Improved Ocean Ecosystem Predictions via Improved Light Calculations

I. Model Descriptions

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Overview

This lecture:

• Overview of the problem

• Features and performance of the EcoLight-S radiative transfer model

• Description of ROMS hydrodynamic and CoSiNE biological models

Next Lecture:

• Example results from use of EcoLight-S in a simple ecosystem simulation
State of the Science

• Predictive ecosystem models are playing an increasingly important role in our understanding of the oceans.

• Applications of such models range from predictions of water clarity for military purposes to management of coastal waters for fisheries and understanding of global climate change.

Currently available ocean ecosystem models often use

• very sophisticated treatments of the physics (e.g., Navier-Stokes solutions in terrain-following coordinate systems)

• increasingly realistic biology (e.g., multiple biological components in complex food webs)

• grossly oversimplified treatments of the optics (often just a single equation parameterizing PAR terms of the chlorophyll concentration and parameters such as the solar zenith angle)
Approach

**HydroLight:** Widely used; very accurate solution of the radiative transfer equation (RTE) for any water composition (Case 1 or 2) and boundary conditions (deep or shallow with reflecting bottom; any sky) to get $L(z, \theta, \phi, \lambda)$

Much too slow for use in ecosystem models with many grid points and time steps.

**Needed:** Just scalar irradiance $E_o(z, \lambda) = \int_{4\pi} L(z, \theta, \phi, \lambda) d\Omega$ to bottom of euphotic zone, or PAR($z$)

Therefore: Can solve

- azimuthally averaged radiative transfer equation (RTE)
- solve RTE only near sea surface where boundary effects are greatest, then extrapolate to greater depths [using $K_o = \mathcal{F}\{\text{absorp. coef } a(z, \lambda)\}$]
- solve RTE at only some wavelengths (get unsolved $\lambda$ by interpolation)
- solve at only some grid points (rescale nearby solution for others)
- solve at only some time steps (rescale most recent solution)

The resulting code is called **EcoLight-S(ubroutine)**.  (details in Mobley, 2011. Optics Express)
EcoLight-S(subroutine) Features

- EcoLight-S solves the azimuthally averaged RTE for any water conditions and for any bottom and sky conditions (same as HydroLight)
- Gives the same irradiances and $R_{rs}$ as HydroLight
- Has various options for wavelength skipping, RTE solution to dynamically determined depths with extrapolation to greater depths, etc. to speed up the run time. Uses a stack of homogeneous layers for IOPs, as do most ecosystem models.
- Runs ~1000 times faster than HydroLight
- Also computes ancillary optical quantities such as $R_{rs}(\lambda)$, $E_d(z,\lambda)$, $E_u(z,\lambda)$, and $L_u(z,\lambda)$, which are not available from analytic models. Having $R_{rs}$ allows for validation of ecosystem model predictions using remotely sensed data without having to convert $R_{rs}$ to Chl via a Chl inversion algorithm. $E_d$ and $L_u$ allow for ecosystem validation from easily made in-water measurements.
- Callable from any other code as a subroutine, with all communication via Fortran 95 modules
Use of EcoLight-S in an Ecosystem Model

Any physical-biological (P-B) ecosystem model

Water-column constituent concentrations as predicted by the P-B model

External environmental information (time and location, wind speed, etc.)

User-written P-B-EcoLight-S interface subroutine:

- defines all IOPs from P-B constituent concentrations
- defines surface and bottom boundary conditions (wind speed, bottom refl., etc)
- sets flags for RTE solution options

Reformats EcoLight-S outputs as needed by the P-B model

The EcoLight-S subroutine:

Solves the RTE given the IOPs and boundary conditions

Returns the irradiances, remote-sensing reflectance, etc. for use by the P-B ecosystem model
Use of EcoLight-S in an Ecosystem Model

Your physical-biological ecosystem model

Model-specific interface routine to
• convert your model output into what EcoLight-S needs to solve the RTE, and then call EL-S
• convert EL-S output into what your model needs, and then return to your model

Your problem

my problem

shared mod_ELS_input

shared mod_ELS_output

EcoLight-S solves the RTE

The interface routine is a “fill in the blank” template (with many options for how to define the needed inputs), which replaces the HydroLight graphical user interface.
The EcoLight-S Input Module

MODULE mod_ELS_input

! nwave: number of computational wavelength bands
! nlayers: number of homogeneous layers in the water column
<snip>

! waveb(1:nwave+1): wavelength band boundaries [nm]
! zgeo(2*nlayers+1): geometric depth array of layer boundaries and midpoints [m]
! acoef(1:nlayers,1:nwave): array of total absorption coefs [1/m]; always used
! bcoef(1:nlayers,1:nwave): array of total scattering coefs [1/m]; always used
! bbcoef(1:nlayers,1:nwave): array of total backscattering coefs [1/m]; used if ibbfracOpt = 2
<snip>

*** The following inputs MUST be defined by the user BEFORE calling EcoLightS.
! This is normally done in the user's main program or interface routine.
! IOPs:
  INTEGER :: nlayers, ibbfracOpt
  REAL, DIMENSION(mxlayer, mxwave) :: acoef, bcoef, bbcoef
  REAL, DIMENSION(mxwave) :: bbfrac ! needed only if ibbfracOpt = 1
<snip>

END MODULE mod_ELS_input
The EcoLight-S Output Module

MODULE mod_ELS_output

USE mod_ELS_dimens, ONLY: mxzgeo,mxwave,mxlayer ! dimensions for arrays

! In arrays Eo, etc, depth index 0 is in air; index 1 is in water at
! zout(1) = 0.0; zout(nzout) is the deepest computed in-water depth in meters
! Wavelengths waveout are in nm
! Irradiances Eo, Ed, Eu are spectral values in W/(m^2 nm)
! Radiances Lu and Lw are nadir-viewing, spectral values in W(m^2 sr nm)

IMPLICIT NONE

INTEGER :: nzout, nwaveout, nlayer ! number of computed depths, wavelengths, and layers
REAL, DIMENSION(mxzgeo) :: zout
REAL, DIMENSION(0:mxzgeo) :: PAR, PAR_Ed
REAL, DIMENSION(0:mxzgeo,mxwave) :: Eo, Ed, Eu, Ld, R, fmud, fmuu, fmu0, Eo_quant
REAL, DIMENSION(mxwave) :: waveout, Rrs, Lw
REAL, DIMENSION(mxwave) :: Kinf, mudinf, muuinf, muinf, Rinf ! asymptotic values, if computed

END MODULE mod_ELS_output
EcoLight-S Philosophy and Optimization

Most current ecosystem models are based on PAR. Simple PAR models can be very inaccurate in some situations and can be an order of magnitude different than PAR computed by HydroLight for the same IOPs.

The goal: Make EcoLight-S run as fast as possible and still get PAR to ~10% at the bottom of the euphotic zone.

Optimizations:
• Solve the RTE at each $\lambda$ only from the sea surface down to the depth where the irradiance has decreased to a fraction $F_o$ of the surface value (e.g., $F_o = 0.1$ solves to the 10% irradiance level), or
• Solve the RTE at each $\lambda$ only from the sea surface down to the depth where the irradiance has decreased to a value of $E_c = F_o$ [e.g., 1 W m$^{-2}$ nm$^{-1}$]
• Solve the RTE at only some wavelengths, and fill in the unsolved wavelengths by interpolation
Dynamic Determination of RTE Solution Depths

The IOPs(z,λ) are known (from the routine that calls EcoLight-S).

\[ E_o(z_o, \lambda) = E_o(0, \lambda) \exp \left[ - \int_0^{z_o} K_o(z, \lambda) \, dz \right] \]

Definition of \( K_o \)

Except very near the sea surface, \( K_o \approx K_d \)

\[ K_d(z, \lambda) = \frac{a(z, \lambda) + b_b(z, \lambda)}{\bar{\mu}_d(z, \lambda)} \]

Single-scattering approx for \( K_d \)

\( b_b \ll a \) and \( \mu_d \approx \frac{3}{4} \), so to a first approximation

\[ F_o = \frac{E_o(z_o, \lambda)}{E_o(0, \lambda)} \approx \exp \left[ - \int_0^{z_o} a(z, \lambda) \, dz \right] \]

Pick \( F_o \) and solve for est. \( z_o \)
est. \( z_o > \) actual \( z_o \)

After the first wavelength, can use actual \( z_o \) depth at previous wavelength to estimate \( z_o \) at the current wavelength. This corrects for errors in neglecting \( \mu_d \), etc.
Depth Extrapolation Below the RTE Solution Depth

Most ecosystem models use homogeneous layers, with layer boundaries \( z_0 = 0, z_1, \ldots, z_N = \text{the bottom} \). After determining the RTE solution depth \( z_o \), solve the RTE to the next deeper layer boundary depth \( z_k \).

The irradiances are then known from solution of the RTE down to depth \( z_k \). Extrapolate to deeper depths using

\[
\overline{\mu}(z_k) = \frac{E_d(z_k) - E_u(z_k)}{E_o(z_k)}
\]

\[
E_o(z, \lambda) = E_o(z_k, \lambda) \exp \left[ - \int_{z_k}^{z} \frac{a(z, \lambda)}{\mu(z, \lambda)} \, dz \right]
\]

The same is done for \( E_d \) using

\[
\overline{\mu}_d(z_k) = \frac{E_d(z_k)}{E_{od}(z_k)}
\]
Depth Extrapolation Example

Depth Extrapolation Example

\[ F_0 = 0.10; \text{ 5 nm bands} \]

circles are in meters
diamonds are optical depths

text:
big computational savings at red \( \lambda \)
because run time is
determined by
optical depth

red = RTE solution depth used
blue = actual \( F_0 \) depth
black = optical depth at 50 m
Effect of Solution Depths

The RTE was solved to various $F_\circ$ depths ($F_\circ$ as a fraction of surface $E_\circ$) at a wavelength resolution of 5 nm. Dots in the second panel show greatest the greatest solution depth (after the first wavelength) for each $F_\circ$. 

![Graph showing the effect of solution depths on chlorophyll and PAR](image)
Effect of Skipping Wavelengths

The RTE was solved to 50 m at a wavelength resolution of 5 nm. Then solved for wavelength intervals of 10 nm (skipping every other 5 nm band), 15 nm (skipping 2 bands) etc.
Combined Dynamic Depths and Wavelength Skipping

Various $F_o$ depths ($F_o$ as a fraction of surface $E_o$) and number of 5 nm bands skipped.
Errors in $E_o(z,\lambda)$ for optimization with $F_o = 0.2$ and 25 nm resolution vs. $F_o = 0$ and 5 nm resolution

Unoptimized:
$F_o = 0$ and 5 nm resolution

Optimized:
$F_o = 0.2$ and 25 nm resolution
# HydroLight vs. EcoLight vs. Ecolight-S Run Times

## Table 1. Simulations of pure water and turbid Case 2 water.

<table>
<thead>
<tr>
<th>model</th>
<th>PAR($z_{max}$) [μ mol m$^{-2}$ s$^{-1}$]</th>
<th>time [seconds]</th>
<th>difference [percent]</th>
</tr>
</thead>
<tbody>
<tr>
<td>HydroLight 5.1 with inelastic</td>
<td>10.1330</td>
<td>427.1 (376.9)</td>
<td>—</td>
</tr>
<tr>
<td>HydroLight 5.1 without inelastic</td>
<td>9.6223</td>
<td>283.6 (268.4)</td>
<td>-5.0</td>
</tr>
<tr>
<td>EcoLight 5.1 with inelastic</td>
<td>10.1090</td>
<td>15.3 (12.8)</td>
<td>-0.2</td>
</tr>
<tr>
<td>EcoLight 5.1 without inelastic</td>
<td>9.1690</td>
<td>5.1 (4.6)</td>
<td>-5.1</td>
</tr>
<tr>
<td>EcoLight-S unoptimized</td>
<td>9.6578</td>
<td>2.71</td>
<td>-4.7</td>
</tr>
<tr>
<td>EcoLight-S with $F_0 = 0.1$, 10 nm</td>
<td>9.6342</td>
<td><strong>0.17</strong></td>
<td>-4.9</td>
</tr>
<tr>
<td>EcoLight-S with $F_0 = 0.2$, 10 nm</td>
<td>9.9650</td>
<td><strong>0.13</strong></td>
<td>-4.3</td>
</tr>
<tr>
<td>EcoLight-S with $F_0 = 0.1$, 20 nm</td>
<td>8.7881</td>
<td>0.08</td>
<td>-13.3</td>
</tr>
<tr>
<td>EcoLight-S with $F_0 = 0.2$, 20 nm</td>
<td>8.8332</td>
<td>0.07</td>
<td>-12.8</td>
</tr>
</tbody>
</table>

Case 2 water: $z_{max} = 20$ m; Secchi depth = 3.7 m

<table>
<thead>
<tr>
<th>model</th>
<th>PAR($z_{max}$) [μ mol m$^{-2}$ s$^{-1}$]</th>
<th>time [seconds]</th>
<th>difference [percent]</th>
</tr>
</thead>
<tbody>
<tr>
<td>HydroLight 5.1 with inelastic</td>
<td>1.6128</td>
<td>198.6 (162.3)</td>
<td>—</td>
</tr>
<tr>
<td>HydroLight 5.1 without inelastic</td>
<td>1.6032</td>
<td>108.3 (89.4)</td>
<td>-0.6</td>
</tr>
<tr>
<td>EcoLight 5.1 with inelastic</td>
<td>1.6068</td>
<td>6.7 (5.5)</td>
<td>-0.4</td>
</tr>
<tr>
<td>EcoLight 5.1 without inelastic</td>
<td>1.5968</td>
<td>2.3 (1.9)</td>
<td>-1.0</td>
</tr>
<tr>
<td>EcoLight-S unoptimized</td>
<td>1.5975</td>
<td>0.98</td>
<td>3.0</td>
</tr>
<tr>
<td>EcoLight-S $F_0 = 0.1$, 10 nm</td>
<td>1.6606</td>
<td><strong>0.28</strong></td>
<td>3.0</td>
</tr>
<tr>
<td>EcoLight-S $F_0 = 0.2$, 10 nm</td>
<td>1.7696</td>
<td><strong>0.21</strong></td>
<td>9.7</td>
</tr>
<tr>
<td>EcoLight-S $F_0 = 0.1$, 20 nm</td>
<td>1.6594</td>
<td>0.15</td>
<td>2.9</td>
</tr>
<tr>
<td>EcoLight-S $F_0 = 0.2$, 20 nm</td>
<td>1.7702</td>
<td>0.11</td>
<td>9.8</td>
</tr>
</tbody>
</table>
HydroLight vs EcoLight-S $R_{rs}$ Spectra

$R_{rs}$ is almost the same for HydroLight vs. optimized EcoLight-S

blue: pure water, Hydrolight with inelastic
green: Case 2 water, Hydrolight with inelastic
open circles: EcoLight–S unoptimized
dots: EcoLight–S with $F_o = 0.2$
ROMS: Regional Ocean Modeling System

• Widely used and very sophisticated and numerically efficient code developed at Rutgers Univ. Single processor or parallelized runs via automatic tiling.

• Free-surface, terrain-following, primitive-equation ocean hydrodynamic model

• In the horizontal, the primitive equations are evaluated using boundary-fitted, orthogonal curvilinear coordinates

• In the vertical, the primitive equations are discretized over variable topography using stretched terrain-following coordinates, which allow increased resolution in areas of interest, such as thermocline and bottom boundary layers

• Includes several coupled models for biogeochemical, bio-optical, sediment, and sea ice applications

See http://www.myroms.org/ for details and links to references
Example Simulation and Timing: ROMS-EcoSim-EcoLight

Initial development and evaluation used **BioToys**:

**Physical model: ROMS** (Regional Ocean Modeling System)
- 6x6 spatial grid with periodic boundary conditions
- variable depth layers from 2 m at the surface to 15 m at 200 m
- daily wind and external irradiance forcing from observations

**Biological model: EcoSim** (Ecosystem Simulation)
- 4 phytoplankton functional groups
- uses spectral irradiance (400 to 700 by 5 nm) to allow for competition between functional groups according to different light- and nutrient-dependent pigment suites
- default light model is a simple chlorophyll-based analytic model:

\[ E_d(z,\lambda) = E_d(0,\lambda) \exp[-K(Chl,\lambda) z] \]  \hspace{1cm} (1)

Initial timing studies applied BioToys to Case 1 water for which (1) is valid.

Replaced Eq. (1) by EcoLight-S for timing comparisons
Example Simulation and Timing: Initialization

BioToys computational grid

daily irradiance forcing

initial chlorophyll profile for 4 phytoplankton functional groups
Example Simulation and Timing: Results

Simulation year 5

Depth = 1.02 m

Total Chl$_a$ [mg m$^{-3}$]

Jan Feb Mar Apr May Jun Jul Aug Sep Oct Nov Dec

time [calendar month]

Analytic light: 32 min/year
EGP, ETS, 5nm, F=0.001
EcoLight, unoptimized: 135.5 hours/year
EGP, ETS, 5nm, F=0.001
EcoLight, optimized: 41 min/year
1GP, 4HR, 25nm, F=0.15
EcoLight, over-optimized: 40 min/year
1GP, 6HR, 50nm, F=0.50
• Analytic light and EcoLight not much different ONLY because this simulation was for Case 1 water, for which Eq. (1) was developed. EcoSim and Eq. (1) cannot simulate Case 2 waters or shallow bottoms.

• When properly optimized, EcoLight requires < 30% greater run time than the analytic model, while giving same results as the exact (unoptimized) calculation to within a few percent.
First law of thermodynamics (conservation of energy)

\[
\frac{\partial T}{\partial t} = - \frac{1}{c_v \rho} \frac{\partial (E_d - E_u)}{\partial z} \approx - \frac{1}{c_v \rho} \frac{\partial E_d}{\partial z}
\]

\[
E_d(z) = \int_{
\begin{array}{ll}
0 & \lambda_1 \\
\lambda_2 & 1 \text{ day}
\end{array}
\int E_d(z, \lambda, t) \, d\lambda \, dt
\]

\[
\Delta T = - \frac{1}{c_v \rho} \frac{E_d(z_1) - E_d(z_2)}{z_1 - z_2}
\]

Paulson & Simpson (1977) parameterized \(E_d(z,400-1000)\) in terms of one of 5 Jerlov water types, based on only 5 measured profiles: 5 sets of \(f, \xi_1, \xi_2\) tabulated values.

\[
E_d(z) = E_d(0) [f \exp(-z/\xi_1) + (1 - f) \exp(-z/\xi_2)]
\]

The P&S model for \(E_d(z)\)

Total irradiance (W m\(^{-2}\)) over 400-1000 nm and 1 day

The P&S irradiance model is simple, computationally fast, easy to use, and almost always wrong as used in ROMS
The P&S model may or may not give good results, depending on the water body. Even if correct at the start of a run, it won’t stay correct as the IOPs change. Even if correct at one location, it won’t be correct at locations with different IOPs.

\[
E(z) = E(0) \left[ f e^{-z/\zeta_1} + (1-f) e^{-z/\zeta_2} \right]
\]

Chl = 1: Jerlov type II

EcoLight: \( \infty \) deep; Case 1

Chl = 1; \( U = 5 \) m/s
CoSiNE: Carbon Silicon Nitrogen Ecosystem

Developed by Fei Chai at the Univ. of Maine and Richard Dugdale at San Francisco State Univ.

- 3 phytoplankton functional groups: picoplankton, diatoms, coccolithophores
- 2 zooplankton functional groups: microzooplankton and mesozooplankton
- Multiple nutrients: nitrate NO$_3$, ammonium NH$_4$, silicate Si(OH)$_4$, phosphate PO$_4$
- Detritus: non-algal particles and biogenic silica bSiO$_2$
- Dissolved organic material: DOC/CDOM, DON
- Phytoplankton take up NO$_3$ and NH$_4$ by photosynthesis. In addition, diatoms utilize Si(OH)$_4$ in the silicification process. Microzooplankton graze on picoplankton. Mesozooplankton feed on diatoms, microzooplankton, and NAP.
- Full carbon cycle via dissolved inorganic C and total alkalinity
- Fe implicitly built in
CoSiNE: Carbon Silicon Nitrogen Ecosystem

Very complex web with many sources, sinks, interactions, rates, etc.
The latest version, CoSiNE-31, has 31 state variables (variables whose values are predicted and describe the biological state of the ecosystem). The IOPs $a(z,\lambda)$, $b(z,\lambda)$, $b_b(z,\lambda)$ are determined from the red variables.

<table>
<thead>
<tr>
<th>Nitrate concentration</th>
<th>Mesozooplankton N</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ammonium concentration</td>
<td>Mesozooplankton C</td>
</tr>
<tr>
<td>Silicate concentration</td>
<td>Bacteria concentration N</td>
</tr>
<tr>
<td>Phosphate concentration</td>
<td>Detritus concentration N</td>
</tr>
<tr>
<td>Small phytoplankton N</td>
<td>Detritus concentration C</td>
</tr>
<tr>
<td>Small phytoplankton C</td>
<td>Biogenic silicate concentration</td>
</tr>
<tr>
<td>Small phytoplankton CHL</td>
<td>Labile dissolved organic N</td>
</tr>
<tr>
<td>Diatom concentration N</td>
<td>Labile dissolved organic C</td>
</tr>
<tr>
<td>Diatom concentration C</td>
<td>Semi-labile dissolved organic N</td>
</tr>
<tr>
<td>Diatom concentration CHL</td>
<td>Semi-labile dissolved organic C</td>
</tr>
<tr>
<td>Coccolithophores N</td>
<td>Colored labile dissolved organic C</td>
</tr>
<tr>
<td>Coccolithophores C</td>
<td>Colored semi-labile dissolved organic C</td>
</tr>
<tr>
<td>Coccolithophores CHL</td>
<td>Particulate inorganic C</td>
</tr>
<tr>
<td>Small zooplankton N</td>
<td>Dissolved oxygen</td>
</tr>
<tr>
<td>Small zooplankton C</td>
<td>Total alkalinity</td>
</tr>
<tr>
<td></td>
<td>Total CO2</td>
</tr>
</tbody>
</table>
Original ROMS-CoSiNE Model

Hydrodynamics & thermodynamics with one light model
Biology with another light model
Physics affects biology, but no feedback from biology to physics

wind, sky $E(400-1000)$ → ROMS hydrodynamics & thermodynamics
\[ \frac{\partial T}{\partial t} = \text{Paulson & Simpson} \]

currents, temp, mixing → CoSiNE biology
\[ PP = f(E(z, 400-700)) \]

concentrations → IOP model
\[ \text{IOPs}(z, \lambda) \]

water IOPs → Analytic light model
\[ E(z, \lambda), 400-700 \]

assumed Jerlov water type
Hydrodynamics, thermodynamics, biology, light are fully coupled via EcoLight.
Conclusions

EcoLight-S enables fast and accurate light computations in coupled physical-biological-optical ocean ecosystem models

- < 30% increase in run time when intelligently called
- valid for both Case 1 and 2 waters; shallow reflecting bottoms
- computes $R_{rs}$, $L_u$, and other quantities that allow validation of ecosystem predictions from remotely sensed imagery and mooring or glider optical measurements

Ecosystem biogeochemical models now can be extended to include resuspended sediments, terrigenous CDOM and particles, and shallow reflecting bottoms, for which there are no simple analytic light models for biological primary production or thermodynamics.

EcoLight-S is also ideal for use as the RTE core of implicit inversion algorithms that recover IOPs from light measurements. This is a promising path to data assimilation in ecosystem model initialization and correction.
Old Woman and Demon, Lhasa