Iterative and FEM methods to solve the 2–D Radiative Transfer Equation with specular reflexion

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Abstract. The present paper deals with iterative algorithms coupled with finite element methods (FEM) to solve the Radiative Transfer Equation (RTE) within semi-transparent heterogeneous materials where specular reflexions occur on their boundaries. As our intention is to use such solution for inversion, the forward model should be solved as fastly as possible. This communication compares, in terms of both accuracy and CPU, the Discontinuous Galerkin (DG) method with the Streamline Upwind Petrov-Galerkin (SUPG) method, both being coupled with the Discrete Ordinate Method. Next, several iteratives methods used to accelerate the convergence are compared. These methods are the Gauss-Siedel (GS), the Source-Iteration (SI) and the Successive Over-Relaxation (SOR) methods.

1. Introduction
The studied forward model commonly used to model the propagation of thermal radiation within heterogeneous semi-transparent media is based on the so-called "Radiative Transfer Equation" (with the acronym RTE). Solving directly the RTE constitutes one of the main task of the inverse methods aiming to accurately retrieve the volumetric radiative properties from experimental measurements. In the field of material science, these measurements (reflectance, transmittance) are today easily performed by Fourier Transform Infrared Spectrometer on centimetric samples with a 1D plan parallel geometry. Specific set-up adapted to spectrometers allows the simulatenous investigation of the spectral and angular dependances of the radiative properties at a given temperature. The solution of the RTE being very time consuming, for both forward and backward integrations, specific numerical tools have been developed to enhance the speed without altering the quality of the solution. At room temperature, the RTE problem consists in searching the radiance $L(x, s)$ satisfying:

$$(s \cdot \nabla + \kappa + \sigma_s) L(x, s) - \sigma_s \oint_{S^{n-1}} L(x, s') \Phi(s, s') \, ds' = 0 \quad \forall (x, s) \in D \times S^{n-1} \quad (1)$$

where $s \in S^{n-1}$ is the direction of propagation of $L$ at the location $x$ ($S^{n-1}$ is the unit circle in 2D), $\kappa$ and $\sigma_s$ are the homogeneized absorption and scattering coefficients, respectively, and $\Phi(s, s')$ is the probability density scattering phase function. The spectral dependance is omitted for more clarity.

In applications considered here, the sample is illuminated with a collimated beam of radiation from the direction $s_{in}$ on the surface boundary $x \in \partial D_0$ as it is the case for bi-directionnal
measurements. Moreover, specular boundary conditions are also considered, as in [1]. This leads to consider the boundary condition formulated as:

\[ L(x, s) = \left[ \tilde{L}_{\text{in}} \times 1_{[s=s_{\text{in}}]} + \rho(n \cdot s_{\text{out}})L(x, s_{\text{out}}) \right] \times 1_{[x \in \partial D_0]} \tag{2} \]

with \( \rho(\cdot) \), the local reflectivity computed on the interface with the Fresnel law. In most situations, the system of equations (1)-(2) cannot be analytically solved due to the integral term \( \int_{S_{n-1}} ds' \) and reflexions \( \rho L(\cdot) \). To cope with such difficulties, the DOM approximates the integral by a quadrature \( \sum_{j=1}^{N_d} w_j \). The RTE (1) becomes the set of semi-discrete system (SDS):

\[ (s_m \cdot \nabla + \kappa + \sigma_s) L_m - \sigma_s \sum_{j=1}^{N_d} w_j L_j \Phi_{m,j} = 0 \quad \forall x \in D, \forall m \in 1, \cdots N_d \tag{3} \]

where we used \( L_m = L(x, s_m) \) and \( \Phi_{m,j} = \Phi(s_m, s_j) \).

2. Iterative methods

The DOM yields to write down, at the end, a linear system of the form \( Ax = b \). The dimension of \( x \) depends on the number of discrete angles \( N_r \) and on the number of degrees of freedom of functional spaces built on the chosen space mesh. Iterative methods may be necessary to reduce the memory capacity:

\[
\begin{align*}
\sum_{j < m} w_j \Phi_{m,j} L_j &+ (\kappa + \sigma_s - w_m \Phi_{m,m} \sigma_s) L_m^N = (1 - r) s_m \cdot \nabla L_m^N \\
(3 - r)(\kappa + \sigma_s - w_m \Phi_{m,m} \sigma_s) L_m^N &+ r \sigma_s \sum_{j > m} w_j \Phi_{m,j} L_j^N + r \sigma_s \sum_{j < m} w_j \Phi_{m,j} L_j^\alpha
\end{align*}
\]

(4)

with \( L_m^0 = \tilde{L}_m, r \in [0, 2] \) is the relaxation parameter, and \( N \) and \( \alpha \) are iteration numbers.

- For \( r = 1 \) and \( \alpha = N \), the iterative scheme is the Source-Iteration (SI). This method uses the radiance at the \( N^{\text{th}} \) iteration in all directions but \( m \) to compute the next iteration \( L_m^{N+1} \). The Source-Iteration method [2] is popular maybe because of its simplicity.

- For \( r = 1 \) and \( \alpha = N + 1 \), the iterative scheme is the Gauss-Siedel (GS). This method uses the radiance at the \( N^{\text{th}} \) iteration in all directions \( j > m \), and the radiance computed at the current \( (N + 1)^{\text{th}} \) iteration for \( j < m \) to compute the next iteration \( L_m^{N+1} \). This Gauss-Siedel method has been applied for the same boundary conditions (2) in [3].

- For \( r \in [0, 2] \) and \( \alpha = N + 1 \), the iterative scheme is the Successive Over-Relaxation (SOR). This method uses both the radiance at the \( N^{\text{th}} \) iteration for \( j \geq m \), and the radiance computed at the current \( (N + 1)^{\text{th}} \) iteration \( j < m \) to compute the next iteration \( L_m^{N+1} \). The SOR method has been applied for non-LTE boundary conditions in [4].

3. Spacial scheme

The Streamline Upwind Petrov-Galerkin (SUPG) scheme [5] uses the lagrangian \( P_k \) basis to build the variational formulation. The \( m^{\text{th}}\)-equation of the semi-discrete system (3) – in short (SDS\(_m\)) – is multiplied by the test function \( s_m \cdot \nabla v \) before integration on \( D \):

\[ \int_D (\text{SDS}_m) s_m \cdot \nabla v \, dx \tag{5} \]

Discontinuous Galerkin schemes are hybrid methods combining FEM and FVM (finite volume method). The cells are connected by an exchange of flux on the boundary on nearby cells. The (SDS\(_m\)) is multiplied by a test function \( v \) and it is integrated on each \( C_i \) before summation:

\[ \int_{C_i} (\text{SDS}_m) v \, dx \tag{6} \]
4. Results
The simulations are performed both on a 4 cm$^2$ square and on a 2 cm radius disk. The collimated beam is a gaussian radiance applied in the $s_{in} = (1, 0)$ direction. We used the following parameters: the refractive indices $n_{out} = 1$, $n_{in} = 1.4$, $\kappa = 0.4$ cm$^{-1}$ and the Heney-Greenstein phase function with $g = 0.5$. The errors $L_2(D)$ of the schemes are compared for different meshes at first for $\sigma_s = 0$ cm$^{-1}$. Specifically, $\mathbb{P}_1$ and $\mathbb{P}_2$ SUPG is compared with $\mathbb{P}_0$ and $\mathbb{P}_1$ DG. Next, the convergence of the iterative methods of the schemes are compared for $\sigma_s = 3$ cm$^{-1}$.

![Figure 1. Left: $L_2$-error between analytical solution and solutions of DG/SUPG schemes as a function of mesh size. Center: convergence error for SI, GS and SOR methods. Right: $L_2$-error at the $r^{th}$ iteration for different meshes and two geometries versus the relaxation parameter $r$.](image)

From Figure 1(a), one can see the error related to the SUPG $\mathbb{P}_2$ scheme is less than for the $\mathbb{P}_0$ and $\mathbb{P}_1$ DG schemes. Moreover, the order of convergence (in space) is greater for the SUPG $\mathbb{P}_2$ scheme. From Figure 1(b), it is seen that the GS method converges faster than the SI method as reported elsewhere in [3]. Moreover, the SOR method, with an appropriate relaxation parameter $r$, can converge even faster than the GS method. From Figure 1(c), one can see that the choice of the optimal parameter $r^*$ does not depend on the mesh fineness for two given geometries.

5. Conclusion
From these numerical tests, one concludes that (i) the SUPG $\mathbb{P}_2$ scheme is even more appropriate than the DG $\mathbb{P}_1$ scheme in terms of errors, with a smaller number of degrees of freedom, (ii) the iterative SOR method with an appropriate relaxation parameter is a promising extension to more classical SI and GS methods, and (iii) the optimal relaxation parameter being independent of the mesh coarseness, it can be searched on a very coarse mesh.

The direct extension of such work is the 3D implementation where the conclusions presented here should be also drawn. Moreover, the multigrid acceleration [3] will be combined with the SOR method to save again CPU-time significantly. At last, this work will open the possibilities to investigate the volumetric radiative properties of samples with a 3D symmetry.

References
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