Dynamic Energy Grouping in Multigroup Radiation Transport Calculations

Brian Macpherson Penfield High School

Advisor: Dr. Reuben Epstein

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Abstract: Radiation is an important energy transport mechanism in laser-plasma interactions. In simulating radiation transport through a medium, the radiation spectrum is currently represented as being divided into photon energy intervals or "groups". The radiation emission and absorption rates are calculated and the equation of transfer is solved for each energy interval to obtain the radiation intensity spectrum. This radiation intensity is then used to calculate useful properties such as matter temperature and energy density. Since some photon energies are very important while other photon energies have little effect on the simulation, the intervals can be re-grouped into a smaller number of intervals to save processing time. The range of important photon energies changes over time, however, so it is desirable to change the groupings accordingly. It is possible to decrease the computation time by dynamically re-grouping the photon energies rather than uniformly resolving the entire spectrum. This reduces the number of groups while preserving much of the accuracy guaranteed by the larger number of energy groups currently used. A program has been written to solve the equation of transfer for a standard test problem. This program allows the user to visualize absorption and emission in space and spectral energy, and automatically chooses new, broader energy groupings at a specified time. The program continues with the new groupings for the rest of the simulation.

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Introduction: Currently at the Laboratory for Laser Energetics, several one and twodimensional hydrodynamic simulation codes such as LILAC and DRACO are used to simulate the conditions of a fusion implosion. These simulations are of paramount importance for scientists and engineers who must simulate nuclear fusion in order to study it. These programs can take hours or days to run, however, which hinders research and progress. Some of the main components of these programs are the energy transport mechanisms such as thermal and radiation transport, which calculate and describe how energy comes and goes within the medium. In my project, only radiation transport and its equation of transfer were dealt with. To evaluate the equation of transfer for radiation transport, opacity and emissivity must be evaluated at all relevant photon energies in order to determine the energy intensity. To accurately represent the integrated photon energies, the spectrum can be at first broken into many small groupings. This method ensures accurate results, but is very taxing on the computation time. A method was proposed to cut down on computation time by analyzing the radiation energy density and/or absorption and emission rates in the simulation at specified times to determine which photon energy ranges have the largest effect on the simulation at these times.¹ The program could then determine new groupings of photon energies which accurately represent the important photon energies with a smaller number of total groupings. This would ensure accurate results while reducing simulation time.

Radiation Transport: Calculating radiation transport is one of the most time-consuming aspects of hydrodynamic simulations at the Laboratory for Laser Energetics. The Equation of Transfer for radiation transport is used to describe the energy radiation intensity, $I_v(s)$, distributed within a medium.²

$$dI_V/ds = \varepsilon_V/4\pi - \kappa_V I_V(s)$$

This describes how energy from a blackbody source enters a medium and travels within it. This transfer of energy is heavily dependent on both emissivity and opacity, properties of the medium. Emissivity is a property which describes how much radiation a medium will emit while opacity describes how much radiation a medium will absorb. Radiation intensity is the rate of energy passing through a unit surface area in a particular direction per unit solid angle per frequency interval. The variable s is the distance traveled by the radiation as described by

$$ds = dx / \cos \theta,$$

 ε_v is the emissivity of the medium, κ_v is the opacity of the medium, and v is the frequency of radiation in Hz. The distance x represents the perpendicular distance from the outside edge of the slab to a point within the slab. The angle θ is oriented so that an angle perpendicular to the edge of the slab would be 0 degrees and an angle parallel to the outside edge would be 90 degrees. My program solved this equation of transfer implicitly for a specified sample problem described by Fleck and Cummings.³ The simulation took into account all propagation directions and a range of photon energies. A 4 cm thick slab is represented by 10 material zones of 0.4 cm thickness. In Ref. 3, a different hypothetical opacity profile is specified for each of several sample problems. For the sample problem used in this project, the radiation source is a blackbody spectrum of 1 keV temperature incident on one side of the slab, and the initial matter temperature was set to 1 eV. The opacity was defined by

$$\kappa_v = 27(1 - e^{-hv/kT})/v^3 cm^{-1}$$
,

where hv and kT are energy in keV, the emissivity is described as

$$\varepsilon_v = 4 \pi B_v \kappa_v$$

where B_{ν} is the Planck Function, and the material specific heat was set to

$$b = 0.5917 a T_o^3$$
,

where T_o is the initial temperature and a is the radiation energy density constant, which is used as a centering parameter between explicit and implicit for the specific heat equation.

The program then ran a simulation in time steps of 0.02 nanoseconds. Several quantities were given as output, including the absorption and emission rates, the radiation energy density per zone and photon energy, and the temperature in each zone.⁴ This output was saved in a data file, then graphed by a plotting program for analysis. By using a looping structure, the simulation was usually run between 40 and 100 time steps, or until equilibrium was met.⁵ The results of these simulations were saved as a model for an accurate, but potentially time-consuming process. The technique of re-grouping was then applied in order to create fewer and broader groups that would potentially save computation time in a program such as DRACO or LILAC.

Re-grouping: Determining new energy groupings that accurately represent the photon energy spectrum at a specific time is crucial for maintaining an accurate simulation of radiation transport. My program determines where the important section of the spectrum is by keeping track of radiation energy density per matter zone and photon energy. The radiation energy density is then analyzed at a specific time, depending on when regrouping is desired. From Fig. 1 it can be seen that at 0.26 nanoseconds the radiation energy density

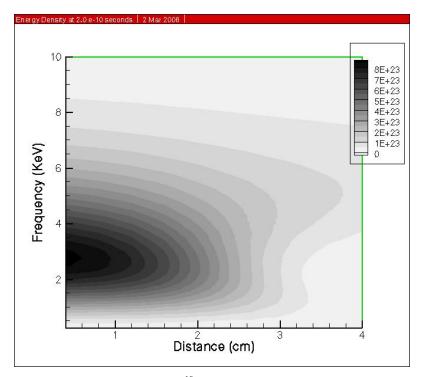


Fig 1: The Energy Density at 2.6×10^{-10} seconds as a function of distance into the slab.

is concentrated at roughly 2.5 keV. In order to divide the energy spectrum into a smaller number of groups, the program goes through a process to determine 5 new boundaries and subsequently 4 new groupings. First, the program finds the spectral density integrated over the whole slab, which gives a good representation of where the energy density is the highest. The program then finds the corresponding hv value at this peak energy density and uses this value as the middle boundary of four new energy groups. The program also determines the mean hv value between the peak energy density and the highest hv value of the spectrum, as well as the mean hv value between the peak energy and lowest hv value of the spectrum. These become two other boundaries of the four new energy groupings. For the last two boundaries of the new groupings, the highest and lowest hv values of the spectrum are used in order to maintain the total range of photon energy. The end result is 4 large groupings where there were once 40 fine groupings.

Results: The program was set up to re-group the photon energies from 40 groups to 4 at a simulation time of 0.3 nanoseconds. It ran in time steps of 0.02 nanoseconds, which was small enough to avoid oscillation in the results. By running the simulation with and without the re-grouping method, and then graphing the temperature of all zones, one can

see the results of re-grouping. At 0.1 ns after re-grouping (Fig. 2), the temperatures with and without re-grouping are very similar. However, at 0.4 ns after re-grouping (Fig. 3), the temperatures with and without grouping differ by a larger margin.

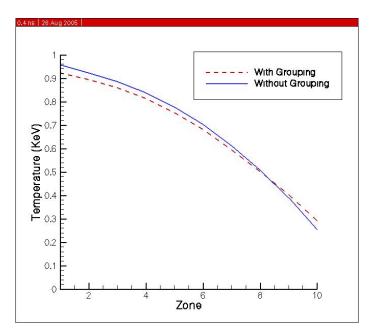


Fig. 2: Temperature profile 0.1 nanoseconds after re-grouping.

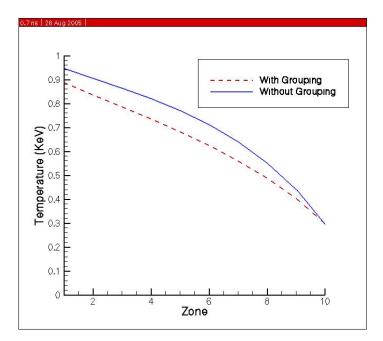


Fig. 3: Temperature profile 0.4 nanoseconds after re-grouping.

It can be seen from these graphs of temperature that as time increases after the regrouping, the accuracy of the simulation decreases. By following the temperature of specific zones of the material over time (see Fig. 4), this correlation is easily seen. Zones 5 and 7 were chosen as representative zones in the simulation because of their deviation seen in Figure 3. The largest deviation between the temperatures with and without regrouping appears in zone 5, making it a good illustration of the worst-case scenario. Zone 7 is very similar to the other zones, making it a good illustration of a normal deviation. There is a direct relationship between time and deviation between the simulations with and without energy re-grouping. As time increases, the accuracy of the simulation using fewer energy groupings decreases.

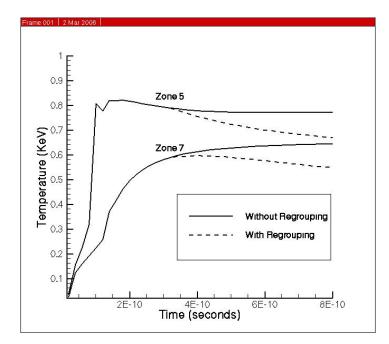


Fig. 4: Time dependence of the temperatures of zones 5 and 7 with and without re-grouping.

Conclusions: By looking at the results from the first test case used with this program, the process of re-grouping is very promising. The spectral resolution was reduced to 10% of its original groupings, yet the simulation remained fairly accurate. After 0.5 nanoseconds, the simulation with re-grouping remained within 15% of the simulation without re-grouping in the fifth and seventh zones of the material (see Fig. 4). Within the initial 0.5 nanoseconds after re-grouping occurs, the fifth zone is seen from Fig. 3 to be

one of the least accurate sections of the material. This means that other zones of the material would probably show better results than 15% agreement within the first 0.5 nanoseconds after re-grouping. While 15% accuracy may not be a desirable accuracy for all purposes, it still gives the user of the program a good idea of the temperature of the material. This result is encouraging considering a 10-fold spectral resolution decrease, which is dramatic. Altering the spectral resolution by a smaller amount would certainly give better results. It could be left to the user of the program to determine how accurate the results need to be. If only a mediocre estimate of the temperature is desired in a small amount of time, a large decrease in spectral resolution could be used. If a very good estimate is desired in less time than is required currently without dynamic re-grouping, a smaller decrease in spectral resolution could be utilized.

Future Work: The most useful conclusion drawn from running the program with photon energy re-grouping is that the accuracy, understandably, decreases by a small amount over time. In the first attempt at re-grouping, there was roughly 85% accuracy in the first 0.5 nanoseconds after re-grouping in one of the least accurate zones. This was accomplished with a ten-fold reduction in spectral resolution, however, which is a relatively large decrease. A decrease in accuracy comes as no surprise. It would be useful to determine the accuracy of re-grouping with a less dramatic decrease in spectral resolution, such as a 1/2 decrease. The results could potentially be much better than the 15% accuracy achieved currently 0.5 nanoseconds after re-grouping.

In a fully realized re-grouping strategy, the code would pick new groupings multiple times after pre-determined intervals instead of just once. This would be accomplished by running one time step with the original fine groupings for all regroupings after the first for the purpose of re-adjusting the groups according to the energy density. The program could re-evaluate the energy density in this one time step, since it shifts over time, and pick new groupings depending on how the spectrum shifted. This method would be more accurate than the previous method of re-grouping because of how the spectrum shifts over time. This could be especially important in simulations where conditions change drastically, such as a more realistic laser-plasma interaction using data from the Laboratory for Laser Energetics. Eventually, the large groupings chosen for

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cooler temperatures fail to accurately represent the photon energy spectrum of hotter material, so shifting the groups accordingly is desired when the material goes from one extreme of temperature to another.¹ The simulation would then run with the large groupings for another pre-determined length of time before re-grouping again. The length of time between re-groupings would have a large effect on simulation accuracy, so that would be adjusted as part of the re-grouping strategy. This method of dynamically re-grouping would slow down the speed of the program only slightly, but could be well worth it if the accuracy of the results improves because of it.

With all of these ideas, as well as the original method of re-grouping, it would be worthwhile to investigate a wider range of test cases in order to see the effects of regrouping on a variety of situations. Different values of radiation temperature, emissivity, opacity and other values could be tested, which would give greater insight into the usefulness and reliability of this dynamic re-grouping method. There are several other test cases in Ref. 3 that could be utilized. If it is determined that the loss of accuracy is worth the time saved in the simulations, dynamic multi-grouping could then be implemented into simulation programs at the Laboratory for Laser Energetics.

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