Planning and developing the Chandra Source Catalog

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ABSTRACT

The Chandra Source Catalog, presently being developed by the Chandra X-ray Center, will be the definitive catalog of all X-ray sources detected by the Chandra X-ray Observatory. The catalog interface will provide users with a simple mechanism to perform advanced queries on the data content of the archival holdings on a source-by-source basis for X-ray sources matching user-specified search criteria, and is intended to satisfy the needs of a broad-based group of scientists, including those who may be less familiar with astronomical data analysis in the X-ray regime.

For each detected X-ray source, the catalog will record commonly tabulated quantities that can be queried, including source position, dimensions, multi-band fluxes, hardness ratios, and variability statistics, derived from all of the observations that include the source within the field of view. However, in addition to these traditional catalog elements, for each X-ray source the catalog will include an extensive set of file-based data products that can be manipulated interactively by the catalog user, including source images, event lists, light curves, and spectra from each observation in which a source is detected.

In this paper, we emphasize the design and development of the Chandra Source Catalog. We describe the evaluation process used to plan the data content of the catalog, and the selection of the tabular properties and file-based data products to be provided to the user. We discuss our approach for managing catalog updates derived from either additional data from new observations or from improvements to calibrations and/or analysis algorithms.

Keywords: catalogs, data archive, data processing, system architecture

1. INTRODUCTION

X-ray astronomy has a long tradition of publishing detected source catalogs. The Einstein IPC catalog[1] demonstrated the utility of catalogs derived from pointed-observation X-ray missions, and catalogs are the primary products from X-ray all-sky surveys such as the ROSAT all-sky survey[2]. The second XMM serendipitous source catalog[3] is a recent example of a state-of-the-art X-ray source catalog. These catalogs provide a uniform reduction of the mission data (to the extent possible), and remove the need for users, who may be unfamiliar with the complexities of the data, to perform detailed reductions for each observation and detected source.

When compared to all previous and current X-ray missions, the Chandra X-ray Observatory breaks the resolution barrier with an arcsecond resolution on-axis point spread function (PSF). Launched in 1999, Chandra continues to provide a unique high spatial resolution view of the X-ray sky in the energy range from 0.1 to 10 keV over a ~60–250 square arcminute field of view. The combination of excellent spatial resolution, a reasonable field of view, and low instrumental background translate into a high detectable-source density, with low confusion and good astrometry. The wealth of information that can be extracted from identified serendipitous sources is a powerful and valuable resource for astronomy.

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The aim of the Chandra Source Catalog (CSC) is to disseminate this wealth of information by characterizing the X-ray sky as seen by the Chandra X-ray Observatory. The CSC will be the definitive catalog of all X-ray sources detected by Chandra, and will provide simple access to Chandra data for individual sources or sets of sources matching user-specified search criteria. The catalog is intended to satisfy the needs of a broad-based group of scientists, including those who may be less familiar with astronomical data analysis in the X-ray regime. For each detected X-ray source, the catalog will list the source position and a detailed set of source properties, including commonly used quantities such as multi-band aperture fluxes, X-ray colors and hardness ratios, spectra, temporal variability information, and source extent estimates. In addition to these traditional elements, the catalog will include file-based data products that can be manipulated interactively by the user, including images, photon event lists, light curves, and spectra for each source individually from each observation in which a source is detected.

The CSC will be released to the user community in a series of increments with increasing capability. The catalog release process is carefully controlled, and a detailed characterization of the statistical properties of the catalog to a well defined, high level of reliability accompanies each release. Key properties included in the statistical characterization include limiting sensitivity, completeness, false source rates, astrometric and photometric accuracy, and variability information.

The first release of the catalog is expected in the winter of 2008. This release will include information for ~200,000 X-ray sources detected in a subset of public imaging observations from roughly the first eight years of the Chandra mission. Only point sources, and compact sources with extents < ~30 arcsec, will be included. Highly extended sources, and sources located in selected fields containing bright, highly extended sources, will be excluded from the first release.

2. CATALOG PLANNING

2.1 Chandra data characteristics

The Chandra X-ray Observatory incorporates two instruments that record images of the X-ray sky. The Advanced CCD Imaging Spectrometer (ACIS) incorporates ten 1024×1024 pixel CCD detectors (any six of which can be active at one time) with an effective pixel size of approximately 0.5 arcseconds on the sky, an energy resolution of order 110 eV at the Al-K edge (1.49 keV), and a typical time resolution of 3.2 s. The High Resolution Camera (HRC) consists of a pair of large format micro-channel plate detectors with a pixel size around 0.13 arcseconds on the sky and a time resolution of ~15.6 μs, but with minimal energy resolution.

Both cameras operate in a photon counting mode, and register individual X-ray photon events. For each photon event, the two dimensional position of the event on the detector is recorded, together with the time of arrival and a measure of the energy of the event. In most operating modes, lists of detected events are recorded over an extended period, typically between 2 ks and 160 ks, and are then telemetered to the ground for subsequent processing.

To minimize the effect of bad detector pixels, and to avoid possible burn-in damage by bright X-ray sources, the pointing direction of the telescope is normally constantly dithered in a Lissajous pattern, with a typical scale length of about 20 arcseconds on the sky and a period of order 1 ks, while taking data. The motion of the telescope is recorded via an Aspect Camera that tracks the motion of a set of (usually 5) guide stars as a function of time during the observation. The coordinate transformation needed to remove the motion from the event (photon) positions is computed from the Aspect Camera data and applied during data processing.

Breaking down the 4-dimensional X-ray data hypercube into spatial, spectral, and temporal axes provides a natural focus on the properties that may be of interest to the general user, but also identifies some of the complexities inherent in Chandra data that must be addressed by catalog construction and data analysis algorithms.

Spatially, the Chandra PSF varies significantly with off-axis and azimuthal angle (with the former variation dominating), as well as with incident photon energy. Close to the optical axis of the telescope, the PSF is approximately symmetric with a 50% encircled energy fraction radius of order 0.3 arcseconds over a wide range of energies, but at 15 arcminutes off-axis angle the PSF is strongly energy-dependent, asymmetric, and significantly extended, with a 50% encircled energy fraction radius of order 13 arcseconds at 1.5 keV (see the example in Figure 1).

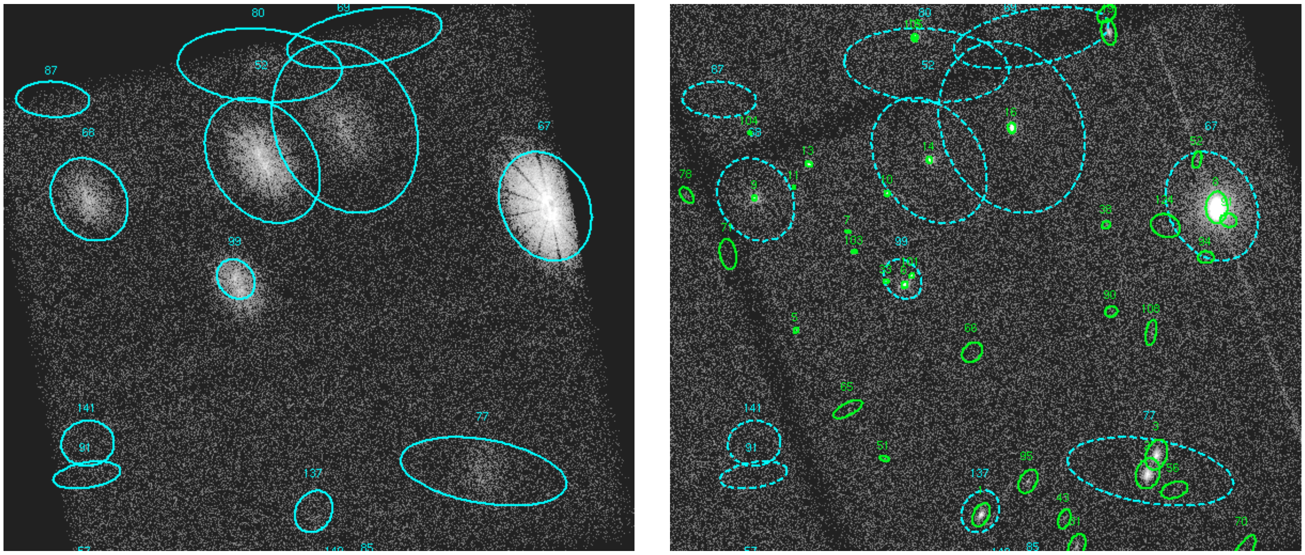

Fig. 1. The variation of the Chandra PSF with off-axis angle is demonstrated clearly in this example. The left panel shows a region of the sky observed well off-axis. The PSF is clearly extended, and the PSF substructure is clearly visible. The detected source regions are indicated with solid ellipses. The right panel shows the same region of the sky observed nearly on-axis. Again, the detected source regions are indicated with solid ellipses. On the same panel, dashed lines indicate the detected source regions from the off-axis pointing. In several cases, a single detected source in the off-axis pointing resolves into multiple distinct sources in the on-axis pointing.

For the widely used ACIS detector, the instrumental spectral energy resolution is of order 100–200 eV, and depends on incident photon energy and location on the detector. Because the energy resolution is significantly lower than the typical energy width of the features and absorption edges that define the effective area of the telescope optics (and therefore the quantum efficiency of the telescope plus detector system), a full matrix formulation that considers the redistribution of X-ray flux into multiple observed spectral bins must be used when performing spectral analyses. This is in contrast to the more familiar scenario from many other wavebands, where the instrumental resolution is much higher than the spectral variation of quantum efficiency, enabling the commonly used implicit assumption that the flux redistribution matrix is diagonal (and is therefore not considered explicitly).

Time domain analyses must consider the impact of spacecraft dither within an observation. Strong false variability signatures at the dither frequency can arise because of variations of the quantum efficiency over the detector, or because the source or background region dithers across a gap between adjacent ACIS CCDs. Corrections for these effects, as well as for cosmic X-ray background flares that can be highly variable over periods of a few ks, must be applied when computing light-curves. The extremely low photon event rates common for many faint X-ray sources typically require time domain statistics to be evaluated using event arrival-time formulations instead of rate-based approaches.

An additional level of complexity occurs because of the many astronomical sources of interest that will be included in the catalog are extremely faint. The flux significance limit for the CSC corresponds to a minimum count limit ~10 detected source photons (on-axis) in the broad band integrated over the total exposure time. Rigorous application of Poisson counting statistics is required when deriving source properties and associated errors, separating X-ray analyses from many other wavebands where Gaussian statistics are typically assumed.

2.2 Design goals

While most astronomers would consider themselves to be at least somewhat familiar with optical telescope data, fewer are familiar with X-ray data. Because of this, many X-ray missions choose in part to meet their obligation to provide reduced data in a form that can be more readily understood by general users by means of a detected source catalog. The CSC, which is intended to be a general purpose virtual science facility, provides this interface to a carefully selected set of generally useful quantities, while at the same time providing more advanced data products suitable for use by astronomers familiar with Chandra data.

The primary design goals for the CSC are to (1) allow simple and quick access to the best estimates of the X-ray source properties and Chandra data for individual sources with good scientific fidelity, and directly support medium sophistication scientific analysis on the individual source data; (2) facilitate easy searches and analysis of a wide range of statistical properties for classes of X-ray sources; (3) provide a user interface that supports searching and manipulating the actual observational data for each X-ray source in addition to the tabular properties that are recorded in the catalog; and (4) include all real X-ray sources detected down to a predefined threshold level in all of the public Chandra datasets used to populate the catalog, while maintaining the number of spurious sources at an acceptable level.

Several secondary design goals follow on from either the primary design goals or from CXCDS infrastructure development requirements. These are (1) the catalog must be source based, and should use all of the available data from multiple observations when extracting the best estimates of the X-ray properties for a source; (2) the actual data from each observation that includes a source should be accessible through the catalog; (3) the catalog must allow for continual updating as new observations become public, as improved calibration data become available, and as new calibration algorithms are developed; and (4) wherever possible the processing software used to build and manipulate the CSC must make use of the existing automated processing infrastructure built in to the Chandra X-ray Center (CXC) Data System[4] (CXCDS), and must use existing analysis tools that are part of the CXCDS and the Chandra Interactive Analysis of Observations[5] (CIAO) portable data analysis package.

Numerous X-ray specific and multi-wavelength science use cases were considered to assess the appropriate catalog content needed to meet the primary design goals of the CSC. While X-ray data mining (including X-ray source classification, source cross-matching with other catalogs, and detailed multiple source studies) is a natural focus for the catalog, sample selection, science project feasibility studies, and proposal preparation support are also priorities. Because the CSC is constructed solely from existing pointed observations, the resulting small sky coverage (of order 1% of the sky), and inhomogeneous statistical properties mean that the catalog is not optimized for science projects that require complete or uniform depth samples.

To evaluate the data content needs of individual science use cases, we first separated them into two broadly distinct categories. The first category includes science use cases that require only tabulated catalog data to support the scientific investigation, possibly combined with access to observation-based (full-field) data products recorded in the Chandra Data Archive[6] (CDA). A significant fraction of the use cases that we identified fall into this category, and can be completed provided that the relevant data content is tabulated.

The second category of science use cases includes those that would only be possible, or would greatly benefit, from direct interactive access to new file-based data products for each detected X-ray source individually. As an example, consider a use case that searches the tabulated catalog data for candidate sources that meet certain selection criteria and that are flagged as being time-variable within the observation, and then retrieves the light-curves for each matching candidate source and manipulates them to search for a specific signature such as rapid flaring. If the search identifies several thousand candidates, then the user may have to retrieve and manipulate full-field data for a significant fraction of the observations stored in the CDA if individual source data-products are not available. These use cases often require further manipulation of individual-source data products in a scripting language environment, and highlight the need for an interface to the catalog that is accessible from such environments. As we transition into the Virtual Observatory (VO) era, we expect that the number of these types of use cases will continue to increase as VO workflows become a mainstream approach to astronomical research.

As part of the design and development cycle for the CSC, an external science and technical review committee was convened to assess the catalog plans after a significant fraction of the preliminary design was completed, but before extensive new algorithm and software development was initiated. This review provided valuable feedback on the catalog goals, priorities, and approach, which were subsequently considered and incorporated into the design and development process.

The most important recommendations of the review committee were in the area of the prioritization of the capabilities to be included in the phased releases of the catalog. The committee reiterated the general feeling shared by the catalog development team that the most important customer was an astronomer wishing to do multi-wavelength work including Chandra data, someone who is not an X-ray expert, but who is reasonably skilled and knowledgeable. The focus of the first release of the CSC is aimed at maximizing the usefulness of the catalog for this type of user, while still completing the catalog on schedule with available resources. However, the CSC also attempts to balance the needs of the general science users with the expectations of the expert Chandra user community, as well as providing some capabilities to support education and public outreach functions.

In some cases methods commonly used within the X-ray astronomy community may not be well known in the broader astronomical community (for example, Bayesian variability analysis such as the Gregory-Loredo method[7]). Since the CSC is intended to be a general user catalog, in these cases the review committee felt that it is important to also include a common analysis that is more easily interpreted by the general community (*e.g.*, a Kolmogorov-Smirnov probability statistic). The complexity that must be addressed in these cases is to ensure that the common analyses are applicable given the known characteristics of Chandra data. Many common statistics assume Gaussian errors and break down in the Poisson regime, for example.

Significant scientific and technical expertise with Chandra data has been developed in-house at the CXC in the ~9 years since launch. Our understanding of the instruments and calibrations has improved to the point that automating bulk processing of Chandra data further along the analysis chain to the level needed to develop the CSC is now feasible. This in-house expertise has proven invaluable in establishing the scientific capabilities and limitations that such automated processing entails, using both existing algorithms or developing new algorithms, and given the resources available to develop the catalog.

3. CATALOG DESIGN

3.1 Data content

The CSC will include detected sources whose flux estimates are at least 3 times their estimated 1σ uncertainties, typically corresponding to about 10 net (source) counts on-axis and roughly 20–30 net source counts off-axis. In the first release, multiple observations of the same field will be linked together with a single source name (see the section on data organization below), but will not be combined prior to source detection. Therefore the flux cutoff applies to each observation separately.

For each source detected in an observation, the catalog will include approximately 160 tabulated properties, mostly falling into the following broad categories:

- Source position and errors,
- Aperture photometry fluxes and confidence intervals measured or inferred in several ways, and in multiple energy bands (ultra-soft, soft, medium, hard, and broad bands for ACIS, and wide band for HRC),
- Spectral hardness ratios,
- Power-law and thermal black-body spectral fits for bright (> 150 net counts) sources,
- Source variability measures (Gregory-Loredo, Kolmogorov-Smirnov, and Kuiper tests),
- Estimate of the raw (measured) extent of the source and the local point spread function, and the deconvolved source extent.

In addition, roughly 90 *master* properties will be tabulated for each distinct X-ray source on the sky, by combining measurements from multiple observations that include the source.

A number of file-based data products will be produced for each source and observation individually, in formats suitable for further analysis in CIAO. These include:

- Source region, background region, and PSF images,
- Source region photon event list,
- Source and background light-curves,
- Limiting sensitivity map in multiple energy bands,
- Auxiliary Response File (ARF),
- Pulse invariant (PI) spectrum and Redistribution Matrix File (RMF) [for ACIS observations].

An estimate of the eventual size of the CSC can be obtained by projecting forwards from the sky coverage observed to-date. Observations obtained during the first 6 years of the Chandra mission covered about 160 square degrees on the sky (including ~80 square degrees down to a flux level of 1.0×10^{-14} ergs cm^{-2} s^{-1}), with an estimated 150,000 detectable sources containing at least 10 counts. These numbers will continue to grow as the mission continues, with a 15 year prediction of ~400,000 sources distributed over ~400 square degrees, or ~1% of the sky.

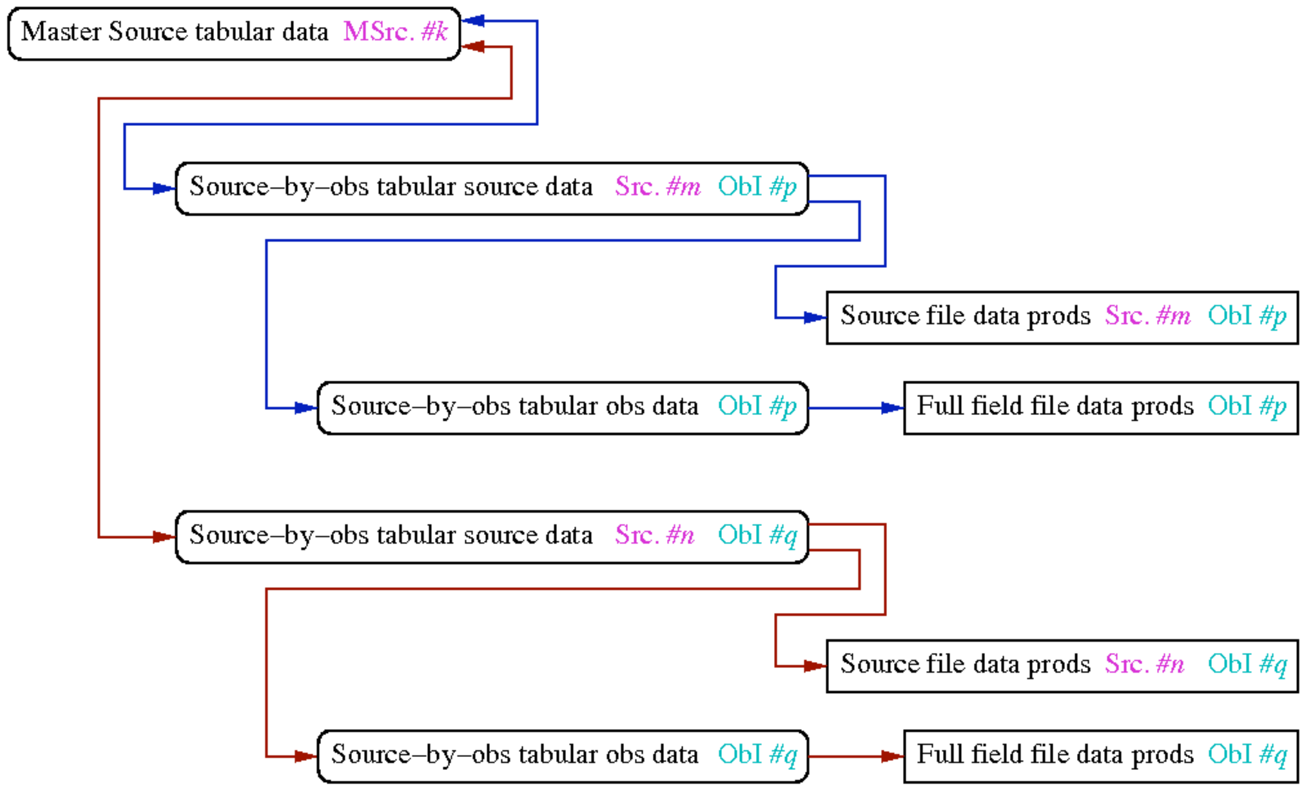

Fig. 2. Conceptually, database records containing tabulated master source properties (one for each identified distinct X-ray source on the sky) are linked bi-directionally to one or more records containing tabulated source-by-observation properties (one for each observation in which the source was detected), which are in-turn linked to both records containing tabulated (source independent) observation information. The source-by-observation database records include pointers to the associated file-based data products.

3.2 Data organization

Each identified distinct X-ray source on the sky is conceptually represented in the catalog by a single *master* catalog entry and one or more *source-by-observation* entries (one for each observation in which the source was detected). The master catalog entry records the "best" estimates of the tabulated properties for a source, derived by combining the data extracted from the set of observations in which the source was detected according to a predefined set of rules. The source-by-observation entries record all of the tabulated properties about a source detection extracted from a *single* observation, and include pointers to the associated file-based data products, which are all observation-specific in the first catalog release (Fig. 2). Conceptually, each source-by-observation object is further split internally into a set of source-specific data and a set of observation-specific, but source-independent, data. The latter are recorded once to avoid duplication of data.

All of the tabulated properties included in both the master catalog and the source-by-observation catalog entries are available for searching via the user interface. Bi-directional links between the master catalog entries and associated source-by-observation entries are managed transparently by the database, so that users can access all observation data for a single source seamlessly.

During catalog processing, source detections in each observation are matched with source detections in observations that overlap the same region of the sky. Subject to certain data quality requirements[8], the source properties extracted from detections that can be matched uniquely are combined to construct the master catalog entry for that source.

As described previously, detections far off-axis in one observation may overlap multiple resolved source detections on-axis in another observation because the Chandra PSF is a strong function of off-axis angle. Such detections are flagged as confused. The source-by-observation entries are linked to the master catalog entries for each overlapped source (and so are accessible to the user), but the data are not used to compute the master source properties. The user will nevertheless be able to identify all of the X-ray sources in the catalog that could be associated with a specific detection in a single observation, and vice-versa. These linkages may be important, for example, when identifying candidate targets for follow-up studies based on a data signature that is only visible in the observation data for a confused source.

3.3 Data access

User access to the CSC will be through a web-based browser interface in the first instance. Through this interface, catalog users will be able to directly query on any of the tabulated master or source-by-observation properties, display the contents of an arbitrary set of properties for matching sources, and retrieve any of the associated file-based data products for further analysis. The user interface will eventually support queries conforming to the VO Astronomical Data Query Language[9] (ADQL) standard, and return query results in accordance in VO standard formats such as VOTable[10]. The ability to perform data queries and retrieval from data analysis scripts executing on the user's home platform, and eventually from VO workflows, is a high priority to support advanced catalog science use cases, as outlined above, and this capability will be added in a subsequent release of the user interface. Further enhancements, such as integrating the catalog user interface with a visual sky browser, are being considered and may be particularly beneficial for education and public outreach, as well as for some science use cases.

Catalog release views provide access to released versions of the catalog. Catalog releases will be infrequent (no more than of order 1 per year) because of the controls built in to the release process, and because of the requirement that each release be accompanied by a detailed statistical characterization of the included source properties. Once data are included in a specific catalog release view, then they are frozen in that view, even if they are superseded or deleted in subsequent catalog release or database views.

Database views provide direct access to the catalog database, including any new content that may not be present in an existing catalog release. Because on-going processing is continually modifying the catalog database, tabulated data and file-based data products in a database view may be superseded at any time, and the statistical properties of the data are not guaranteed. However, since the history of all catalog database updates is recorded, each user can select a database view that reflects the catalog database contents at an arbitrary user-chosen date and time, with the default being the current date and time.

We anticipate that users who require a stable, well-characterized dataset will choose primarily to access the catalog through the latest catalog release view. On the other hand, users who are interested in searching the latest data to identify sources with specific signatures for further study will use the latest database view.

4. CATALOG CONSTRUCTION

4.1 Pipeline processing

Each pointed Chandra observation may include data for a few to upwards of several hundred detectable X-ray sources. Although it is natural to record the tabular catalog information about each source individually, the design goals effectively mandate that the actual observational data (and not just the extracted source properties) for each source individually be extracted from each pointing that includes that source, and be accessible through the catalog.

The bulk of the CSC construction is performed by a set of CXCDS Standard Data Processing (SDP) pipelines[11] that we term the Level 3 pipelines (lower level pipelines includes spacecraft telemetry decommutation, per-pointing science processing, and per-observation science processing). Catalog construction is a multi-part process that is performed by four distinct processing pipelines (Fig. 3), each of which has an appended quality assurance step. First, the observational data for each pointing are recalibrated to ensure that the latest set of processing algorithms and calibration data are used for catalog construction. Next, the full-field data are used to determine the total (cosmic plus instrumental) background during the observation, and a wavelet-based source detection algorithm identifies candidate X-ray sources. Quality assurance criteria reject many false sources at this stage. The two previous steps are performed on the full field of a pointing at one time. Subsequently, each detected source is processed separately to extract per-source data and source properties. Processing source pipelines in parallel allows significant multiplex gains in overall operational performance. Further quality assurance criteria are applied at this point to further reject false sources, and a filter is applied that imposes the catalog flux significance (signal-to-noise) cut-off criterion. After all of the source pipelines complete for a pointing, the master pipeline[12] runs. The master pipeline cross-matches each detected source with all existing sources in the catalog database, and either inserts the derived source properties into the database in the case of a newly identified source, or merges the newly measured source properties with the existing catalog data in the case of an already cataloged source.

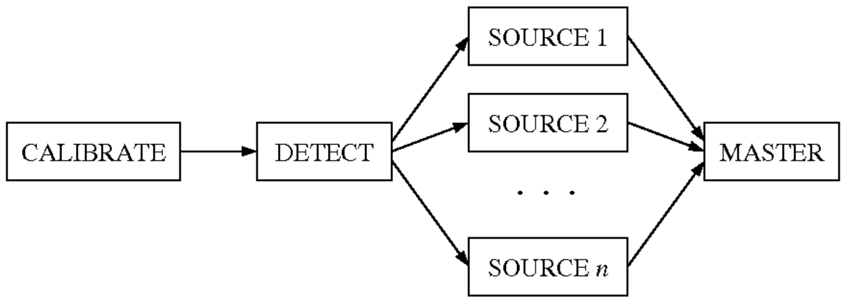

Fig. 3. Catalog processing for a pointing is initiated when the "calibrate" pipeline kicks off to recalibrate the observation data. The "detect" pipeline then identifies sources, which are processed separately by a set of "source" pipelines (one per detected source) to measure source properties. Finally, after all of the source pipelines complete, the "master pipeline" combines the measured source properties with any existing catalog data for the source.

4.2 Processing infrastructure

Unlike other SDP pipelines, which execute solely on a Sun/Solaris platform, for performance reasons much of the compute-intensive Level 3 pipeline processing is performed on a 64-processor Beowulf cluster running a version of the Linux operating system. Level 3 pipeline processing is supervised by the CXCDS Automated Processing (AP) infrastructure[13], which runs on a Sun/Solaris machine that is dedicated to managing Level 3 processing. The Beowulf cluster is configured to allow all of the nodes to access network attached storage (NAS) that is shared with the Solaris-based SDP machines. However, data are copied from the NAS to the local disks on each Beowulf node prior to running a pipeline to minimize the load on the NAS.

Level 3 pipeline processing is triggered manually, by submitting a list ("batch") of observations to be processed to AP. Batches process most efficiently if all nearby and overlapping observations are included in a single batch, although this is not a requirement. Batch construction is performed by the CXCDS Operations group that manages SDP. All observations must satisfy a set of predefined criteria to be candidates for inclusion in a batch, and the Operations group pre-screens the observations to ensure that the criteria are satisfied. The criteria will vary with catalog release. For example, for catalog release 1 observations of bright, extended sources, and observations with highly variable cosmic backgrounds, are excluded. The Operations group maintains a historical record of any anomalies associated with an observation, and has the expertise to evaluate whether an observation should be excluded from the catalog on that basis.

For initial catalog construction, more than 5,000 public observations obtained since launch satisfy the release 1 pre-filters, allowing for efficient batch construction. After the "catch-up" phase, observations will be processed as they are released publicly. The CDA provides a trigger that identifies when observations may be included in Level 3 processing input batches.

4.3 Data storage

Both the tabulated source properties and the individual pointed observation source data (source images, event lists, etc.) that comprise the CSC will physically be stored in the CDA. The former will be recorded in SQL databases, while the latter will be stored as FITS files. Storing the file-based data in FITS format instead of an alternative approach, for example including data blobs in the databases, leverages existing archive software and provides a file-based interface that is compatible with existing CIAO tools[14]. One downside of this approach is that there is more data storage overhead when storing some of the data as FITS files since the volume of the FITS file headers is comparable to the actual data volume. Updates to the catalog database will occur continually as new observations become public. To ensure traceability, a history of updates will be maintained so that the state of the database at any point in time is recoverable.

The catalog release process can only take place when all on-going catalog processing is completed, and any outstanding quality assurance issues are resolved. Consistency checks are applied to the catalog database to ensure that all of the catalog inclusion criteria for the release (*e.g.*, flux significance cutoff) are properly applied. Finally, a "snapshot" of the catalog database is obtained by flagging all of the database entries that should be included in the catalog release. The flagged database entries are identified with the specific catalog release, and internally the database history mechanism ensures that the release contents will remain frozen from that point forward.

5. CONCLUSIONS AND FUTURE PLANS

When completed, the Chandra Source Catalog will be a valuable asset for X-ray astronomy. Users will be able to simply and quickly access the X-ray source properties for a wide range of sources, and will be able to easily search for sources that satisfy their chosen criteria.

The first release of the CSC is scheduled for the winter of 2008, and will include data for roughly 200,000 point and compact X-ray sources detected in public imaging observations obtained by the Chandra X-ray Observatory during the first eight years of the mission. Future releases of the catalog will combine multiple overlapping observations prior to source detection to enable fainter sources to be detected. In the first instance this will be limited to combining multiple pointings obtained with the same instrument, and with nearly identical positions and roll angles to minimize the effects of the spatially variable Chandra PSF, but subsequently these constraints will be relaxed. Eventually, observations including bright, extended sources will be included in the catalog as algorithms for detecting and characterizing the properties of such sources in an automated manner are developed further.

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