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Radiation can have a dramatic effect on the material properties of low density plasmas, altering bulk properties such as energy density and specific heat as well as spectral characteristics such as opacity and emissivity. The response of the material to radiation must be considered when constructing transport algorithms that are intended to provide self-consistent solutions for both the radiation field and plasma properties. It can affect almost every aspect of the numerical solution, from the overall solution strategy down to details of the acceleration algorithms. We discuss these issues in the context of one approach towards improving the stability and convergence of the solution, with examples relevant to high-energy density physics. We also present a direct solution technique for the linearized multigroup radiation transport equations that sidesteps the need for a multigroup acceleration process and can be used to benchmark the performance of iterative algorithms.

Introduction

Radiation transport methods have reached a level of maturity in which they are routinely applied to a wide variety of physical systems, primarily under the assumption of local thermodynamic equilibrium (LTE). However, non-LTE (NLTE) materials, common in high energy density physics applications, respond strongly to radiation in both their energy content and spectral characteristics. In this paper, we discuss the consequences of this response and present an extension to a class of commonly used numerical radiation transport methods to handle such characteristics.

In Section 2, we consider the non-LTE energetics of radiation interacting with matter, determining the relationship between energy density and temperature. The generalization of the LTE relationship separates the dependence of the energy density on the temperature from the direct effect of radiative interactions. A numerical example provides context in terms of the regime in which the radiation spectrum can significantly alter the material response and the magnitude of the effects considered. Section 3 presents the relevant equations and a straightforward linearization scheme, including a natural extension of the scheme that explicitly incorporates the dependence of material properties on radiation. Efficient solutions of these extended equations may require the development of new acceleration methods, and section 4 presents a direct solution technique for the linearized multigroup equations which does not require an accelerated iterative algorithm.

Non-LTE Energetics

For matter that is not in LTE, describing the response to radiation is more complicated than for the corresponding LTE case. We consider the relationship between the material energy density E_m, the material properties and the radiation field:

Here, n_e (n_i) is the number density of the free electrons (ions), which are assumed to have a thermal distribution corresponding to the material temperature T. E_{int} is the material internal energy, which depends not only on the temperature and density, but also on the radiation field, denoted by J_ν, and on the time t. For the remainder of this paper, we ignore the density dependence as unimportant to the discussion and focus on the temperature and radiation. We also adopt a single-temperature description of the material for simplicity of exposition.

For material in LTE, the internal energy depends only on temperature, then the rate of change in material energy density and temperature are related through the specific heat (at constant density) c_V:

Implicit in this formulation is the assumption that either radiative interactions are completely unimportant or that the extant radiation also has a thermal distribution, i.e. $J_\nu = B_\nu$, where B_ν is the Planck distribution. In the more general non-LTE formulation, the rate of change of material energy density is comprised of three different types of terms:

The first term on the RHS of Equation describes the response of the material energy density to a change in temperature, but with fixed radiation densities, while the second term describes the material response to a change in radiation at fixed temperature. The coefficient of the first term plays the part of the non-LTE specific heat, which is related to the LTE specific heat by

The last term on the RHS of Equation arises from evolution of the material at fixed temperature and radiation, and acts as a source or sink of energy. This term can be quite important in following the thermal evolution of matter at very low densities and temperatures, but for the remainder of this discussion we assume this term is negligible and do not consider it further.

Non-LTE effects will become significant at densities low enough for important radiative transition rates to become comparable to the corresponding collisional rates. A numerical example illustrates the relative importance of the temperature and radiative responses to the specific heat. For this example, we calculate the energy density and specific heat of a Xe plasma at three different densities. Figure 1 shows the energy density (per ion) as a function of temperature for an ion number density of 10^{18} cm^{-3}. Both the total energy densities (solid lines) and internal energy densities (dashed lines) are shown, for a case with a Planckian radiation field (blue lines) and no radiation field (green lines). The internal energy densities differ by more than an order of magnitude, reflecting the effect of the radiation on the internal (excited state) structure of the Xe ions. The difference between the internal energy density and total energy density reflects the ionization state of the Xe and differs by a factor of two between the two cases.

Figure 1. Energy density per ion as a function of temperature for a Xe plasma of number density 10^{18} cm^{-3}, in units eV/particle. The solid lines give the total energy density while the dashed lines give the internal energy density only. The blue lines give results in the presence of Planckian radiation field ($T_r = T_e$, where T_e is the material temperature and T_r is the radiation temperature), and the green lines give results with no radiation field (T_r=0).

Figures 2a - 2c show the specific heat as a function of temperature for ion number densities of 10^{18}, 10^{20} and 10^{22} cm^{-3}, respectively. In each figure, the red line gives the LTE specific heat, c_V^{LTE}, while the blue line gives the non-LTE specific heat c_V^{NLTE} evaluated assuming a Planckian radiation field at the given temperature, and the green line gives c_V^{NLTE} evaluated assuming no radiation field.At the highest of the three densities, LTE is a good approximation and the specific heat varies little with the radiation. As the density decreases, the difference between c_V^{LTE} and c_V^{NLTE} increases, and it becomes apparent that the material radiative response dominates the temperature response. Regardless of other considerations, use of the LTE specific heat at low densities in the presence of non-Planckian radiation fields will not describe the material energetics correctly.

(a) (b)

(c)

Figure 2. (a) Specific heat per ion as a function of temperature for a Xe plasma of number density 10^{18} cm^{-3}, in units eV/eV. The red line gives the LTE specific heat, the blue line gives the non-LTE specific heat for a Planckian radiation field ($T_r = T_e$, where T_e is the material temperature and T_r is the radiation temperature), and the green

line gives the non-LTE specific heat with no radiation field (T_r=0). The dashed line gives the specific heat obtained from Eq. (4) using the diagonal approximation. (b) Same as (a) for a number density of 10^{20} cm^{-3}. (c) Same as (a) for a number density of 10^{22} cm^{-3}.

Representative absorption coefficients for two of these cases (assuming zero radiation field) are displayed in Figures 3a and 3b, for temperatures of 100 eV (blue curves) and 500 eV (red curves). Numerous strong bound-bound radiative transitions are apparent for energies between 10^2 and 10^4 eV. At low densities, these transitions couple strongly to the radiation field and poorly to the material temperature.

(a) (b)

Figure 3. Absorption coefficients for a Xe plasma of density (a) $n_i = 10^{18}$ cm^{-3} and (b) $n_i = 10^{20}$ cm^{-3}. The blue curves correspond to a material temperature of 100 eV and the red curves correspond to a material temperature of 500 eV. The calculations assume steady-state conditions with no radiation field.

The new response terms involve all frequencies. These terms do not introduce any new complications into the solution method, but computing all the additional derivatives is extremely expensive. In the low-density regime where we expect strong line radiation to dominate the radiative response, we can make the additional approximation that each bound-bound radiative transition responds to radiation of a single frequency. Implicit in this approximation is the assumption that each strong line is contained within a single frequency bin, and we make no attempt to resolve any of the lines. Under these conditions, we can easily calculate the required derivatives from the atomic kinetics equations. We refer to this as the “diagonal” approximation, as it uses only the diagonal terms from the complete response matrix. Figures (2a) – (2c) demonstrate that this approximation indeed does very well at low densities, but less well near LTE.

A measure of the radiative coupling, in the “diagonal” approximation, is given by , which is displayed in Figures 4a and 4b for the same conditions as Figures 3a and 3b. Large values, , correspond to strong line features in the spectrum.

(a) (b)

Figure 4. Diagonal response coefficients for the same conditions as Figure 3.

Linearized Equations

The system of equations describing energy transport by radiation consists of the radiation transport equation

and the material energy equation

where I_ν is the specific intensity at frequency , α_ν and $_\nu$ are the absorption coefficient and emissivity, Q represents other energy sources, J_ν is the angle-averaged intensity

and is the source function. In LTE, the source function is the Planck function, B_ν, and is a function of temperature only.

A common method of solving this non-linear set of equations is to discretize in time and linearize about the current temperature T^0. Applying these operations to Eq. gives

where

acts as a specific heat for the total system of matter and radiation. Equation can be analytically combined with the linearized and discretized version of Eq. , resulting in

We have assumed a fully-implicit time discretization, since applications usually require at least a partially-implicit treatment for stability. The superscript "0" denotes values at the beginning of the time interval. This treatment can be, and in LTE often is, generalized to an iterative procedure to converge the nonlinear dependence of S_ν on the temperature.

Extending these equations to include the radiation response terms is straightforward. Linearizing the equations about the current temperature and radiation spectrum, using the diagonal approximation, produces

where is defined as in Equation (9) using the NLTE specific heat. Equations and retain the same multigroup structure as before, and may be solved in the same manner.

A numerical implementation of the broadband equations can be extended in a very simple manner. Most of the changes in the implementation are captured by the substitutions:

In the absence of the diagonal approximation, these changes include the obvious sums over frequencies. Besides these substitutions, only the term involving remains to be handled separately.

Omitting radiative response terms from the linearized equations can destabilize a numerical solution, as demonstrated in Scott (2005). Equally worrisome, a solution may appear to have converged by usual criteria while remaining inaccurate. Given the magnitude of these effects, we anticipate that instability or poor convergence will result for other solution methods as well. Unfortunately, the radiative response terms can be extremely expensive to calculate, even more so than the non-LTE opacities and emissivities themselves. One possible avenue towards allowing tabulated information to be used for these calculations is under investigation, as discussed in Scott (2005).

A related issue has to do with the solution technique used for these extended equations, which often employs a grey acceleration (Morel, et al, 1985). This acceleration may become ineffective, both because it uses Planckian weights and because the efficiency depends on the opacity spectrum. Grey acceleration remained effective for the application described in Scott (2005), but this may not hold true for other applications. An alternative procedure is to directly solve Eq. for all frequencies simultaneously. A reduction procedure, described in the next section, makes this quite economical in one dimension and provides a tool to address this issue. This procedure might also serve as the basis for an approximate operator approach in higher dimensionalities.

Direct Solution of the Linearized Equations

The direct solution of the linearized equations is accomplished via a straightforward algebraic reduction. In the following description, we use operator notation for conciseness, while a numerical implementation performs the same operations with matrices. We do not explicity consider boundary conditions, again for conciseness, but note that standard conditions specifying boundary intensities pose no difficulties for the numerical implementation.

We begin by writing the linearized version of the transport equation in terms of the lambda operator λ_ν

The tilde denotes that the absorption coefficient may include the radiative response terms, either in the diagonal approximation or utilizing all derivatives. For simplicity of notation, we drop the tilde from this point on. Substituting for ΔT from the linearized material energy equation and collecting terms produces a single equation coupling intensities for all frequencies, angles and spatial positions:

where

Formally solving Eq. for I_ν and integrating over all angles and frequencies, weighted by α_ν , produces a single equation for the quantity

where

This is the desired result, as substitution of Eq. into Eq. provides the intensities through

The operator algebra employed here reduces to simple matrix operations for discretized equations, and the usual boundary conditions specifying incident intensities are trivially incorporated into the solution.

This technique becomes particularly simple to implement inside an iterative process for converging nonlinearities. We define the iterates through

The intensity corrections are then given by

where

Either formulation isolates a single quantity which couples the radiation intensity to the change in temperature. Equation can be derived more directly by linearizing Eqs. and with respect to **K**.

Each evaluation of λ_ν requires a transport sweep. However, Λ is a full matrix of rank equal to the number of zones that must be inverted once during the solution process. This is a nominal expense for most one-dimensional problems, but becomes quite expensive for higher dimensionalities. Numerical experiments using a small number of diagonals of Λ as an easily invertible approximate operator, similar to the method of Olson, et al (1986), have not proved encouraging. It remains possible that some portion of Λ could be used in this manner, but at present this method remains a useful one-dimensional tool.

A simple test problem demonstrates that efficacy of this method for solving the multigroup equations, even when grey acceleration fails. The physical setup is that of a uniform slab of material of thickness 2 cm with a constant specific heat corresponding to an ideal gas of density 1 g/cm^{-3}, initially at a temperature of 1 eV, which is illuminated by a Planckian radiation field of radiation temperature 1 keV. We consider two frequency distributions for the absorption coefficient:

Case A Case B

where ν denotes the photon energy in keV. The exponential cutoff of the absorption coefficient in case B violates necessary conditions for the effectiveness of grey acceleration, and we expect poor convergence in this case.

Figure 5 shows the (angle-integrated) radiation field within the slab at several positions for two different times. The evolution of both cases is similar in that the radiation gradually “fills in” the optically thick portion of the spectrum as time evolves. Eventually, the material in both cases reaches a uniform temperature of 1 keV and the radiation field becomes a Planckian everywhere. The timescales for this evolution are very similar, but the details of the radiation spectra differ due to the absorption coefficients.

(a) (b)

(c) (d)

Figure 5. Angle-integrated radiation spectrum at several positions within the material. (a) Case A, $t = 1$ ns, (b) Case B, $t = 1$ ns, (c) Case A, $t = 5$ ns, (d) Case B, $t = 5$ ns

The convergence properties of grey acceleration differ dramatically for these two cases, as shown in Figure 6. The blue curves show the iterations required to converge Equations (5) and (6) to the 10^{-4} level using grey acceleration. The dashed curves correspond to solving the linearized versions of these equations, while the solid curves correspond to solving the full nonlinear equations, including the full temperature dependence of the (Planckian) source function. Case A requires at most 10 iterations during the first 10 ns, while case B requires nearly 100 iterations, even with conservatively small timesteps. The direct solution method, with results given by the green curves, does obtain the solution to the linearized equations in a single pass, while requiring only a few iterations to produce the solution to the full nonlinear equations. The red curves show the results obtained using the diagonal of the Λ operator in Equation (21), as an approximate operator that could be easily applied in two- and three-dimensional geometries. The approximate operator improves upon the convergence of grey acceleration when grey acceleration performs poorly, but converges much slower than grey acceleration otherwise.

(a) (b)

Figure 6. Iterations necessary to converge the solution of the equations to 10^{-4} as a function of time for (a) Case A and (b) Case B. The dashed lines correspond to the solution of the linearized equations, while the solid lines correspond to the solution of the nonlinear equations. The blue curves give the results for grey (synthetic) acceleration, and the green curves gives the results for the direct solution method. The red curves give the results obtained using the diagonal of the Λ operator.

To allow for the comparison with grey acceleration, the results presented in Figure 6 were obtained with a diffusion operator rather than a full transport operator. For this problem, the convergence properties of the direct method (full and approximate) observed with the transport operator were very similar to those observed with the diffusion operator.

This example assumes LTE and has none of the NLTE radiative response characteristics discussed above. We only seek to demonstrate that the method does indeed solve the linearized multigroup equations without iterations, and that it can be useful for checking convergence properties (of both the linearized and non-linear equations). This method was applied to a fully NLTE situation in Scott (2005) to confirm that, in this case, grey acceleration did indeed successfully converge to the solution of the extended equations (11) and (12).

Conclusions

Solving the radiation transport equation also involves evaluating material properties that can depend on the radiation field. In NLTE, the material properties can depend directly on the radiation field as well as on the temperature, and the coupling between the material and radiation takes on a different character than in LTE, which should be reflected in the computational algorithms. In this paper, we have discussed some of these issue and presented an extension to a common algorithm, which successfully handles applications with strong NLTE radiation. We have also presented a direct solution algorithm for the linearized multigroup equations that bypasses the need for a multigroup acceleration process and can be used to benchmark the performance of iterative algorithms.

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