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

This function, **gsw_frazil_properties_potential**(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. Henceforth we take that it is sufficiently accurate to assume that the mass-weighted *potential enthalpy* of a mixture of ice and seawater is unchanged when melting or freezing occurs.

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

$$\hbar^{\text{B}} \equiv \left(1 - w^{\text{Ih}}\right)c_p^0\Theta \ + \ w^{\text{Ih}}\hbar^{\text{Ih}}, \tag{1}$$

where we have chosen to write the specific potential enthalpy of seawater, $\hbar\left(S_{\text{A}},t,p\right) \equiv c_p^0\Theta$, in terms of Conservative Temperature. Here the "B" of $\hbar^{\text{B}}$ stands for "bulk" and the symbol $\hbar$ stands for potential enthalpy, so $\hbar^{\text{B}}$ is the "bulk potential enthalpy of the seawater and frazil ice conglomerate". The specific potential enthalpy of ice Ih, $\hbar^{\text{Ih}}$, can be expressed as a function of only the potential temperature of ice $\hbar^{\text{Ih}}\left(\theta^{\text{Ih}}\right)$, or it can be written in the functional form $\hbar^{\text{Ih}}\left(t^{\text{Ih}}, p\right)$ 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 $\hbar^B$. During this first half of the time step the model has advected and diffused $\hbar^B$ 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

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

and the analogous thing for ice is the mass fraction of ice itself, namely w^{Ih}. Note that $\hbar^B$ 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 first half of the model's full time step the model advects and diffuses $\hbar^B$ and S_A^B across the six faces of each of the model's boxes. Also during this first half of the time step, the ice mass fraction w^{Ih} is also advected and diffused across the six faces as a conservative variable. During the second half of the time step, when the seawater and ice phases are brought into thermodynamic equilibrium, $\hbar^B$ 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 raw conservative variables that should be advected and diffused during phase one by an ocean model that admits the presence of frazil ice in each grid cell are

$$\hbar^B \equiv \left(1 - w^{Ih}\right) c_p^0 \Theta \; + \; w^{Ih} \hbar^{Ih}, \quad S_A^B \equiv \left(1 - w^{Ih}\right) S_A \quad \text{and} \quad w^{Ih}.\tag{3}$$

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

$$\hbar_1^B \equiv \left(1 - w_1^{Ih}\right) c_p^0 \Theta_1 \; + \; w_1^{Ih} \hbar_1^{Ih}, \quad S_{A1}^B \equiv \left(1 - w_1^{Ih}\right) S_{A1} \quad \text{and} \quad w_1^{Ih},\tag{4}$$

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

$$\left(1 - w_2^{Ih}\right) c_p^0 \Theta_2 \; + \; w_2^{Ih} \hbar_2^{Ih} \; = \; \left(1 - w_1^{Ih}\right) c_p^0 \Theta_1 \; + \; w_1^{Ih} \hbar_1^{Ih} \; \equiv \; \hbar_1^B,\tag{5}$$

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

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

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

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

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 $f\left(w_2^{Ih}\right) = 0$ where the function $f\left(w^{Ih}\right)$ is given by

$$f\left(w^{Ih}\right) \; = \; \hbar_1^B - \left(1 - w^{Ih}\right) c_p^0 \Theta_{\text{freezing}}\left(S_A, p\right) \; - \; w^{Ih} \hbar_{\text{freezing}}^{Ih}\left(S_A, p\right).\tag{8}$$

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

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

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

$$f'\left(w^{\mathrm{Ih}}\right) = c_p^0 \Theta_{\mathrm{freezing}}\left(S_A, p\right) - \hbar_{\mathrm{freezing}}^{\mathrm{Ih}}\left(S_A, p\right)$$

$$- S_A c_p^0 \left.\frac{\partial \Theta_{\mathrm{freezing}}}{\partial S_A}\right|_p - \frac{S_A w^{\mathrm{Ih}}}{\left(1 - w^{\mathrm{Ih}}\right)} \left.\frac{\partial \hbar_{\mathrm{freezing}}^{\mathrm{Ih}}}{\partial S_A}\right|_p . \tag{10}$$

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

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

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

$$f\left(w_1^{\mathrm{Ih}}\right) = \hbar_1^B - \left(1 - w_1^{\mathrm{Ih}}\right)c_p^0 \Theta_{\mathrm{freezing}}\left(S_{A1}, p\right) - w_1^{\mathrm{Ih}} \hbar_{\mathrm{freezing}}^{\mathrm{Ih}}\left(S_{A1}, p\right). \tag{13}$$

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

$$f'\left(w_1^{\mathrm{Ih}}\right) = c_p^0 \Theta_{\mathrm{freezing}}\left(S_{A1}, p\right) - \hbar_{\mathrm{freezing}}^{\mathrm{Ih}}\left(S_{A1}, p\right)$$

$$- S_{A1} c_p^0 \left.\frac{\partial \Theta_{\mathrm{freezing}}}{\partial S_A}\right|_p - \frac{S_{A1} w_1^{\mathrm{Ih}}}{\left(1 - w_1^{\mathrm{Ih}}\right)} \left.\frac{\partial \hbar_{\mathrm{freezing}}^{\mathrm{Ih}}}{\partial S_A}\right|_p . \tag{14}$$

where the two partial derivatives are both evaluated at $\left(S_{A1}, p\right)$. Note that in Eqn. (10) the largest term is $-\hbar_{\mathrm{freezing}}^{\mathrm{Ih}}\left(S_A, p\right)$, 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 case where we find that $w_2^{\mathrm{Ih}} < 0$ which means that all the frazil ice has actually melted during this total time step. That is, we find that the solution of $f\left(w_2^{\mathrm{Ih}}\right) = 0$ 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, and the solution procedure then is simple. When it is detected that $\hbar_1^B$ is too large ("too warm") then the final ice mass fraction is set to zero, ($w_2^{\mathrm{Ih}} = 0$) and S_{A2} is calculated from Eqn. (6) as $S_{A2} = S_{A1}^B = \left(1 - w_1^{\mathrm{Ih}}\right)S_{A1}$, and with $w_2^{\mathrm{Ih}} = 0$ Eqn. (5) reduces to

$$c_p^0 \Theta_2 = \left[\left(1 - w_1^{\mathrm{Ih}}\right)c_p^0 \Theta_1 + w_1^{\mathrm{Ih}} \hbar_1^{\mathrm{Ih}}\right] = \hbar_1^B, \tag{15}$$

which gives 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 potential (poly)" 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 $w_2^{\mathrm{Ih}} \leq 0$, 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, $\hbar_{\mathrm{limit}}^B$, would be required in order to achieve exactly $w_2^{\mathrm{Ih}} = 0$ at the freezing temperature. In this case (from Eqn. (3)) we see that $S_{A\,\mathrm{limit}} = S_{A1}^B$ and

$\hbar_{\text{limit}}^{\text{B}} \equiv c_p^0 \Theta_{\text{freezing}} \left(S_{\text{A1}}^{\text{B}}, p \right).$ Recapping, if the input bulk potential enthalpy is this value, $\hbar_{\text{limit}}^{\text{B}} \equiv c_p^0 \Theta_{\text{freezing}} \left(S_{\text{A1}}^{\text{B}}, p \right),$ the output of the modified Newton's Method iterations will yield $w_2^{\text{Ih}} = 0.$ Now we note that if $\hbar_1^{\text{B}} > \hbar_{\text{limit}}^{\text{B}}$ then the modified Newton's Method will yield a negative final ice mass fraction, that is $w_2^{\text{Ih}} < 0.$ This can be seen from evaluating $f\left(w^{\text{Ih}} \right)$ of Eqn. (8) with $w^{\text{Ih}} = 0$ noting that because $\hbar_1^{\text{B}} > \hbar_{\text{limit}}^{\text{B}},$ $f\left(w^{\text{Ih}} \right) > 0,$ and then noting that since the derivative, Eqn. (10), is always positive, this implies that $w_2^{\text{Ih}} < 0.$

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

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

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

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

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 $\hbar_1^{\text{B}}$ 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. In the GSW code we first estimate the ice mass fraction using a polynomial with 36 coefficients. This polynomial is in terms of (normalized values of) S_{A}^{B}, func0 and p. Every term in the polynomial contains at least the first power of func0 so that $w^{\text{Ih}} \rightarrow 0$ as func0 $\rightarrow 0$. When we formed this polynomial we up-weighted the region of parameter space in which the ocean model code will most often find itself so as to reduce the number of Newton iterations needed. This polynomial was in fact simply imported from the _poly version of this code.

Because the evaluation of the derivative, $f'\left(w_1^{\text{Ih}} \right)$, involves four separate calls to GSW functions (see Eqn. (14)) it is computationally expensive and we sought to minimize the number of times we needed to evaluate it (we managed to evaluate it only once in the code). Rather than evaluating this derivative at this stage using Eqn. (14) we chose to essentially fit a polynomial to a finite amplitude version of this derivative. The aim of this step was to perform a Newton step using this polynomial form of the derivative so that when the full derivative is calculated, it is calculated at a more accurate point. The finite amplitude derivative, called dfunc_dw_Ih_mean_poly in the code, is a polynomial in S_{A}, w^{Ih} and p with 29 coefficients. This polynomial was in fact simply imported from the _poly version of this code.

Next a Newton step was perfomed using this polynomial form of the derivative but with the func being evaluated with the exact GSW functions (rather than with the _poly versions). Following this, the full derivative $f'\left(w^{\text{Ih}} \right)$ is evaluated (again, with the exact GSW functions rather than with the _poly versions), and the main Newton iteration was begun. For data in the range

```
w_Ih_t >= 0 & w_Ih_t <= 0.20 & SA_t > 15 & SA_t < 60 & p <= 3000
```
only one Newton iteration is needed in order to reach machine precision, while in the range

```
w_Ih_t >= 0 & w_Ih_t <= 0.85 & SA_t > 0 & SA_t < 120 & p <= 3500
```
two Newton iterations are needed, and outside these ranges, three iterations are needed. As noted above, these Newton iterations use the one value of $f'\left(w^{\text{Ih}} \right)$ which we evaluate before entering this Newton loop part of the code.

The GSW (Gibbs SeaWater) codes that solve $f\left(w_2^{\mathrm{Ih}}\right) = 0$ 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).

These codes output the Absolute Salinity and Conservative Temperature, S_{A2} and Θ_2, of the final equilibrium seawater-frazil mixture as well as the final frazil ice mass fraction w_2^{Ih}. It is the "poly" version of this code that we expect to be used in forward ocean models. We also have the 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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