Report of the 6th Argo Delayed-Mode QC workshop for CTD data

John Gilson, Annie Wong, Brian King

2-3 December 2018 Scripps Institution of Oceanography

1. Introduction

An Argo Delayed-Mode QC (DMQC) Workshop was held at the Scripps Institution of Oceanography during 2-3 December 2018. This was the first multi-day DMQC Workshop in 10 years. John Gilson welcomed participants to the workshop and opened it as the 6th Argo Delayed-Mode QC Workshop for CTD data.

Brian King recalled that the 1st Delayed-mode workshop, which was also held at Scripps and also started on a Sunday, had a much smaller number of participants. He emphasized the importance of retaining corporate memory within Argo while the program grew in size and scope.

Annie Wong described the documents that would come out of this workshop: (1) a summary for the ADMT plenary; (2) a workshop report; and (3) an updated QC Manual for CTD data.

2. Overview/review of the DMQC process

An overview of the DMQC process for Argo CTD profile data was presented. Delayed-mode operators were encouraged to follow the various steps of the DMQC process in the following sequence:

- 1. Quality control of the profile position and profile JULD
- 2. Pointwise editing of PARAM_QC and PARAM_ADJUSTED_QC
- 3. Check that the pressure sensor is returning valid data
- 4. Adjust pressures from non-auto-correcting floats
- 5. Apply cell thermal mass adjustment if appropriate
- 6. Assess conductivity sensor drift
- 7. Apply salinity drift adjustment if appropriate
- 8. Generate D-files in Argo V3.1 format

Each of these steps was reviewed briefly.

2.1. Quality control of the profile position and profile JULD

Profile positions should be checked for outliers. Profile JULDs should be checked for chronological order. Erroneous positions and JULDs should be replaced by another telemetered value if available, or by an interpolated value (indicated by QC='8'). It was emphasized that for salinity adjustments, a rough

estimate of positions and JULDs was adequate. However, better estimates would likely aid other uses of the profile data. More accurate assessment of float positions and JULDs could be conducted during evaluation of the trajectory data.

2.2. Pointwise editing of PARAM_QC and PARAM_ADJUSTED_QC

One of the obligations of the DMQC process is to clean up the profile data. Therefore, pointwise errors in PRES, TEMP and PSAL should be flagged appropriately. The QC flags determined in DMQC should replace those determined in real-time QC (RTQC). That is, both PARAM_QC and PARAM_ADJUSTED_QC should contain the same qc flag determined in delayed-mode. For example, both PARAM_QC and PARAM_ADJUSTED_QC should record '4' for bad data. Some of the causes of pointwise errors are pressure inversion, density inversion, salty hook at bottom of profile, biofouling, etc. However, care should be taken in order to not edit out real ocean features.

2.3. Check that the pressure sensor is returning valid data

If an issue with the pressure sensor is detected, all PARAM data should be marked with a flag of '4' and put on the greylist.

2.4. Adjust pressures from non-auto-correcting floats

Some floats (e.g. SOLO, PROVOR) auto-correct the pressure sensor to zero while at the sea surface. Others (e.g. APEX) do not, and their pressure data need to be corrected during processing in real-time and in delayed-mode. Birgit Klein presented on the procedure for APEX pressure adjustment. Delayed-mode operators can refer to the QC Manual for the details.

Some operators reported that there were occasions where PRES_ADJUSTED < 0 in the shallowest bin. In the ensuing discussions, it was thought that these were likely due to outliers in the surface pressure time series that have not been despiked properly before adjustment was made.

Action 1: Birgit, Isabelle, Annie to look into why some PRES_ADJUSTED < 0 in the shallowest bin.

2.5. Apply cell thermal mass (CellTM) adjustment if appropriate

Salinity profile data suffer errors (fresh typically) when there is a temporal mismatch between the water passing through the thermister and the conductivity cell. This salinity error is especially prominent in regions of strong vertical temperature gradient. It was discussed that most delayed-mode groups applied the Johnson et al (2007) thermal lag correction with an assumed constant ascent rate. It is recommended that when information is available, real ascent rates should be used to avoid over-correction in regions where the float slows its ascent. (Note: the CellTM correction may change in the future. Please see Action 6 in Section 3.1.)

2.6. Assess conductivity sensor drift

The general philosophy on how to assess conductivity sensor drift is to inspect the least variable part(s) of the T/S curve for systematic departure of float salinity from background climatology on theta levels. These are usually the deepest isotherms, but in some regions these can be the mode water isotherms (intermediate depths). Care should be taken to not confuse water mass migration with sensor drift. Floats could be moving towards regions of higher/lower background salinity, or crossing fronts, or trapped in eddies, etc. Typically, the sensor drift trend is monotonic in time. The drift rate can vary, but the drift trend does not reverse.

2.7. Apply salinity drift adjustment if appropriate

The OW tool is used in Argo to adjust salinity when it is determined that sensor drift has occurred. Discussions were held on how to assign number of break points in the piecewise linear fit. Most sensor drift trends can be represented adequately with 1 or 2 break points. This can be achieved by setting max_breaks = 1 or 2 in the OW tool. Assigning too many breakpoints will usually fold in ocean variability in the least squares fit and therefore is not recommended. John Lyman suggested an alternative approach, which was to set max_breaks > 20, large enough to allow the AIC to arrive at a minimum number of breakpoints automatically, instead of engaging in subjective decisions.

2.8. Generate D-files in Argo V3.1 format

Delayed-mode operators were reminded to submit D-files in Argo V3.1 format. D-files in old V2.2 or V3.0 formats were to be rejected by the GDACs.

Discussions were held on whether there was a need to standardize the char strings used in the SCIENTIFIC_CALIB section and the HISTORY_ section in the

D-files. It was recognised that without a clear demand, it would be difficult to come up with some kind of arbitrary standardization. However, it was also recognised that operators who were new to delayed-mode activities could benefit from suggestions on how to fill the SCIENTIFIC_CALIB section.

Action 2:

In the QC Manual, Annie to add suggested char strings for filling the SCIENTIFIC_CALIB section of the D-files.

In addition, people who were pursuing machine learning were encouraged to communicate their needs in terms of standardizing the information contained in the HISTORY_ section.

BODC highlighted the potential for the use of a semantic model to populate the SCIENTIFIC_CALIB_COMMENT to limit the variation within the comment field between DMQC operator and over time. Currently there are 251 variations in the BODC database within this field for PSAL. A semantic model would enable standardisation with minimum loss of information using unambiguous names and definitions while enabling automated processes to come first.

3. How to identify floats showing signs of salinity drift

3.1. Community tools

A series of DMQC tools were presented.

Cecile Cabanes presented on the community tool for float salinity calibration: OW and Cabanes et al 2016, hereafter referred to as the OWC tool. This was made available publicly via <u>https://github.com/ArgoDMQC/</u> Updates included some changes to speed up the mapping stage and modified mapping errors. John Lyman suggested further modifications to the error analysis and the Akaike Information Criterion (AIC) analysis in the routine fit_cond.m. Breck Owens suggested including topography in the mapping stage. Giulio Notarstefano suggested some modifications to the routine find_10thetas.m to accommodate the low salinity and small salinity range in the Black Sea. Massimo Pacciaroni suggested modifications to the routine LMA.m.

Action 3:

(a). Recommend all DM groups to upgrade to Cecile's OWC Version 2.0 from the Github site.

(b). Recommend all DM groups to run OWC Version 2.0 with two reference databases separately (CTD, Argo) in their salinity drift analysis.

(c). Cecile, John Lyman, Giulio, Massimo and Breck to work on other updates, then release OWC version 3.0.

John Lyman recapped the Johnson et al (2007) cell thermal mass correction. This error often shows up as a salinity spike at the base of the mixed layer. Kim Martini reported that through experiments conducted at the WHOI stratified tank, Sea-Bird determined that salinity spiking observed in Argo profiles may be caused by alignment errors rather than conductivity cell thermal mass errors. The CTD sampling sequence leads to a mismatch between temperature and conductivity, causing spiking similar to those caused by cell thermal mass. Sea-Bird, in collaboration with the Argo team, is currently working to determine the appropriate corrections for affected data and refine the sampling to minimize these errors in the future.

Action 4:

Susan, Breck, Greg Johnson, John Gilson, Kim Martini to revisit the CellTM correction. Delayed-mode groups to continue following their current practice about applying the CellTM correction.

John Lyman presented the PMEL GUI. The PMEL GUI is written in Matlab and can be used to analyse OWC output. At PMEL, John Lyman runs the OWC tool at night through two reference databases, with 20 break points to find the minimum AIC. His experience suggests that this approach eliminates the need to manually set the number of break points in many floats.

Jenny Lovell presented the CSIRO GUI. The CSIRO GUI is written in Matlab and allows visualisation of a float's data. Salinity drift assessment is done by visual examination against two climatologies. When sensor drift is determined to have occurred, the OW routines are run and salinity adjustment applied.

Susan Wijffels presented on some quick QC assessments tools from WHOI. These include Brunt Vaisala frequency plots and salinity anomaly plots for identify drifting sensors quickly. For CTD with SNs> 2000, plots are at: <u>http://argo.whoi.edu/argo/sbedrift_wmo/</u> Uday Bhaskar presented on a method to QC float salinity data by using neural networks at INCOIS. This method has been trialled at the Arabian Sea and the North Atlantic.

3.2. Recent development of Seabird CTD salty drifts

Dave Murphy explained that the recent uptick in salty drifts in Seabird CTDs was caused by water leaking into the conductivity cell. Seawater intrusion between the glass conductivity cell and the urethane encapsulant caused a parallel resistance path between the signal and ground leads, resulting in a calibration drift toward higher salinity. Seabird was aware of this problem and had been screening their cells since May 2014. The screening process was effective in picking out cells that drift within 12 months of float deployment, but could not pick out cells that may drift after 12 months.

Discussions were held on how best to handle this issue in RTQC and DMQC. It was decided that a moderate approach in RTQC should be taken to ensure that the Argo real-time data set contains the appropriate qc flags and, at the same time, not throw out too much data. Some DM operators raised the concern that some of this salty drift may not be correctable with a pressure-independent offset in delayed-mode. In addition, some salty drifts exhibit trends that are not monotonic in time.

Action 5:

For RT DACs

(1). If there are insufficient resources, assign PSAL_QC='2', but NOT greylist, to all PSAL from cells with SNs 6000-7100.

(2). If there are sufficient resources, examine salinity anomaly plots from Susan, or use other tools, to determine if cells with SNs 6000-7100 show salty drifts. Greylist PSAL from the affected cells with PSAL_QC= '3' or '4'. PSAL from unaffected cells remain with PSAL_QC='1'. Re-check in <6mth intervals if resources allow.

(3). Megan & Susan to check greylist status and append to the Message to Users about what is being done in real-time data.

For DMQC groups

(1). Make it a priority to check cells with SNs 6000-7100, especially those that have been in the water for longer than 2 years, because that is when the salty drift will begin to manifest.

(2). Look out for salty drifts that are not correctable by a simple pressureindependent salinity offset adjustment. These should be considered unadjustable.

(3). Look out for long-term failure patterns that can help SeaBird qualify this pathology.

(4). Pay attention to the more recent cells that are outside the SNs 6000-7100 range. Report suspicious cells to John Gilson, Megan, and SeaBird (Dave, Kim).

4. Background reference datasets

4.1. CTD for DMQC

Christine Coatanoan presented on the issues relating to the CTD reference database for Argo DMQC. There are 3 main sources for this CTD_for_DMQC reference database: Ocean Climate Library, CCHDO, and data directly from scientists. These presented format and data quality difficulties, and checks were needed before data could be added to the reference database. Feedbacks from delayed-mode operators were also needed to improve the data quality.

Steve Diggs presented on the role of CCHDO. He emphasized that CCHDO only acted as a data repository and hence was not responsible for qc-ing the data. Sometimes data quality could improve over time, but it was recommended that Christine should take data in without waiting, as timely reference data were needed in regions of high variability. It was suggested that the reference data qc problem could be coordinated with experts from other ocean observing programs to increase efficiency.

Action 6:

DM operators to note anomalous data in the CTD_for_DMQC reference database and report them to Christine by quoting the version number of the database, the WMO number of the box, and the "source" variable from the mat files.

Christine then pointed out that some areas in the world's oceans have a high concentration of data (>10,000 profiles), such as regions with time series stations. She requested a method to thin out the data in these areas for the reference database. It was also pointed out that the CTD_for_DMQC reference

database excluded CTD casts shallower than 900 dbar, which meant that there were no reference data in shallow regions and marginal seas.

Action 7:

Christine, Isabelle, Annie to work on a method to thin out areas in the CTD_for_DMQC reference database that have a high temporal concentration of spatially co-located profiles. Also, think of a way to include reference data in shallow regions and marginal seas.

4.2. Argo for DMQC

John Gilson presented on the Argo reference database for DMQC. He emphasized that this should be used as a complement to Christine's CTD_for_DMQC database. The Argo_for_DMQC database is made up of good Argo profiles that have passed through a series of filters ("Gilson Rules"):

- 1) Profiles must be 'D' files (passed through DMQC)
- 2) Exclude all profiles that record on descent
- 3) Exclude floats that fail within one year
- 4) No profile within 6 months of last profile (death)
- 5) Profile must not be determined to have salinity drift
- 6) Profile must contain data from below 800dbar
- 7) Profile must contain 90% good salinity values (QC==1)
- 8) No profile within 6 months of deployment
- 9) No profile within 6 months of the onset of salinity drift
- 10) Salinity error must be less than 0.015psu

Discussions were held to modify some of the "Gilson Rules" to take into account the recent development of salty drifts in SeaBird CTDs.

Action 8:

John to modify some of the "Gilson Rules".

Change to "8. No profile within 2 months of deployment." Change to "4. No profile within 12+ months of last profile (death)." Change to "9. No profile within 12+ months of the onset of salinity drift." Also, experiment with modifying Point 6 so that good float data from continental slopes and shallow regions can be included in the DMQC_for_ARGO reference database.

5. DMQC for trajectory files

Megan Scanderbeg presented on DMQC for trajectory files. She suggested some requirements to make a Dtraj file. These included (a) application to the traj file any adjustment made in the profile files to PRES/TEMP/PSAL in D-mode; (b) quality control of cycle number; (c) quality control of surface times and positions; and (d) fill JULD_ADJUSTED. Other optional tasks were also suggested. Discussions were held on who would do DMQC on trajectory files, when it should be done, and what tools might be needed.

Action 9:

(1). Megan to assemble a team to develop community codes for DMQC of trajectory files.

(2). AST to discuss how national programs are to assign resources to implement DMQC of trajectory files.

6. Frequency of DM visits

Brian King led the discussions on how frequently a float should be processed in delayed-mode. During the ADMT18 meeting in November 2017, Action 35 recommended that the first DMQC for a float should be done after one year, then the revisit could be after 2 years for the teams that struggle with DMQC backlog. However, after 2017, identification and characterisation of salty drifts on batches of SBE41 conductivity cells demonstrated the importance of maintaining regular DMQC on all floats. The recommendation as of the time of this workshop (December 2018) was that all floats should have DMQC done after 12 months, and at 12-month intervals thereafter. This was also necessary to identify as yet unknown sensor behaviours.

In addition, it was recognised that scientific users would continue to use RT data, so a high priority was to identify bad or biased RT data in order to improve the quality of the RT dataset. Some examples of triage tools included the altimetry analysis and the objective analysis.

Action 10:

DMQC groups should aim to process data from their floats at 12-month intervals. Where DMQC groups do not have the capacity for annual revisits, near-automatic tools should be used to triage RT data to identify floats that may have drifts, so that biased RT data can be either flagged or adjusted by DMQC.

A question was raised on whether a new DMQC metric was needed to track the percentage of suspicious floats that had been processed in delayed-mode. While it was acknowledged that such a new metric would be useful, it was difficult to implement since there was no reliable method to determine what "suspicious" was. It was therefore concluded that the current metric (percentage of D-files for profiles older than 12 months) should continue to be used for monitoring of the health, or stress, of the DMQC system.

Discussions were then held on how recent a profile could be processed in delayed-mode. In instances of known sensor stability, experienced delayed-mode operators can decide how recent a cycle to send out. When unsure, the recommendation is to keep a 6-month buffer.

Action 11:

Annie to update the qc manual to clarify that there are no eligible cycles; delayed-mode operators to decide how recent a cycle to send out. If unsure, recommendation is to keep a 6-month buffer.

7. Euro Argo DMQC activities

Sylvie Pouliquen presented feedback from the Euro-Argo DMQC Workshop that was held in Brest, 17-18 April 2018. The workshop was dedicated mainly to people who were new to DMQC activities. The objectives of the workshop were to make sure everybody understand the data system, to bring EU countries towards the same level of knowledge, and to share DMQC procedures/tools/methods within the EU. Presentations on the first day included the Argo data system and the Argo delayed-mode process for PRES/TEMP/PSAL. The second day of the workshop was used for practical demonstration and hands-on practice. Overall assessment of the event was very favourable, and it was concluded that such DMQC workshops should be held periodically.

8. Examples of difficult floats and difficult regions

Presentations on examples of difficult floats and difficult regions were made by Tatianna Rykova, Giulio Nostarstefano, Isabelle Gaboury, and Birgit Klein.

9. Discussions on other topics

Discussions were held on ways to preserve and share DMQC knowledge within the Argo community. It was recognised that the DMQC process was one where one-on-one interactions were needed in addition to detailed documentation of the methods. A mentoring system was thus set up where a new operator could reach out to a mentor of his/her choice in order to get acquainted with the DMQC activities. The following people volunteered to be on the mentor list:

Annie Wong (South Pacific, South Indian, South Atlantic, Southern Ocean) Birgit Klein (Nordic Sea, Southern Ocean) Cecile Cabanes (North Atlantic) Giulio Notarstefano (Mediterranean, Black Sea) John Gilson (non-Atlantic) John Lyman (Pacific) Pelle Robbins (Atlantic) Uday Bhaskar (North Indian) Shigaki Hosoda (North Pacific) KiRyong Kang (Yellow and East Seas)

Action 12:

Sylvie and Annie to put the mentor list and the role of a mentor on the argodatamgt webpage. Encourage new operators to work with a mentor.

Action 13: Megan, Sylvie, Annie to look for future ADMT opportunities for half day DMQC interactive sessions.

10. Conclusion

The workshop concluded with a review of the action items.

List of action items

Action 1:

Birgit, Isabelle, Annie to look into why some PRES_ADJUSTED < 0 in the shallowest bin.

Action 2:

In the QC Manual, Annie to add suggested char strings for filling the SCIENTIFIC_CALIB section of the D-files.

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Action 5 (continue):

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may have drifts, so that biased RT data can be either flagged or adjusted by DMQC.

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Action 13:

Megan, Sylvie, Annie to look for future ADMT opportunities for half day DMQC interactive sessions.

List of attendees

First Name	Last Name
Fumihiko	Akazawa
Clare	Bellingham
Henry	Bittig
Cecile	Cabanes
Herve	Claustre
Christine	Coatanoan
Stephen	Diggs
Mingmei	Dong
Sharon	Escher
Isabelle	Gaboury
John	Gilson
Shigeki	Hosoda
Hyeogjun	JO
KiRyong	Kang
Sung-Dae	Kim
Brian	King
Birgit	Klein
Lisa	Lehmann
Zenghong	Liu
Xiaofen	Wu
Jenny	Lovell
John	Lyman
Amaru	Marquez
Kim	Martini
Kristy	McTaggart
Dave	Murphy
Giulio	Notarstefano
Massimo	Pacciaroni
Hyukmin	Park
JongJin	Park
Antoine	Poteau
Sylvie	Pouliquen
Sarah	Purkey
Pelle	Robbins
Dean	Roemmich
Tatiana	Rykova
Raphaelle	Sauzede
Megan	Scanderbeg
Catherine	Schmechtig
Leonardo	Tenorio-Feranandez
Tom	Trull

TVS	Udaya Bhaskar
Pedro	Velez-Belchi
Deb	West-Mack
Susan	Wijffels
Annie	Wong
Jinkun	Yang

Agenda for the 6th Argo Delayed-mode QC Workshop for CTD data

2-3 December 2018, Scripps Institution of Oceanography

Day 1 8h30 to 17h00: Nierenberg Hall Room 101 Day 2 8h30 to 17h00: Martin Johnson House

Day 1

- 1. 8h30 Welcome and local arrangements (J. Gilson)
- 2. 9h00 Overview/review of the DMQC process (J. Gilson, A. Wong, B. Klein)
 - Interpolate missing and/or bad latitude/longitude, check JULD
 - Confirm that pressure sensor is not returning questionable data
 - Edit point wise errors in PRES, TEMP, PSAL for pressure inversions, spikes, density inversions, salty hooks, biofouling, etc. Record in both PARAM_QC and PARAM_ADJUSTED_QC as '4'. Be careful not to edit out real ocean features – these are usually density compensating and can be seen over several cycles.

Coffee break: 10h00 – 10h15

- 2. 10h15 Overview/review of the DMQC process continued (J. Gilson, A. Wong, B. Klein)
 - APEX pressure adjustment, re-compute salinity (pages 30-37 QC Manual) (15min, B.Klein)
 - Apply thermal lag adjustment if appropriate
 - Assess conductivity sensor drift and error bars use least variable (tightest) part of T/S curve, not just the deepest isotherms
 - Generate D-files (V3.1) with emphasis on filling in calibration comment
- 3. How to identify floats showing signs of salinity drift (B. King, A. Wong moderating)
 - 3.1 11h00 General options for correction within netCDF files (20min J. Gilson)
 - Stable and hence need no adjustment, PARAM_QC=1, PARAM_ADJUSTED_QC=1
 - Sensor drift is present and is adjustable, PARAM_QC=1, PARAM_ADJUSTED_QC=1
 - Bad data and unadjustable, PARAM_QC=4, PARAM_ADJUSTED_QC=4
 - 3.2 11h20 Community tools
 - Cabanes et al (2016) and OW (30min, C. Cabanes)
 - Johnson et al (2007) thermal lag correction (20min, J. Lyman)
 - PMEL GUI (20min, J. Lyman)

Lunch break: 12h30 – 13h30

- 3.2 13h30 Community tools continued
 - CSIRO GUI (20min, J. Lovell)
 - WHOI Climatological comparison (15min S. Wijffels)
 - Artificial Neural Networks (ANN) (15min, U.Bhaskar)
 - Discussion of other tools currently available or tools that are needed to be developed to aid the community (25min)

3.3 14h45 Recent development of Seabird CTD salty drifts

- Seabird's understanding of cause (15min D. Murphy)

Coffee break: 15h00 – 15h15

- Characteristics and Discussion on how best to handle this issue in DMQC (45min, J. Gilson)
- 4. 16h00 DM trajectory files: (M. Scanderbeg) : Moved to Day 2

End of Day 1: 17h

Day 2

- 5. 8h30 Issues in correctly identifying salinity drift Background reference datasets
 - CTD for DMQC Is there a need to refine the dataset? Regularity? (20min, C. Coatanoan, 10min S. Diggs, 15min Discussion)
 - Argo for DMQC Present and discuss if a revision of selection criteria is necessary? (45min, J. Gilson)

Coffee break: 10h00 – 10h15

- 6. 10h15 Review frequency of DM visits and submission procedures. Make new proposals to ADMT if necessary (B. King, 45 min)
 - 6.1 How frequently should a float be DMQC'd?
 - 6.2 How recent a profile should be DMQC'd? In instances of known sensor stability, what cycles can be submitted?
 - 6.3 Correcting recent profiles that are identified in near-real time.
- 4. 11h00 DM trajectory files: (M. Scanderbeg, 45 min)
- 7. 11h45 Interaction of CTD delayed-mode data with BGC data (B. King?)
 - How are groups coordinating DMQC experts across ocean state variables?
- 8. 12:15 Euro Argo DMQC activities (S. Pouliquen)

Lunch: 12h30-1h30

9. 1h30 Difficult floats, difficult regions, etc. (Moderated by conveners)
 Participants have a chance to show examples where the standard methodology
 breaks down or gives misleading answer. Discussion/recommendation of how
 these cases should be handled (methodologies, reference data, error estimates).

Participants are asked to bring examples: If none are brought, this will be a short session 3903703 (Tatiana-CSIRO) 3901852 (G. Notarstefano- Black Sea) 4901140 (I. Gaboury-Coastal Environments) 4900494 (I. Gaboury-Inversions) Malvinas Confluence (B. Klein)

Coffee break: 3h00 – 3h15

- 10. 3h15 Further discussion of previous or new topics brought up by attendees
- 11. 4h15 Review of bullet points and Action Items to be sent to ADMT

End of Day 2: 17h