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Application of a fast Newton–Krylov solver for equilibrium simulations of phosphorus and oxygen

Weiwei Fu*, François Primeau

Department of Earth System Science, University of California, Irvine, California

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ABSTRACT

Model drift due to inadequate spinup is a serious problem that complicates the interpretation of climate change simulations. Even after a 300 year spinup we show that solutions are not only still drifting but often drifting away from their eventual equilibrium over large parts of the ocean. Here we present a Newton-Krylov solver for computing cyclostationary equilibrium solutions of a biogeochemical model for the cycling of phosphorus and oxygen. In addition to using previously developed preconditioning strategies – time-averaging and coarse-graining the Jacobian matrix – we also introduce a new strategy: the adiabatic elimination of a fast variable (particulate organic phosphorus) by slaving it to a slow variable (dissolved inorganic phosphorus). We use transport matrices derived from the Community Earth System Model (CESM) with a nominal horizontal resolution of $1^\circ \times 1^\circ$ and 60 vertical levels to implement and test the solver. We find that the new solver obtains seasonally-varying equilibrium solutions with no visible drift using no more than 80 simulation years.

1. Introduction

The concentrations of oxygen and nutrients in the ocean affect marine productivity, ecosystem structure, and biogeochemical transformations that lead to air-sea fluxes of important greenhouse gases such as CO_2 and N_2O. Consequently, most Earth System Models (ESMs) attempt to simulate the biogeochemical processes that control the cycling of oxygen and nutrients in order to predict how their concentrations will be affected by climate change, and in turn, how they feedback on climate. However, models can show trends that are due to tracer initial conditions that are out of balance with the model's physical circulation rather than to changes in external forcing or internal variability. In order to clearly attribute trends in various marine variables to changing climate it is therefore critical to be able to eliminate such spurious 'model drift'.

In principle, a straightforward way to reduce model drift is to integrate the model forward in time until the transients have died out. This process is known as model spinup. Unfortunately, because tracers in the ocean can take thousands of years to equilibrate with their sources and sinks (e.g. Peacock and Maltrud, 2006; Primeau and Deleersnijder, 2009), the length of the required spinup runs can become computationally prohibitive for models of moderate to high resolution – climate modeling centers such as NCAR typically use spinups of only $\sim$300 years to tune biogeochemical parameters by hand. Indeed, inadequate model spinup has been identified as being a possible cause for much of the large differences in the simulated oxygen minimum zones in the suite of CMIP-5 models (Séférian et al., 2016).

There is therefore considerable interest in accelerating the spinup of tracers in ocean models. As an alternative to the direct forward integration as a means of spinning up marine biogeochemical models, Li and Primeau (2008) and Khatiwala (2008) introduced a preconditioned Newton-Krylov (NK) method for iteratively obtaining seasonally-varying periodic equilibriums. They showed that cyclostationary solutions could be obtained with a reduction in computational cost of more than two orders of magnitude. The Newton-Krylov method was also used in Graven et al. (2012) and Bardin et al. (2014) for ^{14}C. Piwonski and Slawig (2016) developed a software package for simulating biogeochemical tracers that includes the option of accelerating the spinup using a Jacobian-free Newton method. They show results for various biogeochemical model formulations and find speedups of about a factor of 6 without applying any preconditioner. Piwonski and Slawig (2016) also gives a brief and selective review of various methods that have been applied to accelerate the spinup of tracers in ocean models.

Bardin et al. (2014) presented a "lump-and-spray" methodology for constructing a more memory-efficient preconditioning strategy that could be applied to an offline version of the ocean component of the Community Earth System Model (CESM-POP2

* Corresponding author.
E-mail address: weiweif@uci.edu (W. Fu).

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Smith et al. (2010)). Here we continue this line of research by documenting the application of the NK methodology to an offline model for dissolved oxygen and the nutrient phosphorus based on the CESM-POP2 circulation.

The slow equilibration time of marine biogeochemical models is due to the long transport time-scales associated with the global overturning circulation rather than the details of the relatively fast chemical transformations catalyzed by phytoplankton. It is our opinion that the challenge for the effective application of the NK methodology to the spinup of marine biogeochemical model does not rest with the nonlinearities that are handled by the Newton part of the solver but rather with the need to accelerate the convergence rate of the iterative Krylov solver. The issues associated with the convergence of the Newton solver are not unique to the ocean spinup problem. For example, Newton's method needs a good initial iterate to converge. For difficult nonlinear problems, such an initial iterate can be obtained by using a continuation method (e.g. Seydel, 1994). See Primeau and Newman (2007) for an application of continuation methods to ocean modeling. We have therefore chosen a relatively simple biogeochemical model formulation to focus on what is important for accelerating the spinup using the NK methodology – the formulation of an effective preconditioner. Indeed Piwonski and Slawig (2016) tested a non-preconditioned NK method to a hierarchy of biogeochemical models and found comparable spinup times (>700 years) for all model formulations.

Our phosphorus-cycling model includes 3 pools: dissolved and particulate organic phosphorus (DOP and POP), and dissolved inorganic phosphorus (DIP), i.e. phosphate. The biological production and regeneration fields diagnosed from the phosphorus-cycling model are then used to force the oxygen model. The previous application of the NK method to the phosphorus cycle, (Li and Primeau, 2008), considered a much coarser resolution model ($\sim 3.8^\circ \times 3.8^\circ$ and 29 vertical levels, compared with $\sim 1^\circ \times 1^\circ$ and 60 vertical levels for CESM-POP2) and did not include an explicit POP pool or oxygen. Here we use tracer transport matrices derived from CESM-POP2 with a monthly resolution to compute the seasonally varying advection diffusion of tracers (Bardin et al. (2014)), but the algorithm could equally be applied to full CESM-POP2 as described in Lindsay (2017). The tracer transport matrix (annually averaged) is only essential for the construction of the preconditioner.

The formulation of our phosphorus and oxygen biogeochemistry model is described in more detail in Sections 2.2.1 and 2.2.2. A review of the Newton–Krylov solver methodology is presented in Section 3 along with our preconditioning strategy, which combines previously introduced strategies, (time-averaging and coarse-graining using lump and spray matrix operators) with a new idea: the adiabatic elimination of the fast variable (POP) by slaving it to the slow variables (DIP). Results, including convergence rates and equilibrium tracer distributions, are presented in Section 4, followed by a discussion of the prospects for utilizing our solver to calibrate uncertain biogeochemical parameters.

2. Model formulation

In this section we describe the formulation of our biogeochemical models. The model's state variables consist of 4 tracer concentrations *DIP*, *DOP*, *POP*, and $[O_2]$, which after being discretized become N-dimensional column vectors with $N = 4,241,988$ being the number of wet gridboxes in the model domain. Uppercase bold letters denote matrix operators and the lowercase bold letters denote discretized scalar fields other than the state variables.

2.1. Transport models

2.1.1. Dissolved tracer transport

The advective-diffusive tracer flux-divergence in our model is computed using tracer transport matrices. We construct these matrices from the physical circulation in the ocean component (POP2) of the Community Earth System Model (CESM) (Smith et al., 2010). The model has a nominal horizontal resolution of $1^\circ \times 1^\circ$ with 60 vertical levels and a dipolar grid with the North Pole displaced into Greenland, with the transition from the Mercator grid starting at the Equator. The transport matrices, like the parent CESM-POP2 dynamical model, have a computational mesh with $N_x = 320$ and $N_y = 384$ tracer grid points in the nominally eastward and northward directions and $N_z = 60$ grid points in the vertical direction, for a total of 4,241,988 wet grid points. The vertical resolution ranges from 10 m for the top 10 layers of the model and increases to 250 m near the bottom. The thickness of the top-most layer is allowed to vary to include regional and temporal variations in sea surface height.

The flux divergence of dissolved tracers is computed using a discretized tracer transport matrix,

$$\nabla \cdot [\mathbf{u}C - \mathbf{K}\nabla C] \rightarrow \mathbf{T}C, \tag{1}$$

where on the left-hand side the operator and the tracer variable are assumed continuous whereas on the right-hand side everything is discretized so that the operator is a matrix **T**, and the tracer is a vector C. C can be either *DIP* or *DOP*. As in Bardin et al. (2014), **T** is decomposed into three parts

$$\mathbf{T} = \mathbf{A} + \mathbf{H} + \mathbf{D}, \tag{2}$$

where **A** is the advective-flux divergence matrix operator, **H** is the horizontal diffusive-flux divergence matrix operator, and **D** is the vertical diffusive-flux divergence matrix operator. This decomposition accommodates a time-stepping scheme in which **D** is treated using an implicit Euler-backward scheme, while **A** and **H** are based on explicit schemes – Euler-forward for **H** and 3rd order Adams-Bashforth for **A**. The seasonality of the physical circulation is represented using 12 matrix operators for each of **A, H**, and **D**, which are held constant within each month. Bardin et al. (2016) showed that monthly averaged matrix operators produced an acceptable representation of the circulation's seasonal cycle for an ideal-age tracer and we assume that this is also the case for our biogeochemistry model, but is something that will need to be tested in future work. More details on the construction of the transport matrices and time-stepping scheme are given in Bardin et al. (2014).

2.1.2. Particulate tracer transport

For the transport of organic phosphorus by sinking particles we use a depth dependent sinking speed, $w(z)$, and create a sinking flux divergence operator **J**, so that

$$\frac{\partial}{\partial z}(w(z)POP) \rightarrow \mathbf{J}\,POP, \tag{3}$$

where on the left-hand side the operator and tracer variables are assumed continuous whereas on the right-hand side everything is discretized using a centered difference scheme. z is the vertical coordinate (positive upward). By assuming that the effect of fluid transport is negligible compared to the transport associated with gravitational settling during the characteristic timescale for POP solubilization, **J** takes the form a block tridiagonal matrix with independent blocks for each fluid column in the model.

The depth dependence of the particle sinking speed is parameterized as

$$w(z) = -az \text{ for } z \le 0, \tag{4}$$

with $z = 0$ corresponding to the sea surface and $a = (4.4625 \text{ days})^{-1}$, which for our chosen *POP* solubilization