Frequency-Dependent Material Motion Benchmarks for Radiative Transfer

Ryan G. McClarren¹, N.A. Gentile²

¹Dept. Aerospace and Mechanical Engineering, University of Notre Dame
Notre Dame, Indiana, USA
²L-38 Lawrence Livermore National Laboratory
Livermore, California, USA
rmclarr@nd.edu, gentile1@llnl.gov

ABSTRACT

We present a general solution for the radiation intensity in front of a purely absorbing slab moving toward an observer at constant speed and with a constant temperature. The solution is obtained by integrating the lab-frame radiation transport equation through the slab to the observer. We present comparisons between our benchmark and results from the Kull simulation code for an aluminum slab moving toward the observer at 2% the speed-of-light. We demonstrate that ignoring certain material motion correction terms in the transport equation can lead to 20-80% errors with the error magnitude growing as the frequency resolution is improved. Our results also indicate that our benchmark can identify potential errors in the implementation of material motion corrections.

KEYWORDS: high-energy density physics, radiative transfer, material motion corrections, special relativity, verification, benchmark solutions

1. Radiation Spectrum in Front of a Moving Slab

We are interested in solving the problem of the radiation spectrum in front of a slab that is moving at a fast speed that is, nevertheless, slow relative to the speed of light. In our notation, the subscript \( L \) denotes a quantity in the laboratory reference frame, and the subscript \( F \) is for the fluid, or co-moving frame.

Considering the observation point \( z = Z \), we compute the solution \( I_L(Z, \mu, \nu_L, t) \). This problem is depicted in Fig. 1. For a photon to reach position \( Z \) at time \( t_Z \) it will have its position \( z(t) \) given by

\[
z(t) = Z + \mu c(t - t_Z). \tag{1}
\]

Given that the back of the slab has position \( z_b = vt \), a photon that leaves the back of the slab and reaches \( Z \) at time \( t_Z \) will be emitted at time \( t_b \) that can be determined from the equation \( z(t_b) = vt_b \) as

\[
t_b = \left( \frac{\mu c t_Z - Z}{\mu c - v} \right)_+, \tag{2}
\]

where \((\cdot)_+\) gives the positive part of its argument (i.e., \((x)_+ = x \) if \( x > 0 \), and \((x)_+ = 0 \) otherwise). Similarly, a photon reaching \( Z \) at time \( t_Z \) emitted from the front of the slab at time \( t_f \):

\[
t_f = \left( \frac{L + \mu c t_Z - Z}{\mu c - v} \right)_+. \tag{3}
\]
Figure 1. Schematic of the problem: a slab of length $L$ moves in the $z$ direction toward the observation point at $z = Z$. The solution $I(Z, \mu, \nu_L, t)$ with $\mu = \cos \theta$ is computed by integrating along the ray over the length $s$, given by Eq. (4).

Additionally, the length of the ray through the slab for a photon is then

$$s = c(t_f - t_b)$$ (4)

Using these relations the solution $I(Z, \mu, \nu_L, t_Z)$ is

$$I(Z, \mu, \nu_L, t_Z) = I_Z(\mu_L, \nu_L) = \frac{B(\gamma D_L \nu_L, T)}{(\gamma D_L)^3} \left[ 1 - \exp \left( -\gamma D_L \sigma_a,_{\text{slab}}(\gamma D_L \nu_L) s \right) \right],$$ (5)

which can be found by using an integrating factor.

2. Analytic Results and Code Benchmarking

We consider a slab of aluminum with density of 0.1 g/cm$^3$, a thickness of $L = 0.4$ cm., and a temperature of $T = 1$ keV. The slab is moving at a speed of 0.5994 cm/ns (about 2% of the speed of light), a speed chosen based on a Mach 45 radiating shock benchmark [3]. The observation point is $Z = 12$ cm and time $t_Z = 10$ ns. We compute the multigroup radiation energy density based on three group structures:

- A coarse structure with 50 logarithmically spaced groups from 0.001 keV to 30 keV,
- A medium structure of 89 total groups based on the coarse set where the extra groups are added between 1 and 10 keV,
- A fine structure of 124 groups based on the medium set where the extra groups are added between 1 and 2 keV.
Frequency-Dependent Material Motion Benchmarks for Radiative Transfer

Figure 2. Group specific opacities, $\kappa_g$ in units of cm$^2$/g for the aluminum slab.

These group structures were chosen to successively capture the spectral lines in the 1 and 2 keV range. The opacities were provided by the TOPS opacity database [4] and are shown in Figure 2.

Our benchmark solution was computed by using Mathematica to compute the solutions. We can also investigate the effects of material motion corrections (MMC) by computing the solution for a stationary slab (i.e., $v = 0$), and when the frequencies in the opacity and blackbody emission terms are not Doppler shifted by $\gamma D_L$ (we call this the no $\nu$ Doppler solution). Even though in our problem $v/c \approx 0.02$, we will be able to show that ignoring MMC leads to errors on the order of 80% for this problem.

We can also compare the benchmark to solutions computed by the implicit Monte Carlo method [5,6] in Kull [7]. We can verify that the MMC is correctly implemented in Kull by comparing its solution to the benchmark. We can also compare Kull solutions with different MMC terms turned off, for example the Doppler shift of $\nu$ and show that the benchmark can elucidate that these terms are missing.

Results for the 50 group problem are shown in Figure 3. In Figure 3(a) the Kull solution with full MMC and $2 \times 10^9$ particles per time step and the benchmark are compared, and reasonable agreement outside of the low-energy groups with few computational particles is observed. The importance of MMC is quantified in Figure 3(b) where the benchmark is compared with solutions where the slab is stationary and without the Doppler shift on $\nu$ via the percent absolute error. Here we can see that errors up to 20% occur in the higher energy groups when the Doppler shift of $\nu$ is ignored. Finally, Figure 3(c) compares the Kull IMC solution with full MMC and the benchmark, as well as the solution lacking the Doppler correction and a solution where the slab is stationary. Figure 3(c) indicates that above photon energies of 1 keV the Kull solution is, on the whole, closer to the benchmark than to the solutions missing MMC corrections. We can conclude from this figure that our benchmark is able to verify if certain MMC terms are correctly implemented in a code.
Figure 3. Comparisons for the 50 group aluminum slab problem: (a) the benchmark solution and the KULL IMC solution with all MMC terms, (b) comparison of the benchmark solution with a solution where the slab is stationary \((v = 0)\) and one where the Doppler correction for the frequency is ignored, and (c) comparison of the KULL IMC solution with full MMC with the benchmark solution, a solution with frequency Doppler shifts ignored, and with the slab stationary.

ACKNOWLEDGEMENTS

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC. LLNL-ABS-813186

REFERENCES

[1] G. C. Pomraning. The Equations of Radiation Hydrodynamics. Dover Publications (2005).

[2] B. A. Clark. “Computing Multigroup Radiation Integrals Using Polylogarithm-Based Methods.” Journal of Computational Physics, volume 70(2), pp. 311–329 (1987).

[3] R. B. Lowrie and J. D. Edwards. “Radiative shock solutions with grey nonequilibrium diffusion.” Shock Waves, volume 18(2), pp. 129–143 (2008).

[4] N. Magee, J. Abdallah Jr, R. Clark, J. Cohen, L. Collins, G. Csanak, C. Fontes, A. Gauger, J. Keady, D. Kilcrease, et al. “Atomic structure calculations and new Los Alamos astrophysical opacities.” In Astrophysical applications of powerful new databases, volume 78, p. 51 (1995).

[5] J. A. Fleck and J. D. Cummings. “An implicit Monte Carlo scheme for calculating time and frequency dependent nonlinear radiation transport.” Journal of Computational Physics, volume 8(3), pp. 313–342 (1971).

[6] R. P. Smedley-Stevenson and R. G. McClarren. “Asymptotic diffusion limit of cell temperature discretisation schemes for thermal radiation transport.” Journal of Computational Physics, volume 286, pp. 214–235 (2015).

[7] N. A. Gentile, N. Keen, and J. Rathkopf. “The KULL IMC package.” Technical report, Lawrence Livermore National Lab. (LLNL), Livermore, CA (United States) (1998).