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Securing The Infrastructure of High-Energy Cross-Calibration

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1 Executive Summary

Scientific results are, now more than ever, obtained as a synergy between observatories, and the physical interpretation relies heavily on good instrumental cross-calibration knowledge, which is bounded by the resources devoted to calibration. A few of the scientific problems that have been limited by instrumental calibration include the neutron star equation of state from X-ray bursts and isolated neutron stars (involving e.g., NICER, Chandra, and RXTE), cosmological contribution of dark matter derived from total masses of galaxy clusters (involving XMM-Newton and Chandra), the contribution of active galaxies to the cosmic X-ray background (involving XMM-Newton, Chandra, and NuSTAR), and atomic processes in astrophysical plasmas in galaxy clusters, stars, and the interstellar medium (involving Hitomi, Chandra, and XMM-Newton). Please refer to the Smith et al. WP on laboratory astrophysics for an extensive discussion of the atomic data problem.

For the last decade, the International Astronomical Consortium for High-Energy Calibration (IACHEC) has performed a crucial role in organizing the high-energy community into a common forum for discussion and solution of calibration and cross-calibration issues. Since 2006, the IACHEC has been hosting annual workshops attended by calibration scientists from past, current, and near-term high-energy observatories. Organized into working groups, IACHEC members cooperate to provide standards and procedures for calibration that are useful for every high energy mission.

The main goal of the IACHEC is to optimize the scientific value of current missions by improving the cross-calibration among existing instruments, creating new standards for analysis, promoting appropriate statistical methods for the interpretation of results, and optimizing calibration plans of future missions. Because of the IACHEC’s past efforts, up-coming and future X-ray mission will benefit from a large knowledge database, which is curated and organized for the benefit of the community. Examples of missions that followed these recommendations were NuSTAR, Hitomi, Astrosat, Insight-HXMT, and most recently, NICER.

The IACHEC is operated without direct funding; it relies on unofficial support of contributing missions and the donation of time by some participating scientists. However, with the increasing ages of missions, there is a constant pressure to decrease the calibration budget (in both time and manpower), due to the perception that mature missions should be well-calibrated, as typically the calibration is more well tested for an aged observatory. However, for some missions the calibration challenges increase with time as the instrument response evolves while the demand for accurate calibration products from the astronomical community persists or even increases. The IACHEC is utilizing its resources on a best effort basis, but with an increasing portfolio of operating missions, resolving cross-calibration issues between observatories is not progressing at the rate desired by the scientific community, based on user group imperatives.

The problem of calibration is therefore presently not just one of data shortage but also of manpower; it is an issue that needs to be addressed more holistically in the next decade. We advocate that calibration should no longer be viewed as just an instrument specific activity, performed within the respective instrument teams only, but as a continual process transitioning from one mission to the next, using knowledge gained from many observatories and the cross-calibration between them. Such a holistic approach has the obvious advantage that the lessons learned from one group are passed on to the next team developing an instrument, but it also has generated new insights and solutions to common problems that the entire community faces.
2 Key Issue and Overview of Impact on the Field

The topic of cross-calibration affects every field of astronomy and astrophysics. In the era of multi-messenger and transient astronomy, it is no longer the exception but the norm that multiple instruments will observe the same event. As such, the results are obtained across a spectrum of energies and instruments, each with their own calibration - in some cases with known offsets, in others not - and the accuracy of the interpretation of the data is dependent on the cross-calibration knowledge. Planned and operating missions have budgets assigned for their instrument calibration, and as long as they meet their requirements as specified in their proposal, there is no mandate to verify their calibration across or against other observatories. The challenges involved in such a task require coordination with other observatories, which can be difficult to achieve given high over-subscription rates and other constraints. Simultaneous calibration data may be obtained and differences identified, but without the interaction of the separate calibration teams, the issues may just be acknowledged but not understood, resulting in confusion in the community about which data to trust.

This problem was realized by the Chandra and XMM-Newton calibration teams some years after the two observatories launched, and enabling direct communication between the Chandra and XMM-Newton calibration teams was the primary motivation for the first IACHEC meeting, held in 2006. Even though the main intent for the first meeting was for increased cooperation between the two specific teams, the calibration representatives from INTEGRAL, RXTE, Swift, and Suzaku also attended as the value of more cooperation on calibration issues was apparent. The IACHEC formed out of this meeting as a collaboration between all calibration teams and has since held a yearly meeting to address these issues. The goal of these meetings has been to publish the results of its investigations and since 2006 more than a dozen papers have been published.

The high-energy community has benefitted immensely from this collaboration, but with increasing demands for improved cross-calibration, the IACHEC is, in its unfunded state, challenged to deliver. In this white paper, We will describe the issues that pertain to the cross-calibration of the high-energy missions (Chandra, INTEGRAL, NICER, NuSTAR, Swift, and XMM-Newton) and their impact on science, and present ways to improve the status, with a long-term goal that it may benefit all future missions. First we will highlight the successes of the IACHEC and then discuss where cross-calibration issues are still not good enough and cause problems for the astrophysical interpretation.

2.1 The Good: The IACHEC Legacy

Differences in the sensitivities of operating instruments require a number of calibration sources with a variety of spectral shapes and flux levels. Unvarying, soft, thermal X-ray spectra, as found in supernova remnants, galaxy clusters, and white dwarfs, are well suited for CCD and grating instruments but not for instruments with their main bandpasses above 5 keV. Hard, bright, non-thermal spectra, such as quasars and blazars, are preferred for calibration above 5 keV, while higher fluxes are required for calibration above 25 keV. The IACHEC is organized into working groups focused on the different types of calibration targets and defining calibration standards. Below we

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1http://iachec.script.scripts.mit.edu/papers.php
2http://iachec.script.scripts.mit.edu/wgs.php
summarize a few examples of this work by the IACHEC to illustrate the importance of this activity.

2.1.1 The ‘steady’ 1E 0102.2-7219
The IACHEC has developed a standard spectral model for the X-ray brightest supernova remnant (SNR) in the Small Magellanic Cloud (SMC) known as 1E 0102.2-7219 (hereafter E0102). This model was created using the high resolution spectral data provided by the “Reflection Gratings Spectrometer” on XMM-Newton and the “High-Energy Transmission Grating” on Chandra in order to improve the response models of the lower resolution CCD instruments on Chandra, XMM-Newton, Suzaku, and Swift. This model was used to provide a simple and direct comparison of the absolute effective area calibrations of the respective instruments in the low energy band of 0.5 to 1.1 keV which is particularly challenging to calibrate given that the detector response is changing rapidly with energy due to absorption edges in the filters and detectors. The model was also used to characterize the accuracy of the time-dependent corrections for the accumulation of a contamination layer on the Chandra/ACIS, XMM-Newton/MOS, and Suzaku/XIS detectors. The model is publicly available on an IACHEC web page and is described in [Plucinsky et al.] (2017). This model has been used by the Astrosat and NICER calibration teams to improve their respective response models and to improve their calibrations. The XRISM and eROSITA calibration teams expect to observe E0102 frequently early in their missions and will use the standard IACHEC model for their analysis.

2.1.2 Clusters of Galaxies
Clusters of galaxies are prime cross-calibration targets for the IACHEC due to their stability, soft X-ray luminosity, continuum-dominated spectra, and large sample of deep science observations across many missions. An early IACHEC project described by Nevalainen, David & Guainazzi (2010) used a small sample of clusters to explore the cross-calibration between the X-ray spectral imagers on XMM-Newton and Chandra, and found that the hard-band (2–7 keV) temperatures differed between the two missions. This work helped to stimulate a reanalysis of Chandra ground data that, with Chandra HETGS data, led to an estimate of hydrocarbon contamination on the mirrors. A revised calibration brought the cluster temperatures into agreement. A recent expansion of this work to include the 64 X-ray-brightest clusters (the HIFLUGCS sample, Reiprich & Böhringer, 2002) has confirmed that the temperatures derived from 2–7 keV spectral fits are now consistent between the imaging instruments on XMM-Newton and Chandra (Schellenberger et al., 2015). However, there are systematic differences among the three XMM-Newton EPIC instruments (pn, MOS1, and MOS2), and between those instruments and Chandra ACIS, in temperatures fit to the soft band (0.7–2 keV) and broad band (0.7–7 keV), as shown in Figure 1. These results were used by Schellenberger et al. (2015) to provide estimates of systematic uncertainties in cosmological parameters derived from galaxy cluster hydrostatic masses, showing that these uncertainties were insufficient to resolve the tension between cosmological constraints derived from Planck CMB measurements and combined SZ–XMM-Newton results. This work continues as an effort to assemble the full sample of galaxy clusters observed by all past and current IACHEC-participating missions and perform a large, multi-mission cross-calibration study.
2.1.3 Coordinated Observations of Blazars

The IACHEC has been responsible for coordinating regular campaigns to observe sources that can be variable on time scales of days. Following on from early campaigns on 3C 273 involving XMM-Newton and Chandra, the yearly campaign now includes nearly every high-energy observatory internationally. Because of the flat, hard, and featureless spectrum, blazars are great calibration targets for continuum measurements across instruments and have become the main resource for defining slope errors across observatories (Ishida et al., 2011; Madsen et al., 2017). The yearly campaign is also used to track well known time-dependent instrumental effects such as contamination buildup. Indeed, at the 2019 IACHEC meeting, Michael Smith (ESAC) showed that the Chandra LETGS flux in the 0.33–0.54 keV band dropped relative to all other instruments after 2008 (see Figure 2). Based on this comparison, the Chandra project will likely re-examine the contamination correction model in this energy range. It is only with annual joint observations that the XMM-Newton and Chandra missions could be compared this way to find such time dependent effects.

2.1.4 Hard X-ray Calibration

Traditionally considered the closest proxy to an X-ray standard candle, the Crab Nebula has been a major calibration and cross-calibration target for many hard X-ray observatories (Kirsch et al., 2005; Weisskopf et al., 2010). The discovery of its long-term flux variability (Wilson-Hodge et al., 2011), led to the search for alternative sources. The most promising thereof has been the pulsar wind nebula G21.5-0.9. A pioneer work by Tsujimoto et al. (2011) unveiled 15-50 keV flux differences of up to 50% among the RXTE/PCA, the Suzaku/PIN, and the INTEGRAL/ISGRI. With the launch of NuSTAR it was discovered to have a spectral break at $\sim 10$ keV (Nynka et al., 2014), later confirmed with Hitomi. The Crab, too, exhibits a spectral break at $\sim 100$ keV (Jourdain & Roques, 2011).

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Figure 2: Comparison of fluxes in nine bandpasses for observations of various blazars before (left) and after (right) 2008 using XMM-Newton and Chandra (M. Smith, 2019 IACHEC). All fluxes are relative to that determined for the XMM-Newton pn detector. This annual campaign shows the value of monitoring cross-calibration with regular coordinated observations, as the model of the Chandra ACIS-S contaminant appears to be insufficient after 2008 for the 0.33–0.54 keV band.

2009), the width of which is uncertain and may potentially impact the calibration of instruments that have assumed an unbroken powerlaw up to 100 keV. A specific IACHEC Working Group is publishing the largest observational sample on these two targets ever compiled (Natalucci et al., Tsujimoto et al., in preparation), to achieve the most comprehensive view of the cross-calibration status above 10 keV after the pioneering paper by Kirsch et al. (2005) almost 15 years ago.

2.1.5 Advances in Analysis and Methods
The IACHEC has consistently encouraged rigorous analysis. This focus has been necessary particularly because it is critical to eliminate biases in calibration estimates and obtain a proper understanding of the uncertainties in the analysis, as they have knock-on effects that affect astrophysical inference. Indeed, IACHEC has facilitated the development and application of methods to incorporate effective area uncertainties in spectral analysis (see Drake et al. 2006; Kashyap et al. 2008; Lee et al. 2011; Xu et al. 2014). This has demonstrated, for example, that uncertainties on spectral indices smaller than $\pm 0.04$ are not achievable given the current knowledge of systematics in the Chandra effective areas. More recently, an IACHEC-led effort has focused on the problem of reconciling a number of disparate measurements of objects observed with different instruments. Each measurement is characterized by a statistical uncertainty, as well as an estimated systematic uncertainty associated with the instrument. These are then combined to generate a shrinkage estimator that best reflects all the available information and can objectively estimate the correction required for each instrument (see Chen et al. 2018). In addition, the IACHEC has strongly encouraged the use of newer and improved methods of X-ray data analysis, including: the use of the cstat statistic (related to the Poisson log-likelihood) over that of $\chi^2$ in the low-counts situations encountered in high-energy datasets; the use of the cstat goodness-of-fit technique pioneered by
2.2 The Bad and the Ugly

Despite the success of the IACHEC in determining and correcting cross-calibration errors, problems still persist as the demand for ever more precise calibration becomes more urgent alongside the new generation of astrophysical models that probe the detailed components of the source physics.

2.2.1 Broad band spectral modeling of X-ray Binaries

One such example is the broad band modeling of the accretion physics of compact objects. These transient events typically result in multi-epoch and multi-mission coverage. The outburst from black hole X-ray binaries allows one to study the complexities of accretion physics, as the BHXRB cycles between quiescence and its Eddington luminosity. It exhibits a wide range of behaviors that include AU-scale steady jets, parsec-scale ballistic jets, X-ray quasi-periodic oscillations (QPOs), and distinct “hard” and “soft” spectral/timing states (Fender, Belloni & Gallo, 2004; Remillard & McClintock, 2006); all of which may be tied to the spin of the black hole. Presently, there is no single instrument that spans the entire thermal and reflection spectrum, and it is necessary to combine multiple instruments as shown in Figure 3 (left). However, slope differences in the overlap regions greatly affect and limit the interpretation of results. The mismatch between instruments made Kühnel et al. (2017) decide to reject the lower energies from NuSTAR, although on its own NuSTAR would have given a perfectly reasonable, but different result. This occurrence is not unique to this source (Bellm et al., 2014) and is observed in other similar type sources as well, though not in others, which may indicate the possibility of a partly astrophysical origin, such as a dust scattering halo. But an instrumental reason, though as yet uncovered, may be part of

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the problem as well. The fact that is is not systematic across sources, indicates the problem has secondary dependencies, such as instrument mode, source spectrum, and source count-rate.

Another example, is the measurement of BH spin, where the critical assumption must be made that the inner edge of the accretion disk is located at the innermost stable circular orbit (ISCO). It has been firmly validated for accretion disk dominated soft states (e.g. Steiner et al., 2010; Zhu et al., 2012), but for Comptonization dominated hard states, it is a matter of dispute, and the measurements of the inner-disk radius \( R_{\text{in}} \) with reflection models and timing techniques appear to be in disagreement by orders of magnitude for the same source (e.g., GX 339-4; García et al., 2015; De Marco & Ponti, 2016). Figure 3 (right) shows a compilation of some such measurements, and the discrepancies have been attributed to a combination of cross-calibration differences, data analysis, and model dependencies. Disentangling these effects foremost requires a precise understanding of the cross-calibration. The question of disk truncation has important ramifications for measurements of black hole spin, given the strong degeneracy between inner radius and spin that arises due to their relations to the strength of gravitational redshift (e.g. Fabian et al., 2014), which limits the confidence with which either parameter can be obtained.

2.2.2 Neutron Star Equation of State

X-ray measurements of isolated neutron stars (INSs) and some neutron stars in X-ray binaries are being used to test models of the equation of state (EOS) of nuclear matter and depend sensitively upon instrument calibration. Young INSs, such as the central compact object (CCO) in Cas A, may be dimming as their cores cool, providing a diagnostic of the structure of nuclear matter in the core. Elshamouty et al. (2013) used a variety of X-ray instruments to assess the cooling of the Cas A CCO to be in the range of 1–3.5% over 10 years, which they say “would indicate extraordinarily fast cooling of the NS that can be regulated by superfluidity of nucleons in the stellar core.” (See also Posselt & Pavlov, 2018). While spatial variations of the SNR wisps make background estimation difficult, systematic differences between X-ray instruments due to calibration monitoring also limits the ability to constrain this CCO’s cooling rate at the 1% level (Posselt et al., 2013).

Measurements of X-ray bursts can also be used to constrain the masses and radii of NSs and, consequently, the nuclear EOS. Several groups have carried out detailed fitting of burst spectra (e.g., Özel et al., 2016; in’t Zand et al., 2017; Nättilä et al., 2017); calibration plays a part in the models as the bursts reach the Eddington limit. One such analysis required cross-calibration between RXTE and the Chandra HETGS or XMM-Newton instruments to estimate that systematic uncertainties in burst fluxes can be of order 15% (Güver et al., 2016). With significant improvements in astrometry via VLBI or optical techniques, absolute calibration will become increasingly important.

3 Strategic Plan

The goal of the cross-calibration effort is to consolidate the understanding of all high-energy observatories, and to provide the science community with the understanding and tools that they need to use any instrument together with any other instrument without having to struggle with cross-calibration differences. The knowledge and the organization exists, but the infrastructure is lacking to ensure the survival of this capability for the future when the founding missions of the IACHEC
To address these challenges, we propose a combination of programs, either nonexistent or unavailable, to assist in the specific activity of cross-calibrations.

### 3.1 Funding channels through APRA or ADAP

In the current formulation of the ROSES Astrophysics Research and Analysis (APRA) and Astrophysics Data Analysis (ADAP) programs, cross-calibration of past and operating instruments fits cleanly in neither. The characterization of working or decommissioned instruments is not considered instrument development, and therefore it cannot be funded by APRA. As a database project, cross-calibration is consistent with the archival work envisioned by ADAP. However, the emphasis for ADAP is on science results; ROSES-2018 (D2.1) reads, "The magnitude and scope of the archival data from those missions enables science that transcends traditional wavelength regimes and allows researchers to answer questions that would be difficult, if not impossible, to address through an individual observing program.” This requires proposals to be primarily science orientated with only secondary goals towards calibration, and as a consequence, proposals focused on calibration tend to rank poorly in panel reviews.

The IACHEC has demonstrated that proper calibration is fundamental for maximizing an instrument’s science return, and proper cross-calibration falls within the realm of enabling difficult science questions to be answered (e.g., [Schellenberger et al. (2015)]). We therefore propose that the ADAP call include an explicit statement that the program can be used to investigate cross-calibration from archival data to generally improve the science return across a wide range of topics, without demanding the need for tying the activity to a specific science question.

### 3.2 Calibration and Knowledge Database

One of the main tasks that motivated the founding of the IACHEC was the creation of a knowledge database. For this purpose it founded the Heritage working group to: facilitating the usage of good practises for the management of pre- and post-flight calibration data and procedures; documenting the best practises in analysing high-energy astronomical data as a reference for the whole scientific community; and ensuring the usage of homogeneous data analysis procedures across the IACHEC calibration and cross-calibration activities. This is mostly a data management problem and has been started using IACHEC web-resources. With the help of AHEAD funding a database has been created for the storage of all the calibration data used in the IACHEC published calibration papers, but there is no location for data procedures yet. It is the vision that many of the cross-calibration procedures be made cloud-based and independent of any specific calibration team. This is inspired by recent emergence of cloud-native workflow management solutions based on portable containerised environment. The IACHEC calibration database could be complemented with a frontend exposing an interface to such an workflow orchestration infrastructure, enabling exploration, re-use, and live deployment of calibration and inter-calibration methods.

A major step in making this effort a success is proper population, maintenance, and access of the database, and without secure funding the logistics of this work risks being lost. Long term stability must be a requirement, and a logical location for such a database could be the high-energy

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5[https://wikis.mit.edu/confluence/display/iachec/IACHEC+Heritage+Working+Group](https://wikis.mit.edu/confluence/display/iachec/IACHEC+Heritage+Working+Group)

6[http://iachecdb.iaps.inaf.it](http://iachecdb.iaps.inaf.it)

7[renkulab.io](http://renkulab.io) ;[www.cosmos.esa.int/web/esac-cmso/sepp](http://www.cosmos.esa.int/web/esac-cmso/sepp); [www.knime.com](http://www.knime.com); [mybinder.org](http://mybinder.org)

8[www.docker.com](http://www.docker.com); [singularity.lbl.gov](http://singularity.lbl.gov); [https://github.com/NERSC/shifted](https://github.com/NERSC/shifted)
data archive HEASARC or similar data center. Another step would be the development of a guiding document that could be endorsed by NASA as a requirement for future missions.

3.3 Research Grants
The main limitation in addressing the pressing needs of the science community for improved cross-calibration is one of manpower. Issues are typically discovered by the community during data analysis, and these are reported on a case by case basis to the individual science teams, which may or may not, be aware of the problem. Many of the remaining cross-calibration issues that persist are not ubiquitous, but only appear in certain types of sources with any number of dependencies on observing mode, countrate, spectral type, orbital parameters, etc. They are also not always easily identified as instrumental, and the analysis of the calibration data is therefore very involved, more so than for general source analysis, since it is addressing the uncertainties in the data responses, which requires extreme care and understanding of the right statistical application. There are indeed projects, initiated at IACHEC meetings, that are many years into their analysis because of the effort. As with any research, part of the problem is prioritization and the difficulties with getting two calibration teams working on the same problem at the same time.

The effort of cross-calibration, and in extension all of high-energy astrophysics, would greatly benefit from a number of grants given to researchers, who are not directly associated with any mission. They could be awarded to researchers who have encountered a calibration issues in relation to their work, and without the resolution of which, the research can not be completed. The grant could cover travel to visit the mission calibration centers and salary for working there directly with the calibration team for a longer period of time to resolve and understand the issue. This would enable an analysis of the problem from an unbiased source, whose view might not be affected by instrument preference. Identifying the issues and quantifying them as related to one or another instrument is half the problem. How to solve the problem would still be up to the individual calibration teams since this may require updates to mission specific responses or pipeline software. A NASA center, with consultation from a panel advised by the IACHEC, could manage such grants.

3.4 Meetings
The backbone of the IACHEC has been the yearly workshop, which has been held now for 14 consecutive years. It is at the workshop, when the different instrument teams can interact and discuss discrepancies raised by their user base, that actions are spawned and cross-calibration research projects defined. The meeting typically obtains some funding, but largely it has been self-funded through registration fees. Because the activity of cross-calibration includes missions from all over the world, the workshop rotates between the US, Europe, and Asia, which limits the participation of some members, and in particular students. The size of the yearly workshop has also grown over the years, with 60 participants at the last workshop held in Shonan Village, Japan, in May 2019. At this modest size, the IACHEC has been able to arrange meetings at low-cost venues, but as we anticipate further growth in the number of active mission and more international participation, the size of the venue must also increase and thus the cost of the venue.

A pressing problem is the communication with the larger community, not all of which is aware of the IACHEC work, and how the community can communicate and report problems of cross-calibration nature to IACHEC. Also, the involvement of students had been low, primarily because of travel costs. A number of travel grants to students, key mission, and science representatives,
who may be unable to attend due to lack of internal funds, would allow the next generation of researchers to gain important insight into the instruments they use, and open the field to outside input.

4 Organization, Partnerships, and Current Status

The IACHEC currently coordinates most of the high-energy cross-calibration activities between the high-energy observatories internationally, and we propose that the IACHEC continues to organize this activity in its present form with yearly meetings. In this paper we advocate an expansion of the cross-calibration infrastructure to assist in improvements to high-energy astrophysical results across the board. International collaborations are important, and the IACHEC continues to pursue partnerships with ESA and JAXA for funding for meetings. Specifically for the US, we search for a more direct collaboration with a NASA center to help with the curation and distribution of the products of cross-calibration in the form of databases and tools through a funded data archive center. The HEASARC would be a natural partner.

5 Schedule

The activity of cross-calibration is on-going and will always be in demand. This effort that we propose aims to address not only the present situation, but to create a structure and knowledge data base for future projects. In the same way that mission data is stored for a lifetime, the data products from cross-calibration should be as well. While NASA requires a detailed data management plan (DMP) in announcements of opportunity (AOs), the specification for the DMP[^9] refers to calibration data only once. The upcoming AO for Explorers and Missions of Opportunity refers to calibrations but often in reference to spacecraft systems. Cross-calibration is not mentioned, so we suggest that language be added either to all AOs or to the DMP specification to explicitly require missions to participate in cross-calibration efforts such as IACHEC and provide calibration data to the IACHEC calibration and knowledge data base to enable cross-calibration by others.

6 Cost Estimates

As the US missions involved in IACHEC are predominantly funded by NASA, we feel that NASA should directly support the effort outlined here. Funding for this effort would not be significant to NASA compared to the costs of the missions supported, likely < $1M/year. The details of how the funding would be allocated would be negotiated or perhaps proposed by the managing NASA center. The funding would support annual meetings that may take place in the US, travel to these meetings for a few guests, salary and research support for visiting calibration scientists, and salary for those who set up and maintain the calibration database.

References


Ishida, M., et al., 2011, PasJ, 63, S657


