Comparison of different formulations for transient radiative transfer problems in absorbing and scattering three-dimensional media

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Thesis to obtain the Master of Science Degree in Mechanical Engineering

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“Research is what I'm doing when I don't know what I'm doing”

Wernher von Braun
Abstract

Four different formulations for the solution of transient radiative transfer in a three-dimensional absorbing and scattering medium are compared in this work. Two of these formulations are frequently used and well-known in the radiative transfer community: the radiative transfer equation, and the diffusion equation, based on the P1 approximation. The other two are based on a multi-scale approach, where the radiative intensity is decomposed into a macroscopic and a mesoscopic components. One of these multi-scale models is called the hybrid transport-diffusion model, while the other is called the micro-macro model. The major difference between the two multi-scale models lies in the way the macroscopic component is defined. These multi-scale models aim to improve the efficiency of the numerical simulation of radiative transfer in transient problems. This kind of problems appears, for example, in optical tomography applications, where the propagation of a laser inside a biological tissue must be simulated efficiently in order to determine the optical properties of the tissue and to detect the presence of tumours or inhomogeneities. The influence of both the discretization schemes (spatial, temporal and angular) and the optical parameters is also investigated. The results show that the discretization schemes and parameters are critical in order to achieve accurate results. The two multi-scale models may improve the accuracy of the results and increase the computational efficiency of the calculations, depending on the optical thickness, albedo and asymmetry factor.

KEYWORDS: Radiative transfer; Discrete ordinates method; P1 approximation; Diffusion equation; Hybrid transport-diffusion model; Micro-macro model.
Resumo

Quatro soluções diferentes para simular a transferência radiativa não estacionária num meio tridimensional com absorção e scattering são comparados. Duas destas formulações são frequentemente usadas e amplamente conhecidas na comunidade: a equação de transferência radiativa, e a equação de difusão, baseada na aproximação P1. As outras duas formulações são baseadas numa abordagem multi-escala, onde a intensidade radiativa é decomposta em duas componentes, uma macroscópica e outra mesoscópica. Um desses modelos multi-escala é denominado modelo híbrido transporte-difusão, enquanto o outro é designado de modelo Micro-Macro. A diferença fundamental entre os dois reside na forma como definem a componente macroscópica da intensidade radiativa. Estes modelos multi-escala visam melhorar a eficiência das simulações numéricas de transferência radiativa em problemas transientes. Este tipo de problemas surge, por exemplo, em aplicações de tomografia óptica onde a propagação de um laser em tecidos biológicos tem de ser precisamente simulada de modo a determinar as propriedades ópticas dos tecidos, permitindo a deteção de tumores e inomogeneidades. A influência dos esquemas de discretização (espacial, temporal e angular) e dos parâmetros ópticos é também investigada. Os resultados mostram que os esquemas e parâmetros de discretização são críticos de modo a obter resultados exactos. Os modelos multi-escala conseguem melhorar a precisão dos resultados e aumentar a eficiência computacional dos cálculos, dependendo da espessura óptica, albedo e factor de assimetria.

PALAVRAS-CHAVE: Transferência de radiação; Método das ordenadas discretas; Aproximação P1; Equação de difusão; Modelo híbrido transporte-difusão; Modelo Micro-Macro
Acknowledgments

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### Notation

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<thead>
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<th>Symbol</th>
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<tbody>
<tr>
<td>( \Delta t )</td>
<td>time step</td>
</tr>
<tr>
<td>( A )</td>
<td>area of the surface of the control volume</td>
</tr>
<tr>
<td>( c )</td>
<td>propagation speed of light</td>
</tr>
<tr>
<td>( c_{fl} )</td>
<td>stability parameter</td>
</tr>
<tr>
<td>( D )</td>
<td>diffusion coefficient</td>
</tr>
<tr>
<td>( F )</td>
<td>temporal derivative of ( I ) at the instant ( t ), divided by ( c )</td>
</tr>
<tr>
<td>( g )</td>
<td>asymmetry factor</td>
</tr>
<tr>
<td>( G )</td>
<td>incident radiation (or photon fluence rate)</td>
</tr>
<tr>
<td>( I )</td>
<td>radiation intensity</td>
</tr>
<tr>
<td>( k_a )</td>
<td>absorption coefficient</td>
</tr>
<tr>
<td>( k_s )</td>
<td>scattering coefficient</td>
</tr>
<tr>
<td>( L )</td>
<td>length of the cubic enclosure</td>
</tr>
<tr>
<td>( L(t) )</td>
<td>radiation absorbed in one of the four lateral boundaries (dimensionless)</td>
</tr>
<tr>
<td>( n )</td>
<td>unitary vector normal to the surface</td>
</tr>
<tr>
<td>( N )</td>
<td>total number of ordinates</td>
</tr>
<tr>
<td>( p )</td>
<td>phase function</td>
</tr>
<tr>
<td>( P )</td>
<td>center node of the control volume</td>
</tr>
<tr>
<td>( q )</td>
<td>radiative heat flux</td>
</tr>
<tr>
<td>( r )</td>
<td>CLAM scheme parameter</td>
</tr>
<tr>
<td>( R(t) )</td>
<td>dimensionless reflectance</td>
</tr>
<tr>
<td>( t )</td>
<td>time</td>
</tr>
<tr>
<td>( T(t) )</td>
<td>dimensionless transmittance</td>
</tr>
<tr>
<td>( t_c )</td>
<td>half duration of the pulse</td>
</tr>
<tr>
<td>( t_p^* )</td>
<td>dimensionless time parameter</td>
</tr>
<tr>
<td>( u )</td>
<td>direction of propagation</td>
</tr>
<tr>
<td>( V )</td>
<td>volume of the control volume</td>
</tr>
<tr>
<td>( w )</td>
<td>quadrature weight</td>
</tr>
<tr>
<td>( x )</td>
<td>location vector ((x, y, z))</td>
</tr>
<tr>
<td>( x, y, z )</td>
<td>cartesian coordinates</td>
</tr>
<tr>
<td>( \delta )</td>
<td>Dirac delta function</td>
</tr>
<tr>
<td>( \Delta x, \Delta x, \Delta x )</td>
<td>length of the control volume in (x, y, z)</td>
</tr>
<tr>
<td>( \varepsilon )</td>
<td>mesoscopic component</td>
</tr>
<tr>
<td>( \epsilon )</td>
<td>emissivity</td>
</tr>
<tr>
<td>( \rho )</td>
<td>reflectivity</td>
</tr>
<tr>
<td>( \tau )</td>
<td>optical thickness</td>
</tr>
<tr>
<td>( \Psi )</td>
<td>Van Leer flux limiter</td>
</tr>
<tr>
<td>( \omega )</td>
<td>albedo</td>
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### Subscripts

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>( b )</td>
<td>black body</td>
</tr>
<tr>
<td>( c )</td>
<td>collimated component of the radiation</td>
</tr>
<tr>
<td>( d )</td>
<td>diffuse component of the radiation</td>
</tr>
<tr>
<td>( D )</td>
<td>downstream node</td>
</tr>
<tr>
<td>( f )</td>
<td>face of the control volume</td>
</tr>
<tr>
<td>( \text{max} )</td>
<td>maximum radiative intensity of the pulse</td>
</tr>
<tr>
<td>( U )</td>
<td>upstream node</td>
</tr>
<tr>
<td>( w )</td>
<td>generic wall location</td>
</tr>
<tr>
<td>Superscripts</td>
<td>Description</td>
</tr>
<tr>
<td>-------------</td>
<td>------------------------------</td>
</tr>
<tr>
<td>'</td>
<td>incident direction</td>
</tr>
<tr>
<td>0</td>
<td>boundary at ((x = 0, y, z))</td>
</tr>
<tr>
<td>lat</td>
<td>lateral boundary</td>
</tr>
<tr>
<td>L</td>
<td>boundary at ((x = L, y, z))</td>
</tr>
<tr>
<td>lim</td>
<td>diffusive limit</td>
</tr>
</tbody>
</table>
Acronyms

**A**
Asymptotic Preserving (AP)

**D**
Diffusion Equation (DE)
Discrete Transfer Method (DTM)
Discrete Ordinates Method (DOM)

**F**
Finite Element Method (FEM)
Finite Volume Method (FVM)

**H**
Hybrid Transport-Diffusion (HTD)

**M**
Method of Lines (MOL)
Micro-Macro (MM)
Monte Carlo (MC)

**O**
One-Dimensional (1D)

**R**
Radiative Transfer Equation (RTE)
Runge-Kutta, 2\(^{nd}\) order (RK2)
Runge-Kutta, 4\(^{th}\) order (RK4)

**T**
Three-dimensional (3D)
Two-dimensional (2D)
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1 Introduction

1.1 Motivation

As widely known, many research fields like heat transfer, astrophysics, nuclear energy, solar energy processes, atmospheric physics are concerned with the numerical simulation of the radiative transfer equation in emitting, absorbing and scattering media. Particularly, in the last few decades, the interest in the study of transient radiative transfer has been increasing mainly because of the advent of numerous engineering and biomedical applications [1], such as optical tomography, laser ablation, laser-tissue interaction, non-destructive biomedical diagnosis and treatment, non-invasive detection in turbid media, laser micromachining, remote sensing, and others that make use of ultra-short pulse lasers, with non-negligible unsteady effects.

The majority of radiative transfer problems allows the disregard of the transient term of the radiative transfer equation, since the time required for the photons to leave the medium is much shorter than the temporal variation of the radiative source/signals. However, with pulse lasers emitted in such a small time scale, that can range from $O(10^{-18}$ s) to $O(10^{-6}$ s) [2], and with characteristic times of travel of the order of 10-100 ps (typical in tissues, for example), the propagation speed must be taken into account and, therefore, a transient radiative transfer application arises. Adding a transient term, to the already highly complex steady-state three-dimensional radiative transfer integro-differential equations, is a very demanding job.

Simultaneously, as stressed by Guo and Kumar [3], thanks to the ultra-short pulse’s small energy content, the temperature of the medium is not significantly affected (Fig 1). So, the media can be regarded as cold, since any emission has no significance when compared with scattering and absorption of the pulse.

![Figure 1: Temperature increase from drilling with nanosecond and femtosecond laser pulses, from [1].](image)

\[\text{Temperature (°C)}\]

\[\text{Time (s)}\]
Because of these phenomena, especially multiple scattering, the ultra-short pulse originates transmitted and reflected temporal signals, longer than the original pulse, which can be a source of information about the optical properties of the medium. This optical diagnosis is used in non-destructive detecting of heterogeneities that can be reconstructed solving an inverse radiation problem [4]. Obviously, the reliability and accuracy of any inverse application is strongly dependent on the direct method. Hence, efficient and precise models are needed.

As proof of its great research interest for a wide range of applications, several methods have been developed over the last decades in order to estimate radiative transfer precisely, with different results and trade-offs [5]. Some of them are based on the linear radiative transfer equation (RTE), such as the Monte Carlo (MC), the discrete-ordinates (DOM) or the finite-volume methods (FVM)\(^1\), while other methods are based on the diffusion equation (DE).

### 1.2 State of the art

Since the early studies in the 80s, the interest in transient radiative transfer has grown continuously, gaining a special momentum in the last 20 years as a result of the development in ultra-short pulse lasers technology [1]. In the following section the evolution in the state of the art is explored, with a special emphasis in biomedical applications.

In 1983, the first works on transient radiative transfer were presented, introducing the two main modelling categories: stochastic and deterministic.

Wilson and Adam [7] applied the stochastic approach, with the Monte Carlo (MC) method, to the study of light propagation in living tissues. This method became popular for its relatively simple algorithm, a consequence of avoiding the complex integro-differential RTE, and still dealing with realistic physical conditions in a flexible way [3]. The MC has provided benchmark results in transient radiative transfer ever since. However, the Monte Carlo method requires a large number of energy bundles to achieve smooth and accurate solutions in order to minimize statistical error due to real finite samplings. This might be computationally expensive and extremely time-consuming.

In contrast, Rackmil and Buckius [8] proposed the so called adding-doubling method to model the transient response of a medium when subject to a unit-step source. This deterministic method allowed to get around those statistical errors, proving to be a very promising approach whit its unique challenges (complicated integro-differential equations, for example). Over the years, numerous deterministic models have been used, with different pros and cons.

\(^1\) The acronym FVM is used for the angular discretization scheme, in order to distinguish it from the spatial discretization scheme with the same name. Both schemes will be further discussed in section 2.2.
Patterson et al. [9] analysed the behaviour of light in tissues by use of the time-dependent DE. The diffusion equation is a (deterministic) macroscopic model where it is assumed that the radiative intensity is almost isotropic (P1 approximation) and, for unsteady problems, that the radiative heat flux scales with the gradient of the incident radiation (diffusion approximation). Basically, the DE is a special case of the first-order spherical harmonics approximation to the RTE [10]. The optical properties of tissues were determined by experimental measurements associated with simple theoretical analyses [4, 11-13]. The participating media in such problems are usually absorbing and anisotropic with strong forward scattering, which could be hard to model using the DE with the P1 approximation. Various drawbacks of the DE have been identified both analytically and experimentally [14].

Alternatively, the transient RTE describes the interactions between scattering and absorption (and emission, when considered) at a mesoscopic scale, i.e. taking into consideration the angular dependence of the radiation, which expectedly offers better accuracy but requires a higher computational (CPU) effort.

The complete (hyperbolic and parabolic) transient RTE was considered and solved by Kumar et al. [15] using the P1 model as a damped wave hyperbolic method. After that, various mathematical models were tested in a series of studies [1,16]. Mitra and Kumar [17] developed and compared the discrete ordinates method (DOM), Pn expansion (P1 and P3 models) and two-flux method in short pulse laser transport. It was concluded that the predicted optical signal is highly influenced by the approximate model chosen, as the P1 model strongly underestimates the light propagation speed, and the discrete ordinates method (DOM) achieves better transient results.

Another take on deterministic models was proposed, separately, by Wu [18] and Tan and Hsu [19] with the integral equation formulation. Their solutions compared well with Monte Carlo simulations, but proved difficult to apply to inhomogeneous and highly anisotropically scattering media.

The studies in transient radiative transfer mentioned so far are restricted to one-dimensional (1D) geometry. In an effort to simulate more realistic conditions, Yamada and Hasegawa [20] applied the finite-element method (FEM) to solve the parabolic diffusion approximation in a two-dimensional (2D) cylindrical medium. In similar media, Wu and Wu [21] solved the integral equation using the quadrature method. Mitra et al. [22] extended also the P1 model to a multidimensional (2D) rectangular enclosure, while, Guo et al. [23] used the Monte Carlo method in a two-dimensional domain subjected to a spatial and temporal Gaussian short pulse laser (closer to reality as opposed to unit-steps). Later, Guo and Kumar [24] adopted the discrete ordinates method (DOM) for an absorbing, emitting and anisotropically scattering two-dimensional medium exposed to diffuse and/or collimated laser irradiation. At this point, their formulation could be easily extended to a three-dimensional (3D) geometry.

Guo and Kumar [3] generalised the parametric studies with DOM to a nonhomogeneous rectangular three-dimensional (3D) enclosure that absorbs, emits and scatters. The influence of grid size, temporal increment and angular discrete order were examined in long known steady-state phenomena
like numerical diffusion (or false scattering) and ray effect, as well as in new transient phenomena like false radiation (which some authors treat, also, as a form of numerical diffusion). Several unique transient features were explored, particularly the thermal wave nature of the propagation induced by the pulsed laser. False radiation results as consequence of the interdependence between the spatial and temporal schemes employed to implement this wave nature. Specifically, they used a finite differencing scheme which relates values (of intensity) at the cell center with those at cell surfaces, assuming an infinite propagation speed. Thus, as they confirmed, the smaller the control volumes, the weaker the false radiation. Similarly, and partially studied in steady-state, finer mesh sizes and smaller time steps decrease numerical diffusion, while increasing the number of discrete ordinates minimizes the ray effect. However, it was concluded that these effects are inevitable, making it hard to predict the sudden rise in transmittance, as calculated in Monte Carlo simulations. It is worth mentioning that the three-dimensional RTE/DOM code developed was validated based on the MC results from [23], with a technique that simulates a “2D” domain.

By the same time, Guo et al. [25] expanded the Monte Carlo method to three-dimensional problems, comparing them with experimental results of 60 ps laser pulse laser transmission in scattering and absorbing media. Besides good agreement between both results, they also demonstrated that the use of scaled isotropic scattering was not precise enough at the early times in a transient simulation. This problem with scaled isotropic scattering was already known [26].

Tsu and Hsu [27] tested the evolution of radiative flux and incident radiation in a homogeneous and inhomogeneous cubic enclosure, with the integral equation method associated with the YIX method or the discrete rectangular volume method. Good agreement between both methods was verified.

Chai et al. [28] presented a finite volume method (FVM), with a fully implicit scheme to discretize the transient term, to compare the solutions obtained with the first-order step (also known as upwind) or second-order CLAM spatial schemes, in a three-dimensional domain. Essentially, the finite volume method (FVM) differs from the discrete ordinates method (DOM) in the angular discretization procedure. The finite volume method (FVM) discretizes the domain into a set of solid-angles, where it integrates the RTE, allowing the direction to vary, but assuming a constant radiation intensity value within a solid angle [29]. Using the same spatial grid, and being second-order, the CLAM scheme predicts penetration depths and steep gradients much more precisely than the step scheme, essentially by reducing the numerical diffusion.

Ayranci and Selçuk [31] have also reported stable, accurate and efficient results provided by Van Leer flux limiters, in three-dimensional (3D) cubic enclosure containing purely scattering media and using a method of lines (MOL) solution to solve the discrete ordinates method (DOM).

Further work in the flux limiters field was done by Rousse [32], applying the finite volume method (FVM) in a one-dimensional environment. He combined a second order Lax-Wendroff spatial
scheme with Van Leer and Superbee flux limiters and compared both with an exponential scheme (first order temporal scheme). The flux limiters bound the significant oscillations near discontinuities (at the front of the pulse), verified in previous studies, by becoming zero and making the Lax-Wendroff scheme degenerate in the step scheme (inherently stable). However, supporting/complementing [3], the results show that flux limiters cannot fully avoid the transmitted flux before the minimum physical time required to get there (basically, numerical diffusion) due to the interdependence between time and spatial discretizations. It is also interesting to stress the reasons, pointed out by Rousse [32], behind his FVM choice: proper angular dependence of the radiation intensity (contrasting with the two-flux method); simple implementation and solution (unlike high-order spherical harmonics); relatively low computational requirements (unlike Monte Carlo); and higher flexibility in angular discretization (comparing to DOM). This last statement, however, is highly questionable since any angular discretization used in the FVM may be readily used in the DOM, while the reverse is not true.

A previous work of Mishra et al. [33] developed and analysed three different models to solve the governing transient RTE, applicable to a 3D participating medium when subject to a short pulse laser: the DOM, the FVM and discrete transfer method (DTM). Similar marching procedure and intensity directions/quadratures were applied in order to fairly compare the models. The models matched very well with each other, as well as with the available literature results. Additionally, the DOM proved to be the most efficient computationally. According to the authors, this is a consequence of the different angular approaches, as FVM spends extra time integrating the RTE over the discrete solid angle and DTM even more time in ray tracing.

Further studies have shown that the computational effort in mesoscopic models (classical methods based on RTE such as DOM, FVM, spherical harmonics and also MC) increases with the optical thickness of the medium and become inefficient in the diffuse regime, converging slowly as stability constraints strictly bound the numerical parameters. At the same time, such conditions are ideal for a macroscopic model (like DE), which is then more efficient than the RTE. Thus, in an effort to improve the performance of simulations in transport physics, a new approach emerged in the last decade: multi-scale models. Among them, two main classes can be distinguished: the domain decomposition methods and the methods where the radiation intensity variable is decomposed.

The first methodology (domain decomposition) splits the domain geometry into sub-regions where different models at different scales are employed. Various applications have been explored since the mathematical formulation behind these models was initially developed [34,35]. Tarvainen et al. [10] were among the first to apply this formulation to a radiative transfer problem. They coupled the RTE with DE to model photon migration. The basic idea was to combine the two different scale models so that each one could overcome each other’s drawbacks and limitations. Gorpas et al. [36], after a first one-dimensional work [37], presented a three-dimensional finite elements approach to solve the coupled RTE and DE model in fluorescent molecular imaging. A special decomposition was employed on the cubic domain, with the RTE being solved near the excitation source on the top and the DE elsewhere (Fig 2). In
this model, the RTE and DE are coupled through the sub-domains boundary conditions (which could problematic). The computational time required for this model to converge was found to be nearly half the time required by the RTE, while still accurate, even near the source.

Roger and Crouiselles [46] developed a new dynamic multi-scale approach for radiative transfer and tested it in stationary and transient one-dimensional cases. To overcome the usually delicate and problematic issue of defining the macroscopic boundary conditions, both in the interface with the mesoscopic sub-domain or in the domain’s frontier, a buffer zone was introduced (proposed in [35]). This buffer zone substitutes the coupling interface by a zone in which both macro and mesoscopic models are solved and coupled, providing a smooth transition zone where both models overlap and degenerate in each other at the buffer zone’s end. Thus, no boundary conditions are needed for the DE. This buffer zone relies on a dynamic transition function, which depends on the time and allows a dynamic control of the transition size. The FVM was used to discretize this multi-scale model (FVM-P1), which was then compared with MC, DE and a simple FVM-RTE. The buffer zone proved to be a robust and easy to handle solution that achieved promising results, in terms of precision and computationally effort (FVM-P1=3.9t vs FVM=6t). In particular, the study suggested that computationally benefit would increase in multi-dimensional cases.

This last dynamic multi-scale [46] approach essentially mixes the two methodologies, being like a transition between the two classes.

The second methodology, i.e. methods where the radiation intensity variable is split into two components, extends the buffer zone concept to the whole domain. The physical unknown, of the considered kinetic equation, is decomposed into a macroscopic and a mesoscopic components, and a coupled system of a macroscopic and a mesoscopic equations is solved. The original transport equation’s solution is recovered as the sum of the solutions of the two components. They are based on the asymptotic preserving (AP) methods where, if a scale parameter goes to zero, the scheme tends to the
classical DE model. Previous studies of unsteady problems showed that these new AP methods are unconditionally stable and accurate [38, 39].

Following previous works [35], Denong et al. [40] developed a different approach solving the DE (macro) together with a localized kinetic (mesoscopic) model that intervenes wherever it is needed. To do that, the so-called, and classical, “micro-macro” decomposition [41] was applied along with a buffer zone and AP schemes. It proved to be easy and flexible to implement, robust and, in contrast with [35], applicable to radiative transfer problems. Denong et al. [42] further improved the micro-macro model with an upgraded dynamic domain control capable of automatically create, move and eliminate as many diffuse, kinetic and buffer zones as required. This feature combined with an enhanced new criterion for the macroscopic collapse, led to better results, in terms of accuracy and computational speed, demonstrating the advantages of this method.

Roger et al. [43] brought the micro-macro formulation to short pulse laser applications, particularly, radiative transport through scattering and absorbing medium in one-dimensional test cases. The micro-macro (MM) model was solved with the DOM, and compared to the RTE (solved with MC and DOM) and DE, with various temporal discretization schemes. The improvement is visible when the scattering optical thickness becomes significant. Moreover, despite similar accuracy between MM and RTE-2nd order schemes, the CPU time of MM is at the level of RTE-1st order schemes, being a serious alternative for both (in terms of CPU efficiency or accuracy, respectively).

An alternative multi-scale model was also proposed and tested by Roger et al. [44]. In the hybrid transport-diffusion (HTD) model, similarly to the MM model, the radiative intensity is decomposed into two components, yielding a macroscopic and a mesoscopic equations. However, unlike in MM, these equations are now uncoupled, as the DE is first solved in the whole time interval throughout the domain, and then the mesoscopic equation estimates the difference between the RTE and DE formulations. Therefore, the model enables to recuperate the original RTE solution, thus keeping the exact boundary conditions. Results for transient radiative transfer with collimated irradiation, related with optical tomography applications, were obtained for HTD (solved with DOM) and compared with RTE (with MC and DOM) and DE. Fig. 3 briefly summarize the conclusions, showing that the model improves the radiative transfer calculations near the diffuse regime.

These last couple of studies done by Roger et al. in [43] and [44] motivated the present work.
1.3 Innovative contribution and objectives

This thesis follows the previous studies developed by Roger et al. [43, 44] and further extended the future work outlined by them, exploring a three-dimensional test case and employing higher-order numerical schemes. Preliminary results were presented in Pereira et al. [45].

Four different formulations for the solution of transient radiative transfer in a three-dimensional absorbing and scattering medium are compared. Two of these formulations are frequently used and well-known in the radiative transfer community: the radiative transfer equation (RTE), and the diffusion equation (DE), based on the P1 approximation. The other two are based on the mentioned multi-scale approaches: the micro-macro (MM) model and the hybrid transport-diffusion (HTD) model. The results are validated and compared with Monte-Carlo simulations.
The various models are employed in a simple hypothetical and academic test case related to optical tomography applications, where an absorbing and scattering cubic enclosure is subjected to a short pulse laser beam (collimated), uniform in space and Gaussian in time. For the first time, these multi-scale models are employed in such unsteady three-dimensional test cases. They aim at improving the efficiency of the numerical simulation of radiative transfer in transient problems.

Supporting and complementing the continuous comparison between the models, the present dissertation:

- Examines the influence of grid sizes, temporal increments and number of ordinates.
- Investigates the impact of the spatial and temporal discretizations.
- Performs a parametric study regarding three key parameters in practical applications:
  - Optical thickness (τ)
  - Albedo (ω)
  - Asymmetry factor (g)
- Analyse the computational effort, in terms of:
  - Time
  - Memory

1.4 Dissertation’s structure

The remainder of this thesis is organized into four main chapters. The mathematical formulation behind the radiative transfer models and the numerical discretization schemes, both spatial and temporal, is presented in the next section. After that, the methodology employed to design a test case and compare the different models and schemes is described. The following chapter presents and discusses the numerical results obtained. Finally, the last section sums up the conclusions and suggests possible future work relevant in this field.
2 Mathematical formulation

2.1 Radiative Transfer Models

2.1.1 Radiative Transfer Equation (RTE)

Radiative transfer is the physical phenomenon of energy transfer in the form of electromagnetic radiation. It plays an essential role in a wide range of applications from astrophysics to telecommunications. In participating media, the radiation propagation is affected by emission, absorption and scattering. The radiative transfer equation mathematically describes these interactions. It can be derived via conservation of energy and, basically, states that as a radiation beam travels in the medium along a given direction, it loses energy by absorption, gains by emission and redistributes energy by scattering.

The transient radiative transfer equation for emitting, absorbing and scattering media can be written as [5]:

\[
\frac{1}{c} \frac{\partial I}{\partial t} + \mathbf{u} \cdot \nabla I = -\left( k_a + k_s \right) I + k_a I_b + k_s \int_{4\pi} p(\mathbf{u} \cdot \mathbf{u}') I' d\mathbf{u}'
\]  

(1)

where \( I = I(\mathbf{x}, \mathbf{u}, t) \) represents the radiation intensity at location \( \mathbf{x} \), propagation direction \( \mathbf{u} \) and time \( t \). The radiation intensity is defined as power per unit area normal to the direction of propagation and per unit solid angle \([\text{W} \cdot \text{m}^{-2} \cdot \text{sr}^{-1}]\). Although the radiation intensity may also depend on the wavelength, such dependence is not addressed in the present work. The speed of light in the medium is represented by \( c \) \([\text{m} \cdot \text{s}^{-1}]\), \( k_a \) is the absorption coefficient \([\text{m}^{-1}]\), \( k_s \) denotes the scattering coefficient \([\text{m}^{-1}]\), \( p \) is the normalized scattering phase function, \( \mathbf{u}' \) is the incident direction and \( I' \) stands for \( I = I(\mathbf{x}, \mathbf{u}', t) \).

The first term on the left size of Eq. (1) describes the rate of change in time of the radiation intensity within an infinitesimal control volume. The other term on the left side represents the radiation intensity transport in the concerned direction due to spatial gradients. On the right side, the first term accounts for the decrease of radiation intensity due to both absorption, which acts like a sink, and out-scattering, which diverts radiation propagating along \( \mathbf{u} \) direction to a direction other than \( \mathbf{u} \). They are directly proportional to the radiation intensity itself and the proportionality coefficients are the absorption and the scattering coefficients, respectively. These coefficients are properties of the medium that depend on its pressure, temperature and molar fractions of the absorbing species [5]. Physically, the coefficients could be seen as the inverse of the average distance travelled by a photon until being absorbed or scattered, respectively. An extinction coefficient can be defined by summing both coefficients. The remainder two terms contribute to increase the radiation intensity. The second term on the right side results from the medium’s emission within the infinitesimal control volume. It is directly proportional to the blackbody radiation intensity at the medium’s temperature, with the absorption
coefficient as proportionality coefficient once again. Finally, the last term represents the in-scattering positive contribution. The integral calculates the probability of radiation travelling along any particular direction being scattered in the considered direction $\mathbf{u}$, which is given by the scattering phase function, weighted by the radiation intensity of the particular direction. This integral times the proportionality coefficient (scattering coefficient) leads to the increase of radiation intensity due to photons travelling in random directions that are scattered into direction $\mathbf{u}$ inside the infinitesimal control volume. Is noted that the $\frac{1}{4\pi}$ factor that usually appears out of the integral, which guarantees that the integrated phase function is equal to one in an isotropic situation, is incorporated in the phase function.

When the medium is subjected to laser irradiance it is convenient, for numerical reasons related with the angular discretization, to decompose the radiation intensity into its collimated component, $I_c$, and its diffuse component, $I_d$, according to $I(x, \mathbf{u}, t) = I_c(x, \mathbf{u}_c, t) + I_d(x, \mathbf{u}, t)$. Simultaneously, according to what has already been discussed (Fig. 1), for the problem under consideration in the present work it is reasonable to neglect any emission and treat the media as cold, without the loss of feasibility. Thus, two equations are obtained [5]:

$$
\frac{1}{c} \frac{\partial I_c}{\partial t} + \mathbf{u} \cdot \nabla I_c = -(k_a + k_s)I_c
$$

(2)

$$
\frac{1}{c} \frac{\partial I_d}{\partial t} + \mathbf{u} \cdot \nabla I_d = -(k_a + k_s)I_d + k_s \int_{4\pi} p(u \cdot u')I_d(u') \, du' + k_s p(u \cdot u_c)I_c
$$

(3)

Subscripts $c$ and $d$ stand for the collimated and diffusive components, respectively. Additionally to the emission term, omitted in both equations, the in-scattering does not appear in Eq. (2) since, by definition, the collimated radiation propagates only along $\mathbf{u}$ direction. The last term that appears in Eq. (3) is directly related with what was just said, as it is due to radiation that is scattered away from the collimated laser irradiance. It is stressed that, from a theoretically point of view, there would be a diffuse radiation direction collinear with the collimated one. However, in numerical methods that is not generally the case, and it is precisely because of it that the radiation intensity is decomposed. This subject will be further discussed later as the spatial discretization is explained.

The collimated intensity $I_c$ is zero in all directions except $\mathbf{u}_c$, and may be found from analytical solution of Eq. (2), which is expressed as [44]

$$
I_c(x, \mathbf{u}, t) = \delta(\mathbf{u} - \mathbf{u}_c)I_c(x_0, \mathbf{u}, t_0) \exp \left(-\int_0^{||x-x_0||} (k_a + k_s) \, dl \right)
$$

(4)

where $\delta$ is the Dirac distribution and $t_0 = t - \frac{||x-x_0||}{c}$ is the time at which the collimated radiation left the boundary point $x_0$.

The general boundary condition for an opaque and diffuse surface can be written as [5]

$$
I_w(x_w, \mathbf{u}, t) = \epsilon_w I_b(x_w, t) + \int_{\mathbf{w} \cdot \mathbf{n} > 0} \rho_w(x_w) I(x_w, \mathbf{u}', t)(\mathbf{u}' \cdot \mathbf{n}) \, d\mathbf{u}'
$$

(5)
where $x_w$ denotes the position at the domain’s boundary, $n$ is the inward surface normal, $\epsilon_w$ is the emissivity and $\rho_w$ is the reflectivity.

The procedure to solve the RTE model is straightforward:

- Solve collimated equation on $I_c$ (Eq.2).
- Solve the transport equation on $I_d$ (Eq. 3) by using the DOM.

However, the large number of variables associated with integro-differential equations make the RTE model difficult to solve and computationally demanding. To avoid/overcome these difficulties some simplifications were developed and applied over the years. A common approximation is the DE, computationally more efficient but less accurate.

## 2.1.2 Diffusion Equation (DE)

The diffusion equation can be deduced by integrating the RTE over the solid-angle space and applying the P1 approximation, which assumes the radiation intensity as nearly isotropic. First of all, Eq. (3) is integrated over $4\pi$ sr leading to [5]:

$$
\frac{1}{c} \frac{\partial G_d}{\partial t} + \nabla \cdot q = -k_d G_d + k_s I_c
$$

where $G$ denotes the incident radiation (or photon fluence rate), defined by $G(x, t) = \langle I(x, u, t) \rangle$, as power per unit of area [W.m$^{-2}$], where $\langle \rangle$ represents the integral over the solid-angle space: $\langle a \rangle = \int_{4\pi} a(u)du$. The quantity $q$ is the radiative heat flux, defined by $q(x, t) = \langle l(x, u, t)u \rangle$ with units of power per unit of normal area [W.m$^{-2}$]. The obtained equation expresses the energy balance of the diffuse component of radiative energy in an elementary control volume. The first term of the left hand side of the equation describes the rate of change of the diffuse component of the incident radiation within the control volume. The second term expresses the net volumetric radiative power entering and leaving the control volume across its boundaries. At the right hand side of the equation, the first term accounts for the radiative power absorbed by the participating medium per unit volume, while the second term represents the increase in volumetric radiative power due to scattering of collimated radiation. Obviously, the angular dependence disappeared and the only scattering contribution comes from the collimated radiation. Scattering caused by the diffuse component does not alter the control volume’s energy level, once in-scattering and out-scattering cancel each other within the volume when all directions are accounted for.

This equation is not closed, so an assumption that relates $G$ with $q$ is necessary. A common approach, detailed in [5], consists in multiplying the RTE by the direction $u$ and integrating it over the solid angle space, leading to
\[
\frac{1}{c} \frac{\partial q_d}{\partial t} + \nabla \cdot (\mathbf{u} \cdot \mathbf{u}) I_d = -\left[ k_a + (1-g) k_s \right] q_d + k_s I_c \mathbf{u}_c
\]

(7)

where the asymmetry factor is denoted by \( g = \langle p(\mathbf{u}, \mathbf{u}') \mathbf{u} \cdot \mathbf{u}' \rangle \) and the phase function depends only on the cosine of the angle between incident and scattered directions, i.e., \( p(\mathbf{u}, \mathbf{u}') = p(\mathbf{u} \cdot \mathbf{u}') \). Then, according to the first order approximation of the spherical harmonics (\( P_N \)-approximation), the P1 approximation for the diffuse radiation intensity states that [5]

\[
I_d = \frac{G_d}{4\pi} + \frac{3\eta_m}{4\pi}
\]

(8)

The first terms describes the isotropic radiation while the second term represents the deviation from isotropy. Introducing Eq. (8) in Eq. (7) and also applying the diffusion approximation, which states that the radiative heat flux remains constant in time, expressed as

\[ \frac{1}{c} \frac{\partial q}{\partial t} = 0 \]

(9)

the additional relation between \( G \) and \( q \) is finally obtained:

\[
q_d^{lim} = -D \nabla \cdot G_d^{lim} + 3D k_a g I_c \mathbf{u}_c
\]

(10)

in which the superscript \( \text{lim} \) means that its validity is restricted to the diffusive limit and \( D \) is called the diffusion coefficient, \( D = 1/[3(k_a + (1-g) k_s)] \). Thus, under these assumptions, combining Eq. (6) and Eq. (10) the following diffusion equation for \( G_d^{lim} \) is obtained:

\[
\frac{1}{c} \frac{\partial G_d^{lim}}{\partial t} - \nabla \cdot \left( D \nabla G_d^{lim} \right) = -k_a G_d^{lim} + k_s I_c - \nabla \cdot \left( 3D k_s g I_c \mathbf{u}_c \right)
\]

(11)

This model is also known as P1 model, since to obtain the macroscopic diffuse model in stationary radiative transfer it just requires the P1 approximation (no diffusion approximation needed).

Because the DE has no angular dependence, the exact boundary conditions of Eq. (5) cannot be employed, since the radiation intensity depends on the direction \( \mathbf{u} \). So the approximate Marshak boundary conditions [47] are used once they proved to be the most accurate [48]. This boundary conditions ensure the conservation of radiative energy at the boundaries and can be written as [5]

\[
\int_{\mathbf{u} \cdot \mathbf{n} > 0} I_d(x, \mathbf{u}, t) (\mathbf{u}, \mathbf{n}) d\mathbf{u} = \int_{\mathbf{u} \cdot \mathbf{n} > 0} \left[ \frac{G_d^{lim}(x, \mathbf{u}, t)}{4\pi} + \frac{3\eta_m}{4\pi} \right] (\mathbf{u}, \mathbf{n}) d\mathbf{u}
\]

(12)

Liu et al. [49] stressed an important shortcoming of the Marshak conditions, the over prediction of surface heat transfer properties.

The procedure to solve the DE model is straightforward:

- Solve the collimated equation on \( I_c \) (Eq.2).
- Solve the macroscopic equation on \( G_d^{lim} \) (Eq. 11).
2.1.3 Micro-Macro (MM)

In the Micro-Macro model the radiation diffuse component is decomposed into a macroscopic and a mesoscopic components, according to

\[
I_d(x, u, t) = \frac{G_d(x, t)}{4\pi} + \varepsilon_d(x, u, t) \tag{13}
\]

Here, the incident radiation \( G_d \) is the macroscopic component (not to be confused with \( G_d^{lim} \)) and \( \varepsilon_d \) is the mesoscopic term, which by definition satisfies \( \langle \varepsilon_d \rangle = 0 \). Noting that the radiative heat flux only depends on \( \varepsilon_d \), i.e., \( q_d(x, t) = \langle \varepsilon_d(x, u, t) u \rangle \), Eq. (6) can be re-written as

\[
\frac{1}{c} \frac{\partial G_d}{\partial t} + \langle u \cdot \nabla \varepsilon_d \rangle = -k_c G_d + k_c I_c \tag{14}
\]

An transport equation for the mesoscopic component can be easily deduced by combining Eq. (13) decomposition with the RTE (Eq. (1)) and then applying Eq. (14), resulting in [43]

\[
\frac{1}{c} \frac{\partial \varepsilon_d}{\partial t} + u \cdot \nabla \varepsilon_d = -(k_a + k_c) \varepsilon_d + k_j \int_{4\pi} \rho(u \cdot u') \varepsilon_d' d\alpha' + k_s I_s \left( \rho(u \cdot u_s) - \frac{1}{4\pi} \right) + \frac{1}{4\pi} \left( (u \cdot \nabla \varepsilon) - u \cdot \nabla G \right) \tag{15}
\]

The system of equations (2), (14) and (15), in which the latter two are coupled, is the so-called Micro-Macro model and is formally equivalent to the transient RTE. However, as mentioned in [43] the exact boundary conditions are not preserved. This is due the equations coupling, since when incoming boundary conditions are prescribed for \( I_d \), they cannot be translated into a boundary condition on \( G_d \) and \( \varepsilon \), since \( I \) is only known for incoming directions, and not for all the directions. In this case, as in [43], artificial boundary conditions of Neumann type are used [58]. It should be stressed that it is possible to develop a different decomposition that matches the exact boundary conditions, as done by Lemou and Méhats [50].

The procedure to solve the MM model is the following:

- Solve collimated equation (Eq. 2).
- Solve simultaneously both the macroscopic equation on \( G_d \) (Eq. 14) and the mesoscopic transport equation on \( \varepsilon_d \) (Eq. 15), using the DOM.
- Estimate the radiation intensity by adding the solution of both equations (Eq. 13).
2.1.4 Hybrid Transport-Diffusion (HTD)

The HTD model relies on a diffuse component decomposition similar to that used in the MM model, according to

\[ I_d(x, u, t) = \frac{G_d^{\text{lim}}(x,t)}{4\pi} + \varepsilon_d(x, u, t) \]  \hspace{1cm} (16)

The difference is that the macroscopic unknown in the HTD model is the incident radiation at the diffusive limit, \( G_d^{\text{lim}} \), which satisfies the diffusion equation (Eq. (11)). Thus, in this case, the mesoscopic component can be regarded as an estimation of the difference between the RTE and the DE. Accordingly, a transport equation for the mesoscopic component \( \varepsilon_d \) can be deduced in an analogous manner to Micro-Macro (but with Eqs. (16) and (11) instead of Eqs. (13) and (14), respectively), yielding:

\[
\frac{1}{c} \frac{\partial \varepsilon_d}{\partial t} + u \cdot \nabla \varepsilon_d = -(k_d + k_s) \varepsilon_d + k_s \int_{4\pi} \rho(u \cdot u') \varepsilon_d' \, du' + k_s I_c \left( \rho(u \cdot u_c) - \frac{1}{4\pi} \right) + \\
\frac{1}{4\pi} \left[ \nabla \cdot \left( D k_s \varepsilon_d + I_c \varepsilon_d^{\text{lim}} - D \nabla G_d^{\text{lim}} \right) - u \cdot \nabla G_d^{\text{lim}} \right]
\]  \hspace{1cm} (17)

Unlike the MM model, the three governing equations (2, 11 and 17) are decoupled, which means that the equations for the HTD model are easier to solve than those for the MM model. Additionally, and consequently, the exact boundary conditions for the radiation intensity are conserved in the HTD model. The boundary conditions for \( \varepsilon_d \) are defined according to that chosen for \( G_d^{\text{lim}} \), in order to match the exact radiation intensity on the boundaries. Just as in the DE model, Marshak boundary conditions were used for \( G_d^{\text{lim}}(x, t) \).

The procedure to solve the HTD model is simple:

- Solve collimated equation (Eq.2).
- Solve the macroscopic DE (Eq. 11) in order to calculate the field of \( G_d^{\text{lim}} \) in the system and for the considered time interval.
- Solve the mesoscopic transport equation on \( \varepsilon_d \) (Eq. 17) by using the DOM.
- Estimate the radiation intensity by adding the solution of both equations (Eq. 16).
2.2 Discretization Schemes

Analytical solutions to the radiative transfer equation exist for simple cases but numerical methods are required for more realistic media with complex multiple scattering effects. When numerical methods are used, the continuous domain of the problem is approximated by a discretized one using discretization schemes.

In the present dissertation, three main discretization categories are defined, corresponding to the RTE (and mesoscopic equations in general) independent variables \( (x, u, t) \): spatial, directional/angular and temporal, respectively.

The discretization schemes may be critical in order to achieve accurate results, depending on the radiative properties of the problem under consideration, as shown by the results presented later.

2.2.1 Spatial Schemes

The spatial discretization of the DE model was performed with the classical central finite-difference method. While for the remaining models, the spatial discretization was carried out using the well-known finite volume method [29] (not to be confused with the directional/angular discretization of similar name, which will be referred to as FVM from now on to avoid confusion – note that FVM usually uses the finite volume method as spatial discretization method, but its use is not restricted to FVM). This method approximates a partial differential equation by a system of linear algebraic equations, whose solution gives the (approximate) numerical solution of the original equation at discrete points on a meshed geometry. Each point is surrounded by an elementary control volume (finite volume) where the properties are assumed to be constant. Integrating the RTE (Eq. (1)) over a control volume and applying the Gauss divergence theorem, the volume integrals are converted to integrals over the boundary of the control volume, as

\[
\frac{1}{c} \frac{\partial I_P}{\partial t} + \sum_{f=1}^{6} \mathbf{s} \cdot \mathbf{n}_f I_f(u) A_f = -k_a V I_P(u) + \frac{k_s}{4\pi} V \int_{4\pi} I_P(u') p(u, u') d\mathbf{u}'
\]

where \( A \) is the surface’s area, \( V \) is the volume of the control volume and the subscripts \( f \) and \( P \) refers to, respectively, the surfaces and the center of the control volume.

These integrals are then evaluated as fluxes at the surfaces of each finite volume. Additionally, because the flux entering an arbitrary volume is identical to that leaving the adjacent volume, the method is conservative.

So, to close the system of equations (as many as the control volumes) the mean radiation intensities at the surfaces of the control volume are required. Once they are not directly calculated, they must be expressed in terms of radiation intensities at the grid nodes. In the present study, this is
accomplished by discretizing the convective-like term using either the step scheme (first-order accurate) or the CLAM scheme (second-order accurate) [30].

The step scheme, also known as upwind, is the most basic approach. The radiation intensity value at the surface \( (f) \) is taken as the same as the radiation intensity at the adjacent upstream \( (U) \) grid node (Fig 4).

\[
\begin{align*}
I_f &= I_A & \text{if} & \quad u \cdot n_f > 0 \\
I_f &= I_B & \text{if} & \quad u \cdot n_f < 0
\end{align*}
\]

Its simplicity, stability and boundedness (it does never yield physically unrealistic solutions, e.g., negative radiative intensities) are the main advantages. The main drawback of this scheme is the poor accuracy, being quite susceptible to phenomena like false radiation and numerical diffusion. The first phenomenon, previously mentioned in section 1.2, results from the interdependence between spatial and temporal schemes. In the step scheme, e.g., the equality \( I_f = I_U \) is assumed to be instantaneous, i.e., the propagation speed is virtually infinite. Obviously this is unrealistic and as a consequence fluxes emerges before the minimum physical time required. The second phenomenon, also called false scattering, occurs when radiation propagates in a direction oblique to the mesh lines and there is a gradient normal to the propagation direction [52]. This causes a spread of the radiation along the gridlines, since these are the directions in which \( I_f = I_U \) is applied. A Taylor series analysis of the step scheme shows that it is first-order accurate. To prevent these phenomena and get more accurate results, higher order method should be employed.

The second-order accurate CLAM scheme is often a solid alternative, offering a good relation between stability, computational effort and accuracy. Developed initially by Van Leer [51] this method relies on the so called flux limiters to avoid the spurious oscillations normally associated with classical high-order schemes. These flux limiters ensure that in the presence of local extreme the CLAM scheme degenerates into the step scheme. So, they act like correction factors that keep the solution monotonic [32]. In this dissertation, the CLAM scheme was formulated based on the total variation diminishing (TVD) schemes, although it also satisfies the normalized variable diagram (NVD) constraints. According to the notation of Fig.5, the radiation intensity at the surface \( I_f \) can be written as
\[ I_f = I_C + \frac{\Psi(r_f)}{2}(I_D - I_C) \quad \text{if} \quad u, n_f > 0 \] (20)

where \( \Psi(r_f) \) is the flux limiter given by \( \Psi(r_f) = (|r_f| + r_f)/(|r_f| + 1) \) and \( r_f \) is a parameter defined as \( r_f = (I_C - I_U)/(I_D - I_C) \).

The influence of both schemes on the results is studied in chapter 4 and phenomena like numerical diffusion and false radiation are discussed.

### 2.2.2 Angular Schemes

The angular discretization in mesoscopic equations is performed using the discrete ordinates method (DOM). In the DOM, the governing integro-differential equation is replaced by a discrete set of \( N \) coupled equations that describe the radiation intensity (or mesoscopic component) field along \( N \) directions. A quadrature replaces the integrals over solid angles, yielding

\[
k s \int_{\Omega} p(u, \mathbf{u}') I' d\mathbf{u}' = k_s \sum_{l=1}^{N} w_l p(u^m, \mathbf{u}') I^l
\] (21)

where \( w_l \) is the quadrature weight of the \( l^{th} \) direction and \( l \) and \( m \) are, analogously to Eq. (1), the incident and the propagation directions. As stressed by Coelho [29] the DOM may not be fully conservative in anisotropic scattering cases due to its formulation, unlike FVM. The FVM is an alternative that differs from the DOM by discretizing the solid angle space and integrating the RTE in each discrete solid angle, allowing the direction to vary within a discrete solid angle but assuming a constant radiation intensity. In this study, an \( S_n \) type quadrature, which has \( N = n \times (n + 2) \) directions, and a DCT111, with 80 directions, were employed.

A particular phenomenon known as ray effect arises from the approximation of a continuously varying angular nature of radiation by a specified set of discrete angular directions, i.e., by a stepwise one. Thus, ray effects tend to enhance the discontinuities or gradients in the domain. It is stressed that this phenomenon can interact with the numerical diffusion, and they may compensate each other, as reported in [52].
Note that no directional dependence exists at a macroscopic scale, so no directional discretization is needed.

### 2.2.3 Temporal Schemes

So far, all the schemes employed are the same as in a steady radiative transfer problem. The extra scheme employed in non-stationary problems comes from the additional transient term.

To carry out this temporal discretization several schemes are applied/tested: Forward Euler (Explicit), 2nd order Runge-Kutta (with two different coefficient weighting approaches) and 4th order Runge-Kutta.

The Forward Euler scheme, also simply referred to as Explicit scheme, is a 1st order accurate method, in which the temporal dependent variable (in this case $I$, $G$ or $\varepsilon$) in the time instant $(t + \Delta t)$ at a given point can be expressed explicitly from the current ($t$) solution values, according to (for the RTE example):

$$
\frac{1}{c} \frac{\partial I}{\partial t} \approx \frac{I^{t+\Delta t} - I^t}{c \Delta t} = F(t, I^t)
$$

where $\Delta t$ is the time step and $F$ is the temporal derivative of $I$ at the instant $t$, divided by $c$. This method is easier to implement and computationally more efficient than the Backward Euler (Implicit) scheme, where the solution $I^{t+\Delta t}$ is found by solving a system of equations involving both the present and latter state, but requires a smaller $\Delta t$ in order to achieve numerical stability.

Aiming to obtain better accuracy, higher order Runge-Kutta methods were developed. The Runge-Kutta family is closely related to the Taylor series expansion and, up to the forth order, uses as many evaluations of derivative as the desired order of accuracy [53]. As a matter of fact, the Forward Euler scheme is the 1st order Runge-Kutta method, where $I^{t+\Delta t}$ is obtained using directly from the estimated derivative in $t$.

Two alternative, slightly different, 2nd order Runge-Kutta schemes are formulated and compared. Firstly, the so called Explicit Midpoint method uses the computed derivative in $t + \Delta t/2$, previously estimated using the derivative in $t$.

$$
\frac{I^{t+\Delta t} - I^t}{c \Delta t} = F(t + \frac{\Delta t}{2}, I^t + \frac{\Delta t}{2} F(t, I^t))
$$

Secondly, in the Heun’s method $I^{t+\Delta t}$ is calculated based on the average slope of the derivatives in $t$ and $t + \Delta t$.

$$
\frac{I^{t+\Delta t} - I^t}{c \Delta t} = \frac{1}{2} \left( F(t, I^t) + F(t + \Delta t, I^t + \Delta t F(t, I^t)) \right)
$$
Both approaches consist of two stages, the difference between the models relies on the specific way the coefficients are weighted. For a more formal definition see a Butcher tableau [54].

Finally, the classical 4th order Runge-Kutta scheme is studied too. This method is a generalization of Simpson’s rule. A weighted average is performed based on four estimated slopes: at the beginning of the interval \( t \), two different slopes (by definition) at the midpoint \( (t + \Delta t/2) \) and at the end of the interval \( (t + \Delta t) \).

\[
\frac{I_{t+\Delta t} - I_t}{c\Delta t} = \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) \tag{25}
\]

\[
k_1 = F(t, I^t) \tag{25a}
\]

\[
k_2 = F(t + \frac{\Delta t}{2}, I^t + \frac{\Delta t}{2} k_1) \tag{25b}
\]

\[
k_3 = F(t + \frac{\Delta t}{2}, I^t + \frac{\Delta t}{2} k_2) \tag{25c}
\]

\[
k_4 = F(t + \Delta t, I^t + \Delta t k_3) \tag{25d}
\]

As a 4th order method, the local truncation error is on the order of \( O(h^5) \), while the total accumulated error is order \( O(h^4) \). This is the most popular Runge-Kutta method since for higher orders the number of evaluations of derivatives is superior to the scheme’s order, making them less computationally attractive.

The stability criteria defines the time step as \( \Delta t = CFL.\Delta x/c \) for RTE, MM and HTD and \( \Delta t = CFL. (\Delta x)^2/(10Dc) \) for DE where \( CFL \) is a stability parameter defined according to [5].
3 Methodology

3.1 Test case

A simple and academically orientated three-dimensional test case was considered to compare the behaviour of the different models and discretization schemes. It consists of a three-dimensional cubic enclosure of side $L = 1\,\text{m}$, schematically shown in Fig. 6, containing a scattering, absorbing and non-emitting homogeneous medium, as often considered in problems of light propagation in biological tissues. The scattering is described by the Henyey-Greenstein phase function \[ p(\mathbf{u}, \mathbf{u}') = \frac{1}{4\pi} \frac{1 - g^2}{1 + g^2 - 2g(\mathbf{u}.\mathbf{u}')^{1.5}} \] (26)

The medium is subjected to an incident laser source in one boundary, specifically, a pulse laser Gaussian in time and uniform in space is simulated according to:

\[ I_c(x_0, \mathbf{u}, t) = I_{\text{max}}\delta(\mathbf{u} - \mathbf{u}_c)\exp \left\{ -4(\ln 2) \left( \frac{t - t_c}{t_p} \right)^2 \right\} \] (27)

where $x_0$ is the emitting wall location ($x = 0, y, z$), $\delta$ is the Dirac delta function and $I_{\text{max}}$ is the maximum radiative intensity of the pulse (set equal to 1), which occurs at $t = t_c = 3t_p$. A dimensionless time parameter defined as $t_p^* = c(k_a + k_s)t_p$ is fixed equal to 0.5. The laser is normal to the boundary (see Fig. 6). After $2t_c$ this surface is free from irradiation. The remaining boundaries are black (absorb all incident radiation) and cold (non-emitting). Thus, the boundary conditions for the diffuse component can now expressed as

\[ \text{RTE} \quad I_{\text{W}}(x_\text{W}, \mathbf{u}, t) = 0 \quad \text{u.n}>0 \] (28a)

\[ \text{DE} \quad \frac{\varepsilon_d}{4\pi}(x_\text{W}, \mathbf{u}, t) = 0 \quad \text{u.n}>0 \] (28b)

\[ \text{Micro-Macro} \quad \varepsilon_d(x_\text{W}, \mathbf{u}, t) = -\frac{G_d(x_\text{W}, t)}{4\pi} \quad \text{u.n}>0 \] (28c)

\[ \text{HTD} \quad \varepsilon_d(x_\text{W}, \mathbf{u}, t) = -\frac{G_d(x_\text{W}, t)}{4\pi} \quad \text{u.n}>0 \] (28d)
where, once more, \( \mathbf{n} \) is the inward surface normal. The RTE boundary conditions are simply obtained from Eq.(5), imposing \( \varepsilon_w = 1 \) and \( \rho_w = 0 \). In the DE case, the boundary conditions appear by combining Eqs.(12) and (28a). Finally, the boundary conditions of both the MM and the HTD models are defined in a similar way where the mesoscopic component \( \varepsilon \) is deduced from the macroscopic variable in order to ensure that the incoming diffuse radiation \( I_d \) (Eqs.(13) and (16), respectively) is null at these boundaries. The MM model relies on Neumann boundary conditions to obtain the macroscopic variable at the boundaries. These conditions prescribe a zero gradient of the diffusive component of the incident radiation. The HTD model relies on the Marshak boundary conditions of the DE model. Unlike the MM model, the HTD model preserves the exact boundary conditions, as discussed in section 2.1.4.

In this work we are concerned with the temporal signature of the incident radiative energy at the boundaries of the cubic enclosure. This is quantified by the dimensionless transmittance \( T(t) \), radiation leaving from the laser’s opposite boundary; the reflectance \( R(t) \), radiation reflected back and leaving the domain through to the laser boundary; and the radiation absorbed in one of the four lateral boundaries \( L(t) \), given by, respectively:

\[
T(t) = T_c(t) + T_d(t) = \int_A \frac{I_c(x_L, \mathbf{u}, t)}{I_{\text{max}}} \mathbf{u} \cdot \mathbf{n} dA + \int_A \int_{2\pi} \frac{I_d(x_L, \mathbf{u}, t)}{I_{\text{max}}} (\mathbf{u} \cdot \mathbf{n}) d\mathbf{u} dA
\]

\[
R(t) = R_d(t) = \int_A \int_{2\pi} \frac{I_d(x_0, \mathbf{u}, t)}{I_{\text{max}}} (\mathbf{u} \cdot \mathbf{n}) d\mathbf{u} dA
\]

\[
L(t) = L_d(t) = \int_A \int_{2\pi} \frac{I_d(x_{\text{lat}}, \mathbf{u}, t)}{I_{\text{max}}} (\mathbf{u} \cdot \mathbf{n}) d\mathbf{u} dA
\]

where \( x_L \) is the boundary located at \((x = L, y, z)\), \( x_0 \) is a boundary at \((x, y = 0 \text{ or } y = L, z)\) or \((x, y, z = 0 \text{ or } z = L)\) and \( \mathbf{n} \) denotes the inward unit vector normal to the surface in question.

A simulation is defined by three main optical parameters: optical thickness, \( \tau \); albedo, \( \omega \); and asymmetry factor, \( g \). The optical thickness, also known as optical depth, is defined as \( \tau = (k_a + k_s) L \) and is a dimensionless parameter that, physically, could be seen as the ratio between the medium’s length and the average distance travelled by a photon until being either scattered or absorbed. It quantifies the ability of the medium to absorb or scatter radiative energy. The albedo is the ratio of the scattering and extinction coefficients, \( \omega = k_s/(k_a + k_s) \).

The influence of each individual parameter on \( T(t) \), \( R(t) \) and \( L(t) \) is investigated. A previously validated Monte Carlo algorithm [44] is used to provide benchmark results. The statistical error associated with it depends on the particular optical scenario, essentially on the albedo. For albedos of 0.5 and 0.9 the errors are inferior to 1% and 6%, respectively, for a 99% confidence interval.
4 Results and Discussion

The three-dimensional test case described above is employed to study the influence of the different models, discretization schemes and parameters, both optical and numerical. The results, and parallel discussion, are organized in two main sections: isotropic and anisotropic.

Firstly, the isotropic scenario, i.e. $g = 0$, is approached to examine the effect of the several models, the spatial and temporal discretization schemes (1st and 2nd order schemes), and the optical parameters, $\tau$ and $\omega$. The numerical parameters remain constant throughout the section. A finer mesh in the collimated $x$ direction is used to discretize the enclosure. This kind of mesh proved to be the ideal compromise between accuracy and computation requirements for a collimated laser beam type application (Appendix-Fig. 24). In this particular case, the medium is divided into fifty control volumes in $x$ direction ($N_x = 50, \Delta x = 0.02\ m$) and twenty in $y$ and $z$ directions ($N_y = N_z = 20, \Delta y = \Delta z = 0.05\ m$). As consequence, taking $cfl$ as 0.5, $\Delta t = 3.33 \times 10^{-11}\ s$ for RTE, MM and HTD, and $\Delta t = 1.70 \times 10^{-12}\ s$ for DE. Finally, for the angular discretization a $S_{12}$ quadrature (168 directions) is employed. These are defined as the standard numerical parameters.

Secondly, the anisotropic scenario is subdivided in moderate and strong forward-peaked scattering. In the first subsection, a study analogous to the anisotropic one and with the standard numerical parameters is undertaken, but now with the additional influence of $g$. And lastly, a highly forward-peaked scattering case is investigated. In this subsection the optical parameters are set constant, defining an extremely demanding scenario where the sensitivity studies of intrinsic numerical parameters are conducted. Finer spatial meshes, smaller time steps, greater number of ordinates, different quadratures and higher order temporal schemes are tested.
4.1 Isotropic Scattering

The influence of the spatial and temporal discretization schemes on the temporal signature of $T(t)$ is investigated, since it is more accentuated there than in $R(t)$ or $L(t)$.

Fig. 7 displays the effects for the base conditions, $\tau = 10$ and $\omega = 0.5$. Since this is a relatively simple case, the 1st order spatial and temporal schemes in Fig. 7(a) already show a close agreement with the MC prediction. Note that when mentioning the 1st order spatial schemes this refers to the Step scheme for RTE, MM and HTD. It is stressed that, although, strictly speaking, the central finite difference scheme used is a 2nd order accurate scheme, the results of the DE are only shown in the figures with the 1st order spatial scheme. This is an arbitrary choice dictated by the poor accuracy of the DE for most cases. In these conditions the DE model proves to be the most accurate while the RTE presents the biggest errors, both in the peak and steep rise regions of the curve, which according to its shape is essentially transmitted collimated radiation. The multi-scale models provide better results comparatively to RTE, in both areas. Increasing the order of the temporal scheme from a 1st order Euler to a 2nd order Runge-Kutta (RK2) has a positive localised effect on the peak value of the models, as visible in Fig. 7(b). However this positive impact is negligible for DE where the results improved less than 1%, probably due to the fact that $\Delta t$ for this model is already so small that a higher order scheme in time has no tangible effect. Meanwhile, using only a 2nd order scheme in space (CLAM scheme), Fig. 7(c), also provides a localised accuracy increase, but now in the abrupt rise region of the curve, basically attenuating the numerical diffusion and false radiation.
phenomena, as verified in previous studies. Finally, in Fig. 7(d), the 2nd order spatial and temporal schemes are combined, providing better results than the simple sum of its individual parts, i.e., the overall impact is greater than the sum of the localised positive effects discussed in Figs. 7(b) and (c). It is important to compare the RTE, MM and HTD models in terms of computational efficient, i.e. the CPU time. To do so, and because what is relevant is to relate the several models, the CPU time is expressed in terms of the RTE’s CPU time. These CPU times vary significantly depending on the schemes used (e.g. $t_{CLAM} \approx 1.2t_{Step}$ and $t_{RK2} \approx 2.3t_{Euler}$) but the differences between the models become smaller for high order schemes (e.g., for Fig. 7(a) $t_{MM} \approx 1.05t_{RTE}$ and $t_{HTD} \approx 1.11t_{RTE}$ while for Fig. 7(d) $t_{MM} \approx 1.01t_{RTE}$ and $t_{HTD} \approx 1.05t_{RTE}$). Despite the results of RTE, MM and HTD being slightly more precise than DE for Fig. 7(d), this last model requires a lower CPU time by several orders of magnitude, being much more attractive for the present case.

In order to study the influence of the optical thickness, the scenario $\tau = 20$ and $\omega = 0.5$ is now addressed in Fig. 8. First, the order of magnitude of the transmittance is highlighted. Doubling the optical thickness results in a transmitted radiation peak four orders of magnitude lower (0.0001!). Despite the probability of a photon being scattered or absorbed has increased in the same proportion, as the total absorbed energy rises, the transmittance peak is much smaller. As the absorbing and scattering phenomena increase, the difficulty of the first order discretization schemes in precisely simulate the concentrated peak is clear in Fig. 8(a). The errors caused by numerical diffusion and false radiation lead to unphysical solutions since the transmittance becomes different from zero well before the first

![Figure 8 - Influence of the spatial and temporal discretization schemes on the transmittance through the boundary opposite to the incident laser pulse for $\tau=20$, $\omega=0.5$, $g=0$.](image-url)
collimated photons reach the boundary $x = L$ at $t = L/c = 3.33 \times 10^{-9}$ s. Both multi-scale models behave better than the RTE, but the (collimated) peak is over predicted in comparison with the results obtained using MC. Such phenomena are virtually non-existing in DE allowing it to more correctly represent the transmittance signature up to its maximum is achieved. However, DE model underestimates the diffuse radiation that reaches the boundary after the collimated peak. To minimize the mentioned phenomena and achieve better accuracy the 2nd order schemes are employed individually, in time (Fig. 8(b)) and in space (Fig. 8(c)). The impact of the higher order spatial scheme is far superior to the temporal one, with a substantial error decrease. Lastly, analysing Fig. 8(d) becomes evident that, for these optical conditions, coupling the CLAM and RK2 schemes is essential to obtain precise results as the oscillations visible in Fig. 8(c) disappear and the peak is more closely estimated. The CPU times for this configuration are $t_{MN} \approx 1.02 t_{RTE}$ and $t_{HTD} \approx 1.07 t_{RTE}$.

Then, to examine the albedo effects the scenario in Fig. 9 is set as $\tau = 20$ and $\omega = 0.9$. The temporal transmittance signature becomes longer, stronger, smoother and the maximum is achieved later than for $\omega = 0.5$, because the average residence time of the photons in the medium is higher due to the increased scattering coefficient. The curves now exhibit two peaks: the first one at $t \approx 3.6 \times 10^{-9}$ s, which is barely visible, is due to the collimated component, while the second peak (global maximum), at $t \approx 7 \times 10^{-9}$ s, is due to the diffuse component. In the case of a large albedo, although the collimated component of transmittance remains constant, it becomes negligible compared to the diffuse one. Once more, Fig. 9(a) shows that, despite the enhanced performance of DE and the multi-scale
models in comparison with RTE, the 1st order schemes are not precise enough. While the RK2 has an insignificant impact on the results (evolution from Figs. 9(a) to (b), or (c) to (d)), the errors became almost inexistent with the CLAM scheme (evolution from Figs. 9(a) to (c), or (b) to (d)). Thus, the three models overlap each other, as well as the MC curve (note that the MC oscillations could be overcome by increasing the number of photon bundles). The relation between the computational times is \( t_{MM} \approx t_{RTE} \) and \( t_{HTD} \approx 1.03 t_{RTE} \).

The isotropic study on transmittance revealed some interesting trends. First, both multi-scale models outperformed the RTE models in terms of accuracy, with a minor computational cost. More specifically, the MM model achieved relatively better results than HTD with slightly lower computational requirements. Secondly, the differences between the models, in terms of precision and CPU, are attenuated as the order of the discretization schemes increase. And finally, the macroscopic DE model with the P1 approximation, which assumes that the radiative intensity is almost isotropic, yields an attractive trade-off, since consistently achieves fairly exact solutions without nearly any computational effort. However, if the interest goes beyond the transmittance at the wall opposite to the laser this could not be true, as it will be discussed next.

The temporal evolution of the incident radiation at the laser boundary, \( R(t) \), and at one of the lateral boundaries, \( L(t) \), is examined with the use of the 2nd order spatial and temporal schemes. Unlike the transmittance, the differences between the discretization schemes are small since phenomena such as numerical diffusion or false radiation are inexistent, for \( R(t) \), or much weaker, for \( L(t) \). So, only the influence of the optical parameters and models is investigated (Fig. 10). Understandably, these temporal signatures start sooner than \( T(t) \) and are several orders of magnitude superior, depending on the particular scenario.

Beginning with the reflectance for \( \tau = 10 \) and \( \omega = 0.5 \), Fig. 10(a) shows a close agreement among the models and the MC solution with exception of the DE model. The performance of the DE is known to be poor near the boundaries, especially near sources, as in this case, because the presence of a source is strongly anisotropic, which leads to a poor accuracy of the P1 approximation. This causes consistent inaccurate estimations for \( R(t) \), and also \( L(t) \), by the macroscopic DE model. When the optical thickness increases in Fig. 10(c) the reflectance peak moves to an early instant but its value remains the same. This is due to the fact that, on average, the photons interact sooner with the participating medium, i.e. the mean free-path is smaller, but at the same time the ratio of the absorption and scattering coefficients remains constant, not changing the maximum value of \( R(t) \). Thus, when the albedo increases from 0.5 to 0.9 the peak value doubles, while occurring at the same time as shown in Figs. 10(c) and (d). The macroscopic DE model has the worst performance, as expected, while for the remaining three models it is only noted the peak overestimation by MM.

The behaviour of \( L(t) \) is very similar to \( R(t) \), with some particular differences. With a larger optical thickness (see Figs. 10(b) to (d)), the peak is also anticipated, but now its value decreases because
\( L(t) \) is due to the successively scattered radiation that eventually reaches the lateral boundaries while \( R(t) \) is only due to the back scattered radiation. The number of extinction occurrences increases when \( \tau \) increases from 10 to 20, so that the probability of a photon being transmitted (not being absorbed) to a lateral boundary is lower yielding a decrease in the peak of \( L(t) \), similarly to \( T(t) \). Meanwhile, increasing the albedo from 0.5, in Fig. 10(d), to 0.9, in Fig. 10(f), does not alter the instant of the peak but approximately doubles its value, analogously to the reflectance. The DE is also inaccurate for \( L(t) \) while the remaining three models are almost coincident and slightly overestimate \( L(t) \). The higher the optical parameters, the higher the overestimation error.
4.2 Anisotropic Scattering

4.2.1 Moderate Forward-Peaked Scattering

In this section, a study similar to the above is conducted, but now in an anisotropic participating medium, described by the Henyey-Greenstein phase function, where the scattering is forward-peaked, i.e., $g > 0$.

Analogously to the isotropic analysis where the base scenario was defined as $\tau = 10$ and $\omega = 0.5$ (Fig. 7), the same optical thickness and albedo are adopted in Fig. 11, the difference being that the asymmetry factor is no longer zero, specifically $g = 0.3$. The first thing to notice by comparing Figs. 7(a) and 11(a) is the increased difficulty of the 1st order schemes to precisely describe the transmittance signal. For different reasons, the various models fail to represent closely the asymmetry of the MC curve. This asymmetry is a consequence of the diffuse component growth, caused by the forward-peaked scattering that extends the signal after the collimated peak. While the mesoscopic/multi-scale models cannot capture the sudden rise of the curve, due to the usual phenomena, the DE model, which performed fairly well in the isotropic case, exhibits considerable peak and post-peak errors, i.e., it underestimates the diffuse component. Once more, Fig. 11(b) shows that the RK2 as no impact in the accuracy of the DE

![Figure 11](image-url)

*Figure 11 - Influence of the spatial and temporal discretization schemes on the transmittance through the boundary opposite to the incident laser pulse for $\tau=10$, $\omega=0.5$, $g=0.3$.***
model but provides a minor localised (peak) improvement for the RTE, MM and HTD. However the major improvement comes from the CLAM scheme (Fig. 11(c)), cancelling much of the false radiation. Of course, associating both spatial and temporal 2nd order methods leads to the best results, with the overlapping of the tested models, but does not completely eliminate the numerical errors. The computational times for case (d) are (from now on, when nothing is said, the CPU times always refer to this case since it is the most accurate): \( t_{MM} \approx 0.99t_{RTE} \) and \( t_{HTD} \approx 1.04t_{RTE} \).

When the optical thickness is raised to 20, maintaining \( \omega \) and \( g \) constant, the differences between the models and the discretization schemes, and the multiple phenomena already discussed, are magnified and the previous analysis becomes clear. The 1st order spatial and temporal schemes in Fig. 12(a) originate very large numerical errors for all the formulations, taking the Monte Carlo solution as reference. As the diffuse component of radiation becomes more important for the overall transmittance, its temporal signature acquires an asymmetric nature that the macroscopic DE model increasingly fails to simulate. For the remaining models, the error in the prediction of the maximum transmittance is of the order of magnitude of the collimated peak itself, resulting in a transmittance curve that has two peaks. In order to diminish the large error due to false radiation, and numerical diffusion, the RK2 and CLAM schemes are employed. Again, the RK2 as a low impact on the results (Fig. 12(b)) while the CLAM scheme largely reduces false radiation (Fig. 12(c)), but the errors remain large. Coupling the two 2nd order schemes is imperative to obtain the most accurate results, as represented in Fig. 12(d). However, in this scenario,

![Figure 12 - Influence of the spatial and temporal discretization schemes on the transmittance through the boundary opposite to the incident laser pulse for \( \tau=20, \omega=0.5, g=0.3 \).](image-url)
they are not enough to achieve good results, and the errors introduced by false radiation, numerical diffusion and, may be, ray effect lead to a peak overestimation, of the order of 25%. There are several possible ways to reduce these errors, e.g., refine the spatial mesh, decrease the time step, employ different quadratures, apply even higher order discretization schemes, among others (this will be further discussed in the next section). The CPU times are $t_{MM} \approx t_{RTE}$ and $t_{HTD} \approx 1.02t_{RTE}$. It is noted that the better performance of the multi-scale models, relatively to the RTE, is diluted with the higher order schemes and since higher order schemes are mandatory in the present case to obtain acceptable results and the CPU times are similar, there seems to be no advantage of the multi-scale models in comparison with the RTE.

Now, similarly to the isotropic investigation, the albedo is increased to 0.9 and its effect is displayed in Fig. 13. The main difference, regarding the isotropic case addressed in Fig. 9, is the substantially higher value of the peak (five times bigger with a change in the asymmetry factor from 0 to 0.3) and its earlier occurrence in time, due to the fact that the photons require less time to leave the domain at $x = L$ once their average travel path became shorter with the forward-peaked scattering. It is also remarked that, unlike the isotropic case, the curve is smooth with only one peak. This happens because the “diffuse radiation curve” grows faster/sooner, overlaying and embodying the collimated one. It is emphasized that, unlike in the previous scenario (Fig. 12), the errors with the 2nd order spatial and temporal schemes are no longer significant and the multi-scale models are an alternative to consider (e.g.

![Figure 13 - Influence of the spatial and temporal discretization schemes on the transmittance through the boundary opposite to the incident laser pulse for $\tau=20$, $\omega=0.9$, $g=0.3$.](image-url)
Fig. 13(c)). This is due to the fact that the transmittance is now smoother and more symmetrical (due to the minor role of the collimated component in comparison with the diffuse one for the present optical parameters), as opposed to the previous case, which is more favourable to the macroscopic component of the multi-scale models. The remaining interpretation of the results is the same as in Fig. 9. The CPU relations are $t_{MM} \approx t_{RTE}$ and $t_{HTD} \approx 1.03t_{RTE}$.

Additionally, to complement the anisotropic investigation, the forward-peaked scattering is intensified by setting as $g = 0.6$ the asymmetry factor. Thus, the scenario $\tau = 20$, $\omega = 0.9$ and $g = 0.6$ is displayed in Fig. 14. The increase of the asymmetry factor yields a narrower transmittance signal, the peak occurs earlier and its value rises. With twice the asymmetry factor the maximum transmittance increases about tenfold. As we move away from the isotropic conditions, the shape of the DE’s curve is increasingly departing from the one predicted by the MC model. Despite the underestimation of the post-peak transmittance, the multi-scale HTD model, along with the MM, performs better than the RTE for the several schemes in Figs. 14 (a), (b) and (c). However, the combination of the CLAM and RK2 schemes does not solve this underestimation problem and the HTD is then outperformed by the RTE, which takes more advantage from the higher order schemes (Fig. 14(d)). The ratio between the CPU times is now $t_{MM} \approx 1.01t_{RTE}$ and $t_{HTD} \approx 1.04t_{RTE}$.

*Figure 14 - Influence of the spatial and temporal discretization schemes on the transmittance through the boundary opposite to the incident laser pulse for $\tau=20$, $\omega=0.9$, $g=0.6.$*
The same general behaviour and trends identified in the isotropic case remain valid for this moderate forward-peaked scattering study. Nevertheless, the scenarios become more demanding. This is true for all the models, but mainly for DE, for special reasons. The assumption on which this model relies, the P1 approximation, as already explained, assumes the radiative intensity as almost isotropic. Evidently, as the anisotropy increases this assumption breaks down and the model becomes useless for precise transmittance results. This analysis is enough to understand the influence of the asymmetry factor and the non-linearity of the transmittance results, as a 0.3 increment, from \( g = 0 \) to \( g = 0.3 \), raise \( T(t) \) by five times and a 0.6 increment, from \( g = 0 \) to \( g = 0.6 \), raise \( T(t) \) by nearly fifty times.

Fig. 15 shows the temporal signature of the incident radiation in the remaining boundaries. Similarly to the previous section, only the 2nd order schemes are used.

Beginning with \( L(t) \), the impact of the anisotropy seems to be practically nonexistent. Although, carefully examining the graphics it could be seen a slight peak delay and a longer lasting signature (more intense for more advanced times) as the photons travel further in space, leaving the domain through its lateral boundaries further away. The response of \( L(t) \) regarding the optical parameters is parallel to the isotropic one.

On the left side of Fig. 15, it is clearly visible that the DE model fails completely in the attempt of describing the reflectance, as the P1 approximation becomes invalid not only because of the proximity to a source but also because the medium itself is now non-isotropic. The behaviour of the reflectance with the optical parametric test is identical to the one observed under isotropic conditions, i.e., a greater optical thickness causes an earlier peak, maintaining its value (Fig. 15(a) and (c), note the different scales) and a higher albedo simply enlarges the peak (Fig. 15(c) and (e)). Additionally, the impact of the asymmetry factor is only related with the magnitude of the peak and not with the instant when it occurs, as shown from Fig. 15(e) to (g) or also from Figs. 10(a), (c) and (e) to Figs. 15(a), (c) and (e). In addition to the peak overestimation by the MM model, noticed earlier in Fig. 10, a new phenomenon appears in the reflectance curve of the multi-scale models: oscillations. These oscillations are intrinsically related with the basic nature of the multi-scale models. Just like DE, the macroscopic component of the radiation is not well predicted near the source and as the anisotropy increases the mesoscopic component correction becomes more and more demanding, especially in the MM model where the equations are coupled. The reflectance solution is then obtained by the sum of two increasingly larger quantities of opposite sign. Thus any small discrepancy by one of the components could generate fluctuations on the overall signal.

In order to further investigate these oscillations a refinement in the time step is carried out for the last scenario, presented in Fig. 14. To do so, the spatial mesh is kept constant and only the stability parameter \( cfl \) is altered. Being a direct proportionality constant between the time step and size of the control volume, when \( cfl \) is halved the time step is also halved. In Fig. 16 the sensitivity to a successively smaller time step is shown. As the time step decreases by one fifth, from the original \( cfl = 0.5 \) to \( cfl = 0.1 \), the oscillations are partially attenuated. However, a further reduction in the time step, by the same
factor, is negligible (the curve for $cfl = 0.02$ overlaps the one for $cfl = 0.1$). This means that these oscillations are only to some extent caused by the temporal discretization.

Figure 15 – Influence of the optical thickness, albedo and asymmetry factor in both $R(t)$ and $L(t)$, with the 2nd order spatial and temporal discretization schemes.
4.2.2 Strong Forward-Peaked Scattering

This final section of the Results and Discussion chapter is devoted to a sensitivity study regarding several numerical parameters. A highly demanding scenario with strong forward-peaked scattering ($\tau = 20$, $\omega = 0.9$, $g = 0.9$) is set to highlight and magnify the differences between them. It is pointed out that a special normalization, developed by Hunter and Guo [55], is employed both for the diffuse and collimated components of the radiation. This type of normalization is essential in highly anisotropic conditions to ensure/force that both the conservation of the scattering energy and the conservation of the asymmetry factor are respected.

Fig. 17 displays the temporal response of $T(t)$, $R(t)$ and $L(t)$ for the various models with the standard numerical parameters (mesh, time step and quadrature/number of ordinates) and the combined
2nd order discretization schemes (except for the DE model, which will not be further discussed and is kept in the graphics only to give an idea of the error associated with it under these conditions).

It becomes clear from Fig. 17(a) that the standard numerical parameters associated with the spatial and temporal 2nd order discretization schemes are insufficient to accurately estimate the transmittance, which shows an hundredfold increase relatively to \( g = 0.6 \). Plenty unphysical radiation and an underestimation of the peak (and the curve in general) is observed. The three models behave similarly and the errors are transverse to all as far as \( T(t) \) is concerned. This suggests that there is nothing wrong with the models themselves, but the discretization parameters are not satisfactory. On the other hand, in contrast to the transmittance, the errors observed for the reflectance (Fig. 17(b)) are particular to the multi-scale models. The oscillations already noticed for \( g = 0.6 \) become stronger, yielding even

![Figure 17](image)

*Figure 17 – Evolution of \( T(t) \), \( R(t) \) and \( L(t) \) pulse for \( \tau=20, \omega=0.9, g=0.9 \), using the 2nd order spatial and temporal discretization schemes.*
negative values in the MM case, as the growing anisotropy generates increasingly larger macroscopic component errors. The HTD model uses the DE model to obtain the macroscopic component, and the DE solution does not fit Fig. 17(b) as the peak is over two orders of magnitude greater than MC’s prediction. This is a major challenge for the mesoscopic component, which rather than finely correct the macroscopic estimation, has to compensate major errors near the source. Still in this figure it is noted that \( L(t) \) is simulated fairly well by the three models (specially the MM). The CPU times for the models are now \( t_{MM} \approx 0.88t_{RTE} \) and \( t_{HTD} \approx 0.92t_{RTE} \). This suggests that as the scenario becomes more demanding, the CPU effort of the multi-scale models decreases, relatively to the RTE model.

To improve the results and understand/trace the source of these errors, the sensitivity of the results to the numerical parameters, examined below.

Following the path started with the time step study, a higher order temporal discretization scheme was implemented and employed: the classic 4th order Runge-Kutta scheme (RK4). The details of this scheme were explained in a previous chapter, however, just like any higher order temporal scheme, the basic idea behind it is to provide an efficient alternative to a smaller time step, mimicking its effects with less computational effort. Fig. 18 displays these results, where the dashed lines represent the simulations with the RK2 scheme and the solid lines are the new ones with the RK4 scheme. As with the smaller \( cfl/time \) step (whose results for the sake of conciseness were only displayed for \( R(t) \) in the case \( \tau = 20, \omega = 0.9, g = 0.6 \)), the impact of the 4th order temporal scheme is negligible in the transmittance evolution (Fig. 18(a)), what is somehow expected since only one of the three phenomena known to be responsible for transmittance errors is influenced by the temporal discretizations, according to [3], i.e., the ray effect only depends on the angular discretization [52], the numerical diffusion on the spatial discretization [3] and, lastly, the false radiation is affected by both the spatial and the temporal schemes [3]. This is not strictly true for reflectance, as some of these phenomena do not apply (false radiation) or become less relevant. This is visible in Fig. 18(b) where the RTE model accurately estimates the reflectance with both Runge-Kutta schemes. However, the multi-scale schemes suffer of the already mentioned oscillations. The RK4 scheme slightly attenuates these fluctuations for the MM model, but it does not improve the predictions of the HTD model. This is probably due to the particularity of the numerical implementation of the HTD implementation, in which the macroscopic component is previously computed using the DE model, over the entire domain for all instants. This means that, unlike in the MM model, the equations are decoupled and therefore the mesoscopic component does not influence/adjust the macroscopic one in the next iteration. Hence, the HTD model is less sensitive, than the MM model to the temporal discretization. However, this is still unexpected and may be due to complex interactions between errors from various sources, e.g., spatial, angular and temporal. The final graphic in Fig. 18 shows the evolution of \( L(t) \) where no measurable difference is noticed between the temporal schemes, excluding the HTD model where the reflectance oscillations seem to contaminate \( L(t) \) at early instants, i.e., near the edges of the cubic enclosure in \( x = 0 \).
The ray effect, one of the phenomena that affects the accuracy of the simulations, is related to the angular discretization. Accordingly, to examine the sensitivity to the angular parameters, a dual test is designed. The test consists in comparing, on the one hand, two similar $S_N$ type quadratures with a different number of ordinates ($S_{16}$ vs $S_{12}$) and, on the other hand, two different kinds of quadrature with the same number of ordinates ($S_8$ vs DCT-111). Specifically, the $S_{16}$ quadrature has 288 directions, the

Figure 18 – Influence of the 4th order Runge-Kutta temporal scheme on $T(t)$, $R(t)$ and $L(t)$ for $\tau=20$, $\omega=0.9$ and $g=0.9$
$S_{12}$, as is known, has 168 directions and both the $S_8$ and the DCT-111 have 80 directions. This last quadrature (double cyclic triangles-DCT), proposed in [56], despite the lower number of ordinates, was claimed to provide a higher accuracy, compared to $S_N$, due to its nearest directions to the $x$, $y$ and $z$ axis [57]. This is obviously desirable since the laser beam is collimated in the $x$ direction. It is remarked that, ideally, a DCT type quadrature with a similar number of directions relatively to $S_{12}$ should be used to more easily draw conclusions, but the directions and weights of such a quadrature are not given in [59], and the calculation of that data is beyond the scope of the present work. The dotted lines in Fig. 19 correspond to $S_{12}$, the dash-point lines represent the DCT-111, the dashed lines are the $S_8$ results and, finally, the solid lines correspond to the $S_{16}$ quadrature.

Starting with the $S_{16}$ quadrature, the impact on $T(t), R(t)$ and $L(t)$, relative to the standard quadrature, is insignificant with a 2%, 1% and 3% improvement, respectively (Fig. 19(a), (b) and (c)). Yet, the transmittance results in Fig. 19(a) show that, despite both quadratures with 80 directions suffer from major unphysical radiation error due to ray effect, the DCT-111 quadrature improves the predictions when compared with $S_8$. The influence of these quadratures on the reflectance is negligible. Finally, Fig. 19(c) shows a fair improvement of $L(t)$ for these two quadratures relatively to the MC’s prediction. At this point, the results suggest that the transmittance errors do not seem to be related with the ray effect, at least in the traditional sense, since a similar $S_N$ quadrature with 70% more ordinates has a minor influence on the results. However, definitive conclusions cannot be drawn since it is known that the evolution of the ray effect with the increase of quadrature directions is not necessarily monotonous. At the same time a different kind of quadrature with ordinates nearest to the axis directions seems to capture much more precisely the collimated nature of the problem. Therefore, there is room for a deeper investigation of the role of the angular discretization on the accuracy of the predicted transmittance.

The CPU times for DCT are $t_{MM} \approx 0.93t_{RTE}$ and $t_{HTD} \approx 0.98t_{RTE}$, and for $S_{16}$ are $t_{MM} \approx 0.73t_{RTE}$ and $t_{HTD} \approx 0.82t_{RTE}$. This supports the hypothesis that as the computational effort increases, the multi-scale models become more favourable in terms of computation time.

The last numerical parameter to be investigated is the mesh size. In Fig. 20, the standard directional $50 \times 20 \times 20$ mesh (dashed line) is successively refined using a $100 \times 40 \times 40$ (dash-point lines) and a $200 \times 50 \times 50$ mesh (solid lines). It is reminded that, as the $cfl$ is kept constant for stability reasons, the time step will also get small. But once the influence of the time step alone was already examined, drawing conclusions about the mesh size will not be problematic. For computational reasons this study can only be carried out using the RTE and the MM models. The HTD model, as explained earlier, uses the DE model to firstly obtain the macroscopic component in the entire time domain, and computationally this means that a 4D matrix is stored to account for the spatial and temporal dependence of the macroscopic variable. The size of the 4th dimension is equal to the number of time steps required by the DE. Allocate this 4D matrix is extremely demanding in terms of computational memory. For example, noting that $\Delta t = cfl.(\Delta x)^2/(10Dc)$ for this macroscopic model, using a $100 \times 40 \times 40$ mesh, with $cfl = 0.5$ and setting the duration of the simulation to $4.5 \times 10^{-9}$ s, a $100 \times 40 \times 40 \times 10588$...
matrix needs to be allocated. With double precision format, more than 13.5 GB would be required. This is highly unpractical for personal computers, and a future optimized version of this model will take this into account, probably storing the DE’s data externally to the program itself.

Figure 19 - Influence of the angular discretization schemes on $T(t)$, $R(t)$ and $L(t)$ for $\tau=20$, $\omega=0.9$, $g=0.9$. 
Fig. 20(a) displays the transmittance’s evolution as the meshes get more refined and the improvement is clear. The unphysical radiation, caused by false radiation and false scattering, practically disappears and the initial steep transmittance rise is captured precisely. However, a small error peak underestimation error remains. This could be due to an inevitable residual ray effect associated with the DOM. The reflectance results in Fig. 20(b) are very interesting, showing that the oscillations of the MM

![Graphs showing T(t), R(t), and L(t) over time.](image)

*Figure 20 - Influence of the mesh refinement on T(t), R(t) and L(t) for τ=20, ω=0.9, g=0.9 (only for the RTE and the MM models)*
model (and probably the multi-scale oscillations in general) are progressively attenuated with a finer mesh. So, the source of these fluctuations is, almost certainly, related with spatial gradients. An even finer mesh would clarify that, and that will be done in the near future. The impact in RTE’s reflectance is negligible since the results were already quite satisfactory. Lastly, the effect on \( L(t) \) is nearly null. Once more, the CPU time is favourable to the MM model with \( t_{MM} \approx 0.90t_{RTE} \) for \( 100 \times 40 \times 40 \) and \( t_{MM} \approx 0.91t_{RTE} \) for \( 200 \times 50 \times 50 \).

4.3 Influence of the optical parameters on the maximum of \( T(t) \)

The present section aims to summarize and compile all the trends exhibited by the transmittance depending on the optical parameters, already discussed above. Despite the small number of simulation points, some effects are clear.

The influence of the optical thickness on the maximum value of transmittance evaluated by the Monte Carlo method is displayed in Fig. 21. The previously mentioned decrease of several orders of magnitude in the transmittance peak when the optical thickness increases is demonstrated in this graphic. Additionally, using a logarithmic scale for the ordinates axis, the results for \((\omega = 0.5, g = 0)\) and \((\omega = 0.5, g = 0.3)\) suggest a linear trend for the results. However for definitive conclusions about the linearity of this trend a greater number of conditions should be simulated and analysed. It is noticed that the rise in the optical thickness leads to a more important role played by the albedo. This is particularly evident in the crossing between the lines of \((\omega = 0.5, g = 0.6)\) and \((\omega = 0.9, g = 0)\), where for \( \tau = 10 \) the first scenario generates the higher peak but for \( \tau = 20 \) the albedo effect superimposes over the higher asymmetry factor leading to a higher transmittance maximum for the last conditions.

*Figure 21 - Influence of the optical thickness on the maximum value of transmittance (logarithmic scale)*
This last conclusion is reinforced by Fig. 22, where it is shown that for $\tau = 10$ the transmittance remains constant with the increase of the albedo. This is not true for $\tau = 20$, where an increase of the albedo leads to several orders of magnitude higher transmittance maximum. Moreover, the greater the asymmetry factor, the greater the increase (slope of the line with the logarithmic scale).

![Figure 22- Influence of the albedo on the maximum value of transmittance (logarithmic scale)](image)

Lastly, the influence of the asymmetry factor is analyzed in Fig. 23. The role of the optical thickness and albedo is well defined, with a higher transmittance peak for either a higher albedo (assuming a constant optical thickness) or a lower optical thickness (assuming a constant albedo). However, when opposite effects are mixed the comparison between two scenarios is no longer straightforward. This is the case with the blue and grey lines, where one scenario has greater albedo (positive effect on the peak) but also a higher optical thickness (negative effect in the peak), and vice-versa. Fig. 23 shows that, as the asymmetry factor increases, the scenario with the highest albedo is the most affected and the difference of several order of magnitude between the blue and grey lines, exhibited with $g = 0$, disappears as those lines merge for $g = 0.9$.

![Figure 23 - Influence of the asymmetry factor on the maximum value of transmittance (logarithmic scale)](image)
5 Conclusions and Future Work

5.1 Conclusions

Four different formulations for transient radiative transfer are compared, in three-dimensional absorbing and scattering media, namely: the radiative transfer equation (RTE), the diffusion equation (DE), the micro-macro model (MM) and the hybrid transport-diffusion model (HTD). The performance of these formulations is investigated using various temporal, spatial and angular discretization schemes and by changing the radiative properties of the medium.

In order to perform this comparison a simple three-dimensional test case was considered. It consists of a three-dimensional cubic enclosure of side L=1 m, schematically shown in Fig. 6, containing a scattering and absorbing homogeneous medium and subjected to an incident laser source in one boundary, while the remaining boundaries are black (absorb all incident radiation) and cold (non-emitting). The medium is cold, as often considered in problems of light propagation in biological tissues, and the scattering is described by the Henyey-Greenstein phase function. Physically, the medium is defined by three optical parameters: the optical thickness, \( \tau \); the albedo, \( \omega \); and the asymmetry factor, \( g \).

The results are organized in three sections according to the asymmetry factor:

- Isotropic scattering (\( g = 0 \))
- Moderate forward-peaked scattering (\( g = 0.3 \) and \( g = 0.6 \))
- Strong forward-peaked scattering (\( g = 0.9 \))

The quantities of relevance in the solution of the selected test case are the temporal signatures at the different boundaries of the domain, i.e., the dimensionless transmittance \( T(t) \), radiation leaving from the laser’s opposite boundary; the reflectance \( R(t) \), radiation reflected back and leaving the domain through to the laser boundary; and the radiation absorbed in one of the four lateral boundaries \( L(t) \). The behaviour of \( T(t) \), \( R(t) \) and \( L(t) \) is a, highly non-linear, function of these parameters. A higher optical thickness, equivalent to a higher extinction coefficient, leads to less intense temporal signals, except for the reflectance where the peak value remains unchanged. Additionally, as opposed to \( R(t) \) and \( L(t) \), the transmittance experiences a longer time variation, i.e., the curve widens. Regarding the albedo, the parametric studies show that its increase causes an overall rise of the incident radiation at the boundaries. Obviously, the higher albedo augments the diffuse radiation and broadens the signals, as the average residence time of the photons grows. Lastly, as the asymmetry factor increases, the reflectance decreases and the transmittance profile gets narrower and its peak increases. Also, \( L(t) \) increases up to a certain point, from which it starts to drop again.

Analytical solutions to the radiative transfer equation exist only for simple cases, therefore numerical methods are required for more realistic media with complex multiple scattering effects. The
discretization schemes and parameters are critical in order to achieve accurate results, depending on the radiative properties of the problem under consideration. The 1st order spatial and temporal discretization schemes, except for relatively undemanding scenarios (low optical parameters), are largely susceptible to several phenomena such as false radiation, false scattering and ray effect, which may yield large errors, and this is why the 1st order schemes are completely omitted from the strong forward-peaked study (i.e. \(g = 0.9\)). These phenomena are inevitable, however they can be minimized and, to do so, several approaches were investigated. The higher order spatial and temporal schemes proved to mitigate these errors. Particularly, the 2nd order spatial scheme has a greater impact on precision than a 2nd order temporal scheme, for the problem under consideration. However, for more demanding scenarios, the 2nd order schemes are not enough and some additional solutions were explored. Regarding the temporal discretization, both the time step decrease and the 4th order Runge-Kutta temporal scheme have almost no tangible effect on the results. The angular discretization study carried out is fairly inconclusive since, while on one hand, a \(S_{16}\) quadrature has a minor effect on accuracy when compared with \(S_{12}\), suggesting a negligible ray effect contribution to the overall errors, on the other hand, implementing a different type of quadrature with nearest directions to the \(x\), \(y\) and \(z\) axis clearly provides a better performance, for a similar number of ordinates (DCT111 vs \(S_8\)), suggesting that a DCT type quadrature with an equivalent number of directions relatively to \(S_{12}\) could improve the predictions. Ultimately, the parametric study showed that, in general, a spatial grid refinement has the greatest impact on precision. The finer mesh significantly decreases the unphysical radiation and, as widely known, the mesh size is related both with the false radiation and false scattering. This suggests that these are the main phenomena affecting the results.

The performance of the four models was analysed and compared under these various conditions. Firstly, in isotropic conditions the DE model can be considered as a feasible alternative to the other models, for applications that do not require much precision regarding the transmittance estimation. But, even for these conditions, the predictions of both \(R(t)\) and \(L(t)\) are poor. Thus, its scope is reduced. In contrast, the multi-scale models consistently out-perform the RTE model with the lower order discretization schemes, and more specifically the MM model achieves the best results. However with the 2nd order discretization schemes this advantage is diluted. Concerning the computational effort, apart from the macroscopic DE model whose CPU time is negligible, all the models have CPU times of the same order of magnitude. Both the MM and HTD require slightly more computation time than the RTE model, about 2% and 6% respectively.

In the moderate forward-peaked scattering case, the difficulty of the DE to simulate the asymmetric nature of the temporal signature of the transmittance is enhanced, in particular when both the collimated and the diffuse components have a visible contribute to the overall radiation intensity or the asymmetry factor becomes significant (\(g = 0.6\)), as both circumstances maximize the transmittance asymmetry. Accordingly, the DE becomes virtually useless for higher asymmetry factors. The performance of the RTE model is surpassed by the multi-scale models when lower order schemes are employed but,
once again, combining the 2nd order spatial and temporal schemes attenuates the differences between them. Also with the 2nd order schemes, the \( L(t) \) predictions of the various models are identical (except the DE), overlapping each other. However this is not the case for \( R(t) \) where the multi-scale models develop peculiar oscillations that introduce errors. In the moderate forward-peaked scattering case, the CPU times are even more uniform with \( t_{\text{MM}} \approx t_{\text{RTE}} \) and \( t_{\text{HTD}} \approx 1.03 t_{\text{RTE}} \), on average.

Finally, the models were compared in a highly demanding strong forward-peaked scattering scenario and their sensitivity to several numerical parameters was investigated. Apart from the DE, whose errors are huge, the behaviour of the several models regarding the numerical parameters are essentially similar. The exception is the estimation of \( R(t) \) where the multi-scale oscillations largely affect the accuracy of the results. For the MM model it is shown that in order to attenuate the oscillations and obtain good predictions for \( R(t) \) this model requires a finer mesh. For more demanding scenarios, like this one, the multi-scale models become faster than the RTE model, with a reduction in CPU time up to 27% for the MM model and 18%, for the HTD model. So, unless a specific application depends solely on the reflectance estimation, the multi-scale models are a desirable alternative, since a finer mesh is necessary to accurately simulate the transmittance either way. In contrast to the MM model, the mesoscopic and macroscopic equations are decoupled in HTD model. However, contrary to what might be expected, the computational requirements of HTD are higher than those of the MM model, not only in terms of CPU time but also of memory allocation. This is due to its more complex algorithm.

5.2 Future Work

For the future, further relevant work regarding the multi-scale models is suggested:

- To better understand the influence of the angular discretization in strong forward-peaked scattering conditions, future work should focus on studying the effect of a DCT type quadrature, with a similar number of ordinates relatively to \( S_{12} \), or on other alternative quadratures.
- According to the results obtained for the optical parameters that lead to higher errors, which suggest that the errors are mainly due to the spatial discretization, implementing a higher order spatial discretization scheme (3rd or 4th order spatial schemes) is quite pertinent, as an alternative to use successively finer meshes.
- Investigate the origin of the oscillations observed in \( R(t) \) for the MM and HTD when the asymmetry factor approaches unity.
- The study of the multi-scale models should be extended to different test conditions. These could include, without being restricted to: media with just diffuse radiation (where the reflectance errors identified with higher asymmetry factors should not occur, since no collimated source
exists to affect the macroscopic component), media with localized inhomogeneities, concentrated lasers, laser pulse trains, and also stationary problems.

- An upcoming version of the HTD model should overcome the memory allocation issues in order to allow the use of finer spatial meshes. Simultaneously, a general computational optimization of the several models should be carried out to accelerate the calculations.
6 References


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Figure 24 - Influence of several meshes on $T(t)$ for the RTE (a), the MM (b) and the HTD (c) models. Optical conditions: $\tau=20$, $\omega=0.9$, $g=0.3$