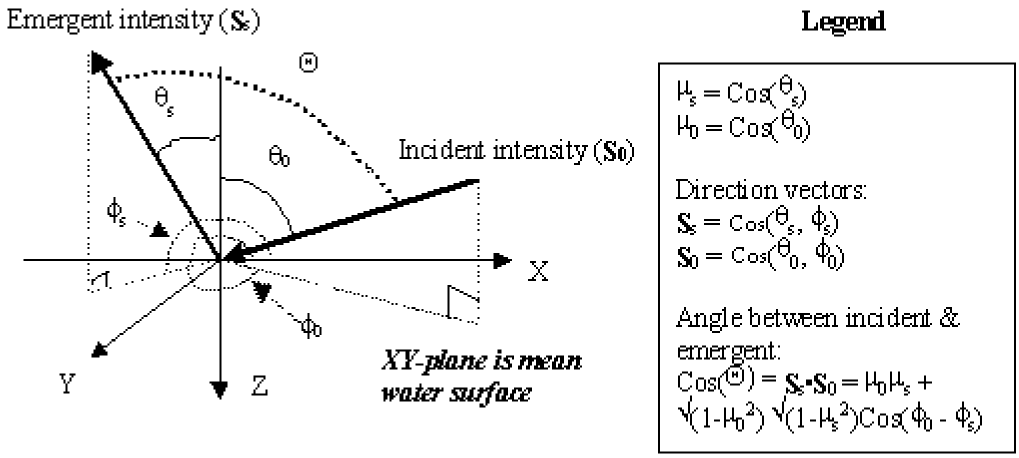
Abstract
We consider the one-dimensional case of radiative transfer in a plane-parallel (semi-infinite) medium. There are two aspects of interest, namely the direct and inverse problems. In the direct problem, physical parameters characterizing the medium are taken as given, certain boundary conditions are assumed for the sources of radiation, and the radiation field in the medium is sought. This paper is concerned with the inverse problem, in which the radiative field is assumed known and it is desired to infer values for the parameters that characterize the medium. The inverse problem is important in remote sensing and, indeed, an eventual objective of the present research is to enable properties of inland water bodies to be inferred from measurements made by airborne instruments. A model is formulated based on a classical solution for the emergent radiation from a medium (part of the direct problem solution), and the model parameters are estimated by a non-linear regression method.

1. Formulation



<u>Figure 1: Incident & Emergent intensities with associated angles</u>

The applicable form of the radiative transfer equation (RTE) [Jerlov, p. 92] is as follows (dependence on wavelength not shown explicitly):

$$\text{Cos}[\theta_s] * \partial_z L[z, \theta_s, \phi_s] == c[z] * L[z, \theta_s, \phi_s] - \beta[\theta_s, \phi_s, \theta_0, \phi_0] * E_i * \text{Exp}[-c[z] * z / \text{Cos}[\theta_0]] - \int_0^{\pi} \int_0^{2*\pi} \beta[\theta_s, \phi_s, \theta, \phi] * L[z, \theta, \phi] * \text{Sin}[\theta] \, d\phi \, d\theta$$

where

$L[x, \theta_s, \phi_s]$ = radiance of photons at depth z propagating in direction (θ_s, ϕ_s)

$\partial_z L[x, \theta_s, \phi_s]$ = change in radiance with depth due to scattering and absorption (*Mathematica* "derivative" notation)

$c[z]$ = beam attenuation coefficient

E_i = irradiance due to direct sunlight on a plane perpendicular to its propagation direction in the water (which is defined by zenith angle θ_s and azimuth angle ϕ_s)

$\beta[\Theta] = \beta[\theta_s, \phi_s, \theta_0, \phi_0]$ = volume scattering function that defines probability that in-water direct visible sunlight will scatter from initial direction (θ_0, ϕ_0) to (θ_s, ϕ_s).

$\beta[\theta_s, \phi_s, \theta, \phi]$ = as above for in-water diffuse visible radiance.

Note (i): The 1st, 2nd and 3rd terms on right of the equation represent, respectively,

- *attenuated radiance in the direction of propagation*
- *direct solar irradiance scattered into the observed direction*
- *diffuse radiance from outside the propagating direction beam scattered into it*

If 3rd term is omitted, one obtains a first approximation for primary scattering only.

Note (ii): The reciprocal of c[z] is called the attenuation length and its value is a key point of distinction between Case 1 and Case 2 waters [Bukata et al , pp. 28, 29]. For Case 1 (say, very clear mid-oceanic) waters one has very low values of c[z] and correspondingly high values of the attenuation length (of the order of 20 metres). On the other hand, for Case 2 (say, very turbid in-shore waters) one has very high values of c[z] with corresponding attenuation lengths ranging from a few metres to only a few centimetres.

It is convenient to express the RTE in terms of the optical depth (τ) which, for the application of interest here, is defined as

$$\tau[z\_] := \int_0^z c[z_d]\, dz_d$$

It turns out that the transformed RTE has the form

$$\mu_s * \partial_\tau L[\tau, \mu_s, \phi_s] == L[\tau, \mu_s, \phi_s] - (F/4) * p[\mu_s, \phi_s, -\mu_0, \phi_0] * \mathrm{Exp}[-\tau/\mu_0] - (1/(4*\pi)) * \int_{-1}^{+1} \int_0^{2*\pi} p[\mu_s, \phi_s, \mu, \phi] * L[\tau, \mu, \phi]\, d\phi\, d\mu$$

where, to align with [Chandrasekhar, p. 22, eqn 126], we have set $E_i = \pi F$ and introduced the scattering phase function p such that $p[\mu_s, \phi_s, \mu, \phi] = (4\pi/c[\tau])\beta[\mu_s, \phi_s, \mu, \phi]$ and $p[\mu_s, \phi_s, -\mu_0, \phi_0] = (4\pi/c[\tau])\beta[\mu_s, \phi_s, \mu_0, \phi_0]$.

Note (iii): The appropriate boundary condition for case of atmospheric radiation [Chandrasekhar, p. 22] for $\mu \in (0, 1]$, is $L[0, \mu_s, \phi_s, -\mu_0, \phi_0] = 0$. Also, it is required that the RTE solution be bounded as $\tau \to \infty$. For the water body application a suitable non-homogeneous boundary condition must be imposed (see "Outlook" below).

Note (iv): The above definition of optical depth is appropriate for the water body application where depth is measured from water surface (z = 0) downwards. In atmospheric applications, *as in [Chandrasekhar] or [Goody & Yung], it is usual to take z to represent vertical height with bottom of the atmosphere as z = 0. Then, the relationship between geometrical height (z) and optical depth (τ) is defined by,*

$$\tau[z\_] := \int_z^\infty c[z_d]\, dz_d$$

An important point to note is that use of the "optical depth" variable ensures that exactly the same mathematical problem is formulated for both applications.

Note (v): Considering the mean water surface z = 0, we see from $\mu = Cos[\theta]$ that

- *$\mu \in (0, 1]$ corresponds to the range $\theta < \pi/2$ to $\theta = 0$. This is the area above the water and is identified by "+μ"*
- *$\mu \in [-1, 0)]$ corresponds to the range $\theta = \pi$ to $\theta > \pi/2$. This is the area below the water and is identified by "-μ"; in fact what is done is to replace μ by - μ and then to use the range $\mu \in (0, 1]$.*

Note (vi): Above, we defined phase scattering function "p" as being a factor 4π/c times volume scattering function β. As expressed by [Maul, p157] "p" is a normalized version of β. However, there is an apparent mismatch between our definition and that of other writers (including [Maul] and [Bukata et al, p. 23]), in that they replace (total) attenuation coefficient "c" by scattering coefficient "b", where c = a + b and "a" is the absorption coefficient. The source of this apparent discrepancy, and its resolution, can be seen in [Goody & Yung, p. 331] where (upper case) "P" is used to denote phase (most generally, phase matrix). Aligning notations, we have that (b/c)P = p. It follows that (b/c)P = (4π/c)β or P = (4π/b)β, which agrees with [Maul] etc.

As an example consider the simplest case of isotropic scattering, namely p = ω_0, a constant [Chandrasekhar, p. 6]. ω_0 represents the "albedo for single scattering", that is, "the fraction of light lost from an incident pencil due to scattering". Hence, [Bukata et al, p. 29], we have that ω_0 = b/c = b/(a + b). Thus, the parameters ω that we introduce in our model (below) provide information only "***on the relative amounts of scattering and absorption occurring within a natural water mass***" and not on the absolute amounts. **Ultimately, a key objective of the present research** is to establish a systematic approach to extracting, from observations, maximum information on the ratio of scattering to total attenuation in order to characterize lakes (and in-shore waters) comprehensively. One test of this approach will be the extent to which it will be able to account for anomalies in some existing research results.

2. Context: Light & Water

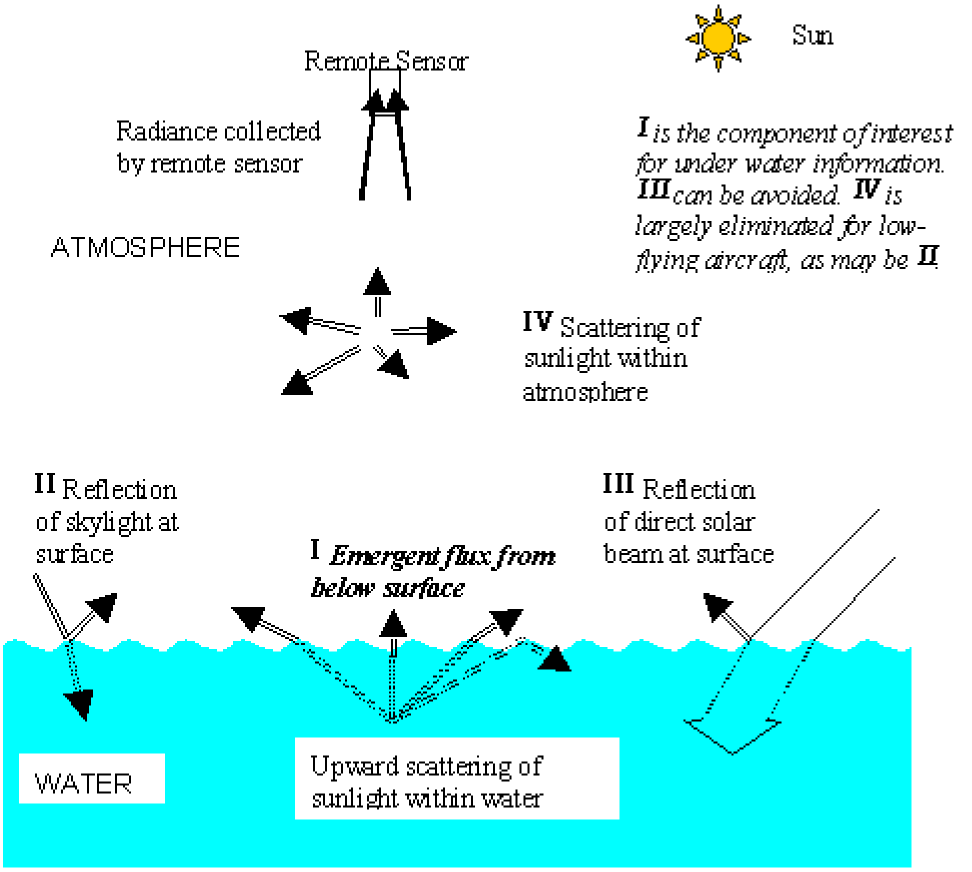


Figure 2: The different origins of the light received by a remote sensor above a water body [Kirk, p. 136]

Aquatic components: There is a wide variety of organic and inorganic materials present in lakes and inshore waters, and at least some of these have particular optical "signatures". For example,

- Both "dissolved yellow pigments" (or Gilvin) and "inanimate particulate matter" have high absorption in blue and low absorption in red [Kirk, pp49-66].
- Scattering is negligible for dissolved aquatic humus [Hakvoort, p52].
- "The absorption peak of chlorophyll at 680nm and a wavelength close by where chlorophyll doe not absorb are used to estimate chlorophyll concentration suspensions" [Hakvoort, p72].

In general, ***absorption data contain chemical information*** whereas ***scattering data contain information on physical characteristics*** of particles [Hakvoort, p. 80].

Volume scattering function β[Θ]: "In the ideal case, β[Θ] is measured from 0 to 180°; this provides not only the angular distribution of scattering for [the water body concerned] but also, by integration, the total, forward and backward scattering coefficients ... Such measurements are in reality difficult to carry out and relatively few natural waters have been completely characterized in this way". [Kirk, p.78]

Pure water: In visible range, $\beta_\lambda[\Theta] = \beta_\lambda[90°](1 + 0.835\mathrm{Cos}^2[\Theta])$ where, at λ = 550nm, $\beta[90°] = 0.93\mathrm{x}10^{-4}\mathrm{m}^{-1}\mathrm{sr}^{-1}$ (result of Morel, [Kirk, p84]). Also, $\beta_\lambda[\Theta] = (\mathrm{constant})\lambda^{-4.32}$. This is fairly close to ***Rayleigh*** molecular scattering predictions.

Natural water bodies: $\beta_\lambda[\Theta]$ differs markedly in shape between natural and pure water. There is an intense concentration of scattering at small forward angles, typical of scattering by particles of diameter greater than λ [***Mie*** theory]. Waters of a given broad optical type (e.g. clear oceanic or moderately turbid) appear to have $\beta_\lambda[\Theta]/b$ curves of rather similar shape [Kirk, p.87]. Dependence on λ is not as strong as for Rayleigh but there is some. "**Particle size** [*not* shape] is the major parameter in (Mie) scattering. ... opaque irregular particles, for which refraction is negligible, behave in the same way as opaque spheres" - result of Hodkinson [Jerlov, p.28].

Relevance to research reported here: Source of comparative data and of initial parameter "guesses" in estimation of ratio of scattering to total attenuation. If either total attenuation (c) or absorption coefficient (a) is estimated separately (e.g. [Hakvoort], [Kirk]) then an estimate of absolute scattering can be deduced.

3. Model

The aim is to estimate phase function p[Cos[Θ]]. Expand in terms of Legendre polynomials, $p[\mathrm{Cos}[\Theta]] = \Sigma\omega_l P_l[\mathrm{Cos}[\Theta]]$. It turns out, for $\{P_0, P_1, ..., P_n\}$, that

$$p[\mu_s\_,\ \phi_s\_,\ \mu_0\_,\ \phi_0\_,\ n\_] := \sum_{m=0}^{n} (2 - \delta_{0,m}) * \left(\sum_{l=m}^{n} \varpi[l] * (l-m)!\,/\,(l+m)! * P[l, m, \mu_s] * P[l, m, \mu_0]\right) * \mathrm{Cos}[m * (\phi_0 - \phi_s)]$$

The quantities to be estimated are the parameters ω_l (l = 0, n). In case of pure water (see above) it would be sufficient to take n = 2.

Solution of the RTE is used to model the radiance L. However, rather than considering the complete solution within the water body, a method originally due to [Chandrasekhar] is used to ***obtain the emergent radiance only*** (see **I** of Figure 2). See [Chandrasekhar] and [Lenoble] for the general approach, which can (though it need not) be based on a physical argument involving embedding a physical invariance. For present purposes, it is enough to present the simplest case of n = 0 and to indicate the form of the more complex models.

The general solution for emergent radiance for the isotropic case of n = 0 is

$$L(\mu, \mu_0)/F = \{\omega_0/4\} \bullet \{\mu_0/(\mu + \mu_0)\} \bullet H[\mu, \omega_0] \bullet H[\mu_0, \omega_0]$$

where function H satisfies the non-linear integral equation

$$H[\mu, \omega_0] = 1 + \{\omega_0/2\} \bullet \mu \bullet H[\mu, \omega_0] \int_0^1 \{1/(\mu + \mu')\} H[\mu', \omega_0] d\mu'$$

Numerical solutions for (above) function H are presented in [Chandrasekhar] and in later literature (such as [Hiroi] or [Steinfelds et al]). In more general cases, one is led to systems of integral equations that can be solved (with some effort!) in terms of "H functions" - for example, for n = 1, one has two "H functions". Each "H function" that arises is itself a solution of a non-linear integral equation of the general form (explicit dependence on parameters ω not shown)

$$H[\mu] = 1 + \mu H[\mu] \int_0^1 \{\Psi[\mu']/(\mu + \mu')\} H[\mu'] d\mu' \text{ where } \int_0^1 \Psi[\mu] d\mu \leq 1/2$$

and $\Psi[\mu]$ is an even polynomial in μ.

The "H function" in the isotropic case model for $L(\mu, \mu_0)/F$ depends on the particular value taken by $\omega_0 \in [0, 1]$. There is a practical issue of efficiency that arises when applying this model while estimating an "optimal" value of ω_0 - whether to numerically solve for H at each step of the estimation or whether to interpolate from previously calculated solutions at particular ω_0 values. Note that, in practice, it will be necessary to solve for several wavelengths concurrently.

4. Estimation Method

In the initial computations performed thus far the approach has been to interpolate between known values of H[μ, ω_0] as calculated in [Chandrasekhar]. A plot of the interpolated function (denoted HiISO) is as follows:

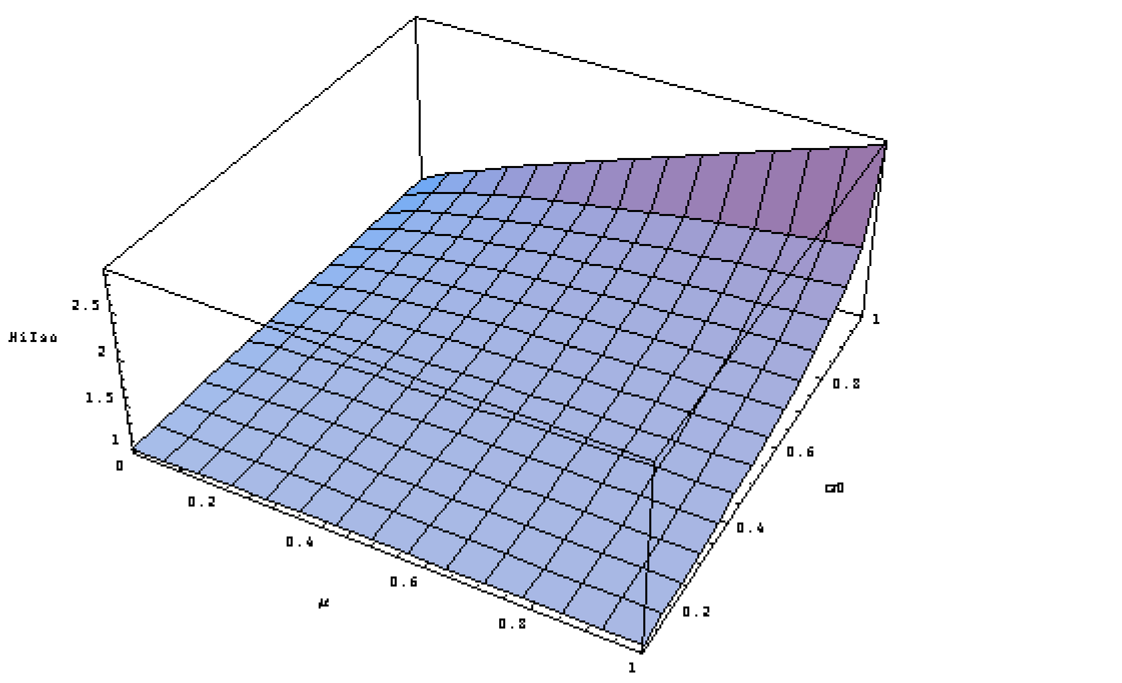


Figure 3: Plot of "H function" for the isotropic case

Thus, our model for L(μ, μ_0)/F is, in fact,

MODEL(μ, μ_0; ω_0) = {ω_0/4}•{μ_0/($\mu + \mu_0$)}•HiISO[μ, ω_0]•HiISO[μ0, ω_0]

The procedure is, essentially, to estimate parameter ω_0 by fitting this model to measured values of L(μ, μ_0)/F. This is a nonlinear fitting problem and to date the method used has been as implemented in the "NonlinearFit" and "NonlinearRegress" functions of *Mathematica*. Within the method a minimum finding algorithm is used to find parameter estimates - to date, in the present research, the default "LevenbergMarquardt" algorithm has been used. Background on the method may be found in [Bates & Watts]. The method has been used largely as a black box up to now but more careful analysis will be required eventually.

5. Validation & Assessment

Several levels of validation and assessment are required, including

- performance of estimation method
- adequacy of model
- assessment for efficiency in extracting information and for information quality.

Initial work has focussed on the first of these by means of the following simulation:

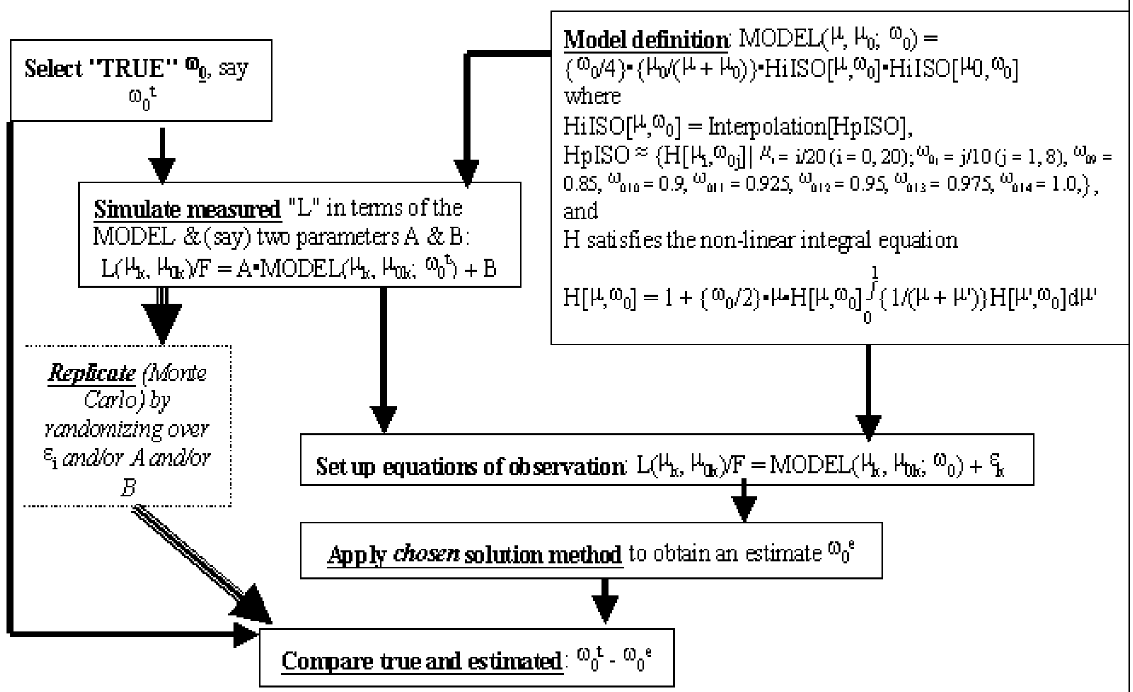


Figure 4: Simulation of estimation process for the isotropic case

6. Initial results (isotopic case)

Results are encouraging in that they suggest that it is indeed possible to estimate ω_0 by means of the chosen method. It appears that ω_0^e is unbiased and that its standard error (SE) is inversely proportional to square root of number of data points.

Some other initial findings:

- ω_0^e does not depend appreciably on the chosen starting value for ω_0.
- SE of ω_0^e is directly proportional to the simulated measurements' σ.
- SE of ω_0^e decreases as ω_0^t increases - minimum at $\omega_0^t = 1$ (conservative case)

More detailed simulations are needed to determine how SE of ω_0^e is affected by choice of data points (for realism). Parameters A and B are included in the simulation for flexibility in adding realism - some suggestive results were obtained but more needs to be done.

7. Outlook

There are several points to be addressed in further work, including:

1. As first steps towards more complex models, include from [Chandrasekhar],

(i) a special linearly anisotropic case ($p[Cos[\Theta]] = \omega_0(1 + xCos[\Theta])$ that involves parameters ω_0 and x, and requires two H functions.

(ii) the (conservative) Rayleigh case ($p[Cos[\Theta]] = ¾(1 + Cos^2[\Theta])$)that involves three H functions.

2. Include models of more than one parameter, possibly using solutions collected in [Lenoble], but eventually incorporating newly calculated solutions for the emergent radiation. Some significant work will be required here, both numerical and analytic.

3. Improve characterization of measurement errors

4 Establish appropriate boundary conditions with corresponding adjustments of model (and maybe of estimation method). (**A key task**)

5. Replace simulated measurements by real data for pure water and then for some (limited number of) natural water bodies. [Initial validation and assessment]

6. Include more real data and compare against results published by others. [Complete validation and assessment]

7. "Production": Routine application of the approach to report on water quality.

References

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