Improving the validity and robustness of a Harmful Algal Bloom model through genetic algorithm-based optimization Arjay C. Cayetano¹, Aletta T. Yñiguez^{2*}, Cesar L. Villanoy³, Laura T. David³, Josephine Dianne L. Deauna¹, Eileen L. Peñaflor⁴, Joseph Dominic H. Palermo⁴, Garry A. Benico⁴ and Rhodora V. Azanza³

ABSTRACT

To study the complex patterns governing Harmful Algal Blooms (HAB), an individual- or agent-based modeling approach was employed. The constructed model was able to mechanistically represent both the biological and the physico-chemical factors involved during events of bloom and decline of the toxic dinoflagellate, Pyrodinium bahamense var. compressum (Pbc), within Sorsogon Bay. An inherent problem with this approach, however, is that as the model complexity increases, it becomes harder to fit the model results to the in situ data during model calibration. The traditional approach to deal with this is to manually tweak the values of model parameters until the model output stabilizes or attains good agreement with field observations. However, this method is time-consuming and does not guarantee accurate results. Hence, automated calibration of the Sorsogon Bay HAB model was designed, which makes use of an optimizer in the form of a genetic algorithm (GA). In this paper, we investigate the effect of variations of the initial vertical distribution of Pbc (distribution of cells among different depths) on the model outcomes of cell increase and transport. The GA approach was used to determine the fit of the model output to field observations expressed as an optimization problem. The genetic algorithm provides values for model parameters during each simulation run and takes the error between the model output and the expected result as the objective for optimization. The GA-provided values for model parameters will then be incorporated into the model resulting to a more robust and valid representation. The calibrated model provides insights into the role of advection and spatial distribution on Pbc dynamics, and can then be more confidently used to explore various scenarios that could provide clues regarding the patterns of HAB and decline within Sorsogon Bay.

Key words: harmful algal blooms, model, Pyrodinium, Sorsogon Bay, genetic algorithm

INTRODUCTION

Harmful algal blooms are recurring events in many bays of the Philippines and other Southeast Asian countries causing considerable losses to the economy and unfortunate fatalities (Azanza and Taylor 2001). The main causative organism involved is a cyst-forming dinoflagellate known as Pvrodinium bahamense var. compressum (Pbc). The species has a complex life cycle having two primary stages: the benthic cyst stage and the motile cell stage (Anderson et al 2005; Azanza et al 2004; Azanza 1997; Usup and Azanza 1998). Each stage is known to be highly influenced not only by internal biological factors but also by external environmental conditions. Data obtained from literature as well as from laboratory experiments showed the complex patterns by which environmental conditions such as light, temperature, salinity, nutrient concentration and water circulation influence the various biological processes such as the encystment of Pbc cells, excystment of Pbc cysts, their mortality as well capability for growth and reproduction (Usup and Azanza 1998; Etheridge and Roesler 2005; Heisler et al 2008; Lim et al 2006; Philips et al 2006; Klausmeier and Litchman 2001). Hydrodynamic conditions, particularly water advection has been found to be a significant influence in the development and dispersion of blooms. Cysts are

able to re-suspend due to particular water velocities at the bottom of the water column (*Villanoy et al 2006*). While the cells can be transported to areas appropriate for growth or accumulated in particular areas depending on water column stability (e.g., *Fauchot et al 2008*; *Stumpf et al 2008*). Thus, in this study, the aim is to investigate the influence of advection on cell distributions and potential bloom formation using a genetic algorithm optimization approach; particularly looking at how spatial distribution is affected by advection, and conversely, how initial distributions in the model affect model outcome. This is relevant as well since information on the spatial distribution of Pbc cells is sparse due to sampling constraints.

The site for this study is Sorsogon Bay, a 20 km by 10 km bay situated at the east side of the Philippines (**Figure 1**). Sorsogon Bay has had intermittent HABs documented since 2002. A HAB agent-based model was constructed (*Yñiguez et al 2012; Cayetano et al 2011*) using the MASON agent-based modelling toolkit (*Luke et al 2004*) for the bay such that spatial and temporal data on Pbc bloom and decline can be easily observed in a manner akin to actual field studies.

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Figure 1. Sorsogon Bay location (Source: Yñiguez et al 2012).

Initial simulation run outcomes on the spatio-temporal abundances of Pbc did not coincide with field observations. Hence, data gathered from field studies conducted during the year 2009 (Azanza, Benico and Baula 2010), were used to calibrate the model spatially and seasonally, in order to provide a more reliable model. The calibration process also allowed for the assessment of the important processes that contribute to making the model capture realistic behaviour. Typically, manually tweaking of specific parameters is conducted but as the number of such parameters grow, the difficulty in calibrating the model drastically increases. Moreover, manual tweaking is open to errors since the choice of values can be arbitrary and fairly user-biased.

Here, we present an automated objective process by which the calibration of the HAB model can be done via an optimization algorithm known as genetic algorithm. In each round or generation of this algorithm, there is a population of candidate solutions corresponding to the sets of values of the decision variables (i.e. model parameters) being tweaked which are evaluated for their fitness expressed in terms of the objective being optimized (*Mitchell 1995*). Fit solutions are then selected which are favored to undergo reproduction in order to produce new candidate solutions. To accomplish this, the solutions basically have two forms: the phenotype and genotype representations. The former corresponds Improving the validity and robustness of a HAB model

to the intended or actual values of the variables, while the latter is where operators in the form of mutation and cross-over are done, which can produce new solutions for the next generation (*Mitchell et al 1991*). This process is repeated until a specific criterion is met such as a good enough solution or after reaching a specific time period. Some of its applications to agent-based model calibration and optimization include the works of *Narzisi et al* (2006) on emergency response systems and *Zhang et al* (2010) on optimizing land use allocation.

In this study, an independent genetic algorithm program runs alongside the model simulation which does the tweaking of the model parameters as well as comparison with the actual field data via least square error computation. In order to study the effects of spatial distribution and advection on model outcomes, the selected parameters for tweaking involve the proportions of Pbc cells for seeding within five specific depth layers. This initial condition of the model can have a large effect on the ensuing outcomes as shown by preliminary simulations. In other words, a key uncertainty in the model is the vertical distribution of Pbc cells among different depths. The set-up for the algorithm therefore not only accomplishes model fitting but also answers an important question regarding how the Pbc cells are distributed at various depths and whether the change of bloom location is mainly due to the advection driven movement of Pbc cells.

MATERIALS AND METHODS

Model Construction



Figure 2. Model events during each time-step (Source: Yñiguez et al 2012).

Updates in the environmental data except circulation occur first followed by updates for the biological processes

associated with both the Pbc cells and cysts. In other layers at hourly intervals while that of vertical velocity words, each simulation grid in the model is updated daily for the new values for light, temperature, nutrient, and salinity before the agents respond based on their known responses and move due to water circulation and their buoyancy. The conceptual framework of the model, as well as how the bay and the Pbc cells and cysts are represented in the model (Figure 3).



Figure 3. Pbc cell (green) and cyst (red) as represented in the model. (Source: Yñiguez et al 2011).

Environmental Updates

A watershed and hydrodynamic model of Sorsogon Bay were developed from which inputs for the biological model were derived (Figure 4). The raster-based watershed model, called Nonpoint-Source Pollution and Erosion Comparison Tool (N-SPECT) (developed by the US NOAA Coastal Services Center) yielded the nutrient load estimate. This model, which runs in a geographic information system (GIS) environment, can be downloaded free of charge at www.csc.noaa.gov/digitalcoast/tools/nspect/. Monthly nutrient (Nitrogen) concentrations were given for each of the rivers flowing into Sorsogon Bay. To be able to determine the concentration at other locations in the bay, a simple diffusion algorithm from MASON (Luke et al 2004) was applied involving assumed uptake rate of nutrients by Pbc as well as assumed diffusion rate via concentration gradient. To have daily values, the process was repeated daily using the monthly averaged value for river mouth nutrient concentration.

For the inputs on the water circulation, temperature and salinity of Sorsogon Bay, a hydrodynamic model was developed using DELFT3D. This hydrodynamic model is influenced by tides, wind and heat fluxes (Deauna et al 2011). Water circulation, temperature fluctuations and salinity changes were simulated from January 2009 to December 2009. The data for water circulation

values have a daily interval. Compared to the spatial granularity of the grid dimensions of the biological model, the velocity data is coarser. Hence, to obtain values for cells in-between, linear interpolation was done.

Since the HAB agent-based model has a daily time step, the horizontal position of agents at one time step is computed by iteratively going through the 24 horizontal velocity values moving from one point to the next.



Figure 4. Snapshots of the environmental data inputted into the agent-based model: a) nitrogen; b) water circulation; c) light; and, d) temperature-salinity plot. (Source: Yñiguez et a, 2012; Yñiguez et al 2011; Cayetano et al 2011; Deauna et al 2011).

The temperature and salinity derived from the DELFT-3D physical model of Sorsogon Bay is also similar to the circulation data in terms of spatial granularity, hence, these also needed to be interpolated. However, the temporal variability was already set to daily, which is in accordance to the agent-based model time step.

Lastly, for the light inputs, MODIS data with a 4 km resolution was obtained from GIOVANNI (Acker and Leptoukh 2007; http://disc.sci.gsfc.nasa.gov/ giovanni/overview/index.html). With this resolution, the bay can be divided into several squares of varying surface light intensities. Values for the different depths involve horizontal velocity values at five different depth were computed using the Beer-Lambert's Law of light

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attenuation. The data is monthly averaged hence such value is used for all the days of the corresponding month.

Biological Updates

There are two distinct agents in the model: the Pbc cell agent and the Pbc cyst agent. As seen in the diagram in **Figure 2**, the Pbc cell agent undergoes four biological events, namely mortality, movement, encystment and reproduction while the Pbc cyst agent undergoes only three events namely mortality, movement and excystment.

Computation of the mortality for both the Pbc cell and cyst makes use of a stochastic rate and is not spatially or temporally variable. Movement is passive for both agents and is basically driven by horizontal as well as vertical water circulation (Villanoy et al 2006). Encystment and excystment depends on the current environmental factors based on known temperature, salinity and nutrient triggers (Usup and Azanza 1998; Villanoy et al 2006; Gedaria et al 2007). Lastly, Figure 5 shows the functions used in the model describing the reproduction potential of Pbc cells against varying values of light, temperature, salinity and nutrient conditions within their immediate environment. The model functions are derived from a meta-analysis of experimental studies and literature values for Pbc and dinoflagellates (Usup and Azanza 1998; Yñiguez et al 2011; Follows et al 2007; Camoying et al 2009; Eppley



Figure 5. Growth response of Pbc cells against varying light (a), salinity (b), temperature (c), and nutrient (d) levels. (Source: *Yñiguez et al 2011 and Yñiguez et al 2012*).

and Thomas 1969; Carpenter and Guillard 1971; Lomas and Glibert 2000). Details on the biological functions and values can be found in *Yñiguez et al* (2012).

Model Calibration

Initial runs of the HAB agent-based model were conducted to assess the stability of simulation outcomes of the bay-wide bloom and decline of Pbc cell populations. Adjustments of model parameters needed to be done to ensure that model outcome is in accordance with field observations.

In lieu of time-consuming manual adjustments of sets of model parameters, this study instead performed an automated calibration via genetic algorithm to provide values for unknown parameters, in particular the initial spatial distribution of Pbc cells. In this way, the calibration performs two things: it aligns the model result to the field observations hence increasing the validity of the model; and it suggests optimum values for the unknown or uncertain parameters that are difficult to provide values for, and allow the model to produce realistic outcomes.

Exploratory Model Fitting

As mentioned earlier, an optimization process in the form of a genetic algorithm is used not only to increase the validity of the model by fitting the result to actual data but also to explore the unknown quantities and parameters. One key unknown parameter is the distribution of Pbc cells with depth (i.e. vertical distribution). Field sampling typically only gives information on a few stations and quantify their abundances only at the surface and bottom of these stations. The genetic algorithm was used to look at the particular influence of water circulation on the actual bay-wide horizontal distributions of Pbc cells. Using the bay-wide horizontal distribution of Pbc cell population from August 2009 to September 2009, this study was able to investigate the influence of the water-circulation driven movement of Pbc cells situated at different depth layers.

To accomplish this, the model was initialized in approximately the same pattern as the bay-wide horizontal percentage distribution observed at the stations during the field study (*Azanza, Benico and Baula 2010*) on August 2009 (**Figure 6a**). To account for the Pbc cell population outside the stations, the whole bay was seeded with 1000 Pbc cell agents at random points in addition to the seed at the stations which sums up to 3000 agents and divided among the stations following the percentage distribution from August 2009 fieldwork. Then, the final simulation result was obtained after one-month equivalent simulation run which was then compared to the bay-wide horizontal distribution of Pbc cell population observed during the field study on Journal of Environmental Science and Management (Special Issue 1-2013)

September 2009 conducted by the same researchers (**Figure 6c**).

Optimization Set-up

The following criterion or objective was set for the genetic algorithm to optimize:

Minimize the least squared error between the model output in terms of the percent distribution of Pbc cells at the different sampling stations (i.e. bay-wide horizontal distribution) for September 2009 against that of actual data.

The following are the model parameters (i.e. decision variables) which were used for tweaking:

Initial percent distribution of Pbc cells for depth layers 1, 2, 3, 4 and 5 (i.e. vertical distribution) at various stations for August 2009.

In the framework of the interaction of the genetic algorithm-based optimizer (available at http://www.iitk. ac.in/kangal/codes.shtml) and the HAB model (**Figure 7**), the genetic algorithm provides the percentages per depth layer by which the initial Pbc cells in the HAB agent-based model will be seeded. The HAB model, in turn, takes those values to run the simulation and then provides the relevant outputs after the run, namely the spatial (horizontal) distribution of Pbc cells throughout the bay. The genetic algorithm then obtains the simulation outputs in order to compute for the next values of the percentages per depth layer needed for



Figure 6. Bay-wide horizontal distribution of Pbc cells in actual data (*Azanza, Benico and Baula 2010*), with the corresponding pattern visualized in the model: a) August 2009 observed cell distributions; b) model representation of this distribution; c) September 2009 observed cell distribution; and, d) expected model result (approximate).



Figure 7. The interaction of the genetic algorithm and the HAB agent-based model. (Source: Yñiguez et al 2011).

initial Pbc cell seeding. The process was repeated until the criterion or objective for optimization specified attains a sufficiently satisfactory value.

RESULTS AND DISCUSSION

The distribution of phytoplankton is recognized as being quite patchy. Scientists have been debating whether physical or biological mechanisms are responsible for this phenomenon (Martin 2003). Horizontal advection, diffusive and turbulent processes are some of the physical processes hypothesized to influence their distribution. The biological processes that can cause patchy plankton distribution are growth, grazing and directed behaviour. Most studies have focused on the role of physical processes although various studies looking at the role of biological processes have recently been conducted (Palermo et al 2009). Those looking at the physical processes have typically investigated the effect of horizontal advection on bloom development and transport (Villanoy et al 2006; He et al 2008; Crespo et al 2011; Dippner et al 2011). The role of vertical patchiness in relation to advective processes in bloom development and transport is not as well understood. Based on field surveys conducted at Sorsogon Bay, horizontal spatial heterogeneity has been observed, the limited surface and bottom samples can only hint at patchiness in vertical distribution as well. However, this vertical distribution can play a large part in the resulting advective trajectories of Pbc cells in the model. The horizontal and vertical water velocities do influence where Pbc cells end up and the environmental conditions they experience since the environmental factors are spatially-explicit. With the combination of physical factors and biological processes represented in the model, this study aided in clarifying their roles in the ensuing spatial distribution of Pbc cells.

It can be easily observed from the model how the general water circulation strongly influences the concentration of Pbc cells at certain locations within the bay. For instance, seeding the cells at various depths and observing the results after three months gives the patterns shown in **Figure 8**.

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Figure 8. The resulting patterns of Pbc cell (green) and cysts (red) after one simulation run equivalent to three months where all cells are seeded at the top depth layer (a), at the middle depth layer (b), and at the bottom depth layer (c) during initialization.

It is therefore important for us to know how the Pbc cells are vertically distributed since this highly influences how they will consequently be horizontally distributed throughout the bay as seen from the HAB model simulations in **Figure 8**.

A total of 120 simulation runs were performed and given such number of runs, the most optimal seeding combination was returned by the genetic algorithm (**Table 1**). Hence, the outcome in **Table 1** give the necessary seeding of Pbc cells at each depth layer during initialization in order to simulate the horizontal distributions seen in the field during the September sampling:

 Table 1. Percent distribution for seeding Pbc cells returned by one round of optimization via genetic algorithm.

Depth Layer	Percent Distribution for Seeding Pbc Cells
1	9.6
2	15.9
3	13.7
4	0.008
5	31.1

The expectation is that if the Pbc cells were seeded using the depth-wise vertical distribution returned by the genetic algorithm, the resulting bay-wide horizontal distribution would be similar to the pattern shown in **Figure 9a** which is the actual bay-wide horizontal distribution for September 2009. However, a different pattern instead emerged as shown in **Figure 9b**.

In the model, there is a greater tendency for Pbc cells to encyst if they are seeded closer to the bottom. Hence, the high Pbc cell population that were initially at the center of the bay decreased not due to advection but by encystment. Since the actual data for September implies that the Pbc cells should be less concentrated at the center of the bay, what happened is that the genetic algorithm opted to seed the cells at the bottom in order to decrease their number via encystment instead of seeding them at the top where their number may hardly lessen.

Although the result seems counter-intuitive, from the point of view of the optimizer, that is the best possible configuration by which the target percent horizontal distribution for September 2009 could somehow be replicated using merely vertical distribution as the changeable parameter and advection as the hypothesized primary driving factor. Hence, the hypothesis that advection alone would transfer the Pbc cells from their August 2009 configuration to the September 2009 configuration is not supported by the result of the optimization. Other factors, not only the physical conditions, may also have strong influence on the pattern of Pbc cell distribution within Sorsogon Bay. This could reflect the important role of biological processes such as growth (as captured in the model) or the effect of grazing pressure in determining the patchy distribution of Pbc. Such a synergy of physical and biological controls on spatial distributions has been highlighted in recent studies (Prairie et al 2011).



Figure 9. a) Expected horizontal distribution of Pbc cell population, and b) horizontal distribution of Pbc cells after a model run using the depth-wise distribution returned by the genetic algorithm.

An agent-based model coupled with hydrodynamic and watershed models has been developed in order to help determine the factors and mechanisms responsible for Pyrodinium bahamense var. compressum bloom initiation, maintenance and decline. A genetic algorithm was linked to this model in order to optimize uncertain or unknown parameters. One of the key unknown parameters are the initial depth distributions of Pbc cells which can have a large influence on their resulting distributions in areas which may or may not be conducive for their growth or encystment. Through the application of the genetic algorithm to optimize Pbc cells vertical distributions, it was observed that even though advection is considered a key factor in harmful algal bloom dynamics it cannot be the sole process affecting their distribution since the optimized result did not satisfactorily fit the observed final distribution. It is suggested, however, that more trials should be conducted involving more rounds and iterations

further.

One possible work-around for the optimization setup in order to improve model fitting is to include in the optimization criteria that the population of Pbc cells should increase from August to September instead of using solely the percent horizontal distribution as basis. That is, percent horizontal distribution is a relative measure so the genetic algorithm ignores the decrease in Pbc cell population due to encystment while trying to adopt the percent horizontal distribution of the different stations for September 2009. Such inclusion of rate of population increase as objective for optimization requires a multi-objective optimizer which is beyond the scope of this study. Other key parameters such as mortality, nutrient response and encystment/excystment rates should also be varied together with layer distributions in order to obtain more holistic optimized results.

Currently, the hydrodynamic and environmental inputs used in the model are still being refined. More realistic mortality rules are also being worked out by computing grazing potentials at various sites. Nevertheless, the model is already showing interesting trends when it comes to investigating the details on the mechanisms and factors of bloom maintenance and clearance. Dynamic models integrating physical and biological processes are important tools to help understand, and possibly manage and mitigate harmful algal blooms. These models are being used to tease out the mechanisms and factors leading to bloom initiation, development and decline. Such models are also being used to help potentially forecast blooms, usually together with other tools such are satellite imagery and real-time data assimilation (Jochens et al 2010). This integrated Pbc model is one of the few models for tropical HAB species and through steps to increase its validity and investigating various factors relevant to blooms, this can provide increased understanding and hopefully options to better manage Pbc-affected areas in the country.

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