Enhancement of Monte Carlo Technique in Absorbing/Emitting Radiating Media for CFD Applications

Paweł Kuczyński

Assessment Report of Ph.D. Thesis

The Monte Carlo method is widely used in science and engineering problems. The present work is concerned with the application of the Monte Carlo method to radiative heat transfer. Although this method has been applied to solve radiative heat transfer problems for about 50 years, there is still room for improvement, as demonstrated in the present work. Hence, the subject of the thesis is scientifically relevant, and adequate for a Ph.D. Thesis. The work is entirely computational. The thesis is organized in seven chapters plus four short appendices. The structure of the thesis and the sequence of presentation are adequate. In general, the thesis is well written, despite a few typos, and the scientific level is quite satisfactory.

The first chapter starts with the motivation of the work, followed by the literature survey and the objectives of the thesis. The references are cited by their number, and listed at the end of the thesis by sequential numbering and in alphabetical order. This option is not common. In fact, when the references are listed in alphabetical order, reference numbers are usually omitted, and the references are cited in the text by the surname of the authors and the year of publication. In contrast, when the references are cited in the text by their number, sequential numbering is usually followed, so that the list of references is not alphabetically ordered. Although the literature survey provides a useful background, it misses a couple of relevant French works, where strategies closely related to those developed in the present thesis were reported, namely Refs. [1-3] listed below. Perez et al. [1] employed an acceleration uniform Cartesian grid enclosing the computational domain, an optimized algorithm for the calculation of the trajectory of the rays, and a multi-level strategy to recursively divide the voxels and create a quadtree/octree data structure. An application of the developed code to an industrial burner prototype is reported in [2]. A space partitioning recursive octree algorithm was used in [3] for radiative transfer in complex geometries bounding a grey medium.

Chapter 2 provides basic theory on radiative heat transfer in participating media, along with a short overview of the governing equations and closure models for turbulence and combustion. This theory is needed to solve turbulent reactive flows with radiative transfer, which are addressed in the applications. Although the turbulence and combustion models employed are relatively simple, they are often used in industrial applications, and their use is further justified by the fact that the thesis is not concerned with those models. It is unclear, however, why Reynolds average decomposition was used to obtain the time-averaged governing equations, since Favre decomposition is far more common in the case of reactive flows.

The most commonly used methods for the solution of thermal radiation problems in participating media are briefly described in chapter 3. The finite volume method is missing, presumably due to the similarity with the discrete ordinates method (DOM).

Chapter 4 constitutes the core of the thesis. It is the longest chapter and describes the developed Monte Carlo method. The emphasis is placed on the main contributions of the author, namely the use of NURBS surfaces to accurately describe the geometry of the boundary, an ortho-Cartesian grid to perform the radiative transfer calculations and thereby reduce the computational requirements, and grid refinement to improve the accuracy of the results at the expense of a small increase of that time. While the use of NURBS does improve the geometrical description of boundaries of complex shape, and is a good topic of research for a Ph.D. thesis, its practical usefulness is questionable. In fact, the vast majority of radiative transfer problems in participating media is characterized by rectilinear or circular boundaries, and a simpler discretization of the boundary is sufficient to obtain accurate results. Moreover, the examples presented in the next two chapters, which illustrate the application of the method, do not demonstrate the advantage of using NURBS in comparison with a simpler discretization procedure. In our view, the use of an ortho-Cartesian coarse grid to simplify the ray tracing procedure and speed-up the calculations is the most important contribution of the thesis. The savings in CPU time are clearly shown in the following chapters. The loss of accuracy that may arise from the use of a coarser mesh for the radiative transfer calculations seems to be negligible in the examples shown in those chapters, but this may not be always the case. The use of grid refinement is somewhat limited by the restriction to a single refinement level, and was little explored in the thesis.

Chapter 5 validates the code developed for the Monte Carlo method by means of application to transparent and participating (grey or non-grey) media, in a few simple problems for which analytical or reliable numerical solutions are available. The selected geometries are quite simple and do not allow either the verification of the code for the description of the boundaries using NURBS or the grid refinement procedure.

Three applications are presented in chapter 6. The first example addresses a pit furnace and assumes a non-participating medium. However, the atmosphere is a mixture of 20% ammonia and 80% nitrogen, and the Planck-mean absorption coefficient of ammonia is comparable to that of water vapour, as shown in Figs. 10.26 and 10.27 of Modest's book (Ref. [81] of the thesis). Therefore, the assumption of transparent medium does not seem reasonable. The second example consists of a cylindrical combustion chamber. The results obtained using Monte Carlo are compared with those calculated using the DOM. Two different spatial and angular discretizations were used in the latter case. The author refers that 1st and 2nd order spatial discretization schemes were employed, but does not specify which schemes were used. As far as the angular discretization is concerned, S_5 and S_{16} quadratures were selected. While the S_{16} quadrature is sometimes used in the literature, odd order quadratures, including S_5, are never employed, because the total number of discrete directions does not allow the use of the same number of directions per octant. This means that odd order quadratures are not invariant to rotations of 90° about the coordinate axes, a property that is recommended when using the DOM. Due to this reason, the direction cosines and the weights for S_5 and not available in the literature, and it is unclear how the author found them. Hence, the poor predictions obtained using S_5 are not surprising, no matter the order of the spatial discretization scheme. The analysis of the CPU time in section 6.2.3 is interesting, but deserves a few comments. First, since a mesh with 100k cells was used for the DOM calculations, it seems that 3D calculations were performed. This is corroborated by the results reported in the thesis. However, 2D axi-symmetric calculations could have been done, and this would greatly reduce the computational requirements for the DOM. A similar simplification is not feasible for the Monte Carlo method. Second, the assumption of temperature independent radiative properties is questionable, but it will depend on the method used to calculate those properties. Finally, the speedup factor (Eq.

6.2) of 1.25 seems too small. We would expect that, after the first call to the radiation solver (n_r=1), only one or two iterations will be needed in the following calls (n_r>1), yielding a significantly higher speedup factor. Therefore, we would expect much higher values of $n_{r,o}$, $n_{r,1}$ and $n_{r,2}$. As far as the mesh refinement is concerned, how confident is the author that the results are insensitive to further refinement? We would like to see a comparison between the Monte Carlo results in Fig. 6.15 and the DOM results. The third example illustrates the application to a laboratory pulverized coal combustor. Since coal particles are present in this problem, scattering will be present, but it is ignored in the present work. However, the additional complication arising from considering scattering appears to be marginal, and therefore it is not clear why the author decided to ignore this phenomenon.

The last chapter summarizes the work carried out and suggests additional work for future research. The four appendices provide complimentary information on the theory presented in the main text.

In conclusion, despite a few weaknesses highlighted above, the present thesis is of good standard, and provides useful original contributions to the Monte Carlo method applied to radiative transfer in participating media, being recommended for the award of a Ph.D.

References

1. Perez P, Paulin M and El Hafi M (2007) Application of a computer graphics technique for radiative transfer simulation in multidimensional combustion systems *Radiative Transfer – V. Proc. Fifth Int. Symp. Radiative Transfer* ICHMT Digital Library, Begell House
2. Joseph D, Perez P, El Hafi M, Cuenot B (2009) *J Heat Transfer*, Vol. 131, 052701.
3. Kahhali N, Rivière P and Soufiani A (2009) Study of an oct-tree based Monte Carlo algorithm for gas radiative transfer in complex geometries, *Computational Thermal Radiation in Participating Media – Proc Eurotherm Seminar 83,* Lisbon, Portugal, 15–17 August.

Pedro Coelho

Prof. Pedro Jorge Martins Coelho

February 6, 2017

Mechanical Engineering Department
Instituto Superior Técnico
University of Lisbon
Av. Rovisco Pais, 1049-001 Lisboa
E-mail: pedro.coelho@ist.utl.pt
Phone: +351-218418194