Notes on the function, gsw_pt_from_entropy(SA, entropy), which evaluates potential temperature with reference pressure of 0 dbar from specific entropy

This function, **gsw_pt_from_entropy**, finds $\theta = \theta(S_A, \eta)$, the potential temperature with respect to the reference pressure $p_r = 0\,\text{dbar}$ for given values of Absolute Salinity and specific entropy. A modified Newton-Raphson iterative solution technique is employed to find the zero of the function

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

which equates the specific entropy of the "bottle", $\tilde{\eta}(S_A, \theta)$, to the input specific entropy η. This function, **gsw_pt_from_entropy** is very similar in its operation to the function **gsw_pt0_from_t**, which calculates the potential temperature referenced to $p_r = 0\,\text{dbar}$ from the inputs (S_A, t, p). The main difference between these functions relates to the way the initial value of potential temperature, θ_0, is evaluated. How this is done for the present function is now described.

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

$$f'(\theta) = \tilde{\eta}_\theta = \frac{c_p^0}{(T_0 + \theta)}\tilde{\Theta}_\theta. \tag{4}$$

Combining Eqns. (3) and (4) we find the following approximate expression for the derivative $f'(\theta)$,

$$f'(\theta) = \tilde{\eta}_\theta \approx \frac{c_p^0}{(T_0 + \theta)}\left[1 - 0.05(1 - S_A/S_{SO})\right]^{-1}. \tag{5}$$

Integrating this expression with respect to θ we find the following approximate expression,

$$\tilde{\eta}(S_A, \theta) \approx c_p^0 \ln\left(1 + \frac{\theta}{T_0}\right)\left[1 - 0.05\left(1 - \frac{S_A}{S_{SO}}\right)\right]^{-1} + \frac{c_p^0}{T_0}\left(1 - \frac{S_A}{S_{SO}}\right)\left[1 - 1.01\left(1 - \frac{S_A}{S_{SO}}\right)\right]. \tag{6}$$

The second part of this expression is a function of only S_A and has been found as a simple fit to entropy at zero potential temperature, that is, a simple fit to $\tilde{\eta}(S_A, \theta = 0°\text{C})$.

The initial value of potential temperature θ_0 is found by equating the right-hand side of Eqn. (6) to the input value of entropy, η, and solving this equation for θ. This initial value of potential temperature, θ_0, is then used in Eqn. (5) to find the initial estimate of the derivative $f'(\theta_0)$.

The modified Newton-Raphson iteration technique

The normal Newton-Raphson technique converges iteratively towards a root of the function $f(\theta) \equiv \tilde{\eta}(S_A, \theta) - \eta = 0$ 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. (5) 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_pt_from_entropy** 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_pt_from_entropy** 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 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 appendix A.10 of the TEOS-10 Manual (IOC *et al*. (2010)).

A.10 Proof that $\theta = \theta(S_A, \eta)$ and $\Theta = \Theta(S_A, \theta)$

Consider changes occurring at the sea surface, (specifically at $p = 0$ dbar) where the temperature is the same as the potential temperature referenced to 0 dbar and the increment of pressure dp is zero. Regarding specific enthalpy h and chemical potential μ to be functions of entropy η (in place of temperature t), that is, considering the functional form of h and μ to be $h = \hat{h}(S_A, \eta, p)$ and $\mu = \hat{\mu}(S_A, \eta, p)$, it follows from the fundamental thermodynamic relation (Eqn. (A.7.1)) that

$$\hat{h}_\eta(S_A, \eta, 0)\, d\eta + \hat{h}_{S_A}(S_A, \eta, 0)\, dS_A = (T_0 + \theta)d\eta + \mu(S_A, \eta, 0)\, dS_A, \qquad (A.10.1)$$

which shows that specific entropy η is simply a function of Absolute Salinity S_A and potential temperature θ, that is $\eta = \eta(S_A, \theta)$, with no separate dependence on pressure. It follows that $\theta = \theta(S_A, \eta)$.

Similarly, from the definition of potential enthalpy and Conservative Temperature in Eqns. (3.2.1) and (3.3.1), at $p = 0$ dbar it can be seen that the fundamental thermodynamic relation (A.7.1) implies

$$c_p^0\, d\Theta = (T_0 + \theta)d\eta + \tilde{\mu}(S_A, \theta, 0)\, dS_A. \qquad (A.10.2)$$

This shows that Conservative Temperature is also simply a function of Absolute Salinity and potential temperature, $\Theta = \Theta(S_A, \theta)$, with no separate dependence on pressure. It then follows that Θ may also be expressed as a function of only S_A and η. It follows that Θ has the "potential" property.

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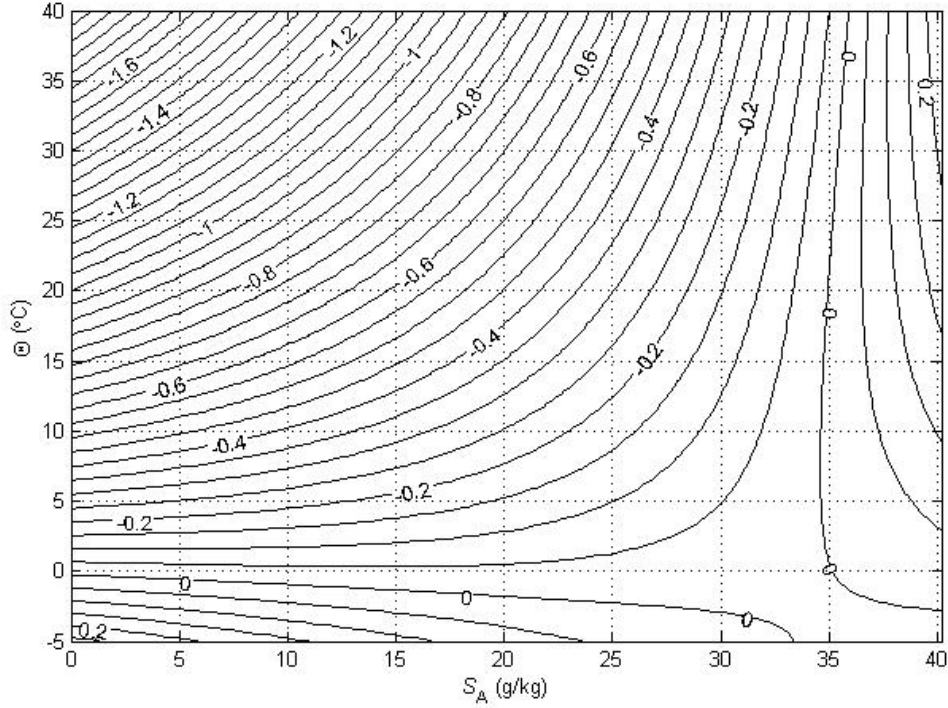
Figure A.17.1. Contours (in °C) of the difference between potential temperature and Conservative Temperature $\theta - \Theta$. This plot illustrates the non-conservative production of potential temperature θ in the ocean.