Biogeosciences Discuss., 6, 10177–10194, 2009
www.biogeosciences-discuss.net/6/10177/2009/

Biogeosciences Discussions

This discussion paper is/has been under review for the journal Biogeosciences (BG).
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A comparison of the variability of biological nutrients against depth and potential density

J. While[1] **and K. Haines**[2]

[1]Met Office, Fitzroy Road, Exeter, Devon, EX1 3PB, UK
[2]ESSC, University of Reading, Reading, RG 6AL, UK

Received: 28 August 2009 – Accepted: 8 September 2009 – Published: 30 October 2009

Correspondence to: J. While (james.while@metoffice.gov.uk)

Published by Copernicus Publications on behalf of the European Geosciences Union.

Abstract

The main biogeochemical nutrient distributions, along with ambient ocean temperature and the light field, control ocean biological productivity. Observations of nutrients are much sparser than physical observations of temperature and salinity, yet it is critical to validate biogeochemical models against these sparse observations if we are to successfully model biological variability and trends. Here we use data from the Bermuda Atlantic Time-series Study and from the World Ocean Database 2005, to demonstrate quantitatively that over the entire globe a significant fraction of the temporal variability of phosphate, silicate and nitrate within the oceans is correlated with water density. The variability of these nutrients with respect to depth and neutral density is estimated and it is shown that in most regions variability against density is significantly reduced. The largest reductions in variability were found within the main pycnocline. This in principle allows nutrient distributions to be inferred from physical hydrographic measurements, a fact that can usefully be applied to modeling, assimilating, and, in the long term, for biogeochemical forecasting.

1 Introduction

The distribution of biological nutrients within the world's oceans is one of the significant determining factors in the distribution of oceanic life (Falkowski et al., 1998). For instance, high nutrient coastal regions are the source of most of the world's fish (Watson et al., 2004), while the nutrient poor subtropical gyres are relatively devoid of life (Sharp et al., 1980). Consequently, our understanding of biogeochemical processes is intimately linked to our knowledge of the behavior of dissolved nutrients. In particular, modeling efforts (see, for example, Palmer and Totterdell, 2001; Le Quéré et al., 2005) of global ocean biogeochemistry need to accurately model nutrient fields in order to simulate ocean biogeochemistry. However, nutrient behavior can be complex as it depends on both the physical circulation of the ocean and on biological activity. Nutrient

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data are usually sparse, both spatially and temporally, and it can therefore be difficult to gain an understanding of the variability.

In this paper we examine the temporal and spatial co-variability of nutrients and potential density. The aim is to determine how much of the nutrient variability in any location can be ascribed to dynamical processes that also affect the variability of water density. In particular, the propagation of internal waves and Rossby waves, both controlled by the potential density distribution, lead to displacements of all Lagrangian water properties, including the nutrients. This can, depending on location, provide a large fraction of the inherent variability of the fields. Temperature, T, and salinity, S, have long been known to co-vary in the physical oceanography literature (see, for example Iselin, 1939), and similar diagnostics to those used here have been presented for looking at S (T) variability in Troccoli and Haines (1999) and Haines et al. (2006).

In previous studies the dependence of nutrients on density has been demonstrated at single observing locations where large amounts of data exist; examples include the work presented in McGillicuddy Jr. et al. (1999) for the BATS (Bermuda Atlantic Time-series) station, and the work in Archer et al. (1996) for the equatorial pacific. However, validity of these relationaships over large regions have not been quantitatively demonstrated before. Nevertheless nutrient distributions are commonly presented plotted along isopycnal surfaces (see, for example, Sarimento and Gruber, 2006, Figs. 5 ,3, 8 and 7, 3, 5) on the assumption that this will give smoother distributions for passively advected tracer quantitites. However, nutrient-density relationships are not guaranteed to hold everywhere as nutrients are affected by biological activity and other sources and sinks, which are highly spatially varying. The aim of this paper therefore is to use all available data to quantitatively assess where nutrient-density relationships exist at global scales.

In this paper we examine how nutrients, generically represented by N, vary both with respect to depth $N(z)$ and with respect to density $N(\rho)$, over different spatial scales. The results therefore give a spatial representation of the goodness of nutrient density relationships for the first time. In consequence, the results show directly where nutrient

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variability can be forecast based on the much better known and observed variability of the water density. At the end of this paper we discuss the potential for use of these results in biogeochemical modeling and data assimilation.

Section 2 of this paper shows, in agreement with McGillicuddy Jr. et al. (1999), how the nutrients nitrate, phosphate, and silicate vary within a water column using data taken from the Bermuda Atlantic Time-series Study, (BATS; Phillips and Joyce, 2007). From these data we show that near Bermuda the variability of $N(\rho)$ is considerably reduced within the main thermocline. More significantly, a global perspective is then considered in Sect. 3 where World Ocean Database (WOD05; Garcia et al., 2006) data are used to show that $N(\rho)$ is of lower variability than $N(z)$ over almost all of the world's oceans. The paper concludes with a section discussing our results and their relevance to biogeochemical modeling and data assimilation.

2 Nutrient time-series at the BATS site

To illustrate how the variability of nutrients changes down a water column at a single site, we repeat some of the work of McGillicuddy Jr. et al. (1999), but including more recently available data. Specifically we present results obtained from an analysis of the BATS data set. The BATS time-series, obtained from approximately 75 km SE of Bermuda, provides a long data record of nutrients that stretches back to 1988, with a sampling interval of approximately one month. As such, the BATS data set contains a high density of measurements in a highly localized area. Crucially for our purposes, measurements taken within BATS include phosphate, nitrate (combined with nitrite), silicate, and potential density (derived from temperature and salinity). Such a large collection of data allows us, with a high degree of accuracy, to quantitatively assess the variability of both $N(\rho)$ and $N(z)$.

Nitrate + nitrite, phosphate, and silicate are plotted against depth and potential density (referenced to 2000 m) in Fig. 1 rows (a) and (b). A visual inspection reveals that the scatter of the data around the "mean" relationship appears much smaller on the

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$N(\rho)$ plots, (b), than on the $N(z)$ plots, (a). This reduction is most obvious where the nutrient concentration increases dramatically with increasing density through the main thermocline. We quantize this reduction in (c) which shows the variance of $N(\rho)$ and $N(z)$ as a function of depth over the top 1500 m of the water column. The variance of $N(z)$ was calculated at 20 m intervals using all data within ±10 m; any interval containing no data was excluded from the result. Conversely, the variance against potential density was obtained by finding the mean density within each 20 m interval and reallocating the nutrient data between the intervals using a nearest in density approach. After this process the nutrient variance was calculated for each depth interval, defined now by its mean density.

Outliers within the data, several of which are clearly visible in Fig. 1b, can severely bias the above variance calculation. As such, outliers were identified and removed prior to calculating the variances. As temperature, salinity, and nutrient errors all contribute to the $N(\rho)$ plots, outliers were identified using these data rather than $N(z)$. Outlier identification was performed by calculating the median absolute deviation of the Nutrient data in an advancing 0.4 kg/m^3 window that moved down the water column; any data point lying more than 3 median deviations from the median was flagged as an outlier. Once flagged, outliers were rejected from the variance calculations of both $N(\rho)$ and $N(z)$.

It is clear from the plots in Fig. 1c that between 300 m and 1000 m there is a very substantial reduction in the variability of all of the nutrients. This is indicative of the nutrient distribution being strongly tied to the vertical density structure of the water within the main thermocline. Here dynamically induced variability associated with vertical heaving of the water column raises the depth level variance, but not the density level variance. At other depths, including depths below 1500 m which we do not show, the variance of $N(\rho)$ is approximately equal to the variance of $N(z)$. In shallow waters the biological processing of nutrients and mixing within the mixed layer will tend to break any Nutrient density relationships. In the deep ocean the dominant variability is less likely to be due to vertical heave of the water column on short timescales and more

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likely to be due to slower processes.

BATS is but a single time-series and its results apply to only one location. However, it is not unreasonable to assume that similar processes are taking place elsewhere leading to similar patterns of variability with depth. In the next section we extend our scope to look at global variability.

3 Global variability

In order to obtain the variability relationships that exist for nutrients on a global scale, we have analyzed nutrient data collected after 1990 available from the WOD05 database. These data give global coverage of the nutrients phosphate, nitrate, and silicate, though there are large gaps in the data set (the data distribution is shown in Fig. 3a). In order to estimate the variability of $N(\rho)$ and $N(z)$ we rejected any data that were flagged – for whatever reason – within the data set. We also rejected any data that didn't consist of concomitant measurements of temperature, salinity, depth, and nutrient. After these initial checks the data were binned into $2^{\circ}\times2^{\circ}$ bins, with each bin treated as representing a single water column.

3.1 Methods

Outliers in each of these bins were again removed using a median based technique; however, as we have far fewer data in a water column, this process needs to be more flexible than for the BATS data. As with BATS, only $N(\rho)$ data were used in the determination of outliers, but once identified outlying points were rejected from both $N(\rho)$ and $N(z)$. To determine whether a data point k was an outlier it was compared to a set of nearby data points. These comparison points were found by gradually increasing the density window $\rho_k \pm \eta\Lambda_k$ until at least 10 data points were found, where ρ_k is the density of k, Λ_k is the full potential density range (referenced to the depth of k) of all data within the bin, and η=0.001, 0.002, 0.003, ..., 0.1. If there were fewer than 10 data

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points available in the largest window (±0.1Λ) then all data points within this window were used down to a minimum of 4. The selected data were detrended and the median and median deviation calculated. If the nutrient value of data point k exceeded 3 median deviations from the median of the window, then k was rejected as an outlier. This method detects most outliers; however, erroneous data points with excessively high densities outside the true density range can be missed. To avoid this problem we also check that the potential density of point k is within 3 median deviations of the potential densities of the other data points within the adaptive window.

With the outliers removed the remaining WOD05 data in each bin were used to estimate the ratio R given by

$$R = \frac{\sum_{j=1}^{M} \left| N_j(\rho_j) - \mu_\rho(\rho_j) \right|}{\sum_{k=1}^{M} |N_k(z_k) - \mu_z(z_k)|}, \quad (1)$$

where M is the number of data points per bin down to a user chosen maximum depth h, N is the amount of a nutrient (either nitrate, silicate, or phosphate) measured at a data point, ρ is the water density, and z is the depth. If R is less than 1 then there is less scatter, hence less variability, in $N(\rho)$ than in $N(z)$ and vice versa if $R>1$. The mean absolute deviation of the data is used because it is a more robust estimator of the variability in the presence of outlying data. This is desirable because we cannot optimize our method for every bin and poor estimates of μ_z and μ_ρ in bins with sparse data can lead to outlying data points.

The functions μ_ρ and μ_z, are the "mean" nutrient profiles with respect to density and depth. It is evident from the BATS data, Fig. 1, that these functions often have a complex structure within a water column. For a data point k, a local estimate of μ_z was calculated from

$$\mu_{zk} = m_k z_k + c_k \quad (2)$$

where z_k is the depth of k and μ_{zk} is the value μ_z takes at k. The parameters m_k and c_k, specific to k, are the gradient and intercept of a local linear regression about

k. The regression was calculated using all data found within the smallest of $z_k \pm \eta \Lambda_z$ that, excluding k, contained 10 data points; here Λ_z is the full depth range of the data, and η is defined as before. If the largest window ($\pm 0.1 \Lambda_z$) contained less then 10 data points, then all data within the window were used down to a minimum of 3 points, otherwise μ_{zk} cannot be estimated and k was rejected. Excluding point k from the estimate ensures that μ_{zk} is independent of k. Since measurements in WOD05 tend to be available at standard depths, it is common to have a lot of data at, or near to, a single depth, with no other nearby data. A linear fit is then ill-conditioned and the data mean was used for μ_{zk}.

The calculation of μ_ρ proceeded in a similar fashion, but using the potential density referenced to the depth of k. However, at large depths (higher densities) a complication arises because the nutrients, especially silicate, can increase very rapidly with potential density, as seen for silicate in Fig. 1a. This makes it hard to determine μ_k, so the maximum depth parameter h is included in the calculation of R. Setting h to a moderate depth (2000 m) avoids this problem while relatively little data are lost, see Fig. 4(b).

3.2 Results

The value of R for the 2° binned WOD05 data down to a maximum depth h=2000 m is shown for phosphate, silicate, and nitrate in Fig. 3b–d. Also given in this Figure are the number of bins $P_{<1}$ that have $R<1$, the number of bins $P_{>1}$ for which $R>1$, and the number of bins $P_{<0.9}$ in which $R<0.9$. While there is a lot of spatial variability in the plots, it is apparent that most bins, by a ratio of 3:1 or more, have $R<1$. Translated into relative area, $R<1$ over 79% of the area for which we have nitrate data, 80% for phosphate data, and 74% for silicate data. More significantly, for all three nutrients $R<0.9$, corresponding to the variability of $N(\rho)$ being at least 11% less than the variability of $N(z)$, more than twice as often as $R>1$. In fact, in terms of relative area, $R<0.9$ over more than half of the area for which we have data (60% for nitrate; 62% for phosphate; 54% for silicate). Thus from the WOD05 data it appears that variations in nutrients are tied to variations in water density over most of the world's oceans.

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There is a lot of scatter in the value of R in Fig. 3, both spatially and between the three nutrients. To get an in-depth and detailed analysis of what is happening would require a bin by bin examination of the data, which is beyond the scope of this paper. Broadly speaking, nitrate and phosphate tend to have smaller values of R than silicate. This is a consequence of differences in the vertical distribution of the nutrients. Nevertheless, in the data rich north Pacific and north Atlantic R is generally less than 0.9 demonstrating a consistent weak but measurable $N(\rho)$ relationship in these waters. It may be that with more high quality data in these regions we would expect to get results similar to BATS, where $R_{\mathrm{BATS}} \approx 0.7$. Interestingly, in the southern oceans below 40°S, R is often fairly low (sometimes less than 0.5) suggesting good $N(\rho)$ relationships; this is despite the somewhat weaker density stratification present at these latitudes. Although data are limited in the southern oceans, a detailed inspection was conducted on a few bins and the results were found to support the idea of lower variability there.

Further to above, we carried out an experiment on WOD05 nitrate data where we varied the width of the data bins used to calculated R. The values of $P_{>1}/P_{<1}$ obtained from this experiment are shown in Fig. 2. A significant reduction in the value of $P_{>1}/P_{<1}$ is seen as the bin size increases. This reduction is probably due to increasing numbers of data points per bin allowing more accurate determinations of the value of R. It is also an indication that, in the mean, nutrient density relationships change relatively slowly across the ocean. If this were not true then horizontal variations in the nutrient-density relationship would counteract the improvement in $P_{>1}/P_{<1}$. However, it appears that the data in Fig. 2 are leveling-off at a bin size of 5 degrees and lateral variations in nutrient-density may be starting to become significant.

Two tests were done to check that the results shown in Figs. 3 and 2 are not due to biases in our analysis method. The first test allowed for a broader data window – $z_k \pm \eta\Lambda_z$ expanded until it contained 40 data points. This test permits more data and allows for more accurate regressions, but is also less local and produces larger errors when μ_z and μ_ρ are strongly non-linear. Applied to WOD05 nitrate data the results from this test were not significantly different to the results obtained above; the new

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values were $P_{>1}$=1081, $P_{<1}$=3954, and $P_{<0.9}$=2999. Such small changes in the results show that our method is relatively insensitive to the size of the local data window and that we can have confidence in the values of R obtained. In the second test we carried out the following experiment. An estimate of R was obtained by applying our method to WOD05 depth and density data, but with the WOD05 nutrients replaced with uniformly distributed random values from 0 to the largest measured nutrient value. Discounting outlier removal, not done in the test, we expect $R>1$ and $R<1$ to be equally likely. The test found a small but distinct bias towards R being greater than 1. This bias is explained by the practice of measuring nutrients on, or as close as possible to, standard depth levels, such as the distinct levels seen on Fig. 1a. Consequently we have a very large number of measurements at relatively few depths and very few measurements elsewhere. This enables μ_z to be determined very accurately at depths where we have data. Conversely, plotted against density the data are spread out along a trend, and thus it is more difficult to determine μ_ρ. This effect is sufficient to bias R. The bias is slight as, excluding bins with less than 1000 points, the mean value of R was 1.01, with a standard deviation of 0.01. That the plots of Fig. 3 show, despite this bias, a very clear signal of $R<1$ almost everywhere, strongly suggests that the variability of nutrients on potential density surfaces is indeed reduced.

As with the BATS data, we wish to know where in the water column the reduction in variability of $N(\rho)$ takes place. We calculated the absolute deviations about μ_z and μ_ρ of all data points in the WOD05 data. These deviations were then collected into 100 m depth bins and their averages taken. The results of this test applied to WOD05 phosphate data (results for nitrate are similar, while silicate follows the same pattern, but has less variability reduction in the near surface) can be seen in Fig. 4a. In the top 1000 m there is a clear reduction of up to 10% in the mean deviation of $N(\rho)$, while below this depth the variability is roughly the same between $N(z)$ and $N(\rho)$. There is some indication that the variability of $N(\rho)$ has been slightly increased at depth, but this effect is small and likely due to the bias of the method. The results seen in the figure are consistent with what is seen at BATS, with upper water column variability

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reduction and then equality of variability at greater depths. This is in agreement with our earlier assertion that an $N(\rho)$ relationship exists where both nutrients and isopycnals are moved up and down by vertical heave of the thermocline. That this appears to happen over a broader range of depths than in the BATS data is indicative of the variation in mean depth of the thermocline across the globe.

4 Summary and discussion

We have shown, through the analysis of in-situ nutrient (nitrate, phosphate and silicate) measurements, that a significant amount of the variability of these nutrient distributions is coupled to the variability of the potential density over most of the ocean. In other words, the nutrient distributions show covariability with the potential density indicating that the variability is of a dynamical origin.

Relationships between nutrients and density have been demonstrated both at a single location, using the data rich BATS time-series, and, more importantly, in a global sense using data from the WOD05 database. In both data sets the variability of the nutrients against potential density was shown to be significantly reduced.

Our results may be explained by the coupling of nutrients to potential density removing the variability due to the dynamical effects of wave propagation. In the case of waves, the vertical motion of water affects the nutrients and potential density in the same way. Other processes, such as surface heating and biological activity, will tend to increase the variability of both $N(\rho)$ and $N(z)$. Nonetheless, our results seem to indicate that vertical motion does play a significant role is determining the nutrient structure of the oceans.

Lateral dynamical transfer of differing water masses will also break the $N(\rho)$ relationship; however, our results indicate that nutrient-density relationships hold over significant areas of the oceans, implying that the effect of lateral transfer will be small. In fact, when testing the $N(\rho)$ relationship with the WOD05 data, results improved as we averaged over larger areas. This improvement continued out to 5°, which was the

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largest bin size used in our experiments. The nutrient-potential density relationships we find in most ocean regions holds most strongly in upper waters, particularly through the main pycnocline, although not necessarily right to the surface. Close to the surface factors such as biological processing break the $N(\rho)$ relationship, while at depth there is relatively little vertical motion of the water and slower processes dominate.

We note that the $N(\rho)$ relationships we have demonstrated can be of importance to practitioners of data assimilation in biogeochemical models. Biogeochemical models can be of very different levels of complexity, but they all share a common dependence on the underlying nutrient distributions, and unfortunately these are often poorly represented in models. In recent studies data assimilation has been used to constrain either the biogeochemical variables themselves (examples include Triantafyllou et al., 2003; Nerger and Gregg, 2007; Hemmings et al., 2008) and/or the physical state of the ocean (Anderson et al., 2000; Eden and Oschlies, 2006). However, in such assimilation schemes nutrients are usually left unconstrained, leading to the breakdown of the nutrient-water mass relationships and a worsening of the modeled nutrient fields. With the results demonstrated here it should now be possible to make adjustments to the nutrient distributions to retain these relationships by introducing nutrient balancing increments similar to the approach used for salinity in Troccoli and Haines (1999). This gives the possibility of considerably improving the reproduction of nutrient distributions in biogeochemical models, which will have a big impact on all areas of model behavior. Experiments using these idea are ongoing and results will be reported in a separate study.

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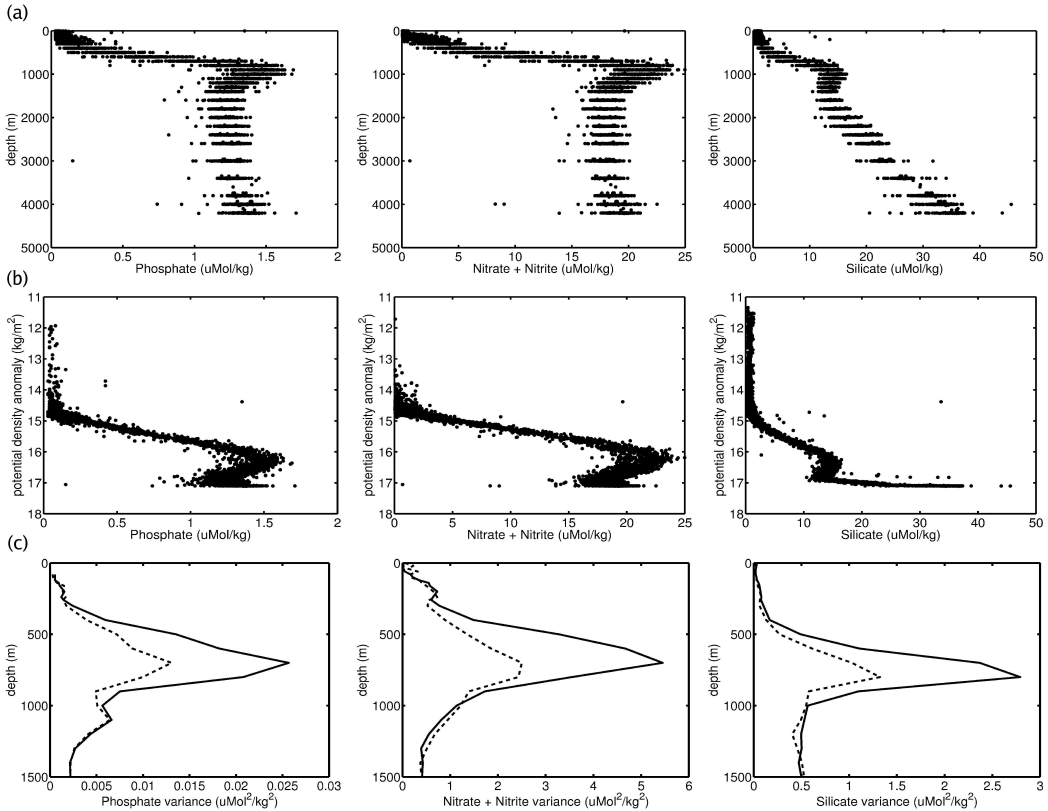

Fig. 1. BATS nutrient concentration data plotted against **(a)** depth and **(b)** potential density anomaly ($\rho - 1020\,\mathrm{kg/m^3}$) referenced to 2000 m. Plots on row **(c)** show the variance of the data with depth down to 1500 m.

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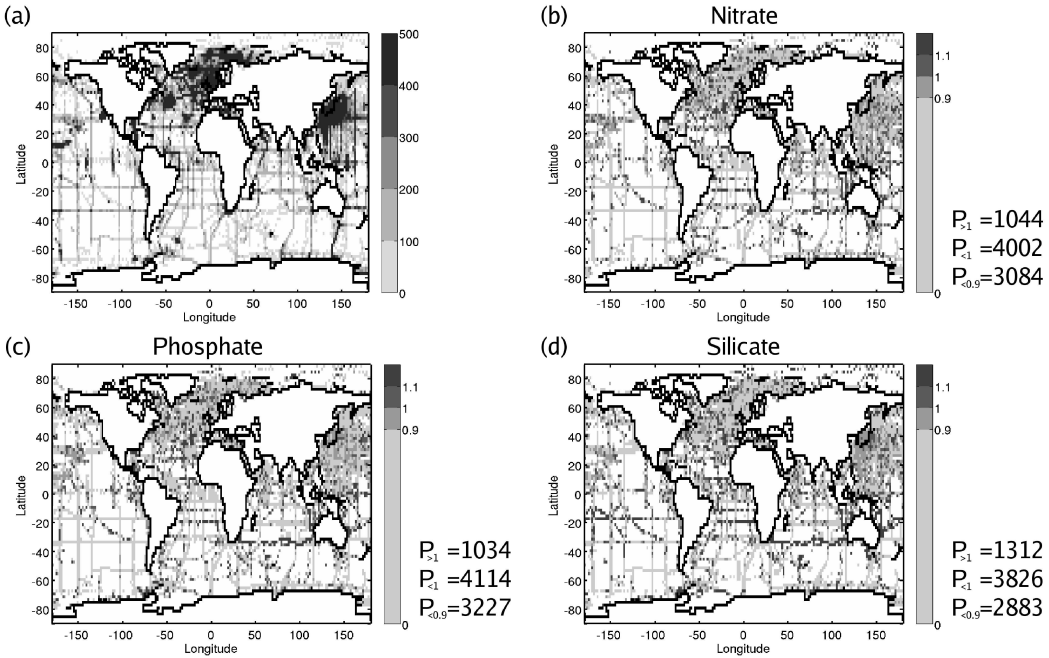

Fig. 2. The value of R, see text, gridded into 2° bins. The nutrients shown are **(b)** Nitrate, **(c)** Phosphate, and **(d)** Silicate. **(a)** Shows the number of data points available to estimate R. The plots were generated from World Ocean Database data measured from 1990 onwards. $P_{<1}$ is the number of bins with $R<1$, $P_{>1}$ is the number of bins with $R>1$, while $P_{<0.9}$ is the number of bins with $R<0.9$. A non-linear scale is used to highlight the structure near the critical value of $R=1$.

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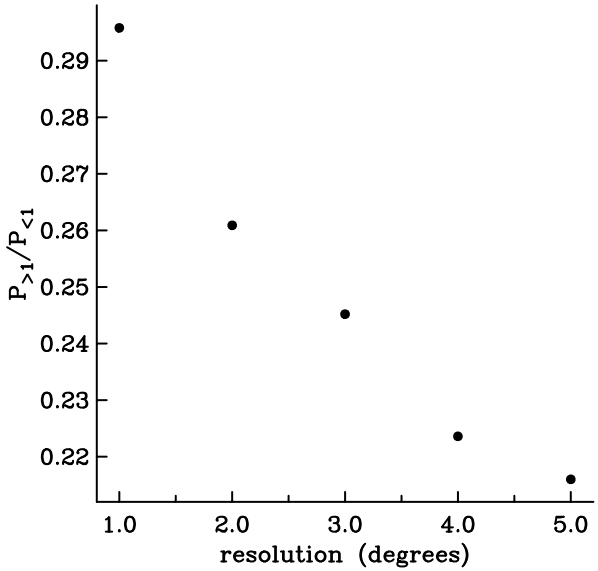

Fig. 3. $P_{>1}/P_{<1}$ for nitrate data as bin size is varied from 1 to 5 degrees.

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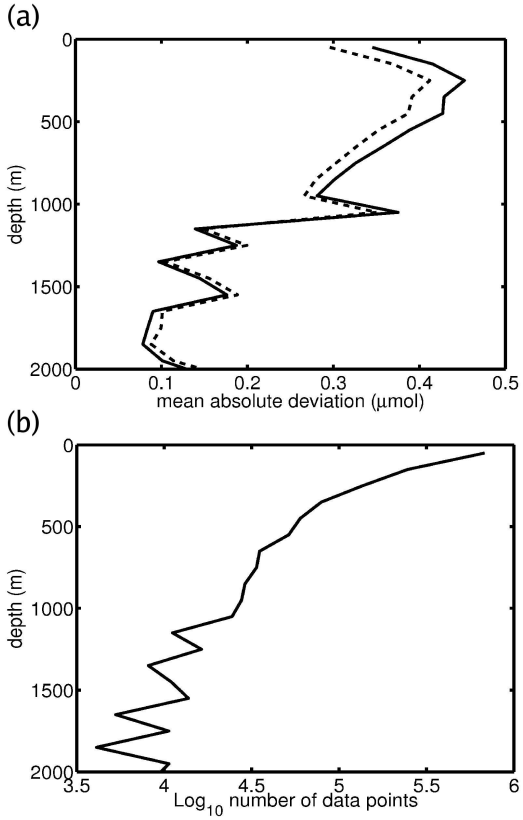

Fig. 4. (a) Mean absolute deviation of WOD05 phosphate down to 2000 m. Solid line: deviation against depth; dashed line: deviation against density. **(b)** the number of data points available to estimate .

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