Calibrating Array Detectors

D. J. Fixsen¹,³, S. H. Moseley², and R. G. Arendt¹

ABSTRACT

The development of sensitive large format imaging arrays for the infrared promises to provide revolutionary capabilities for space astronomy. For example, the Infrared Array Camera (IRAC) on SIRTF will use four $256 \times 256$ arrays to provide background limited high spatial resolution images of the sky in the 3 to 8 $\mu$m spectral region. In order to reach the performance limits possible with this generation of sensitive detectors, calibration procedures must be developed so that uncertainties in detector calibration will always be dominated by photon statistics from the dark sky as a major system noise source. In the near infrared, where the faint extragalactic sky is observed through the scattered and reemitted zodiacal light from our solar system, calibration is particularly important. Faint sources must be detected on this brighter local foreground.

We present a procedure for calibrating imaging systems and analyzing such data. In our approach, by proper choice of observing strategy, information about detector parameters is encoded in the sky measurements. Proper analysis allows us to simultaneously solve for sky brightness and detector parameters, and provides accurate formal error estimates.

This approach allows us to extract the calibration from the observations themselves; little or no additional information is necessary to allow full interpretation of the data. Further, this approach allows refinement and verification of detector parameters during the mission, and thus does not depend on a priori knowledge of the system or ground calibration for interpretation of images.

1. Introduction

The Infrared Array Camera (IRAC) (Fazio et al. 1998) will employ four $256 \times 256$ imaging infrared arrays and the cooled telescope of the SIRTF to produce images of the sky which are

¹Raytheon-ITSS Corp., Code 685, NASA/GSFC, Greenbelt, MD 20771
²Code 685, Infrared Astrophysics Branch, Goddard Space Flight Center, Greenbelt, MD 20771
³email address fixsen@stars.gsfc.nasa.gov
limited by the photon statistics from the natural background, which, in this spectral region (8-25 
μm), is dominated by scattered and emitted light from the zodiacal dust particles. This will be
typical of future applications of infrared detectors in space. In order to produce high quality
images in the presence of this strong background, the relative response of the different pixels
in the detector array must be known to high precision. A technique must be developed that
allows the detector properties to be determined in operation, so that the requisite stability can be
experimentally verified, and changes in response can be measured and included in the analysis of
the data. We present a technique by which the detector properties are determined simultaneously
with the estimates of sky brightness, and formal errors developed for both instrument and sky
parameters.

We observe the same area of the sky with the detector array at a number of spatially offset
positions. These observations are used to set up a system of linear equations involving both sky
brightness and detector properties. In solving this system of equations, we can deduce the sky
brightness and detector gain and offset parameters. By appropriate choices of offset spacings and
sky brightness distributions, this technique allows us to continuously improve our knowledge of
the detector properties or detect changes. This approach embeds the relative calibration of the
detector array into the survey process; all information required to produce an internally consistent
survey can deduced from the survey itself. Since the data on which the calibration is based is
the survey itself, it is the way to calibrate the data which is, in some sense, least susceptible to
systematic errors. In the case that an a priori calibration is used, this technique offers a method
to test internal consistency.

In this paper, we describe this least squares solution for sky and detector properties, and
suggest implementations of the technique for the IRAC instrument. We present the analysis of
synthetic Wide-Field Infrared Explorer (WIRE) data and real Hubble NICMOS data, in which we
derive the sky brightness, detector gain and detector offset. (We had planned a demonstration of
the technique on the Wide-field Infrared Explorer, but its unfortunate demise renders the point
moot.) The results are encouraging, and form the basis of our plans for the analysis of the IRAC
imaging data. Optimization of the observational strategy to produce the best encoding of the
detector parameters in the survey observations is treated in a separate paper (Arendt, Fixsen &
Moseley 2000). This approach can offer significant insurance to the observer, in that regardless
of the availability or applicability of independent relative calibration data for the instrument,
sufficient information is present in the observations themselves to allow the relative calibration of
the data. This provides the capability for the observer to validate the statistical properties of the
data or to calibrate it as required.

Least squares techniques are an important staple of model fitting. In this paper, we use a
least squares technique, combined with sampling over a wide range of spatial scales, to produce an
intensity calibration for the imaging system. Investigators have long used "sky flats" to produce
estimates of system response (e.g. Joyce, 1992). In this process, images are taken at a variety of
positions around the object of interest. These images are often processed using median filtering to
produce estimates of detector response. In this paper, we derive the full algorithm for optimal use of the sampled data for intensity calibration of an imaging detector. This algorithm then allows us to ask more sophisticated questions important for planning observations, such as comparing the relative goodness of different sampling procedures (Arendt et al. 1999). This algorithm provides the optimal tool for calibrating imaging detectors; if the algorithm does not produce reliable results, it is indicative of incompleteness in the sampling of the sky. The algorithm provides an optimal detector calibration based on the data provided it. If a priori information about the detector is known, the algorithm can be adjusted to include it.

Other algorithms have been described in the literature for analyzing dithered image data. The drizzle method (Fruchter and Hook, 1998) is an approach for combining undersampled dithered images to produce a single combined image with improved resolution and signal-to-noise ratio. However, this technique is a means of producing a final image from calibrated data, and is not intended as a method of deriving the detector calibration.

Future observatories will generate survey data. The accuracy of analysis of these data will depend on a clear understanding of the statistical properties of the uncertainties in the data, their level, and spatial and temporal correlations. We present an approach for the analysis of such data, with specific application to the imaging data from the SIRTF IRAC instrument.

This comprehensive least squares approach has been successfully applied to the analysis of the data from the FIRAS instrument on COBE, in which a complex instrument model was required (Fixsen et al. 1994).

2. Overview

The following equations show the derivation of the simultaneous extraction of sky brightness and instrument parameters to the data. The advantages of this system are: 1) It uses the same data for calibration and observation which saves separate observation time for calibration and uses the same time and exactly the same conditions for calibration and observation. 2) It uses a well understood process for calibration allowing for complete error analysis and flexible response in the case that unexpected errors arise. 3) It explicitly includes the uncertainties and correlations introduced in the calibration process in the uncertainties of the resulting data. We focus on an imaging array observing sections of the sky, but the derivation is either directly applicable or easily generalized to other problems.

The underlying process is a simple linear fit which is easily understood, although the matrices involved are unwieldy. The inverses of the matrices are assumed to exist. If there are problems inverting these matrices, it is an indication that information is missing in the calibration process. We do not go into detail about the convergence or singularities of the process, but these need to be addressed as they show key weaknesses in the calibration process and can generally be corrected by improving the measurement strategy (Arendt et al. 2000).
Since the details of the calibration process leave their impact on the noise characteristics of the final data set, the procedure for taking data must be be carefully designed. This is not unique to this particular process for calibration, but this procedure makes the costs of poor measurement strategies obvious.

3. Derivation of the Algorithm

We follow the Einstein summation convention and use different indices for the different vector spaces. Latin indices are used for the raw data and instrument pixels while greek indices are used for the derived solution and the sky pixels. We use the same variable names for the contravariant and covariant cases even though the numerical values are different, because the underlying information is the same (see Table 1).

Consider the general solution, where we have a model of the data, $H^i(\theta^\mu)$, where $\theta^\mu$ is a vector of parameters which includes both detector and sky parameters. First we linearize the equation, about a point $\Theta^\mu$ at or near the solution yielding:

$$H^i(\theta^\mu) \approx H^i(\Theta^\mu) + H^i_\mu \delta^\mu,$$

where $H^i_\mu = \partial H^i/\partial \theta^\mu$. The derivatives are performed at $\Theta^\mu$ and $\delta^\mu$ are perturbations from $\Theta^\mu$ ($\delta^\mu = \theta^\mu - \Theta^\mu$).

Given a data set $D^i$ we define $\Delta^i = D^i - H^i(\Theta^\mu)$. With a symmetric weight matrix, $W_{ij}$, $\chi^2$ is calculated as

$$\chi^2 = (\Delta^i - H^i_\mu \delta^\mu)W_{ij}(\Delta^j - H^j_\nu \delta^\nu)$$

and its minimum is determined by

$$\frac{\partial \chi^2}{\partial \delta^\nu} = -H^i_\omega W_{ij}(\Delta^j - H^j_\nu \delta^\nu) - (\Delta^i - H^i_\mu \delta^\mu)W_{ij}H^j_\omega = -2H^i_\omega W_{ij} \Delta^j + 2H^i_\omega W_{ij}H^j_\nu \delta^\nu = 0.$$ (3)

Thus the solution for $\delta^\mu$ can be expressed as

$$\delta^\mu = (H^i_\mu W_{ij}H^j_\nu)^{-1}H^k_\nu W_{kl} \Delta^l = (H^i_\mu H_{\nu})^{-1}H^k_\nu \Delta_k.$$ (4)

There are several potential pitfalls here particularly if the second derivative, $H^i_{\mu\nu} = \partial H^i_\mu / \partial \theta^\nu$, is ill-behaved in the region of interest. If $H^i_{\mu\nu} \delta^\mu \delta^\nu > 1$ the expansion point $\Theta^\mu$ is too far from the solution. A new $\Theta^\mu$ closer to the solution should be used. If $H^i_{\mu\nu}(H^i_\mu H_{\nu})^{-1}$ is close to 1 or larger a full differential geometric treatment is in order which is beyond the scope of this paper.

The inversion of the matrix $H^i_{\mu\nu}H_{\nu}$ is the hard part of the problem. In what follows we show how properties of this matrix that frequently exist can reduce the problem to one that can be
computed on a modest computer. The inverse of the matrix is also the covariance matrix of the parameters including the sky parameters.

It is also interesting that:

\[ \delta_\mu = H_\mu^i \Delta_i. \]  

(5)

This is a simple mnemonic to remember the solution. It also shows that the covariant form of the solution on the left is like the covariant form of the data on the right. This is the weighted form of the solution needed if one desires to fit this solution to some higher level theory. This can be done even if the matrix cannot be inverted.

To develop a more tractable form of equation (4), we separate the detector parameters from the sky parameters.

\[ \delta^\mu = (X^1 \ldots X^P, \delta S^1 \ldots \delta S^T). \]  

(6)

The parameters are not required to have the same units; the weight matrix has all of the appropriate inverse units. Analogously the parameter weight matrix is separated into 3 parts,

\[ H^i_\mu W_{ij} H^j_\nu = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix}. \]  

(7)

The part dealing with the instrument is \( A = H^i_\mu W_{ij} H^j_\nu. \) The part dealing with the resulting sky map is \( C = H^i_\alpha W_{ij} H^j_\beta. \) And the connections between them are \( B = H^i_\alpha W_{ij} H^j_\mu. \) The covariance matrix (inverse of the weight matrix) is broken into the same sorts of parts. Often, each detector observes only one sky pixel at a time and the weight matrix is simple enough that the large submatrix, \( C = H^i_\alpha W_{ij} H^j_\beta \) can be easily stored and inverted. Let us then consider

\[ (H^i_\mu W_{ij} H^j_\nu)^{-1} = (H^i_\mu H_{\mu\nu})^{-1} = \begin{pmatrix} Q & R \\ R^T & \Psi \end{pmatrix}. \]  

(8)

The inverse or covariance can be calculated by:

\[ Q = (A - BC^{-1}B^T)^{-1} \]  

(9)

\[ R = -QBC^{-1} \]  

(10)

and

\[ \Psi = C^{-1} + C^{-1}B^TQBC^{-1}. \]  

(11)

When the only interest is in the uncertainties in the array parameters, (e.g. when the calibration is used for other data) only \( Q \) is needed. Similarly, if only the sky uncertainties are required, only \( \Psi \) is needed.

The covariance of the derived sky, \( \Psi, \) is composed of two parts. The \( C^{-1} \) is the direct propagation of the measurement errors to the sky. The other part \( C^{-1}B^TQBC^{-1} \) shows the
additional uncertainty due to the calibration. For a well chosen set of observations this part can approach \( (P/PM)C^{-1} \), the limit set by the number statistics.

The matrix, \( Q \), is much smaller than \( H^i_H^j_H^i_{ij} \), but still may be inconveniently large. Equation (4) is really a system of linear equations. By substituting equation (8) into equation (4) and retaining only the first \( P \) equations we have:

\[
X = (QH^i_q + RH^i_i)\Delta_i = QY
\]

where

\[
Y = H^i_q\Delta_i - BC^{-1}H^i_i\Delta_i.
\]

The matrix \( A \) relates the detector parameters to each other. With care these can be chosen so that the matrix can be inverted. With the size and speed of modern computers this can even be accomplished with brute force techniques. In many cases \( A \) will be a multiple of a kernel which is the result of a single observation.

Now to get a form of equation (12) suitable for computing, let

\[
T = A^{-1/2}BC^{-1/2} = (H^i_qH_{qr})^{-1/2}H^i_rH^i_j_\alpha(H^k_\alpha H^k_{k\beta})^{-1/2}.
\]

Then

\[
X = (A-BC^{-1}B^T)^{-1/2}Y = A^{-T/2}(I-A^{-1/2}BC^{-1}B^T A^{-T/2})^{-1}A^{-1/2}Y = A^{-T/2}(I-T T^T)^{-1}A^{-1/2}Y.
\]

Like \( B \), the size of \( T \) is \( P \times \Gamma \), but it is sparse.

Finally, we use \( (I-T T^T)^{-1} = \sum_{n=0}^{\infty} (T T^T)^n \) to get a form that is tractable with a modest computer. Although formally the sum must be carried to infinity the sum converges in tens to hundreds of iterations for well chosen observations. Then,

\[
X = QY = \sum_{n=0}^{\infty} (T T^T)^n A^{-1/2}Y.
\]

The matrix, \( T T^T \), is avoided by defining \( Z_0 = A^{-1/2}Y \), and iterating

\[
Z_{n+1} = Z_0 + T(T^T Z_n)
\]

until \( Z \) is stable. It is trivial then to get the solution \( X = A^{-T/2}Z \). This is only the solution for the detector, but the solution for the sky is then straight forward.

4. Example

Next we show how the algorithm is used in a practical program. Some of the key details are given in the appendix, here we outline the steps of the program and relate them to the previous derivation.
### Table 1. Variable Definitions

<table>
<thead>
<tr>
<th>Variable</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P$</td>
<td>number of Array pixels, e.g. $256 \times 256 = 65536$</td>
</tr>
<tr>
<td>$\mathcal{P}$</td>
<td>number of detector parameters, e.g. $2P = 131072$</td>
</tr>
<tr>
<td>$M$</td>
<td>number of images in the data set, e.g. 100</td>
</tr>
<tr>
<td>$i, j, k$</td>
<td>are indices to data $\in (1 \ldots P \times M)$</td>
</tr>
<tr>
<td>$D^i$</td>
<td>data</td>
</tr>
<tr>
<td>$\Delta^i$</td>
<td>model error</td>
</tr>
<tr>
<td>$V^i$</td>
<td>data variance (assumed to be diagonal)</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>number of observed sky locations, e.g. 500000</td>
</tr>
<tr>
<td>$\alpha, \beta$</td>
<td>indices to sky locations $\in (1 \ldots \Gamma), \Gamma &lt; P \times M$</td>
</tr>
<tr>
<td>$S^\alpha$</td>
<td>set of sky parameters</td>
</tr>
<tr>
<td>$p$</td>
<td>index to pixels $\in (1 \ldots P)$</td>
</tr>
<tr>
<td>$G^p$</td>
<td>set of gain parameters</td>
</tr>
<tr>
<td>$F^p$</td>
<td>set of offset parameters</td>
</tr>
<tr>
<td>$q, r$</td>
<td>indices to detector parameters $\in (1 \ldots \mathcal{P})$</td>
</tr>
<tr>
<td>$X^q$</td>
<td>set of detector parameters $(\delta F^p, \delta G^p)$</td>
</tr>
<tr>
<td>$\mu, \nu, \omega$</td>
<td>indices to all parameters $\in (1 \ldots \mathcal{P} + \Gamma)$</td>
</tr>
</tbody>
</table>
We adopt a simple model for the data, but more complex models are as easily handled as long as they are relatively linear in the range of interest, do not require large numbers of parameters to be determined, and are not undetermined. A formal derivative must be calculated for each of the extra parameters and coded into the algorithm, while this may be messy and clutter the program, small numbers of parameters (e.g. temperature effects) that affect the entire array make only small changes to the required time or the final accuracy of the algorithm. If some part of the parameter space is undetermined the program may not converge.

Our example has a separate gain, \( G \), and oset, \( F \), for each detector that modify the sky intensity, \( S \), as it is detected. The model, \( H^i \) for the data is given by

\[
H^i(G^p, S^\alpha, F^p) = G^p S^\alpha + F^p.
\]

The example is obviously nonlinear and we must be careful to chose an initial point close enough to the solution for the algorithm to converge to the solution. For a particular detector array one would use the algorithm many times so one can use the last solution as the starting point and either add more data to improve the solution or find a new solution with new data. Either way, only once, do we need to start without a previous solution. In that case we can let \( G^p = 1 \), \( F^p = 0 \), and \( V^p = \sum_{i \in p} (D^i - F^p)^2 / M \). Then with the assumption that the uncertainties are a function of pixel only, we have an estimate for \( V^i \). We will return to this estimation in section 6.

We assume a diagonal weight matrix \( W_{ii} = (V^i)^{-1} \) to keep the example simple. However, we emphasize that this is not required. The derivation is completely general and can accommodate a nondiagonal weight matrix. Note that this assumption does not mean that the data are uncorrelated. Indeed, the data are correlated as some of the data are derived from the same pixel or are observations of the same part of the sky with different detectors. If there are other sources of correlation (such as detector temperature) they need to be explicitly included in the model. The assumption here is that the residual errors are uncorrelated.

The first step of the program is to calculate

\[
\Delta_i = W_i(D^i - G^p S^\alpha - F^p).
\]

As there are two types of parameters we divide the matrix \( A \) into its four quadrants for discussion.

\[
A = \begin{pmatrix}
A_G & A_{GF} \\
A_{FG} & A_F
\end{pmatrix}.
\]

Each of the submatrices of \( A \) is diagonal, including the part relating the gain and oset of each pixel. The whole matrix is treated as \( P \ 2 \times 2 \) matrices. There is not a unique \( A^{-1/2} \), mathematically the choice is arbitrary, but the symmetric choice and the choice where the lower left are zero are easier to program. We have used both and found the nonsymmetric version is less susceptible to numerical instability.
Although the size of $H^i$ is $PM \times (P + \Gamma)$ it can be treated as a set of delta functions. With care in the processing, the parts of $H$ that are zero need never be accessed (appendix). There are $3P \times M$ nonzero parts. That is each datum appears 3 times, once associated with $G$, $F$ and $S$.

$$\partial_{G^\alpha} H^i = S^\alpha \delta_{pi}$$

The second step makes use of the following relations: $\partial_{F^\alpha} H^i = \delta_{pi}$ to construct

$$\partial_{S^\alpha} H^i = G^p \delta_{\alpha i}$$

$$\text{diag } A_G = \sum_{i \in P, i \in \alpha} S^\alpha W_i S^\alpha, \quad \text{diag } A_F = \sum_{i \in P} W_i$$

(22)

$$\text{diag } A_{FG} = \sum_{i \in P, i \in \alpha} S^\alpha W_i$$

(23)

and

$$\text{diag } C = \sum_{i \in \alpha, i \in P} G^P W_i G^p.$$  

(24)

$C$ is diagonal as well.

The matrix $B$ is divided into two parts similar to $A$:

$$B_G = \sum_{i \in P, i \in \alpha} S^\alpha W_i G^p, \quad B_F = \sum_{i \in P, i \in \alpha} W_i G^p.$$  

(25)

Finally $Y$ has two parts

$$Y_G = \sum_{i \in \alpha, i \in P} S^\alpha \Delta_i - B_G C^{-1} \sum_{i \in P, i \in \alpha} G^p \Delta_i, \quad Y_F = \sum_{i \in P} \Delta_i - B_F C^{-1} \sum_{i \in P, i \in \alpha} G^p \Delta_i.$$  

(26)

Note that $B$ is $2P \times \Gamma$ but it is sparse. We then calculate $T = A^{-1/2} B C^{-1/2}$. With the elements of equation (16), the program iterates equation (17) until $Z$ is stable. Then the solution $X = A^{-T/2} Z$. This is only the solution for the detector, but the solution for the sky is then:

$$S^\alpha = \sum_{i \in \alpha, i \in P} [(D^i - F^p) G^p W_i] / \sum_{i \in \alpha, i \in P} (G^p)^2 W_i.$$  

(27)

This then is a form which can be handled by a modest computer. The vectors $X$ and $Y$ are each only $2P = 131072$ long. The matrix $A$ is stored as three $P$ long diagonal parts of its submatrices. The matrix $T$ is nominally large ($2P \times \Gamma$) but is sparse and has at most $2P \times M$ nonzero components.

At this point there are two obvious singularities. These correspond to the uniform change in the sky brightness and a cancelling change in the offset, and to a multiplication of the sky by an arbitrary amount and a cancelling effect in the gain term. These two singularities point out what we already know; in order to get an absolute calibration we need an absolute standard. There are
several ways to deal with this issue: 1) An absolute calibration could be done in the laboratory. 2) Certain places on the sky could be determined in some other way and used to impose a condition that would break the singularity. 3) A map could be produced with an arbitrary gain and offset.

The three methods are not mutually exclusive. A map with arbitrary gain and offset can be produced which is subsequently calibrated by laboratory measurements or sky measurements or a combination of sky and laboratory measurements. The absolute calibration can be included in the fit or applied later. We choose to apply it separately as this maintains the uniformity of the algorithm whether viewing a calibration object or not.

Without treating the singularity, the sum in equation (16) does not converge. If there are no dark frames to determine the offset, after each iteration we impose the condition that

$$\sum_p \sqrt{\sum_{i \in p} W_i} \delta F^p = 0.$$

The weight applied to the $\delta F^p$ is only for computational convenience (it is the form of $F^p$ in $Z$). The key is that the net offset is not allowed to change. If dark frames are present we can use them to determine the offset and do not impose this condition. Similarly, a weighted mean gain is held fixed, $\sum_p \sqrt{\sum_{i \in p, i \in \alpha} S^\alpha W_i S^\alpha} \delta G^p = 0$.

This completes the solution for the detector and the sky. The calculation of a single uncertainty vector is completely analogous. However the full covariance matrix $\Psi$ is $\sim 500000 \times 500000$. This matrix is symmetric but it is not sparse. In fact it is likely that all of the elements are nonzero. The $2.5 \times 10^{11}$ components of $\Psi$ are awkward to carry around but they contain all of the information about the correlations imposed by the calibration process. It can be stored more compactly by keeping $T$, and noting that

$$\Psi = C^{-1/2}(I - T^T T)^{-1} C^{-1/2}$$

since $T$ is sparse and $C^{-1/2}$ is diagonal.

Now we return to the issue of variance (weight) estimation. Without a model for the noise we have a hopeless task. However with a simple model we can estimate the variance. An unbiased, but poor, estimation only increases the noise (and the estimate of the uncertainty).

In the model program we assume three sources of error: 1) Poisson statistics, 2) A pixel dependent readout noise, 3) A cosmic ray induced error. The Poisson noise is easily calculated if the approximate gain of the system is known. The readout noise is best estimated by using the RMS of all of the data from that pixel (except the cosmic ray contaminated data). Cosmic rays are identified by seeking large discrepancies. These should not be used in either the sky or variance estimation. Obviously as data are collected a more detailed model can be developed.

After a solution is found, the model program recalculates $\Delta^i$. Data with errors greater than $2.5 \sigma$ are assumed to be cosmic particle hits or other glitches. These data are marked and not used in the next iteration. The remaining $\Delta^i$'s are squared and summed to estimate the noise. The model program noise is treated separately for each pixel. If hundreds or thousands of pictures are available this process could potentially identify subtle problems with particular pixels. If fewer data are available a smooth approximation over entire detector array is more appropriate.
5. Practical Matters

The algorithm described in the preceding sections can produce mosaics of large regions provided that at least some parts of the region (preferably all parts) contain repeated (dithered) observations. The algorithm can be applied to a data set containing spatially separate regions. There is no constraint on the size or geometry of the region(s) in the data set. It is only required that the detector gain and offset and the sky intensity \( G_p, F_p, \) and \( S^\alpha \) are constant for the entire data set. These restrictions can be relaxed by explicitly parameterizing known or suspected variations.

If dark frames are available, they are added to the data set as if they are observations of a region of sky that is separate from the rest of the data and that has an intensity \( S^\alpha \equiv 0 \). The addition of dark frames to the data set allows the algorithm to determine the offset components.

The algorithm can be implemented in a general manner, such that the detector dimensions and number of frames processed are adjustable. A general code can be applied to different data sets from different instruments if a new “front end” is written for each type of data to ingest the data and provide the necessary initial estimates and control parameters.

The selection of the weights \( W_{ii} \) to use in the algorithm can be important. Poor weighting of the data may cause spurious features to propagate through the solutions for \( G_p, F_p, \) and \( S^\alpha \). Cosmic ray hits on the detector also cause spurious features in the results, if not properly handled. Data affected by cosmic rays can be given very low weights or flagged. It is best if the effects of cosmic rays are removed from the data before processing, though this is not always possible. The algorithm can recognize cosmic rays as outliers provided that they are not so numerous that they severely bias the results.

In most cases, the algorithm will be used iteratively for 2 - 5 cycles. Subsequent iterations use the previously derived gain and offset values as inputs, and make use of successively improved weights and exclusions of cosmic rays as well.

An IDL implementation of this algorithm requires free memory \( \sim 15 \) times larger than the size of the data set to be processed. For a data set of 27 256×256 images the algorithm takes \( \sim 450 \) seconds of CPU time on a 300 MHz Pentium II machine running Red Hat Linux 5.2 and IDL 5.0.3. About 270 seconds of that CPU time is spent in the calculation of the summation of equation (16), using the iterative step of equation (17) for 100 terms. The key data arrangements of the program are discussed in the appendix. The time for the procedure is linear with the number of input data elements as long as more iterations are not needed. The number of iterations required is strongly related to the connection map which is determined by the dither pattern of the input data.

Solving only for detector gains in cases where the detector offsets are negligible is a minor simplification of the algorithm and is a more robust procedure. Figure 1 illustrates the results of using this procedure to solve for only the detector gains and sky intensities. The data used is from Wide-Field Infrared Explorer (WIRE) simulations. The model for the sky includes point
sources, cirrus and a zodiacal background. The model for the 128 × 128 detector array included gain variations, bad pixels, and cosmic ray hits. The data set consists of 10 dithered images, one of which is shown in the upper left of Figure 1. The detector gain variations dominate the qualitative appearance of the data. The derived gain compares favorably with the true gain, with the exception of ~ 0.2% of the pixels with remaining artifacts from bad detectors and cosmic rays. There is a small (~ 1.0025) scale factor between the derived and true gains, which reflects the lack of absolute calibration in the procedure. The derived sky is a good representation of the real sky, with the additional noise component indicated by the second term of equation (11).

Figure 2 illustrates the application of the algorithm to real data, namely the HST NICMOS observations of the Hubble Deep Field - South. The raw data used here were 59 good 1152 and 1472 s integrations. The worst effects of cosmic rays were eliminated by calculating linear fits to the multiaccum readouts from each pixel. Fits with poor correlation coefficients were refit using a combination of linear and step functions. Additional pre-processing involved subtracting the median value of each quadrant of each frame from that frame quadrant. This helped compensate for a variable “pedestal” effect which is not modelled by our current algorithm. (The bottom 16 rows of each frame were ignored in the processing to avoid vignetting effects.) The initial gain map was assumed to be flat and unity. The initial offset map was assumed to be flat and zero. A dark file from the NICMOS reference files was used for a simulated dark frame that was processed simultaneously with the sky data. The derived sky after 2 iterations of the algorithm and truncation of the series expansion after 100 terms, is not as clean as the publicly released processed data. Spurious large scale structure is present at low levels. A faint stripe along the detector columns is visible through the brightest star in the field. The gain and offset maps are similar to calibration flat and dark reference files. In our derived gain and offset maps there are residual defects in pixels where the bright sources in the map were observed. The gain and offset maps also contain visible quadrant errors and vertical bars from “shading” because of instrumental effects that are not adequately described by the simple method used here. Clearly there is room for improvement, but the algorithm worked well. The process allowed the simultaneous determination of sky and detector parameters using only sky measurements and dark frames. By inspecting the residuals there are indications that the offsets are not constant from observation to observation. This suggests an improved model for the data could be constructed by parameterizing and fitting these offsets.

In the case of IRAC, such an algorithm is essential. With it, we can continuously derive detector parameters from the normal observations and improve the model of the detectors as well as the model of the sky. Just such a procedure was used on the FIRAS data to improve the sensitivity by a factor of ~ 100 over the initial publication.
6. Uncertainties and Correlations

The algorithm produces a formal estimate of the uncertainties, $\Psi$, based on the derivation and the estimated uncertainties of the input data, $V$. The resulting uncertainties are only as good as the uncertainty estimates of the original data. Those uncertainties, $V$, are checked against the actual deviations from the model to either give an improved estimate of the input data uncertainty or an indication of shortcomings of the model.

Identifying the weight matrix (or metric) as the inverse of the covariance matrix, only defers the question to how to determine the covariance matrix. There are two sorts of ways to attack this problem. The theoretical approach uses \textit{a priori} knowledge about the system to estimate what the noise should be. This includes such things as the Poisson arrival of photons, the Johnson noise of the resistors and other known sources of noise. The empirical approach uses the residuals in the data itself to make an estimate of the noise. Each approach has its strengths and weaknesses. The theoretical approach often underestimates the noise because there are unmodeled noise sources present. The empirical approach often overestimates the noise, as it treats parts of the signal that are not properly modeled as noise. If both approaches lead to the same estimate one has reasonable assurance that the model and estimate are correct. If the approaches differ significantly there are either noise sources that are included in the estimate or signal that is not included in the model. In this example, we assume that the noise variance $V$ is known.

The calibration process introduces correlations into the resulting map, $C^{-1}B^TQBC^{-1}$. The correlations for a single detector are easily generated by using a unit vector in place of the $Y$ in equation (12) and carrying out the calculations as with the data. The process is slightly shorter than for the data (checking for convergence is omitted). Obviously this could be repeated for each of the detectors and then equation (11) could be used to generate the full covariance matrix.

There are two problems with this approach. First, the time required is proportional to the number of detectors (65536 for IRAC or NICMOS data). Second, the space for the final result is $\Gamma^2$, which is $\sim 10^{11}$, for even the modest WIRE example shown here. Storing and using such a large data set is problematical.

Fortunately the correlations for different detectors are nearly identical (see figure 3). This should not be a surprise since the detectors are locked into their relative positions and all move together in each dither move. Bad detectors in the array, cosmic rays, and rotations will obviously break this symmetry but except for the rotations the effects are minor and rather localized. So the correlations can be calculated for typical detectors and the results can be used for the entire data set.
7. Summary

As demonstrated with the simulated WIRE data the program can calculate the gains and offsets to the theoretical limit on the accuracy if it is given a good model of the data. As shown with the NICMOS data the program works reasonably well on real data as well even with the normal complexities of real errors and uncertainties. The uncertainties are calculated, and the correlations can be calculated with minor changes to the program. These allow the user to interpret the result without ad hoc assumptions or guesses about how the errors are related. The speed of the program allows modest data sets to be processed in a few minutes and with the availability of machines with large memories will allow the large data sets of the future to be processed in reasonable times.

8. Acknowledgements

We thank D. Shupe and the WIRE team for supplying simulated WIRE observations for testing the algorithm.

9. References


A. Code Considerations

This appendix points out several details of implementing this least squares calibration procedure in a computer code. The first detail is that a sparse matrix storage and multiplication system must be applied. As presented here, the solution (eq. 16) requires construction of the matrix $T$ which has dimensions $\Gamma \times \mathcal{P}$. For a $256 \times 256$ detector array, $T$ contains at least $256^4 = 17 \times 10^9$ elements, making it difficult to store in memory. However most of the elements of $T$ are 0.0, because a single detector, $p$, observes no more than $M$ of the $\Gamma$ sky pixels. Following the
example presented in §4, we note that $T$ contains the same non-zero elements as $B$. Furthermore, each datum leads to one element in $B_C$ and one element in $B_F$ (eq. [25]). Thus $B$ or $T$ can be stored in an array corresponding to the $P \times M$ data, and replicated for each of the detector parameters (gain, offset, etc.) to be determined. The position within the array indicates the $p \in [1,P]$ index of the element, while the $\alpha \in [1,\Gamma]$ index is stored in a separately constructed array. In this way, the storage requirements are reduced by a factor of $\sim (P/P)M/\Gamma$ which is generally very large as $M \ll \Gamma$ for most datasets.

The second detail is to note that equation (17) is can be implemented as a pair of matrix $\times$ vector multiplications: $TTZ_n$, followed by $T(T^TZ_n)$. This pair of multiplications is much faster and requires negligible storage compared to calculating the matrix multiplication $TTT$ first, and then $(TTT)Z_n$. The $TTT$ matrix is not nearly as compact as the $T$ matrix. Furthermore, with the appropriate juggling of indices both matrix $\times$ vector multiplications are performed using the stored format of $T$ without explicitly calculating the transpose of $T$. An example of this is found in Press et al. (Chapter 2, 1992).
Fig. 1.— The top left image shows one of ten frames of simulated WIRE data. The top center image shows the detector gains derived from the data, while the top right image shows the actual gains used to generate the simulated data. The lower left graph shows the histogram of the differences between the derived and actual gains. The bottom middle and right images show the derived sky intensities and the true sky used to generate the simulated data.

Fig. 2.— The raw data is one of the NICMOS multiaccum frames after fitting linear fits to the readouts from each pixel and removing the worst of the cosmic rays. The other pairs of derived and reference images are each shown on equivalent scales. The derived gain and offset maps only cover the upper 256 $\times$ 240 detectors in the 256 $\times$ 256 array.

Fig. 3.— The panels show six columns of the $2P \times 2P$ matrix $A^{T/2}QA^{1/2}$ for a 256 $\times$ 256 detector array and an idealized data set collected using a dither pattern consisting of 36 pointings evenly spaced along the sides of a Reuleaux triangle. The columns are reformated into 256 $\times$(256+2) arrays. From left to right and top to bottom the columns correspond to those containing the correlations for $G_p$ ($p = [128, 128], [16, 128], [16, 16]$) and $F_p$ ($p = [128, 128], [16, 128], [16, 16]$). Correlations against $G_p$ and $F_p$ map into the bottom and top half, respectively, of each panel. Black indicates strong positive correlations. Displayed ranges for $G_pG_p$, $F_pF_p$, and $G_pF_p = F_pG_p$ correlations are $[1.5 \times 10^{-3}, 1.55 \times 10^{-3}]$, $[1.2 \times 10^{-3}, 2.0 \times 10^{-3}]$, and $[-8 \times 10^{-5}, 8 \times 10^{-5}]$ respectively.