

Reconstruction of Chlorophyll Concentration Profile in Offshore Ocean Water using Ant Colony System

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Abstract.

An inverse hydrologic optics problem is solved using a recent intrinsic regularization scheme coupled to a standard Ant Colony System (ACS). The regularization scheme pre-selects candidate solutions based on their smoothness, quantified by a Tikhonov norm. The Chlorophyll profile is reconstructed from radiance experimental measurements in the ocean water for several depths and single wavelength. Vertical profiles of the absorption and scattering coefficients are estimated from the Chlorophyll profile by means of bio-optical models. The inverse problem is formulated as an optimization problem and iteratively solved by an ACS using the radiative transfer equation as direct model. An objective function is given by the square difference between computed and experimental radiances at every iteration. Each candidate solution corresponds to a discrete Chlorophyll profile. The radiative transfer equation is solved using the Laplace transform discrete ordinate (LTSN) method. A parallel implementation of the Ant Colony System is used and executed in a distributed memory machine. Test results show the suitability of the proposed method.

1 INTRODUCTION

In the last decades, the development of inversion methodologies for radiative transfer problems has been an important research topic in many branches of science and engineering [16, 13]. The direct or forward radiative transfer problem in hydrologic optics, in the steady state, involves the determination of the radiance distribution in a body of water, given the boundary conditions, source term, inherent optical properties (IOPs), 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 previous works, we tried to establish a general methodology to separately tackle the reconstruction of internal

sources [29], IOP estimation [30, 8, 9, 10], the identification of boundary conditions [5, 7, 24], or even a joint inversion scheme [30]. In these works, the inverse model is an implicit technique for parameter and/or function estimation from “in situ” (local) radiometric measurements. 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. An overview of this technique, as well as a survey of the results, can be found in Campos Velho et al. [4] or [6].

This work presents a methodology to reconstruct vertical profiles of the absorption and scattering coefficients in natural waters from *in-situ* radiance measurements in several depths and single wavelength. The inverse problem is iteratively solved using the radiative transfer equation (RTE) as direct model. A former work [30] employed a step-by-step reconstruction methodology, estimating a and b in an alternate manner. A deterministic optimizer was employed to solve the associated inverse problem. In the current work, bio-optical models [17] are employed to correlate the Chlorophyll concentration to a and b . At every iteration, the inverse solver generates a candidate solution that is a set of discrete Chlorophyll concentration values. The inverse problem is formulated as an optimization problem and iteratively solved using the radiative transfer equation as direct model. An objective function is given by the square difference between computed and experimental radiances at every iteration.

At each iteration, the RTE is solved using the candidate set of a and b values by the Laplace transform discrete ordinate (LTSN) method [1, 25, 26]. The associated optimization problem is solved by an Ant Colony System (ACS) [12] implementation. The main contribution of this work is to apply a recent intrinsic regularization scheme that pre-selects candidate solutions based on their smoothness, quantified by a Tikhonov norm. This scheme was proposed in a crystal growth inverse problem to reconstruct the diffusion coefficient [22]. A subsequent Chlorophyll candidate profile is generated and iterations proceed. As hundreds of iterations are typically demanded, a parallel implementation of the ACS is used and executed in a distributed memory machine. The code was parallelized using the Message Passing Interface (MPI) communication library [20]. The parallelization scheme distributes

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the pre-selected candidate solutions of the current iteration among the processors.

Test results show the suitability of the proposed method using noiseless and noisy data. The reconstructed profiles have good agreement to the exact curves. Parallel performance was also evaluated.

2 SOLVING THE RADIATIVE TRANSFER EQUATION

The Radiative Transfer Equation (RTE) models the transport of photons through a medium [27]. 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 absorption (a) and scattering (b) coefficients 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 an optical depth τ that imbeds c . Assuming a plane-parallel geometry, and a single wavelength, the unidimensional integral-differential RTE, can be written as:

$$\begin{aligned} \mu \frac{\partial}{\partial \tau} I(\tau, \mu, \varphi) + I(\tau, \mu, \varphi) = \\ \frac{\varpi_0(\tau)}{4\pi} \int_{-1}^1 \int_0^{2\pi} \Theta(\mu, \varphi; \mu', \varphi') I(\tau, \mu', \varphi') d\varphi' d\mu' \\ + S(\tau, \mu, \varphi) \end{aligned} \quad (1)$$

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 $\Theta(\mu, \varphi; \mu', \varphi')$, 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 finite layers. Boundary conditions are defined between regions, at the surface (incident light) and the bottom of the water. Each layer is denoted as being a region r of the multi-region domain:

$$\varpi_0(\tau) = \varpi_r \quad r = 1, 2, \dots, R \quad (2)$$

There are several resolution methods, most of them adopting the Chandrasekhar's decomposition on the azimuthal angle [11] that generates L integral-differential equations, each one with no dependence on φ . For the discrete ordinate method, the above equations are approximated by a collocation method, where the μ integral is computed by the Gauss-Legendre quadrature formula. This yields a set of N_μ differential equations for each azimuthal mode. Each set (discretized RTE) is solved by the LTSn method [1], that generates a system of equations of order $R \times N_\mu$. In the considered test cases, $R = 10$, $N_\mu = 50$ and there is no dependence on φ ($L = 1$).

This work employs a bio-optical models to correlate the absorption and scattering coefficients of each region to the

chlorophyll concentration. These coefficients are assumed to be constant in each region. Therefore discrete values a_r and b_r can be estimated for each region from the discrete values C_r .

Usually, chlorophyll profiles can be represented according Gaussian distributions [17]. A particular profile, corresponding to the Celtic Sea was considered:

$$C(z) = 0.2 + \frac{144}{9\sqrt{2}\pi} \exp \left[-\frac{1}{2} \left(\frac{z - 17}{9} \right)^2 \right] \quad (3)$$

where z is the depth in meters and C is given in mg/m^3 . This profile can be shown in section 6 of this work, termed *exact profile*. A bio-optical model was formulated by Morel [18] for the absorption coefficient,

$$a_r = [a^w + 0.06 a^c C_r^{0.65}] [1 + 0.2 e^{-0.014(\lambda - 440)}] \quad (4)$$

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, while another was a_g^w formulated by Gordon and Morel [14] for the scattering coefficient,

$$b_r = \left(\frac{550}{\lambda} \right) 0.30 C_r^{0.62} \quad (5)$$

The considered Celtic Sea profile refers to a type of water that present a high concentration of phytoplankton in comparison to organic particles [19]. The values of a^w and a^c depend on the wavelength and can be found in tables [17].

3 ANT COLONY SYSTEM

The Ant Colony System (ACS) is a method that employs a meta-heuristic based on the collective behaviour of ants choosing a path between the nest and the food source [12]. Each ant marks its path with an amount of pheromone and the marked path is further employed by other ants as a reference. As an example of this, the sequence in Fig. 1 shows how ants, trying to go from point A to point E (a), behave when an obstacle is put in the middle of the original path, blocking the flow of the ants between points B and D (b). Two new paths are then possible, either going to the left of the obstacle (point H) or to the right (point C). The shortest path causes a greater amount of pheromone to be deposited by the preceding ants and thus more and more ants choose this path (c).

In the ACS optimization method, several generations of ants are produced. For each generation, a fixed amount of ants (na) is evaluated. Each ant is associated to a feasible path and this path represents a candidate solution, being composed of a particular set of edges of the graph that contains all possible solutions. Each ant is generated by choosing these edges on a probabilistic basis. This approach was successfully used for the Traveling Salesman Problem (TSP) and other graph-like problems [2]. The best ant of each generation is then choosed and it is allowed to mark with pheromone its path. This will influence the creation of ants in the further generations. The pheromone put by the ants decays due to an evaporation rate. Finally, at the end of all generations, the best solution is assumed to be achieved.

A solution is composed of linking ns nodes and in order to connect each pair of nodes, np discrete values can be choosen.

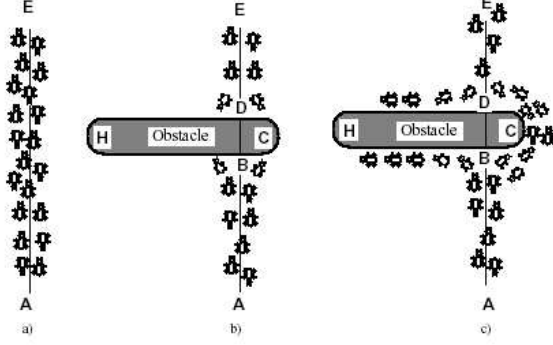


Figure 1. Ants overcoming an obstacle in the trail (from Dorigo et al [12]).

This approach was used to deal with a continuous domain. Therefore, there are $ns \times np$ possible paths $[i, j]$ available. Denoting by ρ the pheromone decay rate and τ_0 the initial amount of pheromone, the amount of pheromone τ_{ij} at generation t is given by:

$$\tau_{ij}(t) = (1 - \rho)\tau_{ij}(t) + \tau_0, \quad (6)$$

In this work, τ_0 is calculated as suggested in [3] using an evaluation Q of the function to be optimized obtained with a greedy heuristics:

$$\tau_0 = 1/(ns * Q), \quad (7)$$

The probability of a given path $[i, j]$ be choosed is then

$$P_{ij}(t) = \frac{[\tau_{ij}(t)]^\alpha [\eta_{ij}]^\beta}{\sum_l \{[\tau_{il}(t)]^\alpha [\eta_{il}]^\beta\}} \quad (8)$$

where $l \in [1, np]$ and η_{ij} is the visibility/cost of each path, a concept that arises from the TSP, where the cost is the inverse of the distance of a particular path. The above equation assumes that all paths are possible for any ant, but the TSP does not allow this assumption. The parameters α and β are weights that establish the trade-off between the influence of the pheromone and the visibility in the probability of each path.

However, there is a further scheme for the choice of a path for a new ant. According to a roulette, a random number in the range $[0, 1]$ is generated for the new ant and it is compared with a parameter q_0 chosen for the problem. If the random number is greater than this parameter, the path is taken according to P_{ij} . If not, the most marked path is assigned.

In the current work, the inverse problem is iteratively solved, being formulated as an optimization problem, solved by the parallel implementation of an ACS. The code was parallelized using calls to the Message Passing Interface (MPI) communication library [20]. At each iteration, candidate solutions are distributed among processors in order to be evaluated.

4 INVERSION SCHEME

This work formulates the inverse problem according to an implicit approach, leading to an optimization problem [15].

$\mathbf{p}$ is the set of parameters to be estimated, in this case, the R discrete values of the chlorophyll concentration C at optical depths τ taken at the upper interface of the regions. Thus $p_r = C(\tau_r)$ for $r = 0, 1, \dots, R - 1$. Experimental data are the discrete radiances $I(\tau_r, \mu_i)$ for $r = 0, 1, \dots, R$ and $i = 1, 2, \dots, N_\mu$. The objective function $J(\mathbf{p})$ is given by the square difference between experimental (exp) and model radiances plus a regularization term. As radiance intensity decays exponentially with depth, a depth correction factor (not shown here) must be employed to weight the influence of the depth-depend radiances [31]. The R discrete values of the concentration are estimated from $(R + 1) \times N_\mu$ radiance values.

$$J(\mathbf{p}) = \sum_{i=1}^{N_\mu} \sum_{r=0}^R [I^{exp}(\tau_r, \mu_i) - I\mathbf{p}(\tau_r, \mu_i)]^2 + \gamma \Omega[\mathbf{p}] \quad (9)$$

$\Omega[\mathbf{p}]$ is the regularization function, that is weighted by a regularization parameter γ . For instance, the 2nd order Tikhonov regularization [32] is defined by

$$\Omega[\mathbf{p}] = \sum_{i=2}^{R-1} (p_{i+1} - 2p_i + p_{i-1})^2 \quad (10)$$

The regularization term is required for noisy data due to the ill-posedness nature of inverse problems. Then, small changes in radiance data cause big changes in the concentration profile. There are some criteria for the choice of γ , but an optimal value can be difficult to adjust, as it requires a choice criteria (Morozov discrepancy principle, L-curve, etc. [5]) that may demand many executions of the inverse solver. A value too small may yield a profile with fluctuations, while the opposite makes the profile flat.

In the current work, a ACS based inverse solver with a recent implicit regularization scheme [22] is proposed and employed without the explicit regularization ($\gamma = 0$). Since here is an *a priori* information about the smoothness of the solution profile, such knowledge is included in the generation of the candidate solutions, by means of pre-selecting the smoother ants.

This information can be used as an alternative for the visibility η_{ij} of each path. First, an overpopulation of ants is generated, making $\alpha = 1$ and $\beta = 0$ in Equation 8 and after, a certain fraction containing the smoother ants/paths is selected. Thus the visibility is assumed to be associated to the smoothness of the path. The criteria choosen to select the paths according to the their smoothness was precisely the 2nd order Tikhonov norm, that is normally used as a regularization function. Actually, a kind of pre-regularization is performed, and the usual regularization term is not required.

It was difficult to find an ACS visibility/cost criteria in this problem since it does not belong to the TSP class and this issue lead to choice of the smoothness for the *ensemble* of paths of each ant. It can be shown that the ACS has poor performance compared to other stochastic optimization algorithms when no visibility information can be defined. In addition, the proposed strategy leads to a reduction of the number of evaluations of the objective function and therefore improves the performance since the direct model demands a significant amount of processing time.

5 PARALLELIZATION SCHEME

In the employed implicit approach, the inverse solver (the ACS) generates successive candidates solutions that are evaluated by the direct model (the LTSN solver). Two levels of parallelization can be devised, corresponding to the inverse and to the direct models, and it is possible to have both.

Concerning the parallelization of the LTSN solver, one or more dimensions (R , N_μ , L) can be chosen to divide the domain among processors. Data dependencies preclude the distribution among processors of radiance calculations according to polar angles or regions. Therefore, a straightforward approach is to assign to each processor a radiance calculations corresponding to a particular azimuthal angle, since each one can be independently computed. This was employed in a previous work [28] with good parallel performance. However, here, $L = 1$ and this scheme is not possible.

The inverse solver can also be parallelized. In the case of an evolutive algorithm, such as a genetic algorithms or ACS, most schemes divide the population in several sub-populations/colonies that evolve independently, except for the migration with specific policies and topologies (*island model*, *stepping-stone model*, etc.) [23]. An alternative, termed *global parallelization*, consider a single population/colony being evolved, but its individuals/ants distributed among processors, thus dividing the evaluation of the population. This scheme is adopted here. The ACS requires that the objective function (the RTE) be evaluated for the pre-selected ants. Therefore, each ant is assigned to a processor, that executes the LTSN solver.

According to the Amdahl's law [21], parallel performance of the code is limited by the sequential part of the code, that depends on the choice of the parallelization scheme. The parallel performance is usually evaluated by two quantities, the speed-up and the efficiency. Speed-up is the ratio of the sequential to the p -processor parallel execution time, while efficiency is defined as the speed-up divided by the number of processors p .

6 NUMERICAL RESULTS

Similarly to other stochastic optimization algorithms, the tuning of parameters in the ACS has a big influence in the results. This implementation required adjustment of parameters like ρ , the pheromone decay rate and q_0 , used in the roulette scheme. Other parameters may influence the quality of the solution, like the the number of np possible paths between each pair of the ns nodes, the number of ants na , or the maximum number of iterations mit . These values are shown in Table 1, and refer to the chosen test cases. In these cases, 15 was found as the minimum number of pre-selected ants that yield a good solution. The parallel inverse solver was tested for a

Table 1. Ant Colony System parameters

seed	ns	np	na	mit	ρ	q_0
33	10	3000	90	500	0.03	0.0

multi-region ($R = 10$) offshore ocean water radiative transfer problem with azimuthal symmetry using both noiseless and

noisy data. In the test cases, synthetic data was used to simulate the experimental values of the Celtic sea case, mentioned in section 2. No “classical” regularization was used ($\gamma = 0$), but smoothness-based pre-selection was performed in the generation of the ants using the 2nd order Tikhonov norm.

The reconstructed profiles shown good agreement with the exact solution. Figure 2 presents the exact Chlorophyll concentration profile and the reconstructed profiles from noiseless and 5% noisy data, using $na = 90$ and pre-regularization.

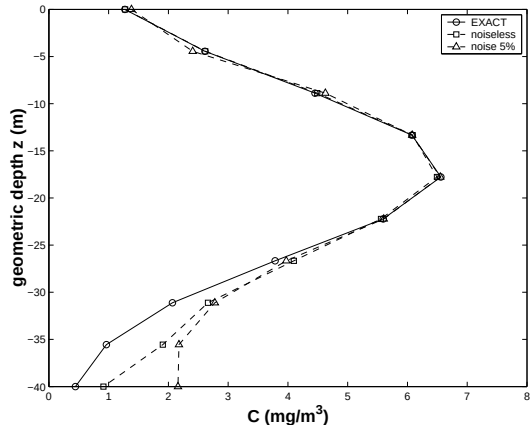


Figure 2. Exact Chlorophyll profile and reconstructed profiles using pre-regularization from noisy and noiseless data.

Figure 3 presents the same test case, using noiseless data, but comparing the reconstructed profiles for the proposed methodology (*pre-regularization*, $na = 90$) and for the ACS without regularization using $na = 15$ (15 ants, i.e. an equivalent number of evaluations of the objective function). Figure 4 presents the same test case, but using $na = 90$ for the ACS without regularization.

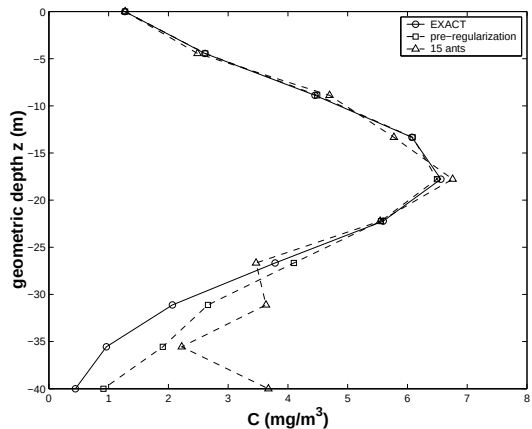


Figure 3. Exact Chlorophyll profile and reconstructed profiles with pre-regularization and without regularization (15 ants) from noiseless data.

Performance results are shown in Table 2. It can be noted

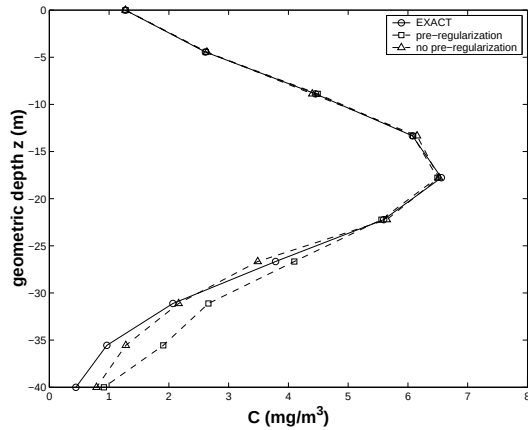


Figure 4. Exact Chlorophyll profile and reconstructed profiles with pre-regularization and without regularization (90 ants) from noiseless data.

that the efficiency decays as the number of processors increase. This is due to the time spent in the sequential part of the code, that remains constant, as the time of the parallel part tends to decay with the increase of the number of processors. Better values can be expected without azimuthal symmetry, since the fraction of time corresponding to the parallel part increases. These results were obtained for a population of 90 ants, but the pre-regularization reduces the number of evaluations since only 15 of these ants are selected at every interaction/generation of the ACS. In the usual scheme, the 90 ants have to be evaluated and the sequential time of the reconstruction is 2323.05 seconds, or 3 times the sequential time that appears in that table (756.98 seconds). The time did not scaled down by 6 times (or 90/15) as the evaluation of the ants represents only a part of the total execution time.

Table 2. Speed-up and efficiency for p processors

p	Time (s)	Speed-up	Efficiency
1	756.98		
3	286.78	2.64	0.880
5	202.20	3.74	0.749
15	118.53	6.38	0.426

7 FINAL REMARKS

This work presents an innovative application of a recent inverse methodology. The inverse solver employed a modified meta-heuristics, that combines a standard ACS algorithm and an intrinsic regularization. Concerning the direct model, the RTE was solved by the LTSN method. A pre-regularization scheme was applied to the ACS in order to include *a priori* information in the generation/selection of the ants. This scheme was used in a previous work [22] in which no good results were obtained with the usual regularization scheme, i.e., the objective function as given by equation 9. In the test cases presented here, results that present good agreement with the

exact solution were obtained using the proposed method. In the case of the standard scheme, the ACS without regularization, good reconstructions are also obtained, but the inverse solutions are less smoother than the proposed ACS. This feature is magnified in the presence of noise in the data. In addition, the proposed scheme significantly reduced the processing time, as fewer evaluations of the objective function had to be performed. This is a very important point in inverse problems, as typically thousands or millions of iterations may be demanded. The ACS with an usual regularization scheme also reconstructed the profile from noisy data. However, this demands to find out the regularization parameter γ . Perhaps the most interesting aspect of the proposed scheme is that γ is not required.

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