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Short Communication

On methods for solving the oceanic equations of motion in generalized vertical coordinates

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Abstract

We note that there are essentially two methods of solving the hydrostatic primitive equations in general vertical coordinates: the quasi-Eulerian class of algorithms are typically used in quasi-stationary coordinates (e.g. height, pressure, or terrain following) coordinate systems; the quasi-Lagrangian class of algorithms are almost exclusively used in layered models and is the preferred paradigm in modern isopycnal models. These approaches are not easily juxtaposed. Thus, hybrid coordinate models that choose one method over the other may not necessarily obtain the particular qualities associated with the alternative method.

We discuss the nature of the differences between the Lagrangian and Eulerian algorithms and suggest that each has its benefits. The arbitrary Lagrangian–Eulerian method (ALE) purports to address these differences but we find that it does not treat the vertical and horizontal dimensions symmetrically as is done in classical Eulerian models. This distinction is particularly evident with the non-hydrostatic equations, since there is explicitly no symmetry breaking in these equations. It appears that the Lagrangian algorithms can not be easily invoked in conjunction with the pressure method that is often used in non-hydrostatic models. We suggest that research is necessary to find a way to combine the two viewpoints if we are to develop models that are suitable for simulating the wide range of spatial and temporal scales that are important in the ocean.
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1. Introduction

Traditionally, ocean models have been written to integrate forward in the time the equations of motion written in just one vertical coordinate at a time, most commonly either height, potential density or some form of terrain-following coordinate. Recently, several models have been developed in a general coordinate framework and specifically to work with hybrid coordinates (for example, Bleck, 2002; Song, 2003; and other references in Griffies et al., 2000b). Hybrid coordinates aim to mimic different types of coordinates in different parts of a model. For example, the expected optimum hybrid coordinate might be similar to potential density in the ocean interior where the flow is nearly adiabatic, then matching to some form of terrain-following coordinate in the bottom boundary and matching either a height or pressure coordinate in the surface mixed layer regions.

One concern about these new classes of models is whether they can produce solutions of the same caliber as the earlier class of single coordinate models. In each category of single coordinate model, much work has been invested in developing techniques for rendering accurate and physically relevant solutions. For example, height coordinate models no longer have a spurious representation of the topography (Adcroft et al., 1997) and isopycnal models can be made truly adiabatic (Oberhuber, 1993). General coordinate models allow the exploration of hybrid coordinates where optimal features of single coordinate models are blended. It is not yet clear whether these optimal features are compatible. The ultimate test will be to compare the new general coordinate models side-by-side with each of the single coordinate models; this has not yet been done.

In this note, we discuss some algorithmic considerations that arise when building a generalized or hybrid coordinate model. We are first concerned with use of the continuity equation in isopycnal models (described, for example, by Bleck, 2002) which has the advantage that it renders isopycnal coordinate models truly adiabatic. The method treats the dynamics as Lagrangian in the vertical, in contrast to the Eulerian algorithms used previously. This distinction was discussed by Bleck (1978). The general notion (with which we agree entirely) is that an adiabatic formulation is preferable for climate scale modeling. However, we also consider how to integrate forward non-hydrostatic equations in general coordinates, appropriate for small scale processes. We find that the Boussinesq non-hydrostatic equations and a Lagrangian treatment of the vertical direction are mutually exclusive. We conclude with more questions than answers and hope that this note will stimulate some research into these issues.

2. Hydrostatic equations in general vertical coordinates

The traditional equations of motion for the ocean (in which the hydrostatic and Boussinesq approximations are made) can be written in terms of a general vertical coordinate $r = r(x, y, z, t)$. We restrict our discussion here to the Boussinesq equations for the purpose of comparison with

the non-hydrostatic equations discussed later. We recognize that we could as easily use the hydro-static non-Boussinesq equations here. The hydrostatic model equations are:

$$D_t \vec{v}_h + f\hat{k} \wedge \vec{v}_h + \frac{1}{\rho_0}\nabla_r p + \frac{\rho}{\rho_0}\nabla_r(gz) = \vec{F}_h \tag{1}$$

$$\partial_r p + \rho\partial_r(gz) = 0 \tag{2}$$

$$\partial_t z_r + \nabla_r \cdot (z_r \vec{v}_h) + \partial_r(z_r \dot{r}) = 0 \tag{3}$$

$$\partial_t(z_r \theta) + \nabla_r \cdot (z_r \theta \vec{v}_h) + \partial_r(z_r \theta \dot{r}) = Q_\theta \tag{4}$$

$$\partial_t(z_r s) + \nabla_r \cdot (z_r s \vec{v}_h) + \partial_r(z_r s \dot{r}) = Q_s \tag{5}$$

$$\rho = \rho(\theta, s, p) \tag{6}$$

$$\partial_t \eta + \nabla \cdot \int \vec{v}_h z_r \mathrm{d}r = P \tag{7}$$

where $\vec{v}_h$ is the horizontal component of the flow vector, f is the Coriolis parameter, ρ_0 is a reference density, ρ is in situ density, g is the constant of gravitational acceleration, z is height referenced to the geoid, $\vec{F}_h$ is an arbitrary horizontal force resulting from the divergence of internal and external stresses on the fluid, p is the thermodynamic pressure, $\dot{r}$ is the vertical flow rate across an r surface and θ is potential temperature, s is the salinity, η is the free-surface height displacement and Q_θ, Q_s and P are general sources and sinks of heat, salt and fresh water, respectively. In all the equations in this note, $\nabla_r = (\partial_x, \partial_y, 0)$ is the gradient operator along r surfaces. The integral in the free surface equation (7) is over the full depth of the fluid and consequently is independent of the choice of coordinate system.

The factor, $z_r \equiv \partial_r z$, is referred to as the "thickness" and is the scale factor describing the vertical coordinate mapping from height. z_r is the principle discriminator between different coordinate systems (choices of r). If we choose $r = z$ then $z_r = 1$ and we recover the conventional height coordinates equations. If we choose $r = \sigma = (z - \eta)/(H + \eta)$, where $z = -H$ is the location of the solid bottom, then $z_r = H + \eta$ and we recover the usual terrain-following coordinate equations. If we choose $r = \rho$ then $z_r = (\partial_z \rho)^{-1}$ and with some small manipulation [2] we can obtain the continuous isopycnal coordinate equations.

The hydrostatic approximation (2) allows the pressure, p, to be found by vertical integration given an appropriate pressure boundary condition at the sea-surface ($p = p_a$ at $z = \eta$):

$$p = p_a + g \int_r^{r_s} \rho z_r \mathrm{d}r'$$

where $r_s = r(z = \eta)$ denotes the coordinate of the free surface. Vertical integration for the pressure is carried out in both classes of model discussed next.

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[2] Isopycnal models are usually formulated using the Montgomery potential, $M = \rho/\rho_0 + \rho gz/\rho_0$, so that in the horizontal momentum equations $\frac{1}{\rho_0}\nabla_\rho p + \frac{\rho}{\rho_0}\nabla_\rho(gz) = \nabla_\rho M$ and the hydrostatic balance equation becomes $\partial_p M = gz/\rho_0$.

2.1. The EVD algorithm: quasi-Eulerian treatment of the vertical direction

In the height coordinate equations, the continuity equation is unambiguously a strong constraint on the flow field and is thus used to diagnose the vertical component of velocity in such a way so as to be exactly non-divergent. The continuity equation is used in essentially the same manner in the more general class of terrain-following coordinate models. Although the continuity equation (3) appears to be prognostic in "thickness", the rate of change of thickness is dictated by the free-surface evolution (7) due to the prescribed functional relationship between the coordinate r and η. Thus, in Eq. (3), the time tendency term is known and the equation may be integrated vertically to diagnose $\dot{r}$:

$$z_r \dot{r} = z_r \dot{r}_{-H} - \int_{r_{-H}}^{r} (\partial_t z_r + \nabla_r \cdot z_r \vec{v}_{\mathrm{h}}) \mathrm{d}r' \tag{8}$$

where $r_{-H} = r(z = -H)$ denotes the coordinate of the ocean floor and $\dot{r} = \dot{r}_{-H}$ denotes the no normal flow boundary condition. Due to the close algorithmic connection between the height and terrain-following coordinate models we refer to this diagnostic use of the continuity equations as the quasi-Eulerian treatment of the vertical direction, or EVD method for short.

In the continuous equations, the free-surface equation (7) is derived by vertically integrating the continuity equation (3) from top to bottom and is consistent with applying Eq. (8) at the free-surface along with appropriate boundary conditions. In the discrete equations, conservation properties typically depend on the relationship between the free-surface equation and the three dimensional continuity equation. However, it simply suffices to ensure that the vertical sum of the time tendencies and horizontal volume fluxes are independently equal to the corresponding terms in the free-surface equation.

We should emphasize that the EVD algorithm refers specifically to the "Eulerian" treatment of the vertical terms in the continuity equation. The horizontal terms could be treated with a Lagrangian or semi-Lagrangian method. Moreover, the vertical advection terms in the thermodynamic and momentum equations could be treated with a Lagrangian method. However, it is typically hard to retain conservation properties of tracers if the tracer equations are treated differently to the continuity equation.

If we choose to use isopycnal coordinates, $r = p$, the algorithm above would appear to work well. However, the procedure of integration differs from the LVD algorithm (described next) used by modern isopycnal models: in the EVD algorithm, we predict the heat and salt (4) and (5), and then diagnose the density. From the density we can diagnose the rate of change of thickness and then diagnose from continuity (3) the cross-coordinate flow, $\dot{r}$. Using this procedure, it is very hard to guarantee that the cross-coordinate flow, $\dot{r}$, is identically zero (adiabatic) in the absence of diabatic forcing.

2.2. The LVD algorithm: quasi-Lagrangian treatment of the vertical direction

In contrast to the EVD algorithm, if we treat the vertical coordinate as Lagrangian, as is the case in modern isopycnal models, then it is more natural to use the continuity equation prognostically:

$$\partial_t z_r = -\nabla_r \cdot (z_r \vec{v}_{\mathrm{h}}) - \partial_r (z_r R) \tag{9}$$

where $\dot{r} = R$ is prescribed. This is especially evident if we consider the adiabatic limit where the cross-coordinate flow vanishes ($\dot{r} = R = 0$). In this case, integrating equations (1)–(3) over layers yields the stacked shallow water equations which represent the archetypal isopycnal model. This conveniently eliminates the need to calculate any vertical fluxes due to advection (there are none) so that all (unforced) prognostic equations appear as strictly horizontal (i.e. terms involving r in Eqs. (3)–(5) vanish). Further, all advective truncation errors are confined to the horizontal coordinate planes and may be entirely masked by epineutral stirring and mixing, to the extent that the coordinate surfaces coincide with neutral surfaces (Bleck, 1998). In this system there is a clear separation of dynamics and thermodynamics; the dynamical modes (internal waves and Rossby mode) are governed by Eqs. (1)–(3) alone. There is no vertical advective signature of linear internal waves; the time tendency of thickness plays that role. Propagation is due to horizontal dynamics and hydrostatic pressure alone.

We will refer to the prognostic use of the continuity equation (9) as the quasi-Lagrangian treatment of vertical dynamics or LVD for short. It specifically refers to the specification of cross-coordinate flow, $\dot{r} = R$, and prognosticated evolution of thickness, z_r. The LVD algorithm is at the heart of modern isopycnal models and some hybrid coordinate models. These models use the "arbitrary Lagrangian–Eulerian" method (or ALE for short) which facilitates non-adiabatic motions—i.e. it allows cross-coordinate flow in an otherwise Lagrangian vertical coordinate system. In the ALE method, the approach is to first integrate the equations forward in a truly Lagrangian phase assuming no cross-coordinate flow and then in a second phase to re-map quantities in the vertical. The re-mapping phase plays the role of cross-coordinate fluxes and can be formulated to re-map to any arbitrary coordinate. In this regard the ALE method is completely general. This use of two distinct phases is generally known as operator splitting. Although the re-mapping phase can account for cross-coordinate flow and render the system as if it were in fixed coordinates (Eulerian), it does not change the algorithmic nature of ALE which is Lagrangian. The ALE method belongs to the class of LVD algorithms because the continuity equation is not used diagnostically. This becomes clear when we later consider how to solve the non-hydrostatic equations in which the three space dimensions are treated symmetrically.

We have ignored many details that are necessary to successfully integrate the isopycnal equations. For instance, a problematic issue is that z_r must be positive definite; using the LVD algorithm, a positive definite advection method is required for thickness. Also, one of the thermodynamic equations is redundant and care must be taken in eliminating this equation consistently with a non-linear equation of state. Here, we assume that such issues are resolvable and not pertinent to this discussion.

2.3. The conundrum

We summarize the essential differences between two basic methods of solution for the hydrostatic primitive equations (also noted by Bleck, 1978) as follows.

The quasi-Eulerian treatment of the vertical direction (EVD), which encapsulates the algorithms used in height and terrain-following coordinate models, has the following features:

- The continuity equation is used in the form of 8 to diagnose the cross-coordinate flow rate, $\dot{r}$,
- the free-surface equation is integrated forward in addition to the three dimensional equations,
- the thickness, z_r, and its time derivative, $\partial_t z_r$, are functionally related to other variables.

The Lagrangian treatment of the vertical direction (LVD), as used in modern isopycnal models that in principle can be exactly adiabatic, has the following features:

- The continuity equation is used in the form of (9) to predict the thickness z_r,
- the cross coordinate flow, $\dot{r} = R$, is specified when used in the continuity equation,
- the free-surface equation is redundant.

It should be self evident that these two algorithms are mutually exclusive; one cannot both supply and diagnose a quantity in an equation.

It has been recognized that spurious diabatic fluxes are a major problem for ocean climate models and these spurious fluxes are particularly large for the height and terrain-following coordinate models (Griffies et al., 2000a). Isopycnal models do not suffer from this problem and can potentially represent truly adiabatic flows.

It is simplest to use the LVD algorithm to solve the isopycnal equations and simplest to use the EVD algorithm when the coordinate is not related to thermodynamic quantities.

The ultimate goal of hybrid coordinate models is to do as well as single coordinate models in particular regions of the ocean. Hybrid coordinate models currently use either the EVD or LVD algorithm. It is not clear whether a hybrid coordinate model using the EVD algorithm can represent adiabatic flows as accurately as a model using the LVD algorithm—this is an open question that needs addressing. On the other hand, it is possible to use the LVD algorithm for a non-Lagrangian coordinate by means of the ALE method (the re-mapping phase accommodates the cross-coordinate flow). To this end, the ALE method would appear to be the best method to achieve optimal fidelity for all coordinate systems.

3. Incompressible non-hydrostatic equations in general coordinates

One aspect of the LVD algorithm is that it explicitly breaks the symmetry between horizontal and vertical direction. This may be justified since in a hydrostatic model the statement of hydrostatic balance breaks the symmetry. However, models such as the MIT general circulation model (Marshall et al., 1997a) have an optional capability to solve the non-hydrostatic equations. A desire to implement general and hybrid coordinates in such a model forces us to consider whether the LVD algorithm can be used for the incompressible non-hydrostatic equations; the current methodology (known as the projection method) used to solve the non-hydrostatic equations falls into the class of EVD algorithms and treats all three space dimensions symmetrically.

The Boussinesq equations are filtered equations and do not exhibit acoustic modes. They differ[3] from Eqs. (1)–(7) by relaxing the hydrostatic approximation (2) which is replaced with the vertical momentum equation

$$D_t w + \left(2\vec{\Omega} \wedge \vec{v}\right) \cdot \hat{k} + \frac{1}{\rho_0} z_r^{-1} \partial_r p + \frac{\rho}{\rho_0} z_r^{-1} \partial_r (gz) = F_w \tag{10}$$

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[3] To be consistent, the approximated Coriolis terms in Eq. (1) must be replaced with the full Coriolis terms, namely the horizontal components of $2\vec{\Omega} \wedge \vec{v}$.

where $w = D_t z$ is the vertical component of velocity in height coordinates. We use the Eulerian vertical flow, w and not $\dot{r}$ to keep the vertical momentum equation simple. Note that the horizontal pressure gradient term (Eq. (1)) now takes the form $\frac{1}{\rho_0}(\nabla_r p - z_r^{-1}\partial_r p \nabla_r z)$. To close the equations we need to relate w and $\dot{r}$. We do this by assuming a limited functional form of $r = (z, \eta, H, \rho)$. Thus, we can write

$$\dot{r} = r_z w + r_\eta D_t \eta + r_H D_t H + r_\rho D_t \rho \tag{11}$$

where

$$r_z \equiv \left.\frac{\partial r}{\partial z}\right|_{\eta,H,\rho}, \quad r_\eta \equiv \left.\frac{\partial r}{\partial \eta}\right|_{z,H,\rho}, \quad r_H \equiv \left.\frac{\partial r}{\partial H}\right|_{z,\eta,\rho} \quad \text{and} \quad r_\rho \equiv \left.\frac{\partial r}{\partial \rho}\right|_{z,\eta,H}$$

Note that r_z should not be confused with the reciprocal of z_r; the first is a functional derivative holding arguments constant while the second is a spatial derivative hold horizontal coordinate and time constant.

Eqs. (1), (10), (3)–(7) and (11) can be solved using the projection method, also known as the pressure method, which is the canonical method for solving incompressible equations (Chorin, 1968; Durran, 1998). Alternative methods, for example a semi-implicit treatment of sound waves, essentially take a similar form. The projection method, as we describe it, assumes an explicit in time treatment of all terms except the pressure gradient (although the method can be generalized).

We summarize the time-discretized momentum and continuity equations with

$$\frac{\vec{v}_h^{(n+1)} - \vec{v}_h^{(n)}}{\Delta t} + \frac{1}{\rho_0}\left(\nabla_r p - z_r^{-1}(\nabla_r z)\partial_r p\right) = \vec{G}_h^{(n)} \tag{12}$$

$$\frac{w^{(n+1)} - w^{(n)}}{\Delta t} + \frac{1}{\rho_0}z_r^{-1}\partial_r p = G_w^{(n)} \tag{13}$$

$$\nabla_r\left(\cdot z_r \vec{v}_h^{(n+1)}\right) + \partial_r\left(z_r \dot{r}^{(n+1)}\right) = -\partial_t z_r \tag{14}$$

where the G's incorporate all the terms that are explicit in time. For convenience, it is useful to define the intermediate quantities

$$\vec{v}^* = \vec{v}^{(n)} + \Delta t \vec{G}_h^{(n)}$$

$$w^* = w^{(n)} + \Delta t G_w^{(n)}$$

$$\dot{z}_r^* = \partial_t z_r + \nabla_r\left(\cdot z_r \vec{v}_h^*\right) + \partial_r(z_r r_z w^*)$$

which simplifies the time-stepping equations to

$$\vec{v}^{(n+1)} = \vec{v}^* - \frac{\Delta t}{\rho_0}\left(\nabla_r p - z_r^{-1}(\nabla_r z)\partial_r p\right)$$

$$w^{(n+1)} = w^* - \frac{\Delta t}{\rho_0}z_r^{-1}\partial_r p$$

Invoking the functional relationship (11) between w and $\dot{r}$ we obtain

$$\dot{r}^{(n+1)} = r_z w^* - r_z \frac{\Delta t}{\rho_0} z_r^{-1} \partial_r p + r_\eta D_t \eta^{(n+1)} + r_H D_t H^{(n+1)} + r_\rho D_t \rho^{(n+1)}$$

Substituting into the continuity equation applied to the future time step (Eq. (14)) we obtain a Poisson problem to solve for p:

$$\nabla_r \cdot (z_r \nabla_r p) - \nabla_r \cdot (\partial_r p \nabla_r z) + \partial_r (r_z \partial_r p) = \frac{\rho_0}{\Delta t} \left[\dot{z}_r^* + \partial_r \left(z_r \left(r_\eta D_t \eta^{(n+1)} + r_H D_t H^{(n+1)} + r_\rho D_t \rho^{(n+1)} \right) \right) \right]$$

(15)

The appearance of the time-derivatives of η and ρ on the right hand side will be troublesome for conservation properties but in principle does not stop us from using the method to integrate the equations forward. Broadly speaking, the pressure equation (15) is an elliptic equation that, in a discrete form and given appropriate boundary conditions, can be solved by various linear algebra methods.

Common sense suggests that pure isopycnal coordinates should not be used for non-hydrostatic modelling because of monotonicity requirements for vertical coordinates and the exclusion of resolution in unstratified regions. This is, of course, pointless since non-hydrostatic effects tend to be associated with over turning (e.g. Kelvin–Helmholtz instabilities). Similarly, terrain-following coordinates can be used for non-hydrostatic modelling but the presence of the cross-terms in the elliptic pressure equation greatly affects the ease with which the equation can be solved. The larger the terms become the harder it is for algebraic solvers to find solutions efficiently. This suggests that a useful strategy for choosing a vertical coordinate for non-hydrostatic modelling is to minimize these cross-terms. Consequently, the most natural choice of vertical coordinate is height (where the terms vanish) or something closely related to height, such as the z^* coordinate (Adcroft and Campin, 2004). The latter choice is still more complicated than height due to the time-dependent source terms in the pressure equation (15).

By construction, the projection method excludes the use of the LVD algorithm of Section 2.2; the LVD algorithm prescribes $\dot{r}$ in the continuity equation and in the projection method this same term should be substituted from the vertical momentum equation. We therefore conclude that non-hydrostatic models using the projection method must use the EVD algorithm (Section 2.1).

4. Discussion

We have considered the general methods for solving the equations of motion in primitive equation form (i.e. prognostic in velocity) in both the hydrostatic and non-hydrostatic limits. We found that the two basic approaches to hydrostatic modelling appear to be exclusive; it is hard to formulate an algorithm that can encompass both approaches. This is of relevance because the isopycnal modelling community has learned that the Lagrangian approach is best suited for modelling adiabatic motions; the EVD algorithm is not sufficiently adiabatic for some important oceanographic applications, even applied in isentropic coordinates (Griffies et al., 2000a). Given the highly adiabatic nature of the interior ocean, the argument is that hydrostatic hybrid coordinate ocean models should use the LVD algorithm to avoid spurious diabatic effects.

In order to construct versatile models that can work efficiently at both the large scales where the flow is hydrostatic and at very small scales in the non-hydrostatic limit (e.g. coastal scale and process studies), we would need to keep the algorithm considerations we have discussed in mind when choosing vertical coordinates and designing algorithms. We argue that it is hard to envision non-hydrostatic modelling in a vertical coordinate that significantly differs from height. Moreover, the projection method used in current non-hydrostatic models of the ocean (Marshall et al., 1997b) excludes the possibility of using the LVD algorithm. Thus, while we might prefer the LVD algorithm for philosophical reasons, future models designed to model a wide range of scales and processes may be forced to use the EVD method.

The differences in solutions invoked by using either the EVD of LVD algorithm in hybrid coordinate models could in principle be evaluated by comparing two such models with the same hybrid coordinate. However, other implementation details (such as the choice of pressure gradient method) are likely to be influenced by the choice of over-arching algorithm and may mask the essential differences. Nevertheless, a comparison may address the question of whether differences due to choice of algorithm are significant at all.

We have considered the non-hydrostatic equations in order to emphasize the difference between the EVD and LVD algorithms. The essential difference is that the EVD algorithm treats all spatial dimensions equally while the LVD algorithm treats the vertical dimension very differently from the horizontal.

The elliptic pressure equation appears in the incompressible non-hydrostatic equations because the acoustic modes have been filtered out of the system. In the unapproximated Navier–Stokes equations the role of the diagnostic elliptic equation for pressure is played by a prognostic equation for pressure; the system is hyperbolic. Here, there appears to be no inherent problems to solving the equations explicitly in general coordinates using either the EVD and LVD algorithm. We speculate that relaxing the incompressible approximation may allow general coordinate non-hydrostatic modelling in the future. This approach is more readily available for use in the atmosphere than in the ocean: the Mach number (U/c_s) is less than one but still of first order while in the ocean the Mach number is of order 10^{-2}.

As computational resources and capabilities increase with time, the resolution of ocean models will be driven ever higher to a point where even global models achieve the resolutions normally associated with regional and process models. At some point, as is happening in meteorology, non-hydrostatic models will become the norm rather than the exception. The current direction that we are heading with the particular algorithms used in hybrid coordinate models may be at odds with this long-term goal. We suggest that a worth-while goal would be to find a non-hydrostatic algorithm that can recover adiabatic properties in the hydrostatic limit. This may require the adiabatic constraint to be enforced in the EVD algorithm or alternatively a non-symmetry breaking form of LVD algorithm be found. We hope that this discussion may stimulate research toward these goals.

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