

Notes on the inverse function, `gsw_pt_from_CT(SA, CT)`, which evaluates θ from Θ

This function, `gsw_pt_from_CT`, finds $\theta = \hat{\theta}(S_A, \Theta)$ by employing modified Newton-Raphson" iteration procedure of McDougall and Wotherspoon (2014) to the (forward) definition of Conservative Temperature Θ in terms of Absolute Salinity and potential temperature, $\Theta = \tilde{\Theta}(S_A, \theta)$. The potential temperature output of `gsw_pt_from_CT` is the potential temperature referenced to $p_r = 0$ dbar.

The first estimate θ_0 is given by the rational function Eqn. (B7) and Table B3 of Jackett *et al.* (2006). This rational function in Jackett *et al.* (2006) was given in terms of Practical Salinity, and in this function this has been taken into account by dividing the input Absolute Salinity by $(35.16504 \text{ g kg}^{-1})/35$. This same rational function for potential temperature is differentiated with respect to Θ to provide the starting estimate of the derivative, $\tilde{\Theta}_\theta = 1/\hat{\theta}_\Theta$.

The modified Newton-Raphson iteration technique

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

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

Notice that in Eqn. (1) 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 a crude estimate 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

$$\theta_2 = \theta_0 - \frac{f(\theta_0)}{f'(0.5[\theta_0 + \theta_1])}. \quad (2)$$

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 would proceed as follows

$$\theta_3 = \theta_2 - \frac{f(\theta_2)}{f'(0.5[\theta_0 + \theta_1])}, \quad \text{then} \quad \theta_4 = \theta_2 - \frac{f(\theta_2)}{f'(0.5[\theta_2 + \theta_3])}. \quad (3a,b)$$

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_CT` we find that the solution converges to machine precision after one and a half iterations, and so the code returns the value θ_3 of Eqn. (3a) above. Hence the function `gsw_pt_from_CT` evaluates f twice (at θ_0 and θ_2) and its derivative f' just once (at $0.5[\theta_0 + \theta_1]$).

The function $f(\theta) = \tilde{\Theta}(S_A, \theta) - \Theta$ involves a call to the function **gsw_CT_from_pt**, while the derivative

$$f'(\theta) = \tilde{\Theta}_\theta(S_A, \theta) = -\frac{(T_0 + \theta) g_{TT}(S_A, \theta, 0)}{c_p^0}, \quad (4)$$

is found using the library function **gsw_gibbs_pt0_pt0** which is a computationally efficient way of finding the second derivative of the Gibbs function with respect to temperature, recognizing that in this case this second derivative is being taken at zero sea pressure.

References

- 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>
- 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.
- 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 section 3.3 of IOC *et al.* (2010).

3.3 Conservative Temperature

Conservative Temperature Θ is defined to be proportional to potential enthalpy according to

$$\Theta(S_A, t, p) = \tilde{\Theta}(S_A, \theta) = h^0(S_A, t, p)/c_p^0 = \tilde{h}^0(S_A, \theta)/c_p^0 \quad (3.3.1)$$

where the value that is chosen for c_p^0 is motivated in terms of potential enthalpy evaluated at an Absolute Salinity of $S_{SO} = 35u_{PS} = 35.165\ 04\ \text{g kg}^{-1}$ and at $\theta = 25\ ^\circ\text{C}$ by

$$\frac{[h(S_{SO}, 25^\circ\text{C}, 0) - h(S_{SO}, 0^\circ\text{C}, 0)]}{(25\ \text{K})} \approx 3991.867\ 957\ 119\ 63\ \text{J kg}^{-1}\ \text{K}^{-1}, \quad (3.3.2)$$

noting that $h(S_{SO}, 0\ ^\circ\text{C}, 0\ \text{dbar})$ is zero according to the way the Gibbs function is defined in (2.6.5). In fact we adopt the exact definition for c_p^0 to be the 15-digit value in (3.3.2), so that

$$c_p^0 \equiv 3991.867\ 957\ 119\ 63\ \text{J kg}^{-1}\ \text{K}^{-1}. \quad (3.3.3)$$

When IAPWS-95 is used for the pure water part of the Gibbs function, $\Theta(S_{SO}, 0\ ^\circ\text{C}, 0)$ and $\Theta(S_{SO}, 25\ ^\circ\text{C}, 0)$ differ from $0\ ^\circ\text{C}$ and $25\ ^\circ\text{C}$ respectively by the round-off amount of $5 \times 10^{-12}\ ^\circ\text{C}$. When IAPWS-09 (which is based on the paper of Feistel (2003), see appendix G) is used for the pure water part of the Gibbs function, $\Theta(S_{SO}, 0\ ^\circ\text{C}, 0)$ differs from $0\ ^\circ\text{C}$ by $-8.25 \times 10^{-8}\ ^\circ\text{C}$ and $\Theta(S_{SO}, 25\ ^\circ\text{C}, 0)$ differs from $25\ ^\circ\text{C}$ by $9.3 \times 10^{-6}\ ^\circ\text{C}$. Over the temperature range from $0\ ^\circ\text{C}$ to $40\ ^\circ\text{C}$ the difference between Conservative Temperature

using IAPWS-95 and IAPWS-09 as the pure water part is no more than $\pm 1.5 \times 10^{-5}$ °C, a temperature difference that will be ignored.

The value of c_p^0 in (3.3.3) is very close to the average value of the specific heat capacity c_p at the sea surface of today's global ocean. This value of c_p^0 also causes the average value of $\theta - \Theta$ at the sea surface to be very close to zero. Since c_p^0 is simply a constant of proportionality between potential enthalpy and Conservative Temperature, it is totally arbitrary, and we see no reason why its value would need to change from (3.3.3) even when in future decades an improved Gibbs function of seawater is agreed upon.

Appendix A.18 outlines why Conservative Temperature gets its name; it is approximately two orders of magnitude more conservative compared with either potential temperature or entropy.

The SIA and GSW software libraries both include an algorithm for determining Conservative Temperature Θ from values of Absolute Salinity S_A and potential temperature θ referenced to $p = 0$ dbar. These libraries also have an algorithm for evaluating potential temperature (referenced to 0 dbar) from S_A and Θ . This inverse algorithm, $\hat{\theta}(S_A, \Theta)$, has an initial seed based on a rational function approximation and finds potential temperature to machine precision ($\sim 10^{-14}$ °C) in one and a half iterations of a modified Newton-Raphson technique (McDougall *et al.* (2011b)).

Also, note Figure A.17.1 below (from IOC *et al.* (2010)) showing the difference between potential temperature and Conservative Temperature.

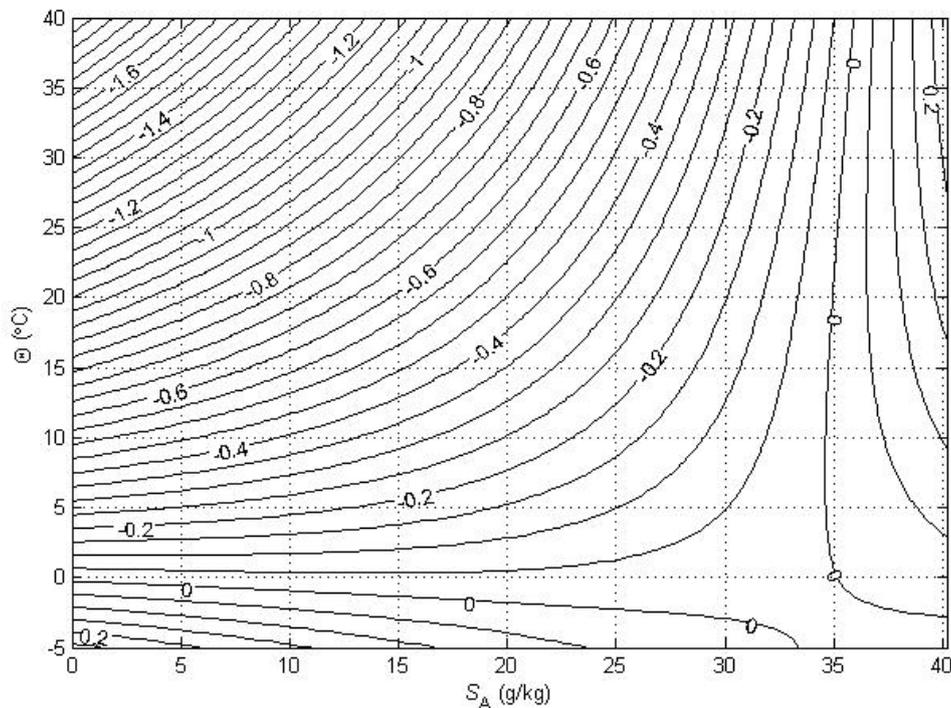


Figure A.17.1. Contours (in °C) of the difference between potential temperature and Conservative Temperature $\theta - \Theta$. This plot illustrates the non-conservative production of potential temperature θ in the ocean.