STScI | SPACE TELESCOPE SCIENCE INSTITUTE EXPANDING THE FRONTIERS OF SPACE ASTRONOMY

Using HTCondor to Calibrate and Archive HST and JWST Data

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The STScI Data Processing & Archive Services (DPAS) Branch 05.23.2018





Our Vision

STSCI | SPACE TELESCOPE SCIENCE INSTITUTE

Our Mission



expanding the frontiers of space astronomy

We help humanity explore the universe with advanced space telescopes and archives

Our Strategic Goals







- **Excel in the science operations of NASA's current and future** astrophysics flagship missions
- **Advance state-of-the-art**
- astronomical data, archives, and
- tools for scientific discovery
- Make the world's astronomical information accessible to all

 \star Proposal (observation) selection \star Planning and scheduling **T**Data calibration **Data** archives

Science Operations for the Hubble Space Telescope (HST)





HST on Twitter





Space Telescope Live

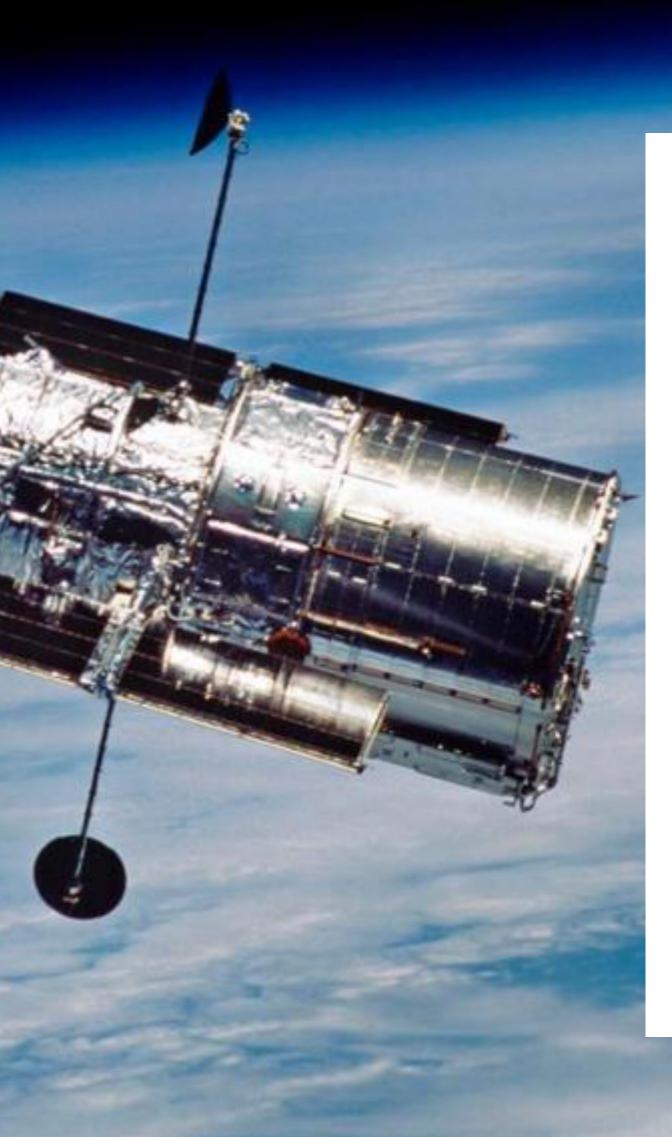
@spacetelelive

What is @HubbleTelescope looking at? -Reference images from @STScI Digitized Sky Survey and Sloan Digital Sky Survey Data Release 13 (not actual Hubble images)

- O Low Earth Orbit
- S spacetelescopelive.org
- Joined August 2016
- © Born on April 24, 1990

Tweet to Space Telescope Live

@spacetelelive





Space Telescope Live @spacetelelive

am looking at the Galaxy NGC0613 with Wide Field Camera 3 for Dr. Peter Erwin. spacetelescopelive.org/2018-05-21T12:...



9:30 AM - 21 May 2018







Spacecraft & Science Operations for the James Webb Space Telescope (JWST) (Scheduled for launch in Spring 2020)

- \star Proposal (observation) selection
- \star Planning and scheduling
- \star Data calibration
- ★ Data archives
- **Mission Operations Center**
- ★ Wavefront Sensing and Control







http://mast.stsci.edu/

- X MAST Observations: Millions of observations from Hubble, Kepler, TESS, GALEX, IUE, FUSE, and more (to include JWST and WFIRST).
- 💢 Virtual Observatory: Search thousands of astronomical data archives from around the world for images, spectra, and catalogs.
- X Hubble Source Catalog: A master catalog with a hundred million measurements of objects in Hubble images.
- MAST Catalogs: Access to catalog data such as Gaia and TESS Input Catalog, with more coming soon.

JWST data < 12 months old

MIKULSKI ARCHIVE & SPACE TELESCOPES

 \propto All data is publicly available except for most HST data < 6 months old and









Data Management System (DMS)

X Multiple data pipelines (workflows):







x Engineering data including spacecraft meta-data and jitter



 χ Mission schedules (planned observations)



Spacecraft ephemerides

- χ The data management system controls the flow of science and engineering data through the data calibration pipelines and into the archive (MAST).

 - \propto New science from the telescope (four active instruments on HST)
 - \propto Reprocessed science data due to changes in software or calibration data









(number of photons emitted).

To solve this problem, one needs to account for:

- Detector bias: counts in a detector readout when no exposure is taken
- Dark current: spurious counts during an exposure due to noise in the detector
- Flat-field: pixel-to-pixel variations in detector efficiency
- CTE correction: pixel-to-pixel charge-transfer efficiency
- Combined/drizzled exposures: Long observations are broken into multiple exposures and combined in processing to increase the signal-to-noise ratio

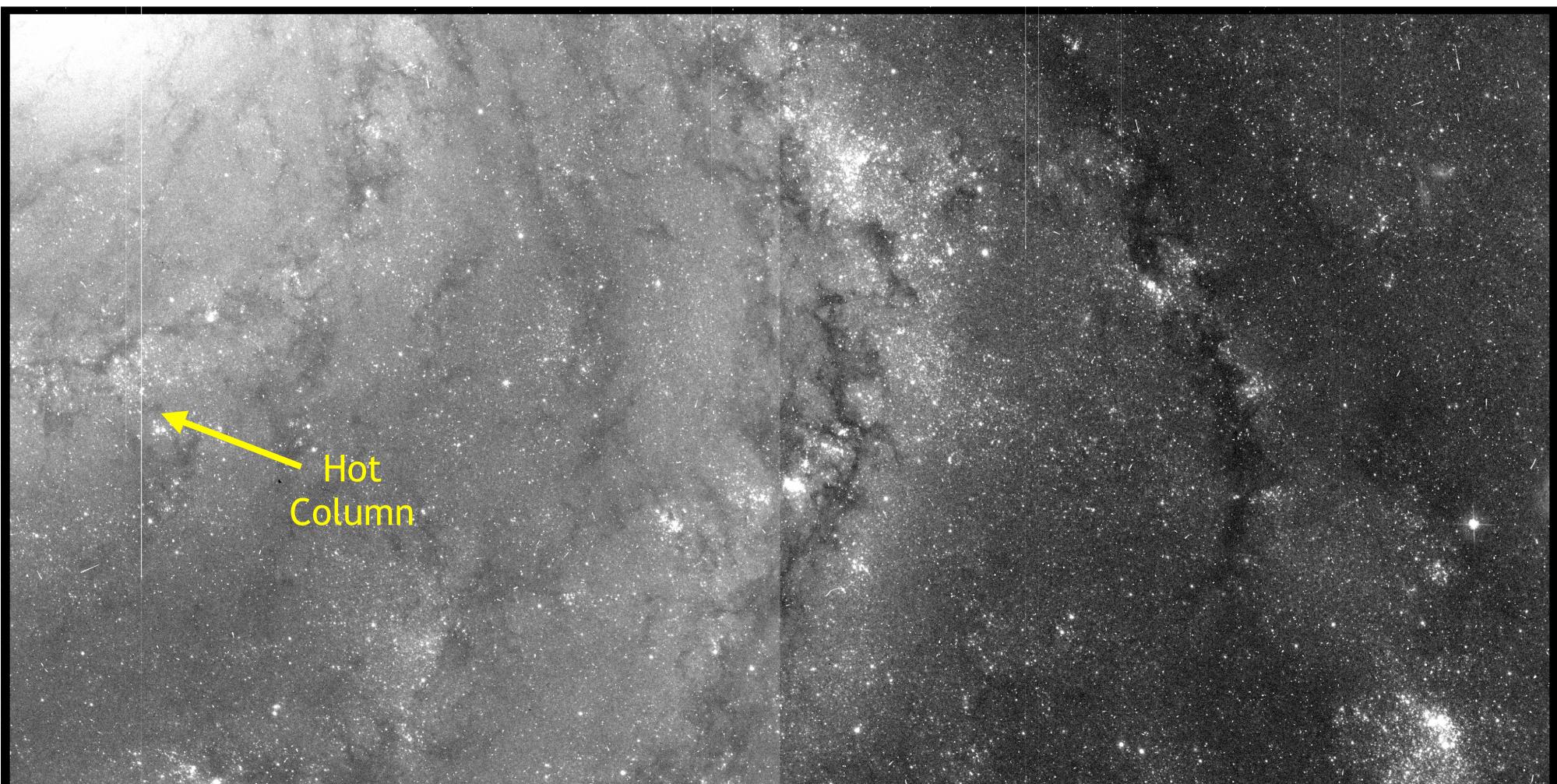
GOAL: Convert an image from raw pixel counts on the detector to a source flux







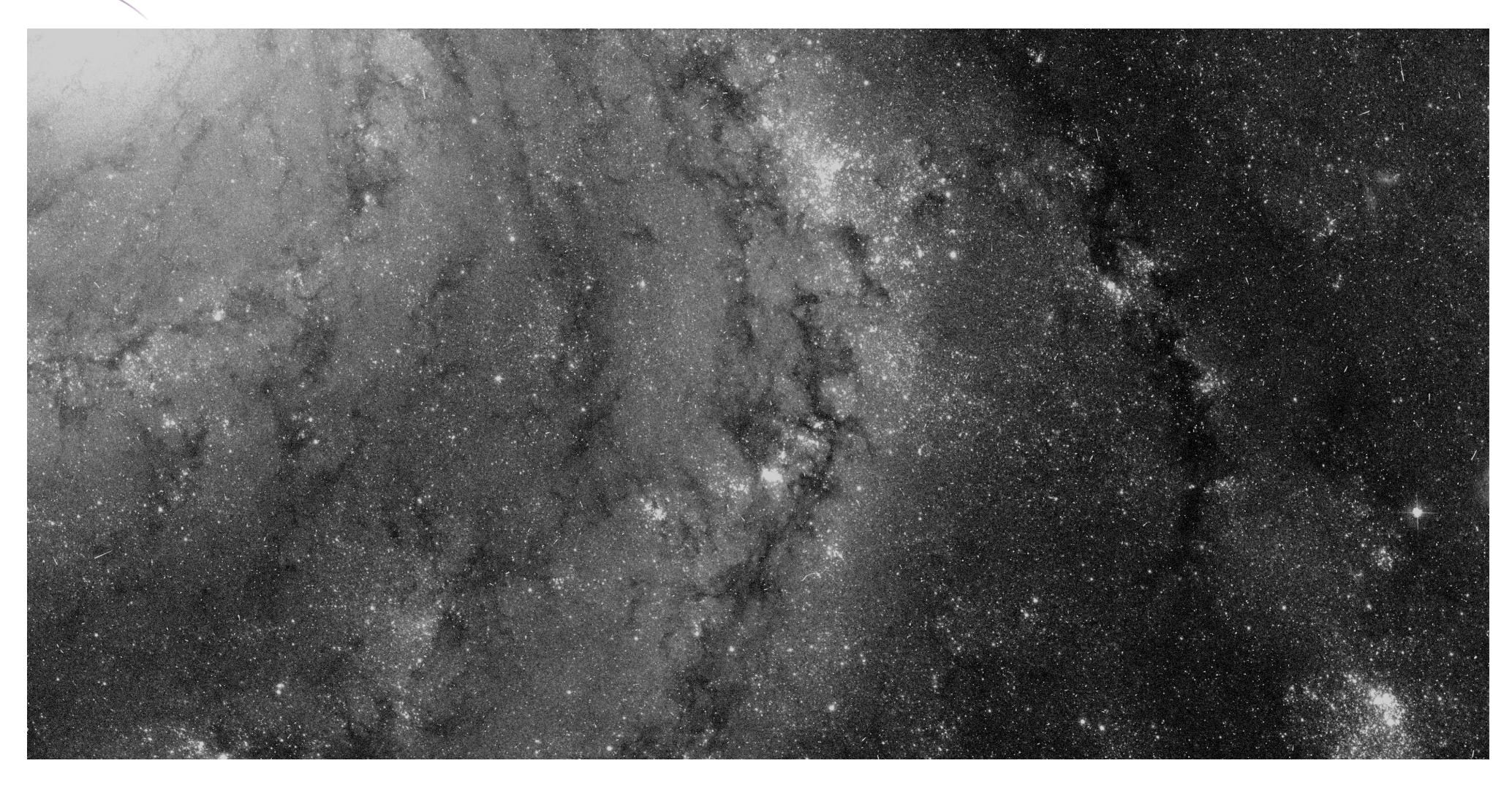
Advance Camera for Surveys (ACS) image of M101 (Pinwheel Galaxy)



Two amplifiers with different bias levels







Cosmetic artifacts in the image have been removed

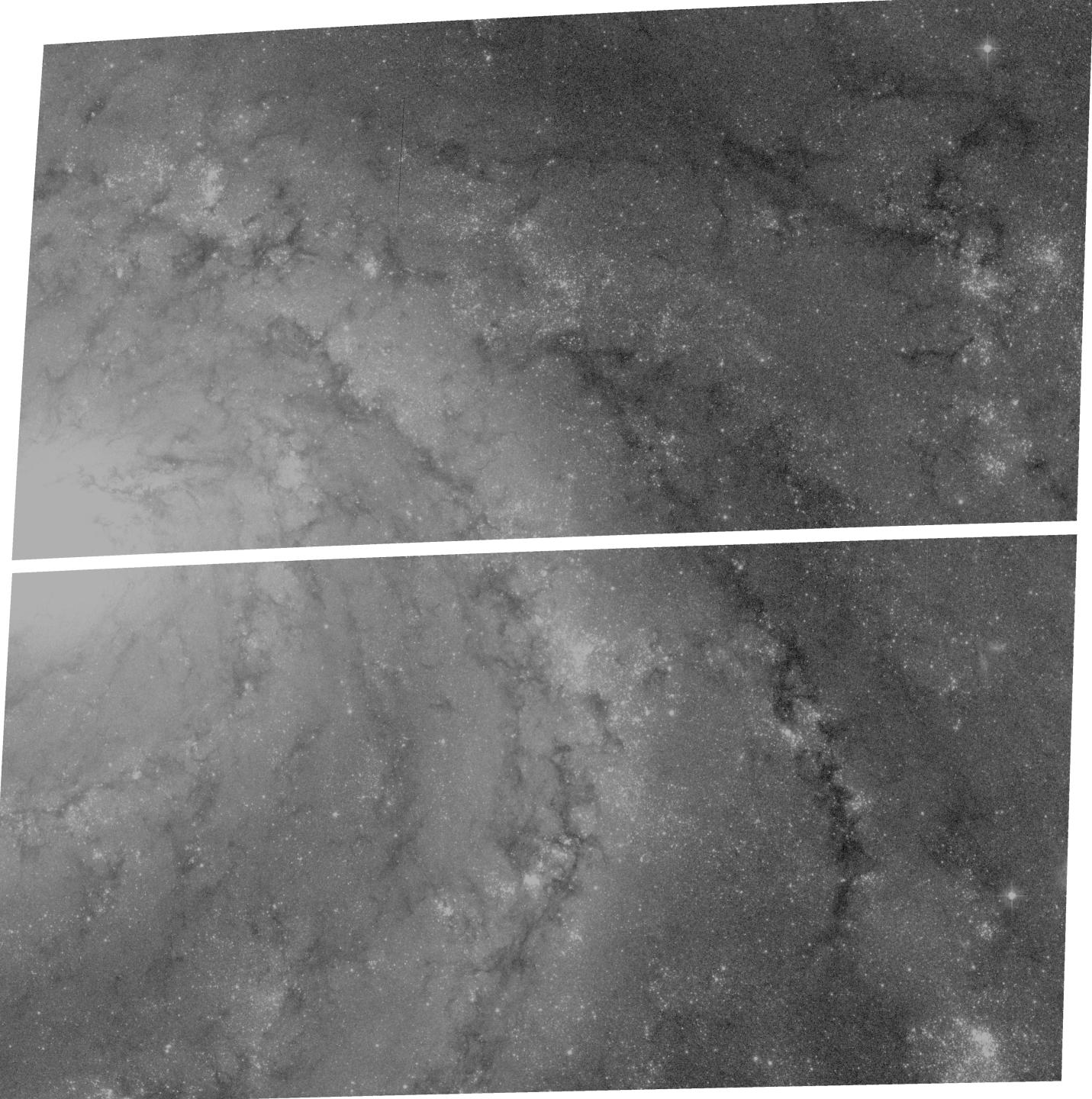




Multiple images are combined to form the final product.

Cosmic ray hits have been removed.

This shows both CCDs in the instrument (previous slides only had the lower one).



HTCondor Use at STScl

- HST previously used an in-house workflow manager called OPUS
- OPUS featured
 - Distributed processing on a pool of machines (shared disk access) • A blackboard paradigm for distributing work
- OPUS was reevaluated under a trade-study in 2011 to choose the workflow management system for JWST
 - HTCondor was chosen for use with custom-made OWL (Orchestrated Workflow Layer) add-on
 - The HST Mission Office decided to allow OPUS to be phased out for HST processing in favor of HTCondor/OWL
- OPUS was gradually phased out and was fully retired in Feb. 2018.



Why HTCondor?

- Better performance and flexibility for large processing runs Capability to add machines when needed, then release them for normal
- operational loads
- A more maintainable, reliable system in the future
 - OPUS was developed in-house, but the expertise had left
 - Huge HTCondor user base (with conferences and everything)
- OPUS could not handle the large data processing needs of JWST. Converting HST to HTCondor had the advantages of
 - Operators and developers only need to know one system
 - Use HST to gain HTCondor expertise before JWST launch and operations



What and Why is OWL?

- OWL = Orchestrated Workflow Layer
- HTCondor manages compute resources extremely well
- Lacks services for managing and tracking the data being processed
- What OWL provides
 - A job-tracking database table (the blackboard) that captures every step in the workflow populated and updated by HTCondor job hooks
 - Template-driven workflow generation ("DAGs on-the-fly") using the Jinja2 template engine



DAGs-on-the-Fly

DAG templates

Job definitions. JOB 2FITS sdp_edt2fits_{{ dataset }}.job JOB RF sdp_bestref_{{ dataset }}.job JOB BC sdp_before_calib_{{ dataset }}.job JOB CA sdp_calibration_{{ dataset }}.job JOB MD sdp_astrodrizzle_{{ dataset }}.job JOB AC sdp_after_calib_{{ dataset }}.job JOB INGEST_SCI archive_submit_{{ dataset }}.job JOB PVW sdp_preview_{{ dataset }}.job JOB CL sdp_clean_{{ dataset }}.job

```
# Relationships.
PARENT 2FITS CHILD RF
PARENT RF CHILD BC
PARENT BC CHILD CA
PARENT CA CHILD MD
PARENT MD CHILD AC
PARENT AC CHILD INGEST_SCI
PARENT INGEST_SCI CHILD PVW
PARENT PVW CHILD CL
```

# Condor	priorities	
PRIORITY	2FITS	50
PRIORITY	RF	55
PRIORITY	BC	60
PRIORITY	CA	65
PRIORITY	MD	70
PRIORITY	AC	75
PRIORITY	INGEST_SCI	85
PRIORITY	PVW	80
PRIORITY	CL	90

sdp_prearch_wf3.dag



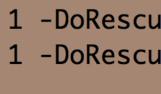


DAGs are created for specific datasets (here WFC3 datasets idkv02010 and idkv02020)

		.> CO	ndor_	-9			•	·			·							
Sche	edd:												@	05/	21/2	18 1	L5:57	7:15
OWNER	BATC	H_NAME									SUB	MIT	TED	D	ONE	F	RUN	ID
	sdp_	prearch	_wf3_	_idkv	0201	0.da	g+56	402	28	5	/21	15	:28		3		1	
	sdp_	prearch	_wf3_	_idkv	0202	0.da	g+56	402	30	5	/21	15	:28		4		1	
4 jobs	; 0 c	omplete	d, 0	remo	ved,	0 i	dle,	4	run	nin	g,	0 h	eld,	0	sus	pend	led	
		.> со	ndor_	_q	noba	tch												
Sche	edd:												@	05/	21/1	18 1	L5:57	7:26
ID		OWNER			SU	BMIT	TED		RU	N_T	IME	ST	PRI	SI	ZE	CME)	
5640228	8.0				5/2	1 15	:28	0	+00	:29	:13	R	0		0.3	cor	ndor_	_dagm
5640230	0.0				5/2	1 15	:28	0	+00	:29	:13	R	0		0.3	cor	ndor_	_dagm
5640362	2.0				5/2	1 15	:29	0	+00	:28	:21	R	65	97	7.0	cal	wf3_	_OWL.
5640525	5.0				5/2	1 15	:56	0	+00	:00	:44	R	70		0.0	md_	_xxx_	_OWL.
4 jobs	; 0 c	omplete	d, 0	remo	ved,	0 i	dle,	4	run	nin	g,	0 h	eld,	0	sus	pend	ded	

DLE TOTAL JOB_IDS 9 5640362.0 9 5640525.0

man -f -l . -Debug 3 -Lockfile sdp_prearch_wf3_idkv02010.dag.lock -AutoRescue 1 -DoRescu man -f -l . -Debug 3 -Lockfile sdp_prearch_wf3_idkv02020.dag.lock -AutoRescue 1 -DoRescu .sh .sh





What and Why is OWL?

- OWL = Orchestrated Workflow Layer
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 - Template-driven workflow generation ("DAGs on-the-fly") using the Jinja2 template engine
 - A web app (OWL GUI) for monitoring dataset processing status and other system features



OWL G

OWL GUI (Data Flow)

	Fileset 🔶	Process Name	Status 🛊	Rescue	StartTime 💡	Completion Time	Controls	State 🔶	Exit Co
Þ	iccz13q0q	INGEST	Ο	RESCUE	2018-05-11 18:33:50.0	1970-01-01 00:00:00.0	II 🔳 🖂 🛍	Starting	
+	lcd903010	REPRO_CL	Ο	RESCUE	2018-05-11 18:33:50.0	1970-01-01 00:00:00.0	II 🗖 🗠 🔟	Starting	
•	iccz13p1q	CL	\odot		2018-05-11 18:33:13.0	2018-05-11 18:33:15.293	<u>∼</u>	Exited	0
+	iccz13ptq	INGEST	\$		2018-05-11 18:33:12.0	1970-01-01 00:00:00.0	II 🗖 🗠 🔟	Running	
•	iccz13psq	INGEST	\$		2018-05-11 18:33:01.0	1970-01-01 00:00:00.0	II 🗖 🗠 🔟	Running	
+	iccz13p2q	CL	\odot		2018-05-11 18:32:59.0	2018-05-11 18:33:04.783	∠	Exited	0
•	iccz13oeq	CL	\odot		2018-05-11 18:32:53.0	2018-05-11 18:32:54.13	<u>∼</u>	Exited	0
•	iccz13pwq	INGEST	\$		2018-05-11 18:32:50.0	1970-01-01 00:00:00.0	II 🗖 🗠 🔟	Running	
•	iccz13ozq	CL	\odot		2018-05-11 18:32:24.0	2018-05-11 18:32:29.06	<u>∼</u>	Exited	0
•	idlx08030	CL	\odot		2018-05-11 18:32:22.0	2018-05-11 18:32:28.147	∠	Exited	0
•	iccz13pqq	INGEST	\$		2018-05-11 18:32:22.0	1970-01-01 00:00:00.0	II 🔳 🗠 🛍	Running	

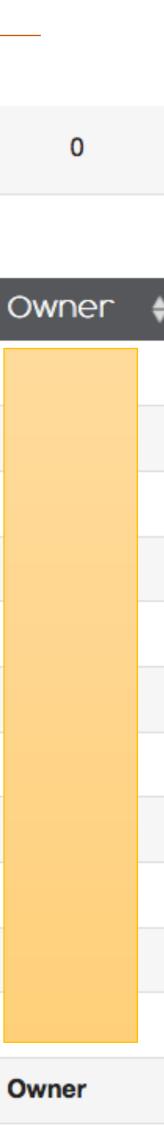


OWL GUI (Data Flow For a Single Dataset)

 \odot CL idlx08030 Show 25 entries Start Time **Process Name** Fileset Status End idlx08030 CL Exited 2018-05-11 18:32:22.0 idlx08030 INGEST 2018-05-11 18:20:36.0 Exited CL 2018-05-11 17:07:09.0 idlx08030 Exited idlx08030 PVW 2018-05-11 17:05:01.0 Exited INGEST_SCI idlx08030 Exited 2018-05-11 17:03:01.0 2018-05-11 17:02:48.0 AC idlx08030 Exited MD 2018-05-11 17:00:06.0 idlx08030 Exited idlx08030 CA Exited 2018-05-11 14:49:43.0 BC 2018-05-11 14:49:30.0 idlx08030 Exited RF idlx08030 Exited 2018-05-11 14:49:09.0 2FITS idlx08030 Exited 2018-05-11 14:48:45.0 Start Fileset **Process Name** Status Start Time

Showing 1 to 11 of 11 entries

		2018-05-11 18:32:22.0	2018-05-11 18:32:28.147	l	~	Exited	ł		
			Searc	:h:					
¢	Comple	tion Time 🛭 👙	Lasted Rescue	ed ♦	State	\$ E>	kit Code	¢	0
	2018-05-1	1 18:32:28.147	None		Exited	0			
	2018-05-1	1 18:32:08.713	None		Exited	0			
	2018-05-1	1 17:07:10.33	None		Exited	0			
	2018-05-1	1 17:07:01.373	None		Exited	0			
	2018-05-1	1 17:04:52.457	None		Exited	0			
	2018-05-1	1 17:02:49.967	None		Exited	0			
	2018-05-1	1 17:02:39.637	None		Exited	0			
	2018-05-1	1 16:59:57.987	None		Exited	0			
	2018-05-1	1 14:49:33.723	None		Exited	0			
	2018-05-1	1 14:49:21.61	None		Exited	0			
	2018-05-1	1 14:48:57.177	None		Exited	0			
	Completio	n Time	Lasted Rescued		State	Ex	it Code		C
				Pr	evious 1	Nex	ct		







- - •

• OWL allows us to specify and feed data processing runs into the system Data Processing Queue (DPQ) database table holds workflow requests



Queue Processing

DESCRIPTION: Shows DPQ_DB.DpQueue table entries for workflows that have not yet been started by the Shoveler task, or for informational message workflowTypes that communicate status of processing where a workflow could not yet be started for a fileset. The Actions column provides a trash icon that, when selected, will result in deletion of the table row from the DPQ_DB.DpQueue database table. This can be used to remove informational message lines that have been looked into and are no longer needed. Once the Shoveler picks up an entry from the DPQ_DB.DpQueue table, the row on this display will disappear, and migrate to the DPQ_DB.DpQueueHist table, and be visible on the History tab.

ιαυ.										+
C Re	Clear Filters		Show 25 rows 🔻		Show/Hide columns	•				
Show 2	5 - entries						Searc	ch:		
Actions	File Set	ŧ	Priority	¢	Workflow Type	▼	Insert Date	ŧ	Shovel Date	\$
Û	idp507czq		15		wf3_single_repro		2018-05-09 20:36:18.7	67		
Û	idp507d0q		15		wf3_single_repro		2018-05-09 20:36:18.9	13		
Û	idp507d1q		15		wf3_single_repro		2018-05-09 20:36:19.0	3		
Û	idp507d2q		15		wf3_single_repro		2018-05-09 20:36:19.1	8		
Û	idp507d3q		15		wf3_single_repro		2018-05-09 20:36:19.32	27		
Û	idp507d4q		15		wf3_single_repro		2018-05-09 20:36:19.4	8		

O Fri, 11 May 2018 18:11:21 UTC ☐ 131 DOY



Managing Datasets

OWL allows us to specify and feed data processing runs into the system • Data Processing Queue (DPQ) database table holds workflow requests

HTCondor — mburger@dmsops1:~ — ssh dmsops1 — 103×25

Last login: Fri May 11 16:48:41 UTC 2018 on pts/7 > shoveler_status.py

DPQ entries	for			as o	f	Fri	May	11	18
priority		type	unsho	ovel	ed	enti	ries		
77		ingest.	_pvw		92	2			
15		cos_as	n_repi	ro	31	L 48			
15		cos_si	ngle_i	repro	0		40	034	
15		reinge	st_pv	N	87	765			
15		wf3_as	n_rep	ro	88	364			
15		wf3_si	ngle_i	repro	0		24	1435	5
0		awaiti	ng_gso	a_ji	t		5		
0		awaiti	ng_sc	i_ji	t		3		
0		collec	ting_d	asn_s	sci	L .	1		
0		collec	ting_e	eng			28	3	

>







- - Data Processing Queue (DPQ) database table holds workflow requests
 - The DPQ is populated by Pollers which watch target directories for new files. When new files are found, workflows are added to the DPQ table.

OWL allows us to specify and feed data processing runs into the system





Start/Stop	Status 🔶	Poller 🔶	Last Update 🔶	Interval 🔹
		repro_manager	2017-09-26 11:04:06.8070000	120
	0	rescue_me	2017-09-26 11:05:26.6630000	120
	—	SHOVELER	2017-09-13 18:19:42.8470000	120
		CRDS	2017-09-25 19:35:13.0600000	60
	—	CSUM_COS	2017-09-26 11:05:18.6400000	60
	—	CSUM_STI	2017-03-17 18:56:40.1270000	60
		dan	2017-09-26 11:05:19.0500000	60
	0	dlg	2000-01-01 00:00:00.0000000	60
		DP_ACS_OWL	2017-09-26 11:05:58.0500000	60
		DP_COS_OWL	2017-09-26 11:05:51.9200000	60
	—	DP_STI_OWL	2017-09-26 11:05:55.4870000	60
	—	DP_WF3_OWL	2017-09-26 11:05:58.0870000	60
	—	jit	2000-01-01 00:00:00.0000000	60
		pnm	2017-09-26 11:05:17.3830000	60
	0	tnm	2000-01-01 00:00:00.0000000	60



Managing Datasets

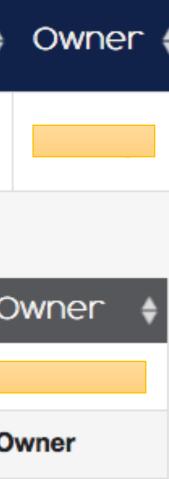
- - Data Processing Queue (DPQ) database table holds workflow requests
 - The DPQ is populated by Pollers which watch target directories for new files. When new files are found, workflows are added to the DPQ table.
 - The Shoveler governs the order and rate at which DPQ entries are sent through the OWL workflow template generator to be transformed into executing DAGMan jobs on the HTCondor pool
- The rescue server receives rescueDAG requests to re-try a failed workflow

OWL allows us to specify and feed data processing runs into the system





	Fil	.eset	¢	 Process Name Statu 		Status	\$	Rescue	cue Start Completion & C Time Time		Controls State 🖨		\$	Exit Code 🕈 R		Remote Host		¢			
•	DAI	N14448		dan_rec	eipt	8		RESCUE 2017- 04:26			2017-09-20 04:26:41.417	<u>~</u>		Exited		1					
			Sho	ow 10 -	entries									Searc	h:						
	≜ F	ileset 🝦	Proces	ss Name	🔶 St	atus 🝦	Sto	art Time	\$	Cor	mpletion Time	¢	Lasted	Rescue	d	🛊 Sto	ite (Exit (Code	\$ O	٧
	D	OAN14448	dan_rece	n_receipt Exited			2017-09-20 04:26:41.0 2			2017	2017-09-20 04:26:41.417 None			Exite			ed	1			
	Fi	Fileset Process Name Status			itus	Start Time Complet			pletion Time	pletion Time Lasted Rescued				Stat	e	Exit Co	ode	0	٨		
			Sho	owing 1 to 1 of	1 entries											Previous	s 1	Next			





Future STScl Operations

scientific observatory in history of the next decade **Expected to launch spring 2020** calibration and archiving operations.

WFC3/UVIS F502N

- **The Hubble Space Telescope is the most successful**
 - **Continue Continue Continue**
- The James Webb Space Telescope will be the premier observatory

 - 16.5 meter segmented mirror optimized for the infrared
- The HTCondor + OWL provide a unified system for the data processing pipelines, allowing for efficient



