

Notes on the function `gsw_CT_from_rho(rho,SA,p)`

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This function, `gsw_CT_from_rho(rho,SA,p)`, calculates the Conservative Temperature Θ corresponding to the input values of *in situ* density, ρ , Absolute Salinity, SA , and pressure, p . The function returns NaNs if

- (i) the input density is too small (which would require Θ to exceed 40 °C), if
- (ii) the input density exceeds the density at the temperature of maximum density (as given by `gsw_CT_maxdensity(SA,p)`), or if
- (ii) the temperature is less than the freezing temperature as given by `gsw_CT_freezing_poly(SA,p)` (implying that we are assuming that at the freezing temperature, the seawater is air free).

This function, `gsw_CT_from_rho(rho,SA,p)`, uses the 75-term expression, $\hat{v}(S_A, \Theta, p)$. This 75-term polynomial expression for specific volume is discussed in Roquert *et al.* (2015) and in appendix A.30 and appendix K of the TEOS-10 Manual (IOC *et al.* (2010)). For dynamical oceanography we may take the 75-term polynomial expression for specific volume as essentially reflecting the full accuracy of TEOS-10.

This function begins by calculating the freezing temperature, `CT_freezing`, and the thermal expansion coefficient, `gsw_alpha(SA,CT_freezing,p)` at this temperature. If this thermal expansion coefficient is positive and exceeds $1 \times 10^{-5} \text{ K}^{-1}$, a “modified Newton-Raphson” iteration procedure of McDougall and Wotherspoon (2014) is performed with an initial Θ value given by solving a quadratic in Θ , given the thermal expansion coefficient at the freezing temperature and the value of density at $\Theta = 40^\circ\text{C}$, as given by `gsw_rho(SA,40,p)`. This quadratic is based on a Taylor series expression for density, expanded about the freezing temperature.

If the thermal expansion coefficient at the freezing temperature is less than $1 \times 10^{-5} \text{ K}^{-1}$ (which occurs only for Absolute Salinities less than approximately 28 g kg^{-1} , depending on pressure), the temperature of maximum density is found from `gsw_CT_maxdensity(SA,p)`. Again a simple quadratic for Conservative Temperature is solved using the density at this value of Θ and the density at $\Theta = 40^\circ\text{C}$. This quadratic gives two solutions, and if the larger of the two solutions exceeds `gsw_CT_maxdensity(SA,p)` by more than 5°C there will be only one non-frozen solution and we find this solution by the modified Newton-Raphson technique.

If the larger of these two quadratic solutions exceeds `gsw_CT_maxdensity(SA,p)` by less than 5°C we avoid using the modified Newton-Raphson method and instead solve for temperature assuming that the variation of density with Θ is a quadratic function of Θ about the temperature of maximum density. This is done iteratively, with each iteration using the previous iteration to effectively estimate $\rho_{\Theta\Theta}$ at the temperature of maximum density. In this part of the code, care is taken to distinguish cases where there are two valid solutions, both of which exceed the freezing temperature, from the situation where this is only one such solution.

When the modified Newton-Raphson method is used, three iterations are performed after which the density of the solution equals that of the input density to machine precision ($1.6 \times 10^{-12} \text{ kg m}^{-3}$). When the iterative quadratic method is used, seven iterations are performed after which the density of each non-frozen solution equals that of the input density to machine precision ($4.6 \times 10^{-13} \text{ kg m}^{-3}$).

This function `gsw_CT_from_rho(rho,SA,p)` is called as

$$[CT,CT_multiple] = gsw_CT_from_rho(rho,SA,p)$$

and if there is a valid second solution, it is returned as `CT_multiple`. When there is only one solution, `CT_multiple` is a NaN. When there are no solutions, both `CT` and `CT_multiple` are NaNs.

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>
- 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. *J. Atmosph. Ocean. Tech.*, **20**, pp. 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>
- Roquet, F., G. Madec, T. J. McDougall and P. M. Barker, 2015: Accurate polynomial expressions for the density and specific volume of seawater using the TEOS-10 standard. *Ocean Modelling*, **90**, pp. 29-43. <http://dx.doi.org/10.1016/j.ocemod.2015.04.002>
- Saunders, P. M, 1981: Practical conversion of pressure to depth. *Journal of Physical Oceanography*, **11**, 573-574.

Here follows appendix A.30 and appendix K of the TEOS-10 Manual (IOC *et al.* (2010)).

A.30 Computationally efficient 75-term expression for the specific volume of seawater in terms of Θ

Ocean models to date have treated their salinity and temperature variables as being Practical Salinity S_p and potential temperature θ . Ocean models that are TEOS-10 compatible need to calculate Absolute Salinity S_A and Conservative Temperature Θ (as discussed in appendices A.20 and A.21), and they need a computationally efficient expression for calculating specific volume (or density) in terms of Absolute Salinity S_A , Conservative Temperature Θ and pressure p .

Following the work of McDougall *et al.* (2003) and Jackett *et al.* (2006), the TEOS-10 specific volume \hat{v} has been approximated by a 75-term polynomial by Roquet *et al.* (2015). This polynomial is expressed in terms of the following three dimensionless salinity, temperature and pressure variables,

$$s \equiv \sqrt{\frac{S_A + 24 \text{ g kg}^{-1}}{S_{Au}}}, \quad \tau \equiv \frac{\Theta}{\Theta_u} \quad \text{and} \quad \pi \equiv \frac{p}{p_u}, \quad (\text{A.30.1})$$

in terms of the unit-related scaling constants

$$S_{Au} \equiv 40 \times 35.16504 \text{ g kg}^{-1} / 35, \quad \Theta_u \equiv 40^\circ\text{C} \quad \text{and} \quad p_u \equiv 10^4 \text{ dbar}. \quad (\text{A.30.2})$$

Their polynomial expression for the specific volume of seawater is

$$\hat{v}(S_A, \Theta, p) = v_u \sum_{i,j,k} v_{ijk} s^i \tau^j \pi^k, \quad (\text{A.30.3})$$

where $v_u \equiv 1 \text{ m}^3 \text{ kg}^{-1}$ and the non-zero dimensionless constants v_{ijk} are given in Table K.1 of appendix K. The specific volume data was fitted in a “funnel” of data points in (S_A, Θ, p) space (McDougall *et al.* (2003)) which extends to a pressure of 8000 dbar. At the sea surface the “funnel” covers the full range of temperature and salinity while for pressures greater than 6500 dbar the maximum temperature of the fitted data is 10°C and the minimum Absolute Salinity is 30 g kg^{-1} . That is, the fit has been performed over a region of parameter space which includes water that is approximately 8°C warmer and 5 g kg^{-1} fresher in the deep ocean than the seawater which exists in the present ocean.

As outlined in appendix K, this 75-term polynomial expression for v yields the thermal expansion and saline contraction coefficients, α^Θ and β^Θ , that are essentially as accurate as those derived from the full TEOS-10 Gibbs function for data in the “oceanographic funnel”. In dynamical oceanography it is these thermal expansion and haline contraction coefficients which are the most important aspects of the equation of state since the “thermal wind” is proportional to $\alpha^\Theta \nabla_p \Theta - \beta^\Theta \nabla_p S_A$ and the vertical static stability is given in terms of the buoyancy frequency N by $g^{-1} N^2 = \alpha^\Theta \Theta_z - \beta^\Theta (S_A)_z$. Hence for dynamical oceanography we may take Roquet *et al.*'s (2015) 75-term polynomial expression for specific volume as essentially reflecting the full accuracy of TEOS-10.

Appendix P describes how an expression for the enthalpy of seawater in terms of Conservative Temperature, specifically the functional form $\hat{h}(S_A, \Theta, p)$, together with an expression for entropy in the form $\hat{\eta}(S_A, \Theta)$, can be used as an alternative thermodynamic potential to the Gibbs function $g(S_A, t, p)$. The need for the functional form $\hat{h}(S_A, \Theta, p)$ also arises in section 3.32 and in Eqns. (3.26.3) and (3.29.1). The 75-term expression, Eqn. (A.30.3) for $v^{75} = \hat{v}^{75}(S_A, \Theta, p)$ can be used to find a closed expression for $\hat{h}(S_A, \Theta, p)$ by integrating $\hat{v}^{75}(S_A, \Theta, p)$ with respect to pressure (in Pa), since $\hat{h}_p = v = \rho^{-1}$ (see Eqn. (2.8.3)). Specific enthalpy calculated from $\hat{v}^{75}(S_A, \Theta, p)$ is available in the GSW Oceanographic Toolbox as the function **gsw_enthalpy**(SA,CT,p). Using **gsw_enthalpy** to evaluate $\hat{h}(S_A, \Theta, p)$ is 7 times faster than first evaluating the in situ temperature t (from **gsw_t_from_CT**(SA,CT,p)) and then calculating enthalpy from the full Gibbs function expression $h(S_A, t, p)$ using **gsw_enthalpy_t_exact**(SA,t,p). (These last two function calls have also been combined into the one function, **gsw_enthalpy_CT_exact**(SA,CT,p).)

Also, the enthalpy difference at the same values of S_A and Θ but at different pressures (see Eqn. (3.32.5)) is available as the function **gsw_enthalpy_diff**(SA,CT,p_shallow,p_deep).

Following Young (2010), the difference between h and $c_p^0 \Theta$ is called “dynamic enthalpy” and can be found using the function **gsw_dynamic_enthalpy**(SA,CT,p) in the GSW Oceanographic Toolbox.

Appendix K: Coefficients of the 75-term expression for the specific volume of seawater in terms of Θ

The TEOS-10 Gibbs function of seawater $g(S_A, t, p)$ is written as a polynomial in terms of in situ temperature t , while for ocean models, specific volume (or density) needs to be expressed as a computationally efficient expression in terms of Conservative Temperature Θ . Roquet *et al.* (2015) have published such a computationally efficient polynomial for specific volume. Their non-dimensional (root) salinity s , temperature τ , and pressure π , variables are

$$s \equiv \sqrt{\frac{S_A + 24 \text{ g kg}^{-1}}{S_{Au}}}, \quad \tau \equiv \frac{\Theta}{\Theta_u} \quad \text{and} \quad \pi \equiv \frac{p}{p_u}, \quad (\text{K.1})$$

in terms of the unit-related scaling constants

$$S_{Au} \equiv 40 \times 35.16504 \text{ g kg}^{-1} / 35, \quad \Theta_u \equiv 40^\circ\text{C} \quad \text{and} \quad p_u \equiv 10^4 \text{ dbar}. \quad (\text{K.2})$$

Their polynomial expression for the specific volume of seawater is

$$\hat{v}(S_A, \Theta, p) = v_u \sum_{i,j,k} v_{ijk} s^i \tau^j \pi^k, \quad (\text{K.3})$$

where $v_u \equiv 1 \text{ m}^3 \text{ kg}^{-1}$ and the non-zero dimensionless constants v_{ijk} are given in Table K.1.

Roquet *et al.* (2015) fitted the TEOS-10 values of specific volume v to S_A , Θ and p in a “funnel” of data points in (S_A, Θ, p) space. This is the same “funnel” of data points as used in McDougall *et al.* (2013); at the sea surface it covers the full range of temperature and salinity while for pressure greater than 6500 dbar, the maximum temperature of the fitted data is 10°C and the minimum Absolute Salinity is 30 g kg^{-1} . The maximum pressure of the “funnel” is 8000 dbar. Table K.1 contains the 75 coefficients of the expression (K.3) for specific volume in terms of (S_A, Θ, p) .

The rms error of this 75-term approximation to the full Gibbs function-derived TEOS-10 specific volume over the “funnel” is $0.2 \times 10^{-9} \text{ m}^3 \text{ kg}^{-1}$; this can be compared with the rms uncertainty of $4 \times 10^{-9} \text{ m}^3 \text{ kg}^{-1}$ of the underlying laboratory density data to which the TEOS-10 Gibbs function was fitted (see the first two rows of Table O.1 of appendix O). Similarly, the appropriate thermal expansion coefficient,

$$\alpha^\Theta = \frac{1}{v} \left. \frac{\partial v}{\partial \Theta} \right|_{S_A, p} = - \frac{1}{\rho} \left. \frac{\partial \rho}{\partial \Theta} \right|_{S_A, p}, \quad (\text{K.4})$$

of the 75-term equation of state is different from the same thermal expansion coefficient evaluated from the full Gibbs function-derived TEOS-10 with an rms error in the “funnel” of $0.03 \times 10^{-6} \text{ K}^{-1}$; this can be compared with the rms error of the thermal expansion coefficient of the laboratory data to which the Feistel (2008) Gibbs function was fitted of $0.73 \times 10^{-6} \text{ K}^{-1}$ (see row six of Table O.1 of appendix O). In terms of the evaluation of density gradients, the haline contraction coefficient evaluated from Eqn. (K.3) is many times more accurate than the thermal expansion coefficient. Hence we may consider the 75-term polynomial expression for specific volume, Eqn. (K.3), to be equally as accurate as the full TEOS-10 expressions for specific volume, for the thermal expansion coefficient and for the haline contraction coefficient for data that reside inside the “oceanographic funnel”.

The sound speed evaluated from the 75-term polynomial of Eqn. (K.3) has an rms error over the “funnel” of 0.025 m s^{-1} which is a little less than the rms error of the underlying sound speed data that was incorporated into the Feistel (2008) Gibbs function, being 0.035 m s^{-1} (see rows 7 to 9 of Table O.1 of appendix O). Hence, especially for the purposes of dynamical oceanography where α^Θ and β^Θ are the aspects of the equation of

state that, together with spatial gradients of S_A and Θ , drive ocean currents and affect the calculation of the buoyancy frequency, we may take the 75-term expression for specific volume, Eqn. (K.3), as essentially reflecting the full accuracy of TEOS-10.

The use of Eqn. (K.3) to evaluate $\hat{v}(S_A, \Theta, p)$ or $\hat{\rho}(S_A, \Theta, p)$ from **gsw_specvol**(SA,CT,p) or **gsw_rho**(SA,CT,p) is approximately five times faster than first evaluating the *in situ* temperature t (from **gsw_t_from_CT**(SA,CT,p)) and then calculating *in situ* specific volume or density from the full Gibbs function expression $v(S_A, t, p)$ or $\rho(S_A, t, p)$ via **gsw_specvol_t_exact**(SA,t,p) or **gsw_rho_t_exact**(SA,t,p). (These two function calls have been combined into **gsw_specvol_CT_exact**(SA,CT,P) and **gsw_rho_CT_exact**(SA,CT,P).)

Table K.1. Coefficients of the 75-term polynomial of Roquet *et al.* (2015).

i	j	k	v_{ijk}	i	j	k	v_{ijk}	i	j	k	v_{ijk}
0	0	0	1.0769995862e-3	0	5	0	-8.0539615540e-7	1	0	2	-5.8484432984e-7
1	0	0	-3.1038981976e-4	1	5	0	-3.3052758900e-7	2	0	2	-4.8122251597e-6
2	0	0	6.6928067038e-4	0	6	0	2.0543094268e-7	3	0	2	4.9263106998e-6
3	0	0	-8.5047933937e-4	0	0	1	-6.0799143809e-5	4	0	2	-1.7811974727e-6
4	0	0	5.8086069943e-4	1	0	1	2.4262468747e-5	0	1	2	-1.1736386731e-6
5	0	0	-2.1092370507e-4	2	0	1	-3.4792460974e-5	1	1	2	-5.5699154557e-6
6	0	0	3.1932457305e-5	3	0	1	3.7470777305e-5	2	1	2	5.4620748834e-6
0	1	0	-1.5649734675e-5	4	0	1	-1.7322218612e-5	3	1	2	-1.3544185627e-6
1	1	0	3.5009599764e-5	5	0	1	3.0927427253e-6	0	2	2	2.1305028740e-6
2	1	0	-4.3592678561e-5	0	1	1	1.8505765429e-5	1	2	2	3.9137387080e-7
3	1	0	3.4532461828e-5	1	1	1	-9.5677088156e-6	2	2	2	-6.5731104067e-7
4	1	0	-1.1959409788e-5	2	1	1	1.1100834765e-5	0	3	2	-4.6132540037e-7
5	1	0	1.3864594581e-6	3	1	1	-9.8447117844e-6	1	3	2	7.7618888092e-9
0	2	0	2.7762106484e-5	4	1	1	2.5909225260e-6	0	4	2	-6.3352916514e-8
1	2	0	-3.7435842344e-5	0	2	1	-1.1716606853e-5	0	0	3	-1.1309361437e-6
2	2	0	3.5907822760e-5	1	2	1	-2.3678308361e-7	1	0	3	3.6310188515e-7
3	2	0	-1.8698584187e-5	2	2	1	2.9283346295e-6	2	0	3	1.6746303780e-8
4	2	0	3.8595339244e-6	3	2	1	-4.8826139200e-7	0	1	3	-3.6527006553e-7
0	3	0	-1.6521159259e-5	0	3	1	7.9279656173e-6	1	1	3	-2.7295696237e-7
1	3	0	2.4141479483e-5	1	3	1	-3.4558773655e-6	0	2	3	2.8695905159e-7
2	3	0	-1.4353633048e-5	2	3	1	3.1655306078e-7	0	0	4	1.0531153080e-7
3	3	0	2.2863324556e-6	0	4	1	-3.4102187482e-6	1	0	4	-1.1147125423e-7
0	4	0	6.9111322702e-6	1	4	1	1.2956717783e-6	0	1	4	3.1454099902e-7
1	4	0	-8.7595873154e-6	0	5	1	5.0736766814e-7	0	0	5	-1.2647261286e-8
2	4	0	4.3703680598e-6	0	0	2	9.9856169219e-6	0	0	6	1.9613503930e-9