Notes on the function, gsw_pt0_from_t(SA, t, p), which evaluates potential temperature with reference pressure of 0 dbar from in situ temperature, t

This function, gsw_pt0_from_t, finds $\theta = \theta(S_A, t, p, 0)$, the potential temperature of "bottle" (S_A, t, p) with respect to the reference pressure $p_r = 0\,\text{dbar}$. A modified Newton-Raphson iterative solution technique is employed to find the zero of the function

$$f(\theta) \equiv \tilde{\eta}(S_A, \theta) - \eta(S_A, t, p) = 0, \tag{1}$$

which equates the specific entropy of the "bottle", $\eta(S_A, t, p)$, to the specific entropy $\tilde{\eta}(S_A, \theta)$ after the adiabatic and isohaline change in pressure to $p_r = 0\,\text{dbar}$. This function, gsw_pt0_from_t, is very similar to the more general function gsw_pt_from_t which calculates the potential temperature $\theta = \theta(S_A, t, p, p_r)$ at the general reference pressure p_r. If the reference pressure is zero, it is 20% faster to use gsw_pt0_from_t rather than gsw_pt_from_t.

The first estimate θ_0 is given by Eqn. (A3) and (A4) of McDougall *et al.* (2003) with the coefficients taken from Table A1 of Jackett *et al.* (2006). This simple seven-term polynomial was given in terms of Practical Salinity, and in this function this has been taken into account by dividing the input Absolute Salinity by (35.16504 g kg⁻¹)/35.

The modified Newton-Raphson iteration procedure needs an initial guess not only of θ_0 but also of the derivative of Eqn. (1) with respect to potential temperature. The plot of $(\theta - \Theta)$ on the $S_A - \Theta$ diagram shown as Figure A.17.1 of IOC *et al.* (2010) (this figure is reproduced below) suggests the following approximation

$$(\theta - \Theta) \approx -0.05(1 - S_A/S_{SO})\Theta, \tag{2}$$

from which we find that $\tilde{\Theta}_\theta$ can be written as

$$\tilde{\Theta}_\theta \approx \left[1 - 0.05(1 - S_A/S_{SO})\right]^{-1}. \tag{3}$$

The derivative of $f(\theta)$ with respect to potential temperature is (from Eqn. (1))

$$f'(\theta) = \tilde{\eta}_\theta, \tag{4}$$

and from Eqn. (P.14a) of IOC *et al.* (2010) we have

$$\tilde{\eta}_\theta = \frac{c_p^0}{(T_0 + \theta)}\tilde{\Theta}_\theta. \tag{5}$$

Combining Eqns. (3) – (5) we find the following approximate derivative $f'(\theta)$ which we use as the initial estimate of this derivative in the modified Newton-Raphson procedure,

$$f'(\theta_0) \approx \frac{c_p^0}{(T_0 + \theta_0)}\left[1 - 0.05(1 - S_A/S_{SO})\right]^{-1}. \tag{6}$$

The modified Newton-Raphson iteration technique

The normal Newton-Raphson technique converges iteratively towards a root of the function $f(\theta) \equiv \tilde{\eta}(S_A, \theta) - \eta(S_A, t, p) = 0$ with each successive iteration being found from the previous one according to

$$\theta_{n+1} = \theta_n - \frac{f(\theta_n)}{f'(\theta_n)}. \tag{7}$$

Notice that in Eqn. (7) the function value and its derivative are evaluated at the same value of θ. For the thermodynamic cases we consider, the derivative $f'(\theta)$ is a slowly varying function of θ, so that we adopt the numerical technique of McDougall *et al.* (2003) (see

pages 731-732 therein) and evaluate the function and its derivative at different values of θ, thereby improving convergence.

Starting from θ_0 and the crude estimate Eqn. (6) of f', an intermediate value of potential temperature, θ_1, is found as $\theta_1 = \theta_0 - f(\theta_0)/f'$. The reason for calculating this intermediate value is so that the derivative can be evaluated at a potential temperature which is close to the mid point between the initial value and the final solution. The derivative is evaluated at $0.5[\theta_0 + \theta_1]$ and the next estimate of potential temperature, θ_2, is found from

$$\theta_2 = \theta_0 - \frac{f(\theta_0)}{f'(0.5[\theta_0 + \theta_1])}. \tag{8}$$

This marks the end of the first iteration of the modified Newton-Raphson method. At this stage we have performed just one evaluation of both f and f'; the same number of such evaluations as are involved in one full iteration of the standard Newton-Raphson procedure. The next two-step modified Newton-Raphson iteration proceeds as follows

$$\theta_3 = \theta_2 - \frac{f(\theta_2)}{f'(0.5[\theta_0 + \theta_1])}, \quad \text{then} \quad \theta_4 = \theta_2 - \frac{f(\theta_2)}{f'(0.5[\theta_2 + \theta_3])}. \tag{9a,b}$$

In this whole process leading to the value θ_4, the function f is evaluated just twice (at θ_0 and θ_2) and its derivative f' is also evaluated just twice (at $0.5[\theta_0 + \theta_1]$ and $0.5[\theta_2 + \theta_3]$).

In the application of this modified Newton-Raphson procedure to the function gsw_pt0_from_t we find that the solution converges to machine precision after two iterations, and so the code returns the value θ_4 of Eqn. (9b) above. Hence the function gsw_pt0_from_t evaluates f twice (at θ_0 and θ_2) and its derivative f' twice (at $0.5[\theta_0 + \theta_1]$ and $0.5[\theta_2 + \theta_3]$).

The function $f(\theta) \equiv \tilde{\eta}(S_A, \theta) - \eta(S_A, t, p)$ involves calling the library function gsw_entropy_part and gsw_entropy_part_zerop which calculate specific entropy except for those terms that depend only on Absolute Salinity, since these terms are common to both $\tilde{\eta}(S_A, \theta)$ and $\eta(S_A, t, p)$ and so cancel in the expression for $f(\theta)$. There is only one call to gsw_entropy_part, being the call to evaluate the "bottle" value at (S_A, t, p). There are two calls to gsw_entropy_part_zerop, once at (S_A, θ_0) and once at (S_A, θ_2).

The derivative $f'(\theta)$ is given by Eqn. (4) above and is evaluated as the second derivative of the Gibbs function,

$$f'(\theta) = \tilde{\eta}_\theta = -g_{TT}(S_A, \theta, 0), \tag{10}$$

this being called twice, once at $0.5[\theta_0 + \theta_1]$ and once at $0.5[\theta_2 + \theta_3]$. Because this second derivative of the Gibbs function is called at zero pressure, a special library function gsw_gibbs_pt0_pt0 has been written to gain computational efficiency by explicitly recognizing that the pressure is zero.

References

Jackett, D. R., T. J. McDougall, R. Feistel, D. G. Wright and S. M. Griffies, 2006: Algorithms for density, potential temperature, conservative temperature and freezing temperature of seawater. *Journal of Atmospheric and Oceanic Technology*, **23**, 1709-1728.

McDougall, T. J., D. R. Jackett, D. G. Wright and R. Feistel, 2003: Accurate and computationally efficient algorithms for potential temperature and density of seawater. *Journal of Atmospheric and Oceanic Technology*, **20**, 730-741.

IOC, SCOR and IAPSO, 2010: *The international thermodynamic equation of seawater – 2010: Calculation and use of thermodynamic properties*. Intergovernmental Oceanographic Commission, Manuals and Guides No. 56, UNESCO (English), 196 pp. Available from http://www.TEOS-10.org

Here follows section 3.1 of IOC *et al.* (2010).

3.1 Potential temperature

The very useful concept of potential temperature was applied to the atmosphere originally by Helmholtz (1888), first under the name of 'heat content', and later renamed 'potential temperature' (Bezold (1888)). These concepts were transferred to oceanography by Helland-Hansen (1912). Potential temperature is the temperature that a fluid parcel would have if its pressure were changed to a fixed reference pressure p_r in an isentropic and isohaline manner. The phrase "isentropic and isohaline" is used repeatedly in this document. To these two qualifiers we should really also add "without dissipation of mechanical energy". A process that obeys all three restrictions is a thermodynamically reversible process. Note that one often (falsely) reads that the requirement of a reversible process is that the process occurs at constant entropy. However this statement is misleading because it is possible for a fluid parcel to exchange some heat and some salt with its surroundings in just the right ratio so as to keep its entropy constant, but the processes is not reversible (see Eqn. (A.7.1)).

Potential temperature referred to reference pressure p_r is often written as the pressure integral of the adiabatic lapse rate (Fofonoff (1962), (1985))

$$\theta = \theta(S_A, t, p, p_r) = t + \int_P^{P_r} \Gamma(S_A, \theta[S_A, t, p, p'], p') \, dP'. \qquad (3.1.1)$$

Note that this pressure integral needs to be done with respect to pressure expressed in Pa not dbar .

The algorithm that is used with the TEOS-10 Gibbs function approach to seawater equates the specific entropies of two seawater parcels, one before and the other after the isentropic and isohaline pressure change. In this way, θ is evaluated using a Newton-Raphson iterative solution technique to solve the following equation for θ

$$\eta(S_A, \theta, p_r) = \eta(S_A, t, p), \qquad (3.1.2)$$

or, in terms of the Gibbs function, g,

$$-g_T(S_A, \theta, p_r) = -g_T(S_A, t, p). \qquad (3.1.3)$$

This relation is formally equivalent to Eqn. (3.1.1). In the GSW computer software θ is found to machine precision ($\sim 10^{-14}\,°C$) in two iterations of a modified Newton-Raphson method, using a suitable initial value as described by McDougall *et al.* (2010b). .

Note that the difference between the potential and *in situ* temperatures is not due to the work done in compressing a fluid parcel on going from one pressure to another:- the sign of this work is often in the wrong sense and the magnitude is often wrong by a few orders of magnitude (McDougall and Feistel (2003)). Rather, the difference between these temperatures is what is required to keep the entropy constant during the adiabatic and isohaline pressure change. The potential temperature θ output of the SIA software is in units of K while the output from the GSW library is in °C .

Also, note Figure A.17.1 below (from IOC *et al.* (2010)) showing the difference between potential temperature θ and Conservative Temperature Θ. In the gsw_pt_from_t function we have approximated the figure below as

$$(\theta - \Theta) \approx -0.05(1 - S_A/S_{SO})\Theta,$$

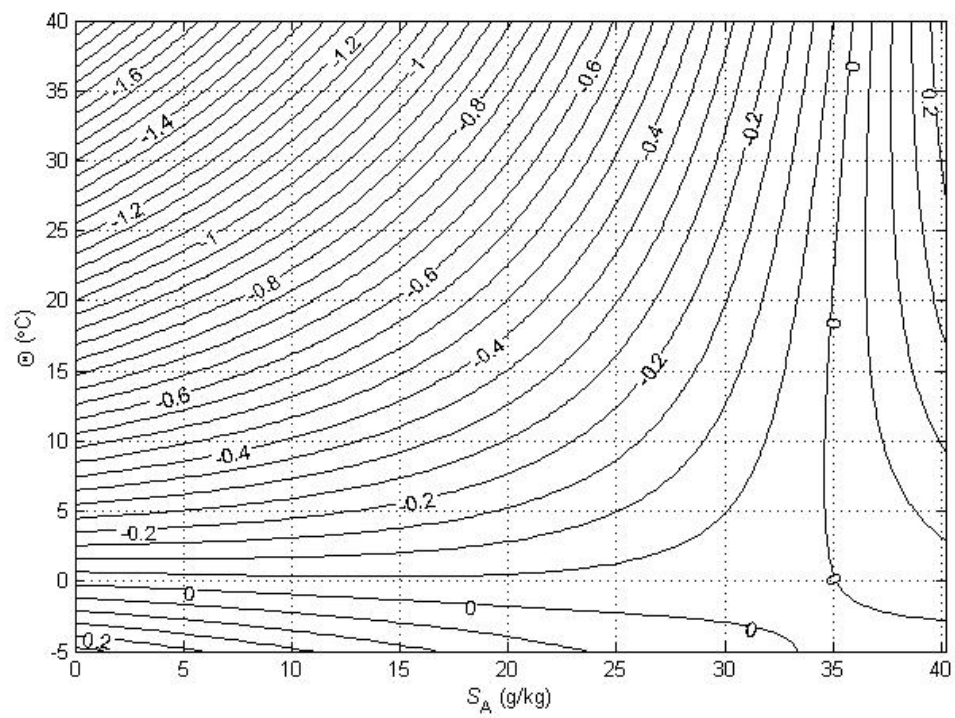in order to obtain an initial estimate for $\tilde{\Theta}_\theta$ in the iterative modified Newton-Raphson procedure.

Figure A.17.1. Contours (in °C) of the difference between potential temperature and Conservative Temperature $\theta - \Theta$. This plot illustrates the non-conservative production of potential temperature θ in the ocean.