

# A finite volume discretization of the pressure gradient force using analytic integration

Alistair Adcroft<sup>a,\*</sup>, Robert Hallberg<sup>b</sup>, Matthew Harrison<sup>b</sup>

<sup>a</sup> *Atmospheric, Oceanic Sciences, Princeton University, NJ 08540, USA*

<sup>b</sup> *NOAA-GFDL, Princeton University, Forrestal Campus, U.S. Route 1, P.O. Box 308, Princeton, NJ 08542, USA*

Received 28 September 2007; received in revised form 23 January 2008; accepted 5 February 2008

Available online 13 February 2008

## Abstract

Layered ocean models can exhibit spurious thermobaric instability if the compressibility of sea water is not treated accurately enough. We find that previous solutions to this problem are inadequate for simulations of a changing climate. We propose a new discretization of the pressure gradient acceleration using the finite volume method. In this method, the pressure gradient acceleration is exhibited as the difference of the integral “contact” pressure acting on the edges of a finite volume. This integral “contact” pressure can be calculated analytically by choosing a tractable equation of state. The result is a discretization that has zero truncation error for an isothermal and isohaline layer and does not exhibit the spurious thermobaric instability.

© 2008 Elsevier Ltd. All rights reserved.

## 1. Introduction

Discretization of the horizontal pressure force has been a notorious source of difficulty for several classes of primitive equation models. Most immediately obvious are the difficulties of dealing with the pressure gradient error in terrain-following coordinates; here, much work has been conducted with the intention of minimizing these errors (Haney, 1991; Shchepetkin and McWilliams, 2003). Less well known to the community at large are the discretization difficulties associated with the non-linearity of the equation of state in layered (isopycnal) models; here, thermobaric effects (compressibility) can lead to spurious numerical instabilities if the compressibility is not handled with care (Sun et al., 1999; Hallberg, 2005). Even in the modern versions of level models (geopotential coordinates) there is the possibility of pressure gradient errors in the bottom-most

cells if the shaved cell or partial step (Adcroft et al., 1997) representation of topography is implemented and treated with anything other than first-order accuracy (Pacanowski and Gnanadesikan, 1998). In other non-natural coordinate systems, such as  $z^*/p^*$  (marginally stretched height or pressure coordinates; Adcroft and Campin, 2004) small pressure gradient errors arise. Hybrid-coordinate models exhibit these errors similarly to models using conventional coordinates.

In this paper, we propose a solution that we originally developed for use in an isopycnal model, but which is an appropriate solution independent of coordinates. Indeed, the finite volume approach applied here is “coordinate-free”, in that the actual vertical coordinate is immaterial to the resulting discretization that we derive. The finite volume (FV) approach has been advocated in earlier papers in various degrees of implementation; for example, Adcroft et al. (1997) applied the FV method principally only to the continuity and tracer equations and applied a pseudo finite-volume interpretation of an essentially finite difference treatment of the momentum equations. A more conventional FV treatment of the momentum equations is described in Lin (1997) for an atmospheric model. As described later, a FV discretization will also

\* Corresponding author. Tel.: +1 609 987 5073.

E-mail address: [Alistair.Adcroft@noaa.gov](mailto:Alistair.Adcroft@noaa.gov) (A. Adcroft).

<sup>1</sup> Supported by the Visiting Scientist Program of the Atmospheric and Ocean Sciences Program at Princeton University and NOAA-GFDL and by the NASA Grant NNG06GC28G, “ECCO II: high resolution state estimates of global ocean circulation and ice”.

suffer from spurious thermobaric instability if used in layered ocean models, although it works quite adequately in pseudo-fixed grid models (Adcroft and Campin, 2004). In the following sections we will briefly describe the origins of pressure gradient errors in general; analyze the nature of thermobaric instability in layered models following Hallberg (2005); briefly discuss the finite volume approach for the pressure gradient force following Lin (1997); and then describe our new approach which exhibits *no pressure gradient errors in isopycnal coordinates even with a full equation of state*. Our approach shares some similarity with that of Shchepetkin and McWilliams (2003) but while theirs strives to minimize the truncation errors in a terrain-following coordinate, ours has strictly no truncation error for isothermal layers, i.e. for layered models.

## 2. The origins of pressure gradient errors in ocean models

The horizontal momentum equations associated with the primitive equations written in a general coordinate,  $r$ , can be summarized as

$$\partial_t \vec{u} + \nabla_r \Phi + \alpha \nabla_r p = \mathcal{F} \quad (1)$$

where the vector  $\mathcal{F}$  represents all other terms (i.e., Coriolis, momentum self-advection, viscosity and forcing). Here,  $\vec{u}$  is the horizontal component of velocity, i.e. the component normal to the vertical.  $\Phi$  is the geopotential (typically written  $\Phi = gz$ ),  $\alpha = \rho^{-1}$  is the specific volume and  $p$  is the pressure (we only consider the hydrostatic equations of motion and thus  $p$  is, hereafter, the hydrostatic pressure). The gradient operator is subscripted  $r$  meaning the gradient along the coordinate surface  $r$ . For particular choices of  $r$ , one of the two gradient terms ( $\nabla_r \Phi$  and  $\alpha \nabla_r p$ ) can trivially disappear. Namely, in geopotential coordinates,  $r = z$ , then  $\nabla_r \Phi = \nabla_z \Phi = 0$  and in pressure or mass coordinates,  $r = p$  so  $\nabla_r p = \nabla_p p = 0$ . However, in an arbitrary general coordinate there will be two terms. Written as is, there is a projection of gravity ( $\hat{\mathbf{k}} \cdot \nabla \Phi$ ) and the vertical gradient in hydrostatic pressure ( $\hat{\mathbf{k}} \cdot \alpha \nabla p$ ) into these two along-surface operators whenever the surfaces are inclined to the horizontal. These projections may be large compared to the dynamically significant signal and will be of opposite sign. Numerical evaluation of these two terms are necessarily inexact and the residual difference between these two terms that should be the actual pressure force acceleration will contain some residual of the vertical projection (the difference will be proportional to the remaining truncation terms in a Taylor series approximation of the difference operators representing the two terms). A simple manifestation of these errors leads to the spontaneous motion observed in terrain-following coordinate models with zero horizontal density gradients over topography.

In isopycnal models, an alternative formulation can avoid these errors. The Montgomery potential, defined as  $M = \alpha p + \Phi$ , proves to be a more natural potential than

$\Phi$  or  $p$  in isopycnal coordinates. A transformation of variables allows the horizontal momentum equation (1) to be written as

$$\partial_t \vec{u} + \nabla_r M - p \nabla_r \alpha = \mathcal{F} \quad (2)$$

where  $\mathcal{F}$  represents the same terms as in Eq. (1). If in situ density,  $\alpha^{-1}$ , is the coordinate, the  $p \nabla_r \alpha$  term vanishes by construction. However, isopycnal coordinate models invariably use a potential density as a coordinate so this term does not vanish. In isopycnal coordinates, it is usually argued that  $\nabla_r \alpha$  will be small and so the Montgomery form will exhibit small pressure gradient errors; this is expected to be the case when  $r = \sigma_2$  (the potential density referenced to 2000 dbars pressure) but obviously is not true throughout the global ocean. Indeed, where  $\sigma_2$  is not monotonically increasing with depth, for example in the haloclines at high latitudes, the solenoidal term,  $p \nabla_{\sigma_2} \alpha$  becomes significant. In general, the Montgomery form will tend to manifest a pressure gradient error when compressibility or the choice of vertical coordinate leads to along surface variations of  $\alpha$ .

## 3. Spurious thermobaric instability in layered models

Sun et al. (1999), and later Hallberg (2005), attempted to account for the effect of compressibility in isopycnal models by constructing a new potential,  $M^*$ , that minimized the size of the analogous solenoidal term  $p^* \nabla_r \alpha^*$ . We will not describe their numerical approach here but will review their analysis that explains why isopycnal models can exhibit spurious thermobaric instability if compressibility is not accurately taken into account.

Following Hallberg (2005), consider an ideal hydrostatic layered fluid with temperature as the only state variable, two layers of which are depicted in Fig. 1. Each layer will be assumed to be isothermal ( $\theta(x, p) = \theta_l$ , where  $l = k - \frac{1}{2}$  for  $p < p_k(x)$  and  $l = k + \frac{1}{2}$  for  $p > p_k(x)$ ) but the specific volume,  $\alpha$ , will be non-constant within the layers due to the pressure dependence of  $\alpha$ . Hydrostatic balance in pressure coordinates is

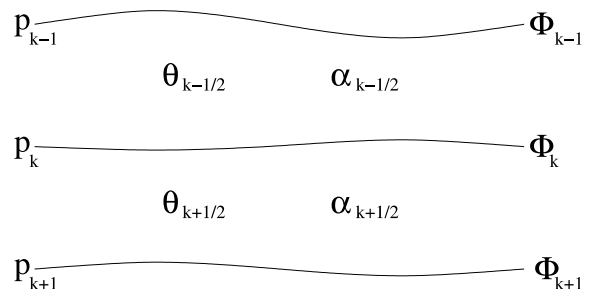


Fig. 1. A schematic of two isothermal layers with variable interface pressures and geopotentials. While  $\theta$  is constant for each layer,  $\alpha$  is variable since it depends on pressure.

$$\frac{\partial \Phi}{\partial p} = -\alpha \quad (3)$$

which can be integrated vertically, starting at the middle interface with pressure  $p_k$ , to obtain the geopotential at any point in the two layers depicted:

$$\Phi(x, p) = \Phi_k - \int_{p_k}^p \alpha(\theta_{k\pm\frac{1}{2}}, p') dp'. \quad (4)$$

The horizontal pressure gradient at any point in the two layers is

$$\begin{aligned} \nabla_p \Phi(p) &= \nabla \Phi_k - \int_{p_k}^{p_{k+1}} \underbrace{\nabla_p \alpha(\theta_{k\pm\frac{1}{2}}, p')}_{=0} dp' \\ &\quad + \alpha(\theta_{k\pm\frac{1}{2}}, p) \times \underbrace{\nabla_p p}_{=0} - \alpha(\theta_{k\pm\frac{1}{2}}, p_k) \nabla p_k \end{aligned} \quad (5)$$

where we have used Leibnitz's rule to bring the gradient operator within the integral. The average horizontal pressure gradient acceleration (PGA) is the vertically average pressure gradient in the layer:

$$\begin{aligned} \text{PGA}_{k\pm\frac{1}{2}} &= \frac{1}{\Delta p_{k\pm\frac{1}{2}}} \int_{p_k}^{p_{k+1}} \nabla_p \Phi dp \\ &= \nabla \Phi_k - \alpha(\theta_{k\pm\frac{1}{2}}, p_k) \nabla p_k \end{aligned} \quad (6)$$

where  $\Delta p_{k\pm\frac{1}{2}} = p_{k+1} - p_k$ , appropriate to each layer. The expression is so simple because the specific volume is only a function of pressure for an isothermal layer. Thus, the difference between the average acceleration in each layer is simply

$$\text{PGA}_{k-\frac{1}{2}} - \text{PGA}_{k+\frac{1}{2}} = \left( \alpha(\theta_{k+\frac{1}{2}}, p_k) - \alpha(\theta_{k-\frac{1}{2}}, p_k) \right) \nabla p_k. \quad (7)$$

A similar analysis of the numerical representation of this term now follows.

In a discrete model, the specific volume of each layer will be represented by a finite number of degrees of freedom, usually just one, corresponding to a piecewise constant representation of  $\alpha$  in the vertical.<sup>2</sup> For simplicity, we choose to evaluate the specific volume using the pressure interpolated to the middle of the level (again, this choice is convenient but does not affect the result) so that the discrete specific volume  $\tilde{\alpha}_{k\pm\frac{1}{2}}(x)$  is

$$\tilde{\alpha}_{k\pm\frac{1}{2}}(x) = \alpha \left( \theta_{k\pm\frac{1}{2}}, \frac{1}{2}(p_k + p_{k+1}) \right) \quad (8)$$

We discretize the pressure gradient acceleration (PGA) in the vertical by finite volume integration, keeping the horizontal continuous to simplify analysis. The layer vertically integrated PGA in each layer is

$$\begin{aligned} \Delta p_{k\pm\frac{1}{2}} \text{PGA}_{k\pm\frac{1}{2}} &= \int_{p_k}^{p_{k+1}} \partial_x \Phi dp \\ &= \partial_x \int_{p_k}^{p_{k+1}} \Phi dp + \Phi_k \partial_x p_k - \Phi_{k+1} \partial_x p_{k+1} \end{aligned} \quad (9)$$

$$\approx \partial_x \left( \Delta p_{k\pm\frac{1}{2}} \frac{(\Phi_k + \Phi_{k+1})}{2} \right) + \Phi_k \partial_x p_k - \Phi_{k+1} \partial_x p_{k+1} \quad (10)$$

where the step from (9) and (10) is the only place where an approximation is made, namely of linear variation of  $\Phi$ , which is a second-order accurate approximation. Hydrostatic balance is discretized as

$$\Phi_{k\pm 1} = \Phi_k - \Delta p_{k\pm\frac{1}{2}} \tilde{\alpha}_{k\pm\frac{1}{2}} \quad (11)$$

and here, the only approximation is in the representation of  $\alpha$  as piecewise constant. Substitution of (11) into (10) and re-arrangement for the difference in accelerations between the two layers gives

$$\begin{aligned} \text{PGA}_{k-\frac{1}{2}} - \text{PGA}_{k+\frac{1}{2}} &= (\tilde{\alpha}_{k-\frac{1}{2}} - \tilde{\alpha}_{k+\frac{1}{2}}) \partial_x p_k \\ &\quad + \frac{1}{2} \left( \Delta p_{k+\frac{1}{2}} \partial_x \tilde{\alpha}_{k+\frac{1}{2}} - \Delta p_{k-\frac{1}{2}} \partial_x \tilde{\alpha}_{k-\frac{1}{2}} \right) \end{aligned} \quad (12)$$

which appears to differ from the continuum analog (7) by an additional term (the last in 12). In fact the first term is also of the wrong form since the pressures used to evaluate the discrete specific volumes are those of the mid-layer and not that of the common interface,  $p_k$ . The Taylor expansion of  $\alpha_{k\pm\frac{1}{2}}$  about  $p_k$  gives

$$\begin{aligned} \tilde{\alpha}_{k\pm\frac{1}{2}} &= \alpha \left( \theta_{k\pm\frac{1}{2}}, p_k + \frac{1}{2} \Delta p_{k\pm\frac{1}{2}} \right) \\ &\approx \alpha \left( \theta_{k\pm\frac{1}{2}}, p_k \right) + \frac{1}{2} \Delta p_{k\pm\frac{1}{2}} \partial_p \alpha_{k\pm\frac{1}{2}} + \mathcal{O}(\Delta p_{k\pm\frac{1}{2}}^2) \end{aligned} \quad (13)$$

and substitution into (12) then yields

$$\begin{aligned} \text{PGA}_{k-\frac{1}{2}} - \text{PGA}_{k+\frac{1}{2}} &= \left( \alpha \left( \theta_{k-\frac{1}{2}}, p_k \right) - \alpha \left( \theta_{k+\frac{1}{2}}, p_k \right) \right) \partial_x p_k \\ &\quad + \frac{1}{4} \left( \Delta p_{k+\frac{1}{2}} \partial_x \left( \Delta p_{k+\frac{1}{2}} \partial_p \alpha_{k+\frac{1}{2}} \right) \right. \\ &\quad \left. - \Delta p_{k-\frac{1}{2}} \partial_x \left( \Delta p_{k-\frac{1}{2}} \partial_p \alpha_{k-\frac{1}{2}} \right) \right) + \mathcal{O}(\Delta p^3) \end{aligned} \quad (14)$$

in which the first term takes a form with appropriate reference pressures and is now identical to that in (7). The second-order term in  $\Delta p$  involves the compressibility,  $\partial_p \alpha$ , and is generally present except for some special choices of layer thickness and compressibility. Use of higher order interpolation for any choices made in this discretization can reduce the magnitude of this term but it can not be made to vanish completely. As pointed out by Hallberg (2005), these terms can lead to exponential growth of interface perturbations and thus numerical instability. The essence of the approach taken by Sun et al. (1999) and Hallberg (2005) was to find a variable transformation that mini-

<sup>2</sup> Piecewise linear representation of  $\alpha$  in the vertical and other higher order representations do not solve the problem about to be described although they do increase the order of accuracy.

mized these terms by careful fitting of the compressibility by an approximate equation of state in the new variables.

There are two reasons for the appearance of the spurious term (14); the first is the discretization of the hydrostatic balance, which leads to the additional terms in (12) and the second is due to the use of a single interpolated pressure within the equation of state that led to the truncation terms in (13). The consequence is that any discrete representation of the specific volume will lead to these spurious compressibility truncation terms, although higher order interpolation may be able to reduce their size. Although similar truncation terms can appear in fixed-grid models (e.g. height-coordinate or terrain-following coordinate models), there is no feedback that leads to an exponential growth because the interfaces are fixed.

Atmospheric models, which are *more* compressible than the ocean, do not appear to suffer from this problem with thermobaric instability. Examination of the literature reveals a subtle trick that at first glance seems unusable in the ocean. The atmosphere can be approximated very well as an ideal gas and this allows the hydrostatic balance equation to be transformed into a linear equation by a transformation of variables. For instance, defining the Exner function as  $\pi = p^k$  allows the hydrostatic balance equation to be re-written as  $\partial_\Phi = c_p \theta$  which is linear. Most atmospheric models work with either  $\log(p)$  or  $\pi$  in the hydrostatic equation; in both cases, compressibility is analytically incorporated and there is no source of the spurious compressibility truncation terms.

#### 4. The analytic-finite volume treatment of pressure gradient force

We are motivated to consider an analytic treatment of the relevant terms in ocean models, and we now describe a treatment using the finite volume method applied in two dimensions. The zonal component of the momentum equations (1), integrated over a finite volume in  $(x-p)$  space, is

$$\begin{aligned} \int dx \int dp \partial_t u &= \int dx \int dp \partial_x |p \Phi \\ &= \int_{p_{br}}^{p_{tr}} \Phi dp + \int_{p_{tr}}^{p_{tl}} \Phi dp + \int_{p_{tl}}^{p_{bl}} \Phi dp \\ &\quad + \int_{p_{bl}}^{p_{br}} \Phi dp. \end{aligned} \quad (15)$$

Fig. 2 shows the placement of variables and integrals for this finite volume PGA calculation. The only approximations that we make are (i) that the potential temperature ( $\theta$ ) and salinity ( $s$ ) can be represented continuously in the vertical within each layer although discontinuities between each layer are allowed and (ii) that  $\theta$  and  $s$  can be represented continuously along each layer. We treat  $\theta$  and  $s$  as piecewise constant in the vertical (the usual assumption for isopycnal models) and use linear interpolation in the horizontal. Higher order representations are possible, but

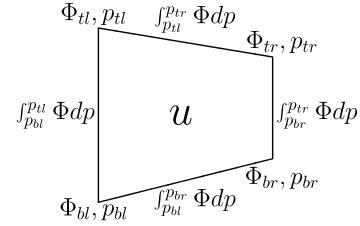


Fig. 2. Schematic of the finite volume used for integrating the  $u$ -component of momentum. The thermodynamic variables  $\theta$  and  $s$  reside on the sides of the depicted volume and are considered uniform for the vertical extent of the volume but with linear variation in the horizontal. The volume is depicted in  $(x, p)$  space so  $p$  is linear around the volume but  $\Phi$  can vary arbitrarily along the edges.

the piecewise constant choice is sufficient to build a dynamic model without spurious thermobaric instability.

We now stipulate the use of the equation of state in the form proposed by Wright (1997), which can be written as

$$\alpha(s, \theta, p) = A(s, \theta) + \frac{\lambda(s, \theta)}{P(s, \theta) + p} \quad (16)$$

where  $A$ ,  $\lambda$  and  $P$  are functions only of  $s$  and  $\theta$ . We choose this equation of state because of the relatively simple analytic form, but our approach can be applied to any equation of state that is in a tractable analytic form. The integral form of hydrostatic balance is

$$\Phi(p_t) - \Phi(p_b) = \int_{p_t}^{p_b} \alpha(s, \theta, p) dp \quad (17)$$

which in the terminology of the finite volume literature, is referred to as the “weak form”. In the finite volume method the objective is to minimize the error in evaluation of the integral. Because of the analytically tractable form of the equation of state we are able to evaluate the integral exactly:

$$\begin{aligned} \Phi(p_t) - \Phi(p_b) &= \int_{p_t}^{p_b} \alpha(s, \theta, p) dp \\ &= (p_b - p_t)A + \lambda \ln \left| \frac{P + p_b}{P + p_t} \right| \\ &= \Delta p \left( A + \frac{\lambda}{(P + \bar{p})} \frac{1}{2\epsilon} \ln \left| \frac{1 + \epsilon}{1 - \epsilon} \right| \right) \end{aligned} \quad (18)$$

which is the exact solution for the continuum *only if*  $\theta$  and  $s$  are uniform in the interval  $p_t$  to  $p_b$ . Here, we have introduced the variables

$$\Delta p = p_b - p_t, \quad \bar{p} = \frac{1}{2}(p_t + p_b) \quad \text{and} \quad \epsilon = \frac{\Delta p}{2(P + \bar{p})}$$

for convenience to simplify the following presentation. We will show later that  $\epsilon \ll 1$ . Note that the series expansion for

$$\frac{1}{2\epsilon} \ln \left| \frac{1 + \epsilon}{1 - \epsilon} \right| = \sum_{n=1}^{\infty} \frac{\epsilon^{2n-2}}{2n-1} = 1 + \frac{\epsilon^2}{3} + \frac{\epsilon^4}{5} + \dots \quad \forall |\epsilon| \leq 1 \quad (19)$$



shows us that the leading order terms in (18) are  $\Phi(p_t) - \Phi(p_b) \approx \Delta p \left( A + \frac{\lambda}{P+\bar{p}} \right) = \Delta p \alpha(\bar{p})$  which is a second-order finite-difference approximation to the hydrostatic equation. Indeed, having the analytic solution to the weak form of the hydrostatic equation allows us to give the exact truncation error of the finite difference approximation to the integral hydrostatic equation. Assuming the same starting value for the integration,  $\Phi(p_b)$ , a simple finite difference approximation for  $\Phi(p_t)$  is

$$\tilde{\Phi}(p_t) = \Phi(p_b) + \Delta p \bar{\alpha} = \Phi(p_b) + \Delta p \left( A + \frac{\lambda}{P+\bar{p}} \right) \quad (20)$$

Taking the difference of (20) and (18) yields the corresponding error

$$\begin{aligned} \tilde{\Phi}(p_t) - \Phi(p_t) &= \Delta p \frac{\lambda}{(P+\bar{p})} \left( 1 - \frac{1}{2\epsilon} \ln \left| \frac{1+\epsilon}{1-\epsilon} \right| \right) \\ &= -\Delta p \frac{\lambda}{(P+\bar{p})} \left( \frac{\epsilon^2}{3} + \frac{\epsilon^4}{5} + \dots \right) \end{aligned} \quad (21)$$

$$\approx -\frac{2}{3} \lambda \epsilon^3 + \mathcal{O}(\epsilon^5) \quad (22)$$

which is, curiously, sign definite, second-order in  $\epsilon$  (referring to the truncation error for a finite difference approximation to  $\partial\Phi/\partial p$ ) and vanishes if the fluid is incompressible ( $\lambda = 0$ ). Recall that these evaluations assume an isothermal layer, which is why it appears there is no error if the fluid is incompressible. Typical values of  $P$  and  $\Delta p$  for an ocean model (using 100 m layer thickness) are  $6 \times 10^8$  Pa and  $10^6$  Pa, respectively, yielding  $\epsilon \sim 8 \times 10^{-4}$  and a corresponding accuracy in the geopotential height calculation of order  $\frac{\Delta p}{g} \sim 10^{-5}$  m. This accuracy might appear to be sufficient for an ocean model and yet, as was shown in the previous section, these small terms ultimately are responsible for the spurious thermobaric instability. For this value of  $\epsilon$ , the series (21) converges to machine precision ( $10^{-15}$ ) with just three terms. In our implementation, we use series rather than the intrinsic log function, since the log is machine dependent and insufficiently accurate. In extreme circumstances,  $\Delta p \sim 6 \times 10^7$  Pa (limited by the depth of the ocean) for which  $\epsilon \sim 0.04$  with geopotential height errors of order 1 m. In this case, the series converges to machine precision with six terms.

The analytic and weak forms of hydrostatic balance give the difference in geopotential across the layer. But the finite volume acceleration (15) is expressed in terms of four integrals around the volume,  $\int \Phi dp$ . The side integrals can be calculated by direct integration of (18), which gives

$$\begin{aligned} \int_{p_t}^{p_b} \Phi dp &= \Delta p \left( \Phi_b + \frac{1}{2} A \Delta p + \lambda \left( 1 - \frac{(1-\epsilon)}{2\epsilon} \ln \left| \frac{1+\epsilon}{1-\epsilon} \right| \right) \right) \\ &= \Delta p \left( \Phi_b + \frac{1}{2} A \Delta p + \lambda \left( 1 - (1-\epsilon) \left( \frac{\epsilon^2}{3} + \frac{\epsilon^4}{5} + \dots \right) \right) \right) \\ &= \Delta p \left( \Phi_b + \frac{1}{2} A \Delta p + \lambda \left( \epsilon - (1-\epsilon) \epsilon^2 \left( \frac{1}{3} + \frac{\epsilon^2}{5} + \dots \right) \right) \right) \end{aligned} \quad (23)$$

where  $\Phi$ ,  $\Delta p$ ,  $P$ ,  $A$  and  $\lambda$  are each evaluated on the left or right side of the volume. Again, for comparison, we can examine the truncation error in a more conventional discretization; the second-order finite-volume method of Lin (1997) approximates the side integrals using linear interpolation from the corner values so that

$$\int_{p_t}^{p_b} \Phi dp \approx \Delta p \frac{\Phi_t + \Phi_b}{2} \quad (24)$$

Using the conventional finite difference discretization (20) for  $\tilde{\Phi}$ , this side integral is approximated as

$$\begin{aligned} \int_{p_t}^{p_b} \tilde{\Phi} dp &\approx \Delta p \frac{\tilde{\Phi}_t + \Phi_b}{2} = \Delta p \left( \Phi_b + \frac{1}{2} \Delta p \left( A + \frac{\lambda}{P+\bar{p}} \right) \right) \\ &= \Delta p \left( \Phi_b + \frac{1}{2} A \Delta p + \lambda \epsilon \right) \end{aligned} \quad (25)$$

for which the truncation error (taking the difference between Eqs. (25) and (23)) is

$$\begin{aligned} \Delta p \frac{\tilde{\Phi}_t + \Phi_b}{2} - \int_{p_t}^{p_b} \Phi dp &= \Delta p \lambda (1-\epsilon) \epsilon^2 \left( \frac{1}{3} + \frac{\epsilon^2}{5} + \dots \right) \\ &= \Delta p \lambda \frac{\epsilon^2}{3} + \mathcal{O}(\epsilon^3) \end{aligned} \quad (26)$$

Dividing by  $\Delta p$  allows us to interpret the truncation error in terms of an average error along the sides in the geopotential height, which for a 100 m layer (as before) is of order  $3 \times 10^{-3}$  m, significantly larger than the point-wise error given by (22).

The top and bottom integrals appearing in (15) must allow for the effect of varying  $\theta$  and  $s$  on  $A$ ,  $\lambda$  and  $P$ . Obtaining these integrals analytically was beyond us (and our skill with Maple or Mathematica software) so we evaluate these integrals numerically using sixth-order quadrature; Bode's rule requires evaluating the coefficients in the equation of state at five points, two of which have already been evaluated for the side integrals. For efficiency, we linearly interpolate the coefficients  $A$ ,  $P$  and  $\lambda$  between the end points, which seems to make very little difference to the solution. We also verified that the use of tenth-order quadrature makes little difference to the solution. The values of the top and bottom integrals are carried upward in a hydrostatic-like integration, obtained as follows:

$$\begin{aligned} \int_{p_{tl}}^{p_{tr}} \Phi_t dp &= (p_{tr} - p_{tl}) \int_0^1 \Phi_t dx = (p_{tr} - p_{tl}) \\ &\quad \times \int_0^1 \left\{ \Phi_b + A(x) \Delta p(x) + \lambda(x) \ln \left| \frac{1+\epsilon(x)}{1-\epsilon(x)} \right| \right\} dx \\ &= (p_{tr} - p_{tl}) \int_0^1 \Phi_b dx + \int_0^1 \Delta p(x) \\ &\quad \times \left\{ A(x) + \frac{\lambda(x)}{P(x) + \bar{p}(x)} \sum_{n=1}^{\infty} \frac{\epsilon^{2n-2}}{2n-1} \right\} dx \end{aligned} \quad (27)$$

The first integral is either known from the top integral of the layer below or the boundary condition at the ocean

bottom. The second integral is the integral evaluated numerically.

All the above definite integrals are specific to the Wright (1997) equation of state; the use of a different equation of state requires analytic integration of the appropriate equations. We have found, however, that high-order numerical integration appears to be sufficient. For example, we have compared the analytic implementations with numerical integration using only numerical integration of the integrals using sixth-order and higher quadrature, in order to verify our mathematical analysis; we found differences comparable to numerical round off at 64-bit precision (Fortran “real \* 8”). Although the numerical implementation is more general (allowing the use of arbitrary equations of state), it is significantly more expensive and so we advocate the analytic implementation for efficiency.

## 5. Results for a global ocean isopycnal model

To illustrate that the new discretization fixes the thermobaric instability we show solutions using the Montgomery-based finite-difference discretization (Hallberg, 2005) and this new finite-volume discretization. The model is global and forced by an atmospheric state and sea-ice model, as described by Griffies et al. (2008), and is otherwise discretized following Hallberg and Rhines (1996). The model has a tri-polar grid, matched at 65°N and uses 1° zonal resolution while the meridional resolution stretched from 1° at mid-latitudes down to  $\frac{1}{3}^\circ$  at the equator. The compressibility is calculated based on Levitus climatology following Hallberg (2005) which is also used for the initial conditions. However, because the model drifts, this compressibility slowly becomes inappropriate and thermobaric instabilities

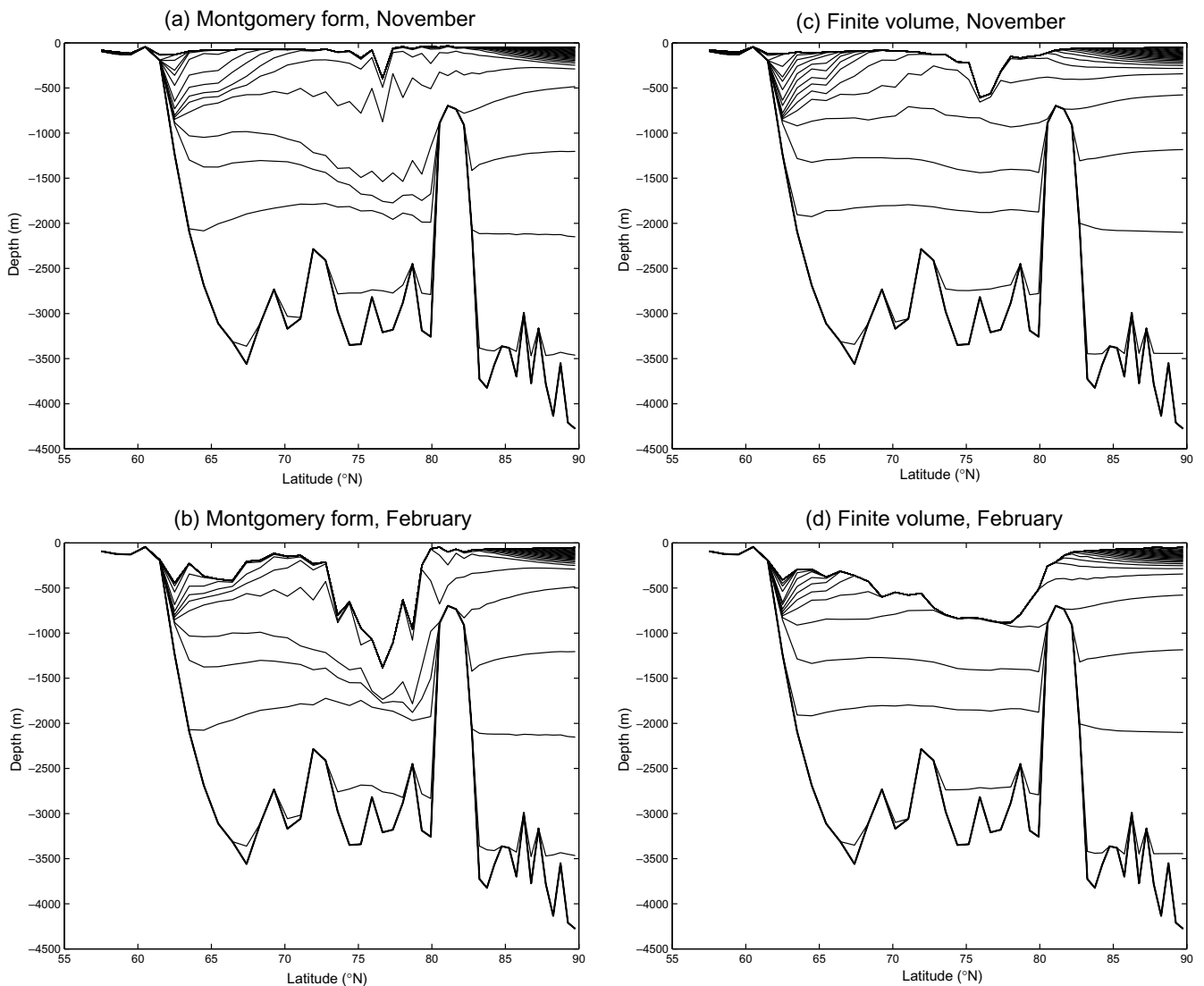


Fig. 3. Interface positions in the Nordic Seas at 0°E in November of year 41 and the following February. On the left are results using the finite difference Montgomery form of pressure gradient and on the right are the results using the new analytic finite volume formulation. The noise apparent in the Montgomery formulation is consistent with spurious thermobaric instability and later leads to deeper mixing as Winter progresses. The new formulation evolves more smoothly and with more realistic mixed layer depths.

begin to appear. Fig. 3 shows the interface depths (isopycnals in the interior) across the Nordic Seas (a) November and (b) February. The grid-scale oscillations grow with time and eventually de-stabilize the water column so that the water column is mixed deeper than in reality. In contrast, the solutions obtained with the analytic finite volume discretization show no such oscillations, and the mixed-layer depth appears well behaved (panels c and d).

The improvement is not only local but has a large impact on water mass formation. Fig. 4a and b shows the ideal age after 48 years at a depth of 2050 m, in the model using the finite difference Montgomery form and

the new finite volume form of pressure gradient, respectively. It is apparent that there is active mixing to great depths in much of the Southern Ocean and far North Atlantic, indicated by young water at this depth in Fig. 4a. In contrast, use of the analytic finite volume discretization shows the result of much more localized regions of deep ventilation of the abyssal ocean (Fig. 4b). Needless to say, use of the new scheme has a major impact on the longer-term climate solution (not shown) because of the systematic reduction in spurious mixing. To the extent that the changes shown in Fig. 4 are typical of all isopycnal models with a realistic equation of state used to date (we

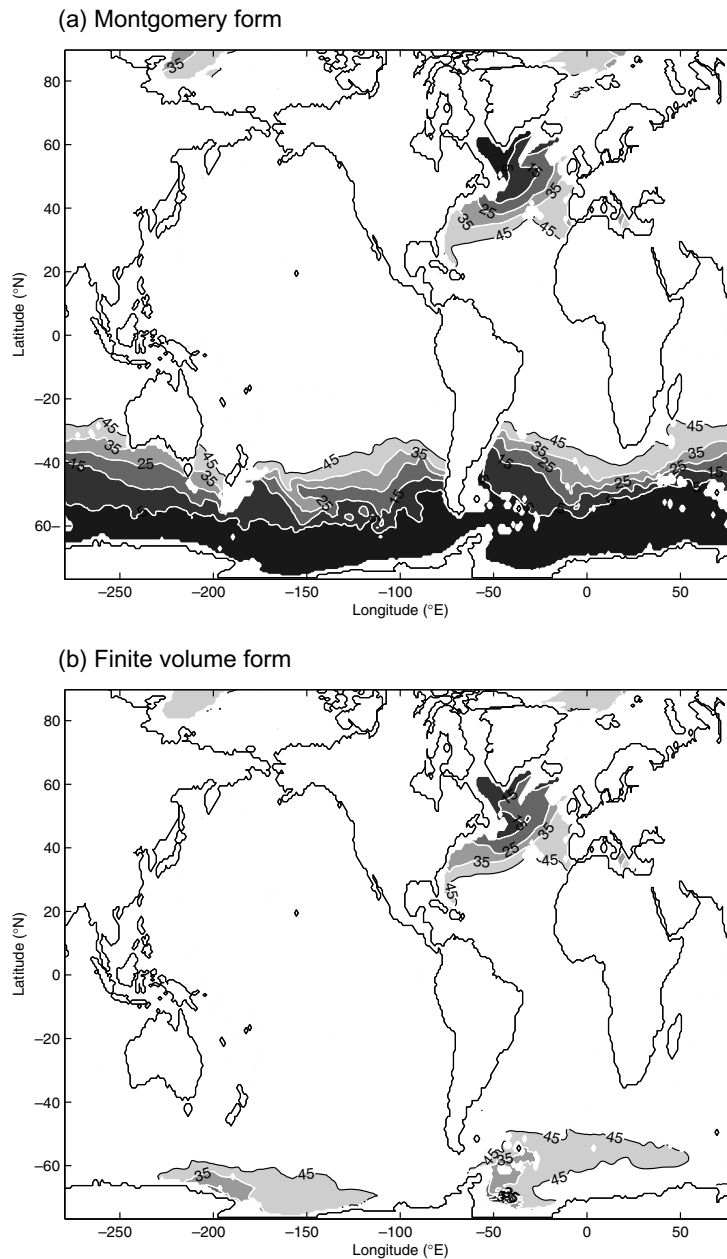


Fig. 4. Distribution of ideal age at 2059 m depth after 48 years of integration: (a) using the finite difference Montgomery form of pressure gradient and (b) using the analytic finite volume formulation. Contours start at 5 years and increment in decades to 45 years. Shaded regions are young water, white regions are older than 45 years.

are aware of nothing that would suggest they are not), the improvements exhibited by the analytic finite volume method would seem to be essential for using an isopycnal model to study long-term ocean climate.

## 6. Conclusions

We have presented the analysis of thermobaric instability in isopycnal models and shown that an analytic finite volume treatment of the equation of state, hydrostatic balance and pressure gradient terms can correctly model a non-linear equation of state with full compressibility. For the simple thought experiment used in the analysis (Hallberg, 2005), this discretization strictly has no truncation error associated with the vertical discretization; this is by construction because the vertical solution structure is found analytically. The horizontal components to the discretization are also treated analytically but here the second-order interpolation for  $s$  and  $\theta$  imply truncation terms with respect to the continuum equations.

Our approach is predicated on the ability to analytically integrate the equation of state. A different choice of equation of state, with a different closed form could therefore require a complete re-working of the mathematics and implementation. We did use numerical integration methods in order to verify our mathematical analysis and to avoid some intractable mathematics in the horizontal direction. However, we note that the analytic approach, as we described here, is simply more efficient than numerical integration at even a moderate order of accuracy. A relatively high-order integration method is required to avoid the truncation errors that gave rise to the thermobaric instability in original layer model, which were of second-order in nature.

The approximations used in our approach are of piecewise constant  $\theta$  and  $s$  in the vertical and linear variation between nodes in the horizontal (along layers). This vertical structure is quite appropriate for isopycnal/layered models and has been a long standing interpretation for such models. Unlike layered models, our approach lends itself to high-order reconstruction in the vertical, for example, piecewise-linear or piecewise-parabolic reconstructions although in that case numerical integration may be preferable to complicated analytic expressions for the vertical integrals. In the horizontal, higher-order reconstruction is also possible and may be more appropriate in strongly inclined layers. Both these modifications may be necessary to apply our approach to non-natural coordinate systems such as terrain-following coordinates. Indeed, our approach shares many similarities with that of Shchepetkin and McWilliams (2003) in that they also analytically integrate the pressure gradient terms. However, they approximate the specific volume by local polynomial fitting which, according to the

authors, can limit the accuracy for strongly inclined interfaces. Our approach does no fitting of functions but the piecewise constant representation of  $\theta$  and  $s$  would not be appropriate in a terrain-following coordinate system. We speculate that high-order reconstruction of  $\theta$  and  $s$ , of the same order and form of Shchepetkin and McWilliams (2003), combined with analytic integration of the equation of state, would yield a system that is at least as accurate or probably more accurate than theirs.

Finally, we have not yet verified that our approach has immediate benefits in other coordinate systems but can see no reasons why it would not work. We are adapting the model used here to use generalized coordinates in the vertical, at which point we will be able to evaluate the utility of our pressure gradient method for other modeling coordinates and classes.

## Acknowledgements

We would like to thank Stephen Griffies and Sonya Legg for their comments on initial drafts of this manuscript and the two anonymous reviewers for their feedback.

## References

- Adcroft, A., Campin, J.-M., 2004. Rescaled height coordinates for accurate representation of free-surface flows in ocean circulation models. *Ocean Modell.* 7, 269–284.
- Adcroft, A., Hill, C., Marshall, J., 1997. Representation of topography by shaved cells in a height coordinate ocean model. *Mon. Weather Rev.* 125, 2293–2315.
- Griffies, S.M., Biastoch, A., Böning, C., Bryan, F., Chassignet, E., England, M., Gerdes, R., Haak, H., Hallberg, R.W., Hazeleger, W., Jungclauss, J., Large, W.G., Madec, G., Samuels, B.L., Scheinert, M., Severijns, C.A., Simmons, H.L., Treguer, A.M., Winton, M., Yeager, S., Yin, J., 2008. Coordinated ocean–ice reference experiments (COREs). *Ocean Modell.*, submitted for publication.
- Hallberg, R., 2005. A thermobaric instability of Lagrangian vertical coordinate ocean models. *OM* 8, 279–300.
- Hallberg, R., Rhines, P., 1996. Buoyancy-driven circulation in an ocean basin with isopycnals intersecting the sloping boundary. *JPO* 26, 913–940.
- Haney, R., 1991. On the pressure-gradient force over step topography in sigma coordinate ocean models. *J. Phys. Oceanogr.* 21 (4), 610–619.
- Lin, S.-J., 1997. A finite-volume integration method for computing pressure gradient forces in general coordinates. *Quart. J. R. Meteorol. Soc.* 123, 1749–1762.
- Pacanowski, R., Gnanadesikan, A., 1998. Transient response in a z-level ocean model that resolves topography with partial-cells. *Mon. Weather Rev.* 126, 3248–3270.
- Shchepetkin, A., McWilliams, J.C., 2003. A method for computing horizontal pressure-gradient force in an oceanic model with a nonaligned vertical coordinate. *J. Geophys. Res.* 5. doi:10.1029/2001JC001047.
- Sun, S., Bleck, R., Rooth, C., Dukowicz, J., Chassignet, E., Killworth, P., 1999. Inclusion of thermobaricity in isopycnic-coordinate ocean models. *J. Phys. Oceanogr.* 29, 2719–2729.
- Wright, D.G., 1997. An equation of state for use in ocean models: Eckart's formula revisited. *J. Ocean. Atmos. Tech.* 14, 735–741.