Sensitivity of a marine coupled physical biogeochemical model to time resolution, integration scheme and time splitting method

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ABSTRACT

Coupled marine biogeochemical models are composed of a hydrodynamic component with a transport model for the ecological state variables and a model for the biogeochemical dynamics. The combination of these components involves the implementation of a numerical coupling method, that performs the spatial–temporal integration of the combined system, introducing an additional source of error to the system (splitting error). In this article we demonstrate the sensitivity of a comparatively complex 1D hydrodynamical biogeochemical model to the coupling method, showing that for an inadequate choice of the coupling method, the splitting error may dominate the numerical error of the system. It is demonstrated that for this type of system the tracer transport time scale clearly dominates over the scale of the biogeochemical processes, that maybe computed on significantly coarser time scales. In between the implemented coupling schemes *Operator Splitting* and *Source Splitting*, the *Source Splitting* method inserting the biogeochemical rates into the transport tracer integration is to be preferred for these type of models.

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1. Introduction

Marine ecosystem dynamics is strongly constrained and, to some extent, governed by the ocean physics. Biogeochemical processes (primary and secondary production, nutrient cycling, etc.) are heavily dependent on physical dynamics, that determines the availability of resources (e.g. nutrients and light for primary producers) and the spatially and temporally variable distribution of individuals and biomass. Moreover, the variability of the ocean temperature field directly affects the metabolic rates of the organisms, as well as all the chemical processes involved in biogeochemical cycling. Thus, adequate understanding and modelling of the marine ecosystem necessarily implies the full consideration of the coupled physical and biogeochemical dynamics. A classical example for temperate waters is given by the so called surface phytoplankton "spring bloom", whose dynamics, unveiled by Sverdrup (1953), is governed by the evolving physical environment (irradiance, vertical stratification, diffusive nutrient flux into the euphotic zone) that determines the conditions for a phytoplankton biomass accumulation near the surface when the seasonal thermocline starts to develop (Mann and Lazier, 1991; Miller, 2006).

Numerical models aiming to capture the coupled ecosystem dynamics have been developed and currently are a widely used tool to investigate biogeochemical cycling in the oceans. The range of applications of these models extends from case studies of particular ecosystem processes in local domains such as harmful algal blooms (Allen et al., 2008) to large scale effects, such as the global carbon budget (Vichi et al., 2011) and ocean acidification (Blackford and Gilbert, 2007). The coupled physical biogeochemical system to be modelled is clearly non linear; moreover the numerical treatment of the resulting complex dynamics adds further problems related to stability and stiffness that are complicated by the choice of an appropriate space and time resolution.

Such models are generally composed of three main components: a spatially resolved (one- or three-dimensional) hydrodynamic model, a model computing the biogeochemical dynamics in a spatial element and a tracer transport model, that determines the transport dynamics of the biogeochemical state variables (non conservative tracers) as a consequence of advection and diffusion. It is common practise to separate the treatment of the physical and biogeochemical processes in order to decouple the spatial

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dimension of the physical sub-model from the state variable dimension of the biogeochemical sub-model and allow for separate numerical treatment.

The artificial partitioning of the ecosystem into a physical and biogeochemical component implies that the modelling system has to combine for each biogeochemical state variable c, usually expressed in terms of concentration, the time dependent changes due to physical transport processes with the changes due to biogeochemical processes (Hofmann, 1998). These changes are then merged to provide the total rate of change:

$$\frac{\partial c}{\partial t} = R_{trp} + R_{bio} \tag{1}$$

where R_{trp} is the rate of change due to transport processes and R_{bio} is the one due to biogeochemical reactions. While most research has been concentrated on the formulation of the hydrodynamical and biogeochemical models, only few studies were dedicated to the appropriate modelling of the transport of biogeochemical tracers (e.g. Levy et al., 2001) in the ocean and very few to the method of coupling of the three main components into one integral modelling system (Burchard et al., 2006). However, the integration of these processes requires some attention, since the involved, closely interacting physical and biogeochemical processes develop on a wide spectrum of temporal and spatial scales (on the physical side ranging from molecular diffusion and small scale turbulence processes to large scale circulation patterns, on the biogeochemical side from individual behaviour and physiological processes to seasonal/decadal variability of biomass and population size). The resulting non-linear character of the coupled dynamics suggests a deeper consideration of the scales dominating the overall dynamics and the coupling technique used to link together the biogeochemical, the hydrodynamical and the tracer transport sub-model.

A considerable amount of work has been dedicated to the argument in the related field of atmospheric chemistry and air-pollution modelling, where stiff chemical dynamics dominate over the atmospheric transport dynamics involving often a split implicit integration on high-resolution time-steps (McRae et al., 1982; Carmichael, 1996; Verwer, 1998). The main two approaches for coupling the chemical processes with the geophysical dynamics to be found are the methods of the so called *Operator Splitting*, e.g. Strang (1968), and *Source Splitting*, e.g. Sun (1996). Both of these techniques are well established in the atmospheric chemistry community and have been extensively tested in examples ranging from simplified analytical and numerical test cases of exponential decay/growth to full scale applications (Sportisse, 2000; Blom and Verwer, 2000; Verwer, 1998; Spee, 1997). The characteristics of these methods will be summarised below.

Although the choice of the coupling method is rarely motivated or even mentioned, essentially all current coupled marine biogeochemical models use, consciously or not, forms of one or the other method to combine the hydrodynamics with the biogeochemical processes (*OperatorSplitting*): i.e. POLCOMS-ERSEM – Allen (2001); GOTM – Burchard et al. (2006); *SourceSplitting*: NEMO – Madec (2008); PELAGOS – Vichi et al. (2007b); POM-BFM – Polimene (2006, 2007).

It is the aim of this work to shed some light onto the sensitivity of a coupled physical biogeochemical model to the method invoked to solve the integration of the combined equation of the geophysical transport for biogeochemical (non-conservative) state variables with respect to time resolution, integration scheme and coupling methods. The fact that there currently exists no mathematical standard for the representation of the marine ecosystem dynamics and the resultant range of structural description of the dynamics with different levels of detail and complexity in current models necessarily limits the scope of a specific study on this subject. In this work we have chosen to focus on a model representative of a comparatively complex representation of the biogeochemical dynamics as

used in numerous previous and recent studies (e.g. Allen, 2001; Zavatarelli and Pinardi, 2003; Holt, 2011; Lazzari, 2010; Siddorn, 2007; Triantafyllou, 2007; Vichi et al., 2011; Ciavatta, in press; Edwards et al., 2012). A series of numerical experiments were performed using a one-dimensional coupled hydrodynamical-biogeochemical model to investigate the required time resolution of the biogeochemical processes, the time scale prevailing in the over-all process and the errors involved with the various schemes and methods used.

2. Coupling methods

Coupled atmospheric or oceanic process models are generally developed by embedding into an established general circulation model (GCM) a chemical or biological model (describing physical–chemical reactions, biogeochemical cycling, population dynamics). This involves the addition of a significant number of state variables. While it is generally possible to insert the process description of the added component into the physical model, often the approach of an external coupling (an interface allowing for the exchanges between the model components) that links the two sub-models is preferred. The motivation for this choice are:

- When dynamics with significantly different time scales and levels of stiffness are involved, the integration method strictly required for one process class (e.g. advanced implicit solvers involving matrix inversions) can become intractable for the rest of the system due to the elevated number of state variables, while an external method offers the possibility to apply tailored integration schemes to each sub-model.
- An external interface allows for the flexibility of applying the same component to different sub-models by simple extension, allowing for inter-comparison of different models and ensembles of structural uncertainty.
- The direct insertion into the GCM may require significant rewriting of the code if not a complete rethinking of the coupled system.

The general solution of a system described by Eq. (1) can be expressed as:

$$c_{n+1} = c_n + \Phi(R_A + R_B, \Delta t), \tag{2}$$

where n is the discrete time index, Φ is the discrete integral operator that advances variable c_n to time $n + 1$ with time step Δt. R_A and R_B can correspond to R_{trp} and R_{bio} of Eq. (1) or to any other rate acting on c.

A variety of strategies to couple the above system can be found in the geophysical modelling literature. However, as stated above, the vast majority of applications concentrate on the *Operator Splitting* and *Source Splitting* methods, which are favourable in terms of implementation and computing resources and shall be presented here in more detail.

2.1. Operator Splitting

The *Operator Splitting* method is widely used in atmospheric chemistry models (McRae et al., 1982; Blom and Verwer, 2000; Verwer, 1998; Strang, 1968), as well as in virtually all general ocean circulation models (e.g. Blumberg and Mellor, 1987), separating advection and horizontal diffusion from vertical diffusion (commonly treated implicitly). The system (2) is therefore divided into two separate subsystems that are solved sequentially:

$$\gamma = \mathbf{c}_n + \Phi_A(R_A(c_n), \Delta t)$$
$$\mathbf{c}_{n+1} = \gamma + \Phi_B(R_B(\gamma), \Delta t). \tag{3}$$