10. A guide to the GSW Oceanographic Toolbox

The key attributes of the three oceanographic variables S_{A}, S_* and Θ may be summarized as follows. Preformed Salinity S_* and Conservative Temperature Θ are the ideal variables for representing the "salt content" and "heat content" of seawater in the standard conservation equations of physical oceanography. However, the thermodynamic properties of seawater (in particular, density) depend not on Preformed Salinity S_*, but rather on Absolute Salinity S_{A}. While Practical Salinity S_{P} is relatively easy to measure accurately, it should now be regarded as a stepping stone on the way to calculating the two more attractive salinity variables, S_{A} and S_*.

The GSW functions are listed on the central four pages of this document. The group of functions "Practical Salinity (SP), PSS-78" contains routines for Practical Salinity in terms of either conductivity *C* or conductivity ratio *R*, as well as their inverse functions. The input temperature to these functions is *in situ* temperature (ITS-90), and the inverse algorithms are iterated until the Practical Salinity is equal to the input value to within $2\text{x}10^{-14}$, that is, to machine precision. These functions incorporate a modified form of the extension of Hill *et al*. (1986) to Practical Salinities between zero and 2. The modification ensures that the algorithm is exactly PSS-78 for $S_{\mathrm{P}} \geq 2$ and is continuous at $S_{\mathrm{P}} = 2$. The function in this group, **gsw_SP_salinometer**, calculates Practical Salinity from the two outputs of a laboratory salinometer, namely R_t and the bath temperature.

The second group delivers the three new oceanographic variables, Absolute Salinity S_{A}, Preformed Salinity S_*, and Conservative Temperature Θ. The first two functions have Practical Salinity S_{P}, pressure, longitude and latitude as input variables. Note that virtually all of the functions which follow this second group require Absolute Salinity S_{A} as an input. Hence it is clear that when analyzing oceanic data, the very first function call must be to **gsw_SA_from_SP**. Hence this function is the most fundamental in the GSW toolbox. This function can be avoided only by ignoring the influence of the spatial variations of seawater composition, in which case the remaining GSW functions would be called with Reference Salinity S_{R} (given by calling **gsw_SR_from_SP**) in place of S_{A}. The function **gsw_CT_from_t** evaluates Conservative Temperature Θ, as a function of Absolute Salinity S_{A}, *in situ* temperature t and pressure p.

The third group contains just the function **gsw_SA_CT_plot** which plots the TEOS-10 version of the "*T-S*" diagram for a series of vertical profiles. The Conservative Temperature at the freezing point for $p = 0$ dbar, and user-selected potential density contours are also displayed on this $S_{\mathrm{A}} - \Theta$ diagram using the 75-term expression for the density of seawater, **gsw_rho**(SA,CT,p).

The fourth grouping of functions has the heading "other conversions between temperatures, salinities, entropy, pressure and height". Some of these functions are the reverse of those in the previous groups (namely **gsw_SP_from_SA**, **gsw_SP_from_Sstar** and **gsw_t_from_CT**) while others perform familiar functions such as **gsw_pt_from_t**(SA,t,p,p_ref) which evaluates the potential temperature of the "bottle" (SA,t,p) referenced to the pressure p_ref.

The next group of functions (the right-hand side of the first page), headed "specific volume, density and enthalpy", are all derived from the computationally-efficient 75-term expression for specific volume, $\hat{v}\left(S_{\mathrm{A}},\Theta,p\right)$ of Roquet *et al.* (2015). This group includes the function **gsw_rho** to evaluate both density and potential density, and **gsw_alpha** to evaluate the relevant thermal expansion coefficient. This 75-term expression for specific volume is essentially as accurate as the full TEOS-10 expression, and this 75-term expression has the advantage that its temperature argument is Conservative Temperature. The functions **gsw_enthalpy** and **gsw_enthalpy_diff** can be used when evaluating various geostrophic streamfunctions, since under isentropic and isohaline conditions, enthalpy is the pressure integral of specific volume. The functions **gsw_SA_from_rho** and **gsw_CT_from_rho** are essentially the inverse functions of the equation of state in that they return the Absolute Salinity (or Conservative Temperature respectively) for given values of density, pressure and either Θ or S_A respectively.

The next group of functions, headed "vertical stability and interpolation", delivers variables which are defined in terms of the vertical gradients of S_A and Θ on an individual vertical profile, and so are inherently water column properties. These functions deliver the square of the buoyancy frequency (**gsw_Nsquared**), the Turner angle, and the ratio of the vertical gradient of potential density to the vertical gradient of locally-referenced potential density. The interpolation functions implement the algorithms of Barker and McDougall (2020) which uses multiply rotated piecewise cubic Hermite polynomials, while the stablisation functions implement the method described by Barker and McDougall (2017).

The following group is for calculating four different geostrophic streamfunctions, and the acoustic travel time for sound up and down a vertical water column. All of these GSW geostrophic streamfunction functions have S_A and Θ as their input salinity and temperature. It is important to realize that a particular geostrophic streamfunction is only accurate when used in the surface for which it is derived. For example, dynamic height anomaly is the geostrophic streamfunction in an isobaric surface while the Montgomery streamfunction is the geostrophic streamfunction in a specific volume anomaly surface. When one is working in some type of approximately neutral surface, the Cunningham geostrophic streamfunction is more accurate than the Montgomery streamfunction, while the "isopycnal" geostrophic streamfunction **gsw_geo_strf_isopycnal** of McDougall and Klocker (2010) is the most accurate (see Figures 1, 2 and 3 of McDougall and Klocker (2010)). The functions in this group all use the 75-term polynomial for specific volume. The function, **gsw_geostrophic_velocity**, calculates the geostrophic velocity in a given surface with respect to the velocity in a reference surface. This function should be called with dynamic height anomaly if the surface in which the geostrophic velocity is required is an isobaric surface. Similarly, **gsw_geostrophic_velocity** should be called with the "isopycnal" geostrophic streamfunction **gsw_geo_strf_isopycnal** if the surface in which the geostrophic velocity is evaluated is an approximately neutral surface (such as a Neutral Density surface (Jackett and McDougall (1997)), an ω-surface (Klocker *et al.* (2010)) or a potential density surface).

The following four groups give properties of ice, of sea ice, and of the thermodynamic equilibrium between seawater and either ice or sea ice. These four groups are followed (on page 3) by a group of functions which gives the latent heats of melting and of evaporation.

The next group "spiciness" delivers the spiciness variable for three different reference pressures. Spiciness is a measure of the change of water-mass properties along a potential density surface.

The next group of functions is concerned with various neutral attributes of the seawater equation of state and returns properties such as the ratio of the gradient of Conservative Temperature in a potential density surface to that in the neutral tangent plane.

The following group "derivatives of entropy, CT and pt" contains functions which use the full TEOS-10 Gibbs function and have a variety of input temperatures, appropriate to the variable being differentiated. The outputs of these functions are used, for example, in evaluating the amount of non-conservative production associated with each variable (entropy, CT and pt) when two seawater parcels are mixed.

The group, "planet Earth properties", delivers straightforward properties of the rotating planet of the solar system on which we presently reside.

The group "TEOS-10 constants" simply returns various constants which are basic to TEOS-10. Note that the constant **gsw_C3515** is not a fundamental constant of either PSS-78 or TEOS-10 but is required to convert a measured conductivity value C into conductivity ratio R (which *is* a fundamental property of PSS-78).

The group of GSW functions, "laboratory functions, for use with densimeter measurements", have *in situ* temperature t as their input temperature variable. All three functions in this group use the full TEOS-10 Gibbs function, namely the sum of the Gibbs functions of IAPWS-09 and IAPWS-08 (rather than the 75-term expression for specific volume). Two of these three functions are also listed on the lower left group of the fourth page; they are also listed here to give them more prominence for those using a densimeter in a laboratory setting.

The group of GSW functions on the right-hand side of the third page, headed "specific volume, density and enthalpy in terms of CT, based on the exact Gibbs function" delivers the same outputs as the corresponding group on page 1, and with the same input variables. The functions on page 1 are based on the 75-term expression for specific volume, $\hat{v}\left(S_{\mathrm{A}},\Theta,p\right)$, whereas the functions on page 3 use the exact Gibbs function for seawater to calculate specific volume. The function names in this group differ from those on page 1 by the additional "_exact" at the end of each function name. These functions can be used to confirm that the use of the 75-term computationally efficient equation of state does not noticeably degrade any output property.

The group "dissolved gases" contains algorithms for the solubility of various gases. This is not work that resulted from SCOR/IAPSO Working Group 127, nor have these algorithms been approved by IOC. These algorithms are included in the GSW Oceanographic Toolbox as they seem to be oceanographic best practice.

The next list, headed "basic thermodynamic properties in terms of in-situ t, based on the exact Gibbs function" contains many of the basic thermodynamic properties of seawater. Each of these functions have in situ temperature as the input temperature variable. The next group contains the library functions used by GSW. These are internal functions which are not intended to be called by users. There is nothing stopping a skilled operator using these programs, but unless the user is confident, it is safer to access these library routines via one of the public functions; for example, there is little or no checking on the array sizes of the input variables in these internal library functions. The data set gsw_data_v3_0 must not be tampered with.

In the *documentation set* the function **gsw_check_functions** confirms that the GSW Oceanographic Toolbox is correctly installed and that there are no conflicts. This function runs three stored vertical profiles through of all the other GSW functions, and checks that the outputs are within predefined limits of the correct answers. These pre-defined limits are a factor of approximately a hundred larger than the errors expected from numerical round-off (at the standard double precision of MATLAB). The user may want to run **gsw_check_functions** periodically to confirm that the software remains uncorrupted. **gsw_demo** runs and displays results from several of the GSW functions, so introducing the user to some of the features of the Toolbox.

The GSW Oceanographic Toolbox is designed to be comprehensive and to be installed in its entirety, even though most users may use relatively few of the functions for routine oceanographic analyses. For example, the most basic use of the GSW Oceanographic Toolbox would begin with a data set of $\left(S_{\mathrm{P}},\, t,\, p\right)$ at known longitudes and latitudes. The first steps are to call **gsw_SA_from_SP** and then **gsw_CT_from_t** to convert to a data set of $\left(S_{\mathrm{A}},\, \Theta,\, p\right)$. With the data set in this form, water masses may be analyzed accurately on the $S_{\mathrm{A}}-\Theta$ diagram, and *in situ* density and potential density are available by calling the computationally-efficient 75-term expression for density, **gsw_rho**, with the pressure input being the *in situ* sea pressure p, and the reference sea pressure p_ref, respectively. That is, in situ density is evaluated as **gsw_rho**(SA,CT,p) and potential density with respect to the reference pressure p_ref is given by **gsw_rho**(SA,CT,p_ref).