Notes on the GSW function gsw_Sstar_from_SP

Notes updated 24th February 2011

Preformed Salinity S_* is designed to be a conservative salinity variable which is unaffected by biogeochemical activity in the ocean; it is defined as Absolute Salinity less the contributions of biogeochemical processes to Absolute Salinity.

The **gsw_Sstar_from_SP**(SP,p,long,lat) function first interpolates the global Absolute Salinity Anomaly Ratio (R^δ) data set using the internal GSW library function **gsw_SAAR** to the (p,long,lat) location and then uses this interpolated value of R^δ to calculate Preformed Salinity S_* according to

$$S_* = \frac{35.165\,04\ \mathrm{g\,kg^{-1}}}{35}\ S_\mathrm{P}\left(1 - r_1 R^\delta\right), \qquad \textit{Non-Baltic} \qquad (1)$$

where r_1 is taken to be the constant 0.35 based on the work of Pawlowicz *et al.* (2011). Note that $\left(35.165\,04\ \mathrm{g\,kg^{-1}}/35\right) S_\mathrm{P}$ is Reference Salinity S_R which is the best estimate of Absolute Salinity for a Standard Seawater sample.

In the Baltic Sea the deviations of Absolute Salinity from Reference Salinity are not due to non-conservative biogeochemical processes but rather are due to the anomalous composition entering the Baltic from rivers. Since these anomalous constituents are conservative, Preformed Salinity S_* in the Baltic Sea is taken to be the same as Absolute Salinity. Equation (1) is the value of Preformed Salinity S_* returned by **gsw_Sstar_from_SP** unless the function detects that the location is in the Baltic Sea (where incidentally the Absolute Salinity Anomaly Ratio (R^δ) internal library function **gsw_SAAR** is arranged to return a value of zero). If the observation is from the Baltic Sea, Preformed Salinity S_* is calculated according to $S_\mathrm{A} - S_\mathrm{R} = 0.087\,\mathrm{g\,kg^{-1}} \times \left(1 - S_\mathrm{P}/35\right)$ (from Eqn. (A.5.6) of IOC *et al.* (2010), following Feistel *et al.* (2010)), so that

$$S_* = S_\mathrm{A} = \frac{\left(35.165\,04\ -\ 0.087\right)\ \mathrm{g\,kg^{-1}}}{35}\ S_\mathrm{P}\ +\ 0.087\ \mathrm{g\,kg^{-1}}. \quad \textit{Baltic Sea} \qquad (2)$$

In summary, the **gsw_Sstar_from_SP** function returns either Eqn. (1) or Eqn. (2) depending on whether the longitude and latitude of the sample put the observation outside or inside the Baltic Sea. Since Practical Salinity should always be positive but there may sometimes be a few negative values from a CTD, any negative input values of S_P to this function **gsw_Sstar_from_SP** are set to zero.

If the latitude and longitude are such as to place the observation well away from the ocean, a flag 'in_ocean' is set to zero as a warning, otherwise it is 1. This flag is only set when the observation is well and truly on dry land; often the warning flag is not set until one is several hundred kilometers inland from the coast. When the function detects that the observation is not from the ocean, R^δ is set equal to zero and **gsw_Sstar_from_SP** returns $S_* = S_\mathrm{R} = \left(35.165\,04\ \mathrm{g\,kg^{-1}}/35\right) S_\mathrm{P}$ in accordance with Eqn. (1).

References

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Below is appendix A.20 of the TEOS-10 Manual (IOC *et al*. (2010)) which discusses the
conservative nature of Preformed Salinity S_* and its use in numerical ocean models.

A.20 The representation of salinity in numerical ocean models

Ocean models need to evaluate salinity at every time step as a necessary prelude to using
the equation of state to determine density and its partial derivatives for use in the
hydrostatic relationship and in neutral mixing algorithms. The current practice in
numerical models is to treat salinity as a perfectly conserved quantity in the interior of the
ocean; salinity changes at the surface and at coastal boundaries due to evaporation,
precipitation, brine rejection, ice melt and river runoff, and satisfies an advection-diffusion
equation away from these boundaries. The inclusion of composition anomalies
necessitates several changes to this approach. These changes can be divided into two
broad categories. First, in addition to fresh water inputs and brine rejection, all sources of
dissolved material entering through the surface and coastal boundaries of the model
should be considered as possible sources of composition anomalies. Second, within the
interior of the model, changes due to the growth, decay and remineralization of biological
material must be considered. Here, we focus on this second issue. While the ultimate
resolution of these issues will involve biogeochemical models, in this appendix we discuss
some practical ways forward based on the approximate relations (A.5.7) - (A.5.12) between
the salinity variables S_R, S_* and $S_A = S_A^{\mathrm{dens}}$. At the time of writing, the suggested
approaches here have not been tested, so it must be acknowledged that the treatment of
seawater composition anomalies in ocean models is currently a work in progress.
    We begin by repeating Eqns. (A.5.11) and (A.5.12), namely

$$S_* \;=\; S_R \left(1 - r_1 R^\delta \right), \tag{A.20.1}$$

$$S_A \;=\; S_* \left(1 + F^\delta \right), \tag{A.20.2}$$

where

$$R^\delta \;\equiv\; \frac{\delta S_A^{\mathrm{atlas}}}{S_R^{\mathrm{atlas}}} \quad \text{and} \quad F^\delta \;=\; \frac{\left[1 + r_1 \right] R^\delta}{\left(1 - r_1 R^\delta \right)} \;. \tag{A.20.3}$$

Recall that the Absolute Salinity Anomaly Ratio, $R^\delta \equiv \delta S_A^{\mathrm{atlas}} \big/ S_R^{\mathrm{atlas}}$, is the ratio of the atlas
values of Absolute Salinity Anomaly and Reference Salinity. The stored values of R^δ are
interpolated onto the latitude, longitude and pressure of an oceanographic observation.
R^δ is bounded between zero 0.001 in the global ocean. With r_1 taken to be 0.35 we note
the approximate expression $F^\delta = S_A \big/ S_* - 1 \approx 1.35 R^\delta$.

A.20.1 Using Preformed Salinity S_* as the conservative salinity variable

Because Preformed Absolute Salinity S_* (henceforth referred to by the shortened name,
Preformed Salinity) is designed to be a conservative salinity variable, blind to the effects of
biogeochemical processes, its evolution equation will be in the conservative form (A.8.1).
When this type of conservation equation is averaged in the appropriate manner (see

appendix A.21) the conservation equation for Preformed Salinity becomes (from Eqn. (A.21.7)),

$$\frac{d\hat{S}_*}{dt} \;=\; \gamma_z \nabla_n \cdot \left(\gamma_z^{-1} K \nabla_n \hat{S}_* \right) + \left(D \frac{\partial \hat{S}_*}{\partial z} \right)_z . \tag{A.20.4}$$

As explained in appendix A.21, the over-tilde of $\hat{S}_*$ indicates that this variable is the thickness-weighted average Preformed Salinity, having been averaged between a pair of closely spaced neutral tangent planes. The material derivative on the left-hand side of Eqn. (A.20.4) is with respect to the sum of the Eulerian and quasi-Stokes velocities of height coordinates (equivalent to the description in appendix A.21 in terms of the thickness-weighted average horizontal velocity and the mean dianeutral velocity). The right-hand side of this equation is the standard notation indicating that $\hat{S}_*$ is diffused along neutral tangent planes with the diffusivity K and in the vertical direction with the diapycnal diffusivity D (and γ_z^{-1} is proportional to the average thickness between two closely spaced neutral tangent planes).

In order to evaluate density during the running of an ocean model, Absolute Salinity $S_A = S_A^{\text{dens}}$ must be evaluated. This can be done from Eqn. (A.20.2) as the product of the model's salinity variable $\hat{S}_*$ and $(1 + F^\delta)$. This could be done by simply multiplying the model's salinity by the fixed spatial map of $(1 + F^\delta)$ as observed today (using $r_1 = 0.35$ and the value of R^δ obtained from the computer algorithm of McDougall *et al.* (2012)). However experience has shown that even a smooth field of density errors can result in significant anomalies in diagnostic model calculations, primarily due to the misalignment of the density errors and the model bottom topography. Indeed, even if the correct mean density could somehow be determined, approximations associated with the specification of the model bottom topography would result in significant errors in bottom pressure torques that can degrade the model solution. One way to minimize such errors is to allow some dynamical adjustment of the specified density field so that, for example, density contours tend to align with bottom depth contours where the flow is constrained to follow bottom topography. This simple idea is the key to the success of the robust diagnostic approach (Sarmiento and Bryan (1982)). To allow dynamical adjustment of the salinity difference $S_A - S_*$ while not permitting $S_A - S_*$ to drift too far from the observed values, we recommend carrying an evolution equation for F^δ so that it becomes an extra model variable which evolves according to

$$\frac{dF^\delta}{dt} \;=\; \gamma_z \nabla_n \cdot \left(\gamma_z^{-1} K \nabla_n F^\delta \right) + \left(D \frac{\partial F^\delta}{\partial z} \right)_z + \tau^{-1} \left(F^{\delta\,\text{obs}} - F^\delta \right). \tag{A.20.5}$$

Here the model variable F^δ would be initialized based on observations, $F^{\delta\,\text{obs}}$ (using Eqn. (A.20.3) with $r_1 = 0.35$ and the interpolated values of R^δ from McDougall *et al.* (2012)), and advected and diffused like any other tracer, but in addition, there is a non-conservative source term $\tau^{-1} \left(F^{\delta\,\text{obs}} - F^\delta \right)$ which serves to restore the model variable F^δ towards the observed value with a restoring time τ that can be chosen to suit particular modeling needs. It should be at least 30 days to permit significant adjustment, but it might prove appropriate to allow a much longer adjustment period (up to several years) if drift from observations is sufficiently slow. The lower bound is based on a very rough estimate of the time required for the density field to be aligned with topography by advective processes. The upper bound is set by the requirement to have the restoring time relatively short compared to vertical and basin-scale horizontal redistribution times.

Ideally one would like the non-conservative source term to reflect the actual physical and chemical processes responsible for remineralization in the ocean interior, but until our knowledge of these processes improves such that this is possible, the approach based on Eqn. (A.20.5) provides a way forward. An indication of how an approach based on

modeled biogeochemical processes might be implemented in the future can be gleaned from looking at Eqn. (A.4.14) for $S_A - S_*$. If a biogeochemical model produced estimates of the quantities on the right-hand side of this equation, it could be immediately integrated into an ocean model to diagnose the effects of the biogeochemical processes on the model's density and its circulation.

In summary, the approach suggested here carries the evolution Eqns. (A.20.4) and (A.20.5) for $\hat{S}_*$ and F^δ, while $\hat{S}_A$ is calculated by the model at each time step according to

$$\hat{S}_A = \hat{S}_*\left(1 + F^\delta\right). \tag{A.20.6}$$

The model is initialized with values of Preformed Salinity using Eqn. (A.20.1) based on observations of Reference Salinity and on the interpolated global database of R^δ from McDougall *et al.* (2012) using $r_1 = 0.35$. This approach applies to the open ocean, but the Baltic Sea is to be treated differently. As described in appendix A.5, the observed Absolute Salinity Anomaly δS_A in the Baltic Sea is not primarily due to non-conservative biogeochemical source terms but rather is due to rivers delivering water to the Baltic with much larger Absolute Salinity than would be expected from the Practical Salinity of the river discharge. In the Baltic Sea, $S_A = S_*$, $r_1 = -1$ and $F^\delta = 0$ (as discussed in appendix A.5) so that in the Baltic region of an ocean model the equation of state should be called with the model's salinity variable, Preformed Salinity S_*. The discharges (mass fluxes) of river water and of Absolute Salinity should both appear as source terms at the edges of the Baltic Sea.

A.20.2 Including a source term in the evolution equation for Absolute Salinity

An alternative procedure would be to carry an evolution equation for Absolute Salinity rather than for Preformed Salinity in an ocean model. Using Eqns. (A.20.4) - (A.20.6), the following evolution equation for Absolute Salinity can be constructed,

$$\begin{aligned}
\frac{d\hat{S}_A}{dt} &= \gamma_z \nabla_n \cdot \left(\gamma_z^{-1} K \nabla_n \hat{S}_A\right) + \left(D\frac{\partial \hat{S}_A}{\partial z}\right)_z - 2K\nabla_n \hat{S}_* \cdot \nabla_n F^\delta - 2DF_z^\delta \frac{\partial \hat{S}_*}{\partial z} + \frac{\hat{S}_*}{\tau}\left(F^{\delta\,\mathrm{obs}} - F^\delta\right) \\
&= \gamma_z \nabla_n \cdot \left(\gamma_z^{-1} K \nabla_n \hat{S}_A\right) + \left(D\frac{\partial \hat{S}_A}{\partial z}\right)_z + \hat{S}^{S_A}.
\end{aligned}$$

$$\tag{A.20.7}$$

Here the non-conservative source term in the evolution equation for Absolute Salinity has been given the label $\hat{S}^{S_A}$ for later use. If the ocean model resolves mesoscale eddies then the term $-2K\nabla_n\hat{S}_* \cdot \nabla_n F^\delta$ in Eqn. (A.20.7) becomes the scalar product of $\nabla_n F^\delta$ and the epineutral flux of S_* plus the scalar product of $\nabla_n\hat{S}_*$ and the epineutral flux of F^δ. In this approach the evolution equation (A.20.5) for F^δ is also carried and the model's salinity variable, $\hat{S}_A$, is used directly as the argument of the equation of state and other thermodynamic functions in the model. The model would be initialized with values of Absolute Salinity using Eqn. (A.5.10) (namely $S_A = S_R\left(1 + R^\delta\right)$) based on observations of Reference Salinity and on the global data base of R^δ from McDougall *et al.* (2012). The production terms involving $\hat{S}_*$ in Eqn. (A.20.7) would need to be evaluated in terms of the model's salinity variable $\hat{S}_A$ using Eqn. (A.20.6).

This approach should give identical results to that described in section A.20.1 using Preformed Salinity. One disadvantage of having Density Salinity as the model's salinity variable is that its evolution equation (A.20.7) is not in the conservative form so that, for example, it is not possible to perform easy global budgets of salinity to test for the numerical integrity of the model code. Another disadvantage is that the air-sea flux of carbon dioxide and other gases may need to be taken into account as the surface boundary condition of Absolute Salinity. Such air-sea fluxes do not affect Preformed Salinity. But perhaps the largest disadvantage of this approach is the difficulty in evaluating the non-

conservative terms $-2K\nabla_n\hat{S}_* \cdot \nabla_n F^\delta - 2DF_z^\delta \partial\hat{S}_*/\partial z$ in Eqn. (A.20.7), especially when meso-scale eddies are present, as discussed above.

A.20.3 Discussion of the consequences if remineralization is ignored

If an ocean model does not carry the evolution equation for F^δ (Eqn. (A.20.5)) and the model's salinity evolution equation does not contain the appropriate non-conservative source term, is there then any preference for initializing and interpreting the model's salinity variable as either Preformed Salinity, Absolute Salinity or Reference Salinity? That is, the simplest method of dealing with these salinity issues is to continue the general approach that has been taken for the past several decades of simply taking one type of salinity in the model, and that salinity is taken to be conservative. Under this approximation the salinity that is used in the equation of state to calculate density in the model is the same as the salinity that obeys a normal conservation equation of the form Eqn. (A.20.4). In this approach there is still a choice of how to initialize and to interpret the salinity in a model, and here we discuss the relative virtues of these options.

   If the model is initialized with a data set of estimated Preformed Salinity S_*, then S_* should evolve correctly, since S_* is a conservative variable and its evolution equation Eqn. (A.20.4) contains no non-conservative source terms. In this approach the equation of state will be called with $\hat{S}_*$ rather than $\hat{S}_A$, and these salinities differ by approximately $(1 + r_1)\,\delta S_A$. The likely errors with this approach can be estimated using the simple example of Figure A.5.1. The vertical axis in this figure is the difference between the northward density gradient at constant pressure when the equation of state is called with $\hat{S}_A$ and with $\hat{S}_R$. The figure shows that when using $\hat{S}_R$, for all the data in the world ocean below a depth of 1000 m, 58% of this data is in error by more than 2%. If this graph were re-done with $\hat{S}_*$ as the salinity argument rather than $\hat{S}_R$, the errors would be larger by the ratio $(1 + r_1) \approx 1.35$. That is, for 58% of the data in the world ocean deeper than 1000 m, the "thermal wind" relation would be misestimated by $\approx 2.7\%$ if $\hat{S}_*$ is used in place of $\hat{S}_A$ as the salinity argument of the equation of state. Also, these percentage errors in "thermal wind" are much larger in the North Pacific.

   Another choice of the salinity data to initialize the model is $\hat{S}_A$. An advantage of this choice is that initially the equation of state is called with the correct salinity variable. However at later times, the neglect of the non-conservative source terms in Eqn. (A.20.7) means that the model's salinity variable will depart from reality and errors will creep in due to the lack of these legitimate non-conservative source terms. How long might it be acceptable to integrate such a model before the errors approached those described in the previous paragraph? One could imagine that in the upper ocean the influence of these different salinity variables is dwarfed by other physics such as air sea interaction and active gyral motions. If one considered a depth of 1000m as being a depth where the influence of the different salinities would be both apparent and would make a significant impact on the thermal wind equation, then one might guess that it would take several decades for the neglect of the non-conservative source terms in the evolution equation for Absolute Salinity to begin to be important. This is not to suggest that the relaxation time scale τ should be chosen to be as long as this, rather this is an estimate of how long it would take for the neglect of the non-conservative source term $\hat{S}^{S_A}$ in Eqn. (A.20.7) to become significant.

   A third choice is to initialize the model with Reference Salinity, $\hat{S}_R$. This choice incurs the errors displayed in Figure A.5.1 right from the start of any numerical simulation. Thereafter, on some unknown timescale, further errors will arise because the conservation equation for Reference Salinity is missing the legitimate non-conservative source terms representing the effects of biogeochemistry on conductivity and $\hat{S}_R$. Hence this choice is the least desired of the three considered in this subsection. Note that this choice is

basically the approach that has been used to date in ocean modeling since we have routinely initialized models with observations of Practical Salinity and have treated it as a conservative variable and have used it as the salinity argument for the equation of state.

To summarize, the approaches of both subsections A.20.1 and A.20.2 of this appendix can each account for the non-conservative effects of remineralization if r_1 is a constant and so long as the appropriate boundary conditions are imposed. The advantage of using $\hat{S}_*$ is that it obeys a standard conservative evolution equation (A.20.4) with no source term on the right-hand side. If an ocean model were to be run without carrying the evolution equation for F^δ and hence without the ability to incorporate the appropriate non-conservative source terms in either Eqns. (A.20.6) or (A.20.7), then the model must resort to carrying only one salinity variable, and this salinity variable must be treated as a conservative variable in the ocean model. In this circumstance, we advise that the ocean's salinity variable be interpreted as Absolute Salinity, and initialized as such. In this way, the errors in the thermal wind equation will develop only slowly over a time scale of several decades or more in the deep ocean.

The use of an existing climatology for F^δ and the introduction of a rather arbitrary relaxation time τ are less than desirable features of this way of treating salinity in ocean models. An alternative strategy is available in an ocean model that includes biogeochemical processes and carries evolution equations for Total Alkalinity (TA), Dissolved Inorganic Carbon (DIC) as well as nitrate and silicate concentrations. Having these quantities available during the running of an ocean model allows the use of the following equation (this is Eqn. (A.4.14), from Pawlowicz *et al.*, 2011) to evaluate Absolute Salinity

$$\left(S_A - S_*\right)/(\mathrm{g\,kg^{-1}}) = \left(73.7\,\Delta\mathrm{TA} + 11.8\,\Delta\mathrm{DIC} + 81.9\,\mathrm{NO_3^-} + 50.6\,\mathrm{Si(OH)_4}\right)\!\Big/(\mathrm{mol\,kg^{-1}}). \qquad \text{(A.20.8)}$$

Under this approach, Preformed Salinity would be carried as the model's conservative prognostic salinity variable as in Eqn. (A.20.4), and the above equation for $S_A - S_*$ in terms of the biogeochemical variables would be used to evaluate Absolute Salinity for use in the model's expression for specific volume.