Lecture 3

Introduction to Thermal Radiation Transport

The purpose of this lecture is to

- Introduce the equations of thermal radiation without material motion.
- Give a brief overview of equilibrium solutions.
- Give a brief overview of how the equations are solved.
- Give a brief overview of the equilibrium diffusion limit.
- Discuss the requirements for numerical schemes used to solve the equations.

1 Basic Equations

The equations of thermal radiation transport consist of a transport equation for the angular intensity $I(\overrightarrow{r}, \overrightarrow{\Omega}, E, t)$ $(energy/area - time - steradian - energy)$:

$$\frac{1}{c}\frac{\partial I}{\partial t} + \overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I + \sigma_t I = \frac{\sigma_s}{4\pi}\varphi + \sigma_a B(T)\,, \tag{1}$$

and an equation for the material temperature $T(\overrightarrow{r}, t)$ $(temperature)$:

$$C_v \frac{\partial T}{\partial t} = \int_0^\infty \sigma_a [\, \varphi - 4\pi B(T) \,]\, dE \ . \tag{2}$$

Here c $(length/time)$ is the speed of light, $\sigma_t(\overrightarrow{r}, E, T)$ $(length^{-1})$ is the total macroscopic cross section, $\sigma_s(\overrightarrow{r}, T)$ $(length^{-1})$ is the Thompson macroscopic scattering cross section, $\varphi(\overrightarrow{r}, E, t)$ $(energy/area - time - energy)$ is angle-integrated intensity, $C_v(\overrightarrow{r}, T)$ $(energy/volume - temperature)$ is the material heat capacity, and $B(E, T)$ $(energy/area - time - steradian - energy)$ is the Planck function:

$$B(E,T) = \frac{2E^3}{h^3c^2}\left[\exp\left(\frac{E}{kT}\right) - 1\right]^{-1} \quad , \tag{3}$$

where h is *Planck's constant* and k is Boltzmann's constant. The angular intensity I, is a photon energy flux rather than a number flux, i.e., it is equal to the angular flux multiplied by the photon energy.

Note that the temperature enters the transport equation through the Planck function. This function serves as an emission source proportional to the absorption cross section. Photons are emitted isotropically with a spectral shape that depends upon temperature. Consequently, absorption of thermal photon energy is quite different from neutron absorption. A fraction of the absorbed photon energy is re-emitted, and what is not re-emitted goes into the material internal energy, thereby increasing the material temperature. Thus in the limit as $C_v \to 0$, all the absorbed energy is re-emitted, resulting in the analog of a pure scattering process. To demonstrate this, we set the heat capacity to zero in Eq. (2)

to obtain

$$\int_0^\infty \sigma_a \varphi \, dE = \int_0^\infty 4\pi\sigma_a B(T) \, dE \,, \tag{4}$$

which states that the total photon energy absorption rate is equal to the total photon energy emission rate.

The analog of the constant solution of neutron transport for radiative transfer is also a time-independent space-independent solution but it is called the equilibrium solution. Setting the time and space derivatives in Eqs. (1) and (2) to zero, we first integrate Eq. (1) over all angles to get solution:

$$\sigma_t \varphi = \sigma_s \varphi + \sigma_a 4\pi B \,. \tag{5}$$

Solving Eq. (5) for φ we obtain

$$\varphi = 4\pi B \,. \tag{6}$$

Substituting from Eq. (6) into Eq. (1), we get

$$I = B(E, T) \,. \tag{7}$$

Equation (7) is valid for any value of T. Thus one can set T and directly obtain I, or one can set I and integrate Eq. (7) over all angles and energies to obtain

$$acT^4 = \int_0^\infty \int_{4\pi} I \; d\Omega \, dE \,, \tag{8}$$

where

$$\int_0^\infty \int_{4\pi} B \; d\Omega \, dE \equiv acT^4 \, , \tag{9}$$

and a $(energy/volume - temperature^4)$ is the radiation constant. Finally solving Eq. (8) for T, we get

$$T = \left[\frac{1}{ac} \left(\int_0^\infty \int_{4\pi} I \; d\Omega \, dE \right) \right]^{\frac{1}{4}} \, . \tag{10}$$

It is appropriate to redefine certain fundamental transport quantities to be consistent with the units of the intensity. We have already defined the analog of the neutron scalar flux, which is the angle-integrated intensity, φ. The analog of the energy-integrated neutron current is the radiative flux:

$$\overrightarrow{\mathcal{F}} \equiv \int_0^\infty \int_{4\pi} \overrightarrow{\Omega} \, I \left(\overrightarrow{\Omega} \right) \; d\Omega \, dE \, , \tag{11}$$

which has units of $(energy/area - time)$. The analog of the neutron number density is the radiative energy density:

$$\mathcal{E} \equiv \frac{1}{c} \int_0^\infty \int_{4\pi} I \left(\overrightarrow{\Omega} , E \right) \; d\Omega \, dE \, , \tag{12}$$

which has units of $(energy/volume)$. The analog of the neutron pressure tensor is the radiation pressure tensor:

$$\mathcal{P}_{i,j} \equiv \frac{1}{c} \int_0^\infty \int_{4\pi} \Omega_i \Omega_j I \left(\overrightarrow{\Omega} , E \right) \; d\Omega \, dE \, , \tag{13}$$

which has the same units as the energy density ($energy/volume$). Note that these units are equivalent to ($force/area$) which are the units of material pressure. Specifically, $force \times length = energy$ and $area \times length = volume$.

The zero'th moment of the radiation equation represents a statement of energy balance rather than particle balance. Integrating Eq. (1) over all angles and energies, we get the radiation energy equation:

$$\frac{\partial \mathcal{E}}{\partial t} + \overrightarrow{\nabla} \cdot \overrightarrow{\mathcal{F}} = \int_0^\infty \sigma_a [\, 4\pi B(T) - \varphi \,]\, dE \,. \tag{14}$$

The first moment of the radiation equation represents a statement of momentum conservation. Note that $h\nu\, \overrightarrow{\Omega}/c$ is the photon momentum where $h\nu$ is the photon energy. Multiplying Eq. (1) by $\overrightarrow{\Omega}/c$ and interating over all angles and energies, we obtain the radiation momentum equation:

$$\frac{1}{c^2} \frac{\partial \overrightarrow{\mathcal{F}}}{\partial t} + \overrightarrow{\nabla} \cdot \overrightarrow{\overrightarrow{\mathcal{P}}} + \frac{\sigma_t}{c} \overrightarrow{\mathcal{F}} = 0 \,. \tag{15}$$

2 Solution of the Equations

Because Eqs. (1) and (2) are nonlinear in T, they are generally solved via Newton's method. To illustrate this technique, we first implicitly difference the equations in time using the

backward Euler scheme

$$\frac{1}{c\Delta t^k}\left(I^{k+\frac{1}{2}} - I^{k-\frac{1}{2}}\right) + \overrightarrow{\Omega}\cdot\overrightarrow{\nabla} I^{k+\frac{1}{2}} + \sigma_t^{k+\frac{1}{2}} I^{k+\frac{1}{2}} = \frac{1}{4\pi}\sigma_s^{k+\frac{1}{2}}\varphi^{k+\frac{1}{2}} + \sigma_a B^{k+\frac{1}{2}}\,, \tag{16}$$

$$\frac{C_v^{k+\frac{1}{2}}}{\Delta t^k}\left(T^{k+\frac{1}{2}} - T^{k-\frac{1}{2}}\right) = \int_0^\infty \sigma_a^{k+\frac{1}{2}}\left(\varphi^{k+\frac{1}{2}} - 4\pi B^{k+\frac{1}{2}}\right) dE \;\;, \tag{17}$$

where k is the time index and the time step $\Delta t_k = t^{k+\frac{1}{2}} - t^{k-\frac{1}{2}}$. We let T^* denote the latest Newton iterate for the temperature. Then the linearized equations for the next Newton iteration are obtained by evaluating the material properties at T^* and linearly expanding the Planck function temperature dependence about T^*:

$$B^{k+\frac{1}{2}} = B^* + \frac{\partial B^*}{\partial T}\left(T^{k+\frac{1}{2}} - T^*\right)\,, \tag{18}$$

where a superscript "*" denotes a quantity evaluated at T^*. Note that this is equivalent to neglecting the contibutions to the Jacobian from the material properties. With the expansion, given in Eq. (17), the material temperature can be eliminated from the transport equation. Suppressing the temporal superscript "$k+\frac{1}{2}$", the linearized temporally-differenced transport equation can be expressed as:

$$\overrightarrow{\Omega}\cdot\overrightarrow{\nabla} I + \sigma_\tau^* I = \frac{1}{4\pi}\sigma_s^*\varphi + \frac{1}{4\pi}\nu\chi\int_0^\infty \sigma_a^*(E')\varphi(E')\,dE' + \xi\,, \tag{19}$$

where:

$$\sigma_\tau = \sigma_t + \tau\,, \tag{20a}$$

$$\tau = \frac{1}{c\Delta t^k}\ \ , \tag{20b}$$

$$\nu = \frac{\int_0^\infty \sigma_a^*(E) 4\pi \frac{\partial B^*(E)}{\partial T}\, dE}{\frac{C_v^*}{\Delta t^k} + \int_0^\infty \sigma_a^*(E) 4\pi \frac{\partial B^*(E)}{\partial T}\, dE}\,, \tag{20c}$$

$$\chi(E) = \frac{\sigma_a^*(E)\frac{\partial B^*(E)}{\partial T}}{\int_0^\infty \sigma_a^*(E')\frac{\partial B^*(E')}{\partial T}\, dE'}\,, \tag{20d}$$

$$\xi = \sigma_a^* B^* + \tau I^{k-\frac{1}{2}} - \frac{1}{4\pi}\nu\chi\left[\int_0^\infty \sigma_a^*(E') 4\pi B^*(E')\, dE' + \frac{C_v^*}{\Delta t^k}\left(T^* - T^{k-\frac{1}{2}}\right)\right]\,, \tag{20e}$$

and the material temperature is given by

$$T^{k+\frac{1}{2}} = T^* + \frac{\int_0^\infty \sigma_a^*(E)\left[\varphi(E) - 4\pi B^*(E)\right]\, dE + \frac{C_v^*}{\Delta t^k}\left(T^{k-\frac{1}{2}} - T^*\right)}{\frac{C_v^*}{\Delta t^k} + \int_0^\infty \sigma_a^*(E) 4\pi \frac{\partial B^*(E)}{\partial T}\, dE}\,. \tag{21}$$

Equation (21) is used to calculate the temperatures after the linearized transport equation has been solved. We note that Eq. (19) has the form of the steady-state neutron transport equation with σ_a playing the role of the fission cross section, ν playing the role of the number of neutrons per fission, χ playing the role of the fission spectrum, and ξ playing the role of the inhomogeneous source. We also note that the scattering process is monochromatic, i.e., photons do not change energy when they scatter.

Equation (19) is generally solved using the standard nested source iteration process. Denoting the iteration index by ℓ, the inner iteration process can be expressed as follows

in multigroup form for energy group g:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I_g^{\ell+1} + \sigma_{\tau,g}^* I_g^{\ell+1} = \frac{1}{4\pi}\sigma_{s,g}^* \varphi_g^{\ell} + \frac{1}{4\pi}\nu\chi_g \sum_{g'=1}^{G} \sigma_{a,g'}^* \varphi_{g'} \ + \xi_g \,, \tag{22}$$

and the outer iteration process can be similarly expressed as

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I_g^{\ell+1} + \sigma_{\tau,g}^* I_g^{\ell+1} = \frac{1}{4\pi}\sigma_{s,g}^* \varphi_g^{\ell+1} + \frac{1}{4\pi}\nu\chi_g \sum_{g'=1}^{G} \sigma_{a,g'}^* \varphi_{g'} + \xi_g \,, \quad g = 1, G,$$

The spectral radius for the inner iteration process is the usual scattering ratio, $c = \sigma_{s,g}^*/\sigma_{t,g}^*$, and the spectral radius for the outer iteration process is given by

$$\rho_0 = \nu \sum_{g=1}^{G} \frac{\chi \sigma_{a,g}^*}{\sigma_{a,g}^* + \tau} \,. \tag{23}$$

The spectral radii observed in a practical problem are the maximum values of c and ρ_0, respectively, evaluated over the problem domain. Any region in which ρ_0 is close to unity will be diffusive.

If desired, one can dramatically reduce the spectral radius for the inner iteration process by roughly a factor of 4 via an acceleration technique known as diffusion-synthetic acceleration. An accelerated inner iteration for group g can be expressed as follows:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I_g^{\ell+\frac{1}{2}} + \sigma_{\tau,g}^* I_g^{\ell+\frac{1}{2}} =$$

$$\frac{1}{4\pi}\sigma_{s,g}^* \varphi_g^{\ell} + \frac{1}{4\pi}\nu\chi_g \sum_{g'=1}^{G} \sigma_{a,g'}^* \varphi_{g'} \ + \xi_g \,, \tag{24}$$

$$-\overrightarrow{\nabla} \cdot \frac{1}{3\sigma_{t,g}} \overrightarrow{\nabla} \delta\varphi_g^{\ell+\frac{1}{2}} + \sigma_{a,g} \delta\varphi_g^{\ell+\frac{1}{2}} = \sigma_{s,g} \left(\varphi_g^{\ell+\frac{1}{2}} - \varphi_g^{\ell} \right) \,, \tag{25}$$

$$\varphi_g^{\ell+1} = \varphi_g^{\ell+\frac{1}{2}} + \delta\varphi_g^{\ell+\frac{1}{2}} \,. \tag{26}$$

Our experience is that acceleration of the inner iterations is not usually required. On the other hand, acceleration of the outer iterations is often essential. The spectral radius for the outer iterations is often very close to unity, making it essential to accelerate convergence of the outer iterations. The spectral radius approaches unity in the limit of strong fluid-radiation coupling, i.e., small heat capacity and large absorption cross section. The technique used to accelerate the outer iterations is a variation on diffusion-synthetic acceleration called the linear multifrequency-grey method. An accelerated outer iteration can be represented in multigroup form as follows:

$$\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} I_g^{\ell+\frac{1}{2}} + \sigma_{\tau,g}^* I_g^{\ell+\frac{1}{2}} =$$

$$\frac{1}{4\pi}\sigma_{s,g}^* \varphi_g^{\ell+\frac{1}{2}} + \frac{1}{4\pi}\nu\chi_g R_a^{\ell} \; + \xi_g \,, \quad g = 1, G, \tag{27}$$

$$-\overrightarrow{\nabla}\cdot\langle D\rangle\overrightarrow{\nabla}\,\delta\Phi^{(\ell+1/2)} + \left[\tau + (1-\nu)\,\langle\sigma_a\rangle\right]\delta\Phi^{(\ell+1/2)}$$

$$= \nu\left(R_a^{\ell+\frac{1}{2}} - R_a^{\ell}\right) \,, \tag{28}$$

$$R_a^{(\ell+1)} = R_a^{(\ell+1/2)} + \langle\sigma_a\rangle\delta\Phi^{(\ell+1/2)} \,. \tag{29}$$

where

$$R_a = \sum_{g'=1}^{G} \sigma_{a,g'}^* \varphi_{g'} \,, \tag{30}$$

$$\langle D\rangle = \frac{1}{3}\sum_{g'=1}^{G} \frac{\varrho_{g'}}{\sigma_{\tau,g'}^*} \,, \tag{31}$$

$$\langle \sigma_a \rangle = \sum_{g'=1}^{G} \varrho_g \sigma_{a,g}^* \,, \tag{32}$$

$$\varrho_g = \frac{\frac{\chi_g}{\sigma_{a,g}^* + \tau}}{\sum_{g'=1}^{G} \frac{\chi_{g'}}{\sigma_{a,g'}^* + \tau}} \,. \tag{33}$$

The linear multifrequency-grey method is generally very effective.

It was thought for many years that diffusion-synthetic acceleration and its variants were unconditionally effective. However, it was eventually discovered that large spatial discontinuities in the cross sections can significantly degrade the effectiveness of diffusion-synthetic acceleration. It is reasonable to assume that its variants suffer the same deficiency. It has recently been shown that solving the neutron transport equation with a preconditioned Krylov technique and recasting diffusion-synthetic acceleration as a preconditioner rather than an acceleration scheme results in an apparently unconditionally effective solution technique.

Krylov methods are beginning to have an enormous impact upon solution techniques for the transport equation. The traditional accelerated solution techniques represent two-level or two-grid methods. As such, they require diffusion discretizations that are consistent with the transport discretizations. This generally leads to non-standard diffusion discretizations that are difficult to solve. Furthermore, high-frequency error amplification for just a single mode can destroy the effectivness of such solution techniques. Preconditioned Krylov methods with traditional acceleration techniques recast as preconditioners are far more

forgiving than traditional accelerated solution techniques. We expect to see great progress made in numerical radiative transfer and radiation-hydrodynamics via Krylov methods.

3 The Equilibrium-Diffusion Limit

The diffusion limit for thermal radiation transport is characterized by:

$$I = B(T)\,, \tag{34}$$

$$(C_v + 4aT^3)\frac{\partial T}{\partial t} - \overrightarrow{\nabla}\cdot\left(\frac{4acT^3}{3\sigma_r}\right)\overrightarrow{\nabla}T = 0\,, \tag{35}$$

where σ_r is the *Rosselund-averaged* total cross section:

$$\sigma_r = \left\{\left[\int_0^\infty \frac{1}{\sigma_t^*(E)}\frac{\partial B(E)}{\partial T}\,dE\right]\Big/\left[\int_0^\infty \frac{\partial B(E)}{\partial T}\,dE\right]\right\}^{-1}\,. \tag{36}$$

We will later derive this limit asymptotically.

4 Numerical Requirements

Although the linearized thermal radiation transport equation is analogous to a particular form of the neutron transport equation, it is generally much more difficult to accurately and efficiently simulate than the neutron transport equation for several reasons:

- Within a specific material region, the cross sections can vary with energy by six or more orders of magnitude.

- The cross sections can change in space by six or more orders of magnitude across a material interface.
- Problems often contain both optically-thin regions and optically-thick regions.
- Optically thick regions may be strongly absorbing or highly diffusive.
- In diffusive regions, the spatial scale-length of the solution can have a thickness of many mean-free paths (e.g., thousands or more).
- The spectral radius of the outer iteration process can be very close to unity, e.g., 0.9999.

As a consequence, the numerical requirements for thermal radiation transport are severe. In particular, spatial differencing schemes must be highly damped in strongly absorbing media, accurate in optically-thin regions, have the thick diffusion limit (produce the correct diffusion solution in diffusive regions where the spatial grid is optically thick), and behave well with unresolved spatial boundary layers. Acceleration of the outer (emission source) iterations is essential in most problems. The numerical implementation of these scheme must be very robust. There are often huge spatial discontinuities in the cross sections. Thus in multidimensional calculations, the diffusion-based acceleration schemes like the linear multifrequency-grey method should be recast as a preconditioner and used in conjunction with a Krylov solution technique.