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" iteration procedure of McDougall and Wotherspoon (2014) 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 $\tilde{\eta}(S_A, \theta = 0°C)$.

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

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McDougall T. J. and S. J. Wotherspoon, 2014: A simple modification of Newton's method to achieve convergence of order $1+\sqrt{2}$. *Applied Mathematics Letters*, **29**, 20-25. http://dx.doi.org/10.1016/j.aml.2013.10.008

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.

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

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

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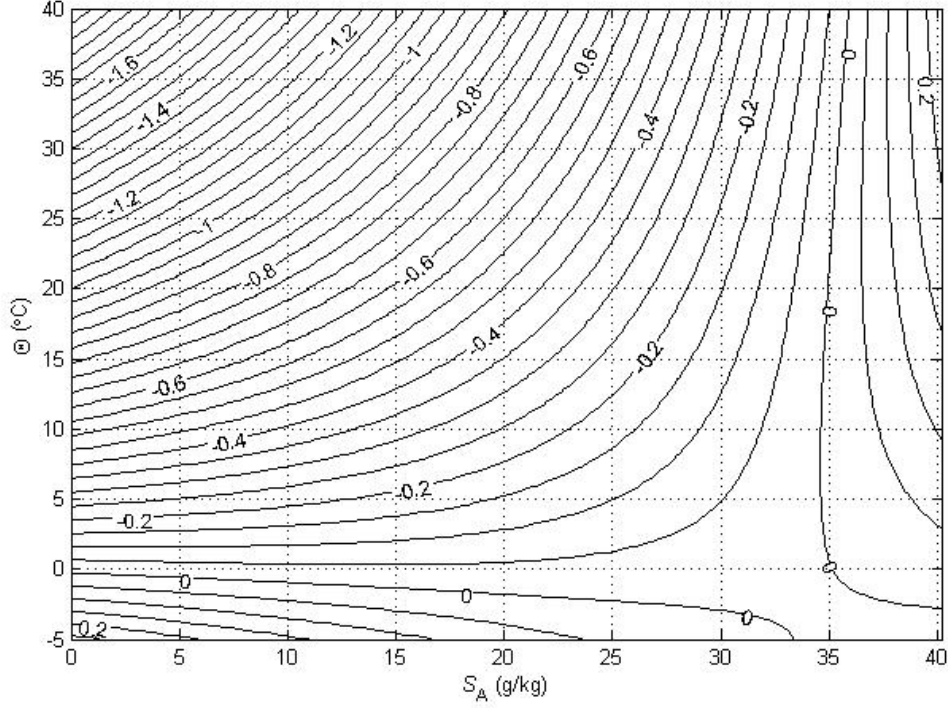

Figure A.17.1. Contours (in °C) of the difference between potential temperature and Conservative Temperature $\theta - \Theta$. This plot illustrates the non-conservative production of potential temperature θ in the ocean.