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A GENERALIZED VERTICAL COORDINATE FOR 3D MARINE MODELS

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ABSTRACT

Vertical coordinate transformation is used in ocean modelling to provide good representation of the flow near bottom and free surface boundaries and to allow the concentration of grid points in regions of high gradient. A natural treatment of impermeability boundary conditions is achieved by considering transformations which fit the surface and bottom boundaries. This paper develops the governing equations of shallow sea hydrodynamics for a generalised vertical coordinate transformation, which embraces all formulations commonly used in ocean modelling, and allows greater freedom to concentrate grid points in regions of high gradient. In addition to the popular σ coordinates, various hybrid "σ-z" coordinate transformations, defined for ad hoc applications, are reviewed. Conservative formulations are proposed for the governing equations, including the pressure gradient and horizontal diffusion terms.

Key words
Vertical coordinate, sigma transformation, 3D modelling
Mots-clés
Coordonnée verticale, Transformation sigma, Modélisation 3D

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INTRODUCTION

Modelling of marine hydrodynamics requires careful treatment of vertical processes such as turbulent mixing of heat and salinity under the influence of tide and wind forcing . The existence and extent of stratified regions is crucial in determining vertical density gradients and the consequent horizontal pressure gradients. Moreover, the presence of a pycnocline strongly influences the dispersion of passive contaminants by limiting vertical diffusion.

For 3D finite difference type models the ability to accurately represent these vertical processes is severely restricted by the constraints of computer memory and time. It is important to optimise the nature and distribution of the vertical grid points so as to minimise errors incurred in the numerical discretisation. The vertical coordinate should, thus:

- provide a good representation of the flow near the bottom and the free surface to allow an accurate evaluation of the boundary fluxes.
- allow the concentration of points in regions of high vertical gradients, such as pycnoclines, where truncation error is greatest.
- avoid distortion of the horizontal pressure force and contamination of the physical vertical diffusion with "artificial" horizontal diffusion.

In this paper the commonly used "z" and "sigma" coordinate systems will be presented within the context of a potentially more powerful "generalised" vertical coordinate.

SHALLOW SEA HYDRODYNAMICS

Governing equations for shallow sea hydrodynamics

The governing equations for shallow sea hydrodynamics are obtained by considering conservation of mass, momentum, energy and salinity. The principal assumptions are : the Boussinesq approximation, the boundary layer approximation (including, in particular, hydrostatic equilibrium) arising from the small aspect ratio of vertical to horizontal length scales, and the representation of unresolved turbulent fluctuations by a turbulent diffusivity, $\lambda_{t(\phi)}$.

The evolution of horizontal velocity, u, the vertical velocity component, w, temperature, T, salinity, S, reduced pressure, q, and buoyancy, b,[†] are given for a Cartesian coordinate system (x_1,x_2,x_3) with horizontal unit vectors $\mathbf{e}_1, \mathbf{e}_2$ and vertical unit vector $\mathbf{e}_3$, (e.g. NIHOUL (1984)):

$$\nabla_h.\mathbf{u} + \frac{\partial w}{\partial x_3} = 0 \quad (3)$$

$$\frac{\partial q}{\partial x_3} = b \quad (4)$$

$$[\mathcal{I} + \mathcal{A}^h + \mathcal{A}^v - \mathcal{D}^h - \mathcal{D}^v](\mathbf{u}) = \mathcal{C}(\mathbf{u}) + \mathcal{Q} \quad (5)$$

$$[\mathcal{I} + \mathcal{A}^h + \mathcal{A}^v - \mathcal{D}^h - \mathcal{D}^v](T) = 0 \quad (6)$$

$$[\mathcal{I} + \mathcal{A}^h + \mathcal{A}^v - \mathcal{D}^h - \mathcal{D}^v](S) = 0 \quad (7)$$

where the horizontal gradient operator is given by,

$$\nabla_h = \mathbf{e}_1\frac{\partial}{\partial x_1} + \mathbf{e}_2\frac{\partial}{\partial x_2} \quad (8)$$

inertia, or time variation, horizontal and vertical advection,

$$[\mathcal{I} + \mathcal{A}^h + \mathcal{A}^v](\phi) = \frac{\partial \phi}{\partial t} + \nabla_h.(\mathbf{u}\phi) + \frac{\partial (w\phi)}{\partial x_3} \quad (9)$$

vertical diffusion,

$$\mathcal{D}^v(\phi) = \frac{\partial}{\partial x_3}(\lambda_{t(\phi)}\frac{\partial \phi}{\partial x_3}) \quad (10)$$

Coriolis,

$$\mathcal{C}(\mathbf{u}) = -f\mathbf{e}_3 \otimes \mathbf{u} \quad (11)$$

pressure gradient,

$$\mathcal{Q} = -\nabla_h q \quad (12)$$

Horizontal diffusion, $\mathcal{D}^h(\phi)$ will be defined later in the transformed coordinate system.

The system of equations (3-7) is closed by a turbulence model to give the turbulent diffusivities, $\lambda_{t(\varphi)}$ and an equation of state giving density as a function of temperature and salinity. The Coriolis frequency, f, is a function of latitude or, for sufficiently small domains, can be considered as constant.

[†]As pointed out by GARY (1973) truncation error is significantly reduced by considering as unknowns the reduced pressure - the pressure relative to a reference atmospheric pressure, $P_{atm,0}$, and reduced by removal of a constant hydrostatic gradient

$$q = \frac{P - P_{atm,0}}{\rho_0} + gx_3 \quad (1)$$

- and the buoyancy relative to a reference density, ρ_0,

$$b = -(\frac{\rho - \rho_0}{\rho_0})g \quad (2)$$

rather than the primitive variables of pressure, P, and density, ρ.

Kinematic boundary conditions

The kinematic boundary conditions representing impermeability of the free surface, $x_3 = +\eta(x_1, x_2, t)$, and the sea bottom, $x_3 = -h(x_1, x_2)$, are given by :

$$[\mathrm{u}.\nabla_h h + w]_{x_3=-h} = 0 \tag{13}$$

and

$$[\frac{\partial \eta}{\partial t} + \mathrm{u}.\nabla_h \eta - w]_{x_3=\eta} = 0 \tag{14}$$

Representation of bottom topography

Conceptually, the simplest mesh, as used for example by BACKHAUS ET AL (1987) consists of plane, orthogonal coordinate surfaces — a "Cartesian mesh" with "z" vertical coordinate as shown in Figure 1 (A). However, this approach may lead to an inefficient use of computational resources for domains with complex bathymetry. Since the array dimensions used in a computer program are fixed, it is necessary either to allocate memory for unused values corresponding to points situated below the sea bottom or to employ an indirect addressing method, which inhibits efficient execution on supercomputers. More importantly, the representation of the sea bottom and associated boundary conditions is poor. In fact, the bottom is discretised as a "staircase" of alternating horizontal and vertical surfaces, which is far from realistic except where the grid spacing is very small.

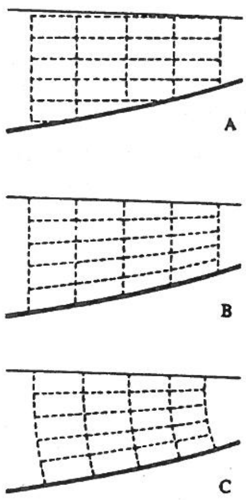

Figure 1: Cartesian (A), non-orthogonal (B), and orthogonal (C) coordinate systems (reproduced from DELEERSNIJDER AND WOLANSKI (1990) after MELLOR AND BLUMBERG (1985))

To overcome these disadvantages, the coordinate system and, hence, mesh, should be chosen to fit the variations of bathymetry. Since the aspect ratio is small, inspiration can be found in the techniques generally used for modelling boundary layers in fluid dynamics. Thus, an orthogonal curvilinear mesh may be defined where the bottom and the surface of the sea are coordinate surfaces as shown in Figure 1. As suggested by MELLOR AND BLUMBERG (1985) this can be approximated by a mesh where two families of coordinate surfaces are vertical to simplify drastically the mathematical, numerical and computational representation. In fact, since the bottom slope usually does not exceed 10^{-2} the meshes B and C are, in reality, very similar.

GENERALIZED VERTICAL COORDINATE

Coordinate transformation

The general form of a boundary fitting vertical coordinate transformation is

$$(\bar{t}, \bar{x}_1, \bar{x}_2, \bar{x}_3) = (t, x_1, x_2, \bar{x}_3(t, x_1, x_2, x_3)) \quad (15)$$

where the new variables appear on the left hand side. With such a transformation, only the vertical coordinate is changed; the horizontal coordinates, x_1, and x_2, remain unchanged, as does the time, t. In other words, in the new space, "a vertical corresponds to a vertical in the physical space". As depicted in Figure 2 the equation of the bottom transforms to $\bar{x}_3 = 0$ while the free surface, which is moving, becomes $\bar{x}_3 = L$ where L is an arbitrary constant length representing the water height in the transformed domain.

The first instance of a variable transformation of this type is normally attributed to PHILIPS (1957) , in the domain of atmospheric simulations, while its application in oceanography goes back to FREEMAN ET AL (1972) .

KASAHARA (1974) shows that the derivative operators transform according to

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial \bar{t}} + \frac{\partial \bar{x}_3}{\partial t}\frac{\partial}{\partial \bar{x}_3} \quad (16)$$

$$\nabla_h = \bar{\nabla}_h + (\nabla_h \bar{x}_3)\frac{\partial}{\partial \bar{x}_3} \quad (17)$$

$$\frac{\partial}{\partial x_3} = \frac{\partial \bar{x}_3}{\partial x_3}\frac{\partial}{\partial \bar{x}_3} \quad (18)$$

and

$$\bar{\nabla}_h = \bar{\mathbf{e}}_1\frac{\partial}{\partial \bar{x}_1} + \bar{\mathbf{e}}_2\frac{\partial}{\partial \bar{x}_2} \quad (19)$$

where $(\bar{\mathbf{e}}_1, \bar{\mathbf{e}}_2) = (\mathbf{e}_1, \mathbf{e}_2)$ are the horizontal unit vectors.

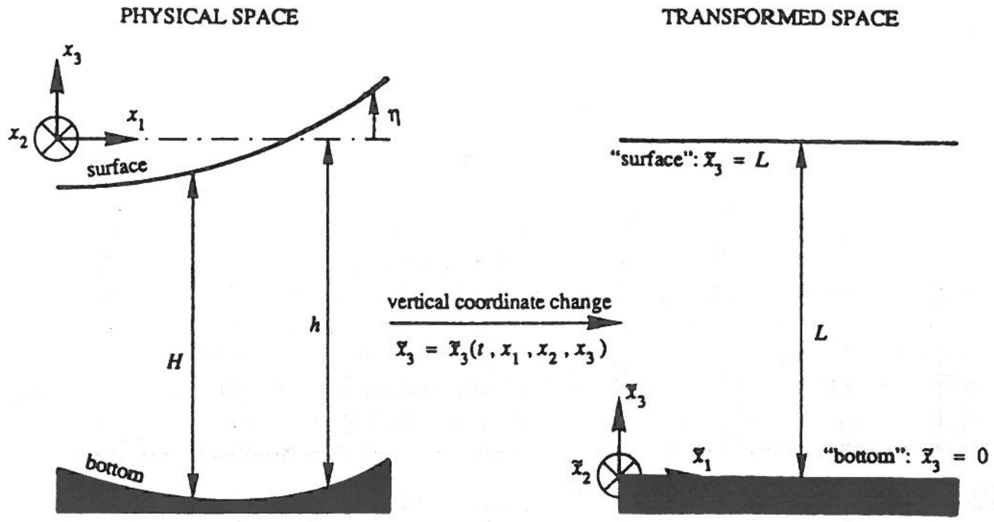

Figure 2: Vertical coordinate in physical and transformed space

The jacobian of the transformation

$$J = \frac{\partial x_3}{\partial \bar{x}_3} = (\frac{\partial \bar{x}_3}{\partial x_3})^{-1} \tag{20}$$

represents the ratio of a unit length in the physical space to a unit length in the transformed space.

A new vertical velocity (the contravariant velocity relative to the moving grid) is defined, as in THOMPSON ET AL (1985) to simplify the equations

$$\bar{w} = D_t \bar{x}_3 \tag{21}$$

where, D_t represents the material derivative,

$$D_t = \frac{\partial}{\partial t} + \mathrm{u}.\nabla_h + w\frac{\partial}{\partial x_3} \tag{22}$$

The identities (23),(24),(26) are used to obtain the equations of motion in the transformed coordinate system,

$$0 \equiv \bar{\nabla}_h x_3 + J\nabla_h \bar{x}_3 \tag{23}$$

$$\bar{\nabla}_h J + \frac{\partial(J\nabla_h \bar{x}_3)}{\partial \bar{x}_3} \equiv \bar{\nabla}_h J + \frac{\partial(-\bar{\nabla}_h x_3)}{\partial \bar{x}_3} \equiv 0 \tag{24}$$

$$
\begin{aligned}
\nabla_h F &\equiv \bar{\nabla}_h F + (\nabla_h \bar{x}_3)\frac{\partial F}{\partial \bar{x}_3} && (25)\\
&\equiv \frac{1}{J}\left[\bar{\nabla}_h(JF) + \frac{\partial (JF\nabla_h \bar{x}_3)}{\partial \bar{x}_3}\right] && (26)
\end{aligned}
$$

which are valid for any function F.

Transformed equations of motion

Transformation of the governing equations according to the relations described in the previous sections, and using the continuity equation to obtain a conservative form for inertia and advective terms, gives:

$$
\begin{aligned}
[\mathcal{I} + \mathcal{A}^h + \mathcal{A}^v](1) &= 0 && (27)\\
\frac{1}{J}\frac{\partial q}{\partial \bar{x}_3} &= b && (28)\\
[\mathcal{I} + \mathcal{A}^h + \mathcal{A}^v - \mathcal{D}^h - \mathcal{D}^v](\mathbf{u}) &= \mathcal{C}(\mathbf{u}) + \mathcal{Q} && (29)\\
[\mathcal{I} + \mathcal{A}^h + \mathcal{A}^v - \mathcal{D}^h - \mathcal{D}^v](T) &= 0 && (30)\\
[\mathcal{I} + \mathcal{A}^h + \mathcal{A}^v - \mathcal{D}^h - \mathcal{D}^v](S) &= 0 && (31)
\end{aligned}
$$

where,

$$
\begin{aligned}
\mathcal{I}(\phi) &= \frac{1}{J}[\frac{\partial (J\phi)}{\partial \bar{t}}] && (32)\\
\mathcal{A}^h(\phi) &= \frac{1}{J}[\bar{\nabla}_h.(J\mathbf{u}\phi)] && (33)\\
\mathcal{A}^v(\phi) &= \frac{1}{J}[\frac{\partial (J\bar{w}\phi)}{\partial \bar{x}_3}] && (34)\\
\mathcal{D}^v(\phi) &= \frac{1}{J}[\frac{\partial}{\partial \bar{x}_3}(\frac{\lambda_{t(\phi)}}{J}\frac{\partial \phi}{\partial \bar{x}_3})] && (35)\\
\mathcal{C}(\mathbf{u}) &= -f\mathbf{e}_3 \otimes \mathbf{u} && (36)
\end{aligned}
$$

The transformed pressure gradient, $\mathcal{Q}$, and horizontal diffusion, $\mathcal{D}^h(\phi)$, terms are described in the following sections.

It is noted that the vertical velocity in the physical space, w, is no longer needed in the governing equations, but can always be recovered in the post-processing of results from

$$
w = J(\bar{w} - \frac{\partial \bar{x}_3}{\partial t} - \mathbf{u}.\nabla_h \bar{x}_3) \qquad (37)
$$

or, if w is desired at scalar cell centres on a staggered grid, the conservative form,

$$
w = \frac{1}{J}(\frac{\partial (Jx_3)}{\partial \bar{t}} + \bar{\nabla}_h.(J\mathbf{u}x_3) + \frac{\partial (J\bar{w}x_3)}{\partial \bar{x}_3}) \qquad (38)
$$

may be used, allowing the surface, bottom and lateral impermeablility boundary conditions to be naturally incorporated.

Pressure gradient

The transformed pressure gradient, $\mathcal{Q}$, contains a component, $\mathcal{Q}_{surf}$, arising from the pressure gradient at the surface and a component, $\mathcal{Q}_{dens}$, representing the "internal" pressure gradient generated by density variations and evaluated by vertical integration of the hydrostatic equation.

$$\mathcal{Q} = \mathcal{Q}_{surf} + \mathcal{Q}_{dens} \tag{39}$$

where,

$$\mathcal{Q}_{surf} = -g\bar{\nabla}_h\eta - \frac{\bar{\nabla}_h P_{atm}}{\rho_0} \tag{40}$$

$$\mathcal{Q}_{dens} = -\frac{1}{J}\left[\bar{\nabla}_h(J q_{dens}) + \frac{\partial(J q_{dens}\nabla_h \bar{x}_3)}{\partial \bar{x}_3}\right] \tag{41}$$

$$q_{dens} = -\int_{\bar{x}_3}^{L} bJ\, d\bar{x}_3 \tag{42}$$

As noted by HANEY (1991) extreme care is required in the formulation and discretisation of the horizontal pressure gradient to avoid the generation of spurious flows. The conservative form (41) has the desirable property , recommended by ARAKAWA AND SUAREZ (1983) , of generating no circulation of vertically integrated momentum around a curve which is a contour of both the bottom ($\nabla_h\eta = 0$) and surface ($\nabla_h h = 0$) topography.

Horizontal diffusion

A consideration of length and velocity scales suggests that the transport of momentum and fluid properties by unresolved sub-grid-scale motions is small compared to transport by vertical diffusion processes. However, horizontal diffusion terms are often included in marine hydrodynamical models, with a diffusion coefficient, κ, chosen much higher than could be justified by physical reasoning based on, for example, the dye plume experiments summarised by LAM ET AL (1984) . It is suggested by MELLOR AND BLUMBERG (1985) and DELEERSNIJDER AND WOLANSKI (1990) that such horizontal diffusion is "artificial", introduced solely to stabilise the numerical scheme and to damp the smallest scale numerical waves which are poorly represented. Thus, it is proposed that for a general vertical coordinate transformation the form (43) be used to apply horizontal diffusion rather than a transformation-invariant form. In addition to the considerable mathematical complexity of transforming a Laplacian-type horizontal diffusion from the Cartesian coordinate system, it is shown by MELLOR AND BLUMBERG (1985) that such a formulation would give unrealistic representation of bottom boundary layers in contrast to forms such as (43), where there is no horizontal diffusion arising from vertical shear

$$\mathcal{D}^h(\phi) = \frac{1}{J}\tilde{\nabla}_h.(J\kappa\tilde{\nabla}_h\phi) \tag{43}$$

Transformed kinematic boundary conditions

Since the sea bottom and surface are impermeable, a fluid particle lying on one of these surfaces must remain on the surface. Therefore, the material derivative of the vertical coordinate in the new space must be zero. Thus, from the definition of $\tilde{w}$

$$[\tilde{w}]_{\tilde{x}_3=0,L} = 0 \tag{44}$$

which is a much simpler form of the kinematic boundary conditions than the corresponding expressions in the physical space.

Effect of coordinate transformation

The introduction of a generalised vertical coordinate thus allows a simple and accurate treatment of the impermeability boundary conditions at the sea bottom and surface, and avoids waste of computational resources, while not complicating significantly the equations. The jacobian can be simply calculated for a cell as the difference in physical vertical coordinate between the top and bottom faces divided by a constant $\Delta\tilde{x}_3$. Use of such a coordinate transformation facilitates the concentration of points in regions of high gradient, such as pycnoclines.

No additional complications in the vertical derivatives would be incurred by the use of coordinate transformation in the horizontal provided that the horizontal and vertical transformations remain uncoupled — i.e. provided that "a vertical in the physical space remains vertical in the transformed space".

REVIEW OF VERTICAL COORDINATES USED IN MARINE MODELLING

Apart from the trivial case of the "z" coordinate system , for which $J \equiv 1$ and which is not boundary fitted, the "generalised" vertical coordinate accomodates all coordinate systems considered useful in oceanography, as outlined in the following sections.

σ coordinate

The most commonly used transformed vertical coordinate (e.g. OWEN (1980), BLUMBERG AND MELLOR (1987), DAVIES (1987)) , the σ coordinate, defined, for example by NIHOUL ET AL (1986) , by

$$\tilde{x}_3 = L\sigma = L\frac{x_3 + h}{H} \tag{45}$$

where H is the total water depth

$$H = h + \eta \tag{46}$$

and L a horizontal length scale, offering an appropriate adimensionalisation of vertical derivatives.

The main advantages of this formulation lies in the fact that the jacobian is constant on the vertical.

$$J = \frac{H}{L} \tag{47}$$

If L is chosen as the characteristic horizontal length scale of the domain the transformed vertical velocity $\tilde{w}$ has the same order of magnitude as the horizontal velocity. DELEERSNIJDER (1989) considers the physical vertical velocity, w, as a sum of an "upwelling" component, $\frac{H}{L}\tilde{w}$, representing vertical motion relative to iso-σ surfaces, and an "upsloping" component arising from bottom and surface topography. This has been exploited by DELEERSNIJDER ET AL (1992) to quantify upwelling phenomena.

Multiple σ coordinate

For regions where bathymetry ranges from shallow sea to deep ocean, a simple σ coordinate is undesirable because of numerical problems associated with greatly varying mesh size, discussed by DELEERSNIJDER AND BECKERS (1992) , and the artificial smearing of pycnoclines, which intersect constant σ surfaces. Figure 3 shows how a double σ coordinate transformation has been used by BECKERS (1991) in the Western Mediterranean to overcome these difficulties by decomposing the domain vertically into shallow and deep regions.

Hybrid σ/"z" coordinate

To avoid artificial horizontal variation in the bottom shear stress, and thus erroneous sediment resuspension, arising from varying grid spacing, a hybrid σ/"z" coordinate has been adopted by DE KOK (1992) to give a horizontally uniform grid spacing, i.e.

$$\tilde{x}_3 = a(x_3 + h) \tag{48}$$

with constant a for the bottom two layers of a five layer model.

Hybrid "z"/σ coordinate

Conversely, constant vertical spacing for the upper layers of a deep ocean model has been used by SPALL AND ROBINSON (1990) with a σ transformation for the lower layers.

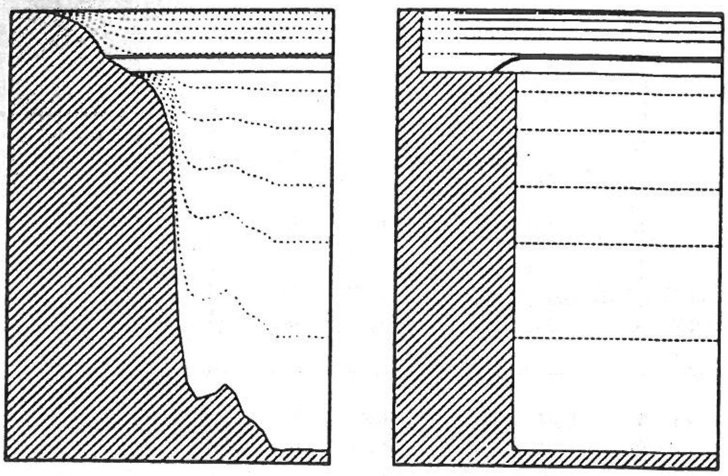

Figure 3: Iso $\bar{x}_3$ lines and idealised thermocline in physical and transformed coordinates using a double σ coordinate transformation (reproduced from BECKERS (1991))

CONCLUSIONS

Building on the work of KASAHARA (1974) in atmospheric modelling, the governing equations for shallow sea hydrodynamics are developed for a generalised vertical coordinate, which embraces all formulations commonly used in ocean modelling. This provides greater flexibility than the popular σ coordinate, since the horizontal variation of internal coordinate surfaces is no longer entirely defined by the surface and bottom topography. The extra freedom enables the use of hybrid "σ-z" coordinates or the concentration of points in regions of high gradient. A simple form is obtained for the governing equations when using the physical horizontal velocities and the contravariant "vertical" velocity relative to the moving grid. This formulation is also valid if dynamically adaptive grid generation is to be attempted. Finally, conservative formulations are proposed for the troublesome pressure gradient and horizontal diffusion terms. While the analysis has been presented here for shallow sea modelling, the general coordinate transformation is clearly also applicable in ocean modelling.

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