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Compact symmetric Poisson equation discretization for non-hydrostatic sigma coordinates ocean model

Roullet Guillaume[a,*], Molemaker M. Jeroen[a,b], Ducousso Nicolas[a], Dubos Thomas[c]

[a] Univ. Brest, CNRS, IRD, Ifremer, Laboratoire d'Océanographie Physique et Spatiale, IUEM, Brest, France
[b] UCLA, Los Angeles, USA
[c] IPSL/Lab. de Météorologie Dynamique, École Polytechnique, Palaiseau, France

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ABSTRACT

In anticipation of relaxing the hydrostatic assumption in a sigma coordinates primitive equations ocean model, we show how a projection method can be designed with the use of a compact symmetric 15-point stencil for the Poisson equation. This is achieved by recognizing that, owing the non-orthogonality of the grid, the velocity has a contravariant and covariant set of components. The two sets play a different role in the primitive equations: the contravariant components enter the definition of the model fluxes, whereas the covariant components experience the forces and in particular the pressure gradient. By treating these two sets separately, the discretized gradient and divergence operators are simple finite differences. The two sets of components are related via a linear transformation, the metric tensor, which is entirely determined by the kinetic energy. We show how the spatial discretization of the kinetic energy fully controls the Poisson equation discretization, including its boundary conditions. The discretization of the Poisson equation is shown to converge at second order and to behave as well or better than alternative methods. This approach is a prerequisite to implement later an efficient Poisson solver, such as a multigrid algorithm.

1. Introduction

With the growing interest on processes at submesoscale (Nikurashin et al., 2013; Molemaker et al., 2015; Callies et al., 2015; Gula et al., 2015) the ocean modelling community needs non-hydrostatic (NH) ocean circulation models. This will allow to investigate in realistic contexts the full range of internal waves, symmetric instability, convection processes, etc. and to bridge the gap with LES (Sullivan et al., 1994). A few circulation models do already handle the non-hydrostatic physics properly: MITgcm (Marshall et al., 1997), POM (Kanarska and Maderich, 2003), ROMS (Kanarska et al., 2007), Symphonie (Auclair et al., 2011), GETM (Klingbeil and Burchard, 2013). However, NH simulations on large grids, in realistic regional configurations are still awaited. It is timely to resolve this. The reason for the NH circulation models rarity is that relaxing the hydrostatic assumption, while keeping the Boussinesq assumption, is not straightforward. At least two levels of difficulties must be faced: i) the requirement to solve a 3D Poisson equation for the pressure at each time step, made more complex in the case of sigma coordinates by ii) the non-orthogonality of the grid. This second difficulty is absent in z-coordinates models. Incidentally, for models with a time-splitting on the free surface, a third difficulty is to properly handle the coupling between the non-hydrostatic pressure and surface waves (Auclair et al., 2011).

The first problem amounts to solving a linear system of equations with as many equations as number of grid points. For the intended purpose of high-resolution turbulent simulations we have in mind grids as large as $2000 \times 2000 \times 1000$ grid points, corresponding to $N \sim 10^9$ coupled equations. It is a classical well known problem of High Performance Computing (HPC). A possible way to circumvent the problem consists in relaxing the incompressibility constraint, which forces to cope with sound waves. The pressure can then be computed by integrating in time the compressible physics using a time-splitting technique. In the atmospheric community, this is the approach implemented in WRF (Skamarock and Klemp, 2008). In the ocean the ratio between advective speed and the phase speed of sound waves is much more unfavorable, leading to a required time split that is two orders of magnitude larger. An approach that uses artificial impressibility to slow down the phase speed of sound waves and hence reduce the required ratio in split time steps is currently under development as part of

* Corresponding author.
E-mail addresses: roullet@univ-brest.fr, guillaume.roullet@univ-brest.fr (R. Guillaume).

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the French regional ocean modeling project CROCO, but not available in a published manuscript (Francis Auclair, private communication). Klingbeil and Burchard (2013) follow a similar approach where a time-splitting on the baroclinic time step is introduced to achieve the incompressibility constraint. These methods trade the price of solving the Poisson problem with accepting a non-strict divergence-freeness of the flow.

Otherwise, the numerical implementation necessarily requires the use of an iterative solver to solve the Poisson equation. Many different numerical methods exist but only a few of them succeed at maintaining a uniform convergence rate for large grids. This is the case of the multigrid technique whose computational cost scales as $N \log N$, which is considered to be the optimal scaling. It has been shown recently to perform very well with large grids on massively parallel cluster, up to 10^{10} degrees of freedom and 65,536 cores, in the context of atmospheric modelling (Müller and Scheichl, 2014). To get the best performances, the stencil for the Poisson equation needs to be symmetric and compact. These two properties reduce the number of floating point operations, the amount of data storage and the data movement between the cpu and the memory. In modern computer architecture, data movement is the bottleneck for high performances (Williams et al., 2009). Any numerical method that reduce data transfer is worth it. In the present study, the compactness means a 15-point stencil, compared to the usual 25-point one (Auclair et al., 2011). The symmetry allows to almost halve the number of coefficients for the matrix since only 8 coefficients are needed for a 15-point stencil (one main and 7 lower diagonals). Overall the present matrix offers a reduction by a factor 3 on the number of matrix coefficients compared to existing methods. In anticipation of implementing such solution into a sigma-coordinates model we present here a way to achieve compactness and symmetry for the Poisson equation.

The second problem is due to the non-orthogonality of the grid. One consequence is that the horizontal pressure gradient cannot be computed as a simple finite difference between two adjacent horizontal grid cells. Chain rule and vertical interpolation should be used (Shchepetkin and McWilliams, 2003) resulting in wide stencils for the gradient operator. The divergence of vertical flux behaves similarly because the vertical flux involves horizontal velocities. Since the Poisson equation arises as the successive action of the gradient and the divergence, the resulting stencil for the Poisson equation is tall in the vertical, involving overall 25 points (Auclair et al., 2011). The Poisson equation couples points over 5 levels in the vertical and 3 in both horizontal directions. The stencil can be made symmetric by defining the gradient as minus the adjoint of the divergence. This is the so-called compatible discretization (Taylor and Fournier, 2010). It is also possible to discretize the Poisson matrix directly and independently of how the gradient and the divergence are discretized (Kanarska et al., 2007). In that case, the stencil is compact with 15 points. The major drawback of such a method is that it fails at maintaining the compatibility between operators which impacts the energy conservation.

In this paper we show how the two problems can be solved jointly. The first step is to recognize that because of the non-orthogonality of the coordinates system, the velocity has two sets of components: a contravariant one and a covariant one. The two sets are related via a linear transformation, the metric tensor, which is invertible. The metric tensor is completely determined by the kinetic energy. The two sets of components play a different role and must be treated distinguishably. The contravariant components appear in the definition of fluxes (volume, tracer, momentum), whereas the covariant components appear in the force budget. Using the framework of the discrete differential geometry (Desbrun et al., 2008) we show that the contravariant components must be discretized at the cell faces of the primal grid whereas the covariant components should be discretized at the edges of the dual grid (the lines joining the cell centers). Such discretization is in line with the C-grid staggering, and the finite volume discretization for tracers. It also completely adheres to Thuburn and Cotter (2012) way to discretize shallow water equations on non-orthogonal grids. The divergence and the gradient operators have then trivial discretization: they are simple finite differences. In the spirit of Molemaker et al. (2005) and Dubos et al. (2015) we then deduce the discrete Poisson equation directly from the discretized kinetic energy and the discretized divergence operator. The price of this approach is to prognose either the covariant components or the contravariant ones. For sake of completeness we present the momentum equations written for the covariant components in both vector-invariant form and in flux-form. The vector-invariant form is similar to a standard Cartesian formulation whereas the flux-form involves additional pseudo-force terms. Up to now, sigma-coordinates models prognose Cartesian components of the velocity, namely horizontal and vertical, which are a blend of contravariant and covariant components. This causes unnecessary wide stencil for the divergence and the gradient and finally a too wide stencil for the Poisson equation. By expliciting and clarifying the subtleties induced by non-orthogonal coordinates, this paper offers a roadmap for an efficient implementation of a projection method.

The paper is organized as follows. We define in Section 2 the contra- and covariant sets of components for the velocity and present the model continuous equations. In Section 3, we present the spatial discretization of the variables, the divergence and the discretized kinetic energy and derive all the other discretizations from them. In Section 4 we discuss the properties of the discretization on a test-case. A conclusion is given in Section 5.

2. Formulation

As stated in the introduction, the objective of this study is to provide a discrete Poisson operator that can be solved efficiently by iterative methods on very large grids. In this section, we will introduce a dual representation of the velocities on the grid, which will prove to be advantageous in arriving at a compact, symmetric, discrete operator. Subsequently, we will present the governing equations of motion for these prognostic variables.

2.1. Flux and momentum

In orthogonal curvilinear coordinates (ξ, η, z), the velocity of a fluid parcel is naturally expressed as $\mathbf{u} = h_\xi \dot{\xi}\,\mathbf{i} + h_\eta \dot{\eta}\,\mathbf{j} + \dot{z}\,\mathbf{k}$, where the dot denotes the Lagrangian time derivative, $\mathbf{i}, \mathbf{j}, \mathbf{k}$ are the unit vectors in horizontal and vertical directions, and (h_ξ, h_η) are the Lamé coefficients in the horizontal directions. We define $(u_c, v_c, w_c) = (h_\xi \dot{\xi}, h_\eta \dot{\eta}, \dot{z})$ and denote them, with a slight abuse of usage, the Cartesian velocity components. The terrain following sigma coordinates are (ξ, η, σ), for which the vertical position is $z(\xi, \eta, \sigma, t)$. The time dependency in z is driven by the sea surface height variations and yields a breathing grid. Using the chain rule, this causes

$$\mathbf{u} = u_c\,\mathbf{i} + v_c\,\mathbf{j} + (u_c\, s_\xi + v_c\, s_\eta + h_\sigma \dot{\sigma} + \partial_t z)\mathbf{k}, \tag{1}$$

where

$$s_\xi = \frac{1}{h_\xi}\frac{\partial z}{\partial \xi}, \qquad s_\eta = \frac{1}{h_\eta}\frac{\partial z}{\partial \eta} \tag{2}$$

are the slopes of σ-surfaces, h_σ is the Lamé coefficient in the vertical direction and $\partial_t z = \partial z / \partial t$ accounts for the breathing of grid. We denote $(U, V, W) = (h_\xi \dot{\xi}, h_\eta \dot{\eta}, h_\sigma \dot{\sigma})$ the sigma coordinate velocity components. They are related to the Cartesian velocity components by

$$u_c = U$$