Enabling Large-Scale Dataset Analytics: Hierarchical Adaptive Tiling Scheme (HATS)

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DATA INTENSIVE RESEARCH IN ASTROPHYSICS AND COSMOLOGY

The LINCC Frameworks Project

LSST Interdisciplinary Network For Collaboration And Computing

To collaboratively develop open computing systems and algorithms needed for large-survey analyses.

Two LINCC-FW hubs:

- Carnegie Mellon University
- University of Washington





The Legacy Survey of Space and Time Deep synoptic optical survey, coming in 2025.

Repeated imaging of the visible sky to ~24th mag. 10 years of operation. 60 PB of raw data. 40 billion stars, galaxies, asteroids. 30 trillion observations.



Objective

Develop a system (format, tools) to deliver and enable end-user analyses on 10TB+ (catalog) datasets

Large-dataset Analytics: Partitioned Files

- Relational databases are not ideal for this type of work. Poor UX, too many bottlenecks.
- Industry state of-the-art is to use distributed analytics tools operating on <u>files</u>.
- Distributed computation achieved through <u>partitioning</u>.



How to partition? Historically, we haven't generally given this much thought...

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GaiaSource_014046-015369.csv.gz	05-May-2022	Parent directory/		We are providing this archive as simple alternative to public event brokers. Full-	"programid3" tarballs; as of this writing the	se are additional observations of
GaiaSource 016241-017018.csv.gz	05-May-2022	1000/		featured event brokers that provide real-time access to these alerts include MARS,	the current 1ESS sector.	
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GaiaSource_021442-021665.csv.gz	05-May-2022	1035/		L] ztf_public_20220808.tar.gz	2 days ago	1.7G
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GaiaSource 022411-022698.csv.gz	05-May-2022	1043/		Di atti publici 20220806 tariga	4 days ago	116
GaiaSource_022699-022881.csv.gz	05-May-2022	1045/		E En_public_coccountinge		
GalaSource_022882=023058.csv.gz	05-May-2022	1045/		T ztf_public_20220805.tar.gz	5 days ago	3.6G
GaiaSource 023265-023450.csv.gz	05-May-2022	1055/	-			
GaiaSource_023451-023649.csv.gz	05-May-2022	1056/		tf_public_20220804.tar.gz	5 days ago	6.3G
GaiaSource_023650-023910.csv.gz	05-May-2022	1057/				
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GaiaSource 024527-025166.csv.gz	05-May-2022	1119/			0 days and	170
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GaiaSource_027107-027517.csv.gz	05-May-2022	1140/				
GaiaSource_027518=027832.csv.gz	05-May-2022	1142/		tf_public_20220730.tar.gz	11 days ago	14G
GaiaSource_027833=028078.csv.gz	05-May-2022	1231/		2012-060-19 10.55		
		1233/		2012-Dec-19 10:33		
		1239/	-	2012-Dec-19 10:33		
		1241/		2012-Dec-19 10:33		
		125/	-	2012-Dec-19 10:33		
		1302/		2012-Dec-19 10:34		
		1220/		2012-Dec-19 10:34		
		1221/		2012 Dec 10 10:34		

There's value in thinking this through, and standardizing

- Users know what to expect and how to handle the dataset
- High quality, shared, analytics tools can be written
- Pre-staging/ETL may be avoided
- Multi-dataset analytics can supported
- Bulk export files == bulk analytics files
- Easier to generate and support for providers
- Can share code and infrastructure (e.g. mirroring, caching)

Think of all the wonderful tools and ecosystems that sprung up around HiPS!



Introducing HATS: Hierarchical Adaptive Tiling Scheme

Gaia DR3

The 1.8Bn sources released in Gaia DR3

A single ASCII file would be about ~680GB in size, (gzip compressed).



1. Partitioning: HEALPix

Partition the sky into NSIDE=1 (order=0) HEALPix tiles, map tiles to files.

Example:

Norder0-Npix0.csv.gz Norder0-Npix1.csv.gz Norder0-Npix2.csv.gz Norder0-Npix3.csv.gz Norder0-Npix4.csv.gz Norder0-Npix5.csv.gz Norder0-Npix6.csv.gz Norder0-Npix7.csv.gz Norder0-Npix8.csv.gz Norder0-Npix10.csv.gz Norder0-Npix11.csv.gz



Problem: Severely unbalanced file sizes

Pixel 4 (Galactic pole) ~ 20GB Pixel 10 (Galactic center) ~ 400GB.

Simple file-based parallelization fails.

Example

Norder0-Npix0.csv.gz Norder0-Npix1.csv.gz Norder0-Npix2.csv.gz Norder0-Npix3.csv.gz Norder0-Npix4.csv.gz Norder0-Npix5.csv.gz Norder0-Npix6.csv.gz Norder0-Npix7.csv.gz Norder0-Npix8.csv.gz Norder0-Npix9.csv.gz Norder0-Npix10.csv.gz Norder0-Npix11.csv.gz



Solution: Partition Hierarchically

If too many sources fall into a pixel, split it into four higher order pixels.

Example

Norder0-Npix0.csv.gz ... Norder0-Npix7.csv.gz ... Norder0-Npix11.csv.gz



If too many sources fall into a pixel, split it into four higher order pixels.

Example

Norder0-Npix0.csv.gz

Norder1-Npix28.csv.gz Norder1-Npix29.csv.gz Norder1-Npix30.csv.gz Norder1-Npix31.csv.gz

Norder0-Npix11.csv.gz



If too many sources fall into a pixel, split it into four higher order pixels.

Repeat.

Example

Norder0-Npix0.csv.gz

Norder1-Npix28.csv.gz Norder1-Npix29.csv.gz Norder1-Npix30.csv.gz Norder1-Npix31.csv.gz

... Norder0-Npix11.csv.gz



If too many sources fall into a pixel, split it into four higher order pixels.

Repeat.

Example

Norder0-Npix0.csv.gz

Norder1-Npix28.csv.gz Norder1-Npix29.csv.gz Norder1-Npix30.csv.gz Norder2-Npix112.csv.gz Norder2-Npix113.csv.gz Norder2-Npix114.csv.gz Norder2-Npix115.csv.gz

Norder0-Npix11.csv.gz



If too many sources fall into a pixel, split it into four higher order pixels.

Repeat until each file size is beneath some pre-defined threshold.

Figure: an overlay of Gaia counts and the partitioning map, taking MAXOBJECTS=1e6

order:

3993 partitions (tiles) for Gaia DR3, with 1M object/partition threshold

2. Serialization: Parquet in HiPS-like Directory Structure

Store the partition files (tiles) into a directory tree.

Parquet files in the leaf nodes.

Norder=0/Dir=0/Npix=0.parquet

•••

Norder=1/Dir=0/Npix=28.parquet Norder=1/Dir=0/Npix=29.parquet Norder=1/Dir=0/Npix=30.parquet Norder=2/Dir=0/Npix=112.parquet Norder=2/Dir=0/Npix=113.parquet Norder=2/Dir=0/Npix=114.parquet Norder=2/Dir=0/Npix=115.parquet

Norder=0/Dir=0/Npix=11.parquet



All together: Hierarchical Adaptive Tiling Scheme (HATS)



Gaia DR2 Catalog Counts (log scale)

Visualization of file storage (color = healpix level) 3933 partitions of similar size (128-256 MB)

gaia/dataset/ metadata gaia/dataset/ common metadata gaia/properties gaia/partition info.csv gaia/point map.fits gaia/dataset/Norder=2 gaia/dataset/Norder=2/Dir=0 gaia/dataset/Norder=2/Dir=0/Npix=20.pargu gaia/dataset/Norder=2/Dir=0/Npix=22.pargu gaia/dataset/Norder=2/Dir=0/Npix=21.parqu gaia/dataset/Norder=2/Dir=0/Npix=23.pargu gaia/dataset/Norder=2/Dir=0/Npix=17.pargu gaia/dataset/Norder=2/Dir=0/Npix=0.parque gaia/dataset/Norder=2/Dir=0/Npix=2.parque gaia/dataset/Norder=2/Dir=0/Npix=19.parqu gaia/dataset/Norder=2/Dir=0/Npix=28.pargu gaia/dataset/Norder=2/Dir=0/Npix=29.pargu gaia/dataset/Norder=2/Dir=0/Npix=34.pargu gaia/dataset/Norder=2/Dir=0/Npix=40.parqu gaia/dataset/Norder=2/Dir=0/Npix=35.pargu gaia/dataset/Norder=2/Dir=0/Npix=42.pargu gaia/dataset/Norder=2/Dir=0/Npix=41.pargu gaia/dataset/Norder=2/Dir=0/Npix=43.pargu gaia/dataset/Norder=2/Dir=0/Npix=44.parqu gaia/dataset/Norder=2/Dir=0/Npix=46.pargu gaia/dataset/Norder=2/Dir=0/Npix=64.pargu gaia/dataset/Norder=2/Dir=0/Npix=65.pargu

Layout on "disk":



Updates since Sydney

Format Updates

- Renaming: HiPSCat -> HATS
- Harmonize metadata file naming/contents conventions with HiPS
- Healpix index made non-unique
- Experimental append support
- VOTable metadata in Parquet

gaia/dataset/ metadata gaia/dataset/ common metadata gaia/properties gaia/partition info.csv gaia/point map.fits gaia/dataset gaia/dataset/Norder=2 gaia/dataset/Norder=2/Dir=0 gaia/dataset/Norder=2/Dir=0/Npix=20.parquet gaia/dataset/Norder=2/Dir=0/Npix=22.parquet gaia/dataset/Norder=2/Dir=0/Npix=21.parquet gaia/dataset/Norder=2/Dir=0/Npix=23.parguet gaia/dataset/Norder=2/Dir=0/Npix=17.parguet gaia/dataset/Norder=2/Dir=0/Npix=0.parquet gaia/dataset/Norder=2/Dir=0/Npix=2.parquet gaia/dataset/Norder=2/Dir=0/Npix=19.parguet gaia/dataset/Norder=2/Dir=0/Npix=28.parguet gaia/dataset/Norder=2/Dir=0/Npix=29.parguet gaia/dataset/Norder=2/Dir=0/Npix=34.parquet gaia/dataset/Norder=2/Dir=0/Npix=40.parguet gaia/dataset/Norder=2/Dir=0/Npix=35.parguet gaia/dataset/Norder=2/Dir=0/Npix=42.parguet gaia/dataset/Norder=2/Dir=0/Npix=41.parquet gaia/dataset/Norder=2/Dir=0/Npix=43.parquet gaia/dataset/Norder=2/Dir=0/Npix=44.parguet gaia/dataset/Norder=2/Dir=0/Npix=46.parguet gaia/dataset/Norder=2/Dir=0/Npix=64.parquet gaia/dataset/Norder=2/Dir=0/Npix=65.parquet gaia/dataset/Norder=2/Dir=0/Npix=70.parquet gaia/dataset/Norder=2/Dir=0/Npix=67.parquet

Code on GitHub/PyPI/conda-forge





Astronomy Data Commons

Software Infrastructure for Science Platforms and Scalable Astronomy on Cloud Resources

Pinned		Customize pins	
axs Public ::	A hats Public		
Astronomy eXtensions for Spark: Fast, Scalable, Analytics of Billion+ row catalogs	Hierarchical Adaptive Tiling Scheme		
● Python ☆ 23 😵 12	● Python 🏠 17 😤 5	Low le	evel format routines
📮 Isdb (Public) 💠	A hats-import Public	:	
Large Survey DataBase	HATS import - generate HATS-partitioned catalogs		
● Python ☆ 19 왕 5	Python 🛱 6 😤 5		
End-user analytics tool		Robu	st importer

https://github.com/astronomy-commons

All of these are also available on PyPI and conda-forge.

LSDB: Python Analytics for HATS

- LSDB: Large Survey Database
- Enable Pandas-like analysis on trillions of observations with thousands of cores
- Build on existing tools: Dask (looking at Ray).
- Full HATS awareness: spatial queries, crossmatching, timeseries, multi-dataset joining.
- Stabilizing the API

Wyatt et al. (2023) https://github.com/astronomy-commons/lsdb

LSDB target APIs: The API center science. Multiprocessing, autoscaling, fail-over, etc. are all implicit. Good user experience.



Nested Pandas: Compact/lazy JOIN evaluation

- Typical catalogs are structured as Object tables, to be joined to Source/Detection tables (time series).
- SQL JOIN-ing Object to Source tends to duplicate fields from Object, and generates a flat table that's inconvenient for the end-user to work with

	а	b	nested
0	0.417022	0.184677	t flux band 0 8.383890 1
1	0.720324	0.372520	t flux band 0 13.704390 1
2	0.000114	0.691121	t flux band 0 4.089045 9
3	0.302333	0.793535	t flux band 0 17.562349 6
4	0.146756	1.077633	t flux band 0 0.547752

 nested_pandas is a memory-efficient pandas extension that presents a "time-series" view to the user, while retaining the speed of evaluation equivalent to that of a flat table.

HATS Datasets @ https://data.lsdb.io

••

- A library of HATSpartitioned datasets to support testing and experimentation with the format
- Download LSDB (the main HATS analytics tool), point it to this website, and immediately start running queries.

•	LSDB × +	
G	e⇒ data.lsdb.io	☆ ♡
	LSDB	Documentati
	GAIA DR3 (GAIA_SOURCE) ZTF DR14 (OBJECTS) ZTF DR14 (SOURCES) DES DR2	Gaia Data Release 3 (GAIA_SOURCE). Gaia Data Release 3 (GAIA_SOURCE table) is a comprehensive catalog released by the European Space Agency (ESA) as part of the Gaia mission, which aims to create a detailed three- dimensional map of our galaxy, the Milky Way. Released in June 2022, Gaia DR3 provides highly precise astrometric data (positions, distances, and motions) for nearly 1.8 billion stars, along with detailed photometric and spectroscopic information.
	TIC V8.2 ALLWISE	<pre>>> lsdb.read_hats('https://data.lsdb.io/hats/gaia_dr3/gaia', margin_cache='https://data.lsdb.io/hats/gaia_dr3/gaia_10arcs')</pre>
	NEOWISE (YEAR 8)	Download with wget
	2MASS (PSC) BAILER-JONES+20	<pre>\$ wget -r -np -nHcut-dirs=2 -R "*.html*" https://data.lsdb.io/hats/gaia_dr3/gaia/</pre>
	ERASS1 MAIN	Metadata information

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HATS Facade @ CDS

- An experiment by FX Pineau et al. to test if CDS catalog holdings can be on-the-fly represented as HATS.
- Converts internal CDS database representation of the catalogs into HATSpartitioned files, served over HTTP.

CDS HATS list × + . vizcat.cds.unistra.fr/hats:n=1000000/ List of CDS's on-the-fly HATS products. HATS stands for "Hierarchical Adaptive Tiling Scheme". It is a "format" developped by the LINCC, see their github repo. The current structure of CDS on-the-fly HATS products is based on the LSDB Gaia example. This prototype will continue evolving to match the evolving LINCC-HATS format. All CDS HATS products are generated on-the-fly from HEALPix indexed data. Although so far the list of available product is limited, all VizieR large catalogues can be added very quickly (matter of adding names in a list). Name a 2MASS/ AllWISE/ GSC 1.1/ HSOY/ SDSS7/ des dr1/ des dr2/ gaia dr2/ gaia dr3/ gaia dr3 astroparams/ gaia dr3 astroparamssupp/ gaia dr3 epochphot/ gaia dr3 rvsmean/ gaia edr3/ aia edr3 dist/

Fornax, SPLUS, ...

- Continuing the integration and testing of HATS/LSDB within Fornax (IPAC & STScI Fornax teams)
- A "HATS/Parquet" server for SPLUS with server-size predicate evaluation (Gustavo Schwarz, Mackenzie U.)

Science Interest Groups Science Analysis Groups Mission Studies Resources **The Fornax Initiative A NASA Astrophysics Science Platform** News NASA's Astrophysics missions generate vast and complex datasets offering immense scientific potential. The vital role of NASA's Astrophysics archives in mission success is evident, as they have demonstrated 13 November 2024 that user-focused, technologically-rich data systems are key science multipliers. As the Astronomy 2020 Habitable Worlds Observatory Decadal Review emphasized, in the coming decade, frontier science will be done with multi-wavelength (HWO) Technology Roadmap and multi-messenger analysis across large, complex data sets, which will only increase the challenges of Webinar accessing big data, maintaining software, and obtaining sufficient computing resources. » Details NASA Astrophysics is developing the Fornax Initiative, a cloud-based system that brings together data, 5 November 2024 software, and computing so that researchers can focus on science PhysCOS Early Career Workshop | November 19th - 21st 2024 The three pillars of the Fornax Initiative project are: 😐 😑 👘 🖉 SPLUS × + splus.iag.usp.br ☆ <u>□</u> | G-PLUS DATA RELEASES INSTRUMENTATION SCIENCE COLLABORATION NEWS Southern Photometric Local Universe Survey

Status and Looking Ahead

- Format is in a reasonably solid draft form now
 - Remains to be done: optimized storage of distributed cross-match margins
- Working or in touch with most major archives/projects.
- Preparing an IVOA Note.
- Application support is maturing for Python (LSDB), but we're looking to expand support in other ecosystems (Rust, Java)
 - E.g. a Spark DataSource for reading HATS would enable advanced support for HATS within Spark
- Field testing within Rubin Commissioning
- Thinking about Iceberg serialization

Where to Try



LINCC Hub: <u>https://lsst.dirac.dev</u>

- LINCC Hub: The LINCC Science Platform for the LSST Science Collaborations (email <u>ncaplar@uw.edu</u> for access)
- NASA Astrophysics Science Platform: Working with the Fornax team at IRSA/MAST/HEASARC to deploy and test.



• Or run conda install -c conda-forge lsdb on your fav. science platform.

Summary and next steps

Mailing list:https://groups.google.com/g/hats-wgRepositories:https://github.com/astronomy-commonsMeetings:10am PT, every third Friday of the month

- Aiming to enable end-user analyses on 1-100T+ catalog datasets. Ad-hoc collaboration of scientists/engineers from LINCC, Rubin, MAST, IRSA, HESARC, LINeA, CDS. Developing formats and tools.
- Lots of progress since last year. Data format and Python tools solidifying. We've gathered enough initial real-world usage to start drafting the formal format spec. Preparing an IVOA Note.
- Next year:
 - Perfect the tools (UX and performance are a priority)
 - Larger scale user deployment
 - Would love to get addt'l feedback and implementations (e.g. Java or Rust)



Carnegie Mellon University



Collaboratively advancing data-intensive astronomy.







AST-2003196

Thank You !

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UNIVERSITY of WASHINGTON