Differentiable modelling and data analysis for the JWST Aperture Masking Interferometer

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ABSTRACT

The Aperture Masking Interferometer (AMI)[1,2] on board the James Webb Space Telescope (JWST)[3,4] has a unique place in observational astronomy as the first imaging interferometer in space, promising highly-precise observations resistant to optical aberrations.[2,5] While the optical system and Point-Spread Function (PSF) are very stable, the infrared detectors on board suffer from a series of non-linearities – primarily charge migration or the "brighter-fatter effect" that, while challenging for other observing modes,[6] are ruinous to the visibility calibration of the AMI mode. Local nonlinear effects produced cannot be straightforwardly corrected in the Fourier domain. Efforts using the existing pipelines have delivered some improvements,[7] but outcomes remain far from the theoretical photon-noise limit of the instrument. This manuscript presents initial work using a fundamentally different approach: the joint implementation of a differentiable physics model of the optics, and a machine-learned Effective Detector Model (EDM), using dLux.[8] These are trained together end-to-end, by gradient descent using the full ensemble of point-source reference targets so far observed by AMI. We infer highly-precise metrology of the AMI and NIRISS optical systems, a preliminary EDM which restores commissioning data to near-ideal precision, and illustrate initial and final residual noise floors representing the present state of this ongoing project.

Keywords: James Webb Space Telescope, JWST, Aperture Masking Interferometry, AMI, Optics, Modelling, Data Analysis, Physical Optics

1. INTRODUCTION

JWST hosts several instruments and modes of interest for high-contrast imaging, with AMI probing the tightest inner working angles.[9] Its non-redundant mask allows it to yield information beyond the classic diffraction limit via interferometric analysis methods. As the first science-driven stellar interferometer hosted on a space observatory, it fulfills a unique role within observational astronomy. The highly stable wavefront combined with moderate baselines should yield unprecedented precision on recovered interferometric observables. In turn, high fidelity complex visibilities enable the study of the immediate circumstellar regions of dusty embedded objects, such as protoplanetary and derbis disks, along with young and hot exoplanets. The remarkable science potential of AMI mode has motivated a coherent push across the field of interferometry to develop robust, capable data analysis pipelines such as ImPlaneIA,[10] AMICAL,[11] SAMpip*, SAMpy,[12] and fouriever.[13] However despite concerted community effort (which has delivered some promising results), no existing pipeline or analysis effort has recovered data at a precision close to the projected limits of the instrument.[2,7,14] To understand why all pipelines, each with unique approaches to data analysis, are incapable of approaching fundamental noise floors, we must examine their commonality: they are all inverse models and reliant on the assumption of shift invariance and linearity inherent to the Fourier transform.

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*https://github.com/cosmosz5/CASSINI

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As an infrared observatory, JWST accepts the wavelength range 0.6 - 28 μm,[4] covering both the near and mid infrared regimes observed from the pristine environment of space with an aperture of unprecedented size and sensitivity. With the extreme optical stability provided by the near cryogenic temperatures and the lack of corrupting atmosphere, the nuances and imperfections of the infrared sensors themselves now dictate the limits of possible science outcomes. AMI mode operates within the Near Infrared Imager and Slitless Spectrograph (NIRISS) instrument[15] and uses a Hawaii-2RG (H-2RG) detector[†] capable of non-destructive reads, providing an 'up the ramp' data product that uses multiple measurements in time as charge accumulates. In the idealized case, these 'ramps' are linear and have a slope fit to them, returning a per-pixel flux value. This type of data product provides resilience to erroneous events such as cosmic rays that would corrupt the kind of long exposures of faint galaxies that JWST uniquely targets. The drawback of these specialised detectors is that they suffer from a series of non-linearities that couple strongly to the science signals targeted by AMI mode. Here we suggest that the primary issue with existing inverse-modelling data pipelines constructed for analysis of AMI mode data is their reliance upon the assumption of linearity. The most harmful nonlinear effect is the Brighter-Fatter Effect (BFE),[6,16] arising from charge migration within the detector. It is so named because observation of brighter sources (and therefore more charge accumulated in the pixel wells) results in stronger electrodynamic forces within the substrate, causing more charge migration and yielding the PSF to appear 'fatter' than its true optical footprint.

The non-linear effect this has on measurements of the PSF can be troublesome for many observing modes,[6] but the *strict* requirement for high precision and stability of the PSF in AMI mode in particular makes it particularly serious. Ignoring anisotropy, non-linear detector sensitivity, data processing pipeline artefacts, and instrumental miscalibrations, any measurement taken with charge migration will strongly couple to both the PSF shape *and* brightness. This is not a pure convolution, and therefore does not appear as a multiplicative term in the Fourier domain that can be calibrated out by comparison to a point source reference.

Forward models take a philosophically different approach to inverse pipelines, rather than making assumptions about a system to derive an algorithm that maps from observations back to observables, forward models directly simulate the physics of a system in order to try and reconstruct an observation, and then fit for parameters of interest by standard Bayesian inference or maximum likelihood methods. Historically, inverse pipelines have been preferential in the sciences for a simple reason: measuring observables directly from data has been far easier than forward-simulating entire systems in sufficient detail to deliver mock data products. While the former can typically be efficiently coded using simple algorithms, the latter generally requires iterative approaches and (previously) suffered the 'curse of dimensionality', wherein the computational complexity of reaching a solution scales with the number of parameters to be solved for, resulting in a computationally intractable problem. Despite this historic understanding, new computational capabilities prompt a reassessment of the forwards model approach. The modern family of Automatic Differentiation (autodiff)[17] algorithms, as implemented for example in JAX,[18] PYTORCH,[19] and JULIA,[20] have given rise to the modern revolution in machine-learning. Iterative application of the chain-rule applied to the primitives of any chain of mathematical operations in a function implemented in one of these frameworks lets us solve for high-dimensional gradients with complexity that scales with the evaluation time of the model itself, *not* the number of parameters to be solved for. This enables extremely high-dimensional problems to be solved very efficiently, enabling entirely novel and simple approaches to classically challenging and computationally complex problems.

Differentiable physics models provide the best of both worlds: flexible, high fidelity models of the physics that can be adapted to real-world complexities such as non-linearities, while still being able to be solved for efficiently. A differentiable forward model of AMI provides a unique way to obtain a data-driven calibration of the *optical* components of the system, jointly solved for with a neural-network EDM detector model including linear and non-linear crosstalk. These models provide a way to improve results from AMI mode while also paving the way for a next generation approach to the calibration and data analysis in *all* observing modes of JWST and other space telescopes.

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2. DATA & METHODS

2.1 Calibration Data

Taking a data driven approach to instrumental calibration necessitates careful curation of a data set to ensure the resulting model is accurate and unbiased. An idealised calibration data set for AMI mode should have 5 characteristics:

1. Complete: Observations in all three filters (F380M, F430M, F480M)
2. Deep: Observations to the max pixel well depth of AMI mode (∼25k e-)
3. Diverse: Sub-pixel pointing dithers
4. Unbiased: Equal signal across all filters and dithers
5. Good time resolution 'up the ramp', ie. many groups

This presents a chicken-and-egg problem for AMI mode: Poor results have prevented further data being taken, and a lack of data prevents the kind of calibration that would leads to good results. However, given the state of the instrument it became clear that a high fidelity training set was required to enable further study and recently a dedicated AMI calibration data set that meets all of these criteria was observed: CAL04481. This will serve as the data set used for calibration in the remainder of this paper.

2.2 Data processing

Given the forward modelling approach in this work, careful consideration of the data processing pipeline is crucial. The default calibration is designed to reduce the raw 4-dimensional data product (integrations × groups × pixels × pixels) into two separate 2-dimensional data products, the PSF and its respective uncertainties. However, various steps in the default data processing pipeline are liable to return a PSF that is not representative of the distribution of incident photons due to non-linearities and miss-calibrations. This poses a problem for forward modelling approaches seeking to reach the fundamental instrumental limit of precision, as we can not build a forward model for pipeline artefacts. Furthermore, these pipelines act as inverse models and break our philosophical approach, we don't want to 'correct' for these effects, we want to include them in our model in order to build a fully coherent end-to-end understanding of our system: 'pixels to planets'.

Presently, we only perform exactly three steps in the default JWST data processing pipeline: bad pixel flagging, super-bias subtraction, and jump detection. All other steps in the pipeline either create artefacts in the data that can not be forward modelled, or introduce new sources of error. From here we perform our own set of custom steps to produce a tractable data product that preserves all the information we need. The key to our approach is its ability to model non-linear effects - ones that vary with *time* as charge accumulates in each pixel. Consequently we produce a 3-dimensional data product, with two spatial and one time dimension, ie. we do not perform a 'ramp fit' in the time domain. This gives rise to a new issue, the H-2RG detectors used have a time varying 'bias voltage', meaning that each pixel resets to a different zero-value from integration to integration. In the regular pipeline this is accounted for using the ramp fitting process, the linear slope that is fit has a free-floating bias value and only returns the slope in each integration, ideally isolating the photons from this drifting bias voltage. We can not use this approach as it throws away our time-evolving nonlinearity; instead we look at *slopes* between each group by taking the difference between each measurement from group to group. This lets us keep fidelity over the non-linearities in time and also circumvents the drifting bias problem. The drawback of this method is that it throws away the photons accumulated from the zeroth to the first group, a loss in signal of $1/N_{\text{ngroups}}$. Using this resulting 'slope' data we directly measure the mean and standard error of the mean for each pixel and slope across integrations. This forms our final 'calslope' data product which simply measures the mean and standard error of the accumulated electrons between each group, crucially maintaining resolution in the time domain.

2.3 Calibration and Optimisation

The calibration method applied to these models is fairly simple from a methodological perspective. Their differentiable nature means that we can efficiently calculate the gradient of all parameters and use simple first order optimisation methods, namely gradient descent, to step towards the maximum likelihood estimate. We use a Bayesian loss: a log-posterior which is the sum of a simple per-pixel log-normal likelihood and optionally any priors over parameters.

3. THE MODEL

This work presents the Aperture Masking Interferometer Generative Observation Simulator (AMIGO) software, currently in development as an open-source Python package. It is built within the differentiable optics framework ∂Lux[21,22] as the optics back-end, with the AMIGO package containing the model components specific to the NIRISS/AMI instrument. It is the highest fidelity end-to-end physical optics and detector model of AMI of any found in the public domain. Functionally every component in this model is differentiable, allowing for any miscalibrations to be learnt directly from the on-sky data, avoiding many of the pitfalls of conventional calibration methods where measurements are made in the lab in a very different environment from where the instrument operates (e.g. in space). The principle is simple: if something affects our data then our model will learn it from that data.

3.1 Optics

The optical model of AMI is fairly straightforward from a physical optics perspective, consisting of only a single pupil plane and focal plane. Each individual wavelength has a series of transformations applied: its amplitude is first multiplied by the JWST primary pupil with a optimisable coherence term on each mirror segment and normalised. It is then multiplied by a dynamic and optimisable aperture mask (the AMI mask). This dynamic aperture mask lets us both calibrate manufacturing errors as well as represent the field-dependent nature of the PSF throughout the focal plane. We do not need to make this a function of field position given that AMI mode can only ever be observed in the SUB80 array which is small enough for field dependent effects to be negligible across it. Optical aberrations are also applied, initially utilising the JWST wavefront sensing measurement nearest in time to the data being fit. We then further apply a set of Zernike aberrations across each mirror to represent both drifts and miscalibrations of the wavefront measurement, as well as field dependent effects. This wavefront is then propagated to the focal plane with an optional oversampling.

3.2 Visibilities

Forward model visibilities are a novel concept in the field and thus we use a novel approach, by identifying splodges of power in the ideal modulation transfer function and multiplying them with a complex visibility mask. Starting with the oversampled PSF in the focal plane, it is Fast Fourier transformed to the uv plane where the splodges can be modified. We pre-calculate a set of Zernike polynomials over each splodge, and multiply each element of this basis with an amplitude and the complex exponential of a phase. This implementation allows us to gain resolution over the splodge in order to build high-fidelity visibility resolution, as opposed to FFT-based methods which typically only sample the central region of the splodge. This splodge map is then inverse Fourier transformed to give us back a PSF with an applied visibility model.

3.3 Detector

The AMIGO detector model is what truly sets it apart in the field and allows for substantially higher precision and accuracy. It accepts a 2-dimensional numerical PSF and produces an output that evolves with *time* due to the previously discussed non-linearities. It is comprised of three distinct components: The linear, non-linear, and read models. Many of the steps included are the forward model counterpart of various 'correction' steps applied in the standard JWST pipeline (recall; we do not apply pipeline processing to our data product).

The linear model is fairly straightforwards and comprises of most steps commonly found in detector models: rotation representing the misalignment of the detector and optical train, the xy anisotropy of the pixels, instrumental jitter, along with the inter- and intra-pixel sensitivities. Next we have the non-linear model, in which we use an 'effective detector model' or EDM - the true physics here is either unknown or too complex to model directly so we instead use a non-parametric model to evolve our electron distribution in time as charge is accumulated. We have explored several diverse approaches to this, but two architectures have stood out: a linear convolution with a set of non-linear polynomial basis vectors built from the data (effectively a non-linear convolution), and a recurrent convolution neural network. These models are still in active development and so are not detailed here, but are at present able to effectively capture the non-linear effects of the H-2RG detectors. They produce a 'ramp' where the third dimension represents the time evolution of the PSF as charge accumulates. Finally we apply the 'read model' that represents the applied transformations to the data as it is transported through the various electronic components. It applies the dark-current to each read, the inter-pixel capacitance, the thermal noise of the amplifier (more commonly known as '1/f' noise), and finally the bias voltage of each pixel. Together these three components provide a highly accurate forward model that maps from the input photons all the way to the final charge in each pixel as read by the electronic components of the detector in time.

4. RESULTS

We train the Amigo model via gradient descent on the log-posterior of the CAL04481 data, we examine two different residuals in the image plane; the mean per-pixel residual and the mean per-pixel χ^2, where the mean is taken along the *time* axis, ie. a mean over the groups. This reduces our 3-dimensional data into a simple 2-dimensional residual image which can then be easily visualised and interpreted for performance.

Figure 1 show the mean per-pixel χ^2 and Figure 2 shows the mean per-pixel residual, both visualising all five dither positions and three filters. Examining these figures provides interesting insight and highly promising results - these models are no longer limited by uncalibrated detector non-linearities. Each sub-figure at all dither positions and filters share a series of common mode features: the residual is not dominated by the central single bright PSF peak, the outer central PSF residual has a fixed pattern, and the outer wings of the PSF show a crescent-shaped residual pattern of speckles that scale with wavelength.

The commonality of the residual between each dither position and filter is a highly significant finding and indicates a model that is not limited by non-linear detector effects, but rather by uncalibrated optical ones. This reveals that the Amigo detectors models are both flexible enough to overcome the complex non-linear interactions of the detector, while not being so unconstrained as to be able to bake in PSF miscalibrations.

5. CONCLUSIONS

The AMI on JWST NIRISS has been an outlier on the observatory and performed substantially below its theoretical limits. This is primarily a consequence of the complex non-linearities within the near-infrared detectors, namely the migration of charge between pixels over the length of an integration. The effect on the measured PSF is much more problematic for AMI mode, due to its strict requirements of *highly* precise PSF knowledge and the assumptions of linearity and translation invariance within the data analysis pipelines. The ability to avoid any potentially harmful assumptions and instead build abstract effective models to bridge the gap between the known and the unknown physics provides a platform to not only improve results from AMI, but also other instruments. Preliminary calibrations efforts on a newly-observed and ideal dataset, CAL04481, have shown that these approaches are able to effectively model the non-linear detector effects without over-fitting to PSF miscalibrations. The high signal in this data and the high angular resolution sensitivity of the AMI PSF has revealed a new optical effect as the current limiting factor within the model.

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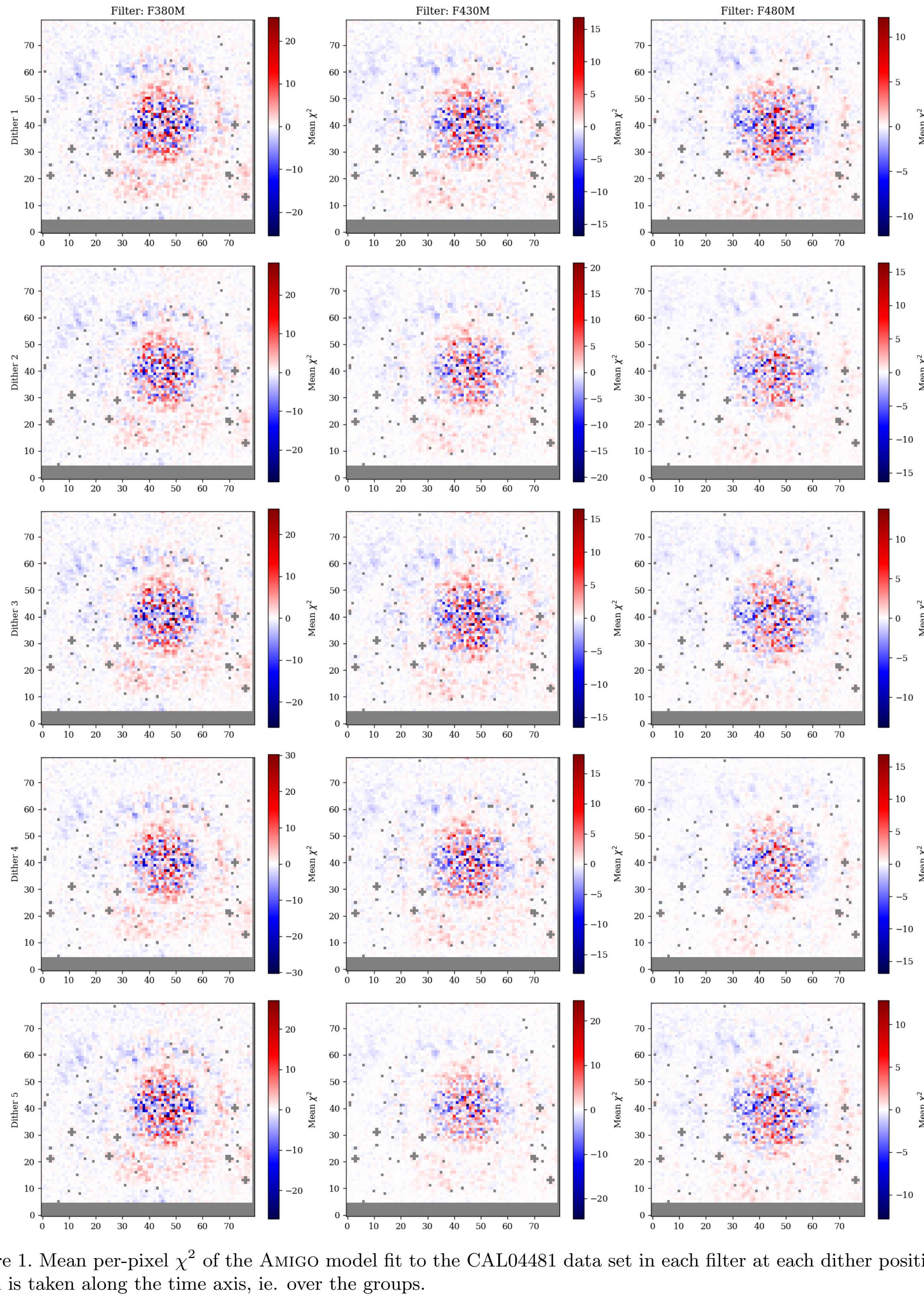

Figure 1. Mean per-pixel χ^2 of the AMIGO model fit to the CAL04481 data set in each filter at each dither position. The mean is taken along the time axis, ie. over the groups.

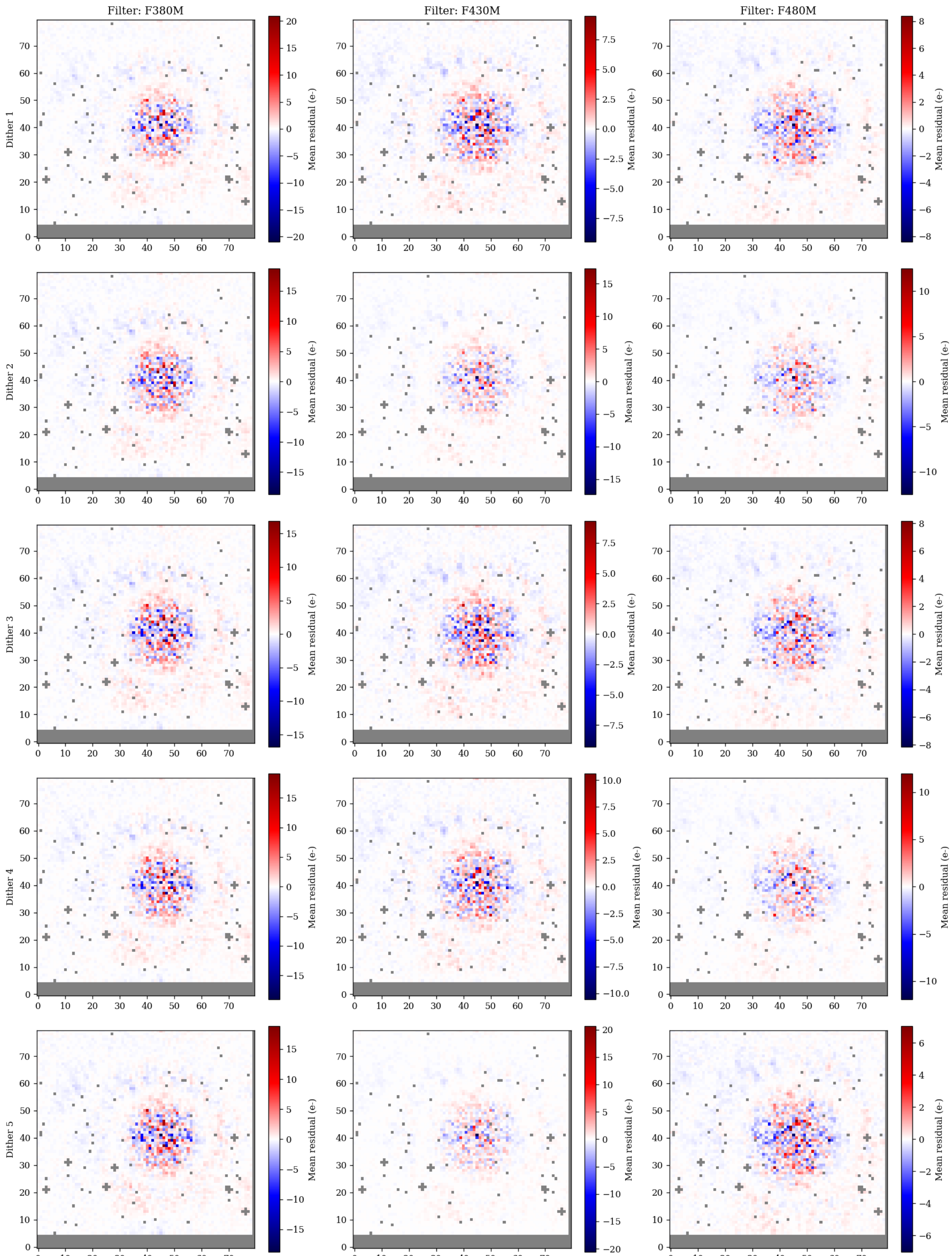

Figure 2. Mean per-pixel residual of the AMIGO model fit to the CAL04481 data set in each filter at each dither position. The mean is taken along the time axis, ie. over the groups.

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