Neutral density revisited

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Abstract

The possibilities of defining and computing an approximately neutral density variable are re-examined in this paper. There are three desirable properties that a neutral density variable should possess. Firstly, the isosurfaces of this variable should coincide with (approximately) neutral surfaces. This would facilitate the analysis of hydrographic data on the most appropriate mixing and spreading surfaces. Secondly, the horizontal gradients of the neutral density should agree with the gradients of the in-situ density, and thirdly the vertical gradient of the neutral density variable should be proportional to the static stability of the water column. A density variable which approximates the latter two properties can be used in ocean circulation models based on layer coordinates, and would reduce substantial errors in present isopycnal models due to the use of a potential density variable.

No variable can possess all the three properties simultaneously. The variable γ_n introduced by Jackett and McDougall [1997] satisfies the first of the properties exactly but is not designed for the use in models. Based on climatological data in the North Atlantic, an alternative neutral density variable $\tilde{\nu}\,(S, \Theta)$ is defined which is shown to approximate the two gradient criteria much better than any potential density. We suggest that this neutral density variable may be useful in isopycnal ocean models as an alternative to potential density, since it could significantly reduce errors in thermal wind relation and vertical stability.

1 Introduction

The nonlinear form of the equation of state and the compressibility of seawater lead to some well-known difficulties in diagnosing and modelling the ocean circulation. A classical oceanographic problem is to find proper surfaces for tracing watermasses. In-situ density surfaces are inappropriate because even under adiabatic conditions the in-situ density of a moving water parcel is not a conserved variable, and changes due to compressibility. Although the potential density introduced by Wüst [1933] is a conserved variable, using a surface of constant potential density for tracing watermasses at large distances away from the reference pressure means to neglect the dependence of the adiabatic compressibility coefficient on salinity and potential temperature, or equivalently to neglect the pressure dependence of the haline and thermal expansion coefficients. These deficiencies of isopycnal surfaces have been known for a long time. To reduce this error, it is common since the work of Kawai [1960] and Lynn and Reid [1968] to use isopycnals with a reference pressure near the investigated depth range. For example, Reid [1994] used isopycnals with ten different reference pressures in the North Atlantic, a procedure which is occasionally called an isopycnal analysis.

The search for adequate surfaces led Ivers [1975] and later McDougall [1987a] to introduce the concept of neutral surfaces. A water parcel undergoing small displacements on these surfaces at constant potential temperature and salinity always has the same density as the surrounding water, hence no restoring buoyancy forces occur, and no energy exchange is required. It is widely accepted that those surfaces would be the appropriate surfaces on which watermasses spread and mix laterally. These surfaces do not exist in a strict mathematical sense, as pointed out by McDougall [1987a] who introduced instead the concept of *approximate* neutral surfaces. The ambiguity in the depth is however only a few meters, whereas a neutral surface can differ from an isopycnal by several hundred meters. The replacement of potential density by a variable which is constant on (approximate) neutral surfaces is therefore obviously very useful. Jackett and

McDougall [1997] have defined such a variable, called γ_n, which can be computed as a function of salinity, potential temperature, pressure and the horizontal position, defined over the whole world ocean. By labeling casts and sections with this variable, one can obtain in an easy and reproducable way most accurate neutral surfaces. This variable has been used e.g. by You and Siedler [1997] to analyze the water mass structure in the South Atlantic Ocean.

There is however another important application of the neutral density concept. Ocean models based on layer coordinates are presently rather popular among oceanographers because they allow simulations with significantly reduced mixing compared to traditional models (Bleck et al. [1992], Oberhuber [1993]). In these models, the horizontal pressure gradient –and hence effectively the vertical shear– is computed from the slope and thickness of layers which are bounded by surfaces of constant potential density, usually σ_0 or σ_2. Consequently, the thermal wind shear in these models is proportional to the horizontal gradient of a potential density, rather than of the in-situ density which alone is dynamically relevant. The error of vertical shear increases with vertical distance from reference level, and can reach a significant magnitude (McDougall [1987b]). Obviously, the replacement of potential density by a neutral density variable in an isopycnal ocean model would be ideal if the horizontal gradients of that variable were equal to the horizontal gradients of the in-situ density.

Static stability is another important parameter for the ocean circulation, it controls the speed of wave propagation and influences the degree of small-scale mixing and other aspects. Up to a constant factor, the static stability coincides with the vertical gradient of potential density at the reference pressure but not at other pressure levels, as was already noted by Ekman [1934]. Hence models based on a potential density have the correct properties only in a restricted depth range near the reference pressure. Obviously, it would be desirable to have a neutral density variable with a vertical gradient which were *everywhere* proportional to the static stability of the water column. Futhermore, as on time scales longer than a few hours the ocean is stably stratified, such a variable varies monotonously with depth, whereas e.g. σ_Θ has inversions over certain regions in the ocean, which could lead to a folding of the coordinate layers in an isopycnal model.

Hence the three properties which a neutral density ideally should possess are that i) it should be constant on (approximate) neutral surfaces, ii) its horizontal gradients should coincide with the horizontal gradients of the in-situ density, and iii) its vertical gradient should be proportional to the static stability of the water column. Of course no variable can satisfy all these conditions, but is possible to define and study approximate neutral densities which constitute a compromise between those properties. The variable γ_n has the first property, and is an optimal choice for the analysis of hydrographic data, but is not immediately useful in the context of layer models.

In this paper we will explore an alternative approach, and focus on the use of a neutral density variable in connection with a layered model where conditions ii) and iii) are more relevant. In a first step, we will determine, from hydrographic data in the North Atlantic, a spatial distribution of a neutral density variable that will indicate the degree to which those conditions can be satisfied by *any* scalar field. For the practical use of a neutral density variable in isopycnal models, a functional representation in terms of potential temperature and salinity is required. We have made an attempt to compute such a functional form which is optimally tuned to the gradient conditions in the North Atlantic.

This paper is organized as follows: In the second section the relevant concepts for describing neutral surfaces are briefly reviewed. In the third section a minimum condition to define an approximate neutral density is introduced, and a distribution of neutral density is calculated numerically for the North Atlantic Ocean, based on the climatology of Levitus [1982]. Subsequently, a second minimization is performed where the neutral density is restricted as a (polynomial) function of potential temperature and salinity. The resulting distributions are discussed, and compared with the performance of other density variables. The last section summarizes and discusses the main results of this paper.

2 Neutral trajectories, neutral surfaces and neutral density

In this section the relevant concepts are reviewed in some detail, in order to introduce in a precise way the terminology which is used in the following.

The adjective *neutral* means throughout the following a neutrally stable static stability. A *neutral trajectory* is a three dimensional path in the ocean, and is defined such that no buoyancy forces act on a water parcel when it is moved a small distance along this path. A neutral trajectory is mathematically well defined but does not generally coincide with a particle trajectory. A *neutral surface element* is an infinitesimally small surface, and again there are no buoyancy forces acting on a water parcel moving a small distance along this surface element which also is mathematically well defined. A *neutral surface* is a surface in the ocean, which one might imagine as being composed of many neutral surface elements. It is however mathematically not uniquely defined. A *neutral density* is a scalar field which should possess the three features mentioned above, i.e. it should be constant along neutral surfaces and have prescribed horizontal and vertical gradients. Because of the ill-defined nature of the neutral surfaces and the neutral density, the reader should keep in mind the adjective *approximate* whenever appropriate.

In the following we will use the equation of state for the in-situ density of seawater in the form

$$\rho = \rho(S, \Theta, p) \tag{1}$$

where S denotes salinity, Θ potential temperature and p the pressure (Gill [1982]). The use of potential temperature rather than the in-situ temperature T is more convenient because it is a conservative variable to a very good approximation. The derivatives are denoted by $\beta = \rho^{-1}\partial\rho/\partial S|_{\Theta,p}$ (haline contraction), $\alpha = -\rho^{-1}\partial\rho/\partial\Theta|_{S,p}$ (thermal expansion), and $\gamma = \rho^{-1}\partial\rho/\partial p|_{\Theta,S}$ (adiabatic compressibility). Note that β and α are numerically very similar but not identical to the usual haline and thermal expansion coefficients defined with the standard equation of state $\rho = \rho(S, T, p)$. For the numerical computations of the state equation and its derivatives in this paper, we have used the polynomial approximation to the Gibbs thermodynamic potential by Feistel and Hagen [1995].

2.1 Neutral trajectories

The change of the in-situ density along a small arbitrary distance $d\mathbf{r}$ can be expressed in terms of the changes of the three thermodynamic state variables along that distance and is given by

$$d\rho = \nabla\rho \cdot d\mathbf{r} = \rho\beta\nabla S \cdot d\mathbf{r} - \rho\alpha\nabla\Theta \cdot d\mathbf{r} + \rho\gamma\nabla p \cdot d\mathbf{r} \ .$$

The definition of a neutral trajectory is such that during an adiabatic displacement of a water parcel, i.e. without a change in salinity and potential temperature, no restoring buoyancy forces appear, and its in-situ density is changed only by the influence of the pressure. In other words, the density of the water parcel must be equal to the density of the surrounding water. Hence the condition for d$\mathbf{r}$ to be an element of a neutral trajectory is

$$\rho\beta\nabla S \cdot d\mathbf{r} - \rho\alpha\nabla\Theta \cdot d\mathbf{r} = 0 \ .$$

If this condition is satisfied everywhere along a certain path, this path constitutes a neutral trajectory. Obviously, for a given horizontal projection (or direction) of $d\mathbf{r}$ there exists exactly one neutral trajectory through any point in the ocean.

All possible directions of $d\mathbf{r}$ define the neutral surface element. Its orientation is described by the normal vector

$$\mathbf{e} = \rho\beta\nabla S - \rho\alpha\nabla\Theta. \tag{2}$$

At any point in the ocean, exactly one neutral surface element exists. The vector $\mathbf{e}$ coincides with the gradient of a potential density which is referenced to local pressure. Hence a neutral surface element lies within an isopycnal surface at reference pressure, but not elsewhere because of the pressure dependence of the expansion coefficients β and α. See figure 1 for a sketch of an isopycnal and the corresponding gradient at the reference pressure, resp. the vector $\mathbf{e}$.

2.2 Neutral surfaces

It is very suggestive to imagine a neutral surface as an envelope of neutral surface elements. All paths in this surface would then obviously be neutral trajectories. The surface should everywhere be orthogonal to the vector $\mathbf{e}$, and therefore the equation $\mathbf{e} \cdot \mathrm{d}\mathbf{r} = 0$, or explicitly

$$e_1(x,y,z)\mathrm{d}x + e_2(x,y,z)\mathrm{d}y + e_3(x,y,z)\mathrm{d}z = 0 \tag{3}$$

has to be satisfied, with $\mathrm{d}\mathbf{r} = (dx, dy, dz)$ lying within the surface. A solution of (3), e.g. in the form $z = \mathcal{N}(x,y)$ exists only if an integrating factor $g(x,y,z)$ can be found which leads to an *exact* differential when multiplied with equation (3). A condition for the existence of the integrating factor is that the *helicity* of $\mathbf{e}$, defined as $\mathbf{e} \cdot \nabla \times \mathbf{e}$, must vanish identically (Bronstein et al. [1995], Jackett and McDougall [1997]). After some algebra, one obtains from (2) and (1) for the helicity

$$\mathbf{e} \cdot \nabla \times \mathbf{e} = \rho(\nabla p \cdot \nabla S \times \nabla \Theta)[\beta(\rho\alpha)_p - \alpha(\rho\beta)_p] \ . \tag{4}$$

Hence a neutral surface can exist only if one of the two brackets in (4) vanishes identically. The condition $\nabla p \cdot (\nabla S \times \nabla \Theta) \equiv 0$ could be satisfied if a $\Theta - S$–relation would hold in a certain region. While this is often a good approximation, it is however not generally true for the ocean. Another possibility for the first bracket in (4) to vanish is that the line of intersection of the S and Θ surfaces, $\nabla S \times \nabla \Theta$, lies in a plane of constant pressure, so that $\nabla p \cdot (\nabla S \times \nabla \Theta) = 0$, as illustrated in figure 3 in McDougall and Jackett [1988]. Since the ocean is nearly in the hydrostatic limit, the weaker condition only for the vertical component of $\nabla S \times \nabla \Theta$ would suffice, i.e. $S_x \Theta_y - S_y \Theta_x = 0$ which however is also not generally satisfied. A possibility for the second bracket in (4) to vanish would require that the pressure dependencies of $\rho\alpha$ and $\rho\beta$ are related, more precisely that

$$\beta(\rho\alpha)_p \equiv \alpha(\rho\beta)_p \tag{5}$$

which is however not satisfied for the equation of state (1). Hence neutral surfaces cannot be defined unambiguously. If one imagines a neutral trajectory in the ocean with a horizontally circular projection, in 3 dimensions the path will normally not be closed but rather have the shape of a helix (McDougall and Jackett [1988]).

Fortunately, the helicity of $\mathbf{e}$ is usually rather small (Jackett and McDougall [1997]), and so is the ambiguity of the neutral surfaces. McDougall and Jackett [1988] has shown that the vertical distance from the start and the end point of the neutral trajectory is less than $10\,m$ for one circuit, if one considers a path around the whole subtropical gyre. Therefore an *approximately* neutral surface may be defined which deviates from the corresponding neutral trajectories by no more than a few meters in the vertical direction. An algorithm to determine an approximate neutral surface which is based on the computation of neutral trajectories has been suggested by McDougall [1987a] and You and McDougall [1990]. A first trajectory is computed from an initial location within the ocean, integrating both towards the north and the south. From the points on this "backbone" trajectory, further trajectories towards the west and east are computed. All points computed in this way form the neutral surface which obviously depends on the chosen trajectory pattern, an unavoidable consequence of the theoretical nonexistence of the neutral surfaces. The depth ambiguity is typically less than 10 meters; see McDougall [1987a] for a detailed discussion.

2.3 Neutral density

For a scalar field $\nu = \nu(x, y, z)$ [1] to denote a neutral density variable, it should be constant on a neutral surface, i.e. its gradient should be orthogonal to the neutral surface. Let $z = \mathcal{N}(x, y)$ denote the depth of a neutral surface. Then we must require that $\nu(x, y, \mathcal{N}(x, y)) = const$, or equivalently $\nabla_h \nu + \nu_z \nabla_h \mathcal{N} = 0$.

The horizontal gradient of the in-situ density is important for creating horizontal pressure gra-

[1] All of the following considerations would remain valid for time-dependent fields.

dients which can drive oceanic motions. From (1) $\nabla_h \rho$ is given by

$$\nabla_h \rho = \rho\beta\nabla_h S - \rho\alpha\nabla_h \Theta + \rho\gamma\nabla_h p \tag{6}$$

Now large-scale oceanic motions are very nearly hydrostatically balanced. Scaling analysis then shows that the relative magnitude of the last term in (6), compared with the first two terms, is of order $gH/c^2 < 0.02$ where H is a vertical scale of motion and $c \approx 1500\, ms^{-1}$ the speed of sound in the ocean. A detailed discussion of the magnitude of this term can be found in Dewar et al. [1998]. With accuracy of 2%, the horizontal components of $\mathbf{e}$ correspond therefore to the horizontal gradient of in-situ density.

The static stability of a water column is described by the stability frequency $N^2 = g(\alpha\Theta_z - \beta S_z)$. The vertical component of $\mathbf{e}$ is hence proportional to the stability frequency, $e_3 = -\rho N^2/g$.

It follows that a variable ν would satisfy the three properties of a neutral density if its gradient were everywhere identical with the vector $\mathbf{e}$. For such a variable to exist, the vector field $\mathbf{e}$ would however have to be irrotational. For the curl of $\mathbf{e}$ one obtains after some manipulations from (2)

$$\nabla \times \mathbf{e} = (\rho\beta)_p \nabla p \times \nabla S - (\rho\alpha)_p \nabla p \times \nabla\Theta \tag{7}$$

Hence the curl of $\mathbf{e}$ would vanish if either the pressure dependence of the coefficients $\rho\alpha$ and $\rho\beta$ could be ignored which is not generally the case, or if S and Θ were constant on surfaces of constant pressure, a rather uninteresting case. Note that the condition $\nabla \times \mathbf{e} = 0$ for the existence of a neutral density is stronger than the condition $\mathbf{e} \cdot \nabla \times \mathbf{e} = 0$ for the existence of neutral surfaces. The existence of a neutral density variable hence would imply the existence of a neutral surface but not vice versa.

To give some examples, let us consider several idealized forms of the equation of state. A neutral density always exists when $\rho = F(S, \Theta) + G(p)$. The neutral density is in this case $\nu = F$, up to an arbitrary constant, and would coincide with a potential density when that constant is chosen as $G(p_r)$. Neutral surfaces and isopycnals would be identical for this form of the equation of state.

Neutral surfaces would also exist when $\rho = F(S, \Theta)G(p)$. The helicity would vanish because the pressure dependency of the expansion coefficients $\rho\alpha = -F_\Theta G$ and $\rho\beta = F_S G$ would satisfy (5), and the neutral surfaces would be surfaces of constant F. These surfaces would be identical with isopycnals since the vector $\mathbf{e}$ would be parallel (though different in magnitude) to the gradient of a potential density $\nabla\rho_r = (F_\Theta \nabla\Theta + F_S \nabla S)G(p_r)$. A neutral density would however not exist because the curl of the vector $\mathbf{e} = F_\Theta G(p)\nabla\Theta + F_S G(p)\nabla S$ would however not normally vanish.

A third idealized form of the equation of state would be a dependency on pressure and temperature alone, $\rho = F(\Theta, p)$. In this case the curl of $\mathbf{e}$ would normally also not vanish but the helicity would do. And again $\mathbf{e}$ would be parallel to the gradient of a potential density, and the neutral surfaces would be identical with isopycnals (in this case isotherms).

The considerations in this section can be summarized as follows: Neither neutral surfaces nor a neutral density variable can strictly exist. Because the helicity of $\mathbf{e}$ is small, it is possible to construct approximate neutral surfaces to a good approximation. While the requirements for a neutral density variable are stronger than those for neutral surfaces, the rotational part of $\mathbf{e}$ is also small, compared to the irrotational one. Therefore, it is worth while to consider neutral density variables which approximate some or all of the postulated properties.

3 Approximate neutral densities

The three desirable properties for an approximately neutral density variable ν can be formulated as

$$\frac{\nabla_h \nu}{\nu_z} = -\nabla_h \mathcal{N} \tag{8}$$

$$\nabla_h \nu = \mathbf{e}_h \tag{9}$$

$$\nu_z = e_3 \tag{10}$$

It is obvious that the three conditions are not independent of each other because the (approximate) neutral surface must obey $\nabla_h \mathcal{N} \approx -\mathbf{e}_h / e_3$ to a very good accuracy. More precisely, if any two of the conditions (8)-(10) would hold exactly, then the third would be automatically also satisfied.

Jackett and McDougall [1997] have constructed a neutral density variable γ_n for the world ocean, using a slightly modified version of the climatology of Levitus [1982] with a resolution of $4° \times 4°$. They computed neutral surfaces starting from a reference profile in the middle of the Pacific Ocean. To label these surfaces they used the local density variable σ_l, as defined by Veronis [1972], i.e. simply the vertical integral of the vertical component of the vector $\mathbf{e}$. The integration constant is chosen so that the variable γ_n coincides with the in-situ density at the surface. It follows that γ_n is constant along neutral surfaces. In terms of the conditions (8)–(10), the variable γ_n exactly satisfies (8), except for the unavoidable ambiguity in the definition of neutral surfaces. Furthermore, relation (10) is satisfied by γ_n at one single position, but no explicit attempt is made to satisfy (9).

As discussed above, the variable γ_n is perfectly suitable for the analysis of hydrographic data, but not designed for the use in layered ocean models. In principle one could attempt to find a compromise between both aspects, but the usefulness of such an approach is not clear. Here we take the alternative approach and focus on the latter aspect, while ignoring the former. Hence we consider only the conditions (9) and (10) which are *linear* and therefore lead to a standard formulation for the following optimization.

3.1 A minimum condition for $\hat{\nu}\,(x, y, z)$

The conditions (9) and (10) can be combined into the 3-d form $\nabla\hat{\nu} = \mathbf{e}$. A straightforward optimization problem is obtained by the minimal condition

$$\frac{1}{2}\,\frac{1}{V}\int_V (\,\nabla\hat{\nu} - \mathbf{e}\,)^2\;\mathrm{d}V = \min \tag{11}$$

where the integration extends over the ocean volume V. The minimization problem (11) is readily solved by means of variational calculus (see for example Courant and Hilbert [1924]) and leads to a Poisson-equation

$$\nabla^2 \hat{\nu} = \nabla \cdot \mathbf{e} \ . \tag{12}$$

From (11) one also obtains the natural (Neumann) boundary condition

$$(\nabla \hat{\nu} - \mathbf{e}) \cdot \mathbf{n} = 0 \tag{13}$$

where the vector $\mathbf{n}$ is normal to the boundary. The problem (12), (13) has a *unique* solution $\hat{\nu} = \hat{\nu}\,(x, y, z)$, except for an arbitrary constant. Hence the gradient of $\hat{\nu}$ consists only of the divergent part of the vector field $\mathbf{e}$. One can expect that the minimum condition (11) would be well satisfied if the rotational part of $\mathbf{e}$ is sufficiently small.

While the above minimum principle is straightforward and has a simple solution, experience with optimization problems suggests that proper weighting of the different contributions to the integral in (11) is essential. In the present problem, this is so because i) the vertical gradients in the ocean are much larger than the horizontal gradients, and ii) the gradients in the upper ocean are much larger that those in the deep ocean. Using (11) without scaling would mean that effectively only the vertical component of $\mathbf{e}$ in the upper ocean would determine the resulting neutral density. Instead of (11) we therefore assume the modified minimal condition

$$\frac{1}{2}\,\frac{1}{V}\int_V \frac{(\nabla_h \hat{\nu} - \mathbf{e}_h)^2 + \delta^{-2}\,(\hat{\nu}_z - e_3)^2}{\Lambda(z)}\,\mathrm{d}V = \min \tag{14}$$

with the solution

$$\nabla_h^2 \hat{\nu} + \frac{\Lambda}{\delta^2}\left(\frac{\hat{\nu}_z}{\Lambda}\right)_z = \nabla_h \cdot \mathbf{e}_h + \frac{\Lambda}{\delta^2}\left(\frac{e_3}{\Lambda}\right)_z \ . \tag{15}$$

Two scaling parameters are introduced in (14), δ and $\Lambda(z)$. The parameter δ which for simplicity is taken to be a dimensionless constant determines the relative weight of the relations (9) resp. (10), with higher values of δ putting stronger emphasis on the relation (9). The parameter

$\Lambda(z)$ weights the vertical structure of the vector field $\mathbf{e}$, and is assumed to be proportional to a power of the mean (horizontally averaged) stability, $\Lambda(z) \sim |\overline{e_3}|^\mu$ (shown in figure 2 for $\mu = 1$). A higher value of μ increases the relative weight of the abyssal ocean. $\Lambda(z)$ is scaled such that its vertical mean is one and becomes dimensionless.

As is often the case in inverse problems, the choice of weighting parameters inevitably is to some extent at the disposal of the investigator. The ratio of the vertical to the horizontal component of $\mathbf{e}$ corresponds to the inverse slope of the neutral surface elements. We hence may expect that δ should resemble a typical value of this inverse slope. Experimentally, it was found that in the interval $2000 < \delta < 10000$ all results were qualitatively rather similar. It also was found that in the range $1 < \mu < 4$ results were not sensitive to the exact value of μ (but were very different for $\mu = 0$). For all following calculations we have used the values $\delta = 5000$ and $\mu = 2$.

In order to have a simple measure for the performance of the resulting density neutral variable, we define the relative errors of horizontal and vertical components according to

$$\epsilon_h(z) = \left(\frac{\overline{(\nabla_h \hat{\nu} - \mathbf{e}_h)^2}}{\overline{\mathbf{e}_h^2}} \right)^{\frac{1}{2}} \tag{16}$$

$$\epsilon_v(z) = \left(\frac{\overline{(\hat{\nu}_z - e_3)^2}}{\overline{e_3^2}} \right)^{\frac{1}{2}} \tag{17}$$

where the overbar denotes a horizontal average. These error estimates describe the relative accuracy to which conditions (9) resp. (10) are satisfied at a given level by the neutral density variable. Both functions (16) and (17) can also be combined into a single number ϵ_0 according to

$$\epsilon_0 = \left(\frac{1}{H} \int_{-H}^{0} \frac{\epsilon_h^2(z) + \epsilon_v^2(z)}{2} \, dz \right)^{\frac{1}{2}} \tag{18}$$

which can be interpreted as an average relative error for both relations (9) and (10). While other measures of error are possible, the definitions (16)–(18) are independent of the particular weighting chosen to minimize (14), and can be defined for any other density variable in an analogous way. Note that all these error estimates are horizontal averages, and that locally errors could be considerably higher.

The scaled Poisson equation (15) with the corresponding boundary conditions has been solved numerically for the North Atlantic Ocean from $0.5^\circ\,S$ to $58.5^\circ\,N$ and from $79.5^\circ\,W$ to $0.5^\circ\,E$, based on the climatology of Levitus [1982]. Only data between $200\,m$ and $5500\,m$ depth have been used, to exclude the surface layer where the neutral density concept is of little use.

Figure 3 shows the relative errors ϵ_h and ϵ_v vs. depth, for various density variables. The horizontal relative error (figure 3a) indicates how accurate the horizontal gradients are related to those of the in-situ density. As to be expected, the density σ_0 performs well at the surface but rather poorly at depth, with an average relative error of up to 80%. The thermal wind relation based on σ_0 is therefore seriously misrepresented in the deep ocean. The error increases not monotonous, however, and there is a pronounced maximum around $1500\,m$ depth. This maximum can be understood by looking at the dominant temperature contribution to the vector $\mathbf{e}_h$. The rms-deviation of the thermal expansion coefficient from its surface value increases almost linearly with depth. On the other hand, the magnitude of the horizontal temperature gradients is largest in the upper kilometer, and strongly decreases with depth. The product of both curves (not shown) very nearly accounts for the shape of the error of σ_0 in figure 3. The presence of Mediterranean Water in the North Atlantic which in this depth range leads both to stronger horizontal temperature gradients and to higher deviations of the thermal expansion α from its surface values also contributes to this maximum, though with lesser magnitude. The overall relative error as given in table 1 is 62%.

The density σ_2 performs perfect at $2000\,m$ but deviates up to 40% not only at large depths but also near the surface. The overall relative error (30%) is smaller than that of σ_0. However, as all gradients are strongest in the upper kilometer, for the overall performance of an isopycnal model near-surface errors may be more critical than errors in the deep ocean.

The relative error of the solution $\hat{\nu}\,(x, y, z)$ of the optimization (15) is much smaller than that of any other field, with an average of 3%. This is to be expected since the relative error resembles the objective function in (14) to a considerable degree. The error exceeds 5% only at great depths and at the level of Mediterranean Water where it stays below 10%.

The relative errors of the vertical components indicate how accurate the vertical gradients are related to the stability frequency, and are shown in figure 3b. For all variables, the errors are similar to those of the horizontal components, both in structure and in magnitude. A difference to figure 3a is that the error of the potential densities has no maximum near $1500\,m$, and decreases more or less smoothly towards the respective reference levels. This behaviour can again be understood from the combination of the pressure-dependence of the thermal expansion coefficient and the vertical stability. The close resemblance between vertical and horizontal errors is not accidental, it indicates that the slopes of the various density surfaces are not very different.

3.2 Comparison with the neutral density γ_N

As discussed above, the neutral density variable γ_n as defined by Jackett and McDougall [1997] satisfies (8) exactly whereas $\hat{\nu}$ is constructed to minimize the deviations from (9) and (10). It is nevertheless instructive to consider the performance of both fields for those aspects for which they were *not* designed. As seen from figure 3 and table 1, the variable γ_n performs better than both potential densities but not nearly as well as the variable $\hat{\nu}\,(x, y, z)$, with an average relative error of 25%. The error is strongly depth-dependent, it is very small at the surface and increases with depth where it reaches a maximum of 35%.

It must however be noted that the comparison of γ_n and $\hat{\nu}$ may be misleading, because γ_n is defined for the whole world ocean while the neutral density $\hat{\nu}$ is defined for the North Atlantic. The reference cast for γ_n which determines the labeling of the neutral surfaces, is located in the Pacific Ocean. Only to the extent that this cast is representative for the whole region, one could expect that relations (9), and consequently also (10), were reasonably satisfied. Most likely, the relative error ϵ_0 would decrease if a reference cast somewhere in the North Atlantic were chosen to define γ_n.

Likewise, it is interesting to compare how well the surfaces of constant $\hat{\nu}$ coincide with neutral surfaces, i.e. how well the condition (8) which has *not* been included in the minimization is satisfied. Figure 4a shows such the neutral surface $\gamma_n = 27.9\,kg\,m^{-3}$ in the North Atlantic, based on the climatology of Levitus [1982]. Its depth is nearly constant at $1500\,m$ south of $35°\,N$, and decreases sharply to less than $700\,m$ north of $50°\,N$.

The isosurface of $\hat{\nu}$ and the neutral surface, shown in figure 4b, coincide at $40°\,W$ and $30°\,N$, marked in the figure with a cross, and their difference in height is over wide areas below $10\,m$, somewhat increasing towards the equator to $25\,m$. In areas of large slopes, the height differences increase to over $100\,m$ north of $55°\,N$ and west of $35°\,W$, an order of magnitude larger than the ambiguity in the definition of neutral surfaces. Different choices for the parameters δ and μ do not improve this result. Hence the neutral density computed via (15) significantly violates the property (8). The error is however much smaller than that of isopycnals. E.g., the height differences of the corresponding σ_0-surface, shown in figure 4d, are in wide areas above $100\,m$, reaching $200\,m$ near the equator, $400\,m$ near the outflow of the mediterranean sea and $700\,m$ in the North Atlantic Current.

3.3 A minimum condition for $\tilde{\nu}\,(S,\Theta)$

In the previous section, we have given a definition for a neutral density as a function of space, $\hat{\nu}\,(x,y,z)$. For the use as a variable in models which could replace the potential density, it is however necessary that the neutral density should be available as a function of temperature and salinity,

$$\tilde{\nu} = \tilde{\nu}\,(S,\Theta) \tag{19}$$

In order to define $\tilde{\nu}\,(S,\Theta)$, we use again the minimum condition (14) but now restrict the solution to be a function of S and Θ. Using (19) to expand the spatial derivatives of $\tilde{\nu}$, it follows that

$$J \;=\; \frac{1}{2}\,\frac{1}{V}\int_V \frac{\left(\,b\nabla_h S - a\nabla_h\Theta - \mathbf{e}_h\right)^2 + \delta^{-2}\left(\,bS_z - a\Theta_z - e_3\right)^2}{\Lambda(z)}\;\mathrm{d}V = \min \tag{20}$$

where the definitions $b = \partial\tilde{\nu}/\partial S$ and $a = -\partial\tilde{\nu}/\partial\Theta$ have been made. We further restrict $\tilde{\nu}\,(S,\Theta)$ to be a polynomial of order six in Θ and S, resulting in 27 unknown coefficients c_j that have to be determined, in addition to an arbitary constant which has been chosen so that $\tilde{\nu}\,(35\,psu, 5^\circ\,C) = 27.0\,kg/m^3$. Note that the derivatives a and b depend on the same coefficients c_j in a linear way.

Evaluating ∇S, $\nabla\Theta$ and the components of the vector $\mathbf{e}$ at every point of the climatological data set, (20) takes on the discrete form

$$(\mathbf{Ac} - \mathbf{y})^T\mathbf{W}(\mathbf{Ac} - \mathbf{y}) = \min \tag{21}$$

where $\mathbf{c}$ is a column vector containing the c_j, and the matrix $\mathbf{A}$ has 27 columns and approximately 165000 rows (three times the number of grid points in the North Atlantic climatology). The row vector $\mathbf{y}$ consists of the observations $\mathbf{e}$ at all grid points. The diagonal matrix $\mathbf{W}$ contains information on the parameters δ and $\Lambda(z)$, and on the grid spacing.

The discrete minimum principle (21) has the standard form of an overconstrained linear inverse problem, and is readily solved for the coefficients $\mathbf{c}$. The resulting function $\tilde{\nu}\,(S,\Theta)$ approximates the conditions (9) and (10) rather well, with an average relative error ϵ_0 of 5%, as compared to 3% for $\hat{\nu}\,(x,y,z)$. An inspection of the function $\tilde{\nu}\,(S,\Theta)$ (not shown) displays however a rather unsatisfactory performance in those regions of the Θ-S-diagram outside the range of the climatological data. Such a behavior is not unexpected as in those regions $\tilde{\nu}\,(S,\Theta)$ is effectively unconstrained, and the polynomial approximation leads to strong undulations here. While that could be acceptable as long as $\tilde{\nu}$ is used only within the presently observed range of Θ and S, such behavior would make it impossible to use a model based on $\tilde{\nu}$ in even the most gentle climate change scenario. Efforts to eliminate this behavior with polynomials of lower orders were unsuccessful.

To further constrain $\tilde{\nu}\,(S,\Theta)$, it is necessary to involve a-priori information which cannot be based solely on the observed Θ-S distribution in the ocean. One possibility is to rely on the properties of the equation of state. The partial derivatives of a neutral density $\nu(S,\Theta)$ with respect to S and Θ should be close to the expansion coefficients $\rho\beta(S,\Theta,p)$ resp. $\rho\alpha(S,\Theta,p)$, as far as that is possible. Now in most parts of the ocean the thermal stratification is dominant, and hence the potential temperature changes monotonically with depth resp. pressure. This allows the possibility to find an approximate average relation between pressure and temperature. Specifically, we have chosen a smoothed fit to the inverse of the horizontally averaged potential temperature

$$\overline{p}(\Theta) = \overline{\Theta}^{-1}(p) \tag{22}$$

which is shown in figure 5. The minimum condition (20) is then modified to

$$J + \frac{1}{2}\,\frac{1}{\Delta\Theta\Delta S}\int \Big(\kappa_S\,[\,b - \rho\,\beta\,(S,\Theta,\overline{p}(\Theta)\,)]^2 + \kappa_\Theta\,[\,a - \rho\,\alpha\,(S,\Theta,\overline{p}(\Theta)\,)]^2\;\Big)\,\mathrm{d}S\mathrm{d}\Theta = \min \tag{23}$$

with J as in (20). In the discrete form, the first sum J is taken again over the climatological dataset of the North Atlantic, and the integral in (23) is evaluated over 775 combinations of S and Θ which form an equidistant grid in the Θ-S-space from $-5^\circ\,C$ to $25^\circ\,C$ with $1^\circ\,K$ spacing ($\Delta\Theta = 30\,K$) and from $32\,psu$ to $38\,psu$ in $0.25\,psu$ spacing ($\Delta S = 6\,psu$).

The relative influence of the a priori information was chosen empirically through the constants κ_S and κ_Θ ($\kappa_S = 0.04\,psu^2\,m^{-2}$ and $\kappa_\Theta = 0.4\,K^2\,m^{-2}$), so that the unrealistic behavior in the outer Θ-S-space was minimized while keeping a reasonable accuracy to approximate the climatological distributions. The polynomial coefficients can be found in the appendix or via internet.

Figure 6 shows isolines of $\tilde{\nu}$ in a Θ-S-diagram together with isopycnals of σ_0 and σ_4 and the Θ-S-combinations of the dataset. Not surprisingly, the isolines of $\tilde{\nu}$ are roughly parallel to the isopycnals of σ_θ at high temperatures, and of σ_4 at low temperatures. Note that the curvature of the isolines of $\tilde{\nu}$ changes sign below $\Theta = 2^\circ C$, an inevitable feature of any neutral density variable due to the fact that the slope of isopycnals in Θ-S-space decreases with higher reference pressure but increases with lower temperature.

The accuracy of the neutral density $\tilde{\nu}$ with respect to conditions (9) and (10) can be seen from figure 3. The relative error for both components, while obviously larger than that of $\hat{\nu}(x, y, z)$, is much lower than that of all other density variables. The overall average relative error ϵ_0 is 6%, maximum values around 10% occur near $1500\,m$ and in the deep ocean. It follows that $\tilde{\nu}(S, \Theta)$, which by definition is a conserved quantity to the same degree than S and Θ, is much better suited than any potential density as a variable in a layered model. As an aside, a solution to (23) *without* the climatological data, based only on the equation of state and relation (22) would have an average error of 14%, still lower than that of any potential density.

The performance of $\tilde{\nu}(S, \Theta)$ with respect to condition (8) which has *not* been explicitly used can be seen from figure 4c. The height difference to the correct neutral surface is over wide regions below $10\,m$, but increases north of $40^\circ N$ up to $150\,m$ north of $55^\circ N$ and west of $45^\circ W$. Overall, the differences, while significantly larger than the theoretical ambiguity, are even slightly lower than those than of $\hat{\nu}$ in figure 4b, and are much lower than those for the isopycnals of σ_0 and σ_2.

4 Concluding remarks

The main purpose of this study has been to illustrate the different possible applications for the concept of a neutral density, and accordingly the different choices that can be made for such a variable. We have identified three desirable properties for a neutral density ν. All three properties which are not independent of each other are satisfied by a potential density at its reference level but not elsewhere. The first property (constancy along neutral surfaces) is optimal for analysing and diagnosing hydrographic observations, while the other two properties (prescribed horizontal and vertical gradients) are optimal in the context of isopycnal layer models.

It has long been known that potential densities are not fully suitable for the first purpose, and that the height differences between potential density surfaces and neutral surfaces can become unacceptably large. Likewise, potential densities are also not fully suitable as a variable in layer models, as was already discussed e.g. by You and McDougall [1990]. As seen from figure 3, the average relative error for the two gradient criteria is on average 30–60%, depending on the reference pressure, and in case of σ_0 reaches up to 80% at great depths. It is our view that an error of this magnitude may significantly restrict the applicability and accuracy of isopycnal models. In order to improve this situation, Rooth et al. [1998] have recently constructed a virtual potential density, which is however definded only on properties of the equation of state and not on any observed $\Theta - S$ distribution in the ocean.

The variable γ_n introduced by Jackett and McDougall [1997] satisfies the first property exactly, and hence is optimally suited for its purpose. The average error for the variable γ_n is around 25%. This number may however at least partly reflect the fact that γ_n is defined globally whereas the comparison was made only for the North Atlantic, and would likely be reduced for an appropriate basin-based definition of γ_n. Nevertheless, γ_n is neither designed nor immediately useful as a variable in isopycnal layer models, not only because it satisfies the two gradient criteria less well (still better than any potential density) but also because due to its spatial dependency γ_n is not a conserved variable.

In this study we have explored variables that satisfy the two gradient criteria as closely as possible, based on the climatological distributions of potential temperature and salinity in the North Atlantic. The variable $\tilde{\nu}(S, \Theta)$ is by construction a conserved variable to the same degree that potential densities are. As shown in figure 3, it satisfies the two gradient criteria with an average relative error of 6%, and at all levels the error rarely exceeds 10%. Only the neutral density $\hat{\nu}(x, y, z)$ which is however irrelevant for use in a model performs better, with an average relative error of 3%. For this reason we believe that $\tilde{\nu}\,(S,\Theta)$, while not unique and far from being perfect, is better suited than any potential density as a variable in a layer model for simulations over the full oceanic depth range. At the same time, the isosurfaces of $\tilde{\nu}\,(S,\Theta)$ approximate the neutral surfaces as defined from γ_n better than isopycnals do, although they are normally not accurate enough for use with hydrographic observations.

Two further remarks are in order. We have looked at one ocean basin only, which is appropriate if one considers use for a model of the North Atlantic. Technically it will not be very difficult to repeat the calculation globally. Due to the larger variance of water masses in different ocean basins, one must expect however that the relative error of a global neutral density variable with respect to the gradient criteria is higher. Whether or not such a variable would still be useful on a global basis remains to be seen, though in any case its performance should remain superior to that of a potential density.

A second remark is that in the construction of $\tilde{\nu}$ we have used the horizontally averaged temperature distribution taken from the present climatology. It is obvious that in case of a substantial climate shift, e.g. warming of the deep ocean, the procedure becomes questionable. For that reason a model based on $\tilde{\nu}$ or a similar variable may be less suitable for simulations of long-term climate change.

Acknowledgment:

We thank Trevor McDougall and an anonymous reviewer for helpful comments.

APPENDIX

Polynomial coefficients for $\tilde{\nu}\,(\Theta, S)$

$$
\begin{aligned}
\tilde{\nu}\,(\Theta, S) = \quad & a_1 + a_2\,S + a_3\,\Theta \\
& + a_4\,S^2 + a_5\,\Theta S + a_6\,\Theta^2 \\
& + a_7\,S^3 + a_8\,S^2\,\Theta + a_9\,S\,\Theta^2 + a_{10}\,\Theta^3 \\
& + a_{11}\,S^4 + a_{12}\,S^3\,\Theta + a_{13}\,S^2\,\Theta^2 + a_{14}\,S\,\Theta^3 + a_{15}\,\Theta^4 \\
& + a_{16}\,S^5 + a_{17}\,S^4\,\Theta + a_{18}\,S^3\,\Theta^2 + a_{19}\,S^2\,\Theta^3 + a_{20}\,S\,\Theta^4 + a_{21}\,\Theta^5 \\
& + a_{22}\,S^6 + a_{23}\,S^5\,\Theta + a_{24}\,S^4\,\Theta^2 + a_{25}\,S^3\,\Theta^3 + a_{26}\,S^2\,\Theta^4 + a_{27}\,S\,\Theta^5 + a_{28}\,\Theta^6
\end{aligned}
$$

$$
\begin{array}{rrlrrl}
a_1 = & 14716.4083300335 & , & a_2 = & -28.9331001608859 & , \\
a_3 = & -3470.91951031568 & , & a_4 = & -157.954300909566 & , \\
a_5 = & 473.289175127584 & , & a_6 = & -4.64974069615661 & , \\
a_7 = & 11.3969084253582 & , & a_8 = & -25.4768804193708 & , \\
a_9 = & -0.389834308335937 & , & a_{10} = & 0.835094681378189 & , \\
a_{11} = & -0.343532351230610 & , & a_{12} = & 0.675628658364396 & , \\
a_{13} = & 5.414334185691196 & \cdot 10^{-2}, & a_{14} = & -6.816453081396268 & \cdot 10^{-2}, \\
a_{15} = & -1.728955910178931 & \cdot 10^{-3}, & a_{16} = & 4.873910348419327 & \cdot 10^{-3}, \\
a_{17} = & -8.806940306192767 & \cdot 10^{-3}, & a_{18} = & -1.695268507497124 & \cdot 10^{-3}, \\
a_{19} = & 1.804453633002675 & \cdot 10^{-3}, & a_{20} = & 1.805489877717028 & \cdot 10^{-4}, \\
a_{21} = & -4.894077892307525 & \cdot 10^{-5}, & a_{22} = & -2.681726391903187 & \cdot 10^{-5}, \\
a_{23} = & 4.499131748650225 & \cdot 10^{-5}, & a_{24} = & 1.645151764773905 & \cdot 10^{-5}, \\
a_{25} = & -1.547343330658305 & \cdot 10^{-5}, & a_{26} = & -3.625108540563305 & \cdot 10^{-6}, \\
a_{27} = & 1.341416007328966 & \cdot 10^{-6}, & a_{28} = & -8.036621802403113 & \cdot 10^{-9},
\end{array}
$$

This polynomial can also be obtained via internet at

http://www.ifm.uni-kiel.de/to/data/pers/ceden.html.

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Table captions

Table 1: Table with the integral relative error ϵ_0 defined by (18) for some density variables.

Figure captions

Figure 1: A sketch of three isolines of in-situ density (solid), an isopycnal (bold) of a potential density with reference pressure p_r, the corresponding gradients at three different locations and a neutral trajectory (dotted). The gradient of the potential density differs at p_r from the in-situ density only by a vertical vector, while at the other depths the difference also has a horizontal component. At p_r the neutral trajectory has the same slope as the isopycnal, while at the other depths the slopes differ.

Figure 2: The horizontally in the North Atlantic averaged (negative) vertical component of $\mathbf{e}$. This is the same as $|\overline{e_3}|^\mu$ with $\mu = 1$.

Figure 3: a) The relative error ϵ_h, defined by (16), in the horizontal components for some density variables. The circles denotes the error for σ_Θ, crosses σ_2, dashed line γ_n, dotted line $\tilde{\nu}\,(\Theta, S)$ and the solid line ϵ_h for $\hat{\nu}\,(x, y, z)$. b) The same for the relative error ϵ_v in the vertical components, defined by (17).

Figure 4: a) Depth of a neutral surface $\gamma_n = 27.9\,kg/m^3$. Contour interval is $100\,m$. b) Difference in depth between the neutral surface from a) and an isosurface of the neutral density $\hat{\nu}\,(x, y, z)$. The surfaces coincide at the at $40^\circ\,W$ and $30^\circ\,N$ in $1500\,m$ depth, marked with a cross. Contour intervals are $5, 10, 25, 50, 100, 150, 200, 250\,m$. Regions where the isosurface of $\hat{\nu}$ is deeper than the neutral surface are contoured with solid lines and vice versa for dashed contours. c) Difference in depth between the neutral surface from a) and an isosurface of the neutral density $\tilde{\nu}\,(\Theta, S)$. The point where the surfaces coincide is also marked with a cross. d) Difference in depth between the neutral surface from a) and an isopycnal $\sigma_\Theta = 27.791\,kg\,m^{-3}$.

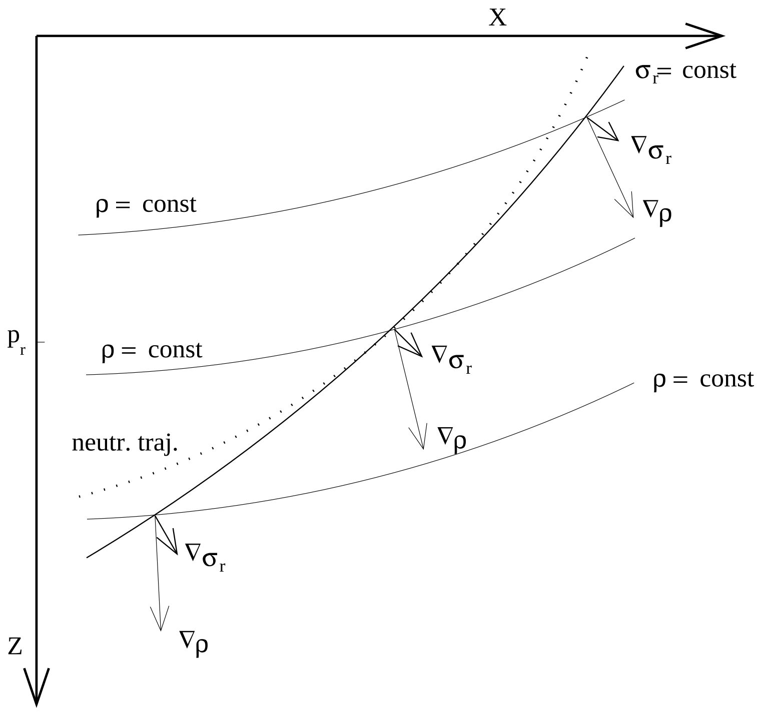
Figure 5: The function $\overline{p}(\Theta)$ (solid) is a fit to the horizontally averaged potential temperatures taken from the data set (circles). It serves as an approximational relationship between pressure and potential temperature to obtain a priori informations from the equation of state.

Figure 6: Θ-S-diagram of the dataset used for the approximation of $\tilde{\nu}\,(\Theta, S)$, isolines of $\tilde{\nu}$ (solid)

and isopycnals of σ_0 (dotted) and σ_4 (dashed) each in $0.2\,kg/m^3$ contour intervalls.

Density variable	ϵ_0
σ_0	0.62
σ_2	0.30
σ_4	0.53
γ_N	0.25
$\nu(x, y, z)$	0.03
$\nu(\Theta, S)$	0.06

Table 1:



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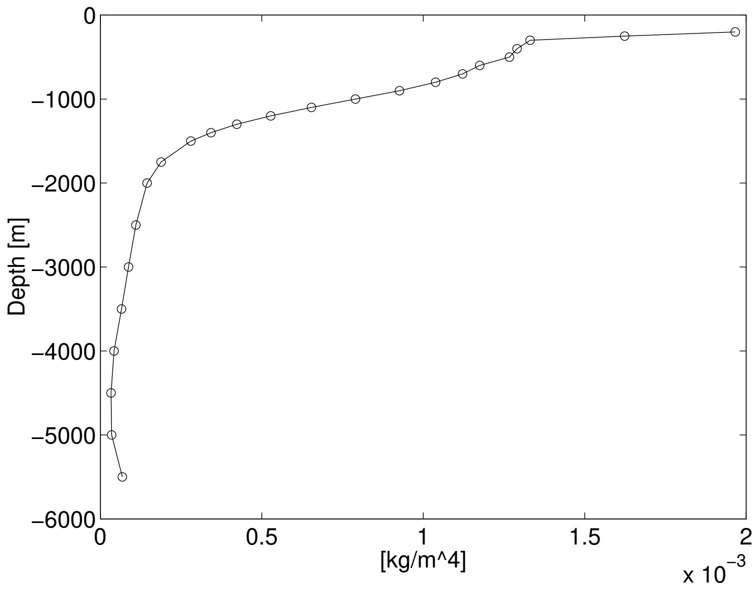
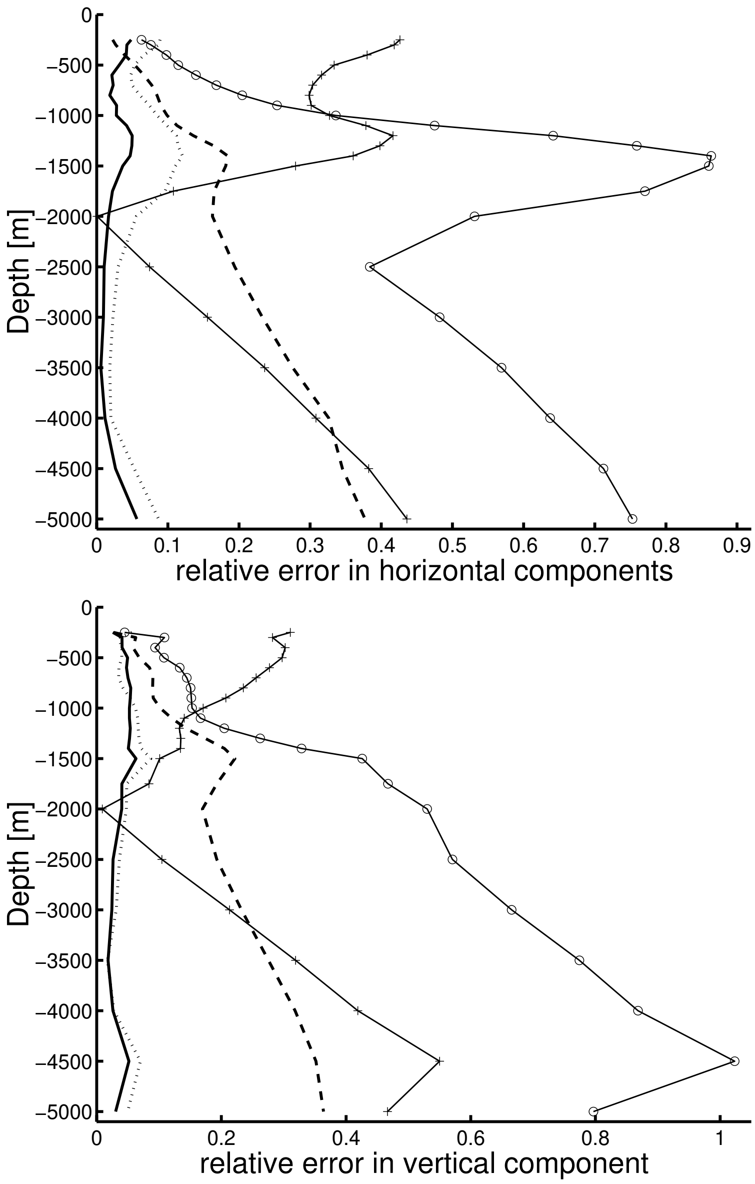


Figure 2: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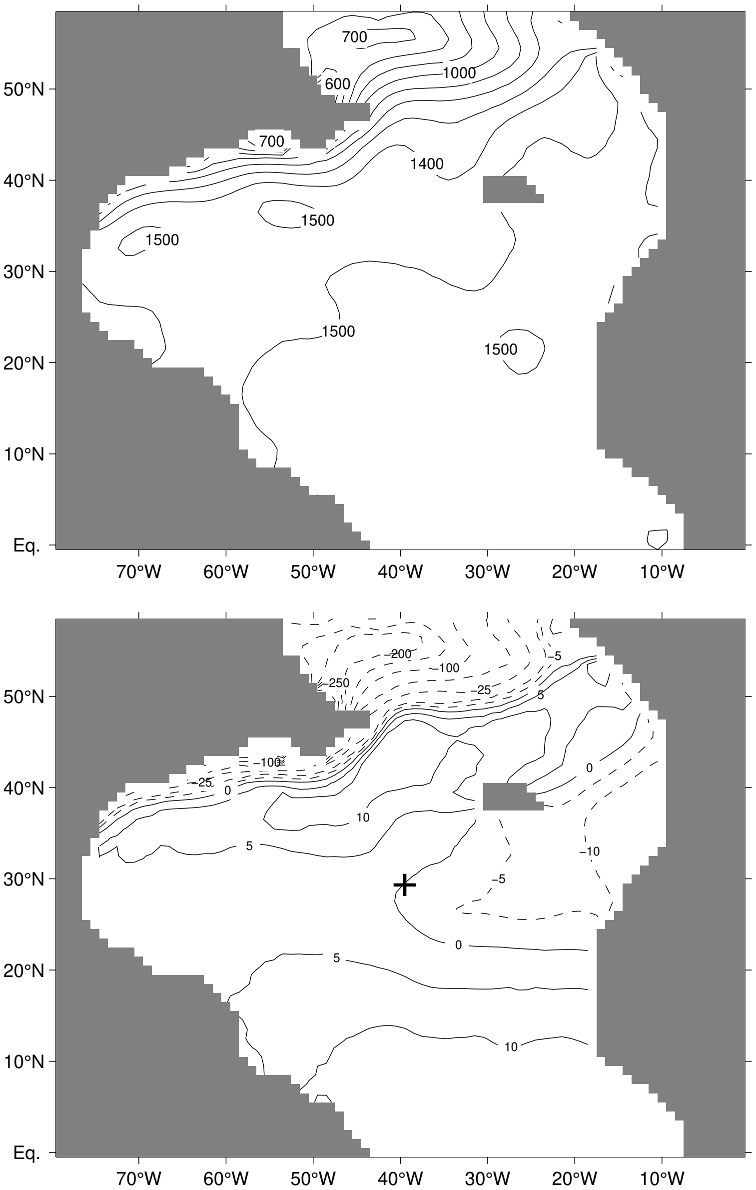
relative error in horizontal components
Depth [m]
relative error in vertical component

Figure 3: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50°W
40°W
30°W
20°W
10°W
-200
-100
-250
25
-5
5
-100
-25
0
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10
5
-10
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10°W

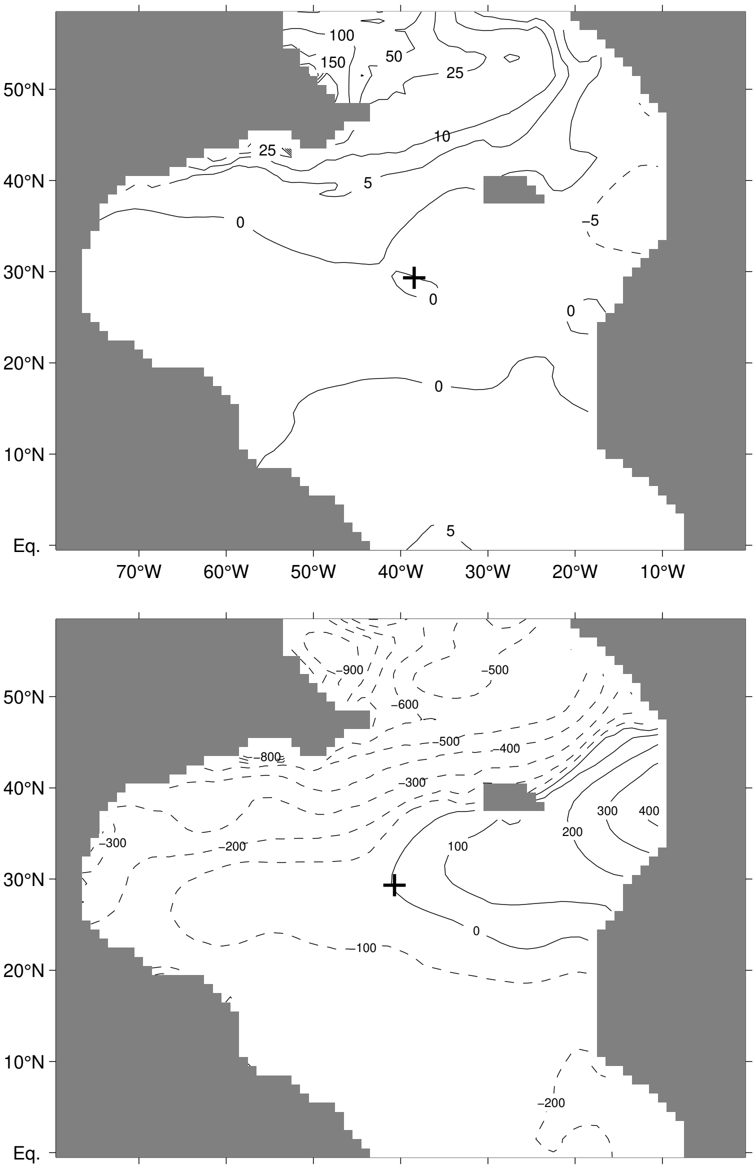
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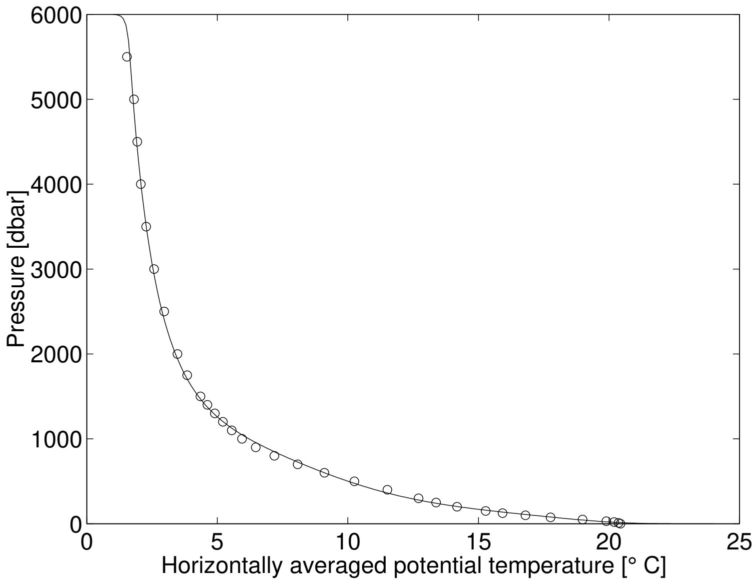
Figure 4:



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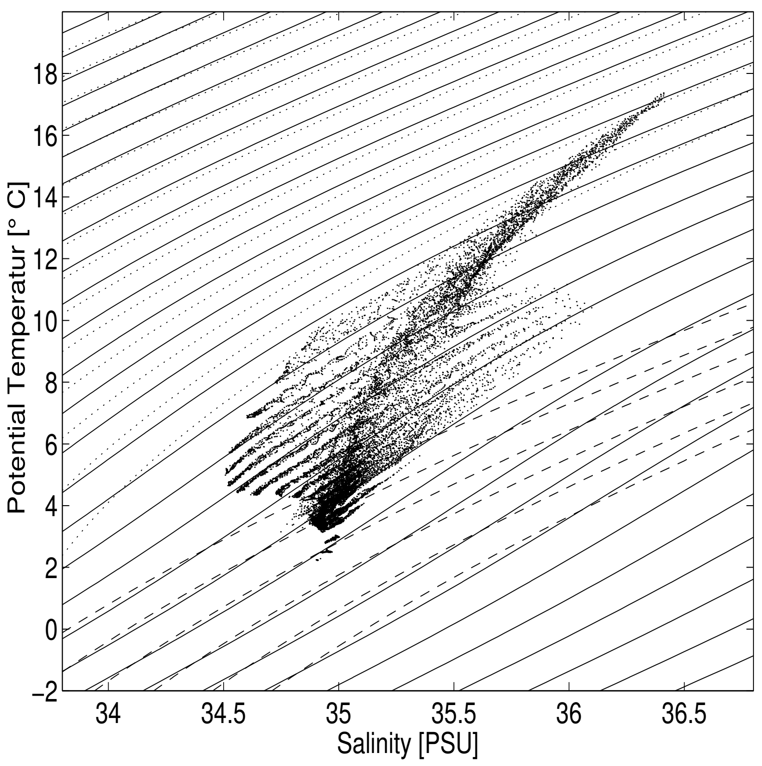

Figure 6: