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## A Bayesian inference approach to account for multiple sources of uncertainty in a macroalgae based integrated multi-trophic aquaculture model



Scott Hadley<sup>a,\*</sup>, Emlyn Jones<sup>b</sup>, Craig Johnson<sup>a</sup>, Karen Wild-Allen<sup>b</sup>, Catriona Macleod<sup>a</sup>

<sup>a</sup> Institute for Marine and Antarctic Studies, University of Tasmania, Private Bag 129, Hobart, Tasmania 7001, Australia

<sup>b</sup> CSIRO Marine and Atmospheric Research, GPO Box 1538, Hobart, Tasmania 7001, Australia

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### ABSTRACT

A Bayesian inference method was employed to quantify uncertainty in an Integrated Multi-Trophic Aquaculture (IMTA) model. A deterministic model was reformulated as a Bayesian Hierarchical Model (BHM) with uncertainty in the parameters accounted for using “prior” distributions and unresolved time varying processes modelled using auto-regressive processes. Observations of kelp grown in 3 seeding densities around salmon pens were assimilated using a Sequential Monte Carlo method implemented within the LibBi package. This resulted in a considerable reduction in the variability in model output for both the observed and unobserved state variables. A reduction in variance between the prior and posterior was observed for a subset of model parameters which varied with seeding density. Kullback–Liebler (KL) divergence method showed the reduction in variability of the state and parameters was approximately 90%. A low to medium seeding density results in the most efficient removal of excess nutrients in this simple system.

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### 1. Introduction

The environmental, economic and social implications of ecosystem disturbances generated by the aquaculture industry have been widely reported (Buschmann et al., 2009). Integrated Multi-Trophic Aquaculture (IMTA) (Troell et al., 2009) involves joint farming of a ‘primary’ species together with other species that take up ‘waste’ (e.g. nutrients, particulates) produced in the farming process. This integrated approach provides both a method of removing problematic waste, as well as offering potential economic benefits through the cultivation of a new crop. Empirical investigations to quantify the effectiveness of IMTA are expensive and the results from small-scale systems do not necessarily extrapolate to large-scale operations because the removal of nutrients involves non-linear interactions between many variables. Models can help our understanding of these interactions whilst avoiding the prohibitive cost of full-scale trial operations. In order to validate model output some of the modelling investigations of IMTA have incorporated results from concurrently run empirical growth

experiments (Broch et al., 2013) or compared results with those from existing IMTA operations (Ren et al., 2012). However methods, which improve model parameterisation and constrain model output to observed values and thereby reduce model uncertainty, have not yet been included in the modelling process.

Bayesian inference provides a robust statistical method to combine information from numerical models and observations in the presence of model error and sparse observations (Wikle et al., 2013). Deterministic biogeochemical (BGC) models are typically assessed against empirical data, and many are highly parameterised, with a degree of uncertainty surrounding parameter values due to varying results from field-based studies (Planque et al., 2014). Furthermore, while the parameters in a deterministic model are constants they in fact often represent processes that in reality vary in time. It follows that useful quantification of model uncertainty provides an envelope of confidence around the model solution, and statistical methods have been developed recently that use observations to objectively reduce model uncertainty (e.g. Parslow et al., 2013; Dowd et al., 2014). This is critical to models such as those used for IMTA, where the results can influence decisions such as whether to undertake expensive full-scale farming operations. Simply perturbing parameters through a range of

\* Corresponding author.

E-mail address: [s\\_hadley@utas.edu.au](mailto:s_hadley@utas.edu.au) (S. Hadley).

possible values may lead to wildly divergent solutions in a non-linear deterministic model. However, by capitalising on Bayesian inference methodologies, observations from empirical experiments can be used to objectively quantify and constrain both model parameters and solutions (Jones et al., 2010; Parslow et al., 2013). Recent advances in statistical methodology and computing allow for the problem to be cast in the Bayesian Hierarchical Modelling (BHM) framework (Cressie and Wikle, 2011), which allows samples of parameters and state variables to be drawn from the posterior distribution that is conditioned on the empirical data.

The use of BHMs (Dowd et al., 2014; Parslow et al., 2013; Jones et al., 2010) is a method currently attracting interest due to its treatment of model uncertainty by incorporating prior knowledge. A BHM is constructed from a state space model (SSM) through a process of reformulating the SSM so that the three main areas of model uncertainty, i.e. observations, process and parameters can be treated individually. In this approach the deterministic BGC model is made stochastic by identifying the time-varying processes in the model and representing them by a random process rather than a constant parameter. In their study, Parslow et al. (2013) replaced a constant parameter representing phytoplankton community structure in a deterministic NPZD model with an autoregressive process. This captured the observed natural variability seen in phytoplankton communities despite the fact that in general the underlying process for this variation is not well understood.

To account for uncertainty in the remaining parameters, constant values are replaced by probability distributions. Finally a data model is constructed from field-based observations. The newly formed process, parameter and data models combine to make the BHM. Once in this format, Bayesian inference techniques are employed to exploit the conditional dependencies between the sub-models to enable a reduction in parameter and process uncertainty. To solve these complex systems, powerful computational techniques are required.

This reformulation into statistical–biophysical models combined with the advancements in distributed node (cluster) architecture supercomputers, has led to powerful new computational techniques that solve complex model systems in a meaningful way. The particle filter Markov Chain Monte-Carlo (pMCMC) (Andrieu et al., 2010) method uses samples from the posterior to calculate a joint distribution of parameter and state. Using a pMCMC approach Parslow et al. (2013) showed learning in parameter space and also that the state variables can be considerably constrained when conditioned on observation. In general this approach can be applied to a range of problems in biogeochemical modelling.

In this study an IMTA approach was employed to examine the capacity of giant kelp (*Macrocystis pyrifera*) to take up excess nitrate released from finfish aquaculture farms. The overall aims of the work are to:

- Reformulate a macroalgae based IMTA (Hadley et al., 2015) model into a BHM and use the method of Parslow et al. (2013) to introduce stochasticity into some of the sub-processes and represent the other parameters using probability distribution functions.
- Use a pMCMC (LibBI) ([www.libbi.org](http://www.libbi.org)) approach to solve this system using observational results taken from a field based IMTA experiment.
- Analyse the posterior distribution to identify the potential of this approach to constrain the model output based on a set of observed data, and to determine the extent to which parameter learning occurs.

## 2. Methods

### 2.1. Governing equations for IMTA model

To simulate the growth of *M. pyrifera* in a near-field arrangement of IMTA we use the model developed by Hadley et al. (2015). It is assumed that nitrogen (N) is the limiting nutrient, and therefore all equations have a common currency of N and are locally mass conserving. The governing equations for the state variables are presented below, while details of the rate process equations are given in Appendix A:

$$\begin{aligned} \frac{d\text{NH}_4}{dt} &= \lambda_R (\text{NH}_{4\text{ref}} - \text{NH}_4) - f(\text{NH}_4, Q)\text{B} + r_L D - r_N \text{NH}_4 \\ \frac{d\text{NO}_3}{dt} &= \lambda_R (\text{NO}_{3\text{ref}} - \text{NO}_3) - f(\text{NO}_3, Q)\text{B} + r_N \text{NH}_4 \\ \frac{d\text{N}_s}{dt} &= f(\text{NX}_x, Q)\text{B} - \mu g(\text{E}, \text{Q}, \text{T})\text{N}_s - d_M \text{N}_s \\ \frac{d\text{N}_f}{dt} &= \mu g(\text{E}, \text{Q}, \text{T})\text{N}_s - d_M \text{N}_f \\ \frac{d\text{D}}{dt} &= \lambda_R (\text{D}_{\text{ref}} - \text{D}) + d_M \text{N}_f - r_L D \end{aligned} \quad (1)$$

The model (1) has 5 state variables all of which are in units of mg N m<sup>-3</sup> seawater. Ambient nitrogen taken up by the macroalgae is in two forms of dissolved inorganic nitrogen (DIN), namely ammonium (NH<sub>4</sub>) and nitrate (NO<sub>3</sub>). Parameters NH<sub>4ref</sub>, NO<sub>3ref</sub> and D<sub>ref</sub> represent the background concentrations of ammonium, nitrate and detritus respectively. The refresh rate λ<sub>R</sub> determines how quickly the external ammonia, nitrate and detritus return to a background concentration in the absence of macroalgae. This term is used in the absence of an advection diffusion model (Dowd, 1997; Aldridge and Trimmer, 2009). Once taken up, DIN is stored as intracellular nitrogen (N<sub>s</sub>), which is then fixed into the macroalgae cellular structure (N<sub>f</sub>). The uptake rate f(NX<sub>x</sub>, Q) is dependent on both ambient concentrations of DIN and the internal quota, Q, of intracellular nitrogen (Solidoro et al., 1997). The instantaneous growth rate μg(E, Q, T) is a product of maximum growth rate, μ, and the environmental variables PAR (E), temperature (T) and Q. N<sub>f</sub> is returned to detritus (D) at a rate determined by the mortality term d<sub>M</sub>. Similarly decaying macroalgae returns N<sub>s</sub> to NH<sub>4</sub> at the same rate. D is remineralised at a constant rate r<sub>L</sub>. Finally NH<sub>4</sub> is nitrified to NO<sub>3</sub> at a constant rate. r<sub>N</sub>.

The height of *M. pyrifera* h<sub>MA</sub> varies according to the allometric relationship (Hadley et al., 2015),

$$h_{\text{MA}} = \left(0.00174\text{N}_f / n_{\text{fronds}}\right)^{1.047} \quad (2)$$

Height change allows kelp to reach the light from depth. Since h<sub>MA</sub> is frond height (m), the parameter n<sub>fronds</sub> is an average of the number of fronds within the unit volume. Observations taken from the IMTA experiment used in the data model were of height and weight. The weight w<sub>MA</sub> (g<sup>-1</sup> dw m<sup>-3</sup>) is given by

$$w_{\text{MA}} = \left(\frac{\text{N}_f}{\text{Q}_{\text{min}}}\right) * h_{\text{MA}} \quad (3)$$

here Q<sub>min</sub> is the minimum amount of structural nitrogen required for the macroalgae cells (Solidoro et al., 1997), while the remainder contributes to growth or respiration. Respiration is not modelled explicitly but is included in the growth term dependent on the internal quota Q. Two changes were made in the present model compared to the original. Firstly, the uptake limiting term min(1, h<sub>MA</sub>/z) (where z is the cultivation depth and h<sub>MA</sub> the algae

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