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VERY LARGE TELESCOPE

From Quality Control Pipelines to Science Grade Data Products

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CHANGE RECORD

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TABLE OF CONTENTS

1 Scope

The Directorate for Operations has as one of its high level goals that the current Quality Control pipelines have to be developed into Science Quality pipelines. In this document we describe the process to be followed to identify, prioritize, carry out and control the developments in the area of generation of science data products for VLT/VLTI instruments.

This procedure, which is detailed in section 5 and rendered graphically in appendix C on page 18, is intended to make a better use of available resources that are already formally available for the scope, but are employed sub-optimally. The aim is to correct the shortcomings of the previous process, as identified in the first two years of operations[1]. Some of these shortcomings are caused by the shift of focus from quality control to scientific data reduction, some others from the lack of common practices across the organization. Ultimately, the goal is to ensure that the activities with a high scientific impact are completed on a reasonable and predictable schedule. This is achieved by focusing on few projects at any given time and by adopting a light, but rigorous approach to project management.

Thorough discussions with and insightful inputs from Pascal Ballester, Christophe Dumas, Wolfram Freudling and Alain Smette are gratefully acknowledged.

2 List of Abbreviations & Acronyms

This document employs several abbreviations and acronyms to refer concisely to an item, after it has been introduced. The following list is aimed to help the reader in recalling the extended meaning of each short expression. Organizational units are in italics; acronyms as they appear in the ERP system are used for them. Instrument names are not reported here, even when they are acronyms.

DFI	Data Flow Infrastructure department, belongs to SDD
DPB	Data Products Board
DPD	Data products Department, belongs to DMO
DMO	Data Management and Operations division, belongs to the Directorate of Operations
INS	INStrumentation division, belongs to the Directorate of Programmes
IOT	Instrument Operations Team
IPD	Instrumentation Projects Department, belongs to INS
LPO	La Silla Paranal Observatory division, belongs to the Directorate of Operations
PDA	Project Definition and Approval
PDAB	Project Definition and Approval Board
PSO	Paranal Science Operations department, belongs to LPO

[1] Counted from the creation of the Data Products Department within DMO on June 1st, 2008, as part of the restructuring of the directorate at large.

PSD	Pipeline Systems Department, belongs to SDD
QC	Quality Control
QCG	Data Processing and Quality Control group, belongs to DPD; it is usually referred to simply as QC
SDD	Software Development Division, belongs to the Directorate of Engineering
SED	System Engineering Department, belongs to SDD
SDP	Science Data Products group, belongs to DPD
USD	User Support Department, belongs to DMO

3 Preamble: the contexts for generation of data products with ESO tools

The generation of data products with ESO tools, which often referred to simply as "ESO pipelines"[2], is performed in different contexts.

- **Online at the observatory**. The focus is on quick-look science processing using static calibrations[3], mainly in support of operations.
- **Offline at the observatory**. Visiting astronomers can process in real time the newly acquired data to assess their quality and adapt the observational strategy accordingly. It is not uncommon that ESO tools are complemented by other data reduction and analysis packages, e.g. IRAF, MIDAS or IDL, and custom scripts.
- **At the Data Processing and Quality Control group in Garching**. This is the center of the quality control loop: raw calibrations are processed into masters, which are, then, used to extract the parameters to monitor the health status of ESO instruments[4]. The results are returned to the observatory within the hour for further action, if needed.

  For pipeline supported instrument modes, as part of the daily workflow the master calibrations are also used to process the science data. The corresponding data products are delivered to the respective PIs and ingested into the Science Archive Facility[5,6]. Science products are also generated

[2] Referring to the data reduction tools as pipelines is, of course, a misnomer, which should solely be used for the sake of brevity. For the actual pipelines, refer to http://www.eso.org/sci/data-processing/software/pipelines.

[3] Note that, at the time of writing, the Data organizer running online at the observatory is being revised to allow the use of dynamic master calibrations.

[4] The QC workflow is thoroughly described in VLT-SPE-ESO-19600-3986. The Health Check Monitor is available at http://www.eso.org/observing/dfo/quality/ALL.

[5] Service Mode science data are processed since several years and are shipped to the corresponding PIs on hard media. Visitor Mode science data are consistently processed since October 1st, 2009 (ESO Observing Period 84). Contrary to Service Mode data, they are not sent to the PIs on hard media. PIs of both Service and Visitor mode runs can download their raw and pipeline processed data from http://www.eso.org/requestHandler/pipacks.

[6] The entry point of the ESO Science Archive Facility is http://archive.eso.org.

offline as part of dedicated campaigns, in which the entire backlog of data for a given instrument is reprocessed in a uniform way. The data products are, then, made public through the Science Archive Facility[7].

- **On the user's desktop**. ESO pipelines can be run offline with Gasgano[8], the EsoRex command line tool[9] or Reflex, an advanced graphical user interface based on a graphical workflow concept[10]. Users are, of course, interested in getting the best science out of their data.

In support of the generation of data products, ESO enforces calibration plans for all of its instruments. That is to say that, for each instrumental mode, a set of calibrations is defined, together with their frequency and accuracy. The calibration plans are made available to ESO users within the respective Instrument User Manuals. Users can apply for supplementary calibrations as part of their scientific Phase 1 proposal, and/or by means of a dedicated calibration proposal[11].

Generally speaking, while in some cases the products generated with ESO pipelines are of adequate quality for immediate scientific analysis, this is generally not the case[12], hence the drive to improve them.

4 The previous *pipeline* prioritization process: an analysis

Before this document, the prioritization of data products was *de facto* identified with the bi-annual Pipeline Priority Meetings. These are described in some detail in appendix A on page 14. Suffice it to say here that the main scope of these meetings is to provide input to the head of the Pipeline Systems Department to plan the work within the department according to priorities of the different stakeholders: the IOTs as represented by the IOT Coordinator, INS, SDP and QCG (a list of acronyms is provided on page 4. Also, see appendix B on page 15 for a more complete list of stakeholders).

While this mechanism has worked fairly well, it is now showing severe limitations, made all the more evident with the focus shift to the enhancement of the scientific data products.

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[7] Examples of such campaigns include UVES (http://www.eso.org/observing/dfo/quality/reproUVES/processing.html) and HARPS (http://archive.eso.org/archive/adp/ADP/HARPS/index.html. Note: the HARPS pipeline is entirely developed and maintained by the HARPS instrument consortium based in Geneva).

[8] http://www.eso.org/sci/data-processing/software/gasgano.

[9] http://www.eso.org/sci/data-processing/software/cpl/esorex.html.

[10] http://www.eso.org/sci/data-processing/software/reflex.

[11] For the different types of proposals and time allocation policies, please refer to the ESO Call for Proposals at http://www.eso.org/sci/observing/proposals/CfP.pdf.

[12] In fact, the answers to the ESO Service Mode Questionnaire indicate that less than a user out of three uses directly for science the pipeline products as received in the PIPacks. The Questionnaire requires authentication with the User Portal and can be accessed at http://www.eso.org/sci/observing/phase2/SMQuestionnaire.php.

- The process was, by its very nature, especially focused on the pipeline development itself.

  Lower attention is, then, devoted to the developments in other areas, e.g. acquisition of test data, definition of new tools and procedures at the observatory and deployment of the changes into the operational environment(s). As a result, there is insufficient coordination among these different activities, all of which are mandatory for enhancing the final science data products.

- The development was mostly organized around individual pipelines. This somewhat limits the exploitation of cross-instrument synergies and tends to fragment the development.

- The input to the development was largely based on individual tickets[13]. While tickets serve very well the need of describing and documenting individual, rather simple changes, more complex developments certainly benefit from a more comprehensive and structured documentation: an articulated description of the relevance and applicability of the development to serve as basis for the selection of the most important projects to be carried out, a requirement document to guide the development, a project plan with timelines and responsibilities to constrain the development within an agreed timeframe, a validation plan for the final deliverables, etc.

  In particular, the input to and goals of the development were frequently vague at the beginning of the project itself and are only focused as the work progresses. This is cause for delays and unpredictable timelines to completion. A better planning and documentation right at the onset of a project is needed to solve this.

  Resources were spread among a somewhat extended list of projects. For as long as there are operational instruments, virtually all pipelines are worked on all of the time. The list of open projects tends to steadily increase with time, as projects take a very long time to complete. Resources are not concentrated enough on a few, well-selected critical developments to bring them to a closure before starting new ones. A solid justification detailing the relevance of a proposed development would allow for a better selection of the valuable projects to invest resources on. Quite naturally, others would have to be "frozen" in order to make such resources available.

5 The new *data products* prioritization process: the procedure

We describe here the new prioritization process conceived to overcome the outstanding points presented above. Please refer to appendix C on page 18 for a Mind Map graphical representation of the concepts expressed here.

[13] Tickets can be accessed (and submitted) at http://support.eso.org/arsys63/shared/login.jsp.

This new procedure is intended to optimize the use of available resources, rather than adding new ones. In fact, the majority of the people involved already have as part of their mandate the enhancement of ESO's data products. An exception comes from the fact that some of the developments are likely to have an impact on the data flow infrastructure itself[14]. These developments would naturally have to be the responsibility of SDD's Data Flow Infrastructure (DFI) department and will likely affect other departments as well, e.g. SDD/SED. The corresponding priorities will have to be evaluated against the global workload and priorities of the affected departments.

The procedure to enhance data products is articulated as follows:

- The prioritization of the developments aimed at enhancing the science quality of the data products generated with ESO tools is decoupled from the Pipeline Priority Meetings. These latter ones should retain their original goal of organizing the work in the Pipeline Systems Department.

  In fact, the developments of the pipelines and of the data reduction algorithms (e.g. to generate new data products, or to enhance the quality of existing ones) are certainly crucial aspects of the endeavour, but they are not the only ones. Other affected areas include data acquisition (what data, e.g. calibrations, are acquired and how), observing templates (e.g. to implement specific acquisition sequences, or to propagate the correct information in the data headers) and validation of the resulting data products. Also, in order for them to be of any use, the new tools and procedures have to be deployed in the appropriate environments, be it at the observatory, be it in Garching or be it on the user's Desktop.

  All areas have to progress in harmony for the resulting data products to improve.

- As global responsible for the enhancement of ESO data products, the Science Data Products group leads the process[15]. Of course, a very close collaboration with all parties involved, and especially the IOT Coordinator and the head of the PSD department, is absolutely crucial (see appendix B on page 15 for a more complete list of stakeholders).

- The development process is based on articulated, comprehensive proposals, rather than on individual tickets concerned with individual features of individual instruments. Of course, at the time of implementation, the analysis of the requirements can lead to the creation of several interdependent tickets, each of which focused on an individual aspect.

[14] Examples include the changes needed to the infrastructure to allow the reuse of data products at a later time, the ability to trigger more than one pipeline recipe per observing template, or further development to Reflex.

[15] See the bullet on SDP in the appendix on page 15.

Proposals for development or enhancement can be submitted at any time and are reviewed periodically. Any proposal aiming at having a significant impact on data products is almost inevitably bound to affect different aspects of the data flow system. These are precisely the kind of projects that should be encouraged and supported the most. The Instrument Operation Teams are, by their very own nature, the point where the large majority of the different relevant competences meet. The IOTs are, then, the natural crib where such proposals should be conceived and defined. Given their broad membership, the IOTs are also the appropriate forums for a realistic assessment of the resources needed to complete a project and of its timeline, thus providing crucial input to the decision making process (see below). A template for proposing a new development is provided in appendix D on page 18.

The individual IOTs are mostly likely to concentrate on projects that affect their respective instrument of responsibility. The IOT Coordinator and the head of SDP should jointly identify and initiate cross instrument projects, where relevant[16]. They should, then, involve the individual IOTs affected to further define and, possibly, execute the projects themselves.

Other groups or individuals are, of course, encouraged to submit proposals, as well, again using the template provided in appendix D.

In addition to these more comprehensive proposals and the tickets that originate from them, individual tickets should be allowed to capture changes that are quite limited in scope and are not necessarily associated to any ongoing major development. However, generally speaking these tickets should not be assigned immediately to pipeline developers. Rather, these incoming tickets should first be evaluated for their pertinence to the approved lines of development before they can be acted upon. Provisions should be made to address urgent operational problems or showstoppers (more on this below).

- Whenever possible proposals for development should favour cross-instrument projects, rather than individual pipelines/instruments.

  This issue is not specific to science data products per se, as testified for example by the DETMON project[17], which was conceived since the onset to

[16] The CALIbration and STAbility (CALISTA) group on Paranal was tasked with "finding and implementing common procedures, tools and means of instrument calibration and stability measurements between different instruments of the VLT/VLTI. [It] searches ways to simplify the calibration of instruments and their stability by identifying common tools, calibration requirements, means of stability measurements between the different instruments available at the VLT/VLTI or for the observatory as a whole". See: http://odyssey5.pl.eso.org/sci/facilities/paranal/sciops/team_only/MediaWiki/index.php/Calibration_and_Instrument_Stability_group

Its activities are now part of the coordination activities of the instrument operation teams, as supervised by the IOT Coordinator.

[17] The DETMON project is thoroughly described in VLT-PLA-ESO-10400-4387.

provide common, cross-instrument tools and procedures to monitor the status of detectors. However, it is certainly exacerbated when it comes to the generation of science data products. This is because, once the basic instrument signatures have been removed, further processing tends to have forgotten about the instrument of origin.

In fact, all of the scientific high priorities for VLT instruments that have emerged from polling ESO astronomers (USD, PSO, QCG, INS) involve cross-instrument developments: multi-OB combination, telluric lines correction, illumination correction, spectrum flux calibration, photometric calibration of IR images (2MASS), error propagation and background subtraction[18].

- Each development is to be organized according to some light, but rigorous project management and control. All parties affected have to be involved and included in the planning since the very beginning, so that showstoppers, e.g. activities on the critical path, can be identified early on and addressed with proper scheduling. Accurate planning since the very beginning avoids confusion of roles and mismatched expectations, whereby it is not clear who should be doing what when.

  A project responsible is appointed for each development project. The project responsible is empowered to access and utilize the agreed resources. At the onset of a project, s/he prepares a project plan and timeline and ensures that all involved parties agree to it. During the project, s/he monitors the progress and ensures that is consistent with the project timeline. Serious deviations from it should be flagged to the head of the Science Data Products group to be brought for discussion to the Data Products Board (see below).

- Setting the global goals and priorities is the responsibility of the Data Products Board. In a resource-limited environment, it is crucial that the incoming proposals are reviewed before they get green light for implementation. In addition to their certified importance, only projects that can be completed in a reasonable, and reasonably certain, timescale should be approved[19].

  The Board approves proposals that deserve to become projects and be implemented. Also, it oversees the deployment of resources by, for example, “freezing” developments in certain areas to make available the appropriate resources to work on, and complete, high priority tasks. Of course, “frozen” areas can be “thawed” at later times, if deemed appropriate by the Board itself.

[18] Regrettably, external users have provided precious little feedback and suggestions through the Data Reduction Forum that was opened in may 2009 for this very purpose at http://www.eso.org/sci/data-processing/forum.html. At the time of writing, only 9 messages from users are posted in the forum. Collecting relevant input from the users is obviously not easy.

[19] The concept of peer review is, of course, commonly accepted among astronomers. It applies to almost any aspect of the scientific work: publication in refereed journals, application for telescope time, applications for grants, etc.

Only projects approved by the Data Products Board are carried out. The exception is constituted by emergency cases with a high impact on operations and/or data quality[20] that cannot wait several months until the next Board meeting. These should be dealt with in the progress meeting described below.

The Data Product Board is chaired by the head of SDP and meets regularly: twice a year seems appropriate, also to match the cycle of ESO Observing Periods. All relevant stakeholders are represented in the Board (see the list of stakeholders on page 15). However, it is not necessary to have all of the stakeholders physically present at the meting. In fact, most of them are part of the Instrument Operation Teams (IOTs): the instrument scientist at the observatory, the user support and quality control scientists in Garching, the pipeline developer and the software developers on the mountain. It seems, then, appropriate that their individual inputs are consolidated at the level of the IOTs and represented at Board meetings by the IOT Coordinator. In addition to the head of SDP and to the IOT Coordinator, the other core members of the Board are the head of LPO/PSO, as direct responsible for the science operations at the observatory, the head of DMO/DPD, as responsible for the different flavours of data products from ESO instruments, the head of SDD/PSD, to provide an overview of the allocation of resource in the critical area of pipeline development, and a representative from INS/IPD. When deemed appropriate, the Board can invite additional participants to provide specific expertise.

- Regular progress meetings are held between meetings of the Data Product Board. The main purpose of a progress meeting is to, well, monitor the progress of the various active projects and make sure that they are in line with the corresponding project plan. Corrective measures should be put in place immediately in case of sizeable deviations. If relevant, affected line managers should be notified at once and should make available the agreed resources.

  Also, as mentioned above, emergency situations should be examined in these progress meetings, possibly even calling them ad-hoc to cope with extremely urgent instances. The emergency case should be presented through the same template as the normal ones (see appendix D on page 18) and should include as much information as possible, so as to allow an evaluation of the impact on the other activities. In this way the disruptions ingrained with such emergencies can be minimized.

  The core participants to these meetings should include the SDP head, as chair, the IOT Coordinator, to represent the main originators of projects, the PSD head, to oversee the deployment of the pipeline developers, and the QCG head, especially if changes in the group's workflow are required. The

[20] For example, it was recently discovered that, after the CCD upgrade of UVES in 2009, a fraction of the order of 10% of the products by pipeline processing the data were affected by reduction problems. Solving this clearly needs immediate attention.

responsibles of selected projects should also participate, as considered appropriate by the core members. The provision of progress reports from all of the active projects should be considered.

6 Harmonization with instrument upgrades

The process described in section 5 focuses on developments motivated by the enhancement of data products, which then affect different aspects of the data flow chain. They are led by the Data Product Department within the Directorate of Operations. Another major component of the normal development of instruments are hardware upgrades. Here the starting point of the project is an evolution of the system hardware, which almost inevitably affects the final data products. They can be fairly large projects and are by nature more episodic than the enhancement of data products, which tends to be a more continuous process. Also, it is not uncommon for instrument upgrade projects to have an impact on data products that extends beyond what is strictly needed to support the new hardware to include general enhancements towards science products. The INS division within the Directorate of Programmes is responsible for driving these upgrade projects.

Instrument upgrades largely draw from the same pool of resources as the enhancement of data products. A useful guideline is provided by the experience in PSD, where accurate time accounting is enforced. If one includes in the instrument development also the commissioning activities and early operations, as it should be the case, in the year 2009 “hardware-driven” projects have absorbed more that 30% of the resources devoted to pipeline development in the Pipeline Systems Department[21].

In order to avoid possible resource conflicts, the impact of instrument upgrades on the activities of data product enhancement has to be carefully evaluated before project approval. To this end, the project team submits to the Data Products Board a plan following the guidelines in appendix D (in particular, the plan should distinguish the developments needed to support the new hardware from the general enhancement to data products). The Data Products Board assesses the impact in the areas of overlap of the proposed activity on the ones currently active or planned. It, then, provides its recommendations, in particular highlighting resource conflicts and possible trade-offs, to the Project Definition and Approval (PDA) Board charged with reviewing the instrument upgrade proposal. These recommendations form an integral part of the PDA’s decision pack.

7 Implementation

The timeline for implementation of the new procedure as described in section 5 is as follows:

- The procedure is operational as of November 1st, 2010.

[21] Pascal Ballester, private communication.

- Proposals for enhancements to data products are submitted at http://w4.hq.eso.org/observing/dfo/sdp/index.html using the template in appendix D.
- The Data Product Board will have its first meeting in January 2011 and regular meetings thereafter.

APPENDIX A: The Pipeline Priority Meetings

The main scope of the Pipeline Priority Meetings is to provide input to the head of the Pipeline Systems Department (PSD) to plan the work within the department according to priorities of the different stakeholders. With time, it has progressively lost its original scope to become the epicentre of the prioritization process for most things concerning the development of data products. The meetings are usually held in June and December to allow for releases in time for the start of the ESO Observing Periods in October and April, respectively.

The head of the Pipeline Systems Department calls the meeting, inviting representatives of the stakeholders: IOT Coordinator, INS, SDP and QCG (a list of acronyms is provided on page 4. Also, see the appendix on page 15 for a more complete list of stakeholders). The meeting is structured by instrument, reflecting the prevailing organization of the work in PSD, whereby each developer is responsible for a given set of instruments (usually a couple of them). The status of tickets submitted to the department is presented by the assignee. In case of conflicts between tickets assigned to the same pipeline developer, stakeholders gathered in the Pipeline Priority Meeting decide on priorities, usually by consensus.

The minutes of the meeting are, then, prepared by the head of PSD and circulated to parties involved. They form the basis for the work of the department in the following six months. Monthly progress meetings are scheduled to evaluate incoming tickets for consistency with the decisions taken in the Pipeline Priority Meeting.

APPENDIX B: Stakeholder analysis

The VLT end-to-end system is complex one, which involves individuals and organizational units across the entire organization. Being one of its components, the process of improving the end products has a similar breadth. The main stakeholders are listed below, in no particular order (organizational units are reported in brackets).

- Science data products astronomers (DMO/SDP). The group was created for and tasked with "providing scientific guidance for the development of pipelines and ensuring their homogeneity concerning use and capabilities as well as the quantification of their scientific grade" [22]. Also, it constitutes "the single interface to SDD for pipeline requirements"[23]. As such, the group holds the overall responsibility and coordination of the process to improve the quality of the ESO data products.
- Instrument scientists at the observatory (LPO/PSO) are responsible for ensuring the day-to-day performance of the instruments and the best exploitation of its data. They chair the Instrument Operation Teams. The Paranal Science Operations department within LPO should channel their "contribution to the science quality data pipeline development through the competence and know how of the instrument scientists"[24].
- Quality control scientists (DMO/QCG). They provide mass processing of data, thus being the power users of ESO pipelines. They have a detailed knowledge of the instrument, the data and of the data processing infrastructure in Garching. The group "should further develop towards science data QC"[25], now that the QC process at ESO is a well mature one, with several tens of instrumental characteristics being computed, scored, trended and monitored[26].
- The Data Products Department, which hosts both Science Data Products group and the Data Processing and Quality Control group. This is to ensure proper coordination and exploitation of the natural synergies between the enhancements of the data products, which forms the core mission of the former group, and their creation within the latter one.
- Instrument scientists in Garching (INS/IPD). They are the main drivers during the development phase of an instrument, including the provision of specs for the data reduction system. Also, they are in charge of subsequent instrument upgrades and interventions.
- User support astronomers (DMO/USD). They are the main interface between

[22] Andreas Kaufer, MM Retreat, March 2008.

[23] Ibid.

[24] Ibid.

[25] Ibid.

[26] See, e.g., Hanuschik et al (2008, SPIE, 7016, 70160Q) and Hummel et al (2008, SPIE, 7016, 70160R).

ESO and its user community. They have a detailed knowledge of the instruments and the science being done with them.

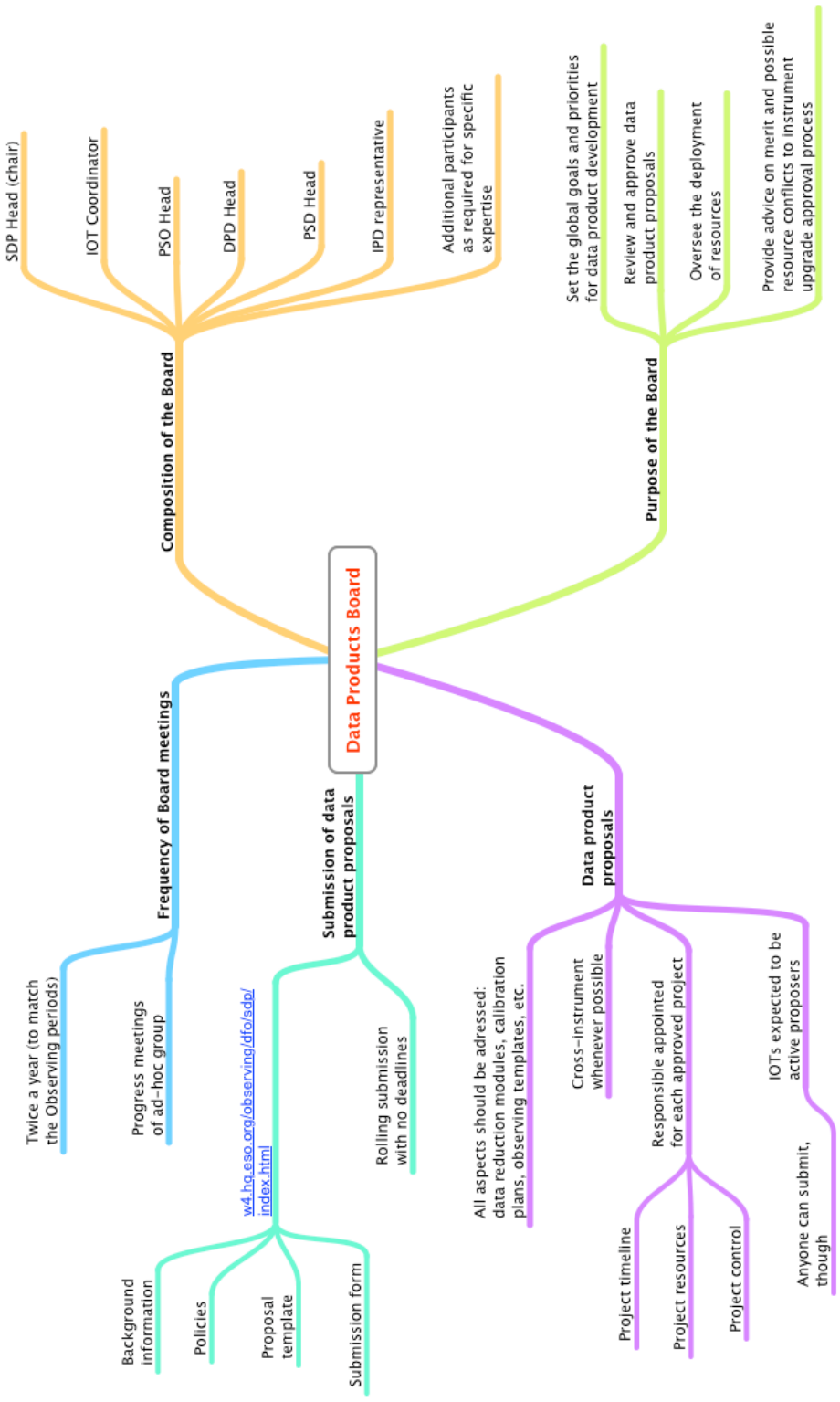
- Pipeline developers (SDD/PSD) are responsible for the development and coding of the pipelines. They are also in charge of developing and maintaining the Common Pipeline Library (CPL[27]), which are the building blocks of the ESO pipelines, the Exposure Time Calculators (ETCs[28]) and the CASA data reduction software for ALMA[29].
- The software group within the Engineering department on Paranal, which is responsible development on site of, e.g. observing templates, etc.
- Most of the stakeholders listed above are part of the Instrument Operation Teams. The IOT Coordinator (LPO/PSO) is, then, a stakeholder as well.
- The DFI department within SDD, which is responsible, among other things, for the data flow infrastructure that supports the data processing.

[27] http://www.eso.org/sci/data-processing/software/cpl.

[28] http://www.eso.org/observing/etc.

[29] http://www.eso.org/sci/facilities/alma/observing/tools/data-reduc.html.

APPENDIX C: Mind Map graphical representation of the Data Products Board



APPENDIX D: Template for data product enhancement proposals
Proposals should be submitted at http://w4.hq.eso.org/observing/dfo/sdp/index.html using the template provided below (also available online at the address above).

- **Project title**
- **Project purpose**
- **Proposer(s) [individual, IOT, etc.]**
- **Project responsible**
- **Instrument/mode(s) affect**
- **Project description**
- **Quantitative assessment of the goals** (e.g. data products to be targeted, expected resulting accuracy)
- **Brief description of the need and/or urgency of the proposed enhancement**
- **Developments needed**
    a. Test data already available
    b. Test data need to be acquired
    c. Development of new tools/procedures at the observatory
    d. Development of new algorithms
    e. Development of new tools/procedures in the QC environment in Garching
- **Project milestones**
- **[Optional] Preliminary estimate of the resources needed**
- **[Optional] Preliminary estimate of the project timeline, including items on the critical path**