Geosci. Model Dev. Discuss., 4, 1941–2010, 2011
www.geosci-model-dev-discuss.net/4/1941/2011/
doi:10.5194/gmdd-4-1941-2011

Geoscientific Model Development Discussions

Addressing the impact of environmental uncertainty in plankton model calibration with a dedicated software system: the Marine Model Optimization Testbed (MarMOT)

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Received: 16 June 2011 – Accepted: 9 August 2011 – Published: 19 August 2011

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Published by Copernicus Publications on behalf of the European Geosciences Union.

Abstract

A wide variety of different marine plankton system models have been coupled with ocean circulation models, with the aim of understanding and predicting aspects of environmental change. However, an ability to make reliable inferences about real-world processes from the model behaviour demands a quantitative understanding of model error that remains elusive. Assessment of coupled model output is inhibited by relatively limited observing system coverage of biogeochemical components. Any direct assessment of the plankton model is further inhibited by uncertainty in the physical state. Furthermore, comparative evaluation of plankton models on the basis of their design is inhibited by the sensitivity of their dynamics to many adjustable parameters. The Marine Model Optimization Testbed is a new software tool designed for rigorous analysis of plankton models in a multi-site 1-D framework, in particular to address uncertainty issues in model assessment. A flexible user interface ensures its suitability to more general inter-comparison, sensitivity and uncertainty analyses, including model comparison at the level of individual processes, and to state estimation for specific locations.

The principal features of MarMOT are described and its application to model calibration is demonstrated by way of a set of twin experiments, in which synthetic observations are assimilated in an attempt to recover the true parameter values of a known system. The experimental aim is to investigate the effect of different misfit weighting schemes on parameter recovery in the presence of error in the plankton model's environmental input data. Simulated errors are derived from statistical characterizations of the mixed layer depth, the horizontal flux divergences of the biogeochemical tracers and the initial state. Plausible patterns of uncertainty in these data are shown to produce strong temporal and spatial variability in the expected simulation error over an annual cycle, indicating differences in the significance attributable to model-data misfits at different data points. An inverse scheme using ensemble-based estimates of the simulation error variance to allow for this environment error performs well compared with

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weighting schemes used in previous plankton model calibration studies. The efficacy of the new scheme in real-world applications will depend on the quality of statistical characterizations of the input data. Practical approaches towards developing reliable characterizations are discussed.

1 Introduction

Ocean biogeochemical general circulation models (OBGCMs) have a key contribution to make to the goal of understanding biogeochemical cycles at global and regional scales. These models are highly simplified "mechanistic" models of a generic plankton ecosystem, coupled with 3-dimensional ocean circulation models that provide the physical environment to which the plankton models respond. Reliable plankton models are needed to make inferences about the potential role of the marine biota in environmental change. However, the contrast between the complexity of biological systems and the limited data available to empirically constrain model structure and parameter values has led to a wide range of different representations of the marine plankton system. Each model is one of a still wider set of competing hypotheses concerning the dominant mechanisms that control the biological response to change in the physical and chemical environment. The level of complexity that can be justified in these models, given the available biogeochemical data, has been a subject of some debate (Anderson, 2005; Le Quéré, 2006). To resolve this we must be able to comparatively evaluate models on the basis of their structure and process formulations. Behaviour of plankton models in OBGCMs is sensitive to the details of the physical dynamics (Sinha et al., 2010). Dependence on a particular physical model in comparative assessments of model designs should therefore be avoided if future biogeochemical simulations are to benefit from improved representations of the physical environment.

Direct comparison of plankton models on the basis of their design is inhibited by parameter uncertainty: behaviour of each model depends on many adjustable parameters

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that are poorly known or difficult to quantify. Although some of these values can be determined experimentally under controlled conditions, the corresponding values in nature are generally highly variable in space and time or across taxa. Fasham and Evans (1995) and Matear (1995) started to address this problem by fitting plankton models to observations from time-series sites in the temperate North Atlantic and subarctic Pacific respectively, using non-linear data assimilation techniques to seek optimal parameter sets. Matear (1995) investigated 3 different ecosystem configurations with 3, 4 and 7 nitrogen compartments and concluded that the data from the study site were insufficient to justify either of the more complex models over the simple nitrate-phytoplankton-zooplankton model. Dadou et al. (2004) compared 3 alternative configurations, spanning a similar range of complexity, at an oligotrophic study site in the eastern North Atlantic and were not able to objectively discriminate between the designs on the basis of their misfit results.

To test models' predictive ability it is necessary to examine their misfit with respect to unassimilated data as in the more recent model inter-comparison experiments of Friedrichs et al. (2006, 2007). In an experiment with 12 models (Friedrichs et al., 2007), data from Arabian Sea and Equatorial Pacific sites were used and models calibrated at one site were cross-validated at the other. Here, the more complex models with multiple plankton functional groups tended to perform better, provided only a small number of parameters were optimized, suggesting greater portability and predictive skill associated with model design.

The results obtained from all of these optimization experiments are dependent on the external inputs to the plankton model. Friedrichs et al. (2006) examined the impact of uncertainty in the physical forcing and demonstrated that likely errors in the physical forcing data can have a major impact on biogeochemical simulations, causing a calibration process to yield inappropriate parameter values. One approach to solving this problem is to improve the physical forcing. Joint assimilation of physical and biogeochemical data, as advocated by Friedrichs et al. (2006), seems likely to be beneficial. However, the inadequacy of data coverage combined with the sensitivity of plankton

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models to their forcing data inevitably makes the problem persistent, motivating a formal treatment of uncertainty.

The uncertainty introduced by horizontal processes poses a further problem for 1-D studies that has yet to be satisfactorily addressed. Flux divergences associated with mesoscale eddy activity are particularly problematical in this respect. The issue does not arise explicitly when calibrating a model to simulate a climatological annual cycle (Matear, 1995; Hurtt and Armstrong, 1996, 1999; Spitz et al., 1998, 2001; Schartau and Oschlies, 2003; Dadou et al., 2004; Losa et al., 2004). In these cases, mesoscale and inter-annual variability are both interpreted as noise superimposed on the average annual cycle. Alternatively, mesoscale variability can be treated as noise superimposed on spatially averaged plankton concentrations. On this basis, Hemmings et al. (2003, 2004) treated all satellite chlorophyll data within either 150 km or 100 km as equally representative of the calibration site. A problem with both approaches is that averaging tends to smooth out features such as blooms, in effect changing the apparent response of the system that we are attempting to model.

Simulating the dynamics for specific years at specific locations seems preferable, particularly if we want plankton models that will benefit from increased resolution in general circulation models, but it requires more supporting data. Year-specific forcing can be derived from in situ observations (Fasham and Evans, 1995; Schartau et al., 2001; Fasham et al., 2006), from a 1-D physical model with appropriate meteorological forcing (Prunet et al., 1996a,b; Faugeras et al., 2003, 2004; Kettle, 2009), from a 3-D circulation model (Fennel et al., 2001; Schartau et al., 2001) or from a combination of in situ and 3-D model data (Friedrichs et al., 2006, 2007). However, the local forcing is only relevant when local effects are dominant. The presence of strong mean flows in some regions, together with the ubiquity of mesoscale patchiness associated with fronts and eddies means that such dominance cannot generally be assumed. Friedrichs et al. (2007) determined that horizontal advective divergence of nutrients could have first order effects on the biogeochemistry at the Equatorial Pacific site and introduced an additional source/sink term computed from a 1/3° coupled

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biological-physical model to account for these, while acknowledging the issue of unknown error in the 3-D model.

Other approaches to the horizontal flux divergence problem have been applied with some success to specific data sets. Fasham et al. (1999) used data from a 3 week North Atlantic spring bloom survey that followed a drogued buoy, deployed within an anti-cyclonic eddy, to minimize contamination of the biological dynamics by non-local effects. In a calibration exercise using data from the SOIREE iron fertilization experiment, Fasham et al. (2006) parameterized diffusive flux divergence effects using a mixing rate based on the dilution of a passive tracer added to the iron enriched water. A novel "variable lag" fitting technique introduced by Wallhead et al. (2006) allows for phase differences associated with mesoscale patchiness. Survey data from a relatively wide area could thereby be combined without explicitly resolving mesoscale processes yet avoiding the risk of smoothing out temporal variability.

It is clear that a thorough investigation of the impact of uncertainty in all factors that contribute to uncertainty in plankton model simulations is a high priority. The associated data management issues, in combination with the need to perform a wide range of computationally expensive model analyses involving many different simulations has been a factor inhibiting rapid progress in this area. The MarMOT software system has been developed as a generic tool applicable to different plankton models with the aim of removing this barrier. The system is first described in Sect. 2 in terms of its key features. In Sect. 3, it is used to evaluate a proposed model calibration method with explicit treatment of environmental uncertainty. In the final section, we discuss some of the practical issues faced in model assessment and and suggest other applications of the MarMOT system.

2 The MarMOT system

The Marine Model Optimization Testbed is essentially a multi-site 1-D simulator for rigorous plankton model evaluation. Following the testbed concept of Friedrichs et

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al. (2006, 2007), MarMOT provides a common physical and computational environment in which different plankton ecosystem models can be calibrated and compared. It is designed to support computationally intensive experiments in which models are evaluated many times with different inputs. A flexible interface makes it easy to apply to a wide range of sensitivity analyses, uncertainty analyses and parameter optimization experiments. MarMOT does not include a 1-D physical model. All physical forcing is instead provided by external input data. Plankton model responses to a wide range of different physical environments can be examined by providing different instances of the forcing data derived from models or observations or a combination of both. With appropriate treatment of uncertainty in these input data ensembles, the plankton ecosystem components of OBGCMs can be assessed independently as hypotheses concerning the dominant biogeochemical processes they are designed to represent.

Figure 1 gives an overview of the MarMOT system in terms of its main components and the data flows between them. Simulations are controlled by data selected from a number of input tables, referred to as "item tables", each containing one or more instances of a particular input item. Different instances of each item are combined according to entries in a further input table: the "case table". Each case table entry defines a simulation case determined by a specific combination of input data and identified by a site name (or number) and an ensemble member name (or number).

A particular case table defines a set of simulations for one or more ensemble members at one or more sites. The set of ensemble members may vary between sites if required. Ensemble configurations for multiple sites can involve site-specific information (e.g. water depth), ensemble-member specific information (e.g. plankton model identifier in a multi-model comparison experiment), information specific to the combination of site and ensemble member (e.g. forcing data) and independent information (e.g. simulation time period). A cross-referencer links the appropriate item instances to the case table, determining the required data for each item either from an explicit reference or from the context implied by the site and/or the ensemble member. Free model parameters can be optimized over all cases in a given case table, so it is straight-forward

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to set up multi-site and calibration experiments. Multi-member calibrations are likewise possible.

The core of the system is the MarMOT Model Evaluator (MME) that performs plankton ecosystem model runs according to the specifications in the case table. It calculates a cost function value dependant on the misfit between simulation variables and a set of observations or other reference values provided as an additional case-dependent input item. It can also provide a range of different output tables that are selected or deselected according to user requirements. Further details of the system design are given in Appendix A.

2.1 Model evaluator

2.1.1 Cost function

The MME outputs a cost function value that is a weighted average of all model-data misfits, over all specified simulation cases (or zero in the absence of any applicable data). Profile variable values are interpolated linearly in depth from level mid-points to the observation depth. The misfit cost is then defined by

$$J = \frac{1}{N} \sum_{k=1}^{C} \sum_{j=1}^{m} \sum_{i=1}^{n_k} p_{ijk} w_{ijk} (x_{ijk} - y_{ijk})^2 \quad (1)$$

$$N = \sum_{k=1}^{C} \sum_{j=1}^{m} \sum_{i=1}^{n_k} p_{ijk} \quad (2)$$

where C is the number of cases, n_k is the number of observation points (in space and time) for case k and m is the number of observed variables; x_{ijk} is the simulated value of the j-th variable at the i-th observation point and y_{ijk} is its observed value. The coefficient p_{ijk} is 1 if the variable is present in the observation set or 0 otherwise. The

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coefficient w_{ijk} is a weight specified in the observation set or 1 if no weight is given. An output table can be produced giving all simulated and observed values, model-data differences, user weights and weighted misfits (squared differences) at each observation point.

Model-data differences may optionally be calculated in log or square root space, in which case x is replaced by $\log_{10} x$ or $\sqrt{x}$, respectively and y is likewise replaced by $\log_{10} y$ or $\sqrt{y}$. Log transformations emphasize relative error and are appropriate for variables that tend to exhibit log-normal distributions. However, in ecological analyses it is often unclear whether absolute or relative errors should be considered. Square root transformations have been applied as a compromise in some studies for this reason (Fasham and Evans, 1995; Evans, 1999; Dadou et al., 2004; Fasham et al., 2006).

Parameter penalty terms are not presently supported in MarMOT. Although such terms have been widely used in the literature to inhibit excessive deviation of parameter values from their prior expected values, their specification normally relies on subjective prior information. Ideally, parameters should be prevented from assuming values far outside their expected ranges by ensuring that the set of adjustable parameters is adequately constrained by the data (Friedrichs et al., 2007). Cases where this doesn't work can potentially provide useful information about deficiencies in the model design. Where parameter bounds are required, prior constraints can be imposed independently of the cost function using optimizer features described in Sect. 2.2.

2.1.2 1-D simulations

The remaining MME features described here relate to each individual simulation case. Case-specific input data include the model selection, fixed model parameter values, forcing and boundary condition data (including initial conditions). In addition the model time-step, vertical grid, advection scheme and photosynthesis sub-model can be varied between simulations, allowing the sensitivity of the solution to these factors to be explored in a single experiment. The available photosynthesis sub-models are described in Appendix B.

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The 1-D equation for the evolution of a biogeochemical tracer concentration C_i in a MarMOT simulation is

$$\frac{dC_i}{dt} = -(w_\mathrm{p} + w_i)\frac{\partial C_i}{\partial z} + \frac{\partial w_\mathrm{p}}{\partial z}C_i + \frac{\partial}{\partial z}\left(K_\rho \frac{\partial C_i}{\partial z}\right) + \mathrm{SMS}_i(\boldsymbol{C}, \boldsymbol{F}) + p_i(C_i, p_i^\star) + r_i(C_i^\mathrm{ref} - C_i). \quad (3)$$

The first three terms represent the vertical flux divergence. w_p is the vertical velocity of the water, w_i is the active vertical velocity of the biological material relative to the water (if any) and K_ρ is the turbulent diffusion coefficient. SMS_i is the source-minus-sink term from the selected plankton model which is a function of the state vector $\boldsymbol{C}$ and a forcing vector $\boldsymbol{F}$. w_i is provided by the plankton model and currently assumed to be constant. The last two terms define the boundary condition: p_i is a perturbation term driven by an applied perturbation $p^\star$, which may be stochastic, and the final term is a relaxation term given by the product of a rate r_i and the deviation of C_i from a reference concentration C_i^ref. In addition, if a non-zero depth is specified for the turbulent upper mixed layer, rapid mixing is parameterized by complete homogenization of tracers above this depth at each time step. Partial mixing of the model level spanning the specified depth is optional.

Forcing data for the model can be periodic, representing a repeating annual cycle, or year specific. The standard forcing variables for a 1-D plankton model simulation determine the light availability at the sea surface and the transport of passive tracers in the water column. In MarMOT, they comprise the downwelling solar radiation incident on the sea surface, either as a daily mean or a point-in-time estimate, the mixed layer depth, the depth-dependent turbulent diffusion coefficient K_ρ and vertical velocity w_p. Additional model-specific forcing variables are also catered for.

In perturbed simulations, the perturbation for an individual tracer can be independent of the concentration C_i or it can be applied to log-transformed or square root-transformed concentration so that p_i becomes a function of concentration. In either

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case, the applied perturbation $p_i^\star$ is given by the sum of a prescribed perturbation μ_i^{pert} and a stochastic term. The latter is modelled as a first order auto-regressive process such that the perturbation at time step n is

$$p_i^\star = \mu_i^{\text{pert}} + q_n \tag{4}$$

where

$$q_n = aq_{n-1} + \epsilon_n. \tag{5}$$

The value a is determined from the auto-correlation coefficient for q at a time lag of 24 h as specified by a fixed simulation parameter. ϵ_n is a normally distributed random variable with zero mean. Its standard deviation is set to give an expected $p_i^\star$ standard deviation matching that prescribed by external data σ_i^{pert} in cases where the process is stationary. The actual perturbation process can be non-stationary: μ_i^{pert} and σ_i^{pert} are handled as forcing variables and both can be time- and depth-dependent. ϵ_n covaries at all depths and is scaled according to the local value of σ_i^{pert}. Any negative post-perturbation tracer concentrations are set to zero.

Each relaxation rate r_i is handled as a forcing variable, as is the reference concentration C_i^{ref} for each tracer. Any of these variables can vary independently in time and/or depth if required. The relaxation rate can be set to fully relax one or more tracers to reference data at each time step. Any of the tracers can thus be held at fixed values or fully determined by external fields. Used in this way, the relaxation scheme is a powerful diagnostic tool that makes it possible to examine the behaviour of individual parts of the model independently. A further option allows relaxation to be restricted to grid points above or below the mixed layer depth, the euphotic zone depth (1 % light level) or the greater of the two.

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2.1.3 Horizontal flux divergence

The appropriate boundary condition for parameterizing horizontal flux divergence depends on the nature of the experiments to be performed. If the aim is to produce the best approximation to the true ocean state at a site then the horizontal flux divergences to be represented, together with their uncertainty, are real-world flux divergences. However for model assessment or calibration they are flux divergences consistent with the model and parameter set under evaluation that would be obtained with a perfect physical simulation.

The perturbation and relaxation terms can be used in combination to provide a suitable boundary condition for representing uncertain real-world flux divergences. A stochastic perturbation rate represents horizontal flux divergence that causes the solution to diverge from a locally forced solution. The relaxation term ensures that, as information from the local solution is lost, the solution tends towards some prior estimate of the system state, provided by C_i^{ref}. The prior state estimate is effectively assimilated during integration. Any cost function value obtained is a measure of the quality of the simulation, rather than the skill of the model. For model assessment or calibration, the required horizontal flux divergences are model-specific and there is no prior state estimate. Flux divergence is then represented solely by the perturbation term.

When both perturbation and relaxation are applied, the magnitude of the relaxation change should be balanced against that of the perturbation change to ensure that information is replaced at a rate consistent with the expected change due to horizontal flux divergence. This can be achieved in MarMOT using a constraint that allows the maximum relaxation rate to be controlled by the perturbation standard deviation.

At each time step, a new perturbation-limited relaxation rate

$$r_i' = \min\left(\frac{R_i}{|C_i^{\mathrm{ref}} - C_i|}, r_i^{\mathrm{ext}}\right) \tag{6}$$

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is determined for each tracer i, where R_i is a maximum permitted magnitude for the rate of change in concentration due to relaxation and r_i^{ext} is the input relaxation rate. The degree of limitation is determined by a relaxation control factor ψ such that

$$R_i = \psi \sigma_i^{\text{pert}} \tag{7}$$

so ψ controls the significance of the relaxation change, relative to the random perturbations. Alternatively, if σ_i^{pert} is defined in transformed variable space

$$R_i = C_i \psi \sigma_i^{\text{pert}} \tag{8}$$

or

$$R_i = 2\sqrt{C_i}\psi \sigma_i^{\text{pert}} \tag{9}$$

for log and square root transformations, respectively.

The maximum permitted relaxation rate is determined separately for each tracer. However, it is desirable to use the same relaxation rate for all tracers to preserve relationships between different tracers in the prior state estimate. At each time step, a universal relaxation rate

$$r_i = \min_i(r_i') \tag{10}$$

is therefore applied to all relaxed tracers.

2.2 Optimizer

The optimizer is well suited to non-linear problems in multi-dimensional parameter space: it includes a genetic algorithm for identifying promising areas of a bounded parameter space and a non-gradient direction set algorithm for bounded or unbounded local minimization. The two algorithms can be used in combination or independently.

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The genetic algorithm is a global method in the sense that it is able to locate multiple minima in the cost function. However, it searches the parameter space in discrete intervals, limiting the accuracy with which it can locate a particular minimum. In contrast, the direction set algorithm navigates towards a local minimum from a given starting point, making it unsuited to finding the global minimum in a cost function with complex topography, but can give greater accuracy. Local algorithms can be applied to global problems by performing repeated searches from different initial points in parameter space to increase the likelihood of locating the global minimum. In MarMOT, the direction set algorithm can be initialized from an input table of parameter vectors or from a set of pre-conditioned parameter vectors output by the genetic algorithm.

The genetic algorithm provided is a micro-genetic algorithm (μGA) (Krishnakumar, 1989), based on an implementation by Carroll (1996). It has been applied to the problem of plankton model optimization by Schartau and Oschlies (2003), Weber et al. (2005) and Kettle (2009) and by Ward et al. (2010) who compared its performance with the local variational adjoint technique employed by Friedrichs et al. (2007). An initial set of parameter vectors is required to define the population for the genetic algorithm to work on. In MarMOT, this can either be from an input table or generated randomly. The bounds for each parameter can be defined in terms of the actual parameter values or log-transformed values.

The direction set algorithm was designed by Powell (1964) to locate a cost function minimum in a continuous free parameter space. The version of Powell's algorithm used is that described in Press et al. (1992), with reference to Acton (1970). Line minimization is performed using Brent's method (Brent, 1973). No gradient information is used so it does not require the provision of an adjoint code for calculating the cost function gradient with respect to the model parameters. It is therefore more straightforward to apply than the variational adjoint method in situations where the formulation of the plankton model is not fixed. The algorithm has been applied in a number of plankton model calibration studies (Fasham and Evans, 1995; Fasham et al., 1999; Evans, 1999; Dadou et al., 2004; Fasham et al., 2006).

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Powell's algorithm treats the parameter space as infinite. However, to support bounded minimizations, transformations can be applied to any parameter value P (in original or log space) to provide an unbounded value $P^\star$ for the optimizer.

$$P^\star = \left\{ \begin{array}{l} \frac{P-P_{\text{mid}}}{P-P_{\text{lower}}} \text{ , } P < P_{\text{mid}} \\ \frac{P-P_{\text{mid}}}{P_{\text{upper}}-P} \text{ , } P > P_{\text{mid}} \end{array} \right\} \quad (11)$$

$$P_{\text{mid}} = \frac{1}{2}(P_{\text{lower}} + P_{\text{upper}}) \quad (12)$$

where P_{lower} and P_{upper} are the required bounds in the original finite parameter space. $P^\star$ tends to infinity as P approaches either bound, so any point $P^\star$ in the infinite space seen by the optimizer maps to a value P where $P_{\text{lower}} < P < P_{\text{upper}}$. The behaviour of the search algorithm with respect to the original parameter space is affected as a consequence of the modified cost function $J'(P^\star) = J(P)$ presented to the optimizer. Transformations are dimension specific, so bounded and unbounded parameters can be optimized simultaneously.

The parameter transformation is based on that introduced by Fasham et al. (1999) for the same purpose. In that study, a parameter penalty term was also included in the cost function formulation to weight against large deviations of the transformed parameters from their prescribed prior values. In MarMOT, prior parameter information is provided purely in terms of allowable ranges so that the value of the cost function $J(P)$ is unaffected by the parameter values, except via the simulation.

The optimizer can output cost function values and corresponding parameter vectors for all function evaluations if required. Any requested simulation output tables are produced for the final optimal parameter vector.

3 Application to model calibration

A potentially robust method for parameter optimization at time-series sites is proposed here and compared with established methods by way of a set of twin experiments in

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which the true parameter values are known. We focus on the design of the cost function. The more general calibration problem normally includes a parameter selection phase guided by a sensitivity analysis to determine which parameters can be independently constrained and/or which parameters are likely to impact on model outputs of particular scientific interest. The required sensitivity analyses can be performed efficiently using MarMOT but are outside the scope of the present demonstration.

3.1 Cost function design

In inverse analyses of plankton ecosystem models, parameter optimization is generally performed by minimization of a cost function. Maximum likelihood methods have also been employed (Hurtt and Armstrong, 1996, 1999), in which an optimizer is applied to the problem of maximizing a function describing the likelihood of the observations conditional on the truth of the model. The two techniques are essentially equivalent and give point estimates of the model parameters. Alternatively, in a fully Bayesian scheme, the likelihood is multiplied by prior probability distributions for the parameters to estimate the complete posterior distributions (Harmon and Challenor , 1997) or combined distributions for the parameters and the system state (Dowd and Meyer, 2003).

The weight given to individual model-data misfits in a particular cost function or likelihood function is fundamental to the effectiveness of data assimilation for controlling model parameter values. As discussed by Evans (2003), a wide variety of different approaches have been used in the literature, having a potentially major impact on parameter estimates and the resultant estimates of key biogeochemical quantities from the calibrated model simulations.

Unweighted misfits have been used (Fasham and Evans, 1995) or sometimes weights have been used in a subjective way to give more influence to observations that are felt to be more reliable or more important to fit (Fasham et al., 1999, 2006). The square root transform used by Fasham and Evans (1995), Evans (1999) and Fasham et al. (2006), while not weighting individual misfits explicitly, has the effect of giving more influence to misfits occurring when values of model and data are low. This

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is a compromise between treatment of absolute and relative errors; absolute errors might be considered more important in the context of estimating total element fluxes, whereas relative errors might be favoured by arguments based on representing ecological structure (Evans, 1999). Hurtt and Armstrong (1996); Fasham et al. (1999); Hurtt and Armstrong (1999) scaled model-data differences relative to the model values at the observation points, giving equal weight to equal relative departures.

More typically, some characteristic scale is determined for each assimilated data type, designed to reflect its variability relative to other data types over the whole data set. Weights w_j (Eq. 1) are chosen to be inversely proportional to the mean of all observations of the same type (Spitz et al., 2001), the square of the mean (Kuroda and Kishi, 2004) or their variance (Friedrichs et al., 2006, 2007; Kettle, 2009; Ward et al., 2010). Friedrichs et al. (2007) and Ward et al. (2010) found it necessary to introduce a subjective up-weighting of misfit to primary production observations due to the high variability of these data. Evans (2003) suggested that if focusing on the cycle of a particular element it may be desirable to give the same weight to all misfits for that element, regardless of the form in which it occurs. Dadou et al. (2004) therefore used a single scaling factor for all nitrogen variables, based on the maximum observed nitrate, and used intuitive arguments to determine relative scaling factors for primary production and particle fluxes based on the maximum observed values of other relevant properties.

In general, characteristic scales are used because of the absence of information required to properly estimate error variances. In some studies though, the variable-specific weight is presented as the reciprocal of an assumed or estimated observation error variance (Prunet et al., 1996a,b; Fennel et al., 2001; Faugeras et al., 2003, 2004); for a particular variable, either absolute or relative error variances are taken to be constant. Schartau et al. (2001) used a combination of constant absolute and relative error variance estimates for chlorophyll and primary production data. Finally, seasonally varying observation error variance estimates have been used in inverse modelling of the annual cycle (Matear, 1995), while Hemmings et al. (2003, 2004) estimated

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error variances specific to individual chlorophyll observations from spatial variances in satellite data.

3.1.1 An uncertainty-based weighting scheme

A formal weighting scheme is developed here, with explicit consideration given to the different sources of error contributing to the model-data misfit. Misfit arises from a combination of error in the observations and error in the simulation. Error in the observations includes both measurement error and error of representativity. The latter is error due to small-scale variability or, more specifically, the mismatch between the volume of water sampled and the minimum scale resolved by the simulation. It includes error due to small-scale variations in both space and time. Error in the simulation is the sum of model error, attributable to deficiencies in the model, and environment error, attributable to error in its environmental inputs (forcing data and boundary conditions). For a model with optimizable parameters, model error can be treated as the sum of parameter error and structural error components. The structural error is the residual error for the true parameter set (assuming such a set exists conceptually). It is the error associated with the model design and includes error attributable to values of any fixed model parameters.

Assuming that errors are additive and independent, the simulated and observed values of variable j at observation point i at site k are then

$$x_{ijk} = x_{ijk\mathrm{T}} + \epsilon_{ijk\mathrm{ENV}} + \epsilon_{ijk\mathrm{P}} + \epsilon_{ijk\mathrm{S}} \quad (13)$$

$$y_{ijk} = x_{ijk\mathrm{T}} + \epsilon_{ijk\mathrm{OBS}} \quad (14)$$

where $x_{ijk\mathrm{T}}$ is the true value (i.e. that for a perfect simulation) and $\epsilon_{ijk\mathrm{ENV}}$, $\epsilon_{ijk\mathrm{P}}$, $\epsilon_{ijk\mathrm{S}}$ and $\epsilon_{ijk\mathrm{OBS}}$ are the environment error, parameter error, structural error and total observation error, respectively. The variance in the model-data difference $x_{ijk} - y_{ijk}$ is

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$$\sigma^2_{ijk} = \sigma^2_{ijk\mathrm{OBS}} + \sigma^2_{ijk\mathrm{S}} + \sigma^2_{ijk\mathrm{P}} + \sigma^2_{ijk\mathrm{ENV}} \quad (15)$$

where the terms on the right hand side are the variances for each error component.

The error variance of interest in a particular analysis depends on the objective. If it is to improve the simulation then the aim is to minimize the total simulation error variance. The residual variance for a perfect solution is the observation error variance $\sigma^2_{ijk\mathrm{OBS}}$, so the estimated observation error variance determines the significance of a given misfit. However, to improve the plankton model we aim to minimize only the model error variance $\sigma^2_{ijk\mathrm{P}} + \sigma^2_{ijk\mathrm{S}}$ and so must determine significance on the basis of estimates of the residual variance $\sigma^2_{ijk\mathrm{OBS}} + \sigma^2_{ijk\mathrm{ENV}}$. This reduces the significance of each individual misfit to take into account the effects of uncertainty in the model's environmental inputs.

For quantifying model error, a normalized model-data misfit statistic is therefore proposed:

$$M_{ijk} = \frac{(x_{ijk} - y_{ijk})^2}{\sigma^2_{ijk\mathrm{OBS}} + \sigma^2_{ijk\mathrm{ENV}}}. \quad (16)$$

Here, the denominator (corresponding to the reciprocal of w_{ijk} in Eq. (1) defines a significance threshold for the square of the model-data difference. The expected value of M_{ijk} for a perfect model is 1; if the model-data difference is no larger than might be expected as a result of observation error and environment error then there is no evidence for model error so the data gives us no cause to reject the model.

In a calibration exercise, the aim is either to find the parameter set that minimizes the model error or to estimate real-world parameter values. Equation 16 is applicable to the first case, parameter optimization, in which parameter values are permitted to compensate for structural error. In the second case, parameter estimation, the aim is to minimize the parameter error variance $\sigma_{ijk\mathrm{P}}$, so the residual variance is $\sigma^2_{ijk\mathrm{OBS}} + \sigma^2_{ijk\mathrm{ENV}} + \sigma^2_{ijk\mathrm{S}}$. Thus the significance of a given misfit for parameter estimation

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is less than that for parameter optimization or model assessment. The appropriate misfit statistic is

$$M'_{ijk} = \frac{(x_{ijk} - y_{ijk})^2}{\sigma^2_{ijk\mathrm{OBS}} + \sigma^2_{ijk\mathrm{ENV}} + \sigma^2_{ijk\mathrm{S}}}. \quad (17)$$

If the model-data difference is no larger than might be expected as a result of observation error, environment error and structural error then there is no evidence for parameter error, given the data, so no cause to reject the parameter set. Parameter estimation is a more difficult problem than parameter optimization because the problem of estimating the varying contribution of structural error between data points is not easily tractable.

A value for $\sigma_{ijk\mathrm{OBS}}$ can in principle be derived from repeat observations, if available. An appropriate value for $\sigma_{ijk\mathrm{ENV}}$ can be obtained from ensemble integrations of the model with different input data. The method of estimating $\sigma_{ijk\mathrm{ENV}}$ relies on a good characterization of uncertainty in forcing data and boundary conditions, requiring a thorough analysis of relevant satellite and in situ data available for the site and its surroundings. Local modelling studies, including data assimilating hindcasts, might provide additional information. For a calibration exercise, ensemble simulations must also provide adequate coverage of the parameter space.

3.1.2 Other weighting considerations

Cases are common in the literature where different numbers of observations are available for different data types. They are generally treated in one of two ways: in some studies, misfits for different variables are weighted by the reciprocal of the number of observations of each type (Hurtt and Armstrong, 1999; Schartau et al., 2001; Schartau and Oschlies, 2003; Faugeras et al., 2003, 2004; Hemmings et al., 2003, 2004; Friedrichs et al., 2007; Kettle, 2009; Ward et al., 2010), while in others, no such weighting is applied (Matear, 1995; Prunet et al., 1996a; Hurtt and Armstrong, 1996; Spitz et

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al., 2001; Friedrichs, 2002; Dadou et al., 2004; Kuroda and Kishi, 2004; Friedrichs et al., 2006). The choice is significant: Fasham and Evans (1995) performed experiments with and without a weighting factor that increased the influence of the small number of zooplankton observations in their data set, obtaining two different optimal parameter sets for which simulated primary production differed by a factor of about 2.

Explicit weighting to balance the contributions of different data types is objectively justifiable if error correlations are much greater between variables of the same type than between different data types. However, this cannot generally be assumed and Evans (2003) argues that, while such balancing has the advantage of emphasizing scarce but important measurements, it may not be desirable in a formal procedure. As discussed by Evans (2003), we can expect simulation errors arising from model error or external factors to introduce both serial correlations and correlations between variables via the model dynamics. This could be allowed for by the use of a non-diagonal covariance matrix in the cost function formulation. However, the issue has not been addressed in previous studies and a full treatment is not presently supported in MarMOT.

Another issue arises when optimizing over multiple sites. Schartau and Oschlies (2003) optimized parameters for three Atlantic sites simultaneously and found with their initial weighting scheme that observations at a particular site had a much greater influence than those at the other sites. This was a consequence of order-of-magnitude variations in property concentrations between sites. The problem was countered by introducing a weight based on variables' mean values at each site, an approach also adopted by Friedrichs et al. (2007) in simultaneous optimizations for sites in the Arabian Sea and Equatorial Pacific. No site-specific weighting was used in the two-site calibration of Hurtt and Armstrong (1999) or the multi-site calibrations of Hemmings et al. (2003, 2004).

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When the objective is to achieve a particular compromise between sites or between variables that is dictated by an application of the model then some subjective weighting can be justified. However, when it is to make inferences about the model such weighting is undesirable. Furthermore, it is possible that improved normalization of model-data misfits could reduce the need for it.

3.2 Twin experiments

A set of identical twin experiments are presented in which synthetic observations are generated from a model with a particular parameter set, taken to represent the true system. The same model with 5 free parameters is then optimized to fit these data in an attempt to recover the original "true" parameter values. Results for the proposed method are compared with those obtained using established weighting schemes. The plankton model is a recent version of the HadOCC (Hadley Centre Ocean Carbon Cycle) model, based on the model of Palmer and Totterdell (2001), in which organic carbon fluxes are controlled by a 4 compartment nitrogen cycle. The state variables are dissolved inorganic nitrogen (DIN), phytoplankton, zooplankton and detritus. A full description of the model's nitrogen cycle is given in Appendix C. The parameters to be optimized are specified in Table 2.

The first step is to create a statistical characterization of the environmental inputs representing a given scenario with reasonably realistic patterns of uncertainty. One realization of this synthetic environment represents the true environment and the corresponding simulation is used to generate the observation set. A second realization is treated as the best available estimate of the true environment and used to drive trial simulations with varying parameter vectors in the optimization experiments. This realization of the environmental data is referred to as the optimization environment. To examine the robustness of the results with respect to environment error, the set of optimization experiments is repeated for different realizations. Estimates of the environment error variances $\sigma^2_{ijk\mathrm{ENV}}$ are determined from ensemble realizations using the same synthetic environment model, so they reflect the impact of known uncertainty in

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the environmental inputs. In a real-world experiment, the reliability of the data assimilation results will depend on how well the environmental uncertainty can be characterized.

The chosen scenario is based on an annual cycle at three sites with 1-D simulations being driven by data from a global ocean biogeochemical general circulation model; the NEMO (Nucleus for European Modelling of the Ocean) model coupled with the MEDUSA (Model for Ecosystem Dynamics, carbon Utilisation, Sequestration and Acidification) biogeochemical model is used to provide physical forcing data and biogeochemical flux divergence statistics. These are derived from 5 day mean fields from a simulation at 1/4° resolution with 64 vertical levels, referred to as ORCA025-N201 (Popova et al., 2010). The run was undertaken at the National Oceanography Centre as part of the DRAKKAR collaboration (Barnier, 2006) with model integration being performed on HECToR, the UK National Supercomputing Centre facility. The selected sites are at 31° N 64° W, 47° N 20° W and 59° N 19° W corresponding to the BATS, NABE and OWS-INDIA sites used by Schartau and Oschlies (2003).

A number of different 1-D simulations were performed at each site in connection with the twin experiments. An overview is given in Table 3. Simulation Group A provides a synthetic climatology used to create an ensemble of initial states. Simulation Group B is an ensemble simulation providing an estimate of the expected environment error variances for a known system as an illustrative example of the impact of environmental uncertainty. Simulation Group C provides parameter-independent environment error variance estimates for the parameter optimization experiments. Simulation Group D provides the true system state for the true environment. This state is used in generating synthetic observations for assimilation in a set of optimization experiments comprising Simulation Group E. The observed variables are DIN, particulate organic nitrogen (PON), phytoplankton chlorophyll and primary production. For the purposes of this experiment, PON is defined as the sum of the organic nitrogen tracers (phytoplankton, zooplankton and detritus).

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3.2.1 Statistical characterization of the synthetic environment

Estimates of the mixed layer depth, the horizontal flux divergences and the initial state at each site are treated as uncertain and represented by input ensembles. The methods for ensemble generation are described below. The potential impact of uncertainty in solar radiation, vertical velocity, interior vertical diffusion and the monthly mean horizontal flux divergence is not explored: the "true" values of these variables are used throughout. The vertical diffusion coefficient is set to zero so that only numerical diffusion occurs below the mixed layer.

For the mixed layer depth, the level of uncertainty is based on the assumption that time-varying mixed layer depth statistics for a 1° square area are known. Mixed layer depth at a given time is described by a log-normal distribution with mean and variance determined from the distribution of turbocline depths over all ORCA025 grid points within a 1° square area centred on each site location, using data from the scenario year (2005). The turbocline depth at each grid point is taken to be an equally likely representation of the depth of the mixed layer at the site. Mixed layer depth values are generated at 5 day intervals with no temporal inter-dependency and linearly interpolated between these times. The characteristics of the mixed layer depth input ensemble are summarized in Fig. 2.

For the horizontal flux divergences it is assumed that depth-dependent monthly means and standard deviations are available from a model-based climatology. In a real-world experiment it would be important to ensure that these statistics were consistent with the model being analyzed. This is not an issue in the twin experiment context, so statistics derived from the ORCA025-N201 output are used despite its dependency on a different plankton model. Inter-annual variability in the actual 3-D simulation provides separate realizations of the circulation, the statistical properties of which are taken be representative of uncertainty in our knowledge of the true circulation affecting conditions in the scenario year. The 3-D model resolution is eddy-permitting, so the advective flux divergences can be expected to represent some limited eddy diffusion effects.

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All perturbations are applied in transformed tracer space so are concentration dependent. A square root transformation was chosen for all tracers at all sites, giving a rate of change for tracer concentration C_i of

$$p_i = 2\sqrt{C_i}p_i^\star \tag{18}$$

in response to a perturbation $p_i^\star$ applied to $\sqrt{C_i}$. The choice of tracer transformation was a compromise supported by a Box and Cox (1964) analysis in which a maximum likelihood method is used to determine the optimum variance-stabilizing transformation from those available in MarMOT (log, square root or none). The applied perturbation was derived from the advective flux divergence of the transformed tracer as determined from the 5 day mean concentration and velocity fields output by the 3-D model, so

$$p_i^\star = -\nabla_\mathrm{h}\cdot(\boldsymbol{u}_\mathrm{h}\sqrt{C_i}) \tag{19}$$

where the subscript h denotes vectors in the horizontal plane and $\boldsymbol{u}_\mathrm{h}$ is the current velocity. Spatial variation in the flow is ignored and taken to be zero, so that the applied perturbation is simply the product of the local flow rate and the horizontal gradient of $\sqrt{C_i}$ in the direction of the flow. This is calculated for all times and depth levels over 15 yr of the 3-D simulation (1991–2005) and binned by month to obtain statistics μ_i^{pert} and σ_i^{pert} for one annual cycle. The resulting tracer perturbation input fields for each site are shown in Figs. 3 and 4. Different realizations of the perturbation rate anomaly, consistent with σ_i^{pert}, are generated internally from different input seed values. A 24 h auto-correlation coefficient of 0.5 is used for all simulations.

There is clearly strong correlation between state variables in the mean flux divergences represented in Fig. 3. Correlation structure arising from the plankton dynamics would likewise be expected in any anomalies, although the present MarMOT system only generates perturbation rate anomalies for different variables independently. Functionality to introduce correlation structure on the basis of input statistics would be a useful extension.

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For the initial state, it is assumed that multi-variate monthly climatological statistics are available for all tracers at depths of 5, 10, 20, 40, 60, 80, 100, 150, 200, 250, 300, 500, 750 and 1000 m. A synthetic climatology is created for each site from a 15 yr HadOCC integration to the start of the scenario year with the true parameter set (Simulation Group A). Excessive model drift due to absent horizontal processes is avoided by relaxing the DIN tracer towards climatology at all depths below the combined mixed layer and euphotic zone, with a 60 day relaxation time scale ($r = 0.0167\,\mathrm{d}^{-1}$). The reference concentrations for relaxation are given by local annual mean nitrate profiles from the World Ocean Atlas (Garcia et al., 2010) and the 15 yr integrations are initialized from a steady state annual cycle obtained from repeat integrations of the first year. Monthly statistics from the resulting climatology are used to construct a probability model for randomly generating system states as needed, preserving vertical covariances and covariances between tracers as characterized by the first 5 principal components of the anomalies. These explain 76 %, 62 % and 74 % of the variance at BATS, NABE and OWS-INDIA sites, respectively. A multi-variate state representative of December or January is selected with equal probability to initialize simulations at the start of the calendar year. The main characteristics of the initial state input ensemble are summarized in Fig. 5.

3.2.2 Environment error for a known system

Given a statistical characterization of the input data, the expected environment error in the simulation is dependent on the plankton model and its parameter values. Estimates of the environment error fields for a known system, specifically the HadOCC model with default parameters (Table C), are given by a 100 member ensemble simulation at each site (Simulation Group B). A square root transformation is applied to each observed variable, on the basis of a Box-Cox analysis (Box and Cox, 1964), to stabilize the ensemble variance. The ensemble standard deviation for each transformed variable gives an estimate of its expected r.m.s. environment error. Estimates are shown in Fig. 6 as a function of depth and time.

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There are particular patterns in Fig. 6 that are directly linked with uncertainty in mixed layer depth (Fig. 2) during seasonal deepening of the boundary layer. At NABE and OWS-INDIA, clear bands of high standard deviation in transformed PON and chlorophyll are evident in the region of the maximum mixing depth from late summer onwards. These are also seen at BATS and NABE from January to March where corresponding bands are present in the DIN plots. In contrast, at OWS-INDIA where there is much greater variability in mixed layer depth over the ensemble, there are no obvious peaks in the depth distributions of the ensemble standard deviation over the winter period. At OWS-INDIA particularly high ensemble variance occurs in transformed DIN as the mixed layer deepens in the autumn. This extends throughout the boundary layer and appears to be the result of high variability in the advective DIN flux divergence (see Fig. 4), much of which is above the mixed layer depth. Variability in DIN flux divergence is similarly high at BATS at this time but below the mixed layer depth, contributing to a sub-surface band of high simulation variance in DIN from spring through to the end of the year. Other high variance patterns in late spring and early summer appear to be associated with the biological response to spring shoaling of the mixed layer. These are symptomatic of more complex interactions between the variance in the input ensemble and the biological dynamics.

Another important point with respect to the transformed DIN ensemble standard deviation is its strong increase over the year at OWS-INDIA. Here, the ensemble variance is much higher over the full depth range at the end of December than at the beginning of the year. The situation is similar at BATS, although less obvious. In contrast, the DIN pattern at NABE is much more suggestive of a repeatable annual cycle. The net growth in transformed DIN error variance at BATS and OWS-INDIA over 1 yr of integration may be due to deficiencies in the statistical representation of the horizontal flux divergences. This should be further investigated with a view to possible refinement of the boundary condition. In particular, the use of a square root transformation in the advective flux divergence calculation (Eq. 19) may not be appropriate over all times and depths at which it is applied. Preliminary analyses of the 3-D biogeochemical simulation suggest

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that the flux divergences might be better represented using a variable power law transformation that adapts to time and depth variations in their probability distributions.

3.2.3 Parameter-independent environment error

In a calibration exercise, the true parameter vector is unknown so parameter uncertainty must be considered. In the experiments presented here, a single standard deviation estimate $s^2_{ijk\mathrm{ENV}}$ is used at each data point for the whole free parameter space to be searched by the optimizer. $s^2_{ijk\mathrm{ENV}}$ was determined by pooling variances calculated for 100 different parameter vectors in the 5-dimensional parameter space, chosen according to a Latin hypercube design (McKay et al., 1979). For improved coverage, a maximin criterion (Johnson et al., 1990) was applied to 500 randomly generated hypercubes, selecting the design minimizing the Euclidean distance between pairs of sample points. For each parameter vector, the error variance estimates were determined using 100 realizations of the environment, requiring 10 000 simulations at each site in Simulation Group C.

The parameter-independent field estimates from the 10 000 member ensemble are shown in Fig. 7. The differences between the error standard deviation patterns shown in Figs. 6 and 7 give an indication of the effect of parameter uncertainty. While the patterns are broadly similar, it is clear that many of the details are sensitive to the parameter values, suggesting that the use of parameter-specific environment error estimates in the cost function could be beneficial. This option would be computationally more expensive and is not explored in the optimization experiments presented here.

3.2.4 Synthetic observations

The observations for the scenario year are generated from a simulation with the true environment (Simulation Group D) by sampling the output and adding observation errors. The resulting observation data set comprises monthly DIN and PON concentrations at depths of 10, 30, 50, 100, 200, 300 and 500 m, monthly chlorophyll concentrations

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and primary production fluxes at 10, 30, 50, 100 and 200 m and upper mixed layer chlorophyll concentrations at 5 day intervals. Plausible errors are applied to square root or log transformed values as specified in Table 1. For the log-transformed biological variables, the error standard deviations are derived from nominal relative errors by averaging positive and negative errors in log space. The actual relative errors are shown in brackets.

3.2.5 Parameter optimization

A set of three experiments is performed with different weighting schemes, one using a characteristic scale for each variable, another based on the known observation error statistics and a third using these in combination with the simulation error variances determined using the environmental input ensemble. The first two schemes are representative of established schemes described in Sect. 3.1.

In Experiment 1, we consider observation error variance estimates based on the inherent variability in the data set and, following Friedrichs et al. (2006), set the uncertainty to 25 % of the standard deviation s for all observations of the same type at the same site. So for variable j at site k the weights in the MarMOT cost function (Eq. 1) are

$$w_{ijk} = \frac{16}{s_{jk}^2}. \tag{20}$$

In Experiment 2, the known observation error statistics are used, so

$$w_{ijk} = \frac{1}{\sigma_{j\mathrm{OBS}}^2}. \tag{21}$$

Model-data differences are calculated in square root space or log space, according to the transformation used for generating observation errors.

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In Experiment 3, the weights are derived following the new method proposed in Sect. 3.1, using environmental simulation error variance estimates $s^2_{ijk\mathrm{ENV}}$. Weights for individual misfits are of the form

$$w_{ijk} = \frac{1}{s^2_{ijk\mathrm{OBS}} + s^2_{ijk\mathrm{ENV}}}. \quad (22)$$

Model-data differences are calculated in square root space. For chlorophyll, PON and primary production, the observation error is specified in $\log_{10}$ space and the expected error in square root space depends on the untransformed observation value $\Omega = y^2_{ijk}$ according to

$$s_{ijk\mathrm{OBS}} = \ln(10)\frac{\sqrt{\Omega}}{2}\sigma_{j\mathrm{OBS}}. \quad (23)$$

For DIN,

$$s_{ijk\mathrm{OBS}} = \sigma_{j\mathrm{OBS}}. \quad (24)$$

While the presence of significant correlation structure in the simulation error is acknowledged, no allowance is made for covariances in the cost function weighting. The adverse effects are reduced by removing duplicate simulation values that occur at multiple sampling depths within the upper mixed layer. Where this occurs, all mixed layer observations below 10 m are excluded.

The optimization procedure was identical for each set of optimization experiments. Initial optimization was performed with the μGA which was run for a minimum of 1000 generations to provide a pre-conditioned set of parameter vectors for local searches with the direction set algorithm. On any convergence in the parameter vector population, defined by uniformity across the population in at least 95 % of the bits in the binary code describing the parameter vectors, a new random population is generated, retaining the best individual. Additional generations after Generation 1000 were

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run until the next convergence. The algorithm was configured with uniform cross-over between bit strings at a probability of 0.5. Bounds are required for the μGA but are removed for the local search to avoid enforcing artificial constraints when locating minima close to the boundaries of the parameter space. Log transformations are used to prevent parameters taking negative values. Details for each parameter are given in Table 2. Within the μGA, each parameter was represented by 8 bits giving 256 possible values prior to refinement by the local searches.

The population size for the μGA was 5, chosen to match the number of free parameters following the recommendation of Schartau and Oschlies (2003). Initial parameter vectors in the original population were distributed in parameter space according to a Latin hypercube design. The direction set algorithm was applied to each unique parameter vector in the final population and the lowest cost result selected. To investigate the sensitivity of the result to the initial parameter vectors, each application of the optimizer was repeated for 5 alternative designs, choosing those with the largest minimum Euclidean distances from a sample of 500 randomly generated hypercubes.

A single set of three optimization experiments is referred to as Simulation Group E. Simulation Group E was repeated for 10 different realizations of the optimization environment. Because the mixed layer depth varies between different realizations of the environment error, a slightly different observation set is used for each set of experiments. A further set of three optimization experiments was performed using the true environment.

3.2.6 Results

Results of the cost function minimization procedure in each optimization experiment are shown in Table 4, together with the cost function value for the true parameter vector $J(\boldsymbol{P}_{\text{true}})$. The initial minima and maxima show the range of the cost J over a super population of 25 parameter vectors, comprising the 5 distinct initializations of the μGA population. The final cost range is that for the 5 output parameter vectors, each being

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the lowest cost vector for one μGA initialization after local minimization. Final cost ranges are small indicating low sensitivity to the details of optimizer initialization.

In Experiment 3, the final cost values $J(\boldsymbol{P}_{\text{opt}})$ and the true parameter costs $J(\boldsymbol{P}_{\text{true}})$ both tend to be close to unity in the presence of environmental error. The costs for the other optimization experiments are consistently larger, indicating that the level of uncertainty present is greater than that allowed for in the cost function design. If the true parameter vector were not known a priori, there would be a risk of such high costs leading to rejection of the true hypothesis. Cost function values are particularly large in Experiment 2. This is a consequence of relative errors in organic tracer concentrations that are much larger than the small observation errors associated with small concentrations. The effect can be attributed to our simple treatment of observation error, which inevitably underestimates expected error as the observed concentration tends to zero. A more sophisticated treatment would be to represent the error as a sum of absolute and relative terms as done by Schartau et al. (2001). Where the true environment is used, Experiment 2 gives cost values close to unity ($J(\boldsymbol{P}_{\text{opt}}) = 1.2$ and $J(\boldsymbol{P}_{\text{true}}) = 1.2$) since the weighting used is consistent with the uncertainty present. In contrast, the corresponding Experiment 3 results show much lower costs ($J(\boldsymbol{P}_{\text{opt}}) = 0.53$, $J(\boldsymbol{P}_{\text{true}}) = 0.54$).

The final costs are always less than $J(\boldsymbol{P}_{\text{true}})$ except when the true environment is used, indicating some degree of over-fitting. This is expected where the cost function is distorted by error in the observations or environmental inputs but should be reduced by an effective weighting scheme. The cost differences $J(\boldsymbol{P}_{\text{opt}}) - J(\boldsymbol{P}_{\text{true}})$ suggest that over-fitting is worst in Experiment 1, with a mean cost difference of -2.8 in the presence of non-zero environment error compared with -1.1 and -0.14 in Experiments 2 and 3, respectively. The Experiment 1 mean cost difference is a factor of 20 greater than that for Experiment 3. This contrasts with factors of about 4 and 6 for the initial cost minima and maxima respectively, so is not simply due to a parameter-independent scaling of the cost function. It should also be noted that for 5 out of 10 environment error realizations, the Experiment 1 cost function is greater at the location of the true parameter vector than the cost function minimum found prior to any application of the optimizer.

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This is a clear indication of a high over-fitting risk not seen in the Experiment 2 or 3 results.

The final parameter values obtained in each experiment for each input environment are shown in Fig. 8. All distinct values are shown for each of the 5 optimizer initialization cases but only the optimal values (those associated with the minimum costs) are highlighted. Table 5 gives summary statistics for the parameter recovery errors over all non-zero realizations of the environment error. Where multiple initialization of the optimizer produced more than final parameter vector with the same cost (to 6 significant digits), parameter values are first averaged to give a single value for each environment error realization.

Parameter recovery is generally improved in Experiment 3, where both error sources are accounted for. There is also less sensitivity in final parameter values to the initial μGA population The Experiment 2 design, where the weights are based on observation error, performs better than the characteristic scale weighting used in Experiment 1, particularly with regard to parameter biases. In Experiment 1, the initial P-E slope α_{surf} is estimated low for all but 1 case of the environment error and has a strong negative bias (−29%). There are also some very high estimates of the sinking velocity parameter w_{D}, leading to a 71 % bias. Furthermore, the r.m.s. errors in the final parameter values show the expected error to be consistently higher than for the other two experiments. In Experiment 2, although the r.m.s. errors are consistently higher than those for Experiment 3, the biases are smaller for 2 of the 5 parameters suggesting some room for improvement in the environment error weighting.

Closer inspection of the values for the parameters g_{max} and m_2 from all experiments shows them to be highly correlated. This is perhaps unsurprising considering their role in the model dynamics, since the maximum grazing rate g_{max} impacts directly on nitrogen transfer into the zooplankton pool and the density-dependent mortality m_2 impacts directly on transfer out. It is thus possible to compensate for excessively high values of one parameter by high values of the other, keeping zooplankton nitrogen stable. This leads to a positive bias in both parameters. High values do increase the throughput of

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nitrogen from phytoplankton food to DIN potentially impacting on chlorophyll and DIN observations but this effect is attenuated by recycling which fuels more phytoplankton growth. Nevertheless, other features of the system make some observational constraint possible. It is notable that the cost function design in Experiment 3 appears more robust in the face of this correlation tendency between parameters than either of the other designs.

To examine the implication of the parameter recovery errors for model estimates of key carbon fluxes, simulations were run with each of the 10 optimal parameter vectors using the true environment. Table 6 gives error statistics, over this 10 member ensemble, for the annual mean primary production integrated over the water column at each site. Corresponding estimates of the export flux of sinking particles to the ocean interior are given in Table 7. The export is represented by the downward flux of particulate carbon at a site-dependent reference depth z_{ref}, given by $w_{\mathrm{D}}\theta_{\mathrm{D}}D(z_{\mathrm{ref}})$. z_{ref} is set at 250, 400 and 100 m for BATS, NABE and OWS-INDIA respectively, just below the maximum depth of winter mixing for all ensemble members. In all experiments, the sinking particle flux r.m.s. errors and biases are consistent across sites and strongly reflect the statistics for the sinking rate parameter w_{D}. While particle flux is also affected by error in the detritus concentration $D(z_{\mathrm{ref}})$, such errors are not consistent over the year so have a relatively small impact on the annual mean.

The r.m.s. errors in both primary production and sinking particle flux are lowest for the Experiment 3 parameter vectors and highest for the Experiment 1 parameter vectors at all sites. In contrast, the biases are generally smallest for Experiment 2, rather than Experiment 3, with the sinking particle flux biases being less than half those given by the Experiment 3 parameter vectors. This underlines the need for further refinements to the new weighting scheme, despite its improved performance generally over both established schemes. The characteristic scale weighting used in the Experiment 1 cost function leads to r.m.s. errors in primary production due to environment error of 14–20 %. The corresponding errors with the new method are reduced by a factor of about 3 at each site. The sinking particle flux errors when the characteristic scale

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weighting is used are more serious at 122–128 %. These are reduced by an order of magnitude in Experiment 3. The twin experiment configuration is of course idealistic. It may not be possible to achieve such improvements in real-world experiments, where characterization of uncertainty is a much more difficult problem. Nevertheless, the poor performance of the widely used characteristic scale method in the presence of a fairly modest amount of synthetic environment error, combined with error in the observation data set, should be seen as a strong motivation for developing reliable statistical characterizations for both sources of uncertainty.

4 Discussion

The MarMOT system has been designed as a tool for plankton model assessment and inter-comparison. The model to be assessed could be the biogeochemical subcomponent of a global or regional OBGCM or the marine biogeochemical module from a complete earth system model. The aim is to provide a facility for evaluating plankton models independently from a particular host model, taking into account uncertainty in their input data.

Model inter-comparison may be performed separately from model assessment or models may be comparatively assessed with reference to observational data. In the first case, MarMOT provides a flexible environment for comparing the responses of alternative model designs to many different instances of their input data. These data include the values of any common parameters together with the models' shared environmental input data: physical forcing, horizontal tracer flux divergences and initial conditions. Such comparisons will lead to an improved understanding of the relationships between models and the implications of different design decisions.

For comparative assessment, MarMOT provides a framework for handling real-world uncertainty in the environmental input data and parameter optimization features to allow models to be calibrated against observations, addressing the issue of parameter

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uncertainty. Effective calibration will allow models to be comparatively assessed, with reference to independent observations, on the basis of their design. The large number of adjustable parameters in most plankton models makes this non-linear inverse problem particularly challenging. Sensitivity analyses are often used as a basis for reducing the size of the adjustable parameter vector prior to formal optimization and are well-supported by the MarMOT framework. The size and dimensionality of the input spaces involved typically limit the effectiveness of Monte Carlo methods. However, drawing on recent developments in the field of Bayesian statistics, output from ensemble integrations performed in MarMOT can be used to build fast statistical emulators (O'Hagan, 2006) with which coverage can be achieved more efficiently.

The twin experiments presented here demonstrate the application of the MarMOT system to the inverse problem of plankton model calibration in an idealized configuration. Specifically, MarMOT features are used to explore the potential of a new cost function weighting scheme that includes a formal treatment of observation and simulation uncertainty, the latter arising as a consequence of uncertainty in the models environmental input data. The new scheme performs well against existing schemes in the presence of environment error. The possibility of further improvements should be investigated by refining the scheme to use parameter-dependent simulation error variances. Ideally, simulation error variances would be computed for all trial parameter vectors in an optimization experiment, but the computational cost of this solution is high. A less expensive alternative would be to use a sample of simulation error variances calculated for different points in the parameter space, as in the analysis of our Simulation Group C, selecting the nearest neighbour for each trial parameter vector. Statistical emulation of the simulation error variance as a function of the parameters might also be considered. A further refinement likely to be beneficial is the inclusion of simulation error covariances in the cost function weighting scheme.

In a real-world context, obtaining reliable statistical characterizations of the required environmental input data will be a major challenge. These are required for all plankton model assessments, with or without parameter optimization. To constrain the

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probability distributions for these inputs we must make use of a much wider range of supporting data than is traditionally used when comparing biogeochemical model outputs with observations.

Background climatological statistics for physical forcing can be based on analyses of 3-D physical simulations. These should ideally be eddy-resolving. Furthermore, it is important that they are evaluated against observational climatologies so that information on biases can be included. Available satellite and in situ observations contemporary with the biogeochemical evaluation data can be used to further constrain the physical forcing statistics. Assimilative physical model output might also be used, although these data may be less reliable than output from free-running simulations if used to infer relationships between observed and unobserved variables. The details will depend on the performance of the balancing schemes use to preserve physical laws in the assimilation process.

Successful application of the horizontal flux divergence scheme depends on obtaining good estimates for the perturbation rate statistics for each tracer. The biogeochemical flux divergences required for model assessment are those for the trial model in a perfect 3-D physical simulation. Thus they do not exist in reality and cannot be derived directly from observations. Furthermore, they are inevitably parameter-dependent. For these reasons we are forced to rely on broad-based statistics derived from biogeochemical simulations. Multiple 3-D simulations should be analyzed to explore sensitivity to model structure and parameters with the aim of developing climatological statistics that are reasonably robust to model differences. This would allow consistent unbiased boundary conditions to be applied to any trial model configuration. The model-based background statistics should be further constrained by observations giving information about the contemporary physical environment. In situ current data can be used, if available. Otherwise, surface geostrophic current estimates derived from satellite altimetry might be used. Evidence of physical gradients from satellite sea-surface temperature or ocean colour measurements is also relevant since horizontal flux divergence is likely to be increased in frontal regions, especially if there is evidence of a cross-frontal velocity

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component. These types of information can be used to modify the climatological flux divergence probability distributions.

In common with the flux divergence boundary condition, the initial conditions in a model assessment could be chosen to be consistent with a spin up of the trial model in a perfect physical simulation. While the idea is conceptually appealing, a reliable characterization of this hypothetical system state is likely to be elusive. A more practical alternative is to use an estimate of the real-world state, explicitly restricting any inferences about the model to its behaviour over relatively short time scales. The state estimate would be based on observational data where possible.

In the absence of observations, initial conditions for 1-D simulations are often determined by a steady state analysis based on a repeating annual cycle. The same approach might be taken in an ensemble simulation, provided that error growth associated with uncertainty in the forcing data and boundary conditions does not prevent achievement of a statistical steady state. The boundary condition would be the real-world flux divergence condition with controlled relaxation to climatology. The relaxation provides an additional constraint, although the climatological reference state for unobserved state variables would be primarily model-based with an appropriately high level of uncertainty.

For some state variables, relevant measurements exist but the relationship between model variables and the real-world observations is uncertain due to a combination of observing system limitations and simplifying assumptions made in model design. In such cases, the observational data can be use to partially constrain model-based estimates. For example, chlorophyll measurements can be used to constrain phytoplankton nitrogen subject to the uncertainty introduced by an unknown nitrogen:chlorophyll ratio. PON measurements might be used to constrain the combined phytoplankton, zooplankton and detritus variables in the HadOCC model. However, they are affected by plankton avoidance of sampling bottles so will tend to under-represent zooplankton. They could therefore be used as an upper bound estimate for the sum of phytoplankton and detrital nitrogen or a lower bound estimate for the total organic nitrogen. A similar

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argument was used by Fasham and Evans (1995) to compare PON observations with values derived from simulated phytoplankton, bacteria, detritus and zooplankton concentrations.

We have focussed on application of MarMOT to model assessment and inter-comparison. Other applications include the comparison of plankton models at the level of individual processes and the provision of 1-D state estimates for specific locations of interest. Comparison at the process level is achieved by holding individual tracer concentrations constant or by fully prescribing their variation using external input fields. This in-built flexibility makes MarMOT a powerful tool for model analysis and development. In addition, the scope of model inter-comparison studies can be reduced to focus on the biogeochemical interactions by applying a common photosynthesis submodel. 1-D state estimates with uncertainty measures can be determined on the basis of one or more plankton models. For these applications, the real-world flux divergence boundary condition allows climatological state estimates to be combined with model responses to year-specific local forcing in a way that takes account of probabalistic horizontal flux divergence estimates contemporary with the forcing data.

MarMOT development is on-going. The software will be adapted to address some of the specific issues identified in this study, including improvements to the boundary condition scheme for better representing horizontal flux divergence statistics and cost function support for parameter-dependent simulation error variances and covariances. In addition, the system is being extended to support models of varying biogeochemical complexity with the aim of establishing a new community resource for plankton model evaluation in global and regional applications.

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Appendix A

MarMOT design concepts

The MME is implemented as a specific application within a system called the Generic Function Analyzer (GFAn). GFAn provides a cross-referencer for input selection and an optimizer for cost function minimization over the model parameter space. It also provides a generic data management framework that adapts to the requirements of the MME application to provide a MarMOT-specific user interface. GFAn is essentially an analysis engine with a well-defined application interface that makes all of its functionality available to any compatible application. The full functionality of both GFAn and the MME can likewise be applied to any plankton ecosystem model for which the basic input requirements are supported. This layered approach ensures the widest possible applicability of on-going improvements to the functionality of both GFAn and the MME. The GFAn code and MME user interface are written in C and the plankton model interface is in Fortran.

A1 Data management

An integrated data management system is essential for efficiently handling the diverse data requirements of different experiments. GFAn handles 3 different kinds of input data item used in MarMOT: parameter set items, gridded domain items and non-gridded domain items. Each instance of a parameter set item consists of a number of individually named values, such as plankton model parameters. There is one parameter set item for each supported plankton model, containing one or more instances of the model's parameter set, possibly augmented by a set of flag values for selecting optional or alternative features of the model. Further parameter set items provide model-independent information such as water column depth, simulation period and a range of other simulation options, including which plankton model to use. Gridded-domain items consist of one or more data arrays defined on a common regular grid

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with axes corresponding to one or more dimensions of the simulation domain. These are used to define the vertical grid, initial conditions, boundary conditions and forcing data. Non-gridded domain items are one or more vectors of values co-located at arbitrary points on the model domain axes. Observations or other reference data for comparison with the simulation output are input in this form.

An important design consideration is the need for the system to support complex experiments while at the same time being easily configurable for simple experiments. Individual items are optional wherever possible. Forcing data can be supplied in a number of different ways: as full-depth time-varying fields or as data fixed in space or in time or simply as environmental constants. Boundary condition data are treated likewise. Time-varying fields can be provided at any regular interval. The interval need not necessarily be the same for all variables: different forcing variables can be distributed arbitrarily among a number of different input item tables, typically one for each user-defined grid. Forcing data interpolated to the model time step is available in the simulation output.

GFAn provides multi-case support in the form of a flexible cross-referencing algorithm that determines the required data for each simulation case. This is done either by context or explicitly by using alphanumeric key variables to identify particular instances of each item. The data instances selected for each case by the cross-referencer are indicated in the log file. For each item having multiple instances, the cross-referencing method is determined by the presence or absence of an item key in the input item table. Items without keys are to be referenced contextually and their instances are identified by one or more variables referred to as case variables. In MarMOT, there are 2 case variables: site and ensemble member. Input data can be associated with a particular site or a particular ensemble member or both. Both case variables are used to identify particular simulations in the input case table and in any output tables produced.

MarMOT is configured by providing a set of input tables and optionally produces a set of output tables, in addition to the cost function value. Each table is contained in an ASCII file. For each input item, a table is expected with one entry for each instance of

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the data. For domain items, this table contains metadata describing the structure of the data and the actual data values are extracted from a separate table. Alternatively, for gridded data items, data can be extracted automatically from one or more NetCDF data sets (Rew and Davis, 1990) to populate a user-defined grid. A case table is needed for any experiment involving more than one simulation. Further input tables are required for setting up optimization experiments and output variable selection where applicable. Finally, an "experiment control table" is used for assigning experiment-specific file names to all other input and output tables. The experiment control table can specify one or more experiments to be run, each either with or without parameter optimization. Batches of experiments are run without the overhead of re-loading resident data. Comprehensive, customizable log output provides a record of the experimental configurations. An example of the input and output for a simple experiment is given in the Supplement.

A2 Plankton model interface

The MarMOT Model Evaluator handles a superset of prognostic and diagnostic variables and the necessary information is transferred between the MME data area and the active plankton model at each time step, allowing plankton models to be implemented with minimal changes to their native variables and code. Each model must provide a specific set of Fortran subroutines. Generic socket subroutines on the MME side of the interface are responsible for calling the appropriate model-specific subroutines, according to the model selected for the current simulation.

A plankton model subroutine "defparm" is required to define variable names and descriptions for the parameters in the model's parameter set item, together with any model-specific option flags therein. Minimum and maximum allowable values for each parameter can also be defined in this routine if applicable. A subroutine "setup" is expected to configure the model to use the model grid, time step and any model-specific options supplied by MarMOT. It is also responsible for requesting any model-specific forcing variables needed by setting the appropriate MarMOT flags. Copying of

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parameter values is done in a separate subroutine "setparm", allowing for the possibility of time-varying parameters in future versions. "setup" also receives from MarMOT a number of mapping vectors for use in other interface subroutines. These index the positions of model variables in the MME arrays. The other mandatory subroutines are "putstate" and "getstate", responsible for copying MME state variables to model variables and back, "biostep" for computing a biological time step and "getdiag" for returning diagnostics. A subroutine "initstate" can be provided to perform any model-specific initialization of the system state that might be applicable. To use the photosynthesis options provided by the MME, a model must provide one further subroutine "getphotin" to output values for the required photosynthetic parameters.

MarMOT maintains two sets of tracers: primary tracers and derived tracers. The concentration of each derived tracer is determined by the concentration of one or more primary tracers and zero or more ratios describing the composition of particular ecosystem components. Derived tracers such as total nitrogen or total carbon are made available for diagnostic purposes only, while other derived tracers can be prognostic variables.

The initial conditions required for a simulation are model-dependent. For a given plankton model the initial state is defined by profiles for each applicable primary tracer and any composition ratios that will vary dynamically. Where tracers are linked by composition ratios, whether variable or fixed, there are alternative sets of prognostic variables and those used within the model may be different from those initialized. MarMOT uses nitrogen variables as the primary tracers for all organic components. Forcing data requirements are also model-dependent. Each model indicates to the MME what forcing data it requires and the MME selects the information from the input data available. Only data relevant to the currently selected model appear in the simulation output.

Two plankton models are currently supported: the 4 compartment nitrogen model of Oschlies and Garçon (1999) and a version of the Hadley Centre Ocean Carbon Cycle model developed by Palmer and Totterdell (2001). Both models are of the NPZD class, representing the nitrogen cycle in terms of fluxes between dissolved inorganic nitrogen

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(DIN), phytoplankton, zooplankton and detritus. The HadOCC model also includes a carbonate system in the form of additional tracers for total dissolved inorganic carbon and alkalinity. A much wider range of models, of varying complexity, will be supported in future versions.

Appendix B

MarMOT photosynthesis options

The MME provides various options for the light limitation of photosynthesis: different parameterizations can be applied independently for the attenuation of photosynthetically available radiation (PAR) in the water column, the chlorophyll-specific absorption of light energy by the phytoplankton and the photosynthetic response.

The PAR attenuation coefficient can be modelled as a linear function of pigment concentration G provided by the plankton model:

$$K_{\mathrm{dPAR}} = k_{\mathrm{water}} + k_{\mathrm{pig}} G \tag{B1}$$

where k_{water} is the attenuation due to water, k_{pig} is the attenuation due to pigment. Although widely used, this formulation ignores the effect of changes in the spectral distribution of the energy in the PAR waveband on the attenuation coefficient as the light quality changes with depth. An alternative option is available that accounts for these changes: an empirical approximation to the 61 wave-band model of Morel (1988), developed by Anderson (Anderson, 1993) for use in OBGCMs. Light penetration is based on a 3 layer model of the attenuation coefficient K_{dPAR}, as a function of a depth-invariant pigment concentration. The three optical layers are divided by layer boundaries at 5 m and 23 m. K_{dPAR} is determined from the local pigment concentration at each depth level. Where the depth level boundaries for the current simulation do not coincide with optical layer boundaries, K_{dPAR} is depth averaged within levels.

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The K_{dPAR} profile from the attenuation model can optionally be adjusted, following Oschlies and Garçon (1999), to allow for the geometric effect of the sun's zenith angle on the path length between the surface and a given depth. The correction factor is based only on the direct path effect, tending to bias K_{dPAR} high. However, a compensating bias is introduced by basing the factor on the zenith angle at noon, when path length is at its daily minimum. The true effect of zenith angle on the attenuation coefficient is strongly wavelength dependent and decreases with depth (Zheng et al., 2002). The depth dependency is not currently modelled.

Chlorophyll-specific light absorption by phytoplankton varies with depth, due to changes in spectral distribution. This directly affects the initial slope of the photosynthesis-PAR curve. In many plankton models, this effect is ignored and a constant value is used for the initial slope. This option is supported in MarMOT, together with an alternative option to use the spectrally-averaged chlorophyll absorption model of Anderson (1993). Like the attenuation coefficient model, this is based on an empirical approximation to a 61 waveband model (Morel, 1988, 1991).

Three alternative parameterizations are provided for the light limitation of photosynthesis: two for calculating the daily mean photosynthetic rate over each simulation level and one for calculating a point-in-time rate for each level that allows the diel cycle to be resolved explicitly when high resolution forcing data are available. The available parameterizations for daily mean photosynthesis are those of Evans and Parslow (1985) and Platt et al. (1990). These are based on different triangular and sinusoidal representations of the diel cycle respectively and use different formulations of the photosynthesis-PAR curve. The point-in-time rate is calculated using the same photosynthesis-PAR curve as Evans and Parslow (1985).

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Appendix C

HadOCC nitrogen cycle simulation

The HadOCC model described here is a modified version of the model of Palmer and Totterdell (2001) incorporating a number of subsequent developments (Totterdell, personal communication, 2005). The nitrogen tracers are phytoplankton P, zooplankton Z, detritus D and dissolved inorganic nitrogen N. The main differences from the original version are the introduction of a variable carbon:chlorophyll ratio and changes to the pathways of material originating from grazing and mortality. In addition, spectrally-averaged photosynthesis is parameterized using the Anderson (1993) approximations (see Appendix B). There is no temperature limitation of photosynthesis and DIN limitation is applied to the photosynthesis-PAR curve maximum, rather than the light-limited photosynthetic rate, reducing its effect at low light levels. A different parameterization of depth variation in the detrital remineralization rate is used and a number of the parameters common to both model versions are assigned different values. Process parameterizations and source-minus-sink terms are defined below. Refer to Table C for parameter values.

Photosynthesis: Daily mean biomass-specific growth rate $\bar{\mu_{\mathrm{P}}}$ is calculated for each model level using the integral approximation of Platt et al. (1990). The photosynthesis-PAR response at depth z and time t is

$$\mu_{\mathrm{P}}(z,t) = P_{\max}\left[1 - \exp\left(-\frac{\alpha_{\mathrm{chl}}(z)E_{\mathrm{d}}(z,t)}{\theta_{\mathrm{chl}}P_{\max}}\right)\right] \tag{C1}$$

where the maximum nutrient-limited photosynthetic rate is given by

$$P_{\max} = V_{\max}\frac{N}{N + k_{\mathrm{N}}}. \tag{C2}$$

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The carbon:chlorophyll ratio is given by the balanced growth photo-acclimation model of Geider et al. (1997):

$$\theta_{\mathrm{chl}} = \min\left(\sqrt{\theta_{\min}\frac{\alpha_{\mathrm{chl}}E_{\mathrm{d}}}{\mu_{\mathrm{P}}(\theta_{\mathrm{chl}})}}, \theta_{\max}\right) \tag{C3}$$

Downwelling PAR E_{d} is determined by the light attenuation coefficient model of Anderson (1993), without the direct path adjustment of Oschlies and Garçon (1999). A ratio of chlorophyll to total pigment concentration of 0.8 is assumed and $E_{\mathrm{d}}(0,t)$ is taken to be 43 % of total downwelling solar radiation at the sea surface. The chlorophyll-specific initial slope α_{chl} is determined from model parameter α_{surf} using the Anderson (1993) chlorophyll light absorption model.

Zooplankton grazing: Phytoplankton and detritus losses due to herbivorous zooplankton activity are $G_{\mathrm{P}} = hP$ and $G_{\mathrm{D}} = hD$ respectively, where h is the grazing rate per unit food concentration:

$$h = \frac{B_Z Z}{F_{\mathrm{tot}}} g_{\max} \frac{F^2}{F^2 + K_{\mathrm{F}}^2}; \tag{C4}$$

$F = \max(0, F_{\mathrm{tot}} - F_{\mathrm{threshold}})$, where $F_{\mathrm{tot}} = B_{\mathrm{P}}P + B_{\mathrm{D}}D$ and $F_{\mathrm{threshold}} = 0.01\,\mathrm{mmol\,N\,m^{-3}}$.

Phytoplankton mortality: $M_{\mathrm{P}} = mP^2$; $m = 0$ for $P <= 0.01\,\mathrm{mmol\,N\,m^{-3}}$, otherwise $m = m_{\mathrm{o}}$.

Zooplankton mortality: $M_Z = m_1 Z + m_2 Z^2$.

Detrital remineralization: $\lambda = 0.1\,\mathrm{d^{-1}}$ for $z < 100\,\mathrm{m}$, otherwise $\lambda = \frac{8.58}{z}\,\mathrm{d^{-1}}$.

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Nitrogen equations:

$$\mathrm{SMS_P} = \bar{\mu_\mathrm{P}} P - M_\mathrm{P} - \eta P - G_\mathrm{P} \tag{C5}$$

$$\mathrm{SMS_Z} = \phi_\mathrm{I}(\beta_\mathrm{P} G_\mathrm{P} + \beta_\mathrm{D} G_\mathrm{D}) - M_\mathrm{Z} \tag{C6}$$

$$\mathrm{SMS_D} = \frac{\theta_\mathrm{P}}{\theta_\mathrm{D}}(0.99 M_\mathrm{P}) + \frac{\theta_\mathrm{Z}}{\theta_\mathrm{D}}(0.33 M_\mathrm{Z}) + \frac{\theta_\mathrm{P}}{\theta_\mathrm{D}} a_\mathrm{PD} G_\mathrm{P} + (a_\mathrm{DD} - 1) G_\mathrm{D} - \lambda D \tag{C7}$$

$$\mathrm{SMS_N} = \left\{0.01 + \left(1 - \frac{\theta_\mathrm{P}}{\theta_\mathrm{D}}\right) 0.99\right\} M_\mathrm{P} + \eta P + \left\{0.67 + \left(1 - \frac{\theta_\mathrm{Z}}{\theta_\mathrm{D}}\right) 0.33\right\} M_\mathrm{Z} + 0.1(1 - \phi_\mathrm{I})(G_\mathrm{P} + G_\mathrm{D}) + \left(1 - \frac{\theta_\mathrm{P}}{\theta_\mathrm{D}}\right) a_\mathrm{PD} G_\mathrm{P} + \lambda D - \bar{\mu_\mathrm{P}} P \tag{C8}$$

where $a_\mathrm{PD} = 0.9(1 - \phi_\mathrm{I}) + (1 - \beta_\mathrm{P})\phi_\mathrm{I}$ and $a_\mathrm{DD} = 0.9(1 - \phi_\mathrm{I}) + (1 - \beta_\mathrm{D})\phi_\mathrm{I}$. The active vertical velocity of detritus relative to the water is equal to the sinking velocity parameter w_D. It is zero for all other tracers.

Numerical configuration: The vertical grid has 63 levels with 35 levels in the top 1000 m. These upper ocean levels have boundaries at approximate depths 6, 12, 19, 25, 32, 39, 46, 54, 62, 71, 80, 90, 100, 112, 124, 137, 152, 168, 187, 207, 229, 254, 281, 312, 347, 386, 429, 477, 531, 591, 656, 729, 809, 896 and 991 m, corresponding to those of the ORCA025 model. Levels spanning the mixed layer depth are partially mixed. The advection scheme is an upstream differencing scheme. The time step is 1 h.

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Supplementary material related to this article is available online at: http://www.geosci-model-dev-discuss.net/4/1941/2011/gmdd-4-1941-2011-supplement.zip.

Acknowledgements. The MarMOT system has been developed with funding from the UK Natural Environment Research Council. We would like to thank Andreas Oschlies for access to code used in the vertical transport schemes and to Rachel Oxlade and Peter Craig for help with system testing and valuable feedback. Thanks are also due to the UK Met Office for access to the HadOCC model code. This work was supported by NERC via the National Centre for Earth Observation (a NERC collaborative centre).

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Table 1. Observation errors.

Observation type	HadOCC equivalent	Transformation	Error std. dev.	Relative error
DIN	N	sqrt	0.05 $(\text{mmol N m}^{-3})^{0.5}$	variable
PON	$P+Z+D$	log	0.239 $\log_{10}$ units	50 % (−42 %, +73 %)
Surface chlorophyll	$12.01\frac{\theta_P}{\theta_{chl}}P$	log	0.159 $\log_{10}$ units	35 % (−31 %,+44 %)
Sub-surface chlorophyll	$12.01\frac{\theta_P}{\theta_{chl}}P$	log	0.088 $\log_{10}$ units	20 % (−18 %,+22 %)
Primary production	$\bar{\mu_P}\theta_P P$	log	0.184 $\log_{10}$ units	40 % (−35 %,+53 %)

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Table 2. Free parameter space.

Parameter	Unit	Symbol	Minimum	Maximum	Transformation	Local Search
Initial slope of photosynthesis-PAR curve	$\mathrm{mg\,C\,(mg\,Chl)^{-1}}$	α_{surf}	0.5	50	log	unbounded
Half-saturation conc. for nutrient uptake	$\mathrm{mmol\,N\,m^{-3}}$	k_{N}	0.01	1	log	unbounded
Maximum grazing rate	$\mathrm{d^{-1}}$	g_{max}	0.1	10	log	unbounded
Zooplankton density-dependent mortality	$\mathrm{d^{-1}(mmol\,N\,m^{-3})^{-1}}$	m_2	0.03	3	log	unbounded
Detrital sinking velocity	$\mathrm{m\,d^{-1}}$	w_{D}	0	100	none	bounded

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Table 3. Overview of 1-D Plankton Model Simulations.

Simulation group id	Product(s)	Time period	Simulations at each site	Model parameters	Initial state	Forcing (ORCA025)	Boundary condition
A	initial state statistics	1990–2004	1	true parameter vector	1990 repeat cycle	on-site data	DIN relaxation to climatology
B	expected environment error for true system	2005	100 member environment ensemble	true parameter vector	initial state ensemble (100 members)	on-site solar rad., w_p MLD ensemble (100 members)	perturbation ensemble (100 members)
C	estimated parameter-independent environment error	2005	100 member environment ensemble × 100 param. vectors	sample from parameter space (100 vectors)	initial state ensemble (100 members)	on-site solar rad., w_p MLD ensemble (100 members)	perturbation ensemble (100 members)
D	observation set	2005	1 (true environment)	true parameter vector	1 initial state realization	on-site solar rad., w_p 1 MLD realization	1 perturbation realization
E	optimal parameter vectors (Expts. 1–3)	2005	1 optimization environment, trial parameter vectors	free parameter space	1 initial state realization	on-site solar rad.,w_p 1 MLD realization,	1 perturbation realization

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Table 4. Cost minimization.

Optimization Experiment	Environment	Initial Cost Minimum	Initial Cost Maximum	Final Cost $J(P_{opt})$	Final Cost Range	True Parameter Cost $J(P_{true})$	Cost Difference $J(P_{opt}) - J(P_{true})$
1	1	6.5	68	3.9	0.0002	4.5	−0.5
1	2	7.5	80	5.1	7e-05	6.2	−1.1
1	3	6.8	73	5.1	0.0005	8.0	−3.0
1	4	5.6	64	3.6	0.02	6.4	−2.9
1	5	10.2	95	8.3	0.004	20.6	−12.3
1	6	7.0	79	4.9	7e-05	8.5	−3.6
1	7	6.5	85	4.6	0.0002	5.7	−1.0
1	8	11.0	102	9.1	0.01	9.7	−0.6
1	9	14.2	91	12.1	0.009	14.4	−2.3
1	10	8.5	81	6.3	0.1	6.8	−0.5
	MEAN	8.4	82	6.3	0.02	9.1	−2.8
1	TRUE	5.3	63	2.6	1e-05	2.9	−0.3
2	1	27.9	99	23.6	0.005	23.7	−0.1
2	2	40.5	108	37.2	0.008	37.6	−0.4
2	3	29.6	98	26.3	0.4	27.2	−0.9
2	4	17.8	89	12.6	0.02	14.5	−1.9
2	5	28.8	112	25.5	0.6	27.7	−2.2
2	6	20.6	85	15.9	0.01	16.2	−0.3
2	7	40.1	108	32.4	0.02	34.9	−2.4
2	8	36.1	98	33.2	0.003	33.5	−0.4
2	9	49.9	115	48	0.1	49.8	−1.8
2	10	24.9	95	20.1	0.0008	20.4	−0.2
	MEAN	31.6	101	27.5	0.1	28.5	−1.1
2	TRUE	5.6	78	1.2	1e-05	1.2	0.0
3	1	1.71	15.1	1.04	2e-05	1.07	−0.03
3	2	1.90	14.9	1.12	2e-05	1.26	−0.14
3	3	1.68	14.4	1.01	1e-05	1.03	−0.02
3	4	1.62	12.7	0.95	0.0002	1.32	−0.38
3	5	2.09	16.3	1.40	2e-05	1.64	−0.24
3	6	1.76	13.7	1.01	2e-05	1.07	−0.07
3	7	1.82	12.7	1.13	1e-05	1.17	−0.05
3	8	2.06	14.3	1.30	0.0007	1.34	−0.04
3	9	2.14	15.0	1.57	0.0002	2.02	−0.45
3	10	1.94	13.0	1.31	0.0009	1.33	−0.02
	MEAN	1.87	14.2	1.18	0.0002	1.33	−0.14
3	TRUE	1.43	13.5	0.53	3e-06	0.54	0.00

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Table 5. Posterior parameter errors.

Parameter	True	Unit	R.M.S. Error			Bias		
	Value		Expt. 1	Expt. 2	Expt. 3	Expt. 1	Expt. 2	Expt. 3
α_{surf}	5.56	mg C (mg Chl)$^{-1}$ (E m^{-2})$^{-1}$	1.80 (32 %)	0.78 (14 %)	0.48 (8.7 %)	−1.62 (29 %)	+0.11 (2 %)	−0.41 (−7 %)
k_N	0.1	mmol N m^{-3}	0.056 (56 %)	0.045 (45 %)	0.021 (20 %)	−0.016 (16 %)	−0.002 (2 %)	+0.001 (1 %)
g_{max}	0.8	d^{-1}	0.55 (68 %)	0.48 (60 %)	0.39 (48 %)	+0.37 (45 %)	+0.24 (30 %)	+0.18 (23 %)
m_2	0.3	d^{-1}(mmol N m^{-3})$^{-1}$	0.59 (195 %)	0.41 (136 %)	0.31 (103 %)	+0.45 (149 %)	+0.20 (66 %)	+0.16 (52 %)
w_D	10	m d^{-1}	12.1 (121 %)	1.8 (18 %)	1.4 (14 %)	+7.1 (71 %)	−0.3 (3 %)	+0.9 (9 %)

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Table 6. Error in annual mean primary production.

	Production (mmol C m^{-2} d^{-1})					
	R.M.S. Error			Bias		
Optimization Experiment	BATS	NABE	INDIA	BATS	NABE	INDIA
1	1.7 (14 %)	8.5 (20 %)	4.4 (20 %)	−1.3 (−11 %)	−7.3 (−18 %)	−3.6 (−16 %)
2	1.0 (8 %)	3.7 (9 %)	2.6 (12 %)	+0.3 (2 %)	+0.6 (1 %)	+0.7 (3 %)
3	0.5 (4 %)	2.4 (6 %)	1.5 (7 %)	−0.3 (−2 %)	−1.7 (−4 %)	−0.7 (−3 %)

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Table 7. Error in annual mean sinking particle flux.

Optimization Experiment	Particle Flux at Reference Depth (mmol C m^{-2} d^{-1})					
	R.M.S. Error			Bias		
	BATS (250 m)	NABE (400 m)	INDIA (1000 m)	BATS (250 m)	NABE (400 m)	INDIA (1000 m)
1	0.154 (125 %)	0.879 (122 %)	0.825 (128 %)	+0.089 (73 %)	+0.512 (71 %)	+0.48 (74 %)
2	0.022 (18 %)	0.128 (18 %)	0.116 (18 %)	−0.004 (−3 %)	−0.024 (−3 %)	−0.021 (−3 %)
3	0.016 (13 %)	0.093 (13 %)	0.086 (13 %)	+0.010 (8 %)	+0.056 (8 %)	+0.051 (8 %)

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Table C1. HadOCC model parameters.

Parameter	Symbol	Value
Minimum C:Chl ratio	θ_{min}	20 g C (g Chl)$^{-1}$
Maximum C:Chl ratio	θ_{max}	200 g C (g Chl)$^{-1}$
C:N ratio for phytoplankton	θ_P	6.625
C:N ratio for zooplankton	θ_Z	5.625
C:N ratio for detritus	θ_D	7.5
Maximum photosynthetic rate	V_{max}	2 d^{-1}
Initial slope of photosynthesis-PAR curve	α_{surf}	5.56 mg C (mg Chl)$^{-1}$ (E m^{-2})$^{-1}$
Half-saturation conc. for nutrient uptake	k_N	0.1 mmol N m^{-3}
Phytoplankton density-dependent mortality	m_o	0.05 d^{-1}(mmol N m^{-3})$^{-1}$
Phytoplankton specific respiration	η	0.05 d^{-1}
Maximum grazing rate	g_{max}	0.8 d^{-1}
Half-saturation conc. for grazing	k_F	0.5 mmol N m^{-3}
Fraction of grazed material ingested	ϕ_I	0.77
Assimilation efficiency for phytoplankton	β_P	0.9
Assimilation efficiency for detritus	β_D	0.65
Zooplankton specific mortality	m_1	0.05 d^{-1}
Zooplankton density-dependent mortality	m_2	0.3 d^{-1}(mmol N m^{-3})$^{-1}$
Detrital sinking velocity	w_D	10 m d^{-1}
Parameters derived from C:N ratios (above):		
Biomass-equivalent:N ratio for phytoplankton	B_P	1
Biomass-equivalent:N ratio for zooplankton	B_Z	0.87
Biomass-equivalent:N ratio for detritus	B_D	1.11

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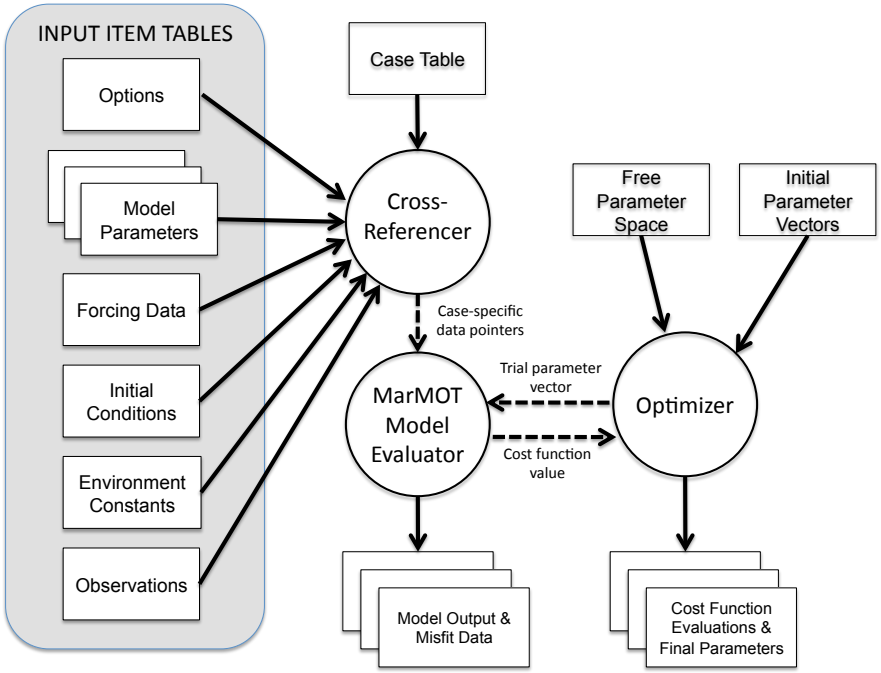

Fig. 1. Simplified schematic of the MarMOT system, showing the main system components and data flows. Data flows shown by dotted lines are purely internal.

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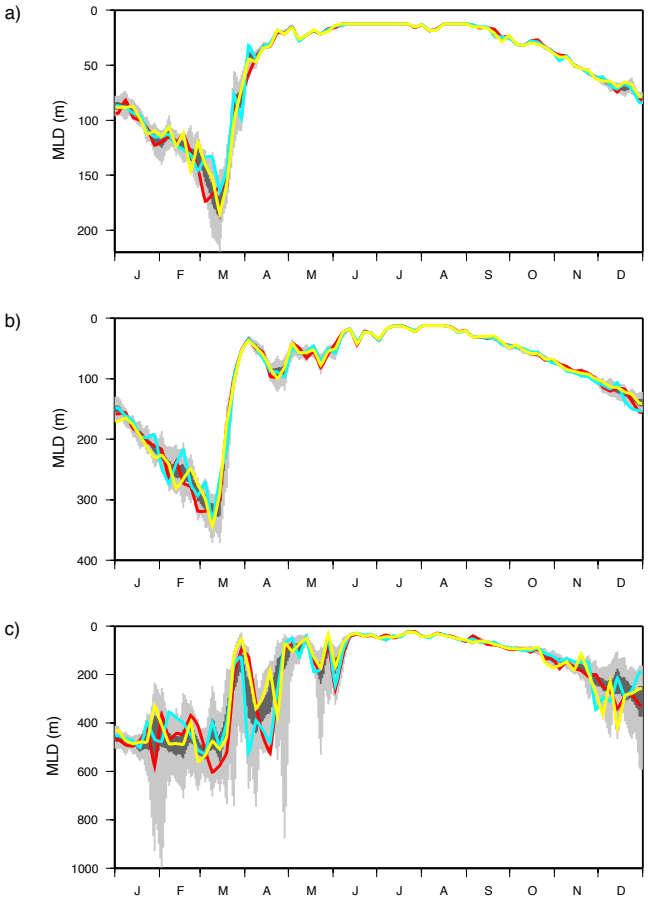

Fig. 2. Illustration of 100 member mixed layer depth ensemble at **(a)** BATS, **(b)** NABE and **(c)** OWS-INDIA sites, showing full ranges (light grey), inter-quartile ranges (dark grey) and three example members (coloured).

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Uncertainty in plankton model calibration

J. C. P. Hemmings and P. G. Challenor

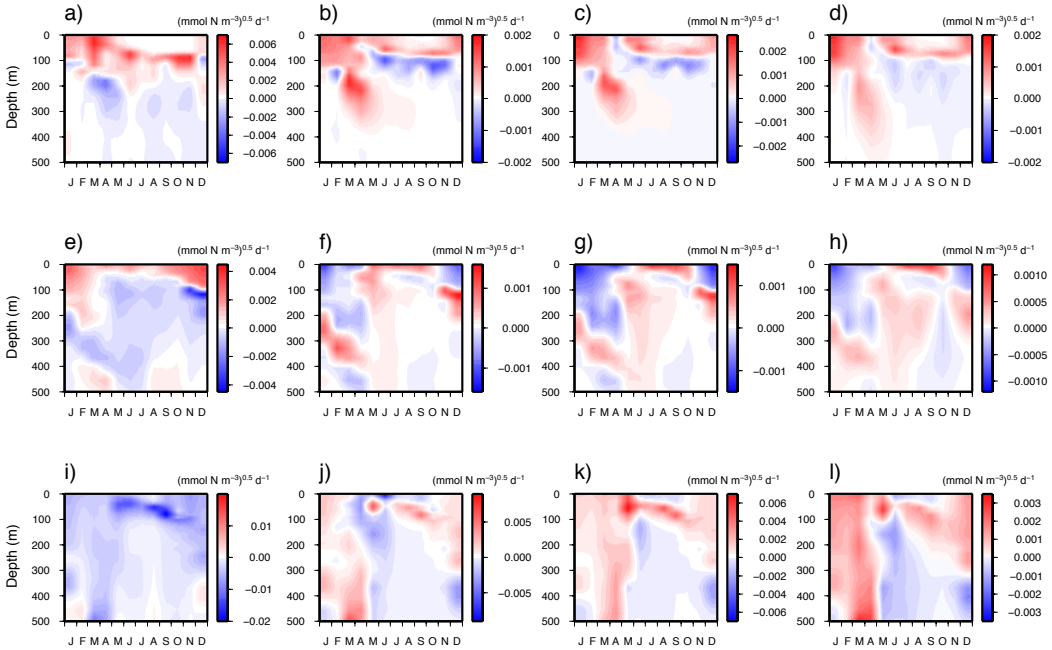

Fig. 3. Perturbation rate mean μ_i^{pert} for transformed state variables. For the BATS site: **(a)** DIN ($\sqrt{N}$), **(b)** phytoplankton ($\sqrt{P}$), **(c)** zooplankton ($\sqrt{Z}$) and **(d)** detritus ($\sqrt{D}$). **(e–h)** Same variables at the NABE site. **(i–l)** Same variables at the OWS-INDIA site.

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Uncertainty in plankton model calibration

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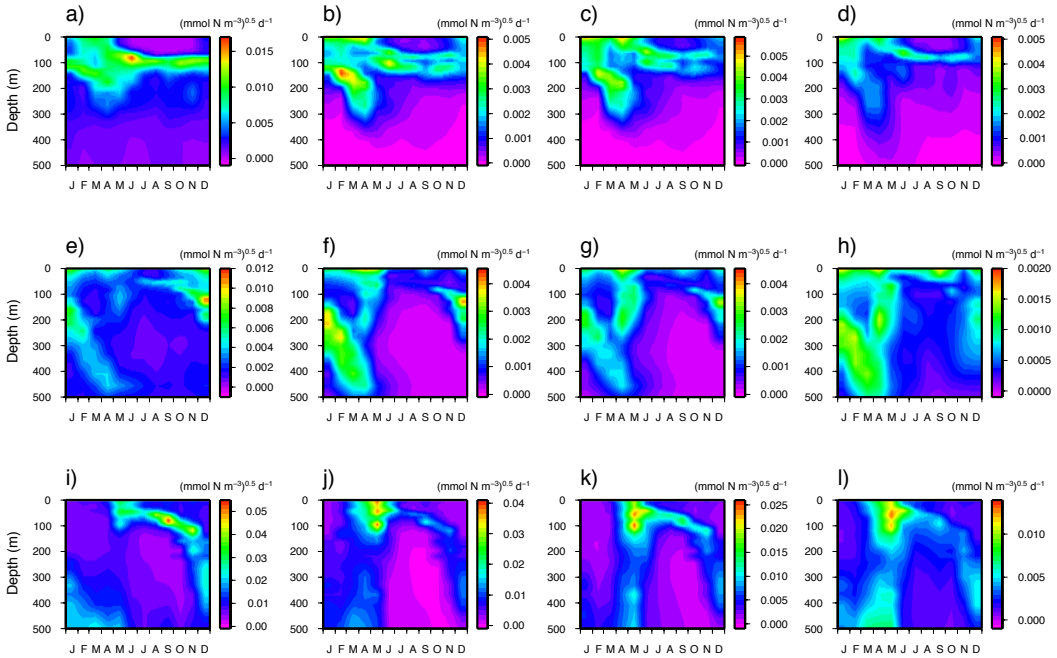

Fig. 4. Perturbation rate standard deviation σ_i^{pert} for transformed state variables. For the BATS site: **(a)** DIN ($\sqrt{N}$), **(b)** phytoplankton ($\sqrt{P}$), **(c)** zooplankton ($\sqrt{Z}$) and **(d)** detritus ($\sqrt{D}$). **(e–h)** Same variables at the NABE site. **(i–l)** Same variables at the OWS-INDIA site.

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Uncertainty in plankton model calibration

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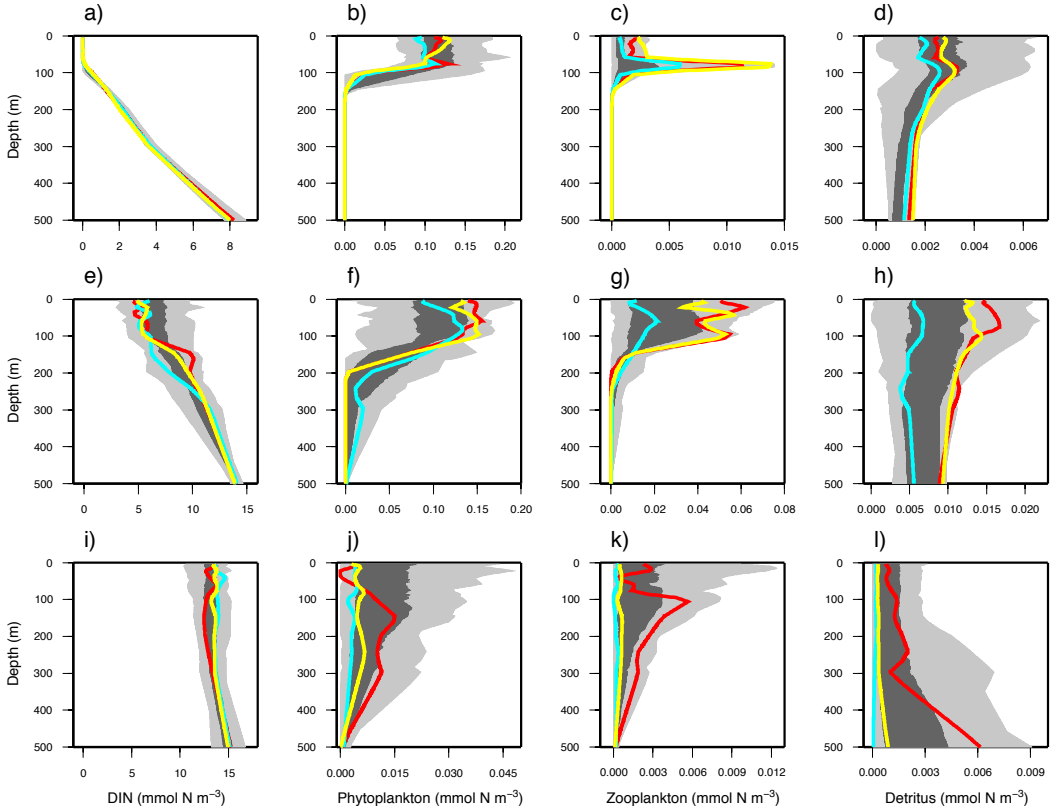

Fig. 5. Illustration of the 100 member initial state ensemble. For the BATS site: **(a)** DIN (N), **(b)** phytoplankton (P), **(c)** zooplankton (Z) and **(d)** detritus (D). **(e–h)** Same variables at the NABE site. **(i–l)** Same variables at the OWS-INDIA site. Full ranges (light grey), inter-quartile ranges (dark grey) and three example members (coloured) are shown.

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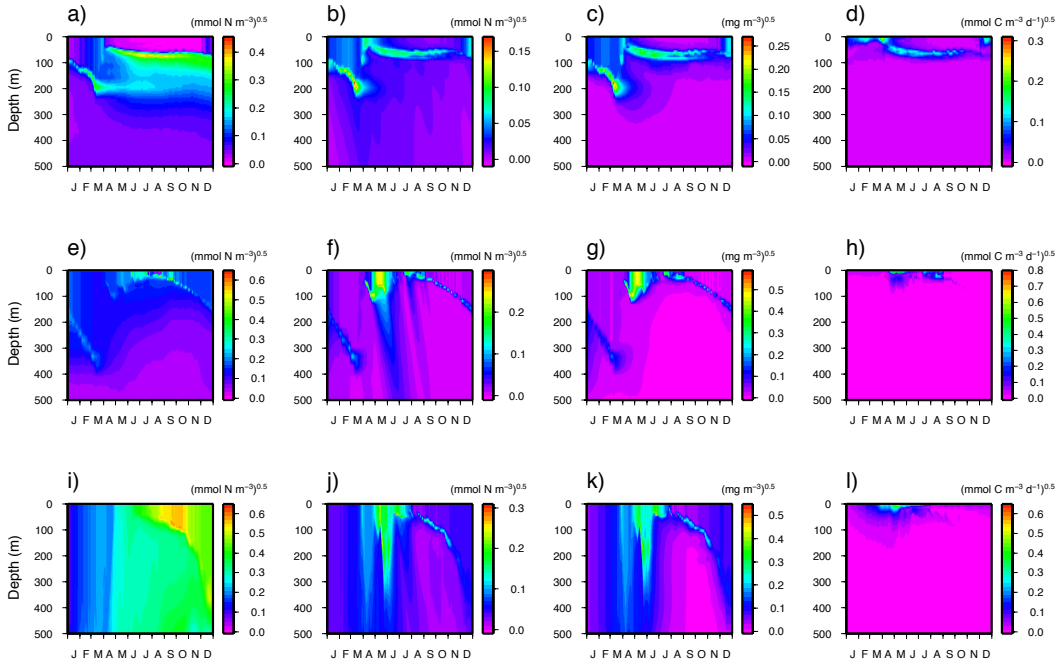

Fig. 6. Ensemble standard deviation of square-root transformed variables from Simulation Group B: estimated environment error for the HadOCC model with the default parameter set. For the BATS site: **(a)** DIN ($\sqrt{N}$), **(b)** PON ($\sqrt{P+Z+D}$), **(c)** Chlorophyll ($\sqrt{12.01(\frac{\theta_P}{\theta_{chl}})P}$) and **(d)** primary production ($\sqrt{\bar{\mu}_P \theta_P P}$). **(e–h)** Same variables at the NABE site. **(i–l)** Same variables at the OWS-INDIA site.

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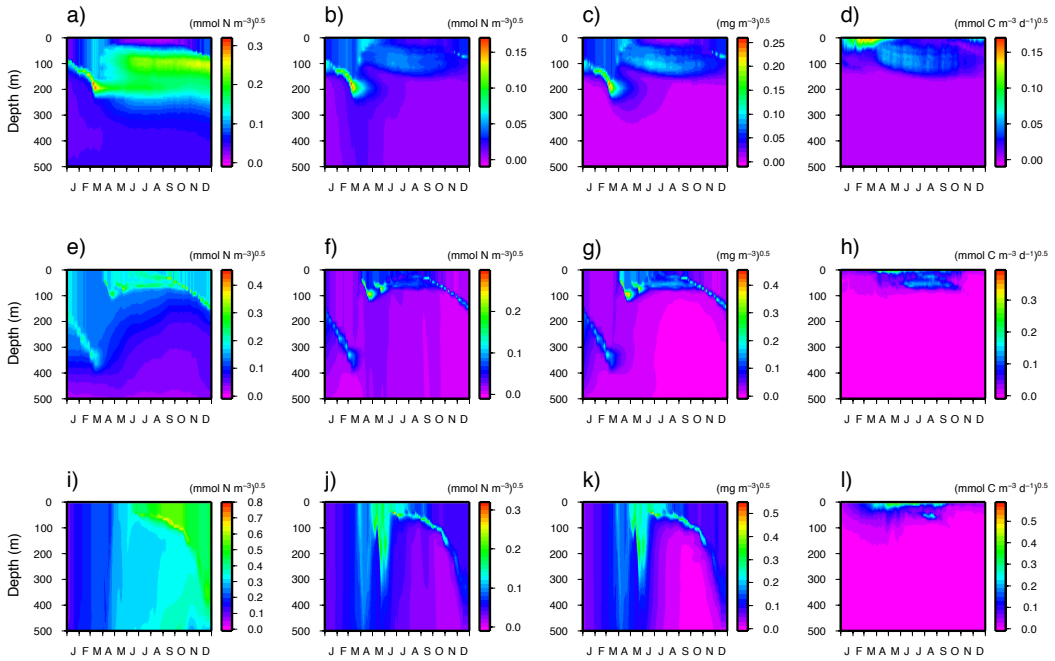

Fig. 7. Ensemble standard deviation of square-root transformed variables from Simulation Group C: estimated environment error $s_{ijk\mathrm{ENV}}$ applicable to the HadOCC free parameter space defined by the μGA optimizer bounds. For the BATS site: **(a)** DIN ($\sqrt{N}$), **(b)** PON ($\sqrt{P+Z+D}$), **(c)** Chlorophyll ($\sqrt{12.01(\frac{\theta_\mathrm{P}}{\theta_\mathrm{chl}})P}$) and **(d)** primary production ($\sqrt{\bar{\mu}_\mathrm{P}\theta_\mathrm{P}P}$). **(e–h)** Same variables at the NABE site. **(i–l)** Same variables at the OWS-INDIA site.

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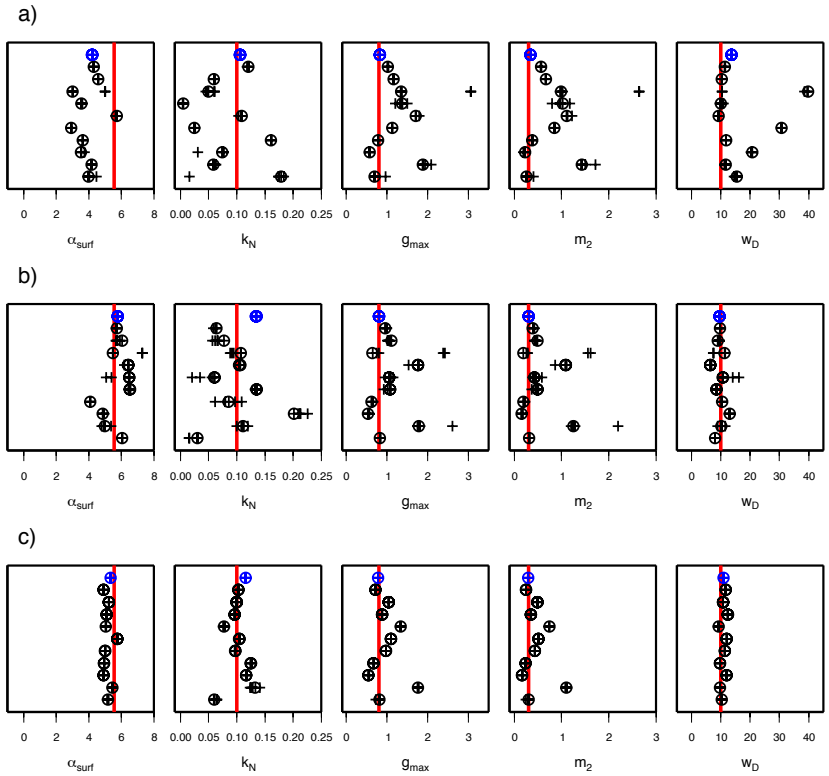

Fig. 8. Parameter recovery results for **(a)** Experiment 1, **(b)** Experiment 2 and **(c)** Experiment 3. Red lines represent the true values for each parameter. Crosses in each row show optimizer output parameter values for the true environment (blue) and for each of the 10 realizations of the optimization environment (black). One cross is shown for each distinct parameter value obtained with 5 different optimizer initialization cases. Optimal values are circled. Crosses not highlighted thus are values associated with higher cost function values.

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