - \gamma_{ei} \left(T_e - T_i\right) &= 0, \end{cases}$$

+ e.o.s
$$(E_{e,i} = \frac{p_{e,i}}{(\gamma_{e,i}-1)\rho} = C_{v\{e,i\}}T_{e,i}).$$

 F_r radiative flux, Q_r radiative energy \Leftarrow radiative transfer equation S laser energy drop

$$\gamma_{ei} = \rho C_{ve} \frac{m_e}{m_i} \frac{1}{\tau_{ei}}, \quad \tau_{ei} \propto T_e^{3/2}, \quad \chi_e \propto T_e^{5/2}.$$

Radiative transfer

 $I = I_{\nu}(x, t, \Omega)$: specific radiative intensity (Jm^{-2}) ν frequency, Ω direction of propagation.

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$$\frac{\rho}{c}\frac{d}{dt}\left(\frac{I_{\nu}}{\rho}\right) + \Omega \cdot \nabla I_{\nu} + \sigma_a \left(I_{\nu} - B_{\nu}(T_e)\right) + \kappa_{\mathrm{Th}}\left(I_{\nu} - \int_{S^2} \frac{3}{4} \left(1 + \left(\Omega \cdot \Omega'\right)^2\right) I_{\nu}(\Omega')\frac{d\Omega'}{4\pi}\right) = 0,$$



Coupled system

$$\begin{cases} \frac{d\rho}{dt} + \rho \operatorname{div}(u) &= 0, \\ \rho \frac{du}{dt} + \nabla \left(p_e + p_i\right) &= F_r, \\ \rho \frac{dE_e}{dt} + p_e \operatorname{div}(u) - \operatorname{div}\left(\chi_e \nabla T_e\right) + \gamma_{ei}\left(T_e - T_i\right) &= Q_r + S, \\ \rho \frac{dE_i}{dt} + p_i \operatorname{div}(u) - \operatorname{div}\left(\chi_i \nabla T_i\right) - \gamma_{ei}\left(T_e - T_i\right) &= 0, \end{cases}$$

(+ equation of state)

$$\frac{\rho}{c}\frac{d}{dt}\left(\frac{I_{\nu}}{\rho}\right) + \Omega \cdot \nabla I_{\nu} + \sigma_a \left(I_{\nu} - B_{\nu}(T_e)\right) \\ + \kappa_{\rm Th} \left(I_{\nu} - \int_{S^2} \frac{3}{4} \left(1 + \left(\Omega \cdot \Omega'\right)^2\right) I_{\nu}(\Omega')\frac{d\Omega'}{4\pi}\right) = 0,$$

$$F_r = \int_{S^2} \int_0^\infty \Omega \left(\sigma_a + \kappa_{\rm Th} \right) I_\nu(x, t, \Omega) d\nu \frac{d\Omega}{4\pi},$$

$$Q_r = \int_{S^2} \int_0^\infty \sigma_a \left(I_\nu(x, t, \Omega) - B_\nu(T_e) \right) d\nu \frac{d\Omega}{4\pi}.$$

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Radiative transfer: theory

Without hydro



$$\frac{1}{c}\frac{\partial I_{\nu}}{\partial t} + \Omega \cdot \nabla I_{\nu} + \sigma_a \left(I_{\nu} - B_{\nu}(T)\right) + \kappa_{\mathrm{Th}} \left(I_{\nu} - \int_{S^2} \frac{3}{4} \left(1 + \left(\Omega \cdot \Omega'\right)^2\right) I_{\nu}(\Omega') \frac{d\Omega'}{4\pi}\right) = 0,$$

$$C_{\nu}\frac{\partial T}{\partial t} = \int_{S^2} \int_0^\infty \sigma_a(\nu) \left(I_{\nu}(x,t,\Omega) - B_{\nu}(T)\right) d\nu \frac{d\Omega}{4\pi} \,,$$

Initial conditions: $I_{\nu}(x, 0, \Omega) = I_{\nu}^{0}(x, \Omega), \quad T(x, 0) = T^{0}(x).$ Boundary conditions:

$$\forall x \in \partial \mathcal{D}, \quad \forall \Omega / \Omega \cdot n(x) \le 0, \quad I_{\nu}(x, t, \Omega) = I_{\nu}^{\text{ext}}(x, t, \Omega),$$

Theorem: (Golse, Perthame, 1986) Under "suitable hypotheses", the radiative transfer system is well- posed.

Radiative transfer: theory

Remark on the hypotheses: one of them reads



 $\forall \nu > 0, T \mapsto \sigma_a(\nu, T)$ is nonincreasing, and $T \mapsto \sigma_a(\nu, T) B_{\nu}(T)$ is nondecreasing.

Physically, this is not relevent. But implies accretiveness of semi-group.

More realistic results on simpler system (Bardos, Golse, Perthame, Sentis, 1988)

Coupled system: local in time existence: Lin (2007), Zhong, Jiang (2007).

- radiation almost isotropic \Rightarrow P1 approximation in Ω
- radiation is **not** Planckian (M-band of gold)





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P1 approximation in Ω : $I_{\nu} \approx cE_{\nu} + \frac{1}{3}\Omega F_{\nu}$.

$$E_{\nu} = \frac{1}{c} \oint_{S^2} I_{\nu} d\Omega, \quad F_{\nu} = \oint_{S^2} \Omega I_{\nu} d\Omega.$$

$$\begin{cases} \frac{dE_{\nu}}{dt} + \operatorname{div}(F_{\nu}) + \sigma_a(cE_{\nu} - B_{\nu}(T)) = 0, \\ \frac{1}{c}\frac{dF_{\nu}}{dt} + \oint_{S_2}\Omega\Omega \cdot \nabla I_{\nu}d\Omega + \sigma_a F_{\nu} = 0. \\ \underset{\approx \frac{c}{3}\nabla E_{\nu}}{\overset{\sim}{\longrightarrow}} \end{cases}$$

Stationary approximation for the second equation: $c \ll 1$.

$$\frac{dE_{\nu}}{dt} - \operatorname{div}\left(\frac{c}{3\sigma_{\nu}}\nabla E_{\nu}\right) + \sigma_a(cE_{\nu} - B_{\nu}(T)) = 0.$$

Nonlinear diffusion equation.

Diffusion approximation – boundary condition

Boundary condition on $I_{\nu}(x,t,\Omega) \Rightarrow$ boundary condition on $E_{\nu}(x,t)$?

$$\forall x \in \partial \mathcal{D}, \quad \forall \Omega / \Omega \cdot n(x) \le 0, \quad I_{\nu}(x, t, \Omega) = I_{\nu}^{\text{ext}}(x, t, \Omega),$$

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$$\int_{\Omega \cdot n \leq 0} |\Omega \cdot n| I_{\nu}(x, t, \Omega) d\Omega = \int_{\Omega \cdot n \leq 0} |\Omega \cdot n| I_{\nu}^{\text{ext}}(x, t, \Omega) d\Omega := F_{\nu}^{\text{in}}(x, t),$$

$$\frac{c}{4\pi}E_{\nu}\int_{\Omega\cdot n\leq 0}|\Omega\cdot n|d\Omega + \frac{3}{4\pi}\left(-\frac{c\nabla E_{\nu}}{3\left(\sigma_{a}(\nu)+\kappa_{\mathrm{Th}}\right)}\right)\cdot\int_{\Omega\cdot n\leq 0}|\Omega\cdot n|\Omega d\Omega = F_{\nu}^{\mathrm{in}}.$$

$$E_{\nu} + \frac{2}{3\left(\sigma_a(\nu) + \kappa_{\rm Th}\right)} \frac{\partial E_{\nu}}{\partial n} = \frac{4}{c} F_{\nu}^{\rm in}.$$

Marshak boundary condition

Dimensional analysis:

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mean free path $\frac{1}{\sigma_a + \kappa_{Th}} \approx \varepsilon$, mean free time $\frac{1}{c(\sigma_a + \kappa_{Th})} \approx \varepsilon^2$. Asymptotic analysis: $t \to \varepsilon^2 t$, $x \to \varepsilon x$ (Larsen, Badham, Pomraning, 1983).

$$\frac{\varepsilon}{c}\frac{\partial I_{\nu}}{\partial t} + \Omega \cdot \nabla I_{\nu} + \frac{\sigma_a}{\varepsilon} \left(I_{\nu} - B_{\nu}(T)\right) + \frac{\kappa_{\rm Th}}{\varepsilon} \left(I_{\nu} - \int_{S^2} \frac{3}{4} \left(1 + \left(\Omega \cdot \Omega'\right)^2\right) I_{\nu}(\Omega') \frac{d\Omega'}{4\pi}\right) = 0,$$

$$\varepsilon C_v \frac{\partial T}{\partial t} = \int_{S^2} \int_0^\infty \frac{\sigma_a}{\varepsilon} \left(I_\nu(x, t, \Omega) - B_\nu(T) \right) d\nu \frac{d\Omega}{4\pi}$$

Hilbert expansion:

$$I_{\nu} = I^{0} + \varepsilon I^{1} + \varepsilon^{2} I^{2} + \dots,$$
$$T = T^{0} + \varepsilon T^{1} + \varepsilon^{2} T^{2} + \dots.$$

$$\frac{\varepsilon}{c}\frac{\partial I_{\nu}}{\partial t} + \Omega \cdot \nabla I_{\nu} + \frac{\sigma_a}{\varepsilon}\left(I_{\nu} - B_{\nu}(T)\right) + \frac{\kappa_{\rm Th}}{\varepsilon}\left(I_{\nu} - \mathcal{K}(I_{\nu})\right) = 0,$$

order ε^{-1} :

$$\sigma_a \left(I_{\nu}^0 - B_{\nu}(T^0) \right) + \kappa_{\rm Th} \left(I_{\nu}^0 - \mathcal{K}(I_{\nu}^0) \right) = 0 \implies I_{\nu}^0 = B_{\nu}(T^0).$$

order ε^0 :

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$$\Omega \cdot \nabla I_{\nu}^{0} + \sigma_{a} \left(I_{\nu}^{1} - \frac{c}{4\pi} B_{\nu}'(T^{0})T^{1} \right) + \kappa_{\mathrm{Th}} \left(I_{\nu}^{1} - \mathcal{K}(I_{\nu}^{1}) \right) = 0.$$

$$\Omega \cdot \nabla I_{\nu}^{1}(\mathbf{x}, t, \Omega) = \Omega \cdot \nabla \left(\frac{1}{\sigma_{a} + \kappa_{\mathrm{Th}}} \Omega \cdot \nabla I_{\nu}^{0} \right) + \Omega \cdot \nabla (...).$$

$$\int_{S^{2}} \Omega \cdot \nabla I_{\nu}^{1}(\mathbf{x}, t, \Omega) d\Omega = \operatorname{div} \left(\frac{1}{3(\sigma_{a} + \kappa_{\mathrm{Th}})} \nabla I_{\nu}^{0} \right).$$

order ε^1 :



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$$\frac{1}{c}\frac{\partial I_{\nu}^{0}}{\partial t} + \Omega \cdot \nabla I_{\nu}^{1} + \sigma_{a} \left(I_{\nu}^{2} - \frac{c}{4\pi}B_{\nu}'(T^{0})T^{2} - \frac{c}{4\pi}B_{\nu}''(T^{0})\frac{(T^{1})^{2}}{2} \right) + \kappa_{\mathrm{Th}} \left[I_{\nu}^{2} - \mathcal{K}(I_{\nu}^{2}) \right] = 0,$$

$$C_{\nu}\frac{\partial T^{0}}{\partial t} = \int_{S^{2}} \int_{0}^{\infty} \sigma_{a} \left(I_{\nu}^{2} - \frac{c}{4\pi} B_{\nu}'(T^{0})T^{2} - \frac{c}{4\pi} B_{\nu}''(T^{0})\frac{(T^{1})^{2}}{2} \right) \frac{d\Omega}{4\pi} d\nu.$$

Integrate over Ω and ν , sum:

$$\frac{1}{c}\frac{\partial}{\partial t}\left(C_{v}T^{0}+ac(T^{0})^{4}\right)+\int_{S^{2}}\int_{0}^{\infty}\Omega\cdot\nabla I^{1}(\mathbf{x},t,\Omega)d\nu\frac{d\Omega}{4\pi}=0,$$

Using the expression of $\int \int \Omega \cdot \nabla I^1$,

$$\frac{1}{c}\frac{\partial}{\partial t}\left(C_vT^0 + ac(T^0)^4\right) - \operatorname{div}\left(\frac{1}{3\sigma_R}\nabla\left[ac\left(T^0\right)^4\right]\right) = 0.$$

Rosseland model

$$\frac{1}{c}\frac{\partial}{\partial t}\left(C_vT + ac(T)^4\right) - \operatorname{div}\left(\frac{1}{3\sigma_R}\nabla\left(acT^4\right)\right) = 0.$$



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$$\frac{1}{\sigma_R(T)} = \left(\int_0^\infty B'_\nu(T)d\nu\right)^{-1} \int_0^\infty \frac{B'_\nu(T)}{\sigma_a(\nu,T) + \kappa_{\rm Th}}d\nu$$

Theorem: (Bardos, Golse, Perthame, 1987) Under "suitable hypotheses", the solution to the radiative transfer equation converges, as $\varepsilon \rightarrow 0$, to the solution to the Rosseland equation.

Remarks:

with

- Hypotheses similar to the existence theorem for radiative transfer (accretiveness).
- If initial or boundary conditions are not Planckian, boundary layer.

Frequency-dependent diffusion

Rosseland approximation \Rightarrow planckian distribution. Frequency-dependent diffusion:



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$$\frac{\varepsilon}{c}\frac{\partial E_{\nu}}{\partial t} - \operatorname{div}\left(\frac{1}{3(\sigma_{a} + \kappa_{\mathrm{Th}})}\nabla E_{\nu}\right) + \frac{\sigma_{a}}{\varepsilon}\left(E_{\nu} - \frac{4\pi}{c}B_{\nu}(T)\right) = 0,$$
$$\varepsilon C_{\nu}\frac{\partial T}{\partial t} = \frac{c}{4\pi}\int_{0}^{\infty}\frac{\sigma_{a}(\nu)}{\varepsilon}\left(E_{\nu} - \frac{4\pi}{c}B_{\nu}(T)\right)d\nu.$$

Theorem: As $\varepsilon \to 0$, the solution to the above system converges to the Rosseland equation.



Frequency-dependent diffusion

Another approach: $\frac{1}{c} \ll 1$, $\sigma_a \ll 1$, $\kappa_{Th} \gg 1$.



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$$\frac{\varepsilon}{c}\frac{\partial I_{\nu}}{\partial t} + \Omega \cdot \nabla I_{\nu} + \varepsilon \sigma_a \left(I_{\nu} - B_{\nu}(T)\right) \\ + \frac{\kappa_{\rm Th}}{\varepsilon} \left(I_{\nu} - \int_{S^2} \frac{3}{4} \left(1 + \left(\Omega \cdot \Omega'\right)^2\right) I_{\nu}(\Omega') \frac{d\Omega'}{4\pi}\right) = 0,$$

$$C_{\nu}\frac{\partial T}{\partial t} = \int_{S^2} \int_0^\infty \sigma_a \left(I_{\nu}(x,t,\Omega) - B_{\nu}(T)\right) d\nu \frac{d\Omega}{4\pi}$$

Theorem: (Buet, Depsrés, 2009) As $\varepsilon \to 0$, the solution to the above system converges to the frequency dependent diffusion equation, with a diffusion coefficient equal to $\frac{1}{6\pi r}$.

Then,

$$\frac{1}{\kappa_{\rm Th}} \approx \frac{1}{\kappa_{\rm Th} + \sigma_a}$$

$$\frac{1}{c}\frac{\partial}{\partial t}\left(C_vT + ac(T)^4\right) - \operatorname{div}\left(\frac{1}{3\sigma_R}\nabla\left(acT^4\right)\right) = 0.$$



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Simplification: $C_v T \ll acT^4$, $\sigma_R \propto T^{-\alpha}$. $u = acT^4$:

$$\frac{\partial u}{\partial t} - \operatorname{div}\left(u^{\alpha/4}\nabla u\right) = 0,$$

up to change of variables. Porous media equation

Explicit solutions:

$$u(x,t) = \left(\frac{4t}{\alpha} - x_i\right)_+^{4/\alpha}.$$

Front propagating at speed $v = \frac{4}{\alpha}$.

$$T(x,t) \propto \left(\frac{4t}{\alpha} - x_i\right)_+^{1/\alpha}.$$



Grey case:



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$$\begin{cases} \frac{\partial E}{\partial t} - \operatorname{div}\left(\frac{1}{3\sigma}\nabla E\right) + \sigma\left(E - aT^{4}\right) = 0,\\ C_{v}\frac{\partial T}{\partial t} = \sigma\left(E - aT^{4}\right). \end{cases}$$

Another particular case: σ independent of T and $C_v = \alpha T^3$ (physically questionable).

Then, setting $u \propto E$, $v \propto T^4$,

$$\begin{cases} \frac{\sigma}{\alpha} \frac{\partial u}{\partial t} - \Delta u = v - u, \\ \frac{\partial v}{\partial t} = u - v. \end{cases}$$

In dimension one, explicit solution with Laplace transform (Pomraning, 1978, Marshak, 1958).

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Explicit solution (Olson, Su, 1996)

Flux limitation

Recall definitions of energy E_{ν} and flux F_{ν} :



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Consequence:

 $|F_{\nu}| \le cE_{\nu}.$

 $E_{\nu} = \frac{1}{c} \oint_{S^2} I_{\nu} d\Omega, \quad F_{\nu} = \oint_{S^2} \Omega I_{\nu} d\Omega.$

But, in the diffusion approximation,

$$F_{\nu} = -\frac{c}{3\left(\sigma_a + \kappa_{\rm Th}\right)} \nabla E_{\nu}.$$

Use flux limiter:

$$\frac{F_{\nu}}{cE_{\nu}} = X(|R_{\nu}|)R_{\nu}, \quad R_{\nu} = \frac{1}{\sigma_a(\nu) + \kappa_{\rm Th}} \frac{\nabla E_{\nu}}{E_{\nu}},$$

with $X(r) \leq \frac{1}{r}$.

Flux limitation

$$\frac{F_{\nu}}{cE_{\nu}} = X(|R_{\nu}|)R_{\nu}, \quad R_{\nu} = \frac{1}{\sigma_a(\nu) + \kappa_{\mathrm{Th}}} \frac{\nabla E_{\nu}}{E_{\nu}},$$



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with $X(r) \leq \frac{1}{r}$. Want to recover:

• Diffusion limit: $X(r) \sim \frac{1}{r} \text{ as } r \to \infty$,

• Free streaming limit:
$$X(r) \rightarrow \frac{1}{3}$$
 as $r \rightarrow 0$.

Examples (Levermore, 1984, Levermore, Pomraning, 1981, ...):

• Minerbo:
$$X(r) = \frac{1}{3+r}$$
.

• Sharp cut-off:
$$X(r) = \min\left(\frac{1}{r}, \frac{1}{3}\right)$$
.

Extends the validity of diffusion approximation.

Flux limitation



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Discretization: frequency

 N_g frequency groups $G_k = [\nu_{k-1}, \nu_k], 1 \le k \le N_g$.



Integration over group k:

$$\frac{\partial E_k}{\partial t} - \operatorname{div} \left(\int_{\nu_{k-1}}^{\nu_k} \frac{c}{3\left(\sigma_a(\nu) + \kappa_{\mathrm{Th}}\right)} \nabla E_\nu d\nu \right) + c \int_{\nu_{k-1}}^{\nu_k} \sigma_a(\nu) E_\nu d\nu - 4\pi \int_{\nu_{k-1}}^{\nu_k} \sigma_a(\nu) B_\nu(T_e) d\nu = 0,$$

where

$$E_k := \int_{G_k} E_{\nu} d\nu.$$

Discretization: frequency

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$$\frac{\partial E_k}{\partial t} - \operatorname{div} \left(\int_{\nu_{k-1}}^{\nu_k} \frac{c}{3\left(\sigma_a(\nu) + \kappa_{\mathrm{Th}}\right)} \nabla E_\nu d\nu \right) + c \int_{\nu_{k-1}}^{\nu_k} \sigma_a(\nu) E_\nu d\nu - 4\pi \int_{\nu_{k-1}}^{\nu_k} \sigma_a(\nu) B_\nu(T_e) d\nu = 0,$$

$$E_k := \int_{G_k} E_{\nu} d\nu.$$

Hypothesis: E_{ν} "not too far" from $B_{\nu}(T_e)$

$$\frac{\partial E_k}{\partial t} - \operatorname{div}\left(\frac{c}{3\sigma_k^R}\nabla E_k\right) + c\sigma_k^P\left(E_k - b_k a T_e^4\right) = 0,$$

 σ_k^R group Rosseland opacity ("harmonic mean"), σ_k^P group Planck opacity (arithmetic mean).
Discretization: frequency

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$$\frac{\partial E_k}{\partial t} - \operatorname{div}\left(\frac{c}{3\sigma_k^R}\nabla E_k\right) + c\sigma_k^P\left(E_k - b_k a T_e^4\right) = 0,$$

$$\frac{1}{\sigma_k^R} = \left(\int_{\nu_{k-1}}^{\nu_k} B'_{\nu}(T_e) d\nu\right)^{-1} \int_{\nu_{k-1}}^{\nu_k} \frac{B'_{\nu}(T_e)}{\sigma_a(\nu, T_e) + \kappa_{\rm Th}} d\nu,$$

$$\sigma_k^P = \left(\int_{\nu_{k-1}}^{\nu_k} B_{\nu}(T_e) d\nu\right)^{-1} \int_{\nu_{k-1}}^{\nu_k} \sigma_a(\nu, T_e) B_{\nu}(T_e) d\nu,$$

$$b_{k} = \frac{\int_{\nu_{k-1}}^{\nu_{k}} B_{\nu}(T_{e}) d\nu}{\frac{acT_{e}^{4}}{4\pi}} = \frac{\int_{\nu_{k-1}}^{\nu_{k}} B_{\nu}(T_{e}) d\nu}{\int_{0}^{\infty} B_{\nu}(T_{e}) d\nu}.$$

Discretization: frequency



An example of cross section as function of frequency.

Discretization: time

Explicit: stability condition $\Delta t \lesssim (\Delta x)^2$



Implicit discretization:

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$$\frac{E_k^{n+1} - E_k^n}{\Delta t} - \operatorname{div}\left(\frac{c}{3\sigma_k^R}\nabla E_k^{n+1}\right) + c\sigma_k^P\left(E_k^{n+1} - b_k a(T_e^{n+1})^4\right) = 0.$$

Semi-implicit with $\theta = 1/2 \Rightarrow$ second order in Δt .

$$\frac{E_k^{n+1} - E_k^n}{\Delta t} - \frac{1}{2} \operatorname{div} \left(\frac{c}{3\sigma_k^R} \nabla E_k^{n+1} \right) + c\sigma_k^P \left(E_k^{n+1} - b_k a (T_e^{n+1})^4 \right)$$
$$= \frac{1}{2} \operatorname{div} \left(\frac{c}{3\sigma_k^R} \nabla E_k^n \right).$$

Discretization: space

Implicit diffusion \Rightarrow elliptic (nonlinear) problem.



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- Constraints:
 - Lagrangian deformed mesh
 - Piecewise constant unknowns.

 $-\operatorname{div}\left(D\nabla u\right)=f.$



Discretization: space

Implicit diffusion \Rightarrow elliptic (nonlinear) problem.



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- Constraints:
 - Lagrangian deformed mesh
 - Piecewise constant unknowns.

 $-\operatorname{div}\left(D\nabla u\right)=f.$



Diffusion schemes

The most simple scheme: five-point scheme, D = 1.



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$$\int_{K} -\Delta u = \int_{\partial K} \nabla u \cdot \mathbf{n} = -\int_{K} f.$$

Approximate gradient on each face: $\forall \mathbf{x} \in K | L$, $\nabla u(\mathbf{x}) \approx \frac{u(\mathbf{x}_L) - u(\mathbf{x}_K)}{|\mathbf{x}_L - \mathbf{x}_K|} \frac{\mathbf{x}_L - \mathbf{x}_K}{|\mathbf{x}_L - \mathbf{x}_K|}$,

$$\frac{\partial u}{\partial n_{K|L}} \approx \frac{u(\mathbf{x}_L) - u(\mathbf{x}_K)}{|\mathbf{x}_L - \mathbf{x}_K|} \frac{\mathbf{x}_L - \mathbf{x}_K}{|\mathbf{x}_L - \mathbf{x}_K|} \cdot \mathbf{n}_{K|L} = \frac{u(\mathbf{x}_L) - u(\mathbf{x}_K)}{|\mathbf{x}_L - \mathbf{x}_K|} \cos(\theta_{K|L}),$$



Five-point scheme



 $|K|f_K = \sum_{L \in \mathcal{N}(K)} \ell(K|L) \frac{u_K - u_L}{|\mathbf{x}_K - \mathbf{x}_L|} \cos(\theta_{K|L}).$

nergie atomique - energies alternatives $\mathcal{N}(K)$ neighbouring cells of K, $\ell(K|L)$ length of edge $K|L = \overline{K} \cap \overline{L}$.



Number of cells

Five-point scheme



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Example:
$$(\varphi = \frac{\pi}{3})$$

$$\begin{cases} -\Delta u = 0 \text{ in } \mathcal{D}, \\ u = x_2 \text{ on } \partial \mathcal{D}. \end{cases}$$



Solution:

 $u(x_1, x_2) = x_2.$



Five-point scheme

Tilted mesh:



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Fixed *u*, compute approximate flux:

$$\frac{u(\mathbf{x}_L) - u(\mathbf{x}_K)}{|\mathbf{x}_L - \mathbf{x}_K|} \cos(\theta_{K|L}) = \frac{\partial u}{\partial x_1}(\mathbf{y})\sin(\varphi) + O(h).$$

Compute exact flux:

$$\nabla u(\mathbf{y}) \cdot n = \frac{\partial u}{\partial x_1}(\mathbf{y}) \sin(\varphi) - \frac{\partial u}{\partial x_2}(\mathbf{y}) \cos(\varphi).$$

If $\varphi \neq 0$, fluxes ar not consistent.

Kershaw mesh



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Kershaw-type (sheared) mesh.

Five point scheme



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Five point scheme on Kershaw mesh

Five point scheme

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Comparison five-point scheme – reference solution

Diffusion schemes

Elliptic equation

 $-\operatorname{div}(D\nabla u) = f$



on a deformed mesh. f, u piecewise constant.

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The ideal scheme:

- Convergent (order 2?)
- Stable
- Maximum principle
- Symmetric matrix (if *D* is symmetric)
- Linear (?)
- Unstructured polygonal meshes
- Recover 5 point scheme on orthognal meshes

Diffusion schemes on deformed meshes

(centered) finite volume:

- Kershaw (1981)
 Pert (1981)
 Faille (1992)
 Morel, Dendy, Hall, White (1992)
 Jayantha, Turner (2001, 2003, 2005)

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- Mixed (hybride) finite elements:

 Raviart, Thomas (1977)
 Burbeau, Roche, Scheurer, Samba (1997)
 Arbogast, Wheeler, Yotov (1998)
- Discrete Duality Finite Volumes (DDFV):
 Hermeline(1998, 2000, 2003,2007,2009)
 Domelevo, Omnes (2005)
- Mimetic Finite Difference (MFD):
 - Shashkov, Steinberg, Morel, Lipnikov, Brezzi (1995, 1997, 1998, 2004).
- Multi-point flux approximation (MPFA):
 Aavatsmark, Barkve, Boe, Mannseth (1996, 1998)
 Le Potier (2005)
 Breil, Maire (2008)
- Scheme Using Stabilisation and Harmonic Interfaces (SUSHI):
 Eymard, Gallouët, Herbin, 2010.

Split each cell in subcells:

 $K = \bigcup K_s, \quad s \text{ vertices of } K$

Kershaw scheme:

 $\mathcal{T} = \{K = K_i, 1 \leq i \leq N\}$ set of cells of the Lagrangian mesh



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$$\int_{\mathcal{D}} u \left(-\operatorname{div}(D\nabla u) \right) = \int_{\mathcal{D}} (\sqrt{D}\nabla u) \cdot (\sqrt{D}\nabla u) = \sum_{K \in \mathcal{T}} \int_{K} (\sqrt{D}\nabla u) \cdot (\sqrt{D}\nabla u).$$



$$\int_{\mathcal{D}} u \left(-\operatorname{div}(D\nabla u) \right) = \sum_{K \in \mathcal{T}} \sum_{s \in K} \int_{K_s} (\sqrt{D}\nabla u) \cdot (\sqrt{D}\nabla u).$$



and flux continuity:

$$\lambda_{K|L} = \sqrt{\frac{2}{\ell(K|L)}} \sqrt{\left(\frac{|x_k - y_{K|L}|}{D_K} + \frac{|x_L - y_{K|L}|}{D_L}\right)^{-1}}.$$

Kershaw scheme induces coupling with cells sharing a node.



Kershaw, J. Comp. Phys. 39, p 375, 1981.

- Consistent of order 2, stable
- Does not satisfy the maximum principle

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Nine-point scheme – Violation of the maximum principle



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x 10⁶ 21 4 18 15 12 2 - 9 - 6 - 3 0 x 10⁶ 21 18 15 -2 12 - 9 6 - 3 -40.3 0.0 0.1 0.2

Comparison nine-point scheme – five-point scheme

Idea : use the Voronoïmesh of the cell centers $\mathcal{T} = \{K = K_i, 1 \le i \le N\}$ set of cells of the Lagrangian mesh $\forall K \in \mathcal{T}, x_K$ center of mass of *K*.

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Step 1. Compute the Voronoïmesh $\tilde{\mathcal{T}}$ if the points x_K :

$$\forall K \in \mathcal{T}, \quad \tilde{K} = \{\mathbf{x} \in \mathcal{D}, \forall L \neq K, |\mathbf{x} - \mathbf{x}_K| \leq |\mathbf{x} - \mathbf{x}_L|\}.$$



Kershaw mesh



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Voronoïmesh

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Shestakov (random) mesh and Voronoï mesh.

Step 2. Use "five-point" scheme on $\tilde{\mathcal{T}}$:



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$$\begin{aligned} \left| \tilde{K} \right| (-\Delta u)(\mathbf{x}_{\tilde{K}}) \approx \int_{\tilde{K}} -\Delta u &= -\int_{\partial \tilde{K}} \nabla u \cdot n = -\sum_{\tilde{L}} \int_{\tilde{L}|\tilde{K}} \nabla u \cdot n \\ &\approx -\sum_{\tilde{L}} \ell(\tilde{K}|\tilde{L}) \frac{u(\mathbf{x}_{K}) - u(\mathbf{x}_{L})}{|\mathbf{x}_{K} - \mathbf{x}_{L}|}. \end{aligned}$$

$$|K|(-\Delta u)(\mathbf{x}_K) \approx \int_K -\Delta u \approx \frac{|K|}{|\tilde{K}|} \int_{\tilde{K}} -\Delta u.$$



Step 3. Symmetrize the matrix :

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$$\forall K \neq L, \quad A_{KL} = -\frac{|K|}{|\tilde{K}|} \frac{\ell(\tilde{K}|\tilde{L})}{|\mathbf{x}_K - \mathbf{x}_L|}, \quad B_{KL} = -\frac{1}{2} \left(\frac{|K|}{|\tilde{K}|} + \frac{|L|}{|\tilde{L}|}\right) \frac{\ell(\tilde{K}|\tilde{L})}{|\mathbf{x}_K - \mathbf{x}_L|}$$

 $B_{KK} = \frac{|K|}{|\tilde{K}|} \sum_{L} \frac{\ell(\tilde{K}|\tilde{L})}{|\mathbf{x}_K - \mathbf{x}_L|}.$

Step 4. Modify diagonal terms tos that the sum of each line vanishes:

$$\tilde{B}_{KK} = \sum_{L} \frac{1}{2} \left(\frac{K|}{|\tilde{K}|} + \frac{|L|}{|\tilde{L}|} \right) \frac{\ell(\tilde{K}|\tilde{L})}{|\mathbf{x}_{K} - \mathbf{x}_{L}|}.$$

The matrix $C = \gamma I + B$ is an *M*-matrice, for any $\gamma > 0$

$$\begin{aligned} -\Delta u + u &= \mathbf{1}_{\{x_1 \leq 0\}} & \text{in } \Omega = (-1, 1)^2, \\ \nabla u \cdot n &= 0 & \text{on } \partial \Omega. \end{aligned}$$



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Explicit solution:

$$u(x_1, x_2) = \begin{cases} 1 - \frac{\cosh(x_1 + 1)}{2\cosh(1)} & \text{if } x_1 \le 0, \\ \frac{\cosh(x_1 + 1)}{2\cosh(1)} & \text{if } x_1 \ge 0. \end{cases}$$





LapIn scheme is:

- Linear.
- Symmetric.
- Convergent of order 1.
- Satisfies the maximum principle.
- Five-point scheme on orthogonal meshes.

P1 model

Use P1 approximation: $I_{\nu} = \frac{c}{4\pi}E_{\nu} + \Omega \cdot F_{\nu}$.



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$$\begin{cases} \frac{\partial E_{\nu}}{\partial t} + \operatorname{div}(F_{\nu}) + c\sigma_{a}(\nu) \left(E_{\nu} - \frac{4\pi}{c}B_{\nu}(T_{e})\right) = 0, \\ \frac{1}{c}\frac{\partial F_{\nu}}{\partial t} + \frac{c}{3}\nabla E_{\nu} + (\sigma_{a}(\nu) + \kappa_{\mathrm{Th}})F_{\nu} = 0. \end{cases}$$

Hyperbolic system:

- Define convergent scheme on deformed mesh.
- Recover diffusion limit (asymptotic preserving scheme).

See Buet, Després, Franck (2010), Jin, Levermore (1993), Gosse, Toscani (2004). PN model (1D)

Assume that I_{ν} is a polynomial of degree N in Ω .



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$$I_{\nu}(x,t,\mu) = \sum_{n=0}^{N} J_n(x,t,\nu) P_n(\mu).$$

 $P_n = n^{\text{th}}$ Legendre polynomials.

$$\frac{1}{c}\frac{\partial J_n}{\partial t} + \frac{\partial}{\partial x}\left(\frac{n+1}{2n+1}J_{n+1} - \frac{n}{2n+1}J_{n-1}\right) + (\sigma_a(\nu) + \kappa_{\rm Th})J_n$$
$$= \sigma_a(\nu)B_\nu(T_e)\delta_{n0} + \kappa_{\rm Th}\delta_{n0}J_0,$$

with the convention that $J_{-1} = J_{N+1} = 0$.

Scheme on deformed mesh...

M1 model

Set
$$E_{\nu} = \frac{1}{c} \oint_{S^2} I_{\nu} d\Omega$$
, $F_{\nu} = \oint_{S^2} \Omega I_{\nu} d\Omega$, $P_{\nu} = \frac{1}{c} \oint_{S^2} \Omega \otimes \Omega I_{\nu} d\Omega$.



System

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$$\begin{cases} \frac{\partial E_{\nu}}{\partial t} + \operatorname{div}(F_{\nu}) + c\sigma_{a}(\nu) \left(E_{\nu} - \frac{4\pi}{c}B_{\nu}(T_{e})\right) = 0, \\ \frac{1}{c}\frac{\partial F_{\nu}}{\partial t} + c\operatorname{div}(P_{\nu}) + (\sigma_{a}(\nu) + \kappa_{\mathrm{Th}})F_{\nu} = 0. \end{cases}$$

Closure relation

$$P_{\nu} = \mathcal{F}(E_{\nu}, F_{\nu}).$$

 $P_{\nu} = \frac{1}{3} E_{\nu} Id$: P1 model.

Definition of \mathcal{F} : entropy minimization. Dubroca, Feugeas (1999), Coulombel, Golse, Goudon (2005), Hauck, Levermore, Tits (2008), Levermore (1997), Morel (2009).

If the boundary condition of radiative transfer is



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 $\forall x \in \partial \mathcal{D}, \quad \forall \Omega / \Omega \cdot n(x) \le 0, \quad I_{\nu}(x, t, \Omega) = I_{\nu}^{\text{ext}}(x, t, \Omega),$

with I_{ν}^{ext} independent of Ω , then idem for diffusion. If not, need a boundary layer analysis:

$$I_{\nu}(x,\Omega) = J_{\nu}^{0}\left(x,\frac{x_{1}}{\varepsilon},\Omega\right) + \varepsilon J_{\nu}^{1}\left(x,\frac{x_{1}}{\varepsilon},\Omega\right) + \varepsilon^{2} J_{\nu}^{2}\left(x,\frac{x_{1}}{\varepsilon},\Omega\right) + \dots ,$$

$$T(x) = S^{0}\left(x,\frac{x_{1}}{\varepsilon}\right) + \varepsilon S^{1}\left(x,\frac{x_{1}}{\varepsilon}\right) + \varepsilon^{2} S^{2}\left(x,\frac{x_{1}}{\varepsilon}\right) + \dots$$

Incoming flux

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OT.

$$\frac{\varepsilon}{c}\frac{\partial I_{\nu}}{\partial t} + \Omega \cdot \nabla I_{\nu} + \varepsilon \sigma_a \left(I_{\nu} - B_{\nu}(T)\right) + \frac{\kappa_{\rm Th}}{\varepsilon} \left(I_{\nu} - \int_{S^2} \frac{3}{4} \left(1 + \left(\Omega \cdot \Omega'\right)^2\right) I_{\nu}(\Omega') \frac{d\Omega'}{4\pi}\right) = 0,$$

$$I_{\nu}(x,\Omega) = J_{\nu}^{0}\left(x,\frac{x_{1}}{\varepsilon},\Omega\right) + \varepsilon J_{\nu}^{1}\left(x,\frac{x_{1}}{\varepsilon},\Omega\right) + \varepsilon^{2} J_{\nu}^{2}\left(x,\frac{x_{1}}{\varepsilon},\Omega\right) + \dots ,$$

Milne problem for $J_0 = J_0^{\nu}(x, s, \mu)$, $\mu = \Omega \cdot e_1$:

$$\begin{cases} \mu \partial_s J^0_{\nu} + \kappa_{\rm Th} \left(J^0_{\nu} - \mathcal{K}(J^0_{\nu}) \right) = 0 & s > 0, \\ J^0_{\nu} \left[(0, x_2, x_3), 0, \mu, \nu \right] = \int_{S^1} I^{\rm ext}_{\nu} \left(\Omega \right) d\Omega_T & \mu > 0. \end{cases}$$

Boundary condition for I_{ν}^{0} : $I_{\nu}^{0} = \overline{J_{\nu}^{0}(x, \infty, \mu)}$

$$\mu \partial_s J_{\nu}^0 + \kappa_{\rm Th} \left(J_{\nu}^0 - \mathcal{K}(J_{\nu}^0) \right) = 0 \qquad s > 0,$$

$$J_{\nu}^0 \left[(0, x_2, x_3), 0, \mu, \nu \right] = \oint_{S^1} F_{\nu} \left(\Omega \right) d\Omega_T \qquad \mu > 0.$$

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Theorem: (Dautray-Lions 1988, Chandrasekhar 1950, Case-Zweifel 1967, Williams 1971) The Milne problem is well-posed, and its solution J_{ν}^{0} satisfies the convergence

$$J^0_{\nu}(x,s,\mu) \xrightarrow[s \to \infty]{} \oint_{S^1} I^{\text{ext}}_{\nu}(\Omega') d\Omega'.$$

<u>Remark:</u> Here, use that \mathcal{K} is self-adjoint, and that 1 is a simple isolated eigenvalue, with constant eigenvector.

Boundary condition:
$$E_{\nu} = \int_{S^2} I_{\nu}^{\text{ext}}(\Omega) d\Omega$$

In the Rosseland approximation, boundary layer:



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$$\frac{\varepsilon}{c}\frac{\partial I_{\nu}}{\partial t} + \Omega \cdot \nabla I_{\nu} + \frac{\sigma_a}{\varepsilon} \left(I_{\nu} - B_{\nu}(T)\right) + \frac{\kappa_{\rm Th}}{\varepsilon} \left(I_{\nu} - \int_{S^2} \frac{3}{4} \left(1 + \left(\Omega \cdot \Omega'\right)^2\right) I_{\nu}(\Omega') \frac{d\Omega'}{4\pi}\right) = 0,$$

$$\varepsilon C_v \frac{\partial T}{\partial t} = \int_{S^2} \int_0^\infty \frac{\sigma_a}{\varepsilon} \left(I_\nu(x, t, \Omega) - B_\nu(T) \right) d\nu \frac{d\Omega}{4\pi}$$

Milne problem $J^0_{\nu} = J^0_{\nu}(x, s, \mu)$:

$$(\mu \partial_s J^0_{\nu} + (\sigma_a + \kappa_{\rm Th}) (J^0_{\nu} - B_{\nu}(S^0)) = 0 \qquad s > 0,$$

$$\int_{0} \int_{-1} \sigma_a \left(J_{\nu}^0 - B_{\nu}(S^0) \right) d\mu d\nu = 0 \qquad s > 0,$$

$$\int_{\Omega} J^{0}_{\nu} \left[(0, x_{2}, x_{3}), 0, \mu, \nu \right] = \int_{S^{1}} I^{\text{ext}}_{\nu} \left(\Omega \right) d\Omega_{T} \qquad \mu > 0$$

Milne problem $J^0_{\nu} = J^0_{\nu}(x, s, \mu)$:



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$$\begin{cases} \mu \partial_s J_{\nu}^0 + (\sigma_a + \kappa_{\rm Th}) \left(J_{\nu}^0 - B_{\nu}(S^0) \right) = 0 & s > 0, \\ \int_0^{+\infty} \int_{-1}^1 \sigma_a \left(J_{\nu}^0 - B_{\nu}(S^0) \right) d\mu d\nu = 0 & s > 0, \\ J_{\nu}^0 \left[(0, x_2, x_3), 0, \mu, \nu \right] = \int_{S^1} I_{\nu}^{\rm ext} \left(\Omega \right) d\Omega_T & \mu > 0. \end{cases}$$

Theorem: (Golse 1987, Sentis 1987, Clouet-Sentis, 2009) The above Milne problem has a unique solution, which satisfies

$$\lim_{s \to \infty} S^{0}(s) = T^{*}, \quad \lim_{s \to \infty} J^{0}_{\nu}(s, \mu, \nu) = B_{\nu}(T^{*}).$$

 T^* is the boundary data for T^0 in Rosseland model.

Rosseland approximation for the non-equilibrium diffusion model: boundary layer

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$$\begin{cases} \frac{\varepsilon}{c} \frac{\partial E_{\nu}}{\partial t} - \operatorname{div} \left(\frac{1}{3(\sigma_a + \kappa_{\mathrm{Th}})} \nabla E_{\nu} \right) + \frac{\sigma_a}{\varepsilon} \left(E_{\nu} - \frac{4\pi}{c} B_{\nu}(T_e) \right) = 0, \\ \varepsilon C_v \frac{\partial T}{\partial t} = \frac{c}{4\pi} \int_0^\infty \frac{\sigma_a(\nu)}{\varepsilon} \left(E_{\nu} - \frac{4\pi}{c} B_{\nu}(T) \right) d\nu. \end{cases}$$

Milne problem $E_0 = E_0^{\nu}(x, s, \mu)$:

$$\begin{cases} -\partial_s \left(\frac{1}{3(\sigma_a + \kappa_{\rm Th})} \partial_s E_{\nu}^0 \right) + \sigma_a \left(E_{\nu}^0 - B_{\nu}(S^0) \right) = 0 \quad s > 0, \\ \int_0^{+\infty} \int_{-1}^1 \sigma_a \left(E_{\nu}^0 - B_{\nu}(S^0) \right) d\mu d\nu = 0 \quad s > 0, \end{cases}$$

$$E_{\nu}^{0}\left[(0, x_{2}, x_{3}), 0, \mu, \nu\right] = \oint_{S^{1}} I_{\nu}^{\text{ext}}\left(\Omega\right) d\Omega_{T} \qquad \mu > 0.$$
Boundary conditions (continued)

Milne problem $E_0 = E_0^{\nu}(x, s, \mu)$:



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$$-\partial_{s} \left(\frac{1}{3(\sigma_{a} + \kappa_{\mathrm{Th}})} \partial_{s} E_{\nu}^{0} \right) + \sigma_{a} \left(E_{\nu}^{0} - B_{\nu}(S^{0}) \right) = 0 \quad s > 0,$$

$$\int_{0}^{+\infty} \int_{-1}^{1} \sigma_{a} \left(E_{\nu}^{0} - B_{\nu}(S^{0}) \right) d\mu d\nu = 0 \qquad s > 0,$$

$$E_{\nu}^{0} \left[(0, x_{2}, x_{3}), 0, \mu, \nu \right] = \int_{S^{1}} I_{\nu}^{\mathrm{ext}} \left(\Omega \right) d\Omega_{T} \qquad \mu > 0.$$

Theorem: The above Milne problem has a unique solution, which satisfies

$$\lim_{s \to \infty} S^0(s) = T^*_{\text{diff}}, \quad \lim_{s \to \infty} J_0(s, \mu, \nu) = B_{\nu}(T^*_{\text{diff}}).$$

 T^*_{diff} is the boundary data for T^0 in Rosseland model.

Question: how to ensure $T^* = T^*_{\text{diff}}$?