Notes on the implementation of the *Alexandrium fundyense* biological model into a 3D Hydrodynamic Model

Charles Stock

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Introduction

This document outlines the steps necessary for implementing the *Alexandrium fundyense* model developed during the ECOHAB-Gulf of Maine program into a 3D hydrodynamic model. The codes included in this directory are the core routines used for implementation into the model ECOM3D (Blumberg and Mellor 1987). Routines and some other aspects of the implementation will need to be modified depending on the hydrodynamic model used, model inputs, and the details of the application. The intent of this document and the codes included is to summarize the primary steps in the implementation, highlight a few of the pit-falls to avoid, and provide some sections of code that may save some time and effort. It is stressed that care should be taken to ensure consistency in units, time stepping, and other details that can vary according to the model used. It is also recommended that the germination model and growth model descriptions as well as associated publications (mentioned below) be read before implementing and applying the codes herein. Questions should be directed to Charlie Stock (cstock@whoi.edu) and Dennis McGillicuddy (dmcgillicuddy@whoi.edu).

The implementation of the model falls naturally into four sections:

1. Input of biological model forcing and biological model parameter values
2. Temporal cycling of the biological model forcing
3. Solution of the *A. fundyense* advection, diffusion, reaction (ADR) equation
4. Specification and creation of model output

While this document will discuss all the steps, the majority of time will be spent on steps 1 and 3. During the discussion, reference will be made to the various fortran codes included in this directory and having printed copies of these may be handy.

I. The biological model input

Necessary input for the *A. fundyense* model includes:

1. Values for the parameters of the biological model

2. Cyst concentration (cysts/cm^3) specified for each model grid point
3. Nutrient data (μM) for specification of the nutrient fields
4. Values of daylight averaged irradiance (watts/m^2). This should be averaged over 14 hours to be consistent with the laboratory data on which the model is based.
5. Any observations for model/data comparison

Most of the work for this section is accomplished in the routine biodat.f, which includes subsections for each of the inputs above. This routine also initializes the endogenous clock function by explicitly setting the values of the germination potential for each month. The details of the input for items 2-5 are flexible according to the way in which the fields and forcing are specified. The specification of the biological model parameters is a bit more particular, as values must be in the correct order and have the correct units if the germination and growth functions are to calculate rates and fluxes correctly. Table 1 provides a summary of this input, and an example is given in the file 'params'.

Table 1: Biological model parameters. Values and ranges listed are those considered in Stock et al. (submitted). Note that attenuation coefficients are given + values

Parameter	Description	Units	Value (Range)
$\mu_{max}(T_{opt},S_{opt})$	The maximum growth rate at optimal temp./salinity	$days^{-1}$	0.58 (0.46-0.70)
d_g	The germination depth	cm	1.0 (0.5-1.5)
K_N	Nutrient Half-saturation constant	μM	0.0-3.0
m	mortality	$days^{-1}$	0-0.3
α_g	The growth efficiency	$watts^{-1}\ m^2\ day^{-1}$	0.36 (0.17-0.56)
μ_o^r	The maintenance respiration rate	$days^{-1}$	0.2 (0.15-0.25)
k_w	The diffuse attenuation coefficient in water	m^{-1}	0.2 (0.15-0.25)
k_s	The diffuse attenuation coefficient in sediment	mm^{-1}	3.5 (2-5)
E_{lgt}	The "light" germination threshhold	watts/m^2	2.4 (1.2-3.6)
E_{drk}	The "dark" germination threshhold	watts/m^2	1% of E_{lgt}, (0.1-10% E_{lgt})
w_a	The *A. fundyense* vertical swimming rate	m/day	10 (5-15)

The biodat.f routine should be placed in the initialization phase of the hydrodynamic model (i.e. before time-stepping begins). Many of the parameters defines in biodat.f will be needed within subsequent functions. While some are passed directly in the function calls to aid modularity of the code, others benefit from inclusion in an 'include' file or other construct which allows sharing of the biological model variables between different routines. The file dino.inc was used for this purpose in the present implementation. Opening of input files and assignment of relevant file identifiers (e.g. IUBIO, IUCYS, IUNIT etc.) should be done prior to calling this function.

II. Temporal cycling of biological model forcing

The values of environmental variables relevant to the biological model must be set during each time step prior to solving for the transport, sources and sinks of *A. fundyense*. Within the present formulation, this requires that the temperature (^{o}C), salinity (ppt), irradiance (watts/m^2), and nutrients (μM) be set for each model grid cell. The hydrodynamic model provides the temperature and salinity, but short codes must be written to cycle through the irradiance and nutrients specified by the input section above.

III. Solution of the *A. fundyense* advection, diffusion, reaction equation

Once the biological model forcing has been set, the evolution of the *A. fundyense* populations within the model can be calculated. This requires the inclusion of the *A. fundyense* concentration as an additional prognostic variable. Many ocean models already allow for a passive tracer, and this can often be easily adapted to *A. fundyense*. In the present formulation, the following steps are taken:

1. The routine endoclock.f calculates the germination potential
2. The routine cellflux.f is called to determine the flux of new cells from the sediment via germination from resting cysts.
3. The flux is added to existing concentrations and cells are advected and diffused by the currents and mixing fields provided by the hydrodynamic model.
4. Cell concentrations are enhanced or attenuated according to the net growth rate calculated by the routine dinogrow.f.

The precise order of steps 2-4 is flexible (i.e. one could solve for the growth first, then transport cells, and then update concentrations according to the germination). The details of the growth and germination function can be found in the function descriptions (see web page), or in publications of Anderson et al.(submitted) and Stock et al. (submitted). Reading these publications before applying this model is highly recommended, as they give a sense for the strengths and weaknesses of the model.

Routines for the transport of temperature and salinity are easily adjusted for transport of *A. fundyense*. If vertical swimming behavior is desired, this can be accomplished by augmenting the vertical fluid velocity within the advection routine. Specification of boundary conditions can also be done in parallel with the temperature and salinity calculations. However, it is important that careful attention be paid to the details of the time stepping (e.g. if a leap-frog type scheme is used for advection, make sure you adjust the fluxes for 2 time steps, this is the case with the dinogrow.f from the website). ***Also, it is highly recommended that a positive definite advection scheme be used.*** It is quite likely that simulations will produce relatively sharp fronts between areas of high concentrations very low concentrations. Under these conditions, some non positive-definite schemes (e.g. centered differences) will create oscillations between negative and positive values that. If such negative values are corrected at each step, there is a potential that significant addition of cells will occur, invalidating the mass balance.

This section ends with a short discussion of scalability. Often times it may be desired to run multiple biological simulations with each hydrodynamic simulation. This is possible using the codes provided, although it takes a bit of effort. First, additional rows must be added to the "params" file and the input loops in biodat.f must be expanded to accommodate such additional input. Then, additional state variables (table 2) need to be added. This can be done by incrementing the numeric value at the end of the state variables accordingly. Also, each step in the ADR calculation must be duplicated for each set of biological model parameters. This is facilitated by the subroutine passing formats. Each routine allows the passage of specific state variables from biological model setting "n" (e.g. CYSTINITn, CYSTBEDn, where n = 1, 2, 3...) in generic

variables (CYSTINIT, CYSTBED, ...) within the subroutines (see codes included). An integer value (II) is also included in the variables passed as a reference to the correct row in the parameter file. For example, the germination related variables for the first biological model setting are passed to the routine cellflux.f via:

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CALL CELLFLUX(CYSTINIT1,CYSTBED1,GRATE1,CELLFLX1,CCELLFLX1,...
                    GRMADD1,PGERM1,1)
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within cellflux.f, they are passed to CYSTINIT, CYSTBED, etc. and II = 1. The II references a row in the array BIOMOD, which is used to set the values k_w, k_s, E_{lgt}, E_{drk}, and d_g for the first biological model setting. If one is simulating many different biological model settings, it is fairly straightforward to expand this to any desired number of settings. This avoids the necessity of resolving for all of the hydrodynamic state variables for each perturbation in biological model parameters.

IV. Output

Within the codes provides, several variables are tracked for the primary purpose of providing output suitable for interpretation of results. These are summarized in the table 2 below. It is left to the user to write the code necessary to store these variables at desired time increments and in desired formats (CDF, HDF etc.).

Table 2: State variable arrays within the biological model. First biological model setting uses CYSTINIT1, CYSTBED1, GRATE1..., second biological model setting uses CYSTINIT2, CYSTBED2, GRATE2, ..., the N^{th} uses CYSTINITN, CYSTBEDN etc. All the variables below are 2D, with the exception of GROW, which is 3D.

Variable	Description	Units
CYSTINIT(1..N)	The initial number of cysts	cysts in top d_g cm m^{-2}
CYSTBED(1..N)	The present number of cysts	cysts in top d_g cm m^{-2}
GRATE(1..N)	The germination rate	%/day
CELLFLX(1..N)	The cell flux	cells m^{-2} time $step^{-1}$
CCELLFLX(1..N)	cumulative flux of cells	cells m^{-2}
GRMADD(1..N)	Number of cells added via germination per time step	number of cells time $step^{-1}$
PGERM(1..N)	The percentage of cysts germinated	% of initial cysts germinated
GROW(1..N)	The growth rate	day^{-1}
GROADD(1..N)	The number of cells added by growth per time step	number of cells time $step^{-1}$

ANDERSON, D. M. and others submitted. Experimental and modeling observations of *Alexandrium fundyense* cyst dynamics in the Gulf of Maine. Deep Sea Research II.

BLUMBERG, A. F., and G. L. MELLOR. 1987. A description of a three-dimensional coastal ocean circulation model, p. 1-16. *In* N. Heaps [ed.], Three-Dimensional Coastal Ocean Models. American Geophysical Union.

STOCK, C. A., D. J. MCGILLICUDDY, A. R. SOLOW, and D. M. ANDERSON. submitted. Evaluating hypotheses for the initiation and development of *Alexandrium fundyense* blooms in the western Gulf of Maine using a coupled physical-biological model. Deep Sea Research II.