Rubin Observatory

Crafting big data systems for astronomy

William O'Mullane, AURA/Rubin Observatory
DM Project Manager

March 6, 2020

what did and did not work ..

Or

the good

the bad

and

the ugly.

A little about myself

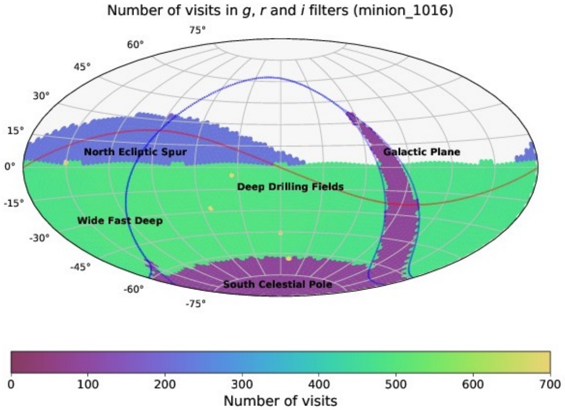
- 1985ish started with BASIC on a Commodore
- 1993 MSc BSc Computer Science, University College Cork, Ireland
- 1993 - 1997 Spacecraft Control Systems (C++), ESA ESOC Germany
- 1997 - 2001 Hipparcos, Integral, Planck, Gaia, Bepi-Sax (C,Java,Oracle, HTM, HEALPix), ESA ESTEC Netherlands
- 2001-2003 Commercial programming - some Astronomy (Java)
- 2003-2005 The Johns Hopkins, SDSS and National Virtual Observatory (C,C#,Java,Sqlserver)
- 2005-2014 Gaia Astrometric Solution and Science Operations (Java, Oracle, Intersystems Cache)
- 2012 PhD on Implementing the Gaia Astrometric Solution, Barcelona University
- 2014-2017 ESA SCI-OD division head - all science ground segments in development
- 2017- LSST Data Management Project Manager (Python,C++), Deputy Project Manager for Software (control systems and IT)

LSST:uniform sky survey

An optical/near-IR survey of half the sky in ugrizy bands to r 27.5 (36 nJy) based on 825 visits over a 10-year period: *deep wide fast*.

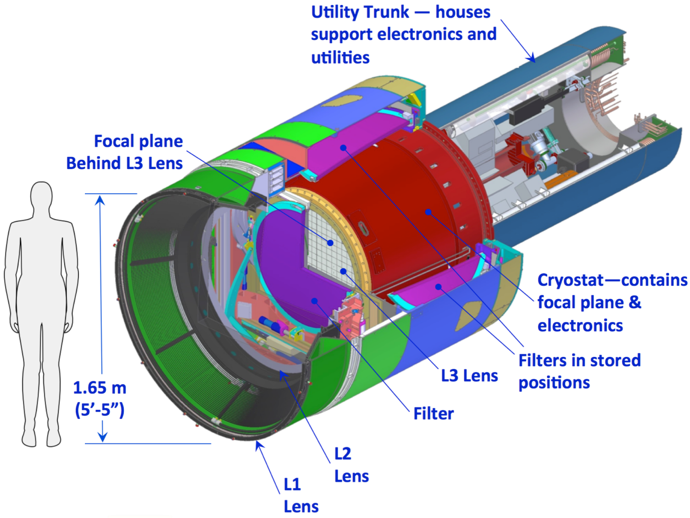
- 90% of time spent on uniform survey: every 3-4 nights, the whole observable sky scanned twice per night
- 100 PB of data: about a billion 16 Mpix images, enabling measurements for 40 billion objects!

see also `http://www.lsst.org` and Ivezić et al. (2019)-arXiv:0805.2366



10-year simulation of LSST survey: number of visits in u,g,r band (Aitoff projection of eq. coordinates)

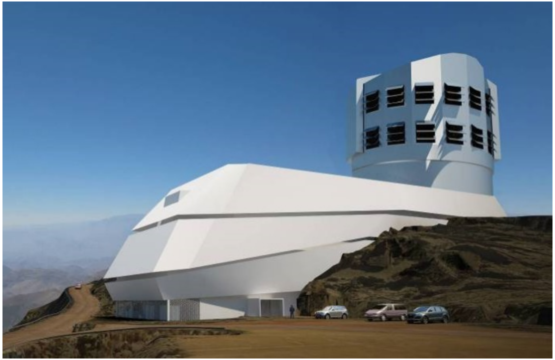
LSST Camera

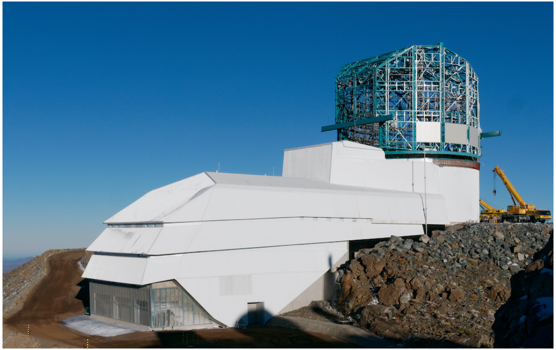


The largest astronomical camera:

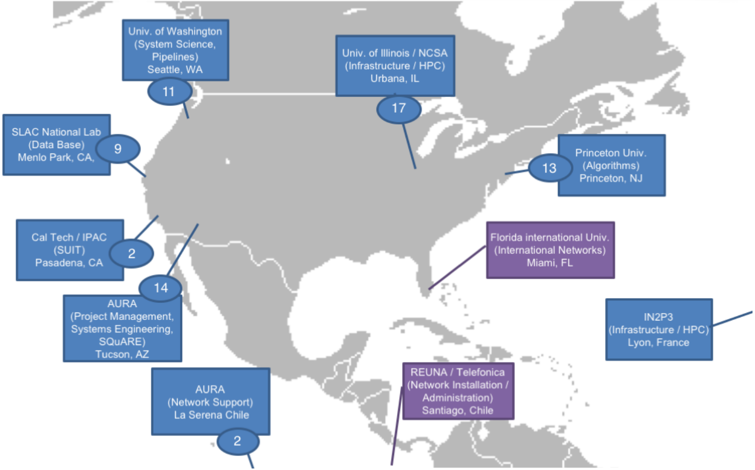
- 2800 kg
- 3.2 Gpix

Site as imagined and in March 2019





Data Management Mission Statement



DM’s mission:

Stand up operable, maintainable, quality services to deliver high-quality LSST data products for science, all on time and within reasonable cost.

Development is distributed across the Americas.
Plus we have partners like IN2P3 (France).

About 100 individuals ≈80 FTE

Communication is difficult and important I

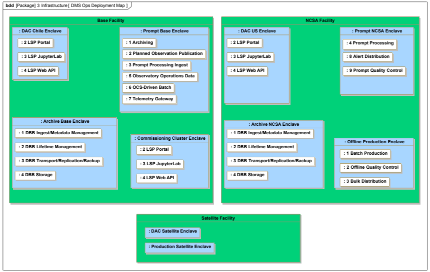
Have a code of conduct.

- Internal
  - Data Management Leadership meeting every Monday (30 minutes) - 4 times a year longer 2.5 days (2 now virtual with moderators and 5 hour days to match time zones).
  - Gaia DPAC executive similar (2 times physical meeting per year) - technical focus.
  - Both Rubin and DPAC have newsletters excellent and (DPAC) well contributed to
  - (Few) Focused working groups and working meetings
  - DPAC First consortium meeting Nov 2015; 10 years perhaps late .
  - Rubin have one every year it seems too much
  - Though stressful personally Rubin putting all software under one leader is good - Done rather late hence stress .
  - As for any project cost of entry for new people is very high — no obvious solution
- ESA policy initially to reduce contact between DPAC and Astrium (now AirbusDS who constructed Gaia) not good

Communication is difficult and important II

- External
  - Perhaps could have had a better DPAC website - Rubin is somewhat ok .. would really like a git backed Pull Request driven site .. but we have Drupal..
  - ESA PR also not great (ok as they point out they have a tiny fraction of NASA budget)
  - A bit better on Rubin (also fraction of NASA budget).
  - DPAC Publication policy was dealt with very late
  - Publication policy clearly in place on Rubin

DM build and deploy - already challenging



DM must build everything to get LSST products (see `http://ls.st/dpdd`) to the users.

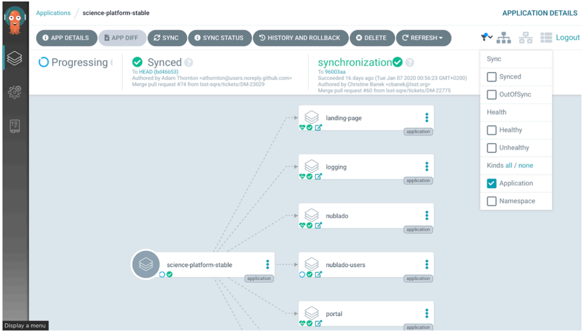
- large data sets (20TB/night)
- complex analysis
- aiming for small systematics
- Science Alerts in under 2 minutes .. (aiming for 1 minute)

About $\frac{1}{2}$ million lines of code (C++/python) all open source on github

diagram K.T. Lim

Kubernetes-based services with ArgoCD

- Kubernetes provides powerful container orchestration and management of resources available to services
- ArgoCD provides a framework for deploying and monitoring Kubernetes-based services with configuration management via GitOps
- Vault provides secrets management
- Combined, these three allow us to have automated, reproducible deployments



Frossie Economou frossie@lsst.org

Rubin Observatory Catalog 2035

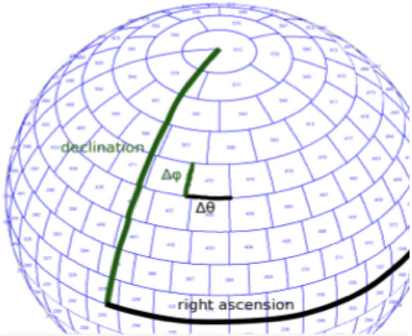
Astronomy catalogs tend to be highly structured, tabular, somewhat predictable access.

- Data, by DR11:
  - 60T rows (mostly ForcedSource)
  - 10PB (mostly Source + ForcedSource + Object extra)
- Breakdown of most significant tables (rows x cols, storage):
  - Object: 47B x 330, 100TB
  - Object extra: 1.5T x 7,600, 1.2PB
  - Source: 9T x 50, 5PB
  - ForcedSource: 50T x 6, 2PB

- Get an object or data for small area - <10 sec
- Scan through billions of objects - ≈ 1 hour
- Deeper analysis (Object_*) - ≈ 8 hours
- Analysis of objects close to other objects - ≈ 1 hour, even if full-sky
- Analysis that requires special grouping - ≈ 1 hour, even if full sky
- Source, ForcedSource scans - ≈ 12 hours
- Cross match & anti-cross match with external catalogs - ≈ 1 hour

Qserv (slides from Fritz Muller)

- Shared-nothing MPP RDBMS (SQL, throughput, horizontal scaling)
- Spherical partitioning with overlap (near-neighbor self-joins)
- Shared scans (concurrent query load)
- Replicated data (resiliency)
- Fixed-purpose, dedicated hardware (cost, predictability)



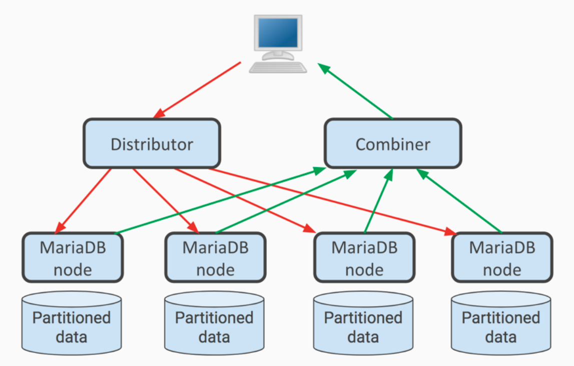
Tessellation not O'Mullane et al. (2001)

Design optimized for use case + hardware efficiency LDM-135

Built on project at SLAC, leverage existing tech within Stanford (MariaDB, MySQL Proxy, XRootD, Google protobuf, Flask)

100% open source `https://github.com/LSST/Qserv`

Shared Nothing Massively Parallel Processing



Recent scale tests:

`https://dmtr-071.lsst.io`

Perf and BigQuery: Document-31100

- Ultimate target platform 300 nodes in 2 international data-centers
- Development cluster (CC-IN2P3):
  - 400 cores, 800 GB memory, 500 TB storage
  - 100 TB synthetic dataset on 2 x 25 nodes
- Prototype Data Access Center (NCSA):
  - 500 cores, 4 TB memory, 700 TB storage
  - 100 TB science dataset (SDSS Stripe 82 + WISE) on 30 nodes
  - + HSC reprocessing + GAIA DR2 coming up

Guidelines, tools, conventions

- Its great having extensive guidelines - it was also something super on Gaia
- DPAC had full engineering Guide from early on (WOM-011) - how to Mantis, SVN, Java guide . . .
- `http://developer.lsst.io` is a full developer guide - everything from git commit messages to style guides for Python and C+.
- `http://pipelines.lsst.io` documents the main software release(s)
  - worst of both worlds - it is a monolithic release - but made up of > 120 git repos
  - Still using *in house* tools like EUPS `https://github.com/RobertLuptonTheGood/eups`
  - moving toward conda-forge
  - All open source (GPL) on github.com
- Language (spoken/written) and conventions are also super important
  - Single language projects (like US or UK) fall more easily in the trap of *believing* they speak about the same topics because they speak language X.
  - RubinObs lacks something like BAS-003

Software (and data) licensing

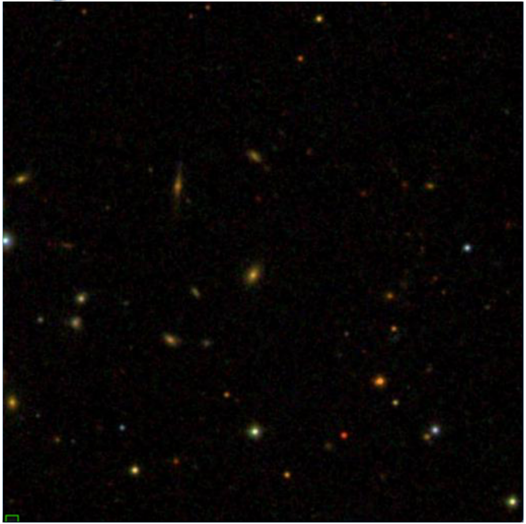
- Protect intellectual property — grant use to the consortium
- Often forgotten or not well dealt with - or worse ignored!

- DPAC agreed to LGPL (WOM-019) - some institutes e.g. ESA, do not allow GPL code
- LGPL in ESA involved lawyers and directors and time Now ESA have own open license.
- Rubin GPL .. would prefer APL.
- Gaia Data license only after DR1 (open with attribution).

You may use up to seven (7) cartoons per year at no costs as part of our fair use policy.

Have only mentioned Data license on Rubin

SDSS image

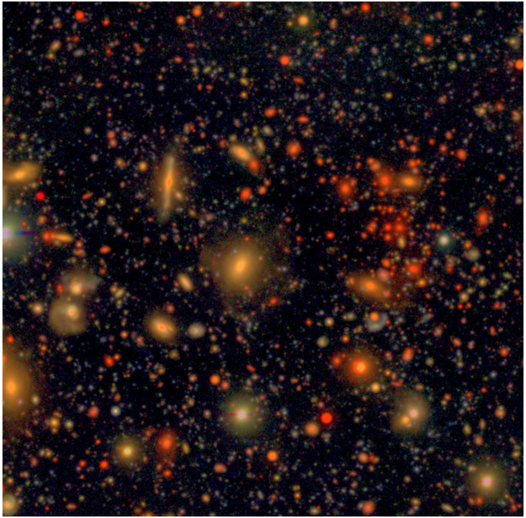


Nice colors Lupton et al. (2004)

$\approx 3.5'$

Image Robert Lupton

Hyper Suprime Cam (HSC) on Subaru



HSC image (COSMOS) from g,r(1.5 hrs) ,i(3 hrs)

PSF matched co-add ($\approx$ 27.5)

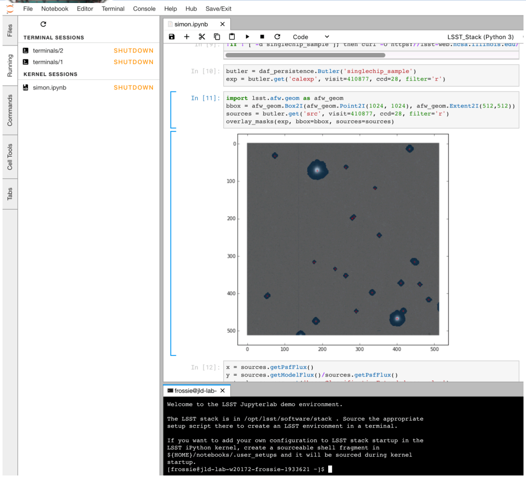
Challenges:

- Unknown statistical distributions, Truncated, censored and missing data, Unreliable quantities (e.g. unknown systematics and random errors)
- PSF - short exposure - atmosphere dominated ?
- Photometry challenging - will Gaia help ..
- Everything is blended!!

Processed with *LSST Stack* `https://pipelines.lsst.io/`

Image HSC collaboration, Robert Lupton

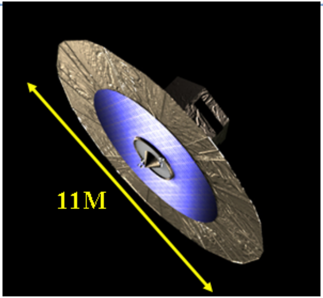
Catalog extraction



- Identifying sources and disentangling them becomes more difficult as we have deeper images.
- Left our typical Jupyter setup runs
  - Insrtrument signature removeval
  - calibration
  - source extraction
  - overlay extracted information on cleaned image
- This helps users understand how catalogs are produced.

Satellite overview

- Mission:
  - ESA Corner Stone 6
    - ESA provided the hardware and launch
      Mass: 2120 kg (payload 743 kg)
      Power: 1631 W (payload 815 W)
  - Launched December 19th 2013
  - Stereoscopic Census of Galaxy over 5 years
    - Extended 2 yrs - request for five
  - μarcsec Astrometry $G < 20$ (10^9 sources)
  - Radial Velocities $G < 16$
  - Photometry millimag $G < 20$



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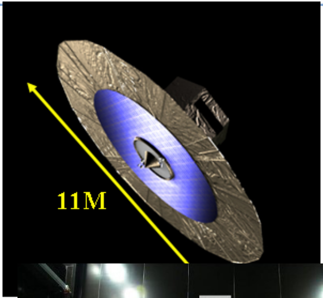
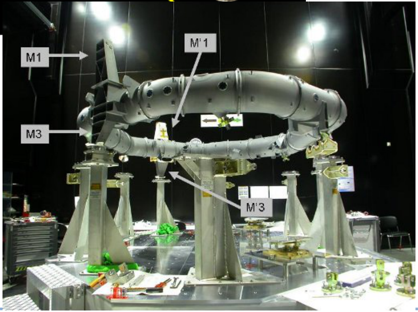
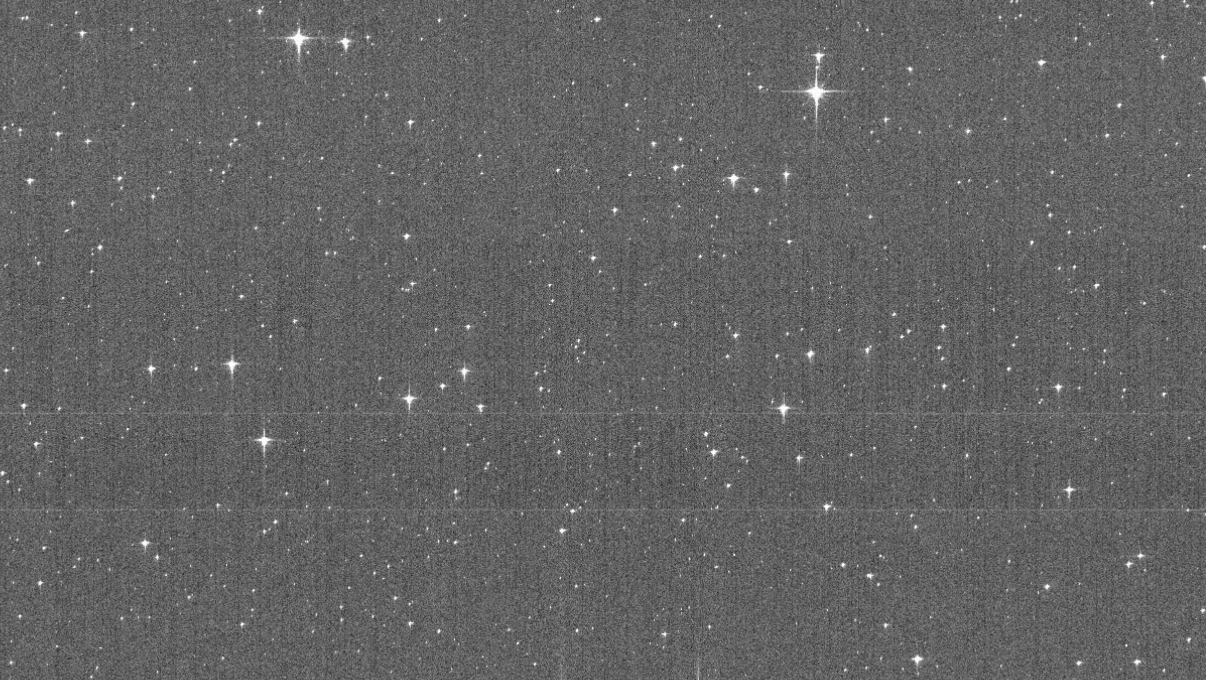
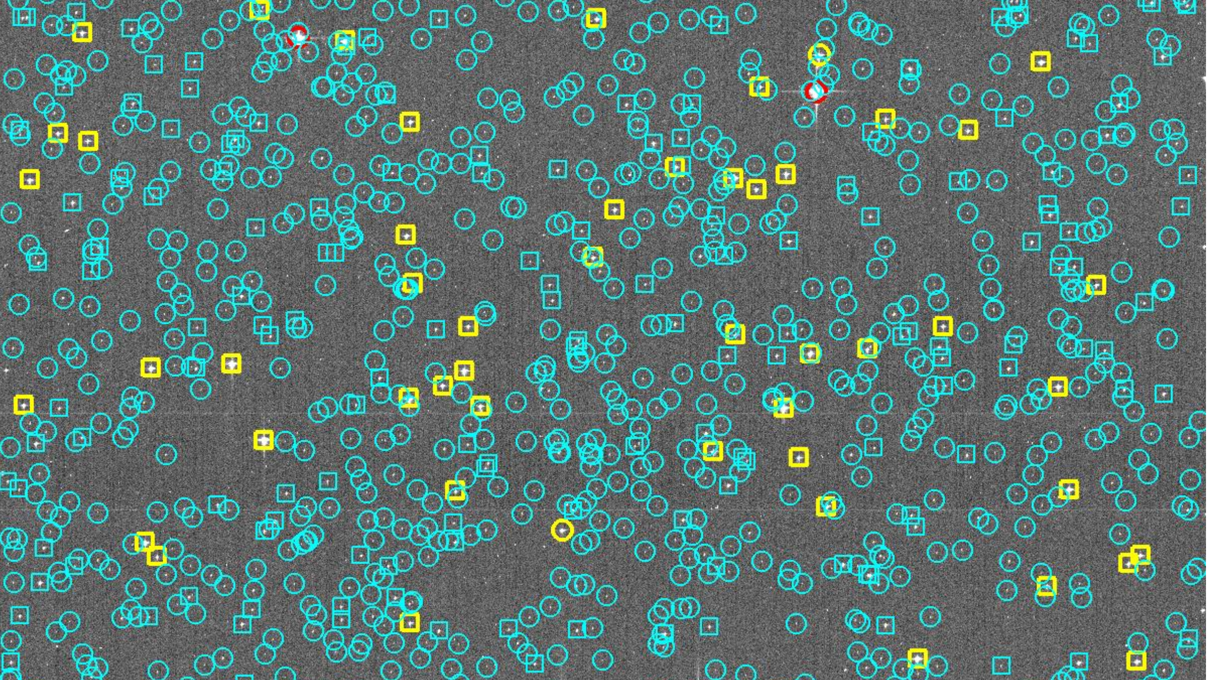
  - Photometry millimag $G < 20$
- Final catalogue $\approx$ 202?









Data processing - challenging complex data

- Astrometric centroid of the CCD image to be determined to an accuracy of 1% of the pixel size!
  - There will be 10^{12} images $\approx$ 100TB downlink need to handle $\approx$ 1PB
  - At 1 millisecond each that is $\approx$ 30 years
- Reconstructed attitude is required to order 10 μarcsec
  - Path of light through instrument needed to nanometre level
  - System must be extremely stable
  - Must consider relativistic light bending from solar system objects.

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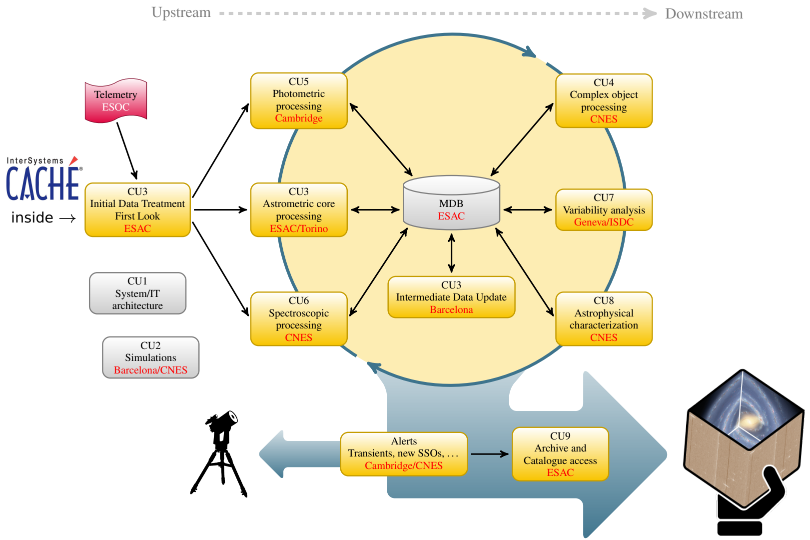
  - Must consider relativistic light bending from solar system objects.
- Attitude and Geometric calibration can only by done using Gaia's own observational data. (AGIS) (O'Mullane et al., 2011a; Lindegren et al., 2012)
  - this requires a significant portion of the data to be processed iteratively

Simplified processing overview



CU=Coordination Unit

Daily 50 – 100*GB* compressed

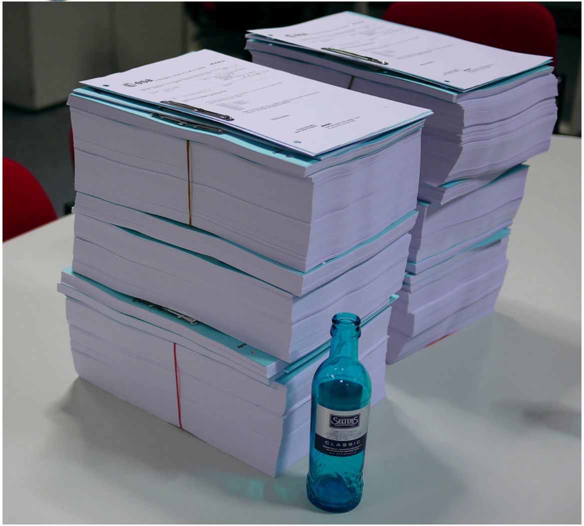
5yrs 1*PB*

(see also O'Mullane et al. (2006), O'Mullane et al. (2009))

Parameters and data models

- Avoid different values of constants in peoples code . . .
- The Gaia Parameter Database was set up early on for this (de Bruijne et al., 2005)
  - all constants in one place; web searchable configuration controlled (Only updated by Jos De Bruijne)
  - published as constants for Java (can also do C, Fortran. . .) so you may refer to a particular version
- then the actual data model — what exactly is an AstroElementary?
  - entire data model defined in multi-user dictionary tool; includes Units on each field.
    - good for astronomers — computer people find it harder to handle
  - from it we generate data instance classes and schemas for storage.
  - ONLY data model not processing — all objects are dumb (had discussion with KT and Mario on this)
  - This was in UML (Rose) in the 90s but it was impractical to continue..
  - Rubin Obs also had Rational Rose and still have Magic Draw .. but the Data model is in python now more or less.
- These are logical extensions of having agreed conventions. . .

Flight Operations Procedures

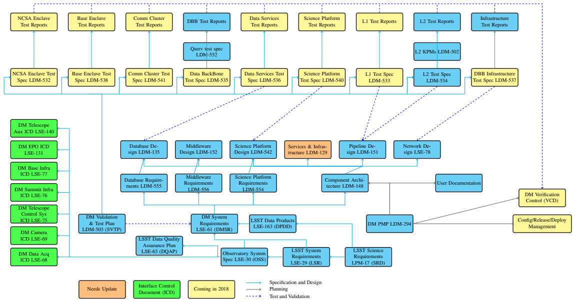


The FOP is followed by the spacecraft operators - the paper copy is just in case the computers fail - could be useful!

But we should avoid *write only* documents.

Have a standard: DPAC follows ECSS, Rubin MBSE

Rubin Observatory



Rubin Obs DM Doctree (LDM-294) Rubin less rigorous than DPAC - but then its on the ground

European Cooperation for Space Standardization

- Standards need to be tailored
  - LaTeX Templates/examples provided
  - Documents are iterated — All of this is done for all products.
  - It is very good to have a standard set of documents augmented by technical notes and streamlined
  - Some still found it too heavy — other reports requested beyond the standard ones.
- DPAC had sufficient QA people ($\sim 1/$CU) from the start (Rubin NONE)

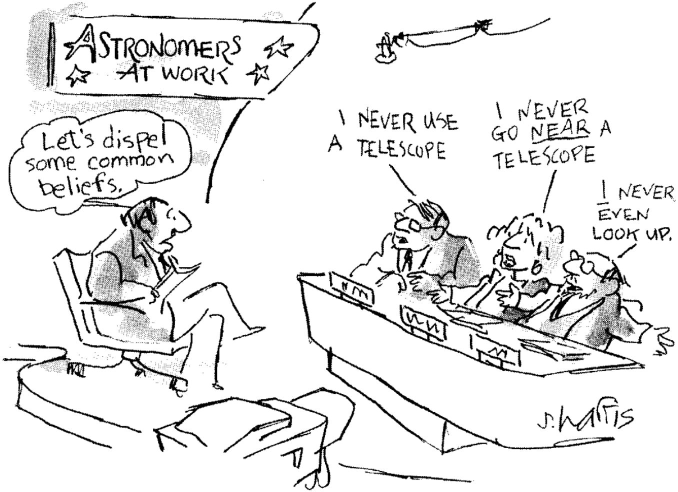
Development tools

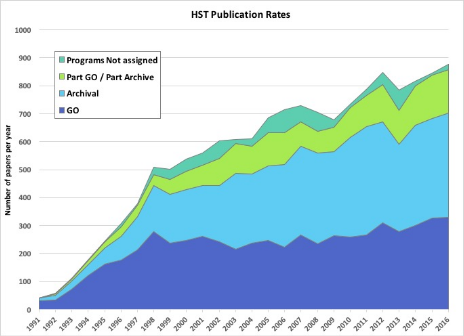
- All DPAC code and docs in Subversion, Rubin in GitHub.
  - Access control according to Group membership in the LDAP
- Centralized issue tracking (includes risks and actions)
  - DPAC - Mantis eventually Jira. Rubin Jira

Development tools

- All DPAC code and docs in Subversion, Rubin in GitHub.
  - Access control according to Group membership in the LDAP
- Centralized issue tracking (includes risks and actions)
  - DPAC - Mantis eventually Jira. Rubin Jira
- Having one language is good (O'Mullane et al., 2011b) Gaia agreed on Java 2006, Rubin Python/C++ (2009 perhaps earlier)
  - Can have a library of standard routines GaiaTools (Relativity, Field Angle Calculator, Ephemeris handling. . .)
    - The set of routines were not defined hence GaiaTools is a bit of hodgepodge mess. . .
    - Counter argument for common tools is (unnecessary) interdependence. . . we have that on Rubin
  - virtual machines make some reasons for Java invalid
  - Rubin builds take a long time ..

The Era Of Surveys and Archives





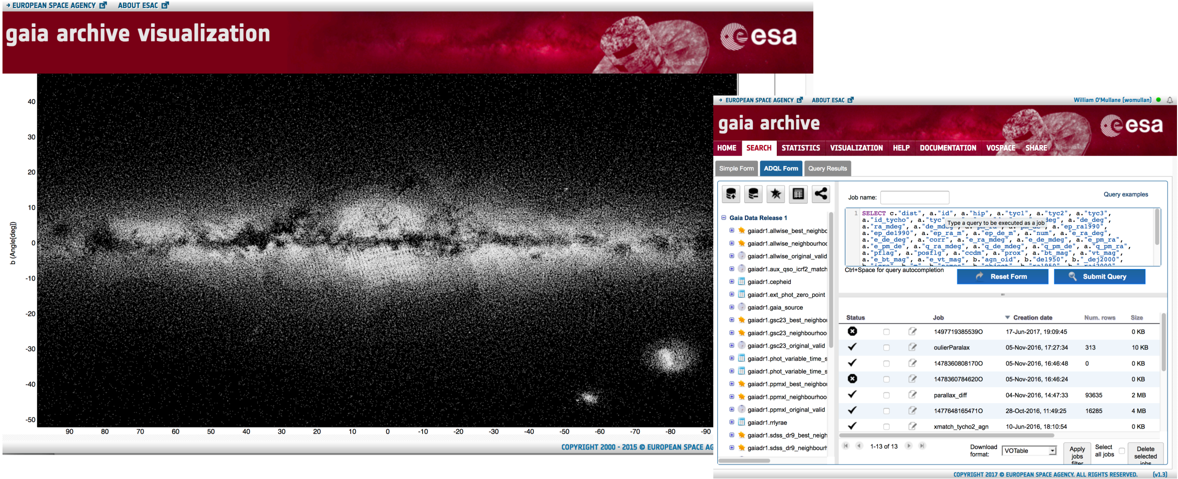
https:

//archive.stsci.edu/hst/bibliography/pubstat.html

...indicates archival research probably play an important role in the scientific success of XMM-Newton

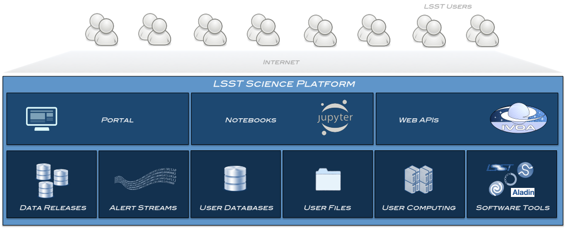
Ness et al. (2014)

Gaia Archive



All Gaia data is publicly accessible at `https://gea.esac.esa.int/archive/`

LSST Science Platform



For DR2:

- Computing:2,400 cores ($\approx$ 18 TFLOPs)
- File storage: $\approx$ 4PB (VOSpace)
- Database storage: $\approx$ 3PB (MYDB)

The Science Platform has three user facing aspects: the Portal (novice), the JupyterLab (intermediate), and the Web APIs (expert and remote tools).
Vision: LSE-319 — Design: LDM-542 — Test: DMTR-51

This is the sort of environment users now *expect* to have - it is no longer novel. We are finally Bringing code to the data - almost did with GAVIP Vagg et al. (2016)

General Challenge : Data volume

See also Bauer et al. (2019)

Soon, if not already, Data will be looking for astronomers not vice versa. Looking at Hubble archive 7K datasets have no publications.

- Proprietary data may have had its day .. if we want people to look at data we need to remove barriers.
- Networks and infrastructure are improving but more needs to be done
- Who looks after all the data ?
    - For space science in Europe ESAC preserves data - it is relatively small
    - IPAC, HEASARC and STScI pretty much deal with NASA data - still not one location.
    - Who looks after all the ground based data ?
    - There is no long term preservation plan for LSST or other big telescopes in the USA (Alex wil probably have more to say on this)

Its all team work on big projects

The End

Acronyms I

Acronym	Description
AGIS	Astrometric Global Iterative Solution
Archive	The repository for documents required by the NSF to be kept. These include documents related to design and development, construction, integration, test, and operations of the LSST observatory system. The archive is maintained using the enterprise content management system DocuShare, which is accessible through a link on the project website www.project.lsst.org.
CAOM	Common Astronomical Observation Model
CCD	Charge-Coupled Device
CI	Continuous Integration
CU	Coordination Unit
Camera	The LSST subsystem responsible for the 3.2-gigapixel LSST camera, which will take more than 800 panoramic images of the sky every night. SLAC leads a consortium of Department of Energy laboratories to design and build the camera sensors, optics, electronics, cryostat, filters and filter exchange mechanism, and camera control system.
DM	Data Management
DMTR	DM Test Report
Data Backbone	The software that provides for data registration, retrieval, storage, transport, replication, and provenance capabilities that are compatible with the Data Butler. It allows data products to move between Facilities, Enclaves, and DACs by managing caches of files at each endpoint, including persistence to long-term archival storage (e.g. tape).
Data Management	The LSST Subsystem responsible for the Data Management System (DMS), which will capture, store, catalog, and serve the LSST dataset to the scientific community and public. The DM team is responsible for the DMS architecture, applications, middleware, infrastructure, algorithms, and Observatory Network Design. DM is a distributed team working at LSST and partner institutions, with the DM Subsystem Manager located at LSST headquarters in Tucson.
Data Release	The approximately annual reprocessing of all LSST data, and the installation of the resulting data products in the LSST Data Access Centers, which marks the start of the two-year proprietary period.

Acronyms II

ESA	European Space Agency
ESAC	European Space Astronomy Centre
ESOC	European Space Operations Centre
ESTEC	European Space Technology Engineering Centre
FGCM	Forward Global Calibration Model
GAVIP	Gaia Added Value Interface Platform
GB	Gigabyte
HEALPix	Hierarchical Equal-Area iso-Latitude Pixelisation
HEASARC	NASA's Archive of Data on Energetic Phenomena
HSC	Hyper Suprime-Cam
HTM	Hierarchical Triangular Mesh
IPAC	No longer an acronym; science and data center at Caltech
IR	Infra Red
ISSI	International Space Science Institute
IVOA	International Virtual-Observatory Alliance
LDM	LSST Data Management (Document Handle)
LSE	LSST Systems Engineering (Document Handle)
LSST	Large Synoptic Survey Telescope
MPP	Massively Parallel Process
NASA	National Aeronautics and Space Administration
NCSA	National Center for Supercomputing Applications
Operations	The 10-year period following construction and commissioning during which the LSST Observatory conducts its survey
PB	PetaByte
PSF	Point Spread Function

Acronyms III

Project Manager	The person responsible for exercising leadership and oversight over the entire LSST project; he or she controls schedule, budget, and all contingency funds
Qserv	Proprietary Database built by SLAC for LSST
SDSS	Sloan Digital Sky Survey
Science Platform	A set of integrated web applications and services deployed at the LSST Data Access Centers (DACs) through which the scientific community will access, visualize, and perform next-to-the-data analysis of the LSST data products.
Subsystem	Aăset of elements comprising a system within the larger LSST system that is responsible for a key technical deliverable of the project.
TAP	Table Access Protocol
TB	TeraByte
XMM	X-ray Multi-mirror Mission (ESA; officially known as XMM-Newton)
arcmin	arcminute minute of arc (unit of angle)
arcsec	arcsecond second of arc (unit of angle)
astrometry	In astronomy, the sub-discipline of astrometry concerns precision measurement of positions (at a reference epoch), and real and apparent motions of astrophysical objects. Real motion means 3-D motions of the object with respect to an inertial reference frame; apparent motions are an artifact of the motion of the Earth. Astrometry per se is sometimes confused with the act of determining a World Coordinate System (WCS), which is a functional characterization of the mapping from pixels in an image or spectrum to world coordinate such as (RA, Dec) or wavelength.
calibration	The process of translating signals produced by a measuring instrument such as a telescope and camera into physical units such as flux, which are used for scientific analysis. Calibration removes most of the contributions to the signal from environmental and instrumental factors, such that only the astronomical component remains.
camera	An imaging device mounted at a telescope focal plane, composed of optics, a shutter, a set of filters, and one or more sensors arranged in a focal plane array.

Acronyms IV

metric	A measurable quantity which may be tracked. A metric has a name, description, unit, references, and tags (which are used for grouping). A metric is a scalar by definition. See also: aggregate metric, model metric, point metric.

References

[BAS-003], Bastian, U., 2007, *Reference systems, conventions and notations for Gaia*, GAIA-CA-SP-ARI-BAS-003, URL http://www.rssd.esa.int/cs/livelink/open/358698
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