Notes on the function
[SA_final, CT_final, w_Ih_final] = …
gsw_frazil_properties(SA_bulk, h_pot_bulk, p)

This function, **gsw_frazil_properties**(SA_bulk, h_pot_bulk,p), evaluates the final interstitial seawater Absolute Salinity, interstitial seawater Conservative Temperature, and the final ice mass fraction of the seawater and frazil mixture that exists at the equilibrium freezing temperature for given input values of the bulk Absolute Salinity, SA_bulk, bulk potential enthalpy, h_pot_bulk, and pressure, p. The "bulk" variables, h_pot_bulk and SA_bulk are defined in Eqns. (1) and (2) below.

Consider a box in a Cartesian z-coordinate model that advances the conservation equations for "heat" "salt" and "ice". Imagine these three quantities being advanced one time step by the processes of advection and diffusion and boundary fluxes [including the air-sea boundary fluxes and the ice-sea boundary fluxes] and the vertical Stokes drift velocity of the frazil ice size classes, migrating vertically between model boxes. After this advection/diffusion step, the variables need to be brought back into thermodynamic equilibrium at the freezing temperature, and during this second part of the time step, there is no transfer of heat, salt or water across the faces of the box.

In this second part of the model time step we consider a mixture of small ice Ih crystals (frazil ice) suspended in seawater, and we ignore any relative vertical velocity that the ice crystals might have with respect to the seawater. In section 5 of McDougall *et al*. (2014) we considered what happened when the pressure of this seawater-frazil ice mixture changed. In section 3 of that paper we dealt with the melting of ice Ih into seawater at fixed pressure, and we compared panels (a) and (b) of Figure 6 to show that at a pressure of 500 dbar the assumption that the sum of the *potential* enthalpies of ice and seawater is conserved leads to an error of 0.15% (the correct thing that is conserved is the sum of the *in situ* enthalpies of ice and seawater). Most of this error is due to ice, not seawater, since an error of 0.15% for seawater alone occurs at a much larger pressure of 4000 dbar . Graham and McDougall (2013) proved that the error involved in treating Conservative Temperature as totally conserved is very small. The arguments to prove this were rather complicated, and are to be found in section 3b of that paper; essentially it is based on the realization that for a turbulent mixing process occurring at a particular pressure, the potential enthalpy referenced to that pressure is both a "potential" and a "conservative" variable. Figure 6(a) and 6(b) of our ice paper does the same thing for the interaction of ice Ih and seawater. In the present code we conserve enthalpy (rather than the ***potential enthalpy***). In so doing, this code will not be as computationally efficient as if we made the approximation of conserving potential enthalpy.

Let the mass fraction of ice be w^{Ih}; the mass fraction of seawater in the ice-seawater mixture is then $\left(1 - w^{Ih}\right)$. The total enthalpy per unit mass of the ice-seawater mixture at any stage is the weighted sum of the specific enthalpies of the two phases, namely

$$h^{B} \equiv \left(1 - w^{Ih}\right)h + w^{Ih}h^{Ih}. \tag{1}$$

Here the "B" of h^{B} stands for "bulk". The specific enthalpy of ice Ih, h^{Ih}, can be expressed in the functional form $h^{Ih}\left(t^{Ih}, p\right)$ in terms of the *in situ* temperature of the ice.

After the first part of the two-stage time-stepping procedure one gets an updated value of h^{B}. During this first half of the time step one can imagine the model to have advected and diffused h^{B} across the six faces of each of the model's boxes.

The analogous salty thing that should be advected and diffused by the model is the "bulk salinity", that is, the "Absolute Salinity of the mixture", defined by

$$S_A^B \equiv \left(1 - w^{\mathrm{Ih}}\right)S_A,\tag{2}$$

and the analogous thing for ice is the mass fraction of ice itself, namely w^{Ih}. Note that h^B and S_A^B are conservative variables while w^{Ih} is not a conservative variable during the process of adjustment to a new thermodynamic equilibrium. That is, during the second half of the time step, when the seawater and ice phases are brought into thermodynamic equilibrium, h^B and S_A^B are both conserved but w^{Ih} is not (and neither is the interstitial Absolute Salinity S_A of the seawater component).

That is, the variables that should be conserved during the thermodynamic equilibration phase are

$$h^B \equiv \left(1 - w^{\mathrm{Ih}}\right)h + w^{\mathrm{Ih}}h^{\mathrm{Ih}}\quad\boxed{\text{and}}\quad S_A^B \equiv \left(1 - w^{\mathrm{Ih}}\right)S_A.\tag{3}$$

At the end of the first phase of each time step we will have the subscript 1 values

$$h_1^B \equiv \left(1 - w_1^{\mathrm{Ih}}\right)h_1 + w_1^{\mathrm{Ih}}h_1^{\mathrm{Ih}},\quad S_{A1}^B \equiv \left(1 - w_1^{\mathrm{Ih}}\right)S_{A1}\quad\text{and}\quad w_1^{\mathrm{Ih}},\tag{4}$$

and our job is to invent a phase two procedure of this time step that brings the ocean and ice properties back into equilibrium at the freezing temperature. During this phase two, the mass fraction of ice will change and the constraints are that there is no exchange of heat with the environment, that is that

$$\left(1 - w_2^{\mathrm{Ih}}\right)h_2 + w_2^{\mathrm{Ih}}h_2^{\mathrm{Ih}} = \left(1 - w_1^{\mathrm{Ih}}\right)h_1 + w_1^{\mathrm{Ih}}h_1^{\mathrm{Ih}} \equiv h_1^B,\tag{5}$$

that the total amount of salt is conserved, that is that

$$\left(1 - w_2^{\mathrm{Ih}}\right)S_{A2} = \left(1 - w_1^{\mathrm{Ih}}\right)S_{A1} \equiv S_{A1}^B,\tag{6}$$

and that the total amount of H_2O is conserved, that is, that

$$\left(1 - w_2^{\mathrm{Ih}}\right)\left(1 - S_{A2}\right) + w_2^{\mathrm{Ih}} = \left(1 - w_1^{\mathrm{Ih}}\right)\left(1 - S_{A1}\right) + w_1^{\mathrm{Ih}}.\tag{7}$$

This H_2O constraint is the same constraint as the salt constraint Eqn. (6), so we can ignore it.

So we have the two constraints Eqns. (5) and (6) as well as the fact that either (i) the final values are at the freezing temperature, or (ii) that there is no ice present. So our aim is to find the value of the ice mass fraction w_2^{Ih} that solves $f\left(w_2^{\mathrm{Ih}}\right) = 0$ where the function $f\left(w^{\mathrm{Ih}}\right)$ is given by

$$f\left(w^{\mathrm{Ih}}\right) = h_1^B - \left(1 - w^{\mathrm{Ih}}\right)h\left(S_A, \Theta_{\mathrm{freezing}}[S_A, p], p\right) - w^{\mathrm{Ih}}h^{\mathrm{Ih}}\left(t_{\mathrm{freezing}}[S_A, p], p\right).\tag{8}$$

During the evaluation of $f\left(w^{\mathrm{Ih}}\right)$ the interstitial seawater Absolute Salinity is given by

$$S_A = \frac{S_{A1}^B}{\left(1 - w^{\mathrm{Ih}}\right)}.\tag{9}$$

The zero of $f\left(w^{\mathrm{Ih}}\right)$, namely finding the value of w_2^{Ih} at which $f\left(w_2^{\mathrm{Ih}}\right) = 0$, is found using the modified Newton-Raphson method of McDougall and Wotherspoon (2014) using the following expression for the derivative of $f\left(w^{\mathrm{Ih}}\right)$ with respect to w^{Ih} (using the w^{Ih} derivative of Eqn. (9)),

$$f'\left(w^{\mathrm{Ih}}\right) = h\left(S_A, \Theta_{\mathrm{freezing}}[S_A, p], p\right) - h^{\mathrm{Ih}}\left(t_{\mathrm{freezing}}[S_A, p], p\right)$$

$$- S_A\left[\left.\frac{\partial h}{\partial S_A}\right|_{\Theta, p} + \left.\frac{\partial h}{\partial \Theta}\right|_{S_A, p}\left.\frac{\partial \Theta_{\mathrm{freezing}}}{\partial S_A}\right|_p\right] - \frac{S_A\, w^{\mathrm{Ih}}}{\left(1 - w^{\mathrm{Ih}}\right)}c_p^{\mathrm{Ih}}\left(t_{\mathrm{freezing}}, p\right)\left.\frac{\partial t_{\mathrm{freezing}}}{\partial S_A}\right|_p.\tag{10}$$

So how do we proceed to solve $f\left(w^{\mathrm{Ih}}\right) = 0$ and so proceed from the intermediate time step 1 to arrive at the values labeled 2 at the end of the full model time step; values labeled 2 that solve $f\left(w_2^{\mathrm{Ih}}\right) = 0$? Answer, we do a Modified Newton Raphson iterative procedure (McDougall and Wotherspoon (2014)), and the first value of $f\left(w^{\mathrm{Ih}}\right)$ is the value of f at w_1^{Ih}. We can calculate the value of the interstitial Absolute Salinity at the half time step (at time 1) from Eqn. (6), namely

$$S_{A1} = \frac{S_{A1}^B}{\left(1 - w_1^{Ih}\right)}, \tag{12}$$

where we are confident that the ice mass fraction never approaches unity because when it gets greater than say 0.2, a very large vertical diffusion coefficient kicks in to the model code to ensure that the interstitial salinity does not get too large and that the ice mass fraction never ever exceeds 0.5. The initial value of f is then

$$f\left(w^{Ih}\right) = h_1^B - \left(1 - w_1^{Ih}\right)h\left(S_{A1}, \Theta_{\text{freezing}}[S_{A1}, p], p\right) - w_1^{Ih} h^{Ih}\left(t_{\text{freezing}}[S_{A1}, p], p\right). \tag{13}$$

The initial value of the derivative f' is similarly evaluated at S_{A1} as

$$f'\left(w_1^{Ih}\right) = h\left(S_{A1}, \Theta_{\text{freezing}}[S_{A1}, p], p\right) - h^{Ih}\left(t_{\text{freezing}}[S_{A1}, p], p\right)$$

$$- S_{A1}\left[\left.\frac{\partial h}{\partial S_A}\right|_{\Theta, p} + \left.\frac{\partial h}{\partial \Theta}\right|_{S_A, p} \left.\frac{\partial \Theta_{\text{freezing}}}{\partial S_A}\right|_p\right] - \frac{S_{A1} w_1^{Ih}}{\left(1 - w_1^{Ih}\right)} c_p^{Ih}\left(t_{\text{freezing1}}, p\right) \left.\frac{\partial t_{\text{freezing}}}{\partial S_A}\right|_p. \tag{14}$$

where the partial derivatives are evaluated at (S_{A1}, p). Note that in Eqn. (10) the largest term is $- h^{Ih}\left(t_{\text{freezing}}[S_A, p], p\right)$, and in fact the top line of Eqn. (10) is very similar to the latent heat of melting.

What to do if all the ice melts by the end of this time step? This paragraph addresses the situation where we find that $w_2^{Ih} < 0$. That is, we consider the situation where we find that the solution of $f\left(w_2^{Ih}\right) = 0$ corresponds to the mass fraction of ice w_2^{Ih} being negative. This indicates that during this equilibration phase all of the ice will melt. This means that one is left with pure seawater rather a conglomerate of seawater and ice. When this is detected we set the final ice mass fraction to zero, ($w_2^{Ih} = 0$) and S_{A2} is calculated from Eqn. (6) as $S_{A2} = S_{A1}^B = \left(1 - w_1^{Ih}\right)S_{A1}$, while with $w_2^{Ih} = 0$ Eqn. (5) reduces to

$$h_2 = h\left(S_{A1}^B, \Theta_2, p\right) = \left(1 - w_1^{Ih}\right)h_1 + w_1^{Ih}h_1^{Ih} \equiv h_1^B, \tag{15}$$

which can be inverted using gsw_CT_from_enthalpy_exact to yield the Conservative Temperature of the final mixture, Θ_2.

How do we detect that we are in a sufficiently warm piece of seawater that we do not need to spend the computer time in this "frazil properties" code? It makes sense to have a simple method to detect when we are in a box that is sufficiently warm that if we entered this thermodynamic code, the output would be $w_2^{Ih} \leq 0$, because then we know that in fact the answer is warm seawater with no frazil ice and the answer is very simple to write down.

The way to detect this situation is to consider the situation where the output ice mass fraction w_2^{Ih} is exactly zero and the seawater is exactly at the freezing temperature. We ask what value of the input bulk potential enthalpy, $\hbar_{\text{limit}}^B$, would be required in order to achieve exactly $w_2^{Ih} = 0$ at the freezing temperature. In this case (from Eqn. (3)) we see that $S_{A\,\text{limit}} = S_{A1}^B$ and $\hbar_{\text{limit}}^B \equiv c_p^0 \Theta_{\text{freezing}}\left(S_{A1}^B, p\right)$. Recapping, if the input bulk potential enthalpy is this value, $\hbar_{\text{limit}}^B \equiv c_p^0 \Theta_{\text{freezing}}\left(S_{A1}^B, p\right)$, the output of the modified Newton's Method iterations will yield $w_2^{Ih} = 0$. Now we note that if $\hbar_1^B > \hbar_{\text{limit}}^B$ then the modified Newton's Method will yield a negative final ice mass fraction, that is $w_2^{Ih} < 0$. This can be seen from evaluating $f\left(w^{Ih}\right)$ of Eqn. (8) with $w^{Ih} = 0$ noting that because $\hbar_1^B > \hbar_{\text{limit}}^B$, $f\left(w^{Ih}\right) > 0$, and then noting that since the derivative, Eqn. (10), is always positive, this implies that $w_2^{Ih} < 0$.

The upshot of this detection method is simply that we test whether $\hbar_1^B > c_p^0 \Theta_{\text{freezing}}\left(S_{A1}^B, p\right)$ and if it is, we avoid doing the computationally expensive modified Newton's Method iterations and instead we put

$$w_2^{\text{Ih}} = 0, \qquad S_{A2} = S_{A1}^B \qquad \text{and} \qquad \Theta_2 = \hbar_1^B / c_p^0. \tag{16}$$

In more detail, in the code we evaluate a variable we call func0 defined by

$$\text{func0} \equiv \hbar_1^B - c_p^0 \Theta_{\text{freezing}}\left(S_{A1}^B, p\right), \tag{16A}$$

and if this variable is positive (or zero) we determine the three outputs of the algorithm using Eqn. (16). In this way the computationally expensive Newton iterations are avoided for all the data that is "too warm" to contain any frazil ice at the end of the iterations.

The initial value of w^{Ih} in the code. For data values that have func0 < 0 (which means that $\hbar_1^B$ is "sufficiently cool" that some frazil ice will co-exist in thermodynamic equilibrium with the interstitial seawater at the end of the time step) we proceed as follows. We realize that $w^{\text{Ih}} \to 0$ as func0 $\to 0$ and we find an initial estimate of the ice mass fraction w^{Ih} as being func0 divided by a very simple four-term polynomial in func0 and pressure. With this initial value of w^{Ih} the modified Newton's method of McDougall and Wotherspoon (2014) is employed to find the root of $f\left(w_2^{\text{Ih}}\right) = 0$ using the expression Eqn. (10) or (14) for the derivative of this function. The method converges to machine precision within three iterations.

There are three similar GSW (Gibbs SeaWater) codes that solves $f\left(w_2^{\text{Ih}}\right) = 0$. These are called

[SA_final, CT_final, w_Ih_final] = gsw_frazil_properties_potential(SA_bulk,h_pot_bulk,p)
and

[SA_final, CT_final, w_Ih_final] = …

 gsw_frazil_properties_potential_poly(SA_bulk,h_pot_bulk,p).
It is this "poly" version of this code that we expect to be used in forward ocean models. We also have the present code

[SA_final, CT_final, w_Ih_final] = gsw_frazil_properties(SA_bulk,h_bulk,p)
where the quantity that is input is enthalpy rather than potential enthalpy. This code is very computationally expensive compared with the other two.

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