RADIATIVE PROPERTIES ESTIMATION IN TWO-LAYER PARTICIPATING MEDIA WITH THE LUUS-JAAKOLA METHOD

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Abstract. *Implicit formulations for inverse problems of parameter estimation, in which a cost function is minimized, have largely been employed in several applications related to heat and mass transfer. Gradient based methods have been used in most cases, but it has been observed an increasing interest in the use of stochastic methods for the solution of inverse problems. In the present work we are interested in the estimation of the scattering and absorbing coefficients in two-layer participating media. The direct radiative transfer problem is solved using a combination of Chandrasekhar's discrete ordinates method and the finite difference method. For the solution of the inverse problem we propose the use of the Luus-Jaakola method, a random search optimization method that has been successfully employed mainly in chemical engineering problems. This method has been used previously by the authors for the solution of the inverse problem of radiative properties estimation in single-layer participating media, and in the present work it is intended for multi-layer media with relevant applications in remote sensing and biology, among others.*

Keywords*: radiative transfer, inverse problems, two-layer participating media, optimization, Luus-Jaakola*

1. INTRODUCTION

The inverse analysis of radiative transfer in participating media has several practical applications such as optical tomography (Kim and Charette, 2007), computerized tomography (Carita Montero *et al*., 2004), coupled atmospheric-ocean models (Zhang *et al*., 2007), hydrologic optics (Chalhoub and Campos Velho, 2001) and radiative properties estimation (Nenarokomov and Titov, 2005, Hespel *et al*., 2003, An *et al*., 2007). Most of the published works in direct and inverse radiative transfer problems deal with one-dimensional plane-parallel media, but a good number of papers have also been published looking at radiative transfer in composite layer media, with applications, for example, in regional and global climate models (Hanan, 2001, Tanaka *et al.*, 2009), Solar System bodies research (Hillier, 1997, Morishima *et al.*, 2009), Earth remote sensing (Verhoef and Bach, 2003, Weng, 2009, Toomey *et al.*, 2009) and multi-layer clouds studies (Bennartz and Preusker, 2006, Boesche *et al.*, 2009).

In the present work we focus on the implicit formulation and solution of an inverse radiative transfer problem in a two-layer plane parallel medium. When formulated implicitly, inverse problems are usually written as optimization problems, and the main focus becomes the minimization of a cost function, for example the one given by the summation of the squared residues between a calculated and a measured quantity. For the direct problem solution we use the well known Chandrasekhar's discrete ordinates method combined with the finite difference method.

For the solution of the inverse problem we propose the use of the Luus-Jaakola method, a random search optimization method that has been successfully employed mainly in chemical engineering problems. This method has been used previously by the authors for the solution of the inverse problem of radiative properties estimation in single-layer participating media (Knupp *et al.*, 2007, Knupp, 2008). In the present work the LJ method is used for the estimation of the scattering and absorbing coefficients in two-layer participating media.

2. MATHEMATICAL FORMULATION AND SOLUTION OF THE DIRECT PROBLEM

Consider the problem of radiative transfer in a composite medium with two plane-parallel, isotropically scattering, gray layers, with diffusely reflecting boundary surfaces and interface, as shown in Fig. 1. The medium is subjected to external irradiation on both sides with intensity F_1 at $x=0$ and F_2 at $x=L_1+L_2$. L_1 and L_2 represent the thickness of layers 1 and 2, respectively.

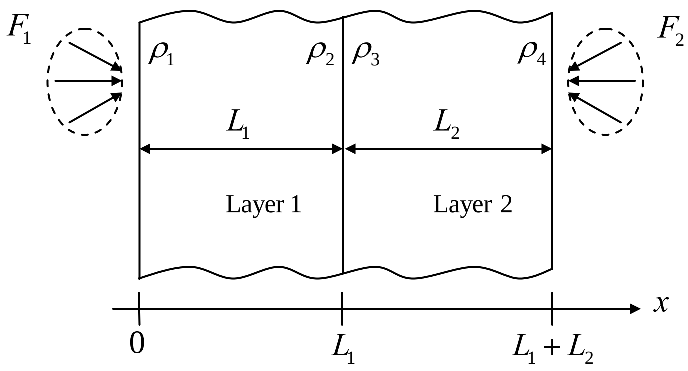

Figure 1. Two-layer semitransparent medium

The mathematical formulation of the direct radiative transfer problem with azymuthal symmetry is given by

Layer 1:

$$\mu \frac{\partial I_1(x,\mu)}{\partial x} + \beta_1 I_1(x,\mu) = \frac{\sigma_{s1}}{2} \int_{-1}^{1} I_1(x,\mu')\, d\mu', \ 0 < x < L_1 \text{ e } -1 \le \mu \le 1 \tag{1a}$$

$$I_1(0,\mu) = F_1 + 2\rho_1 \int_0^1 I_1(0,-\mu')\,\mu' d\mu', \ \mu > 0 \tag{1b}$$

$$I_1(L_1,\mu) = (1-\rho_3) I_2(L_1,\mu) + 2\rho_2 \int_0^1 I_1(L_1,\mu')\,\mu' d\mu', \ \mu < 0 \tag{1c}$$

Layer 2:

$$\mu \frac{\partial I_2(x,\mu)}{\partial x} + \beta_2 I_2(x,\mu) = \frac{\sigma_{s2}}{2} \int_{-1}^{1} I_2(x,\mu')\, d\mu', \ L_1 < x < L_1 + L_2 \text{ e } -1 \le \mu \le 1 \tag{2a}$$

$$I_2(L_1,\mu) = (1-\rho_2) I_1(L_1,\mu) + 2\rho_3 \int_0^1 I_2(L_1,-\mu')\,\mu' d\mu', \ \mu > 0 \tag{2b}$$

$$I_2(L_1+L_2,\mu) = F_2 + 2\rho_4 \int_0^1 I_2(L_1+L_2,\mu')\,\mu' d\mu', \ \mu < 0 \tag{2c}$$

where $I_i(x,\mu)$ represents the radiation intensity in layer i, with $i=1$ or 2. β_i is the total extinction coefficient.

$$\beta_i = \kappa_{ai} + \sigma_{si} \tag{3}$$

κ_{ai} is the absorption coefficient, σ_{si} is the scattering coefficient, μ is the cosine of the polar angle and ρ_j are the diffuse reflectivities, with $j = 1, \cdots, 4$.

When the geometry, the radiative properties, and the boundary conditions are known, problem (1-2) may be solved yielding the values of the radiation intensities $I_1(x,\mu)$, for $0 \le x \le L_1$ and $-1 \le \mu \le 1$, and $I_2(x,\mu)$, for $L_1 \le x \le L_1 + L_2$ and $-1 \le \mu \le 1$. This is the direct problem.

In order to solve the direct problem we have used Chandrasekhar's discrete ordinates method (Chandrasekhar, 1960). The polar angle domain and the spatial domain are discretized as shown in Figs. 2 and 3, respectively. The integral terms on the right hand side of Eqs. (1-2) are replaced by gaussian quadratures. We then used a finite-difference approximation for the terms on the left hand side of Eqs. (1-2). With that, $I_1(x,\mu)$ and $I_2(x,\mu)$ are determined for all spatial and angular nodes of the discretized computational domain.

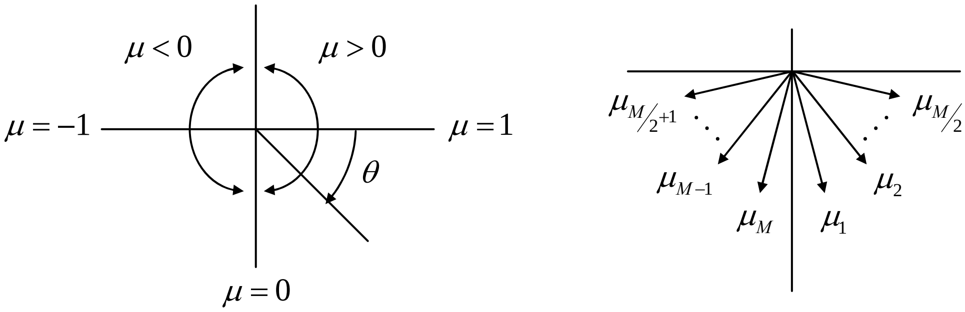

Figure 2. Angular domain discretization

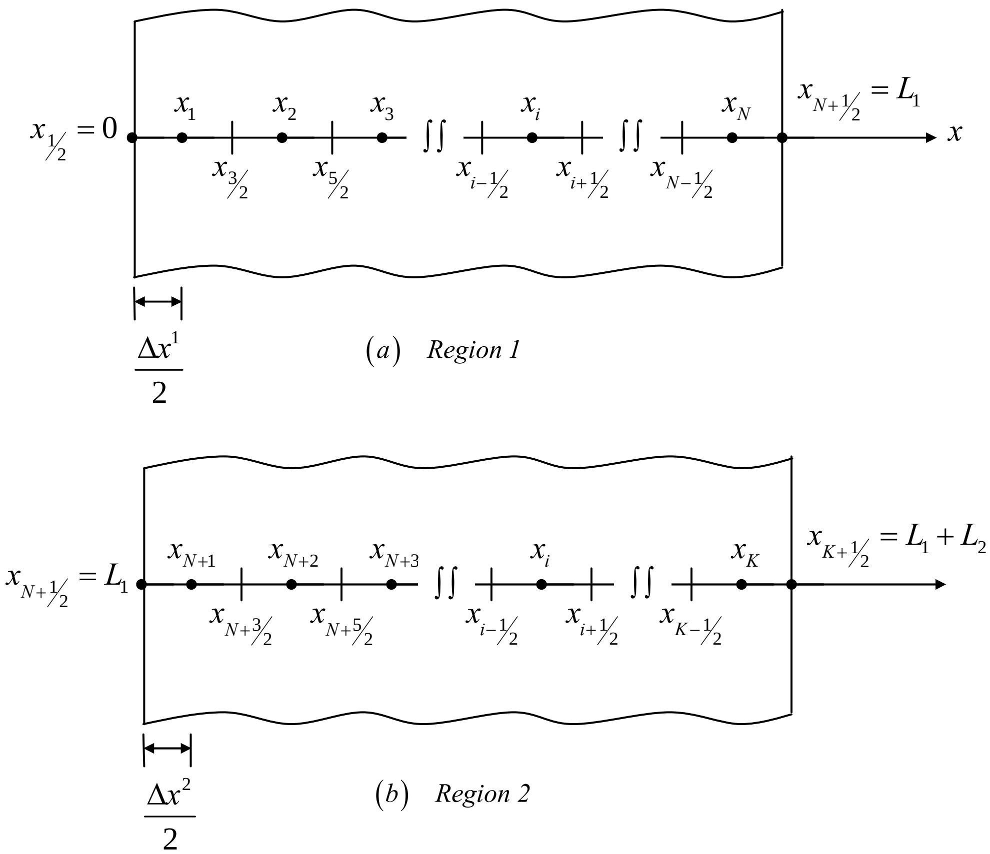

Figure 3. Spatial domain discretization

The discretized equations are not presented here and can be found in details in (Soeiro and Silva Neto, 2006, Knupp, 2008).

3. MATHEMATICAL FORMULATION OF THE INVERSE PROBLEM

In the present work we are interested in obtaining estimates for the vector of unknowns

$$\vec{Z} = \{\sigma_{s1}, k_{a1}, \sigma_{s2}, k_{a2}\}^{T} \tag{3}$$

using measured data on the emerging radiation intensity at $x=0$ and $x = L_1 + L_2$, Y_i, with $i = 1, 2, \cdots, N_d$, being N_d the total number of experimental data.

As real experimental data was not available, we generated sets of synthetic experimental data with

$$Y_i = I_{\exp_i} = I_{\mathrm{calc}_i}\left(\vec{Z}_{\mathrm{exact}}\right) + \sigma_e r_i \tag{4}$$

where I_{calc_i} represents the calculated values of the radiation intensity using the exact values of the radiative properties, $\vec{Z}_{\mathrm{exact}}$, which in a real application is not available and we want to determine with the inverse problem solution, σ_e simulates the standard deviation of the measurement errors, and r_i is a pseudo-random number in the range [-1, 1].

In the present work it is considered $N_d = M$, and half of the experimental data is acquired at $x=0$, at the polar angles corresponding to μ_m with $m = \frac{M}{2}+1, \frac{M}{2}+2, \cdots, M$, and half at $x = L_1 + L_2$, at the polar angles corresponding to μ_m with $m = 1, 2, \cdots, \frac{M}{2}$.

When internal detectors are also considered, there is a total of $N_d = 2M$ experimental data, being half of it acquired at $x=0$ and $x = L_1 + L_2$ as described before, and half at the interface $x = L_1$, at the same polar angles with μ_m, $m = 1, 2, \cdots, M$.

As the number of measured data, N_d, is usually much larger than the number of parameters to be estimated, $N_u = 4$, the inverse problem is formulated as a finite dimensional optimization problem in which we seek to minimize the squared residues functional

$$Q\left(\vec{Z}\right) = \sum_{i=1}^{N_d}\left[I_{\mathrm{calc}_i}\left(\vec{Z}\right) - Y_i\right]^2 \tag{5}$$

where I_{calc_i} represents the calculated value of the radiation intensity (using estimates for the unknown radiative properties $\vec{Z}$) at the same boundary, and at the same polar angle, for which the experimental value Y_i is obtained.

4. SOLUTION OF THE INVERSE PROBLEM WITH THE LUUS-JAAKOLA METHOD

Random search methods for optimization are based on a random exploration of a domain to find a point that minimizes an objective function. They were originally introduced by Anderson (1953), and then developed by Karnopp (1963) and Matyas (1965), among others.

Random search methods have been widely employed in chemical engineering for continuous optimization as, for example, those proposed by Luus and Jaakola (1973), Gaines and Gaddy (1976), and Salcedo *et al*. (1990). The most popular of these techniques is the Luus-Jaakola algorithm (LJ, Luus and Jaakola, 1973), which has been used not only in chemical engineering (Luus and Jaakola, 1973, Lee *et al*., 1999, Luus and Hennessy, 1999, for example), but also in control problems (Luus, 2001), in optics (Al-Marzoug and Hodgson, 2006), in electrical engineering (Singh, 2005), and in chromatography (Poplewska *et al.*, 2006), among other applications.

As stated by Liao and Luus (2005), the idea behind the Luus-Jaakola algorithm is very simple: random solutions are selected over a region that is decreased in size as iterations proceed.

Our implementation of LJ is described in Fig. 4. It differs from the original algorithm proposed by Luus and Jaakola (1973) in one point: while, originally, **x*** was replaced by a possible improved solution only after the internal loop was completed, we replace **x*** immediately if a better solution is found, as suggested by Gaines and Gaddy (1976) in their optimization algorithm.

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Choose an initial search size r^(0) .
Choose a number of external loops n_out and a number of internal loops n_in.
Choose a contraction coefficient ε.
Generate an initial solution x* .
For i = 1 to n_out
  For j = 1 to n_in
    x^(j) = x* + R^(j) r^(i-1) , where R^(j) is a diagonal matrix of random numbers between -0.5 and 0.5.
    If Fitness ( x^(j) ) < Fitness ( x* )
      x* = x^(j)
    End If
  End For
  r^(i) = (1-ε) r^(i-1)
End For
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Figure 4. The Luus-Jaakola (LJ) pseudo code

5. RESULTS AND DISCUSSION

For our test case we consider a two-layer medium composed of two different plane-parallel medium with the properties shown in Table 1.

Table 1. Properties considered for the test case

Property	Value
$L_1\,(\mathrm{cm})$	0.8
$L_2\,(\mathrm{cm})$	3.2
$\sigma_{s1}\,(\mathrm{cm}^{-1})$	0.8
$k_{a1}\,(\mathrm{cm}^{-1})$	0.5
$\sigma_{s2}\,(\mathrm{cm}^{-1})$	0.9
$k_{a2}\,(\mathrm{cm}^{-1})$	0.3
ρ_1	0.1
ρ_2	0.0
ρ_3	0.0
ρ_4	0.6

This situation corresponds to two different adjoint layers with the following dimensionless radiative properties

$$\omega_1 = \frac{\sigma_{s1}}{\kappa_{a1} + \sigma_{s1}} = 0.61, \quad \omega_2 = \frac{\sigma_{s2}}{\kappa_{a2} + \sigma_{s2}} = 0.75 \tag{6}$$

$$\tau_{01} = \left(\kappa_{a1} + \sigma_{s1}\right) L_1 = 1.04, \quad \tau_{02} = \left(\kappa_{a2} + \sigma_{s2}\right) L_2 = 3.84 \tag{7}$$

The external radiation was considered as $F_1 = 0.3$ and $F_2 = 1.0$ in Eqs. (1b) and (2c), respectively.

These properties were intentionally chosen equally to those considered in (Soeiro and Silva Neto, 2006), where the same problem is solved using the Levenberg-Marquardt method (LM, Marquardt, 1963) and a hybridization of the Simulated Annealing method (SA, Kirkpatrick *et al.*, 1983) with LM (SA-LM).

The LJ was set with $n_{in} = n_{out} = 100$, $\varepsilon = 0.05$ and the search space was considered [0,1] for all unknowns. All LJ runs were performed on a PC with the processor AMD Turion™ 63 X2 Mobile (1.60 GHz with 1.37 GB of RAM).

Starting with the initial guess

$$\vec{Z}^0 = \left\{\sigma_{s1}^0, \kappa_{a1}^0, \sigma_{s2}^0, \kappa_{a2}^0\right\}^T = \{0.18,\, 0.93,\, 0.30,\, 0.81\}^T \tag{8}$$

neither the LM nor the hybridization SA-LM converge, as shown in Tables 2 and 3.

Table 2. Results obtained with the LM using only external detectors. $\sigma_e = 0.002$ (5%)
(Soeiro and Silva Neto, 2006)

Iteration	σ_{s1}	κ_{a1}	σ_{s2}	κ_{a2}	$Q(\vec{Z})$
0	0.18	0.93	0.30	0.81	1.94E-01
10	0.0284	0.0404	22.77	9.23	4.10E-02
20	0.0	0.0	115.31	115.51	1.40

Table 3. Results obtained with the hybridization SA-LM using only external detectors. $\sigma_e = 0.002$ (5%).
(Soeiro and Silva Neto, 2006)

Iteration	σ_{s1}	κ_{a1}	σ_{s2}	κ_{a2}	$Q(\vec{Z})$
0	0.928	0.599	0.923	0.294	5.16E-04
5	0.519	0.346	0.995	0.331	5.19E-05
10	0.519	0.346	0.995	0.331	5.19E-05

In Table 4 are presented the results obtained with the LJ in 10 independent runs. It is also shown the average, μ_Z, the standard deviation, σ_Z, and the CPU time. The last run started with the initial guess in Eq. (8), the others started with random initial guesses in the search space. It can be seen that even though the average of the runs led to estimates that are very close to the exact values, the standard deviation is relatively high, what happens because the estimates are not accurate. The unknown κ_{a2} was the only one that was able to be well recovered in all runs.

Table 4. Results obtained with the LJ using only external detectors. $\sigma_e = 0.002$ (5%)

# Run	$\sigma_{s1} = 0.8$	$\kappa_{a1} = 0.5$	$\sigma_{s1} = 0.9$	$\kappa_{a2} = 0.3$	$Q(\vec{Z})$	CPU Time (min)
1	0.846	0.514	0.916	0.303	6.61E-05	120.7
2	0.735	0.448	0.936	0.311	8.25E-05	126.4
3	0.600	0.387	0.980	0.326	7.72E-05	118.2
4	0.932	0.548	0.898	0.297	3.60E-05	114.1
5	0.976	0.617	0.810	0.273	5.41E-05	116.6
6	0.816	0.518	0.886	0.294	3.47E-05	118.8
7	0.679	0.438	0.936	0.312	3.51E-05	118.9
8	0.676	0.442	0.940	0.311	5.46E-05	118.0
9	0.704	0.460	0.936	0.311	5.92E-05	115.8
10	0.922	0.538	0.903	0.299	1.05E-04	114.8
μ_z	0.789	0.491	0.914	0.304		
σ_z	0.128	0.068	0.045	0.014		
$\frac{\mu_z}{\sigma_z}\times 100\%$	16.3%	13.8%	5.0%	4.7%		

In Fig. 5, the same results of Table 4 are shown in graphics. The confidence bounds have been included.

As the sample size is relatively small (10 runs), the confidence bounds have been calculated based on the Student's T distribution as

$$\left(\mu_Z - t_{(n-1),(1-C)} \times \frac{\sigma_Z}{\sqrt{n}}, \mu_Z + t_{(n-1),(1-C)} \times \frac{\sigma_Z}{\sqrt{n}}\right) \tag{9}$$

where $t_{(n-1),(1-C)}$ is the critical value for the Student's T distribution with n data points, i.e., $n-1$ degrees of freedom, and C% confidence. For this case, we have 10 runs, i.e. $n=10$. Considering 99% confidence, $t_{(n-1),(1-C)} = t_{(9),(0.01)} = 3.250$.

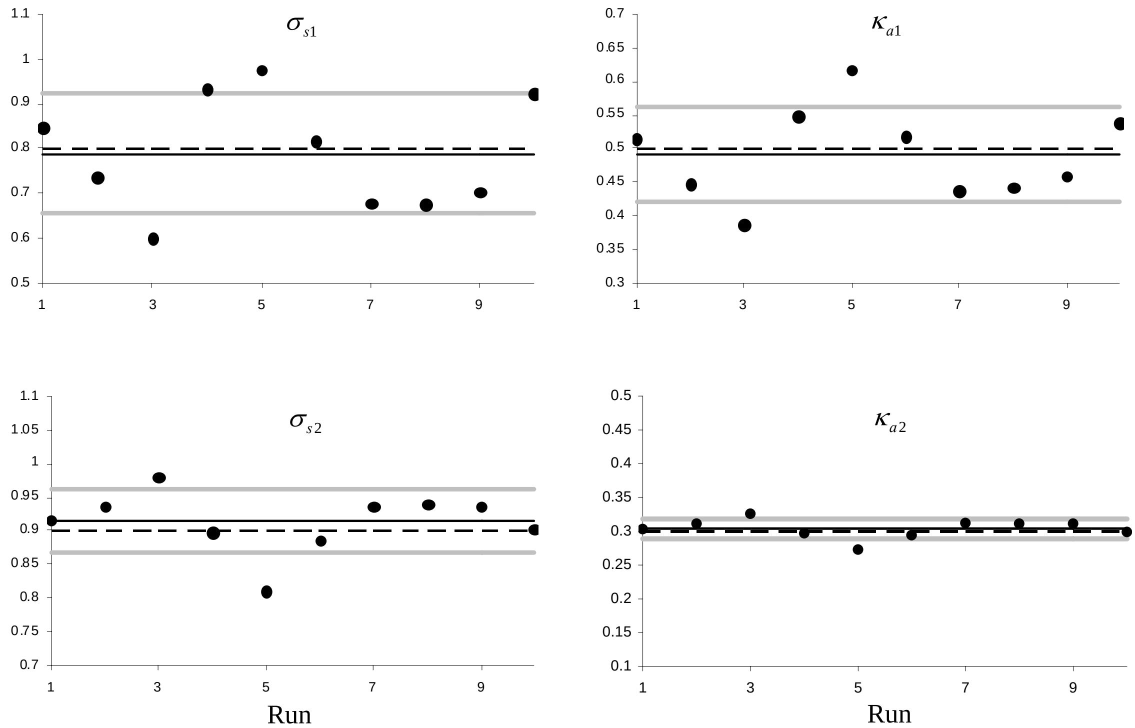

Figure 5. Results obtained with the LJ using only external detectors. $\sigma_e = 0.002$ (5.0%).
______ , average; _ _ _ _ _ _ _ , exact values; ________ , confidence bounds; • , estimates.

In Fig. 5 it is clear that, with exception of κ_{a2}, all the confidence bounds are relatively wide, i.e., the estimates are not accurate. Nevertheless, the performance of LJ for this test case with $\sigma_e = 0.002$ was better then the performance of LM and the hybridization SA-LM (Tables 2 and 3, respectively).

In Tables 5 and 6 are presented the results obtained with the hybridization SA-LM and with the LJ, respectively, considering external and internal detectors, for the same situation $\sigma_e = 0.002$ (errors up to 5%). The hybridization SA-LM and the last run of LJ started with the initial guess in Eq. (8). The other runs of the LJ started with random initial guesses in the search space.

Table 5. Results obtained with the hybridization SA-LM using external and internal detectors. $\sigma_e = 0.002$ (5%). (Soeiro and Silva Neto, 2006)

Iteration	σ_{s1}	κ_{a1}	σ_{s2}	κ_{a2}	$Q(\vec{Z})$
0	0.928	0.599	0.923	0.294	3.38E-03
5	0.7938	0.4988	0.8940	0.297	8.96E-05
10	0.7938	0.4988	0.8940	0.297	8.96E-05

Table 6. Results obtained with the LJ using external and internal detectors. $\sigma_e = 0.002$ (5%)

# Run	$\sigma_{s1} = 0.8$	$\kappa_{a1} = 0.5$	$\sigma_{s1} = 0.9$	$\kappa_{a2} = 0.3$	$Q(\vec{Z})$	CPU Time (min)
1	0.816	0.504	0.899	0.300	1.35E-04	111.8
2	0.788	0.502	0.891	0.298	7.15E-05	111.9
3	0.792	0.499	0.893	0.300	1.17E-04	111.8
4	0.809	0.504	0.893	0.299	1.05E-04	111.7
5	0.808	0.500	0.894	0.300	1.53E-04	111.8
6	0.802	0.500	0.900	0.298	1.06E-04	111.9
7	0.788	0.504	0.897	0.299	1.45E-04	114.2
8	0.783	0.497	0.913	0.301	1.08E-04	117.2
9	0.812	0.495	0.891	0.301	2.04E-04	118.1
10	0.797	0.501	0.895	0.298	1.16E-04	122.4
μ_z	0.800	0.501	0.897	0.299		
σ_z	0.012	0.003	0.007	0.001		
$\frac{\mu_z}{\sigma_z} \times 100\%$	1.4%	0.6%	0.7%	0.4%		

In Fig. 6, the results of Table 6 are shown in graphics. The confidence bounds have been calculated with Eq. (9). In this case, when external and internal detectors are used, it can be seen that all the 10 runs yielded good estimates and the confidence bounds are much narrower.

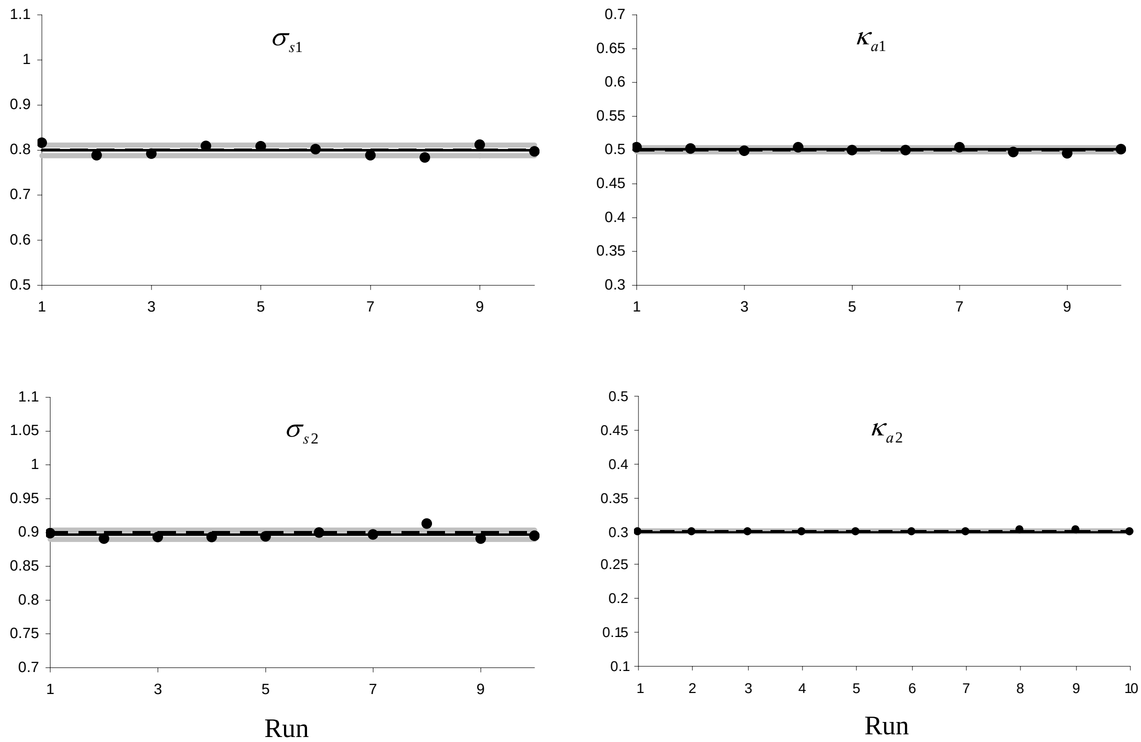

Figure 6. Results obtained with the LJ using external and internal detectors. $\sigma_e = 0.002$ (5.0%).
______ , average; - - - - - - - , exact values; ________ , confidence bounds; • , estimates.

When external and internal detectors are used, both the hybridization SA-LM and the LJ were able to recover all unknowns of the inverse problem.

6. CONCLUSIONS

From the results presented in this work, it can be concluded that the LJ, despite its simplicity, yields good estimates for the inverse radiative transfer problem for the estimation of the scattering and absorption coefficients in a two-layer plane-parallel medium. Even when only external detectors are used (and consequently non-uniqueness of the solution arises), the averages of the runs are close to the exact values of the unknowns (obviously with relatively wide confidence bounds).

7. ACKNOWLEDGEMENTS

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