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 $L(z,\theta,\varphi,\lambda)$

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

Needed: Just scalar irradiance $E_o(z,\lambda) = \int_{4\pi} L(z,\theta,\varphi,\lambda)\,d\Omega$ 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 λ 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(ubroutine) 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 $L_{\underline{u}}(z,\lambda)$, 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 consituent 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

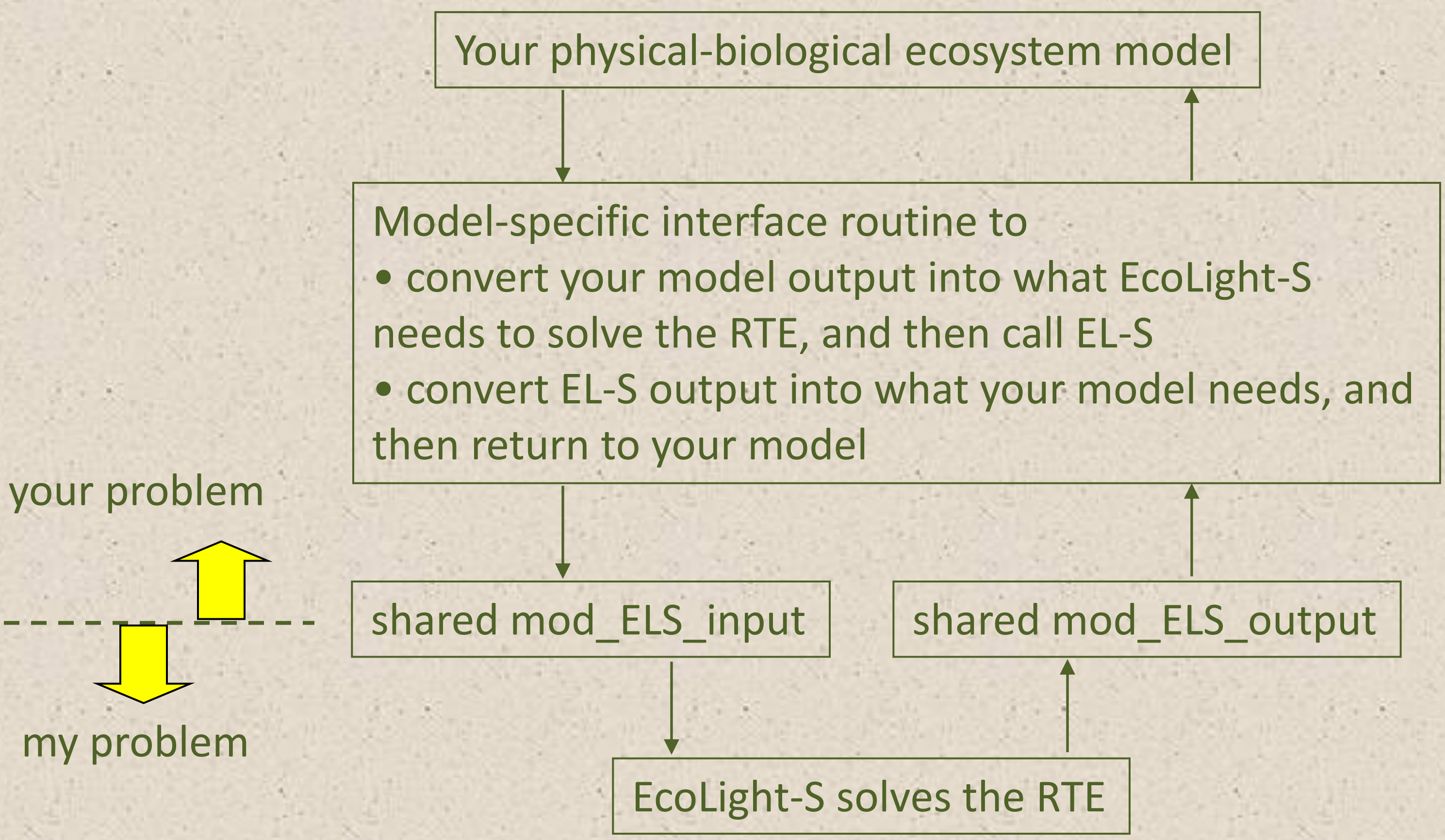
Reformats EcoLight-S outputs as needed by the P-B model

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



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)
   <snip>

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, Lu, 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
   <snip>

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 λ 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 λ 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 $\mu_d \approx 3/4$, 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 μ_d, etc.

Depth Extrapolation Below the RTE Solution Depth

Most ecosystem models use homogeneous layers, with layer boundaries z_0 = 0, z_1, ..., z_N = 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

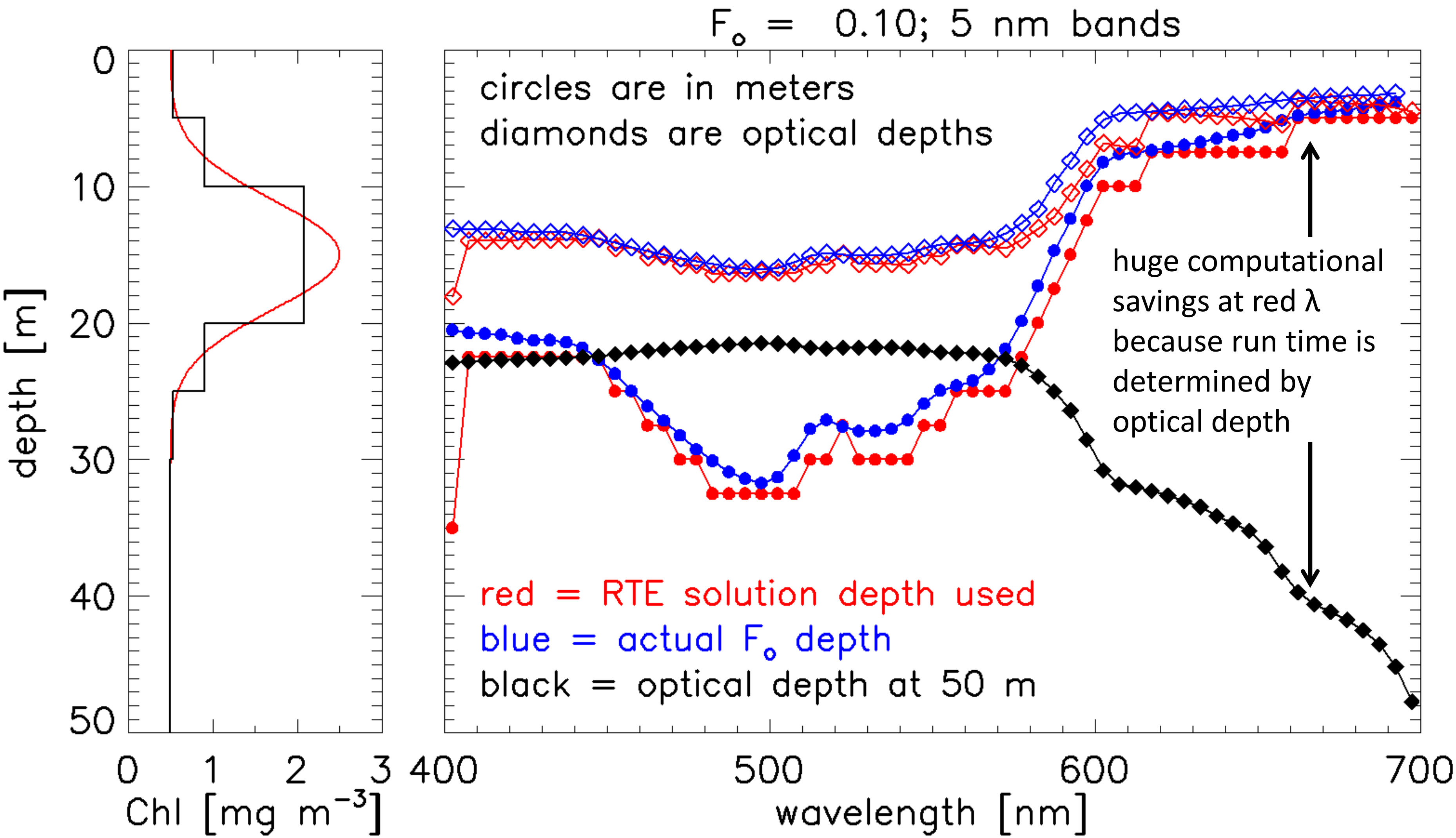
$$\overline{\mu}(z_k) = \frac{E_\mathrm{d}(z_k) - E_\mathrm{u}(z_k)}{E_\mathrm{o}(z_k)}$$

$$E_\mathrm{o}(z,\lambda) = E_\mathrm{o}(z_k,\lambda)\exp\left[-\int_{z_k}^{z}\frac{a(z,\lambda)}{\overline{\mu}(z_k,\lambda)}\,\mathrm{d}z\right]$$

The same is done for E_d using

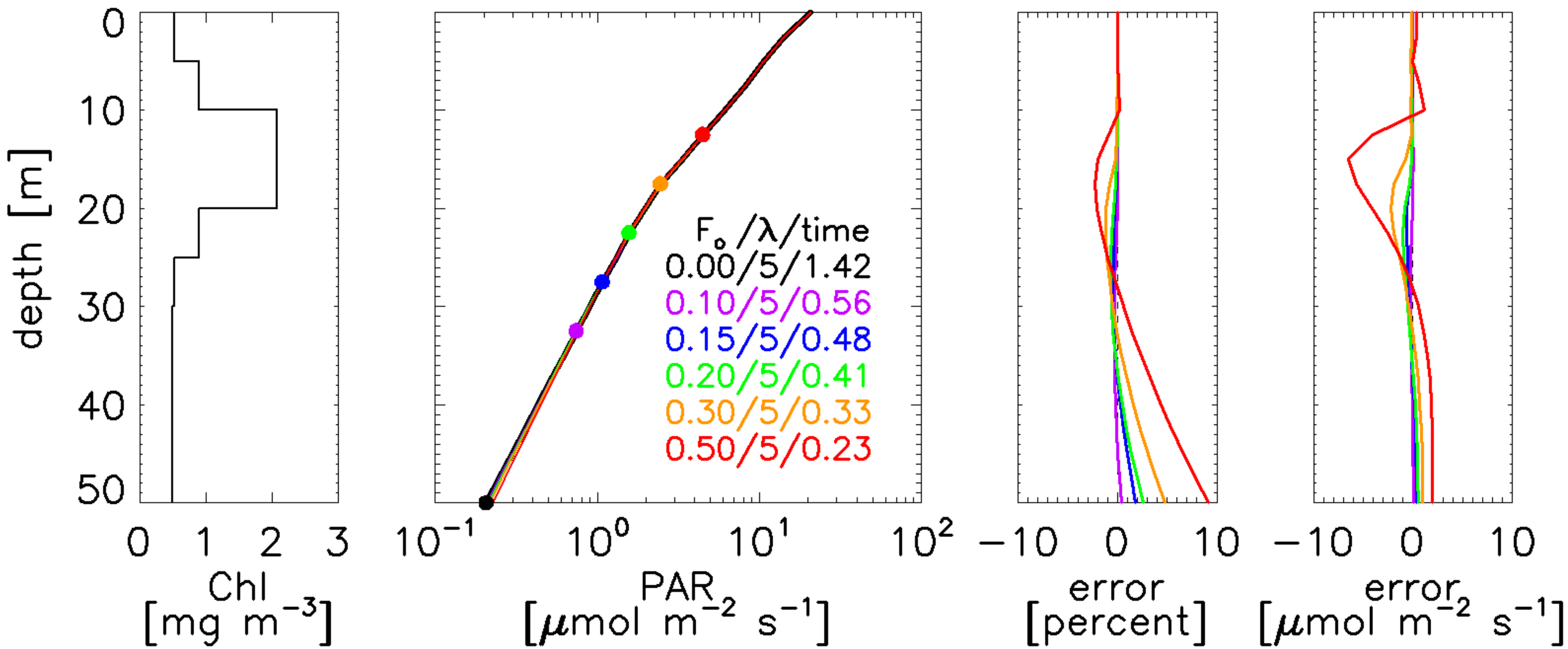
$$\overline{\mu}_\mathrm{d}(z_k) = \frac{E_\mathrm{d}(z_k)}{E_\mathrm{od}(z_k)}$$

Depth Extrapolation Example



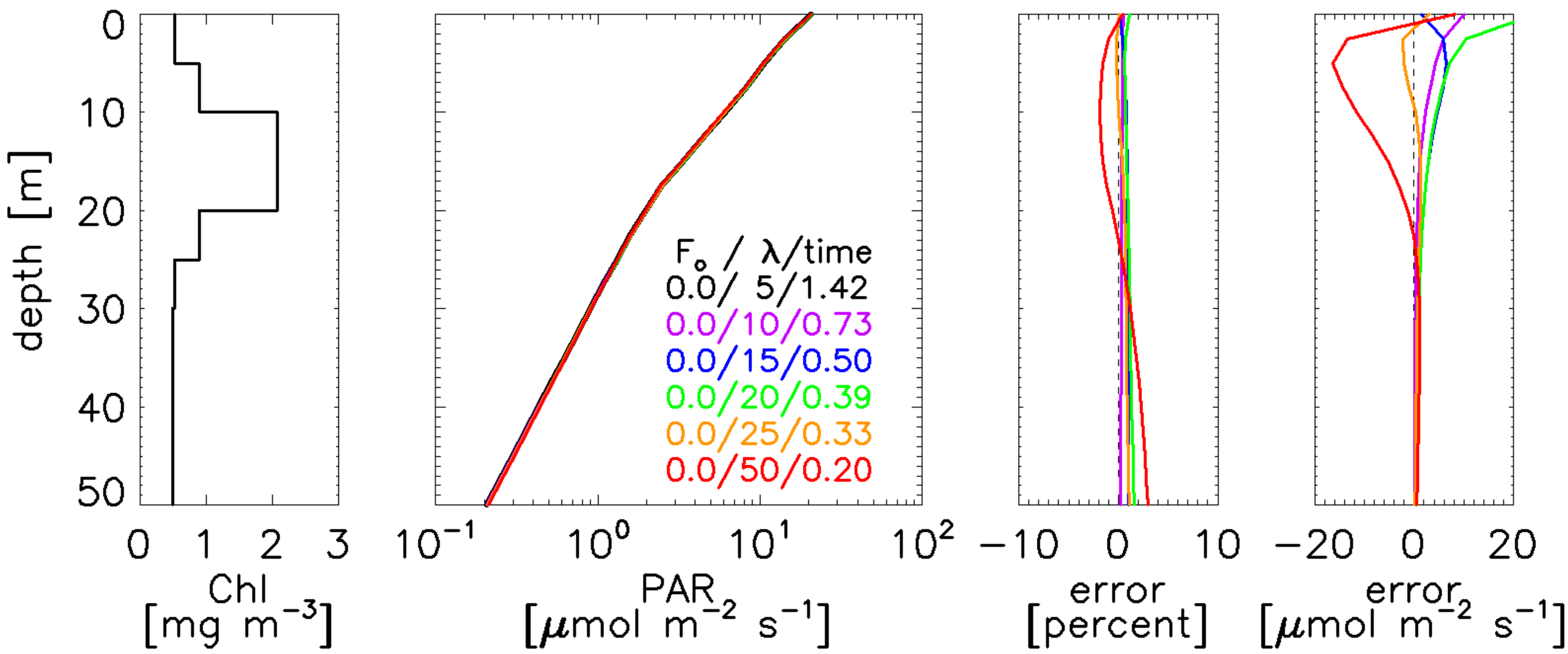
Effect of Solution Depths

The RTE was solved to various F_o depths (F_o as a fraction of surface E_o) 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_o.



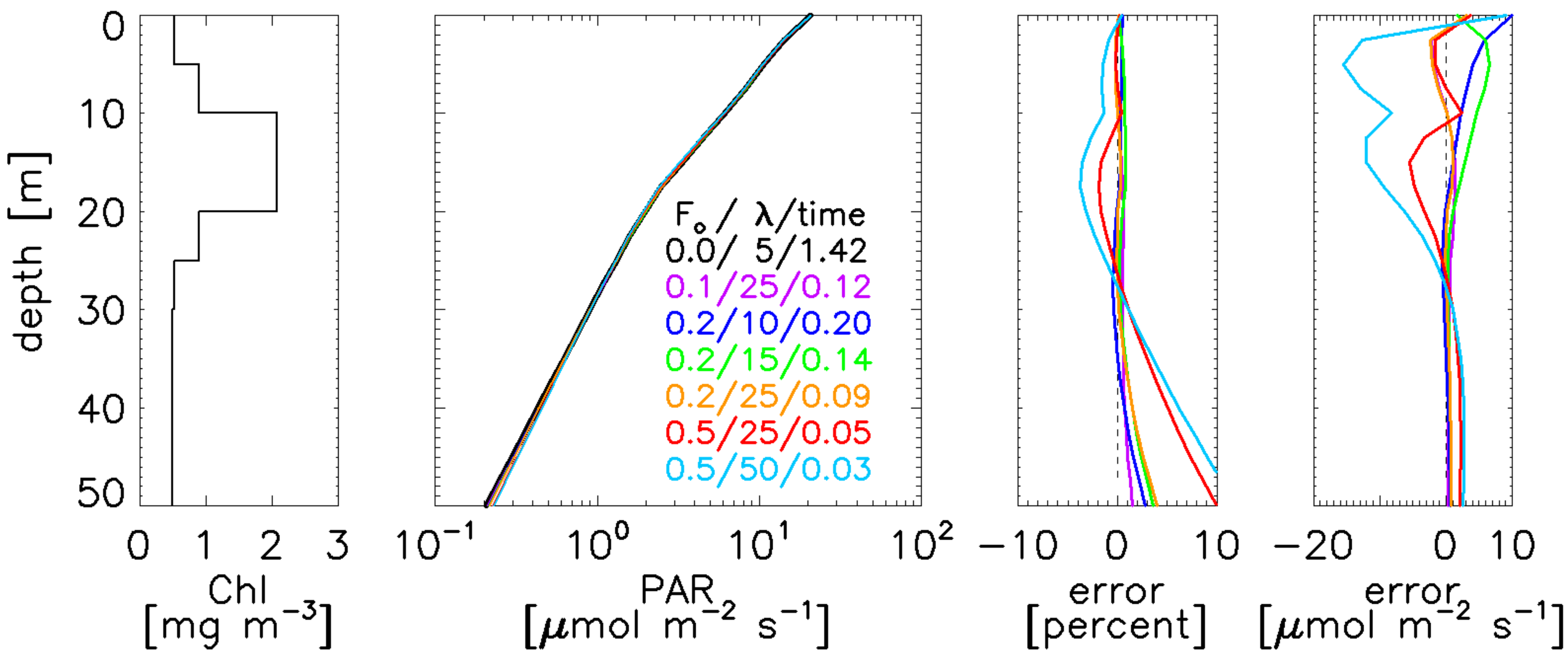
Effect of Skipping Wavelengths

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

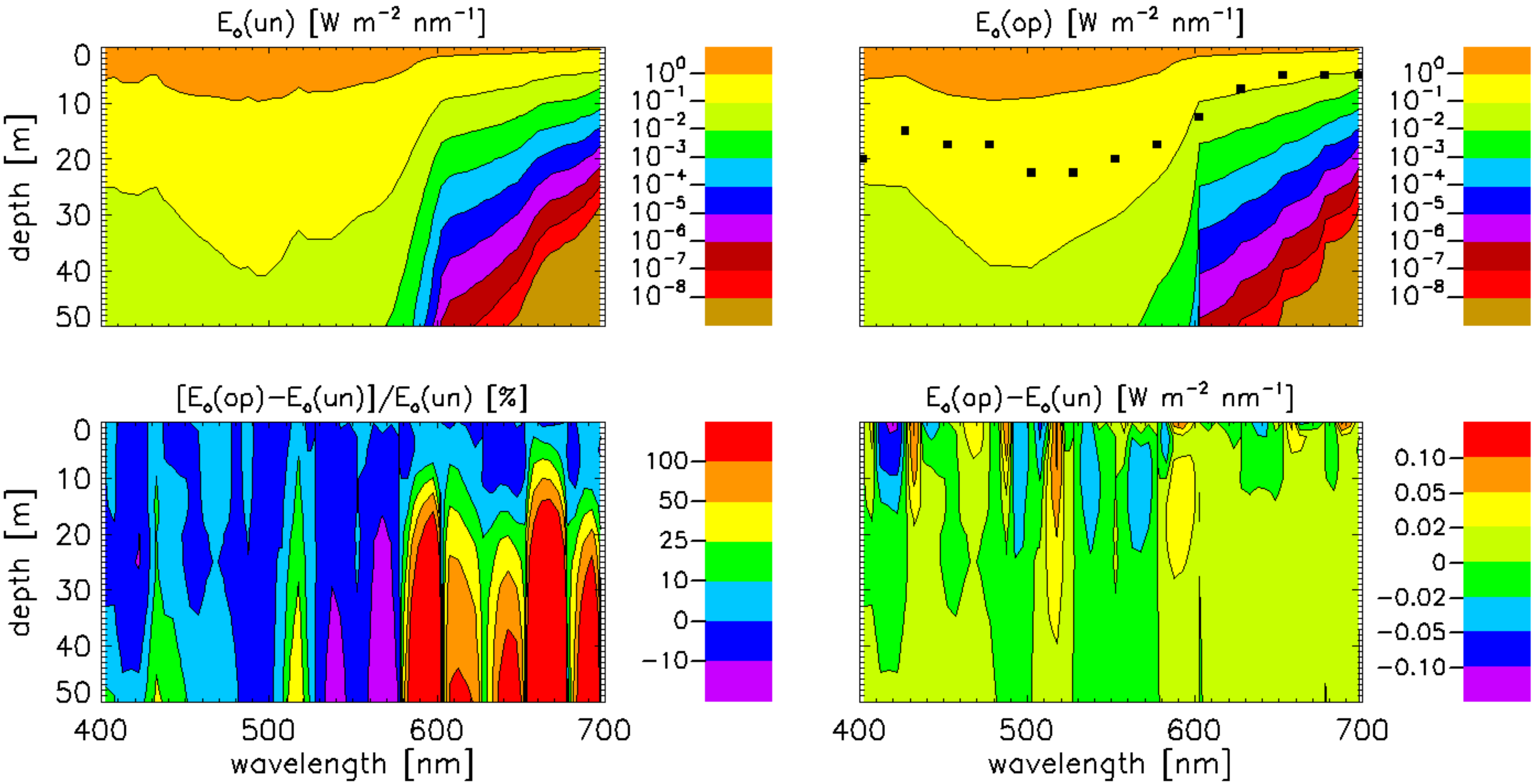
Various F_o depths (F_o as a fraction of surface E_o) and number of 5 nm bands skipped



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



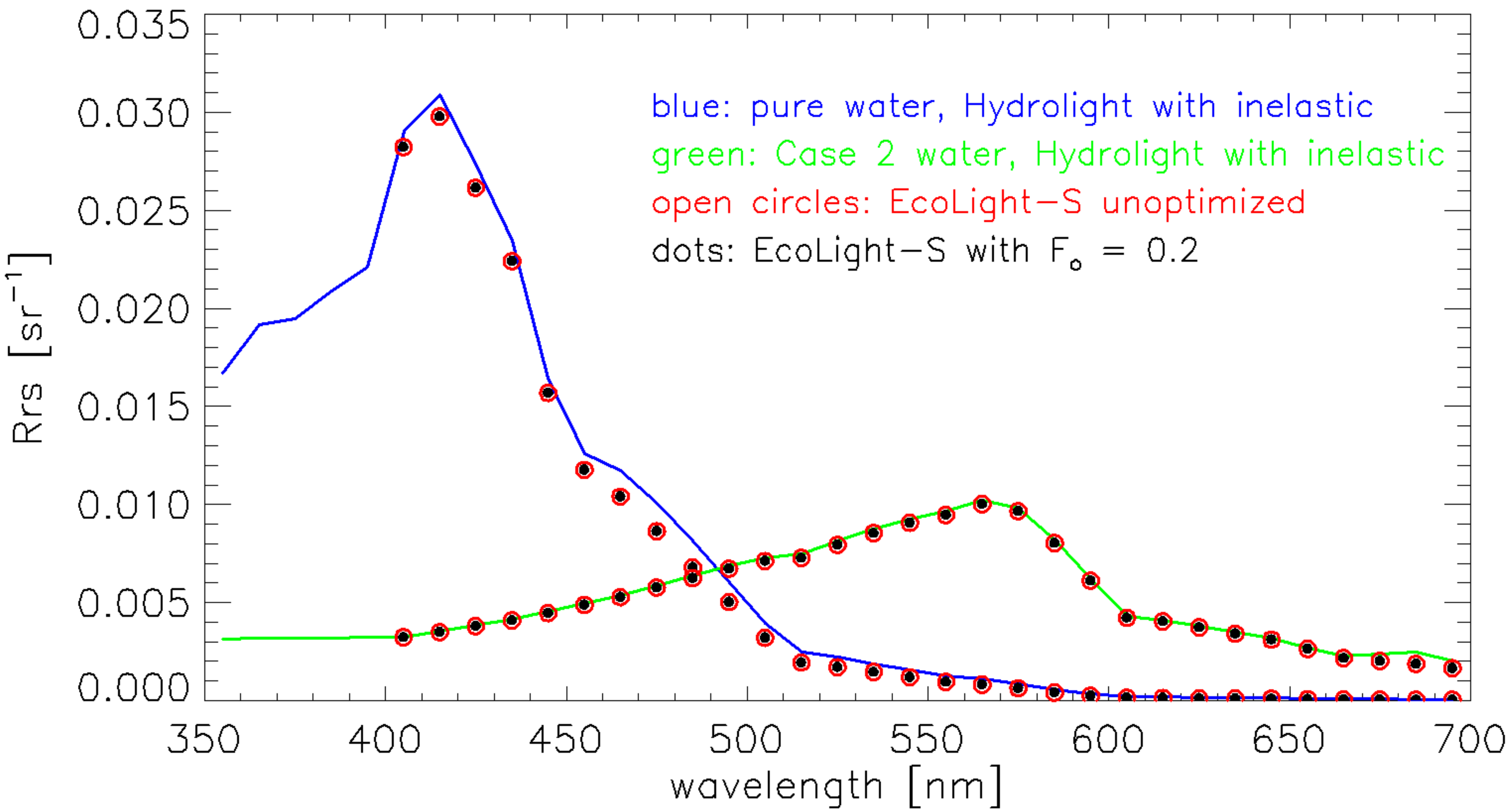
HydroLight vs. EcoLight vs. Ecolight-S Run Times

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

Pure water: $z_{max} = 400$ m; Secchi depth = 120 m			
model	PAR(z_{max}) [μ mol m^{-2} s^{-1}]	time [seconds]	difference [percent]
HydroLight 5.1 with inelastic	10.1330	427.1 (376.9)	—
HydroLight 5.1 without inelastic	9.6223	283.6 (268.4)	-5.0
EcoLight 5.1 with inelastic	10.1090	15.3 (12.8)	-0.2
EcoLight 5.1 without inelastic	9.1690	5.1 (4.6)	-5.1
EcoLight-S unoptimized	9.6578	2.71	-4.7
EcoLight-S with $F_o = 0.1$, 10 nm	9.6342	0.17	-4.9
EcoLight-S with $F_o = 0.2$, 10 nm	9.9650	0.13	-4.3
EcoLight-S with $F_o = 0.1$, 20 nm	8.7881	0.08	-13.3
EcoLight-S with $F_o = 0.2$, 20 nm	8.8332	0.07	-12.8
Case 2 water: $z_{max} = 20$ m; Secchi depth = 3.7 m			
HydroLight 5.1 with inelastic	1.6128	198.6 (162.3)	—
HydroLight 5.1 without inelastic	1.6032	108.3 (89.4)	-0.6
EcoLight 5.1 with inelastic	1.6068	6.7 (5.5)	-0.4
EcoLight 5.1 without inelastic	1.5968	2.3 (1.9)	-1.0
EcoLight-S unoptimized	1.5975	0.98	3.0
EcoLight-S $F_o = 0.1$, 10 nm	1.6606	0.28	3.0
EcoLight-S $F_o = 0.2$, 10 nm	1.7696	0.21	9.7
EcoLight-S $F_o = 0.1$, 20 nm	1.6594	0.15	2.9
EcoLight-S $F_o = 0.2$, 20 nm	1.7702	0.11	9.8

HydroLight vs EcoLight-S R_{rs} Spectra

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



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)

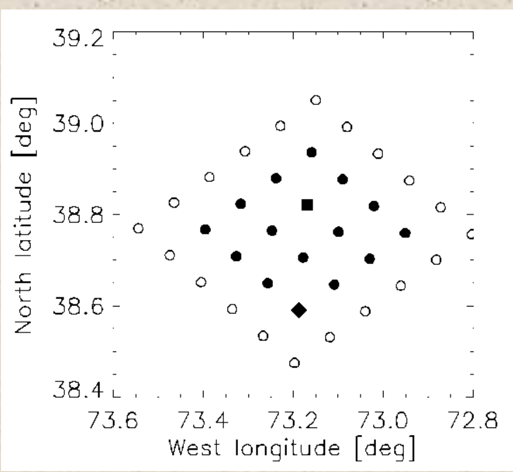
- 4 phytoplankton functional groups
- uses spectral irradiance (400 to 700 by 5 nm) to allow for competition between functional groups according to different light- and nutrient-dependent pigment suites
- default light model is a simple chlorophyll-based analytic model:

$$E_d(z,\lambda) = E_d(0,\lambda) \exp[-K(Chl,\lambda)\, z] \qquad (1)$$

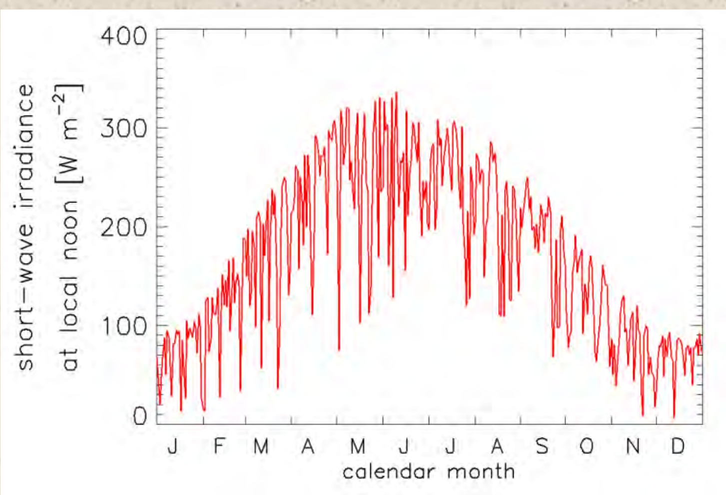
Initial timing studies applied BioToys to Case 1 water for which (1) is valid.

Replaced Eq. (1) by EcoLight-S for timing comparisons

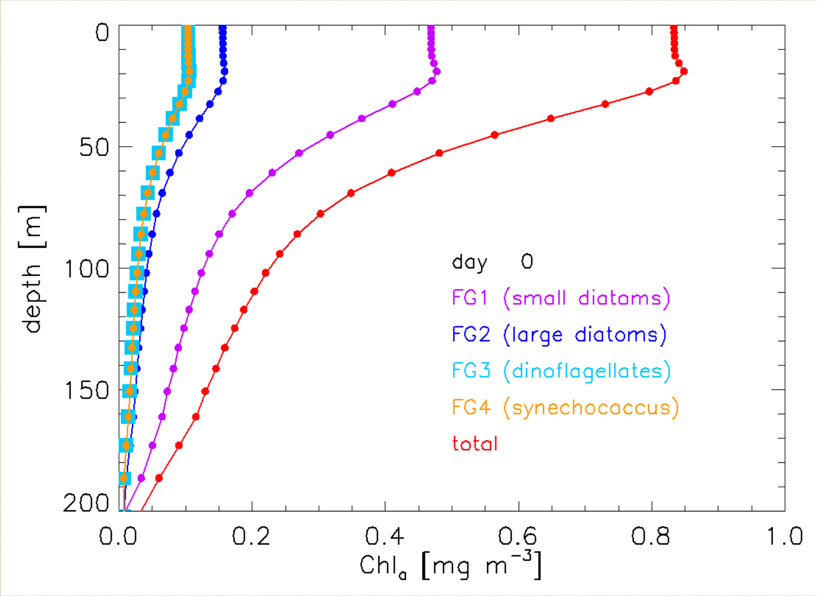
Example Simulation and Timing: Initialization



BioToys computational grid

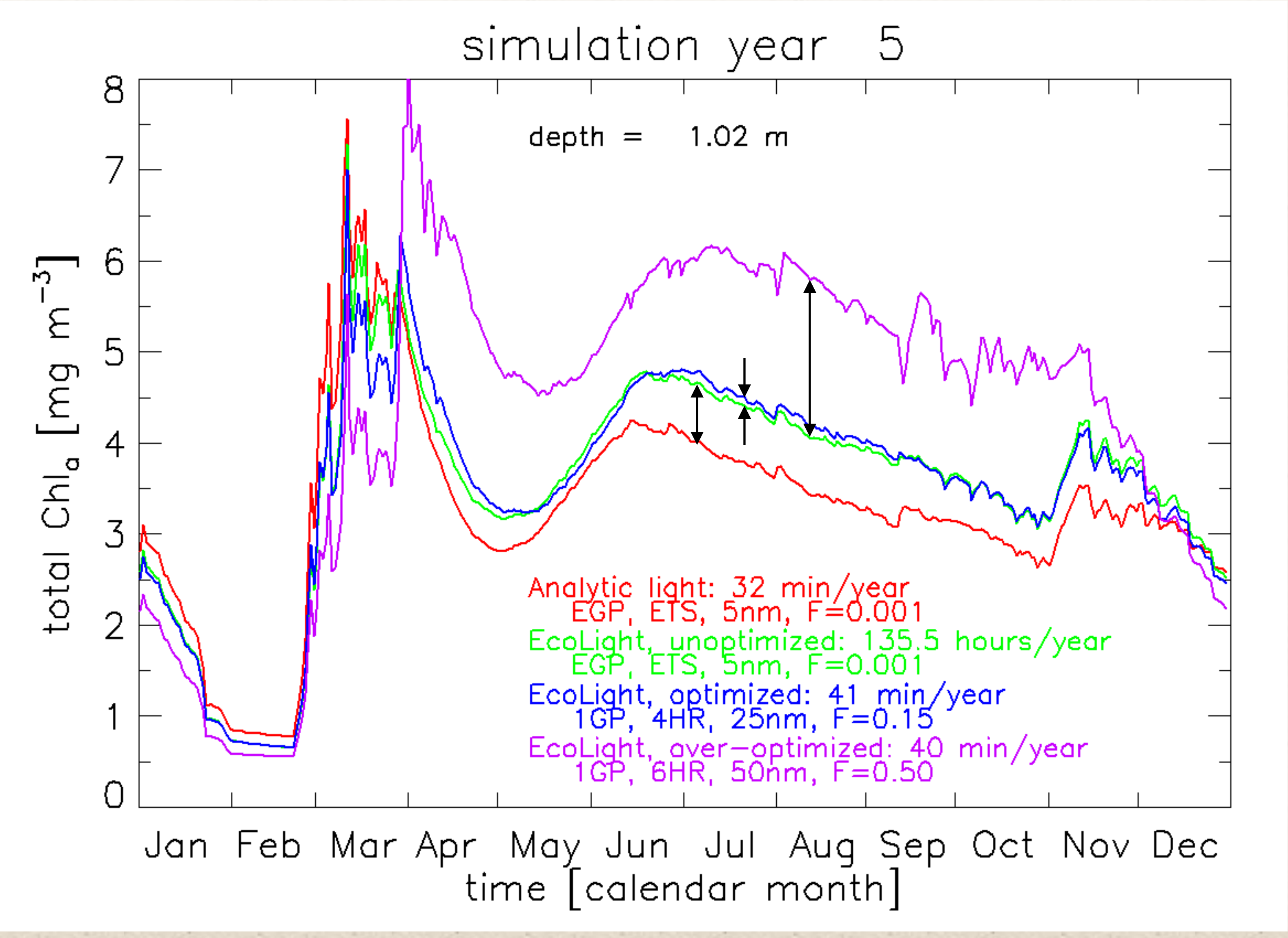


daily irradiance forcing

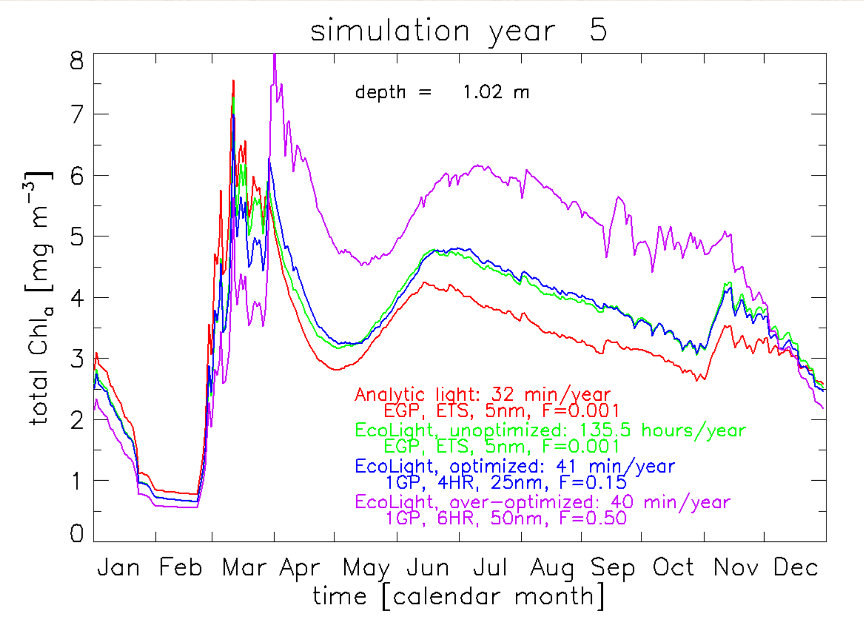


initial chlorophyll profile for 4 phytoplankton functional groups

Example Simulation and Timing: Results



Example Simulation and Timing: Results



- 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

ROMS Heating (standard version)

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

First law of thermodynamics (conservation of energy)
c_v = 3900 J/(kg K)
ρ = 1025 kg/m^3

$$\bar{E}_d(z) = \int_0^{1\text{ day}} \int_{\lambda_1}^{\lambda_2} E_d(z,\lambda,t)\, d\lambda\, dt$$

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

$$\Delta T = -\frac{1}{c_v \rho} \frac{\bar{E}_d(z_1) - \bar{E}_d(z_2)}{z_1 - z_2}$$

Change in temp (deg C) over 1 day for water between depths z_1 and 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, ξ_1, ξ_2 tabulated values.

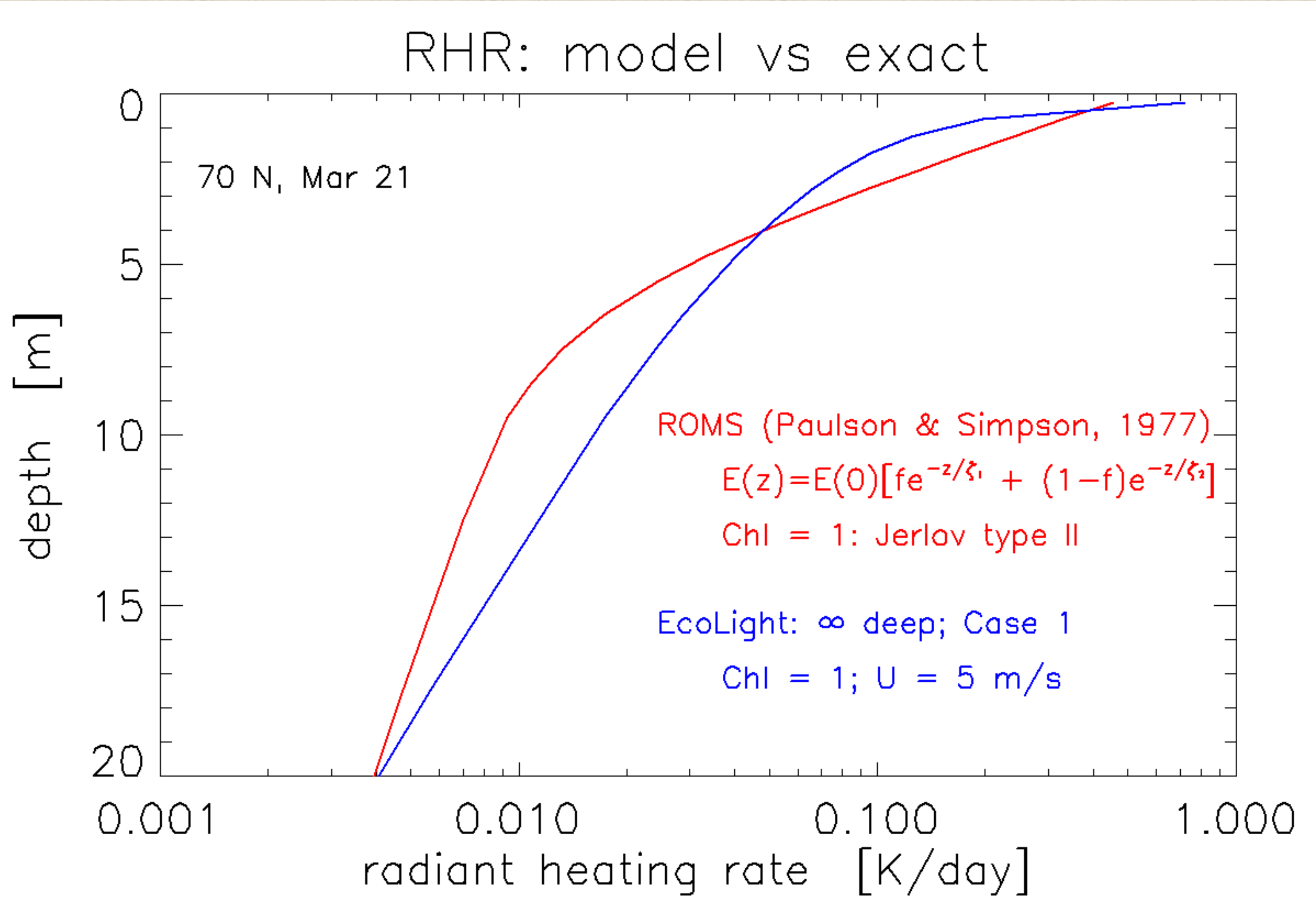
$$\bar{E}_d(z) = \bar{E}_d(0)\,[f \exp(-z/\xi_1) + (1-f)\exp(-z/\xi_2)]$$

The P&S model for E_d(z)

The P&S irradiance model is simple, computationally fast, easy to use, and ***almost always wrong as used in ROMS***

ROMS Heating: P&S vs EcoLight

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.



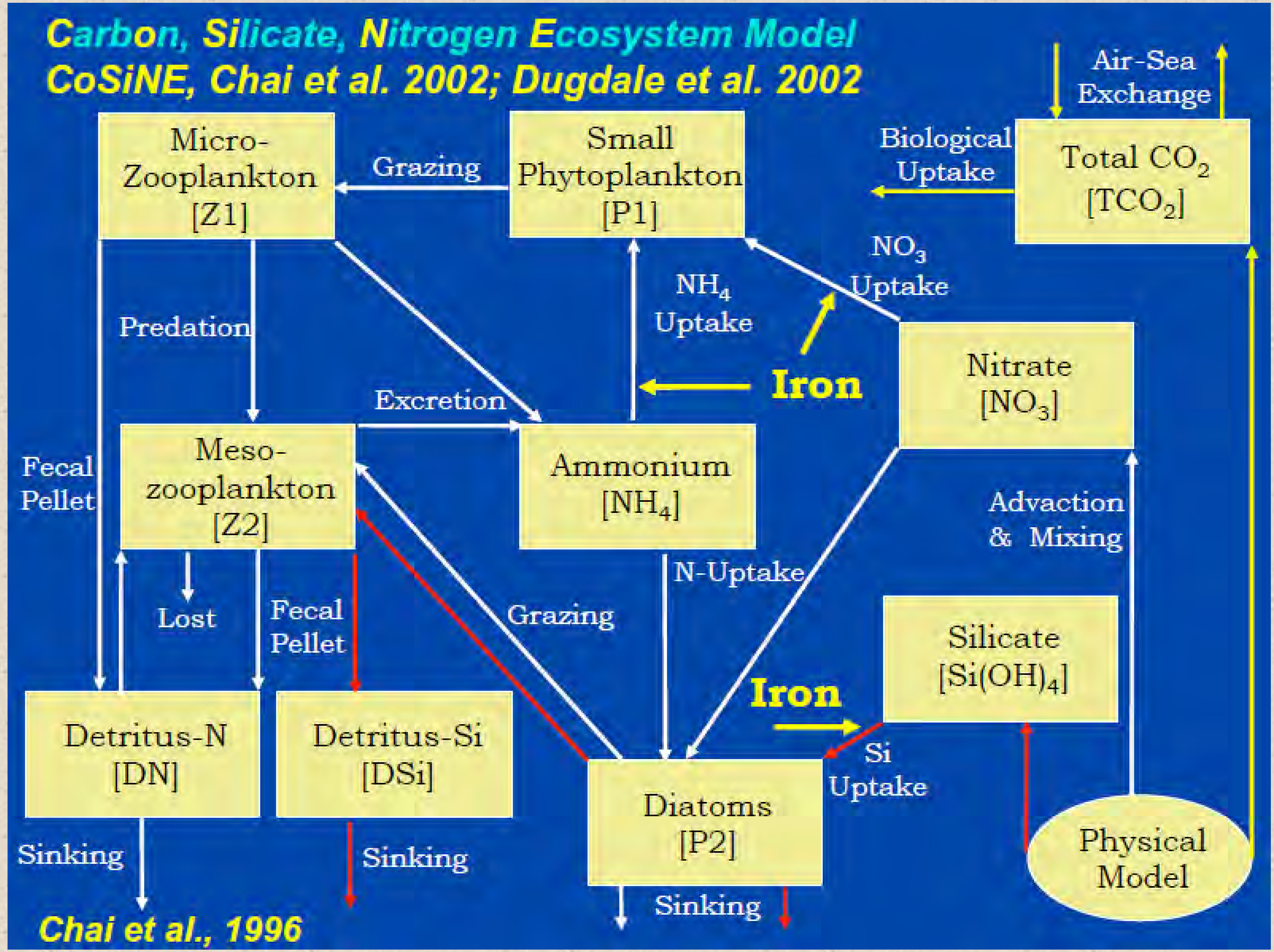
CoSiNE: Carbon Silicon Nitrogen Ecosystem

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 mesozooplantkon
- 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.



CoSiNE: Carbon Silicon Nitrogen Ecosystem

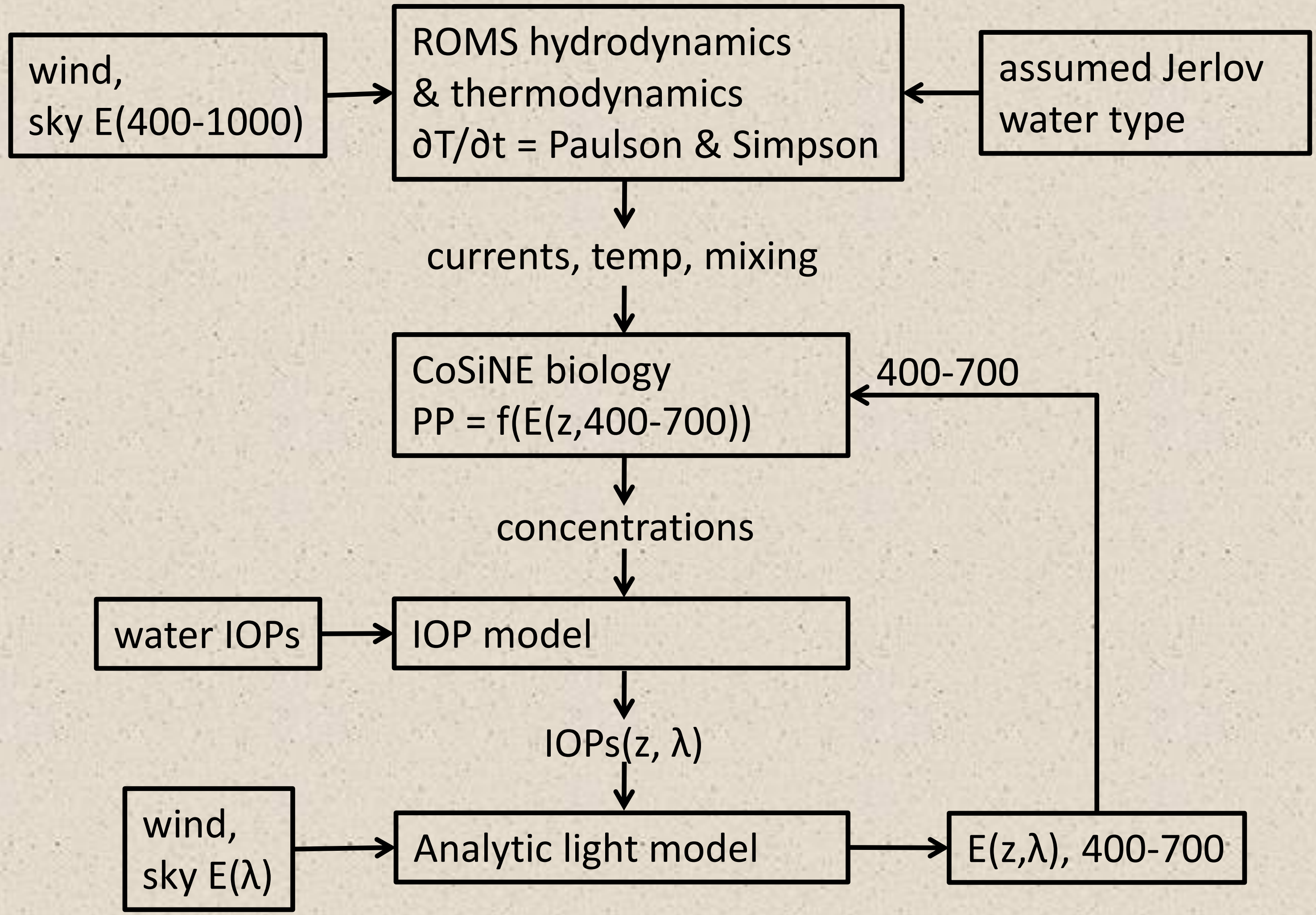
The latest version, CoSiNE-31, has 31 state variables (variables whose values are predicted and describe the biological state of the ecosystem).
The IOPs $a(z,\lambda)$, $b(z,\lambda)$, $b_b(z,\lambda)$ are determined from the red variables.

Nitrate concentration
Ammonium concentration
Silicate concentration
Phosphate concentration
Small phytoplankton N
Small phytoplankton C
Small phytoplankton CHL
Diatom concentration N
Diatom concentration C
Diatom concentration CHL
Coccolithophores N
Coccolithophores C
Coccolithophores CHL
Small zooplankotn N
Small zooplankotn C

Mesozooplankotn N
Mesozooplankotn C
Bacteria concentration N
Detritus concentration N
Detritus concentration C
Biogenic silicate concentration
Labile dissolved organic N
Labile dissolved organic C
Semi-labile dissolved organic N
Semi-labile dissolved organic C
Colored labile dissolved organic C
Colored semi-labile dissolved organic C
Particulate inorganic C
Dissolved oxygen
Total alkalinity
Total CO2

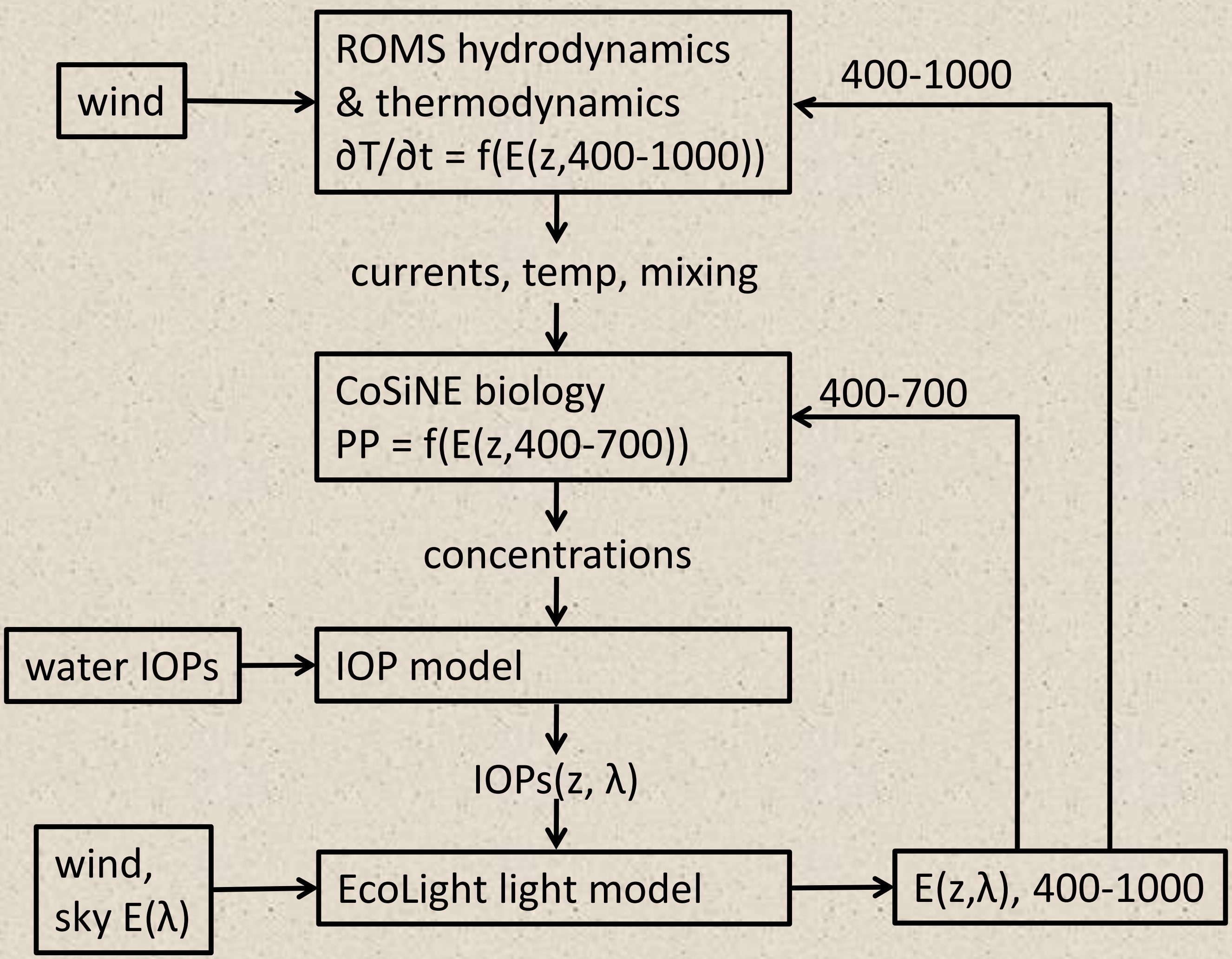
Original ROMS-CoSiNE Model

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



ROMS-CoSiNE-EcoLight Model

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