# Software and big data from astronomy

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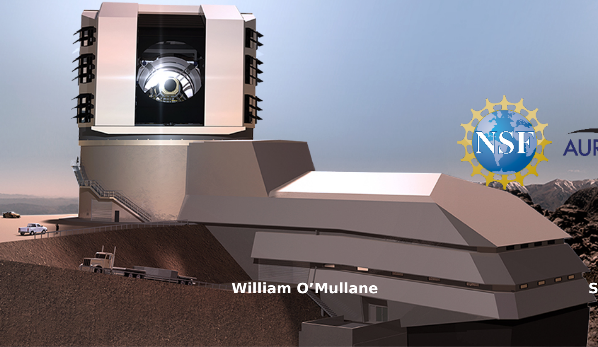
DM Project Manager

March 2, 2020



# 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)

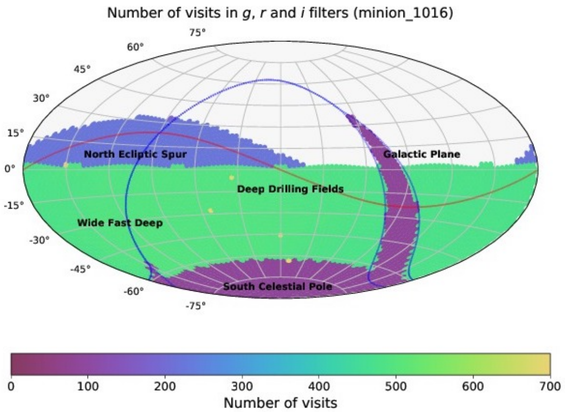
# LSST:uniform sky survey

Rubin Observatory

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*.

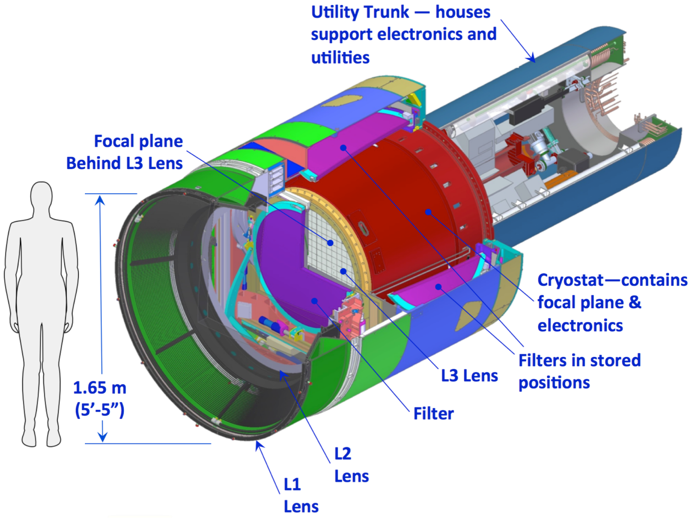
- 90% of time spent on uniform survey: every 3-4 nights, the whole observable sky scanned twice per night
- 100 PB of data: about a billion 16 Mpix images, enabling measurements for 40 billion objects!

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)**

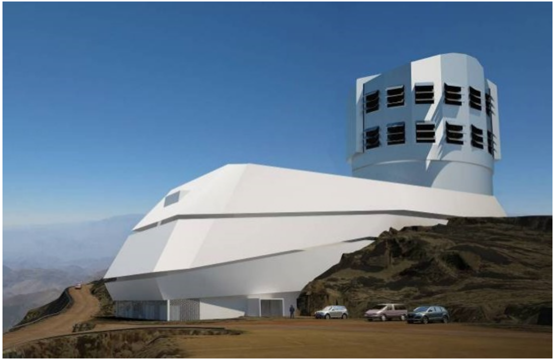
# LSST Camera



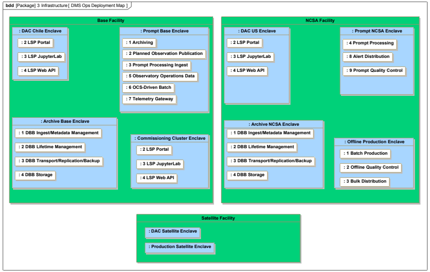

**The largest astronomical camera:**

- 2800 kg
- 3.2 Gpix

# Site as imagined and in March 2019



# DM build and deploy - already challenging



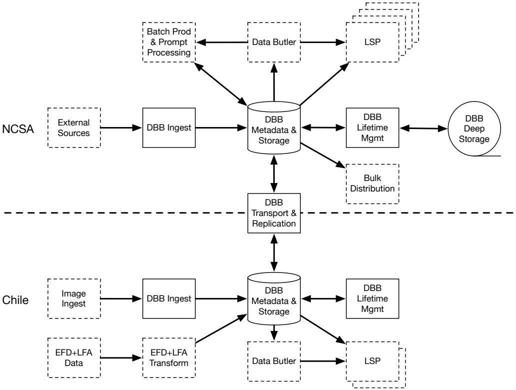

DM must build everything to get LSST products (see `http://ls.st/dpdd`) to the users.

- 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**

# Data Backbone




One small box on the previous slide was Data Backbone.

That hides several things

- Qserv - the LSST end user database
  - Custom Massive Parallel Processing (MPP)
  - allow queries on $\approx$ 20 Petabytes of tabular data
  - $4 \times 10^{10}$ objects, $4 \times 10^{13}$ sources (observations)
- All the networks : we now have fiber to the mountain and from La Serena to NCSA (two routes)

**diagram K.T. Lim**

# Rubin Observatory Catalog 2035

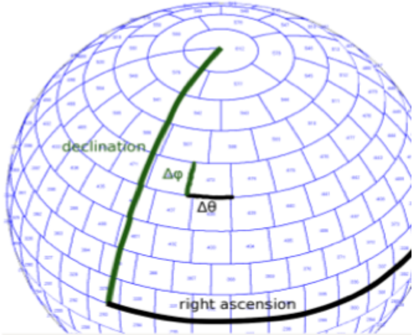
Astronomy catalogs tend to be highly structured, tabular, somewhat predictable access.

- 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)



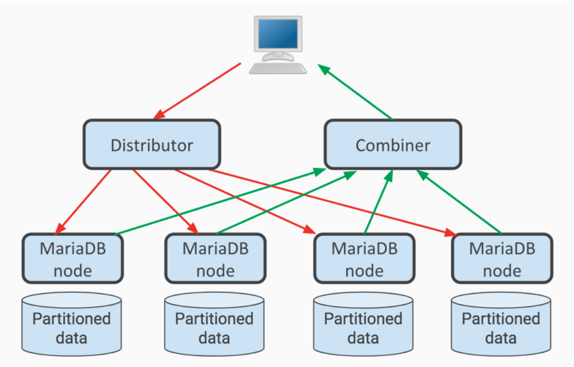

Tesselation see O'Mullane et al. (2001)

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



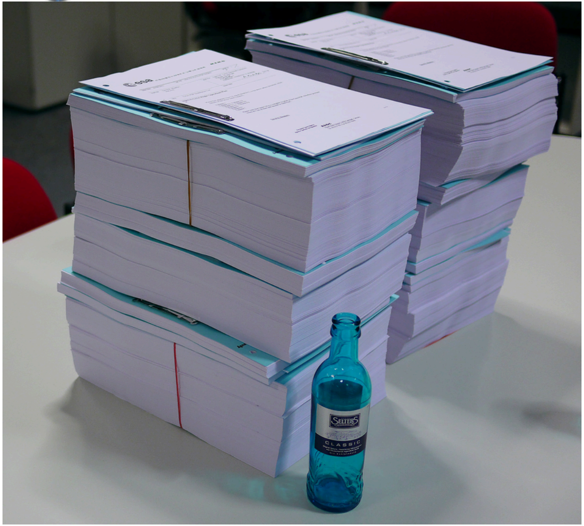

Recent scale tests:

`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

# Flight Operations Procedures



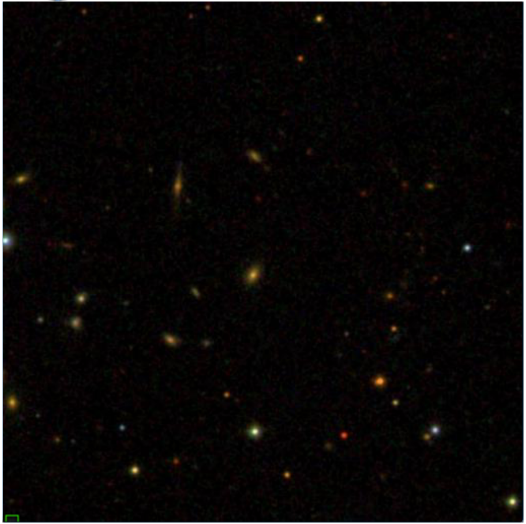

The FOP is followed by the spacecraft operators - the paper copy is just in case the computers fail - could be useful!

But we should avoid *write only* documents.

# Guidelines, tools, conventions

- Its great having extensive guidelines - it was also something super on Gaia
- `developer.lsst.io` is a full developer guide - everything from git commit messages to style guides for Python and C+.
- `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.
  - - on RubinObs we lack something foundational like BAS-003

# SDSS image

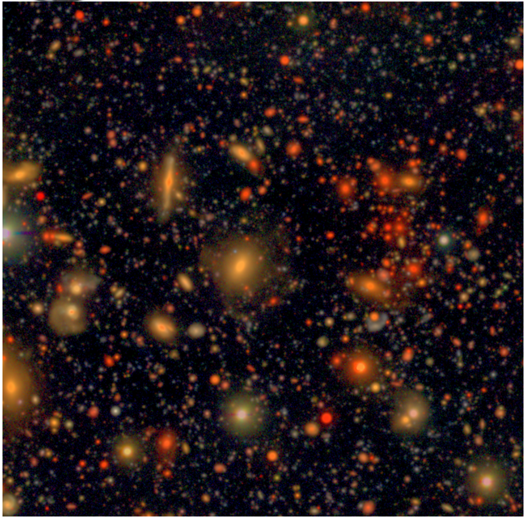


Nice colors Lupton et al. (2004)

$\approx 3.5'$

**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 (≈ 27.5)

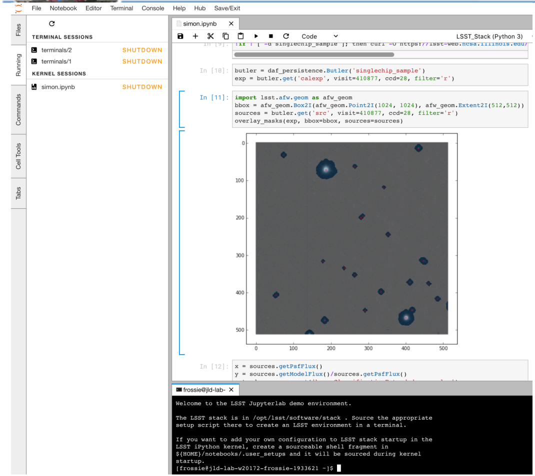
Challenges:

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

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

**Image HSC collaboration, Robert Lupton**

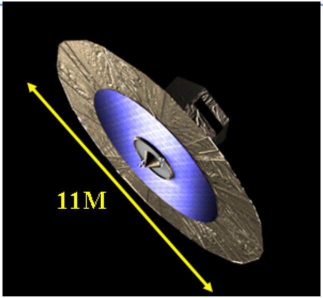
# Catalog extraction




– 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

# 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 19$^{th}$ 2013
  - Stereoscopic Census of Galaxy over 5 years
    - Extended 2 yrs - request for five
  - $\mu$arcsec Astrometry $G < 20$ ($10^9$ sources)
  - Radial Velocities $G < 16$
  - Photometry millimag $G < 20$



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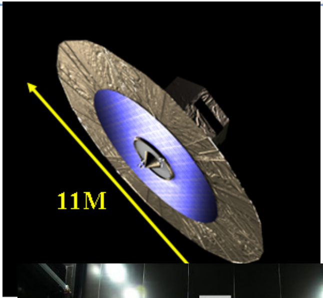
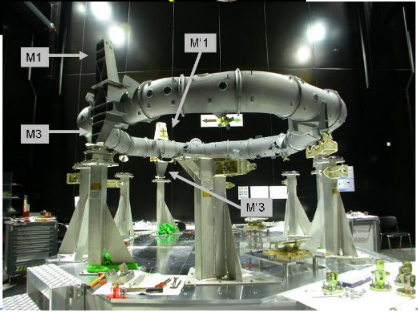
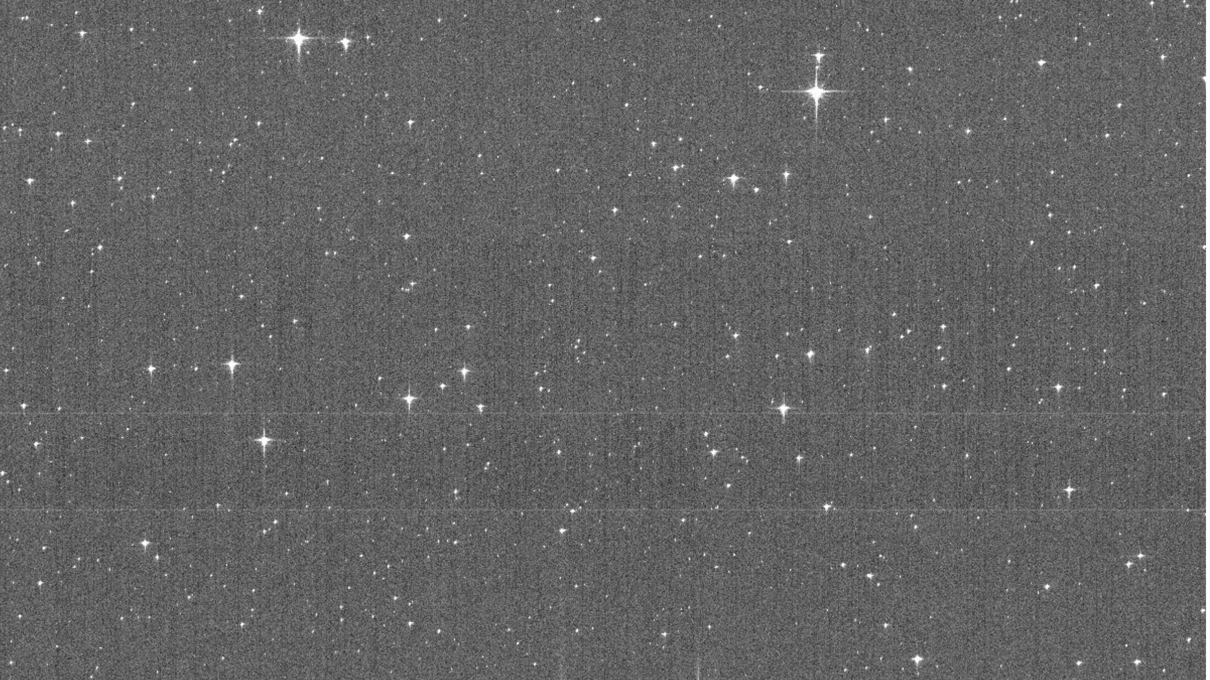
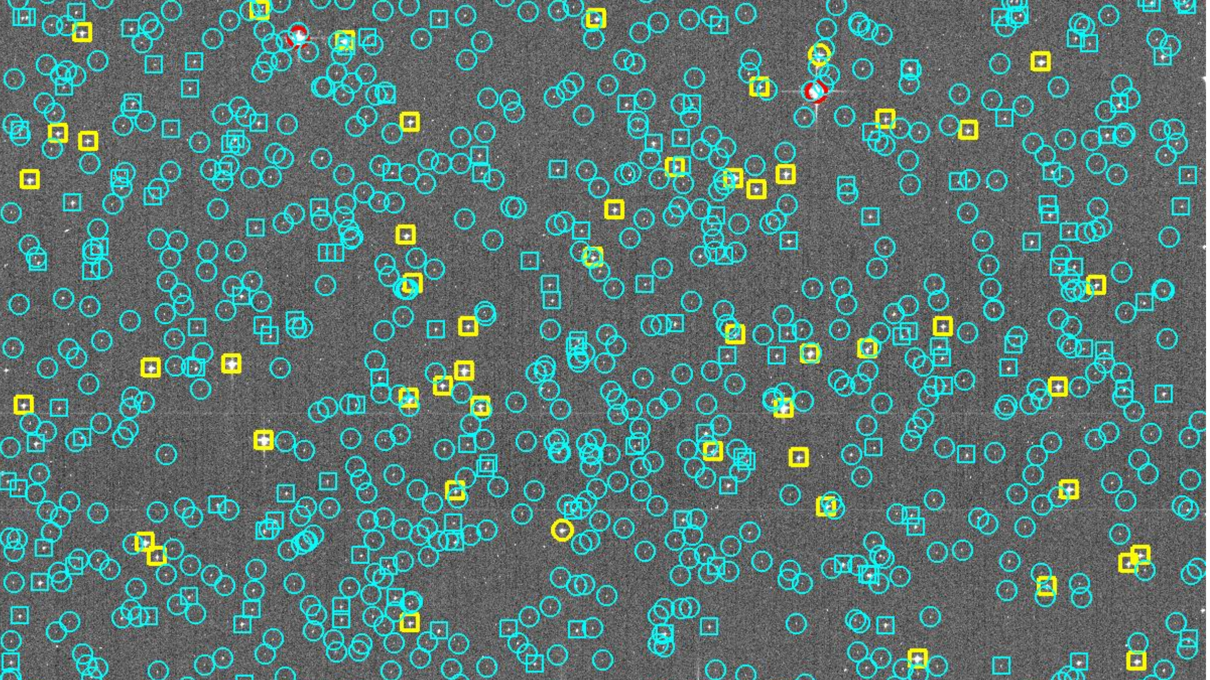
  - Photometry millimag $G < 20$
- Final catalogue $\approx$ 202?







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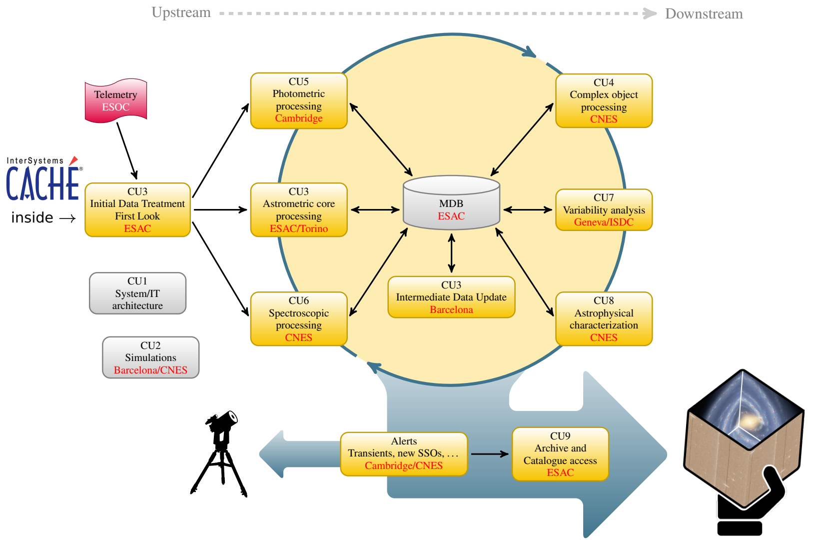
  - Must consider relativistic light bending from solar system objects.
- Attitude and Geometric calibration can only by done using Gaia's own observational data. (AGIS) (O'Mullane et al., 2011; Lindegren et al., 2012)
  - this requires a significant portion of the data to be processed iteratively

# Simplified processing overview



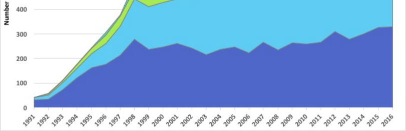

CU=Coordination Unit

Daily 50 — 100$GB$ compressed

5yrs 1$PB$

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

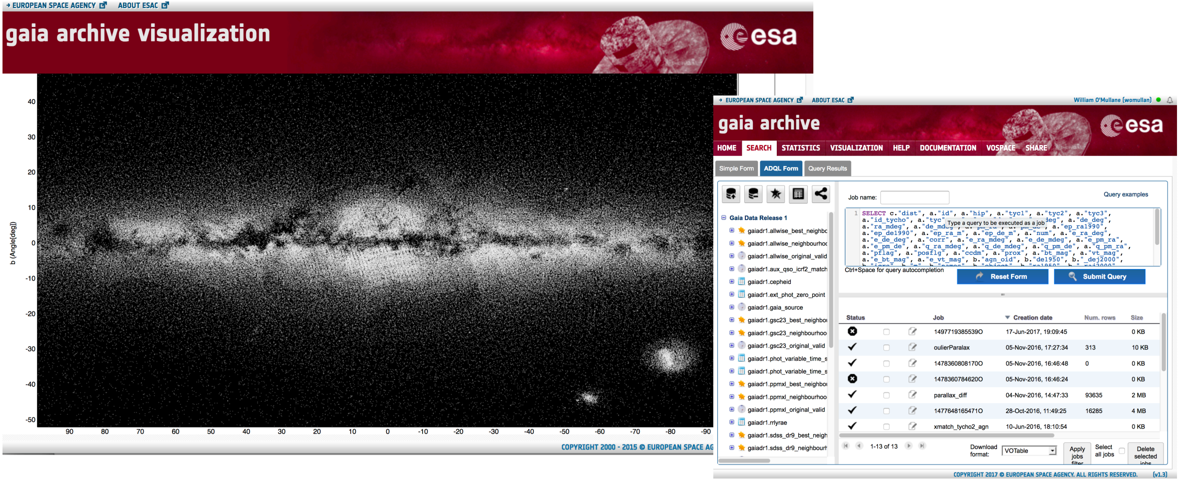
# The Era Of Surveys and Arc


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

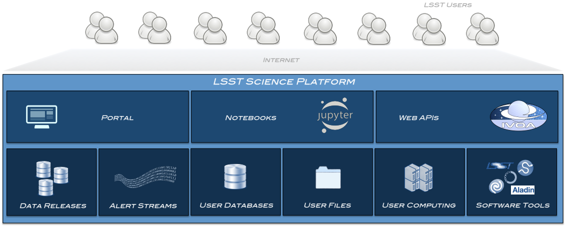
. . . indicates archival research probably play an important role in the scientific success of XMM-Newton Ness et al. (2014)

# Gaia Archive




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

# LSST Science Platform




For DR2:

- Computing:2,400 cores (≈ 18 TFLOPs)
- File storage: ≈ 4PB (VOSpace)
- Database storage: ≈ 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)
**Bruno will have more to say on this topic.**

# General Challenge : Data volume

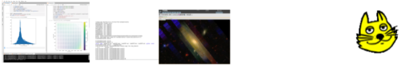
See also Bauer et al. (2019)

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)

# Architecture

We all constantly redesign and rebuild wheels, this will become too expensive as data volume grows ..



Notebook | Cmd Line | Portal | Alert Filtering | Pipelines | TopCat/Other | Developer Services

ASTRONOMICAL DOMAIN ENABLING SERVICES

Astro APIs (UWS,TAP+ etc.), Data Access (Butler, Rucio) Identity/Group services, AstroPy

SYSTEM SOFTWARE AND COMPONENTS

Helm/Terraform, Kubernetes, Pegasus, Condor, Docker, CDN, Jupyter Hub, Jenkins CI

HARDWARE RESOURCES

Compute (HPC,GPU), Storage, Database services

– We should agree a component based cyber infrastructure model and work on improving specific components to plug in - right now we are all building TAP, Designing Databases , deploying Jupyter . . .

– Data models like CAOM from IVOA are going to be essential going forward so we can inter-operate on data

**Filesystems are End Of Life** - object stores should not be confused with the object databases many of us struggled with in the 90s and 00s .. Google and Amazon do not run filesystems they run object stores.

# Processing patterns

- LSST allows 9 months for a Data Release Processing Cycle - probably about 6 months actual processing.
- The original requirement for Gaia astrometric solution was three months.
- Traditional batch systems and shared nothing architecture may not always work
  - Gaia Astrometric Solution required temporal spatial access and had global matrices
  - There are processes for LSST which will have similar problems e.g. Forward Global Calibration Model (FGCM) `https://github.com/lsst/fgcmcal` (Burke et al., 2018)
- preparing and staging for tasks can take ever longer as our processing becomes more sophisticated
- And then there is machine learning!
  - Automated discovery - need it great !
  - Reproducibility, understandability ..

# Software is no longer an afterthought

- In ESA (personal opinion) Gaia was a game changer - the Software was seen as critical - I had to fight to keep it off the Launch Critical Items List. We still had a meager 10% or so of the budget.
- LSST recognized early on that the processing was as important as the telescope - DM is one of 4 Subsystem with about 20% of the project budget
- We need to consider long term software support and the software eco system
  - Open source and publicly scrutinized algorithms
  - Agree community cyber infrastructure model (previous slide)
  - Though I made my career in astronomy/computing .. its not easy .. and I really had to do the management thing
- Education and outreach - How do we do better?
  - Does everyone need to be a data scientist/programmer ?
  - Educate astronomers/managers on how to *open source*
  - How do we foster inclusion ?

# 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. |

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