1. INTRODUCTION

The interaction of the ocean with the rest of the earth system happens primarily at the sea-surface through air-sea fluxes that imprint on fluid parcels the current physical or chemical state of the atmosphere. When fluid parcels are transported below the surface, they become shielded from the atmosphere until they resurface at a later time to communicate past physical or chemical climate conditions to the atmosphere. The delay between successive visits to the surface mixed layer imparts to the climate system an important long-term memory. Since the properties of fluid parcels get reset by air-sea interactions during each visit to the surface mixed layer, the “memory” of a fluid parcel does not extend to times earlier than its last contact with the surface layer, nor does it persist beyond its next contact with the surface layer. In light of this, the distribution of times for fluid parcels to have had their last contact with the surface layer, as well as the distribution of times when fluid parcels will have their first (or next) contact with the atmosphere provide a useful description of the transport characteristic of ocean models. Our approach is to characterize the transport characteristics using transit-time-distribution functions as described in Holzer and Hall (2000).

1.1 Probability For Transport From One Grid Box To Another

As a preliminary step, we seek to understand in a probabilistic sense where fluid parcels come from and where they are going. More precisely we seek answers to the following two questions (see figure 1):

1. Where do fluid parcels come from? What is the probability that a fluid parcel located in grid-box $i$ at time $t$ was transported from grid-box $j$ during the preceding time interval from $t_0$ to $t$? In other words we want to determine

$$p_{ij}(t, t_0) = \mathbb{P}(j \mid x(t) = i, t_0 < t < t_1)$$

2. Where are fluid parcels going? What is the probability that a fluid parcel located in grid-box $i$ at time $t$ will be transported to grid-box $j$ during the time interval between $t$ and $t_1$? In other words we want to determine

$$p_{ij}(t, t_1) = \mathbb{P}(j \mid x(t) = i, t_1 > t)$$

In the absence of sources or sinks, the advection-diffusion equation describing the transport of tracers in the ocean is

$$\frac{\partial C}{\partial t} + \nabla \cdot (u C + K \nabla C) = 0$$

where $u$ is the fluid velocity field and $K$ is the diffusion tensor. For a numerical ocean model, the tracer distribution, $c(t)$, can then be described with an $n$ dimensional vector whose elements are the tracer concentration in each grid-box of volume $w_i$. For the discrete model, the time evolution of an initial tracer distribution $c(t_0)$, is given by

$$c(t) = P(t, t_0) c(t_0)$$

where $P(t, t_0)$ is the state transition matrix (Padulo and Arbib 1974) given by the solution to

$$\frac{d}{dt} P(t, t_0) + T(t) P(t, t_0) = 0$$

$$P(t_0, t_0) = I$$

In equation (5), $T(t)$ is the discrete advection-diffusion transport operator written as an $n \times n$ matrix and $I$ is the $n$-dimensional identity matrix. The $i$th row of $P(t, t_0)$ tells us in what proportion the fluid from each model grid-box at time $t_0$ gets mixed to form the fluid mixture in grid-box $i$ at time $t$. The rows of $P(t, t_0)$ can thus be thought of as probability mass functions of the location, $x$, at some time $t_0$ of fluid parcels conditioned on their position at some later time $t$. In other words, the $ij$th element of $P(t, t_0)$ is $p_{ij}(t, t_0)$ that appears in (1). Thus for the case where $t > t_0$, the rows of $P(t, t_0)$ answers the question of where fluid parcels come from. If we interchange the time arguments of $P$ such that the first argument is smaller than the second we get $P(t_0, t)$ with

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The probability that a fluid parcel located in grid-box \( i \) at time \( t \) was transported from grid-box \( j \) at time \( t_0 \) immediately following \( t_0 \) without making contact with the surface layer during the time interval of length \( t - t_0 \) leading up to \( t \). If, however, \( t < t_0 \), then the \( j \)th element of \( P_{ij}^* (t, t_0) \) gives the probability that a fluid parcel in grid box \( i \) at time \( t \) will be transported to grid box \( j \) without making contact with the surface layer during the time interval of length \( t_0 - t \) immediately following \( t \).

For the case where \( t > t_0 \) the \( j \)th element of \( P_{ij}^* (t, t_0) \) can be interpreted as the probability that a fluid parcel in grid-box \( i \) at time \( t \) was transported from grid-box \( j \) at time \( t_0 \) without having made contact with the surface layer during the preceding time interval of length \( t - t_0 \) leading up to \( t \). To obtain the new equation we partition the transport equation into interior, (10) except that fluid parcels should get “untagged” when they reach the surface layer. To obtain the new equation we partition the transport equation into interior, (11) and then “untag” fluid parcels in the surface layer by setting \( P_{ii}^* = 0 \) and \( P_{ii}^* = 0 \), to get an equation for the interior boxes only

\[
\begin{align*}
\frac{d}{dt} P_{ii}^* (t, t_0) &= -T_i (t) P_{ii}^* (t, t_0) \\
P_{ii}^* (t_0, t_0) &= I_i
\end{align*}
\]
Differentiating (18) with respect to $t$, we obtain the probability density (per unit time) that a fluid parcel in grid-box $i$ at time $t_0$ will make its first contact with the surface layer at time $t$. Similarly, differentiating equation (19) with respect to $t_0$ we obtain the probability density (per unit time) that a fluid parcel in grid-box $i$ at time $t$ made its last contact with the surface layer at time $t_0$. Thus the distribution of first passage times is

$$ f(t|x(t_0) = i) = -\frac{\partial}{\partial t} s_i(t_0, t) = -\sum_j \frac{\partial}{\partial t} p^*_j(t, t_0) \frac{w_j}{w_i}. $$

(20)

and the distribution of last passage times is

$$ f(t_0|x(t) = i) = -\frac{\partial}{\partial t_0} s_i(t, t_0) = -\sum_j \frac{\partial}{\partial t_0} p^*_j(t, t_0). $$

(21)

In vector form, equation (20) can be written as follows

$$ f(t_0, t) = -\frac{\partial}{\partial t} s^T(t_0, t) $$

$$ = -1^T W_1 \left( \frac{\partial P^*_i}{\partial t} \right) \frac{t}{W_i^{-1}} $$

(22)

and (21) can be written as

$$ f(t, t_0) = -\frac{\partial}{\partial t_0} P^*_i t(t, t_0) $$

$$ = -\frac{\partial}{\partial t_0} P^*_i (t, t_0) \mathbf{1} $$

$$ = \left( 1^T W_1 \frac{\partial P^*_i}{\partial t} W_1^{-1} \right)^T $$

(23)

(24)

(25)

(26)

where the $i$th component of $f(t_0, t)$ is $f(t|x(t_0) = i)$ and the $i$th component of $f(t, t_0)$ is $f(t_0|x(t) = i)$. In equation, (26) we have made use of (12) to replace $P^*(t, t_0)$ with $P^*(t, t_0)$ since we need to compute the derivative with respect to the second time argument and as we will see in the next section we can use the adjoint equation to compute $P^*(t, t_0)$ as a function of its second time argument whereas equation (11) allows us to compute $P^*(t, t_0)$ only as a function of its first time argument.

2.0.1 ADJOINT TRANSPORT EQUATION

To derive the adjoint equation we first note that fluid parcels that have not made contact with the surface layer during the time interval from $t_0$ to $t$ must be in one and only one grid-box at an intermediate time $t$ between $t_0$ and $t$. Consequently, the conditional probabilities given by the elements of $P^*_i(t, t_0)$ must satisfy the following condition

$$ p_{x(t_0)}(j|x(t_1) = i) = \sum_{k \in i} p_{x(t_1)}(k|x(t_1) = i) p_{x(t_0)}(j|x(t) = k); $$

(27)

which can be expressed in words as follows, the probability of being transported from grid-box $j$ to grid-box $i$ is equal to the sum of the probabilities of being transported first from grid-box $j$ to an intermediate grid-box $k$ and then from grid-box $k$ to grid-box $i$ for each possible intermediate grid-box not in the surface layer (see figure 2).

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{figure2.png}
\caption{Schematic diagram showing how the probability $p_{ik(t_0,t_1)}$, that a fluid parcel going from grid box $j$ to grid box $i$ during the time interval from $t_0$ to $t_1$ is equal to the sum over all $k$ of going first from $j$ at time $t_0$ to $k$ at time $t$ and then from $k$ at time $t$ to $i$ at time $t_1$.}
\end{figure}

In matrix form this gives

$$ P^*_i(t_1, t_0) = P^*_j(t_1, t) P^*_k(t, t_0). $$

(29)

Differentiating equation (29) with respect to $t$ we get

$$ 0 = \frac{\partial P^*_i(t_1, t)}{\partial t} P^*_k(t, t_0) + P^*_k(t_1, t) \frac{\partial P^*_i(t, t_0)}{\partial t} $$

(30)

and then using equation (11) to eliminate the time derivative in the second term on the right hand side of (30) we get

$$ 0 = \frac{\partial P^*_i(t_1, t)}{\partial t} P^*_k(t, t_0) - P^*_k(t_1, t) T(t) P^*_i(t, t_0). $$

(31)

Finally, pre-multiplying equation (31) by the diagonal matrix $W_i$, with the interior grid-box volumes $w_i$ down the main diagonal and post-multiplying by $P^{-1}_i(t, t_0) W_i^{-1}$ and taking the transpose we get

$$ 0 = W_i^{-1} \frac{\partial P^*_i(t_1, t)}{\partial t} W_i - W_i^{-1} T^T(t) W_i W_i^{-1} P^*_i(t_1, t) W_i. $$

(32)

which we can rewrite as

$$ \frac{\partial}{\partial t} T^*_i(t, t) = T^*_i(t) P^*_i(t, t), $$

(33)

where

$$ T^*_i(t) = W_i^{-1} \frac{1}{T(t)} W_i $$(34)

$$ P^*_i(t_1, t) = W_i^{-1} P^*_i(t_1, t) W_i. $$

(35)

Equation (33) is the adjoint tracer transport equation. Since equation (29) is valid only for $t_1 > t$, equation (33) should be integrated back wards in time starting from the "final" condition

$$ P^*_i(t_1, t_1) = I. $$

(36)
The advantage of equation (33) is that it can be used to solved for $F^*_n(t, t_0)$ as a function of the second time argument as is needed to compute the distribution of last passage time from the surface using equation (26).

3. Steady Transport Operator

For the special case where the transport operator is independent of time, expressions (23) and (26) for the first and last passage time distributions simplify considerably because $F^*_n(t, t_0)$ becomes a function of only the time difference between $t$ and $t_0$. We can then write, $F^*_n(t, t_0) = P^*_n(\tau)$ and $P^*_n(t_0, t) = P^*_n(-\tau)$. Property (12) obtained from Bayes’ theorem then reduces to

$$P^*_n(\tau) = \left( W_i P^*_n(\tau) W_i^{-1} \right)^T = P^*_n(-\tau) \quad (37)$$

Equation (15), for the probability that a fluid parcel will not make contact with the surface layer in the next time interval of length $\tau = t - t_0$ then reduces to

$$s(-\tau) = 1^T W_i P^*(\tau) W_i^{-1} = (P^*(\tau) 1)^T, \quad (38)$$

and the probability density for the first passage time to the surface layer reduces to

$$f(-\tau) = -\frac{d}{d\tau} s^T(-\tau). \quad (39)$$

where $s^T(\tau)$ is obtained by solving

$$\frac{d}{d\tau}s^T(-\tau) = T^*_n s^T(-\tau) \quad (40)$$

Equation (16) for the probability that a fluid parcel did not make contact with the surface layer in the previous time interval of length $\tau$ reduces to

$$s(\tau) = (P^*(\tau) 1)^T, \quad (41)$$

and the probability density for the last passage time to the surface layer reduces to

$$f(\tau) = -\frac{d}{d\tau}s^T(\tau) \quad (42)$$

where $s(\tau)$ is obtained by solving

$$\frac{d}{d\tau}s^T(\tau) = -T^*_n s^T(\tau) \quad (43)$$

The great computational advantage of equations (40) and (43) is that only two single-tracer simulations are needed (one with the forward model and one with the adjoint model) in order to obtain the full distribution of first and last passage times for every interior grid-box in the model.

3.1 Moments of the First and Last Passage Time Distributions

For the case where the transport operator is independent of time, the moments of the first and last passage time distributions can be obtained recursively by inverting the transport operator without having to time-step the transport equation.

As a first step to obtaining the recursive formula for the moments, we first establish the normalization condition for the first passage time distribution

$$\int_{0}^{\infty} f(-\tau)d\tau = -s^T_{\tau}(-\in\infty) + s^T_{\tau}(0) = 1. \quad (44)$$

Multiplying equation (39) by $\tau^{n+1}$, and integrating with respect to $\tau$ from 0 to $\infty$ using integration by parts gives

$$\tau^{n+1}f(-\tau) \equiv \int_{0}^{\infty} \tau^{n+1}f(-\tau)d\tau \quad (45)$$

$$= (n+1) < \tau^n s^T(-\tau) > \quad (46)$$

Similarly, multiplying the top equation in (40) by $\tau^n$ and integrating with respect to $\tau$ from 0 to $\infty$ using integration by parts gives

$$-n < \tau^{n-1}s^T(-\tau) >= T^*_n < \tau^n s^T(-\tau) > \quad (47)$$

Equations (47) and (46) can then be combined to give

$$T^*_n < \tau^{n+1}f(-\tau) >= -(n+1) < \tau^n f(-\tau) > \quad (48)$$

Setting $n = 0$ and using (44) we can obtain the mean first-passage time by directly inverting the adjoint transport operator

$$< \tau f(-\tau) >= -(T^*_n)^{-1}1. \quad (49)$$

The variance can then be obtained by setting $n = 1$ in (48) and solving

$$< \tau^2 f(-\tau) >= -2(T^*_n)^{-1} < \tau f(-\tau) >, \quad (50)$$

and standard deviation of the distribution

$$std = \sqrt{< \tau^2 f(-\tau) > - < \tau f(-\tau) >^2} \quad (51)$$

The other moments can be obtained recursively. For the moments of the last passage times a similar approach yields the following recursive formula

$$T^*_n < \tau^{n+1}f(\tau) >= (n+1) < \tau^n f(\tau) >, \quad (52)$$

in which one inverts the forward transport operator to obtain the moments.

4. Application To An OGCM

In this section we apply the theory to the time-averaged transport operator of a 3-dimensional global ocean general circulation. We use a version of the ocean component of the Canadian Centre for Climate Modelling and Analysis climate model (NCOM). The model has 29 levels in the vertical ranging in thickness from 50 meters near the surface down to 300 meters near the bottom. The horizontal resolution has 48 grid-points meridionally and 96 grid-points zonally for an approximate resolution of $3.75' \times 3.75'$. The KPP (Large et al. 1994) vertical mixing scheme as well as the GM (Gent and McWilliams 1999) isopycnal mixing scheme are used. Tracers are advec ted using a second order centered difference scheme.
The dynamical model is forced by a prescribed monthly freshwater and heat fluxes obtained as output from the atmospheric component of the climate model together with a restoring to observed surface temperature with a 30 day timescale and to observed surface salinity with a 180 day timescale.

The model was spun-up for over 8000 years and the flow field and the diffusion tensor fields were averaged over a period of 5 years at the end of the simulation. These time averaged fields were then used to construct the time averaged advection-diffusion transport operator.

In figure 4 the mean last-passage time from the surface layer and the mean first-passage time to the surface layer are shown for a depth of 2615 m. The presence of deep water formation in the North Atlantic and its absence in the North Pacific are apparent in figure 4 by the much older water in the North Pacific compared to the North Atlantic. Also apparent in the North Atlantic is the presence of a deep western boundary current carrying young water southward.

**Fig. 3:** Mean last-passage time from the surface layer (upper panel). Mean first-passage time to the surface layer (lower panel).

The upper panels of figure 4 show vertical cross sec-
tions of the mean last-passage time to the surface in the Atlantic Ocean at 30W, as well as the standard deviation of the distribution. The lower panels of figure 4 show the same cross sections for the mean first-passage time to the surface layer.

Surface waters are generally younger deep waters and the distribution for the deeper waters is generally broader except in the polar regions where the distributions are younger with smaller standard deviations.

4.0.1 GLOBAL INVENTORY FUNCTION

The volume integral, $K(t)$, of the last-passage time distribution

$$K(t) = \int \mathbf{1}^T \mathbf{W} f(t)$$

(53)

gives a global inventory of when fluid parcels made their last contact with the surface layer. Figure 4 shows a plot of the global inventory function. For short times, $K(t)$ scales as $t^{-1/2}$. Such a scaling is consistent with the dominance of the diffusive terms for short times. More surprising is that the $t^{-1/2}$ scaling persists out to approximately 900 years (figure 4 upper panel). For large times, $K(t)$ scales as $e^{t/\tau_1}$ where $1/\tau_1$ is the lowest eigenvalue of the transport operator. The time scale $1/(1/\tau_1 - 1/\tau_2 u_2) = 918$ years (where $\tau_1 = 797$ and $\tau_2 = 427$), associated with the difference between the two lowest eigenmodes gives a rough estimate of the transition time between the two regimes. The first moment of $K(t)$ is 658 years and the standard deviation of $K(t)$ is 360 years.

5. Discussion

The concept of age and age distribution is becoming a familiar concept in oceanography because of its importance for understanding the ventilation properties of the ocean (e.g. England 1995, Hall and Haine 2002). The distribution of first-passage times to the surface has received much less attention, but it also characterizes oceanic transport. It may also have application to the anthropogenic CO2 problem because of current proposals to inject CO2 captured at the source directly into the deep ocean – the time-scale for the transport of fluid parcels from the deep ocean to the surface will determine in part the efficiency of the deep ocean as a reservoir of anthropogenic carbon.

In this study we have used a direct matrix inversion of a time-averaged OGCM transport operator to efficiently compute the first few moments of the first and last passage time distribution without having to explicitly time step the model.

6. References


