

Notes on the GSW library function `gsw_delta_SA`

Notes made 27th September 2010 regarding version 2 of this function which looks up version 2 of the global δS_A data base.

The thermodynamic properties of seawater are functions of Absolute Salinity S_A (rather than of Practical Salinity S_P). If a seawater sample has Standard Composition (that is, the sample is a sample of Standard Seawater, SSW) then its Absolute Salinity S_A is equal to its Reference Salinity S_R which is proportional to its Practical Salinity S_P according to

$$S_R = \left(\frac{35.165\,04\text{ g kg}^{-1}}{35} \right) S_P . \quad (1)$$

When a seawater sample has non-standard composition, the relationship between Practical Salinity and Absolute Salinity is more complicated, and the difference between Absolute Salinity and Reference Salinity is called the Absolute Salinity Anomaly δS_A .

The most direct way of evaluating δS_A is via measuring the density of a seawater sample, for example, by using a vibrating beam densimeter in the laboratory. Another method of estimating δS_A is via measurements of total alkalinity (TA), dissolved inorganic carbon (DIC), silicate and nitrate, together with a model of seawater properties (such as that of Pawlowicz *et al.* (2010)) to relate these measurements to δS_A . Due to the relative paucity of these measurements, a method for estimating the Absolute Salinity Anomaly δS_A has been developed based on spatially interpolating a global data base of δS_A which is stored as a function of longitude, latitude and pressure. The GSW function `gsw_delta_SA` does this interpolation.

This GSW algorithm for calculating Absolute Salinity from Practical Salinity, `gsw_SA_from_SP`, takes the form (see McDougall *et al.* (2010a))

$$S_A = S_R + \delta S_A = \left(\frac{35.165\,04\text{ g kg}^{-1}}{35} \right) S_P + \delta S_A(\lambda, \phi, p) = S_A(S_P, \lambda, \phi, p), \quad (2)$$

where λ is longitude (degrees east, ranging from 0°E to 360°E), ϕ is latitude (degrees North), p is sea pressure, and the Absolute Salinity Anomaly δS_A is obtained from the `gsw_delta_SA` algorithm of McDougall *et al.* (2010a). In this algorithm the Baltic Sea is treated separately, following the work of Feistel *et al.* (2010), because some rivers flowing into the Baltic are unusually high in calcium carbonate. In fact, in the Baltic Sea the Absolute Salinity Anomaly is a function of only Practical Salinity S_P , namely $S_A - S_R = 0.087\text{ g kg}^{-1} \times (1 - S_P/35)$ (from Eqn. (A.5.6) of IOC *et al.* (2010), following Feistel *et al.* (2010)), so that Absolute Salinity S_A in the Baltic Sea is given by

$$S_A = \frac{(35.165\,04 - 0.087)\text{ g kg}^{-1}}{35} S_P + 0.087\text{ g kg}^{-1}. \quad \text{Baltic Sea} \quad (3)$$

The Absolute Salinity Anomaly of the GSW function `gsw_delta_SA` is illustrated in Figure 1 (a) at a pressure of 2000 dbar, and in a vertical section through the Pacific Ocean in Figure 1 (b). As described in appendix A.5 of the TEOS-10 Manual (IOC *et al.* (2010)), the values of Absolute Salinity Anomaly in the global data set underlying the `gsw_delta_SA` function have been obtained by correlating densimeter-based measurements of δS_A with silicate concentrations in the different ocean basins. Heuristically the dependence of $\delta S_A = S_A - S_R$ on silicate can be thought of as reflecting the fact that silicate affects the density of a seawater sample without significantly affecting its conductivity or its Practical Salinity. In practice this explains about 60% of the effect and the remainder is due to the correlation of other composition anomalies (such as nitrate) with silicate.

The silicate data that underpins the global data base of δS_A in the gsw_delta_SA function is stored with horizontal resolution of $4^\circ \times 4^\circ$ in longitude and latitude, and this has been taken from the Gouretski and Koltermann atlas of hydrographic data by adopting the deepest cast in the Gouretski and Koltermann atlas within $\pm 2^\circ$ of latitude and longitude of the final grid. The resulting $4^\circ \times 4^\circ$ global data has rather more ocean and less land than does the planet. This has been done to ensure that any sample from the real ocean will definitely be processed by the function. This is illustrated in Figure 2 which indicates how the ocean is allowed to spill over into the continents.

If the latitude and longitude are found by the gsw_delta_SA function to place the observation well away from the ocean, a flag 'in_ocean' is set to zero as a warning, otherwise it is 1. This flag is only set when the observation is well and truly on dry land; often the warning flag is not set until one is several hundred kilometres inland from the coast.

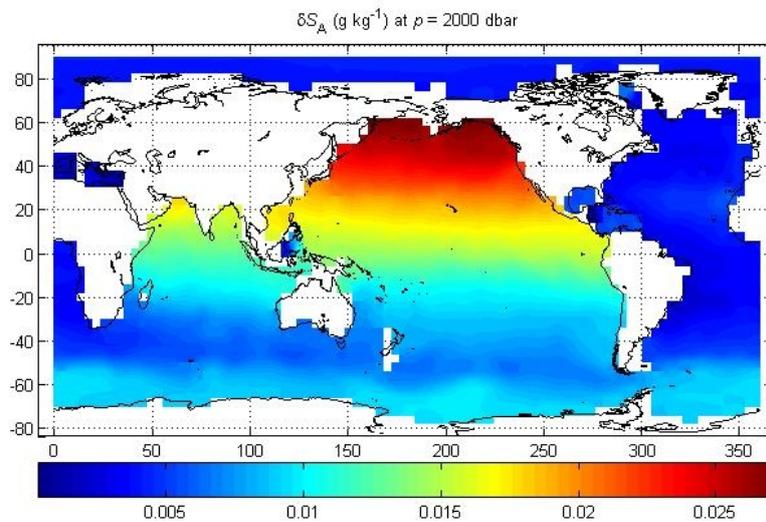


Figure 1 (a). Absolute Salinity Anomaly δS_A at $p = 2000$ dbar.

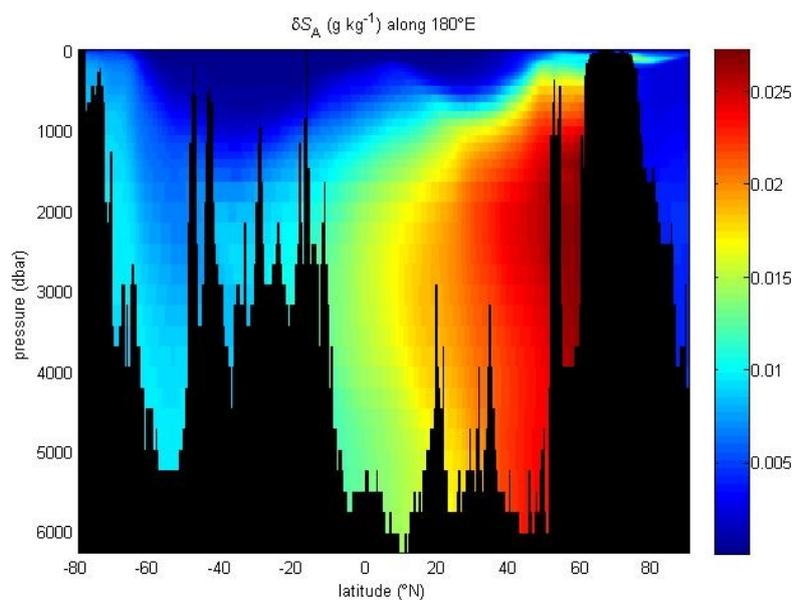


Figure 1 (b). A vertical section of Absolute Salinity Anomaly δS_A along 180°E in the Pacific Ocean.

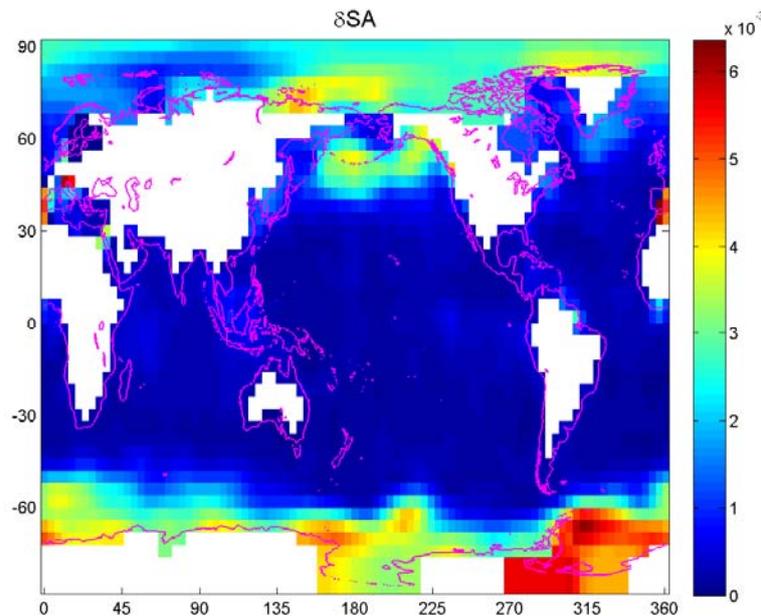


Figure 2. Values of the Absolute Salinity Anomaly (g kg^{-1}) of the gsw_delta_SA global data set at the sea surface. The gsw_delta_SA function returns the flag 'in_ocean' as zero in the white regions of this figure, otherwise the 'in_ocean' flag is set to 1.

During the interpolation of the underlying data set, care is taken not to interpolate between different ocean basins in the vicinity of the Panama Canal and the Indonesian Throughflow. Also, if the input data point is deeper than any of the surrounding four vertical atlas profiles, the deepest "bottle" of the reference profile is used (that is, the reference profile is effectively extended deeper at the δS_A value of its deepest bottle).

The first version of this function was made available in early 2009. The second version (version 2) is being released in October 2010. This version calls version 2 of the global δS_A data set which is almost identical to the data set of version 1. The changes are that (i) two regions adjacent to the Antarctic continent where there previously was no data have been filled in, (ii) the data set has been formed from the deepest vertical profiles in the Gouretski and Koltermann atlas within $\pm 2^\circ$ of latitude and longitude of the final grid rather than simply sub-sampling to the $4^\circ \times 4^\circ$ grid, and (iii) the flag 'in_ocean' has been added.

References

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- Feistel, R., S. Weinreben, H. Wolf, S. Seitz, P. Spitzer, B. Adel, G. Nausch, B. Schneider and D. G. Wright, 2010: Density and Absolute Salinity of the Baltic Sea 2006–2009. *Ocean Science*, **6**, 3–24. <http://www.ocean-sci.net/6/3/2010/os-6-3-2010.pdf>

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- Pawlowicz, R., D. G. Wright and F. J. Millero, 2010: The effects of biogeochemical processes on oceanic conductivity/salinity/density relationships and the characterization of real seawater. *Ocean Science Discussions*, **7**, 773–836.

Below is appendix A.5 of the TEOS-10 Manual (IOC *et al.* (2010)) which discusses the spatial variations in seawater composition.

A.5 Spatial variations in seawater composition

When the oceanographic data needed to evaluate Eqn. (A.4.10) for $S_A^{\text{dens}} - S_R$ is not available, the look-up table method of McDougall *et al.* (2010a) is recommended to evaluate $\delta S_A \equiv \delta S_R^{\text{dens}} \equiv S_A^{\text{dens}} - S_R$. The following paragraphs describe how this method was developed.

In a series of papers Millero *et al.* (1976a, 1978, 2000, 2008b) and McDougall *et al.* (2010a) have reported on density measurements made in the laboratory on samples collected from around the world's oceans. Each sample has had its Practical Salinity measured in the laboratory as well as its density (measured with a vibrating tube densimeter at 25 °C and atmospheric pressure). The Practical Salinity yields a Reference Salinity S_R according to Eqn. (A.3.3), while the density measurement ρ^{meas} implies an Absolute Salinity $S_A \equiv S_A^{\text{dens}}$ by using the equation of state and the equality $\rho^{\text{meas}} = \rho(S_A^{\text{dens}}, 25 \text{ °C}, 0 \text{ dbar})$. The difference $S_A^{\text{dens}} - S_R$ between these two salinity measures is taken to be due to the composition of the sample being different to that of Standard Seawater. In these papers Millero established that the salinity difference $S_A - S_R$ could be estimated approximately from knowledge of just the silicate concentration of the fluid sample. The reason for the explaining power of silicate alone is thought to be that (a) it is itself substantially correlated with other relevant variables (e.g. total alkalinity, nitrate concentration, DIC [often called total carbon dioxide]), (b) it accounts for a substantial fraction (about 0.6) of the typical variations in concentrations (g kg^{-1}) of the above species and (c) being essentially non-ionic; its presence has little effect on conductivity while having a direct effect on density.

When the existing data on δS_A , based on laboratory measurements of density, was regressed against the silicate concentration of the seawater samples, McDougall *et al.* (2010a) found the simple relation

$$\delta S_A / (\text{g kg}^{-1}) = (S_A - S_R) / (\text{g kg}^{-1}) = 98.24 (\text{Si(OH)}_4 / (\text{mol kg}^{-1})). \quad \text{Global (A.5.1)}$$

This regression was done over all available density measurements from the world ocean, and the standard error in the fit was 0.0054 g kg^{-1} .

The dependence of δS_A on silicate concentration is observed to be different in each ocean basin, and this aspect was exploited by McDougall *et al.* (2010a) to obtain a more accurate dependence of δS_A on location in space. For data in the Southern Ocean south of 30°S the best simple fit was found to be

$$\delta S_A / (\text{g kg}^{-1}) = 74.884 (\text{Si(OH)}_4 / (\text{mol kg}^{-1})), \quad \text{Southern Ocean (A.5.2)}$$

and the associated standard error is 0.0026 g kg^{-1} .

The data north of 30°S in each of the Pacific, Indian and Atlantic Oceans was treated separately. In each of these three regions the fit was constrained to match (A.5.2) at 30°S and the slope of the fit was allowed to vary linearly with latitude. The resulting fits were (for latitudes north of 30°S , that is for $\lambda \geq -30^\circ$)

$$\delta S_A / (\text{g kg}^{-1}) = 74.884(1+0.3622[\lambda / 30^\circ + 1]) (\text{Si(OH)}_4 / (\text{mol kg}^{-1})), \quad \text{Pacific (A.5.3)}$$

$$\delta S_A / (\text{g kg}^{-1}) = 74.884(1+0.3861[\lambda / 30^\circ + 1]) (\text{Si(OH)}_4 / (\text{mol kg}^{-1})), \quad \text{Indian (A.5.4)}$$

$$\delta S_A / (\text{g kg}^{-1}) = 74.884(1+1.0028[\lambda / 30^\circ + 1]) (\text{Si(OH)}_4 / (\text{mol kg}^{-1})). \quad \text{Atlantic (A.5.5)}$$

These relationships between the Absolute Salinity Anomaly $\delta S_A = S_A - S_R$ and silicate concentration have been used by McDougall, Jackett and Millero (2010a) in a computer algorithm that uses an existing global data base of silicate (Gouretski and Koltermann (2004)) and provides an estimate of Absolute Salinity when given a seawater sample's Practical Salinity as well as its spatial location in the world ocean. This computer algorithm accounts for the latest understanding of Absolute Salinity in the Baltic Sea, but it is silent on the influence of compositional variations in other marginal seas. The Absolute Salinity Anomaly in the Baltic Sea has been quite variable over the past few decades of observation (Feistel *et al.* (2010c)). The computer algorithm of McDougall *et al.* (2010a) uses the relationship found by Feistel *et al.* (2010c) that applies in the years 2006-2009, namely

$$\delta S_A = S_A - S_R = 0.087 \text{ g kg}^{-1} \times (1 - S_R / S_{SO}), \quad (\text{A.5.6})$$

where $S_{SO} = 35.16504 \text{ g kg}^{-1}$ is the standard-ocean Reference Salinity that corresponds to the Practical Salinity of 35.

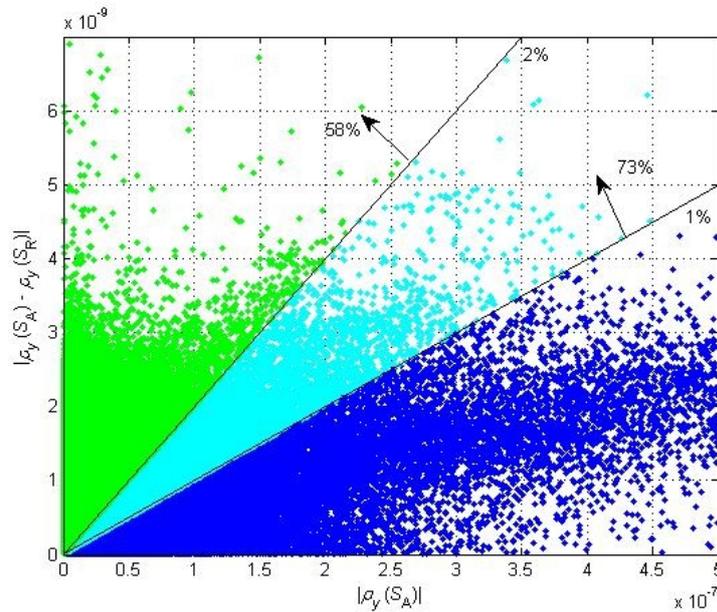


Figure A.5.1. The northward density gradient at constant pressure (the horizontal axis) for data in the global ocean atlas of Gouretski and Koltermann (2004) for $p > 1000$ dbar. The vertical axis is the magnitude of the difference between evaluating the density gradient using S_A versus S_R as the salinity argument in the TEOS-10 expression for density.

In order to gauge the importance of the spatial variation of seawater composition, the northward gradient of density at constant pressure is shown in Fig. A.5.1 for the data in a world ocean hydrographic atlas deeper than 1000m. The vertical axis in this figure is the magnitude of the difference between the northward density gradient at constant pressure when the TEOS-10 algorithm for density is called with $S_A \equiv S_A^{\text{dens}}$ (as it should be) compared with calling the same TEOS-10 density algorithm with S_R as the salinity argument. Figure A.5.1 shows that the “thermal wind” is misestimated by more than 2% for 58% of the data in the world ocean below a depth of 1000m if the effects of the variable seawater composition are ignored.

The importance of the spatial variations in seawater composition illustrated in Fig. A.5.1 can be compared with the corresponding improvement achieved by the TEOS-10 Gibbs function for Standard Seawater compared with using EOS-80. This is done by ignoring spatial variations in seawater composition in both the evaluation of TEOS-10 and in EOS80 by calling TEOS-10 with S_R and EOS-80 with S_p . Figure A.5.2 shows the magnitude of the improvement in the “thermal wind” in the part of the ocean that is deeper than 1000m through the adoption of TEOS-10 but ignoring the influence of compositional variations. By comparing Figs. A.5.1 and A.5.2 it is seen that the main benefit that TEOS-10 delivers to the evaluation of the “thermal wind” is through the incorporation of spatial variations in seawater composition; the greater accuracy of TEOS-10 over EOS-80 for Standard Seawater is only 18% as large as the improvement gained by the incorporation of compositional variations into TEOS-10 (i. e. the rms value of the vertical axis in Fig. A.5.2 is 18% of that of the vertical axis of Fig. A.5.1). If the Atlantic were excluded from this comparison, the relative importance of compositional variations would be even larger.

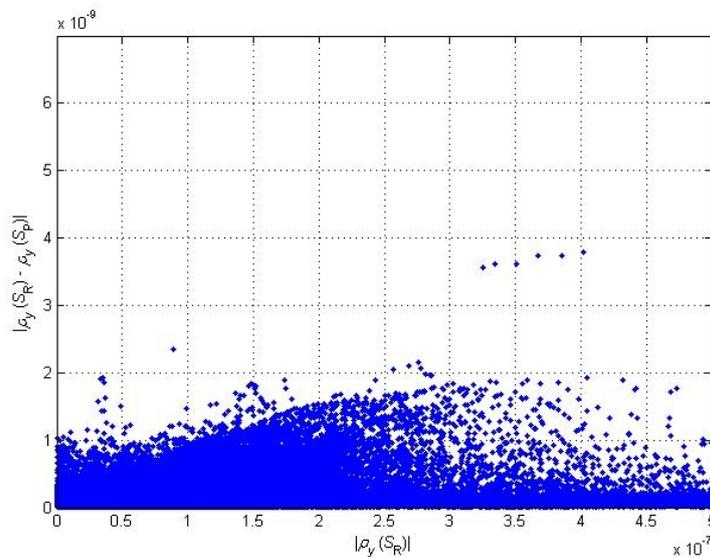


Figure A.5.2. The northward density gradient at constant pressure (the horizontal axis) for data in the global ocean atlas of Gouretski and Koltermann (2004) for $p > 1000$ dbar . The vertical axis is the magnitude of the difference between evaluating the density gradient using S_R as the salinity argument in the TEOS-10 expression for density compared with using S_p in the EOS-80 algorithm for density.

The thermodynamic description of seawater and of ice Ih as defined in IAPWS-08 and IAPWS-06 has been adopted as the official description of seawater and of ice Ih by the Intergovernmental Oceanographic Commission in June 2009. The adoption of TEOS-10

has recognized that this technique of estimating Absolute Salinity from readily measured quantities is perhaps the least mature aspect of the TEOS-10 thermodynamic description of seawater. The present computer software, in both FORTRAN and MATLAB, which evaluates Absolute Salinity S_A given the input variables Practical Salinity S_p , longitude λ , latitude ϕ and sea pressure p is available at www.TEOS-10.org. It is expected, as new data (particularly density data) become available, that the determination of Absolute Salinity will improve over the coming decades, and the algorithm for evaluating Absolute Salinity in terms of Practical Salinity, latitude, longitude and pressure, will be updated from time to time, after relevant appropriately peer-reviewed publications have appeared, and such an updated algorithm will appear on the www.TEOS-10.org web site. Users of this software should state in their published work which version of the software was used to calculate Absolute Salinity.