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New developments on reconstruction of high resolution chlorophyll-a vertical profiles

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Abstract: *We present a methodology to reconstruct vertical profiles of chlorophyll-a pigment concentration in open-ocean waters based on radiance values at different depths. The inverse problem is formulated here as an optimization problem and iteratively solved by an Ant Colony System (ACS) meta-heuristic. An objective function is given by the square difference between computed and experimental radiances at each iteration. The Laplace transform discrete ordinate (LTSN) method is used to solve the radiative transfer equation (direct problem) in order to compute the radiances. In a first approach, this methodology was not able to reconstruct profiles with two or more peaks of chlorophyll-a concentration. This result can be partially explained by the relatively low number of sampling points (11 points), that limits the geometric resolution of the vertical profile to be reconstructed. Alternatively, we propose the reconstruction vertical profile using a higher geometric resolution, lower than one meter, in order to evaluate the ability of identifying any peak in chlorophyll-a concentration. A hybrid methodology is adopted: initially, the original inverse ACS methodology is employed to retrieve a high resolution profile (81 points), and then this result is used as an initial guess for the deterministic method of optimization Levenberg-Marquardt to refine the profile.*

Keywords: *radiative transfer equation, ant colony system, Levenberg-Marquardt, hydrologic optics, chlorophyll-a profile*

1 Introduction

The direct radiative transfer problem in hydrologic optics involves the determination of the radiance distribution in a body of water, given the boundary conditions, source term, inherent optical properties, as the absorption a and scattering b coefficients, and the scattering phase function. The corresponding inverse radiative transfer problem arises when physical properties, internal light sources and/or boundary conditions must be estimated from radiometric measurements of the underwater light field.

In this work, the inverse model is an implicit technique for function estimation from synthetic radiometric measurements in several depths and single wavelength. The algorithm is formulated as a constrained nonlinear optimization problem, in which the direct problem is iteratively solved for successive approximations of the unknown parameters. Iteration proceeds until an objective

function, representing the least-square fit of model results and experimental data added to a regularization term, converges to a specified small value.

The RTE is solved by the Laplace transform discrete ordinate (LTS_N) method [1, 7, 8]. The associated optimization problem is solved by an Ant Colony System (ACS) [3] implementation. A intrinsic regularization scheme that pre-selects candidate solutions based on their smoothness is applied, quantified by a Tikhonov norm [11]

It is proposed a hybrid inversion scheme, where the ACS solution provides an initial guess to the deterministic Levenberg-Marquardt (L-M) method. The spatial domain is discretized in a number of regions (R). The coefficients and thus the chlorophyll-a concentration are assumed as being constant in each region. The discrete chlorophyll-a profile is then defined by $(R+1)$ points.

For a low vertical resolution (ie, $R+1=11$ levels of depth), the ACS was not able to identify some details of the chlorophyll-a profile. Better results for the ACS inversion are then obtained using a higher resolution (ie, $R+1=81$ levels of depth) in the discrete vertical domain. However, depending on the choice of the step-size for the finite-difference method, the aftwerwards application of the L-M inversion did not improve the profiles reconstructed by the ACS using 11 or 81 levels of depth, as previouly showed in [9].

2 Radiative transfer equation in hydrologic optics

The Radiative Transfer Equation (RTE) models the transport of photons through a medium. Light intensity is given by a directional quantity, the radiance I, that measures the rate of energy being transported at a given point and in a given direction. Considering a horizontal plane, this direction is defined by a polar angle μ (relative to the normal of the plane) and a azimuthal angle φ (a possible direction in that plane). At any point of the medium, light can be absorbed, scattered or transmitted, according to the coefficients a and b and to a scattering phase function that models how light is scattered in any direction. An attenuation coefficient c is defined as $c=a+b$ and the geometrical depth is mapped to a optical depth τ that imbeds c. Assuming a plane-parallel geometry, and a single wavelength, the unidimensional integral-differential RTE, can be written as:

$$\mu\frac{\partial}{\partial\tau}I(\tau,\mu,\varphi)+I(\tau,\mu,\varphi)=\frac{\varpi_0(\tau)}{4\pi}\int_{-1}^{1}\int_{0}^{2\pi}\beta(\mu,\varphi;\mu',\varphi')I(\tau,\mu',\varphi')d\varphi'd\mu'+S(\tau,\mu,\varphi) \quad (1)$$

where $\mu\in[-1,1]$ and $\varphi\in[0,2\pi]$ are the cosine of the incident polar angle θ and the incident azimuthal angle, respectively. $\varpi_0(\tau)=b(\tau)/c(\tau)$ is the single scattering albedo. The scattering phase function $\beta(\mu,\varphi;\mu',\varphi')$, gives the scattering beam angular distribution, mapping the incident beam direction (μ,φ) to the scattered direction (μ',φ'), and the source term is $S(\tau,\mu,\varphi)$. The heterogeneous medium, in this case offshore ocean water is then modeled as a set of R homogeneous parallel finite layers with boundary conditions between layers. Each layer is denoted as being a region r of themultiregion domain:

There are several resolution methods, most of them adopting the Chandrasekhar's decomposition on the azimuthal angle [2] that generates $L+1$ integral-differential equations, each one with no dependence on φ. For the discrete ordinate method, the above equations are approximated by a colocation method, where the μ integral is computed by the Gauss-Legendre quadrature formula. This yields a set of N differential equations for each azimuthal mode. Each set (discretized RTE) is solved by the LTS_N method, that generates a system of equations of order $(R+1)\times N$. For the considered test cases, it was assumed $R=10$ and $R=80$, with $N=20$ and $L=0$ (azimuthal simmetry on φ).

This work employs bio-optical models that correlate coefficients (a) and (b) of each region to he chlorophyll concentration. These coefficients are assumed to be constant in each region. Therefore discrete values ar and br can be estimated for each region from the discrete values C_r.

The adopted bio-optical model for the absorption coefficient was formulated by [6]:

$$a_r = \left[a^w + 0.06\ a^c\ C_r^{0.65}\right]\ \left[1 + 0.2\ e^{-0.014(\lambda - 440)}\right] \tag{2}$$

where a^w is the pure water absorption and a^c is a nondimensional, statistically derived chlorophyll-specific absorption coefficient, and λ is the considered wavelength. The adopted bio-optical model for the scattering coefficient was formulated by [4]:

$$b_r = \left(\frac{550}{\lambda}\right)\ 0.30\ C_r^{0.62} \tag{3}$$

3 Inversion scheme

This work formulates the inverse problem according to an implicit approach, leading to an optimization problem. the set of parameters to be estimated, is given by $\boldsymbol{p}$, in this case, the $R+1$ discrete values of the chlorophyll concentration C at optical depths τ taken at the interface of the regions. Thus $p_r = C(\tau_r)$ for $r = 0, 1, ..., R$.

Experimental data are the discrete radiances $I(\tau_r, \mu_i)$ for $r = 0, 1, ..., R$ and $i = 1, 2, ..., N$. The objective function $J(\boldsymbol{p})$ is given by the square difference between experimental and model radiances plus a regularization term:

$$J(\boldsymbol{p}) = \sum_{i=1}^{N} \sum_{r=0}^{R} \left[I^{exp}(\tau_r, \mu_i) - I_{\boldsymbol{p}}(\tau_r, \mu_i)\right]^2 + \ \gamma\, \Omega(\boldsymbol{p}) \tag{4}$$

The $R+1$ discrete values of the concentration are estimated from $(R+2) \times N$ radiance values. $\Omega(\boldsymbol{p})$ is the regularization function, that is weighted by the 2nd order Tikhonov regularization parameter γ:

$$\Omega[\boldsymbol{p}]\ =\ \sum_{i=2}^{R-1} \left(p_{i+1} - 2p_i + p_{i-1}\right)^2\ . \tag{5}$$

The regularization term is required for noisy data due to the ill-posedness nature of inverse problems. The influence of radiance data of higher depths can be underestimated since radiances decay nearly exponentially with depth. Therefore, a depth correction factor may be used in the objective function (4). This correction factor is given by the ratio between the mean radiance related to the polar angle at each vertical level and the mean radiance at the surface. This is done separately for upward and downward polar directions.

4 Results

Chlorophyll-a concentration was measured on the Brazilian coast using a sensor for natural fluorescence (PNF, Biospherical instruments), on board of the oceanographic campaing at the fall 2003 [10]]. The radiative transfer problem is considering $N = 20$ polar angles and $L = 0$ (azimuthal symmetry). In this test case, synthetic data was used to simulate the experimental radiance values, but this data was corrupted with 1%, 2% and 5% Gaussian noise.

The inverse solver, based on a ACS implementation, was tested for this offshore ocean water. Instead of the *classical* regularization, the smoothness-based pre-selection was employed in the generation of the ants. The 2nd order Tikhonov norm was used as smoothness criterion. Figure 1(a) shows the inverse solution obtained from a realization of the ACS for a 11-depths vertical resolution profile (called ACS_{11}), using **5% noisy** radiance data. It was not able to identify the two peaks of the exact chlorophyll-a profile. As is illustrated in Figure 1(b), a improved solution is reached applying the Levenberg-Marquardt deterministic method (called L-M_{11}), with ACS_{11} solution as its initial guess.

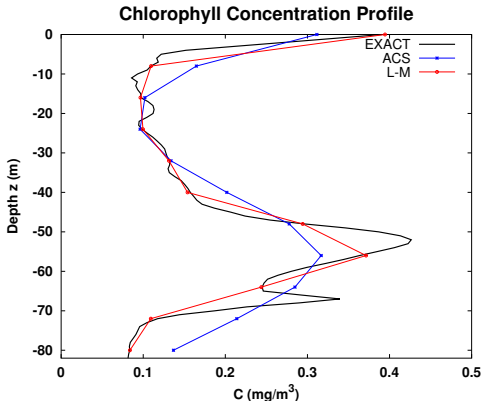
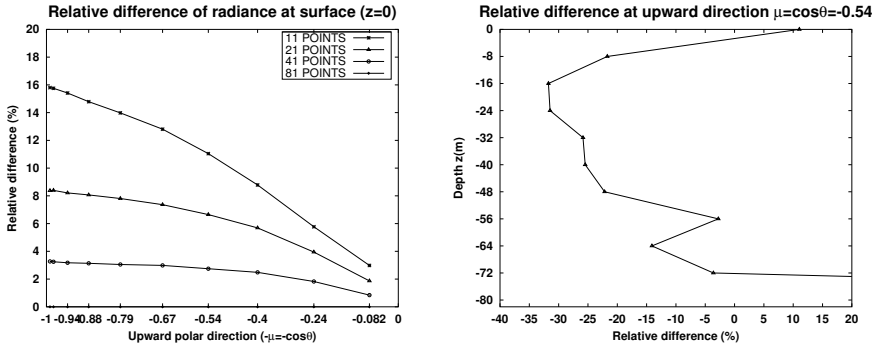


Figure 1: Reconstruction of the 11 depths chlorophyll-a vertical profile obtained with Levenberg-Marquardt (L-M_{11}), with ACS_{11} as initial guess, from **5% noisy** radiance data.



(a) (b)

Figure 2: Relative difference between radiances:
(a) at surface (z=0), generated with 11, 21 and 41 points, compared to 81 levels resolution.
(b) between radiances generated with 11 and 81 points, for polar upward direction $\mu = cos\theta = -0.54$. At z = 80m (out of figure), this difference is near 178%

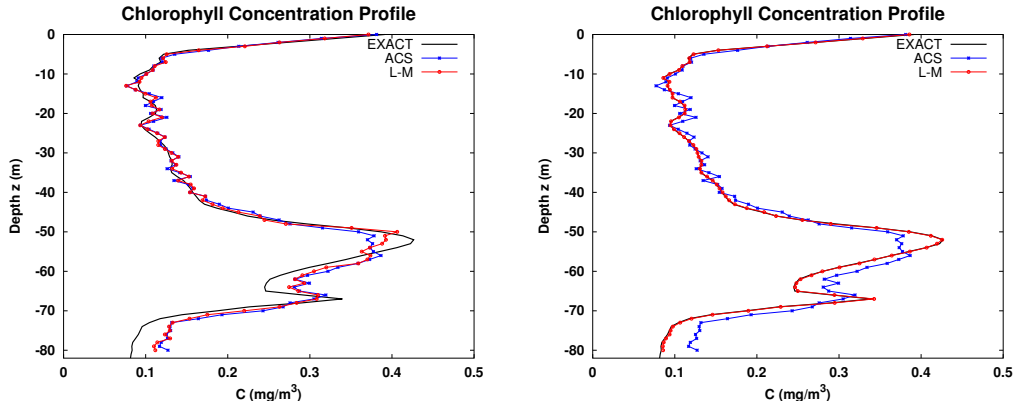
4.1 Higher resolution profile

However, although the solution in each 11 depths have values very close to exact solution, the amount of points adopted to form the vertical profile of the solution is not enough to identify two peaks of concentration.

Another limitation when adopting low-resolution refers to the modeling error that is being added to the radiance generated. To illustrate this, Figure 2 shows the percentage error between the radiance values calculated by LTSN model with a resolution of 11 vertical levels, compared with the values in these same points, but with a resolution of 81 levels deep.

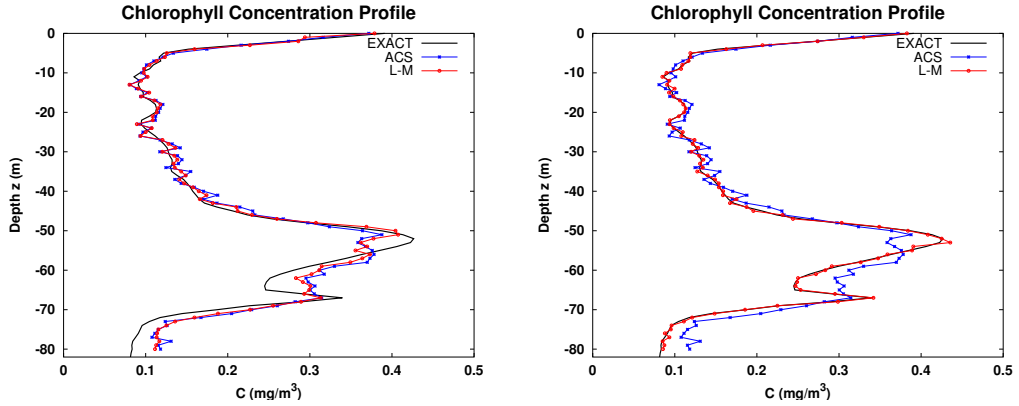
Although we have no available field measurements of radiance data for this vertical profile, we take as true the hypothesis that the higher the resolution adopted, the model generates radiances closer to the real value. Consequently, a lower resolution implies radiances farther from the truth. Therefore, when dealing with observed data, it is strongly recommended to be used the highest resolution possible. We decided to recover the concentration values of chlorophyll-a in each meter of the profile depth, ie, in 81 levels deep.

For noiseless data, at this higher resolution, as seen in Figure 6(a) the result obtained in ACS was able to identify the two maximum concentration with reasonable accuracy. However, it also shows that L-M was not able to find the exact position of these peaks, as could be expected. This is due the relatively small value of step-size (h) used for obtaining first derivative by forward



(a) (b)

Figure 3: Reconstruction of the 81 depths chlorophyll-a vertical profile, obtained with Levenberg-Marquardt (L-M), with ACS as initial guess, from **noiseless** radiance data:
(a) finite difference step-size is $h = 10^{-9}$ for L-M
(b) finite difference step-size is $h = 10^{-6}$ for L-M



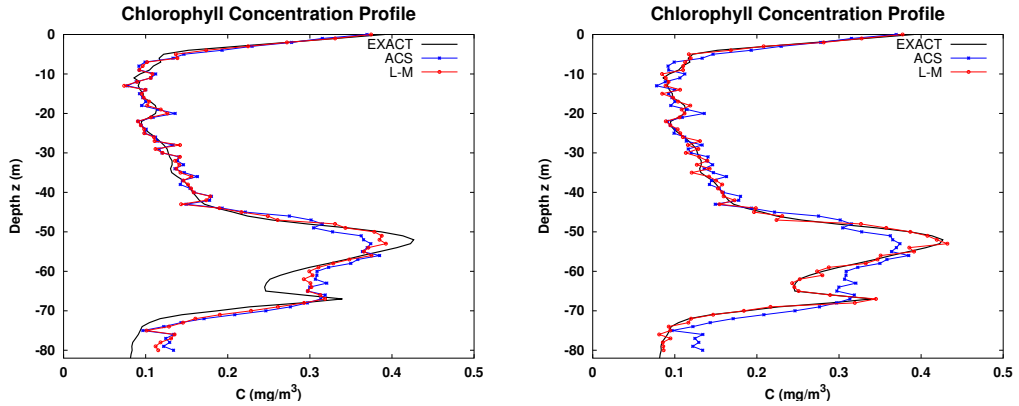
(a) (b)

Figure 4: Reconstruction of the 81 depths chlorophyll-a vertical profile, obtained with Levenberg-Marquardt (L-M), with ACS as initial guess, from **1% noisy** radiance data:
(a) finite difference step-size is $h = 10^{-9}$ for L-M
(b) finite difference step-size is $h = 10^{-6}$ for L-M

differences approximation in the L-M algorithm (Eq. 6).

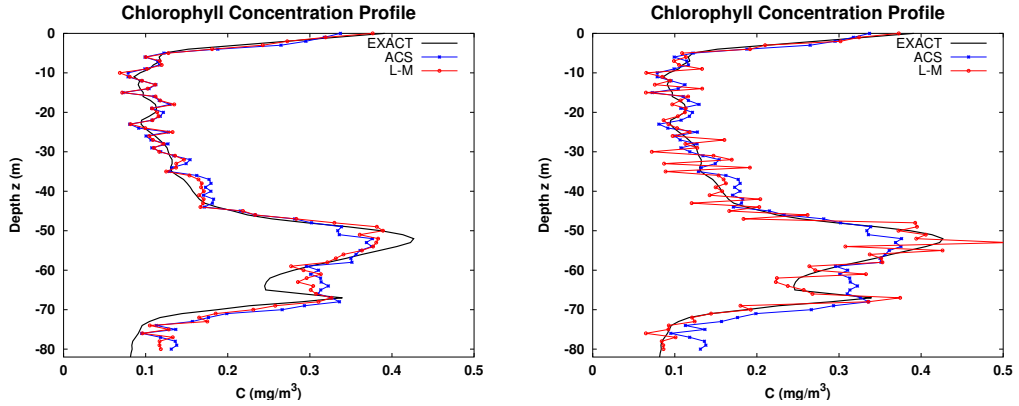
$$f'(x) = \frac{f(x+h) - f(x)}{h} \tag{6}$$

Indeed, the choice of a suitable step-size parameter (h) is essential for gradient-based optimization methods [5], like Levenberg-Marquardt. A trial-and-error approach resulted in a value of $h = 10^{-6}$. As shown in Figure 6(b), the resulting profile is very close to the exact solution. Although we know that the step-size depends on the objective function and hence the noise embedded in the data, we decided to test the same value of step-size for radiance data with 1%, 2% and 5% of noise. As expected, the results for 1% and 2% are not as good as the noiseless one. Nevertheless, can also be observed that there is a good improvement in the quality of solution achieved when it is compared with the result obtained with step-size equal to $h = 10^{-9}$ On the other hand, the results achieved through the use of 5% noisy data was much worse than the previous. The inverse problem becomes increasingly ill-posed with the increase of the noise,



(a) (b)

Figure 5: Reconstruction of the 81 depths chlorophyll-a vertical profile, obtained with Levenberg-Marquardt (L-M), with ACS as initial guess, from **2% noisy** radiance data:
(a) finite difference step-size is $h = 10^{-9}$ for L-M
(b) finite difference step-size is $h = 10^{-6}$ for L-M



(a) (b)

Figure 6: Reconstruction of the 81 depths chlorophyll-a vertical profile, obtained with Levenberg-Marquardt (L-M), with ACS as initial guess, from **5% noisy** radiance data:
(a) finite difference step-size is $h = 10^{-9}$ for L-M
(b) finite difference step-size is $h = 10^{-6}$ for L-M

especially for this problem with a high number of points. Recall that for the case with only 11 points, this noise level was no impediment for a good recovery to be achieved. In addition to that the L-M method implemented does not use any regularization, as the one used in ACS method.

5 Final remarks

This work presented an inverse methodology for enhancing the estimation of the vertical profile of chlorophyll-a concentration in natural waters from radiance data in different depths. The ACS-based inverse solver yielded an initial estimation of the chlorophyll vertical profile using a depth correction factor for the input radiances for the test cases with noiseless and noisy radiance data. The objective function did not require a standard regularization term, since a pre-regularization scheme was employed.

Considering a profile with 11 levels of depth, even the hybrid inversion approach (Ant Colony

System + Levenberg-Marquardt) was not able to reconstruct a profile identifying the two peaks of concentration of chlorophyll-a of the original profile. Therefore, a vertical profile with 81 levels of depth (1-meter resolution) allowed the reconstruction of the concentration profile with the two peaks with the sole use of the ACS inversion.

It was expected that the hybrid inversion approach with these 81 levels of depth would result in a more accurate reconstruction of the profile. However, this was not the case. It can be concluded that this requires further sensitivity analysis of the objective function for each level of noise in the data. The step-size of the finite-difference method was defined by a trial-and-error scheme and yielded good results using noiseles data. For data with up to 2% the result achieved was not as good, but most of the profile points was recovered. The worst result was for the profile with 5% of noise, since it was not able to reconstruct none part of this profile. In a future work, we intend to develop an adpative scheme for deriving the optimal step-size for each level of noise.

References

[1] L. B. Barichello and M. T. Vilhena. A general approach to one-group one-dimensional transport equation. *Kerntechnik*, 58(3):182–184, 1993.

[2] S. Chandrasekhar. *Radiative transfer*. Dover, New York, 1960.

[3] M. Dorigo, V. Maniezzo, and A. Colorni. The ant system: optimization by a colony of cooperating agents. *IEEE Transactions on Systems, Man, and Cybernetics–Part B*, 26(2):29–41, 1996.

[4] H. R. Gordon and A. Morel. Remote assessment of ocean color for interpretation of satellite visible imagery, a review. In *Lectures Notes on Coastal Estuarine Studies*, page 114. Springer-Verlag, New York, 1983.

[5] J. Iott, R. T. Haftka, and H. M. Adelman. Selecting step sizes in sensitivity analysis by finite differences. *NASA Technical Memorandum*, 86382, 1985.

[6] A. Morel. Light and marine photosynthesis: a spectral model with geochemical and climatological implications. *Progress in Oceanography*, 26(3):263–306, 1991.

[7] C. F. Segatto and M. T. Vilhena. Extension of the ltsn formulation for discrete ordinates problem without azimuthal symmetry. *Annals of Nuclear Energy*, 21(11):701–710, 1994.

[8] C. F. Segatto, M. T. Vilhena, and M. G. Gomes. The one-dimensional ltsn solution in a slab with high degree of quadrature. *Annals of Nuclear Energy*, 26(10):925–934, 1999.

[9] R. P. Souto, P. L. Silva Dias, H. F. CamposVelho, S. Stephany, and M. Kampel. Reconstruction of chlorophyll-a vertical profiles with enhanced resolution. In *Proceedings of 10th World Congress on Computational Mechanis*, São Paulo, 2012.

[10] R. P. Souto, M. Kampel, F. Brandini, H. F. CamposVelho, and S. Stephany. Análise comparativa de medições in situ e orbital de radiâncias do oceano na estimativa de concentração de clorofila-a. In *Anais do XII Simpósio Brasileiro de Sensoriamento Remoto*, pages 3679–3686, São José dos Campos, 2005.

[11] S. Stephany, J.C. Becceneri, R.P. Souto, H.F. de Campos Velho, and A.J. Silva Neto. A pre-regularization scheme for the reconstruction of a spatial dependent scattering albedo using a hybrid ant colony optimization implementation. *Applied Mathematical Modelling*, 34(3):561–572, 2010.

