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Sea Surface Temperature Global Area Coverage (GAC) Processing

Version 4.0

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Foreword

This document describes the processing steps involved in generating global daily fields of sea surface temperature (SST) values from data collected by the Advanced Very High Resolution Radiometer (AVHRR)*, an infrared radiometer aboard polar-orbiting satellites of the NOAA series. The processing is part of the AVHRR Pathfinder Oceans program. The global SST products described here correspond to Version 4.0.

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Pathfinder Processing

Processing of the Version 4.0 Pathfinder AVHRR data occurs in a four step process:

1. Ingestion, calibration and navigation of Global Area Coverage (GAC) data
2. Pathfinder SST calculation
3. Spatial binning
4. Temporal binning.

All Pathfinder GAC 4.0 data distributed by the JPL DAAC has been processed at the University of Miami by these four steps before release t for distribution. Most end users will find the information provided in sections 1 through 4 valuable for understanding the use and application of Pathfinder sea surface tempreature products. More detailed information on the methods used in calibration and navigation of the raw AVHRR sensor data are provided in Appendix A for user's who may be considering processing the raw AVHRR data by an alternative method

1. Data Ingestion

AVHRR data are received in files containing approximately one orbit of GAC coverage. An orbit file contains about 90 minutes of raw digital counts from the AVHRR sensor aboard the spacecraft. For ease of processing, the large orbit file is split into 6-8 "processing pieces" (or "pieces, for brevity). The orbit file is first scanned (through procedure SCAN), to obtain information on the times of the first and last scan lines of the orbit file, and the time and scan line number of any pole crossings. Pole crossings define the transition between ascending and descending data, which are processed separately. The information collected by SCAN is used during the ingestion step (INGEST) to split the orbit file into several ascending and descending pieces, and to reformat the data for input to the atmospheric correction and SST calculation procedure (ATCOR).

1.1 Calibration and counts-to-radiance conversion

During ingestion, the raw AVHRR digital counts are converted to calibrated radiance values. This is achieved during the calibration stage. AVHRR calibration methods have changed through the years, and various groups had historically used different calibration procedures. However, one of the results of the AVHRR Pathfinder project is a consensus AVHRR Pathfinder calibration protocol. Briefly, the goal of NOAA/NASA AVHRR Pathfinder calibration procedure is to minimize spurious trends in the long-term records of AVHRR-derived geophysical products, and to ensure homogeneity across geophysical products derived from AVHRR sensors aboard NOAA-7, -9, 11, and -14 spacecraft. A detailed explanation of the sensor calibration method is beyond the scope of this document. Interested readers are referred to Appendix A and Rao and Chen (1995, 1996) for visible and near-infrared channels 1 and 2, and Walton et. al (1993) for infrared channels 3 4 5. Additional information and pointers can be found in section 7.1 of the NOAA KLM User's Guide* located at http://www2.ncdc.noaa.gov/docs/klm/index.htm*.

1.2 Navigation, clock, and attitude correction

Following the conversion of counts to calibrated radiance, the geo-referencing information associated with each piece is obtained by the procedure SECTOR. The position on Earth of any pixel on the AVHRR data can be determined from an orbital model and a sensor model. The orbital model determines the precise location of the satellite along the orbital track, using the time code embedded in each processing piece. The sensor model determines the direction in which the AVHRR instrument is pointing. The major sources of error in geo-locating AVHRR data are (a) drift in the spacecraft clock (which causes errors in the estimated along-track position), and (b) uncertainty errors in spacecraft and sensor attitude.To minimize error in the along track position estimated by the orbital model a satellite a clock correction factor is applied to the time code imbedded in each piece. The method used to determine these clock correction factors is presented in Appendix A for users who desire more detailed information.

After clock correction, a nominal attitude correction is then applied to minimize the uncertainty in regard to the direction in which the spacecraft is pointing. The nominal attitude correction applied was determined by averaging the absolute attitude of the spacecraft over many geographic locations and times along the orbital track. The atitude corrections factors applied and details of the method used to determining these factors may also be found in Appendix A .

2. SST Calculation

Once the calibrated pieces and the navigation information are completed, the ATCOR procedure is executed. This procedure reads the navigation and radiance data of all five AVHRR channels contained in a piece, and then applies the algorithm to calculate the Pathfinder sea surface temperature value (PFSST). The PFSST atmospheric correction algorithm is a statistical algorithm which relies on coefficients derived from co-located, co-temporal satellite and *in situ* SST observations ("matchups"). Coefficients are estimated on a monthly basis, and for two separate atmospheric regimes (dry and medium to moist atmospheres). A full description of the Pathfinder SST algorithm and a listing of the appropriate coefficients for each satellite, month, and atmospheric regime is available on this site.

The AVHRR Oceans Pathfinder SST algorithm is based on the NLSST (Non-Linear SST) algorithm developed by C.Walton, formerly of NOAA/NESDIS [Walton et al., 1998], and has the following form:

$$SST_{sat} = a + b\ T4 + c\ (T_4 - T_5)\ SST_{guess} + d\ (T_4 - T_5)\ (\sec(theta) - 1),$$

where SST_{sat} is the satellite-derived SST estimate, T_4 and T_5 are brightness temperatures for AVHRR channels 4 and 5 respectively, SST_{guess} is a first-guess SST value, and theta is the satellite zenith angle. Coefficients a, b, c, and d are estimated from regression analyses using co-located in situ and satellite measurements (or "matchups") for a given month and atmospheric regime.

Computation of the PFSST requires a first-guess SST. The first-guess reference SST used in Version 4.0 of the Pathfinder GAC products was derived from the weekly global Optimally Interpolated SST (OISST) fields produced by R. Reynolds. These fields are derived from both *in situ* (ships and buoys) and satellite data. The Reynolds OISST fields can be found at http://www.cdc.noa.gov/cdc/data.reynolds_sst.html*. The OISST files have a nominal one-degree resolution. A week starts on Sunday and ends on Saturday. To reduce noise, three weekly fields are averaged using a 1:2:1 weighting scheme to create an SST reference field centered on the middle week. A 3-week averaged Reynolds reference file is created for each week. The naming convention for the Reynolds reference file was set to the middle week. During the PFSST computation, the appropriate Reynolds reference field is selected by matching the date of the satellite data associated with the middle week in the reference file.

Users should be aware that the relatively low temporal and spatial resolution of the Reynolds reference fields may introduce errors in SST calculations for coastal or frontal regions. In these regions, significant SST changes over short distances may not be well represented by the smooth Reynolds fields. Errors may also arise in regions away from main shipping lanes or not well monitored by *in situ* buoys (e.g., high latitudes, equatorial Atlantic, Indonesia, etc.); in these regions the Reynolds values are derived solely from possibly biased satellite data. Nevertheless, the PFSST algorithm is not very sensitive to the first-guess SST, as long as values are reasonable. As the Reynolds fields are also used to determine SST quality flags, data may be incorrectly flagged in coastal or frontal regions. More detail on this topic is given in the following section.

2.1 Pixel-by-Pixel Science Quality Flags

One of the main goals of the Pathfinder AVHRR Oceans project is to produce global SST fields of a quality as good as possible. Nevertheless, raw data availability and processing errors (cloud flagging, SST algorithm) may result in SST estimates known to be suspect. The next step in the processing is to perform a series of tests to assess the likelihood that a pixel contains an SST value of suspect quality. The various tests are then combined to define eight overall quality levels for a pixel. Finally, the overall pixel quality levels are taken into account during the spatial binning stage (details below); the outcome is an overall bin quality level. The various steps involved are described in subsequent paragraphs.

First, a series of SST quality tests are applied on a pixel-by-pixel basis. The outcome of each individual test is separately stored in a bit contained within two 8-bit variables called `mask1` and `mask2`. In both variables, each bit is independently set to 1 *if a given test fails.* That is, the flag is set (bit value=1) for pixels that fail the test. The quality flags associated with each bit in mask variables 1 and 2 are described in Tables 1 and 2, respectively.

Table 1. Quality flags associated with each bit in variable Mask 1.

Bit No.	Test Name	Description
Bit 1	*Brightness temperature test*	Brightness temperatures for AVHRR channels 3, 4 and 5 must be greater than, or equal to -10°C

		and less than or equal to 35°C. This test identifies sensor digitizer errors or very cold pixels associated with high cloud tops.
Bit 2	*Cloud test*	Pixel must pass a suite of cloud flagging tests, arranged as a decision tree and defined for the given satellite and year (Figure 2). The cloud-flagging decision trees are discussed in detail in the description of the Pathfinder matchups.
Bit 3	*Unused*	Always set to 0. Reserved for future development.
Bit 4	*Unused*	Always set to 0. Reserved for future development.
Bit 5	*Uniformity test 1*	Maximum and minimum brightness temperature values are calculated for channels 4 and 5, for a 3x3 box centered around the pixel being classified. The difference between maximum and minimum brightness temperatures for both channels must be less than 0.7°C. This test seeks to identify contamination by small clouds, and is based on the assumption that SSTs are relatively uniform at small scales (e.g., 3x3 pixels). The 0.7°C threshold was selected by testing different threshold values in the matchup database. For uniformity thresholds below 0.7°, no significant bias was detected in SST estimates, and the rms of SST residuals was relatively uniform.
Bit 6	*Uniformity test 2*	This test was similar to that described for bit 5, but the threshold was set as 1.2°C. That is, differences between maximum and minimum brightness temperatures must be less than 1.2°C to pass this test. A higher uniformity threshold allows more pixels to pass the test, at the expense of accepting pixels with a higher SST bias.
Bit 7	*Zenith angle test 1*	Satellite zenith angle must be less than 45 degrees to pass this test. At higher zenith angles, radiation emitted by the ocean has to go through a longer atmospheric path before reaching the AVHRR instrument, with consequently higher chances of being attenuated. The received radiance, therefore, is likely to have a lower proportion of radiance originating from the ocean's surface (the signal of interest) and a greater proportion of radiance re-emitted by the atmosphere. The negative side of limiting zenith angles is the loss in geographic coverage.
Bit 8	*Reference test*	The absolute difference between the Pathfinder SST for the pixel considered and the reference Reynolds SST field (see discussion above) must be less or equal to 2°C.

Table 2. Quality flags associated with each bit in variable Mask 2.

Bit No.	Test Name	Description
Bit 1	*Zenith angle test 2*	Satellite zenith angle must be less than 55 degrees. This is similar to the test in bit 7 of variable mask1, but it allows a larger range of

		acceptable zenith angle values, with the goal of gaining geographic coverage.
Bit 2	*Stray sunlight test*	An examination of data stratified by satellite zenith angle and by side of the AVHRR scan line (left and right of nadir) revealed potential problems under certain Earth-Sun-satellite configurations. This flag identifies configurations in which problems may potentially occur. The problem is probably associated with stray solar radiation entering the radiometer and it occurs only in the middle to high latitudes in the Southern Hemisphere. For that reason, in the Northern Hemisphere this flag is always set to 0 (pass). In the Southern Hemisphere, the flag is set to 1 (fail) when (a) the satellite zenith angle is greater than 45 degrees, and (b)the pixel is located on the Sun side of the AVHRR scan line. For an ascending pass (spacecraft flying from south to north), the Sun side of the scan line is located left of nadir; for a descending pass, the Sun side of the scan line is right of nadir. The latitude in the Southern Hemisphere at which stray sun light becomes a problem is a function of season. During the austral summer, this problem may potentially reach the mid-latitudes, whereas in austral winter, it is confined to very high latitudes. For speed of processing, we have disregarded the seasonality of the latitude dependence, which may result in "good" pixels being erroneously flagged as failing this test. As this test is later used to define overall quality levels (see below), mid-latitude Southern Hemisphere pixels at high scan angles have the potential of being assigned to the lowest quality level during austral winter.
Bit 3	*Unused*	Always set to 0. Reserved for future development.
Bit 4	*SST test*	To pass test, the estimated Pathfinder SST must be within geophysically reasonable boundaries: 2^{o}CPathfinderSST35^{o}C.
Bit 5	*Unused*	Always set to 0. Reserved for future development.
Bit 6	*Ascending/descending test*	Result is set to 0 for descending (nightime) AVHRR passes; set to 1 for ascending (daytime) passes.
Bit 7	*Edge test*	Pixels must not be on the first or last scan lines of a piece, or on the first or last pixels in a scan line. Pixels along edges are not surrounded by pixels so that tests based on 3x3 boxes can be performed. Important: if this test is failed (i.e., if pixel is on an edge), bit values for all other tests (in mask1 and mask2) are set to 1. Also, the number of lines or pixels along edges rejected can be adjusted if the size of the homogeneity box is changed: for instance, if a 5x5 box is adopted, the edge test will reject the first and last *two* pixels in a scan line.
Bit 8	*Glint test*	Glint index must be < 0.005 sr^{-1}. The glint index is computed using the Cox and Munk (1954) formulation, assuming a nominal surface wind speed of 6 m s^{-1}. A value greater than 0.005sr

-1 generally indicates significant presence of sunglint.

2.2 Overall Quality Levels of Global SST Fields

The outcomes of the individual quality tests described above are subsequently combined into an overall quality level for each pixel. There are eight possible overall quality levels (levels 0 to 7) to which a pixel may be assigned. A quality level of 0 indicates very bad SST data, while level 7 is the highest quality.

Pixels of the poorest quality (level 0) are identified through a few initial tests likely to identify potential gross SST errors. These initial tests are illustrated in Figure 2. For brevity, a short name (listed in the previous section) is given to each test. The location of the test result in the appropriate mask variable is indicated (in parentheses) as "MXBY", where X is 1 or 2, indicating whether test result is in `mask1` or `mask2`, and Y is the bit number (1–8) in the corresponding mask variable. Whether a test is passed or failed is noted respectively

A pixel is automatically assigned to the lowest quality (0) if *any* of the following four quality mask bits are set to 1 (i.e., if tests are failed):

1. Brightness temperature test (`mask1`, bit1)
2. Uniformity test 2 (`mask1`, bit 6)
3. Zenith angle test 2 (`mask2`, bit 1)
4. Stray sunshine test (`mask2`, bit 2)

The seven remaining possible quality levels are assigned by evaluating various combinations of the bits in variables `mask1` and `mask2`. These combinations are illustrated in Figure 2. Test names and location of test outcomes are given as in Figure 2.

Figure 1. Initial tests to identify lowest quality pixels (quality level 0) in GAC data. The mask bit and test numbers for each test result are listed in parentheses. FOr example, M1B1 indicates mask 1, bit 1.

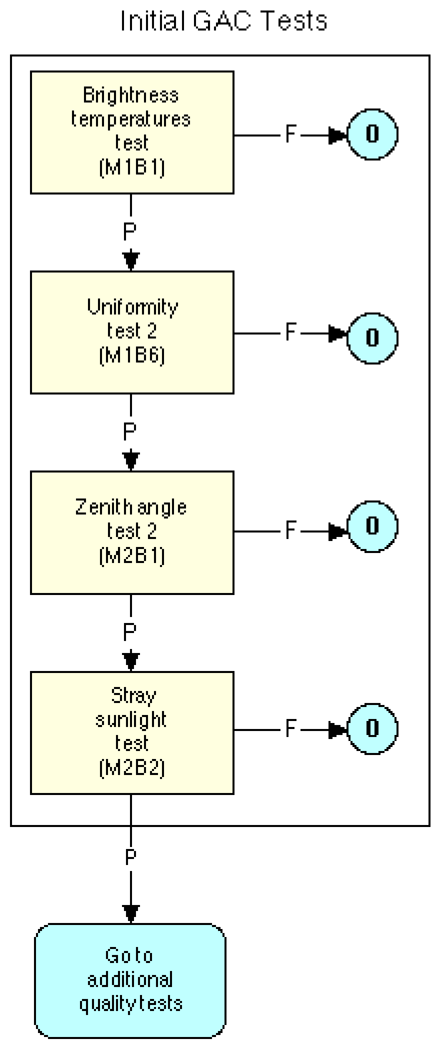
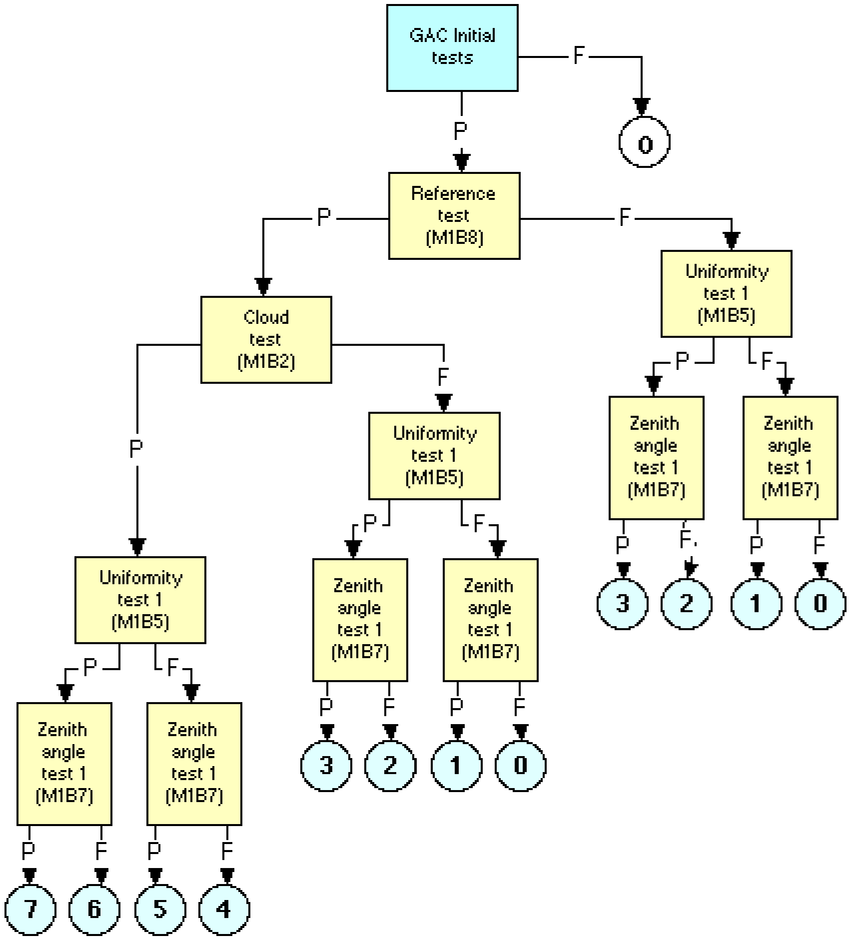


Figure 2. Combination of individual quality tests to derive an overall pixel quality level. Final quality levels are indicated in the circles.



We stress that overall quality levels are provided only as guidance to users, and that they are not associated with any specific error levels in SST estimates. Further, the quality scale is arbitrary and it does not involve any proportionality (e.g., pixels with quality level 4 are not twice as bad as those with quality level2).

Once overall quality levels are defined for all pixels in a processing piece, the next step is to combine these values into a bin quality level when the pixels are spatially binned. This step actually takes place during the spatial binning stage, described in detail below. For the sake of conceptual continuity, however, we discuss here how the quality level is set for a bin.

Suppose pixels in a given piece are being binned into the Pathfinder equal-area 9-km grid (described below). More than one GAC pixel can be assigned to the same bin. Which pixels are included in the binning, however, is a function of the overall quality levels for all candidate pixels. Only pixels of the highest available quality are aggregated into a bin value; pixels of lower quality are not included during the binning. This is best illustrated with an example. Suppose three pixels could be assigned to bin N; two of these pixels have a quality of 3, and the remaining pixel has a (higher) quality level 5. In this case, only the pixel with quality 5 is binned and the two quality 3 pixels are discarded. That is, the binning procedure considers only the "best" data available for a given bin.

Users of binned data may select what SST bin quality levels they may wish to consider in their specific application. For instance, if quantitative analyses are being performed on SST values (e.g., for climate studies), users will probably want to use bins holding only the best quality SST estimates. On the other hand, if the goal is to monitor patterns (e.g., frontal features), users may be willing to accept lower quality level bins, trading off SST quality for a more complete coverage.

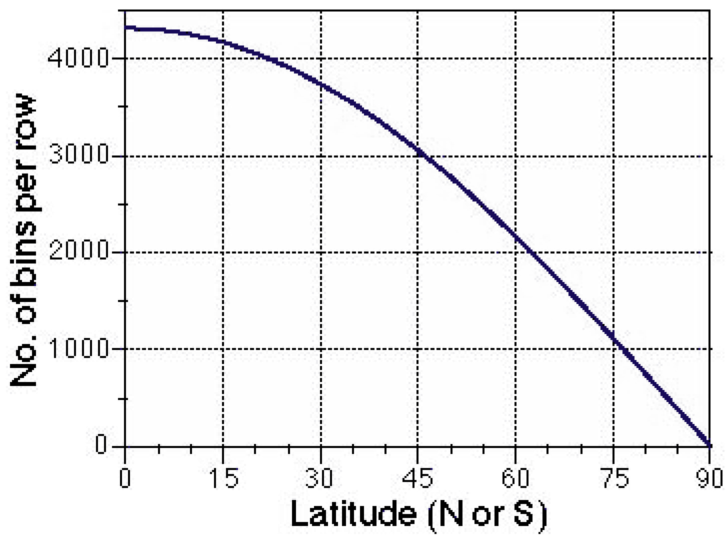
3. Spatial Binning

The next step in processing involves spatially binning all pixels in a piece into an equal-area global grid. During this step, each GAC pixel in a processing piece is assigned to a bin in an equal-area grid.

3.1 Pathfinder equal-area grid

The spatial gridding scheme adopted for AVHRR Pathfinder Oceans processing is based on the equal-area grid adopted by the International Satellite Cloud Climatology Project (ISSCP). The equal-area grid adopted consists of rectangular bins or tiles, arranged in zonal rows. These bins are approximately 9.28 km per side at the Equator (for brevity, they will be referred to as 9-km bins). This results in 2160 zonal rows of tiles from pole to pole (1080 in each hemisphere). There are a total of 5,940,422 bins in the global grid. The bins are arranged in rows beginning at 180^o longitude and circumscribing the Earth eastward at a given latitude. The number of tiles per row varies with latitude. The rows immediately above and below the equator have 4320 bins; at the poles the number of tiles is always three. Between these two extremes, the number of bins in a zonal row decreases as an approximate cosine function of latitude. The number of bins per row as a function of latitude is shown in Figure 3.

Figure 3. Number of 9.28 km tiles per zonal row as a function of latitude(North or South). The number of tiles is 4320 at the equator and decreases to 3 at the poles.



The number of bins in each zonal row is always an integer. To ensure an integer number of bins, the width of each bin must vary slightly from row to row. The bins, however, are always 9.28km along the meridians. That is, only one of the bin dimensions changes. Because the x-length of the bin is adjusted, the equal-area characteristics of the binning scheme are not rigorously preserved. However, variations in bin size are negligible throughout much of the globe and only become relevant at very high latitudes, where there are fewer bins per row. As the number of bins per row increases with distance from the poles, the difference between bin sizes rapidly becomes practically unnoticeable. To illustrate the magnitude of the size fluctuation, the worst possible case occurs when half a bin remains uncovered after filling a zonal row with an integer number of bins. Once a row has 100 bins (approximately 16 rows, or 148km, from the poles), the worst possible difference between the actual length and the standard length of 9.28 km is of the order of 0.5% (half a bin length redistributed over 100 bins). For a 9-km bin this represents a difference in the x-length of 45m. A row with 50 bins (80km from the poles) has a 1% variation with respect to a standard bin.

The gridding scheme used for Pathfinder products has various desirable features. One of them is that the number of rows of 9-km bins in each hemisphere is divisible by many numbers (e.g., 2, 3, 4, 5, 6). Therefore, it is extremely easy to generate an integer number of rows at many useful spatial resolutions. For example, 12 rows can be combined to generate zonal bands of 1^o resolution (1^o of latitude is equal to 111.12km; 12 bins would form a band 111.20km wide). Another example is the use of 30 rows to generate zonal bands of about 2.5^o, a typical grid size for atmospheric circulation models. In addition, because the total number of rows is even, the bins never straddle the equator, i.e., there are equal numbers of rows above and below the Equator. This avoids situations where the Coriolis factor is zero, a characteristic that numerical modelers expect from any gridding scheme. On the other hand, the equal-area scheme has some disadvantages. Although the equal area characteristic of the grid allows for more meaningful statistical analyses, displaying or visualizing the data becomes more cumbersome than for an equal angle projection.

As stated above, during assignment to a given spatial bin only pixels of the highest available quality level are summed. Repeating the example given above, suppose three pixels could be assigned to bin N; two of these pixels have a quality of 3, and the remaining pixel has a (higher) quality level 5. In this case, only the pixel with quality 5 is binned and the two quality 3 pixels are discarded. That is, the binning procedure considers only the "best" data available for a given bin.

The bits of the two bin quality masks for a given bin are set if the corresponding pixel mask bits of any of the individual summed pixels in the bin were set. For each bin, the following items are stored: bin number, bin quality masks, overall quality level, SSST, $SSST^2$, and count (number of pixels used in bin) are stored. The SST value for a given bin is then calculated from the count and the sum of the SST and represents the average of all pixels accumulated.

In addition, during the spatial binning stage, pieces are assigned to the appropriate data-day. Pieces assigned to given data-day are later assembled into a daily field during the time binning process.

A detailed description of the Pathfinder equal-area grid can be found elsewhere in this WWW site. Coding details of the spatial gridding algorithm used in the RSMAS binning procedure can be found in Appendix b of the SeaWiFS Technical Memorandum Vol. 23 (Campbell et. al. 1995).

3.2 Data-day definition

The basic products to be generated by the NASA Pathfinder SST project are global daily fields of sea surface temperature. To construct the daily fields, however, one should address the question of what exactly constitutes a day's worth of AVHRR data. This section introduces a consistent definition of a Pathfinder data-day.

A full discussion of various alternative definitions of a data-day and their respective implications is presented in Podesta (1995) for the SeaWiFS Sea Star spacecraft, which has orbital characteristics similar to the NOAA satellites. An on-line version of this document (in PDF format) with examples for the NOAA spacecraft can be found elsewhere on this WWW site. Because it is fairly difficult to discuss the data-day topic without a step-by-step graphical explanation of the various alternatives, readers are strongly encouraged to refer to these documents.

Perhaps the most intuitive choice is a 24-hour data-day. Such a definition, however, has problems such as possible gaps in coverage, large temporal discontinuities between sampling at adjacent locations, and changing locations for the 24-hour data-day boundaries. Another alternative is a spatial definition of a data-day, in which the boundary between data-days is not defined by time, but by a fixed geographic reference (e.g., the 180° meridian).

A spatial definition of a data-day is adopted for Pathfinder global SST daily fields. The start of a data-day is defined as the time at which the satellite crosses the 180^{o} meridian closest to the equator (there are several crossings of this meridian in a day, most of them at high latitudes). The data-day end is the next crossing of the 180^{o} meridian closest to the equator. The time of these crossings varies as a function of the satellite orbit.

The spatial definition solves some of the problems associated with a 24-hour data-day. Nevertheless, some of the problems remain. A remaining problem associated with the spatial definition is the occurrence of large temporal discontinuities between geographically adjacent data near the meridian data-day boundary. Typically, these discontinuities are associated with the first and last orbits in a data-day. Some of the data that give rise to discontinuities can be removed, but that may leave gaps in the spatial coverage. To eliminate gaps, the previous data-day definition is extended to include data taken up to 2 hours before or 2 hours after the data-day start and end times resulting from the previous definition.

We must note that data from ascending and descending orbits are processed separately in the Pathfinder project. The NOAA satellites cross the equator at the 180^{o} meridian on the descending orbit approximately 12 hours prior to the ascending crossing. The start and end times for a data-day of descending orbit data, therefore, occur 12 hours prior to the corresponding times for the ascending orbit data-day

4. Temporal binning and the accumulation of daily global fields

The spatially binned ascending or descending pieces for a given data-day are then binned in time to produce interim global ascending or descending fields at daily or other resolutions. In low latitudes, there is no spatial overlap between consecutive ascending or descending passes in a given data-day, therefore bins in a daily product only have pixels from a single piece. At higher latitudes, on the other hand, there may be spatial overlap between passes. In this case, the selection of data to be binned in time (e.g., bins from two consecutive passes) is performed in the same way as during the spatial binning. That is, only the "best" bins of equal quality level are summed and the equivalent quality mask bits set.

The interim daily fields are temporarily stored until the bin quality levels can be re-evaluated using a 3-week PFSST reference (not to be confused with the Reynolds OISST reference fields). The 3-week PFSST reference is created by time-binning seven global daily files into a week, and subsequently binning three consecutive weekly files. Empty bins in the 3-week reference are then filled using a smoothed distance-weighted interpolation of surrounding bins. A new 3-week reference file is produced for each week. A given 3-week reference file is then used to reevaluate the quality level of the daily fields associated with the middle week of the reference file. The final quality level for each of the global daily bins is determined by comparing the interium daily field to the 3-week reference. If the difference between the daily and the 3-week reference is greater than +/- 2 ^{o}C, then the bin's quality is demoted one level.

The quality-controlled daily fields are then output to a global daily PST file (an intermediate file format) and delivered to the DAAC at NASA's Jet Propulsion Laboratory*, where they are reformatted for distribution. The NOAA/NASA AVHRR Oceans Pathfinder SST data are distributed by the JPL DAAC in several spatial and temproal resolutions. Data are made available via ftp and through subsetting routines. The products are in HDF format as raster images. These data products are distributed as daily and monthly files, which are defined as spatially and temporally averaged bins of all temperature retrievals. There are four main products 1)best_sst 2) all-pixel sst 3) equal-area 4) the matchup database. The products are available at the different spatial resolutions including 9km.18km and 54km spatial resolution. Details of the processing at JPL and a description of products available to users is provided in http://podaac-www.jpl.nasa.gov/sst/*.

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