Authors' response to the comments of Referee #2 on “In-operation Field of view Retrieval (IFR) for satellite and ground-based DOAS-type instruments applying coincident high-resolution imager data” by H. Sihler *et al.*

We would like to thank Referee #2 for the review of our submission to AMTD and for contributing helpful comments and suggestions to improve the quality and clarity of our manuscript.

For reference, the original Referee comments below are typeset in black, our responses in blue. Modifications of the original manuscript (green) are indicated in red.

The paper presents a method for in-operation field of view retrieval (IFR). The method is based on the correlation of the instrument with a higher resolution accompanying instrument. Three applications of this LR/HR system are studied: GOME-2 and AVVHR; OMI and MODIS; MAX-DOAS and an SO_2 camera.

I recommend the paper for publication, the main reason being the usefulness of the method: IFR seems good in monitoring in-flight changes in the FOV.

However, some aspects, in particular in the method section, could be improved.

General comments

1) Number of measurements m. The several usages of m throughout the paper are confusing:

On the one hand, m is described as the minimum number to achieve a square linear system: m = n+1, where n is the number of HR pixels in one LR pixel. On the other hand, m is allowed to be smaller than n (p13 l5). Further, m is also a parameter that is easily varied in a study to obtain an error (Appendix). And m is often chosen very large, probably to get a massive over-determined system to cancel out noise.

We understand the Referee's confusion and decided to reformulate the entire IFR description in Sect. 2.3. The changes can be found in the latexdiff-document, but are too voluminous to repeat here.

Furthermore, a top level definition of m is added to the reformulated last paragraph of the introduction: “set of *m* inhomogeneous HR measurements“

Does m need to be large because a lot of LR measurements are not independent?

In principle, all LR and HR measurements are numerically independent. However, noise virtually diminishes the rank of the LES because the tiniest input error inevitably changes the result of the inversion. Therefore, large m is favourable in order to decrease noise contributions in the result.

Changes applied to the manuscript (p.12, l.27):

contains errors – statistical as well as systematic – and different approaches exist to increase the stability of the solution contains errors – statistical, systematic, and numeric – and different approaches exist to increase the stability of the solution

In p13, l1-11 two cases are mentioned. It seems to me, at first sight that in general, m » n as desired by the authors. An matrix with many more rows than columns has a good chance of having adequate rank, and thus of giving a well-defined solution. And, giving the number of HR pixels in a LR pixel (GOME-2: 30x40=1200, see fig 7); OMI: 60x40=2400, see fig 14), an m=1E5 seems sufficient.

However, the second case (p13, r5) is then confusing: m < n will, given enough measurements, not be the case. Perhaps it is meant that rank(H) < n+1 ?

Please clarify.

In order to clarify the relevance of the second case, p.13, l.5-7 are reworded as follows:

Sometimes it is not possible to acquire a sufficiently large set of measurements, and thus the previous approach is not applicable. Then, however, it is still possible to calculate a solution for c under an additional regularisation constraint in the underdetermined m < n case

Sometimes, it may not be possible to acquire m >= n+1 measurement pairs rendering the previous approach non-applicable. Then, however, it is still possible to calculate a solution for c under an additional regularisation constraint.

Specific comments

p4, l 13: the along-track size of 40km is not explained (I assume 100 minute orbit, so 40km in 6s)

The along-track FOV size is a result of the instantaneous FOV (IFOV) of GOME-2, which has probably be designed to match the distance the satellites travels during one scan in order to obtain a seamless coverage at nadir. However, the along-track size is not due to the satellite's movement in the first place.

We applied the following changes to the manuscript (p.4, l.11):

The IFOV in across-track direction is 4 km (Munro et al., 2016).

The IFOV in across-track and along-track direction are 4 km and 40 km, respectively (Munro et al., 2016).

p4, l 33: Does this technique of 9 measurements use (partly) the same HR signals? In what sense does this provide 8 extra, original measurements, or is there a large dependence between them?

It is true that this approach uses partly the same HR signals, but also the regular approach uses HR data overlapping in along-track direction. Errors in the HR data may therefore result in periodic structures in the IFR results, e.g. in Fig. 16 in along-track direction.

We added this information to the results section for OMI (p.20, l.8):

Compared to pixel 3, the sensitivity of pixel 56 seems to be more heterogeneous and the background noise is larger. The FOV maximum approximates at x=-30 km.

Compared to pixel 3, the sensitivity of pixel 56 seems to be more heterogeneous and the background noise is larger. Both results reveal background structures, which are periodic in along-track direction and probably caused by the multiple use of overlapping HR data corresponding to neighbouring LR pixels. The FOV maximum in Fig. 16(b) is approximately at x=-30 km.

and to the discussion of GOME-2 results after p.26, l.11:

Periodic structures, as in Fig. 16 for OMI, are neither evident in along- nor across-track direction, even though always nine neighbouring pixels within one scan were used.

p6, l 13: Here pixel size is defined as along x across, while for GOME-2 it was across x along.

13×24 km^2 is changed to 24×13 km^2

p11, l 1-10: A bit confusing. It seems that (A,C) and (B,D) also have the same y-offset. But I am happy to believe that the resampling has been done in an sensible way, and that some constraints (whether and when ABDC is a perfect rectangle, for example) do or do not hold and that adequate (bi-)linear interpolation of the transformed HR pixel-centers is done. I suggest to be either more specific or less specific.

We understand the Referees conclusion about the shape of the ABCD based on Fig. 6 on page 11. However, Figs. 8 9, and 16 illustrate that a rectangular shape is exceptional, and, therefore (A,C) and (B,D) do not have the same y-offset in general. Therefore, we decided to use a robust approach to align different pixel shapes as applied.

We added (p.11, l.9):

The definitions of the rotations of step 2 apply for any common quadrangular pixel shape.

to the manuscript. Furthermore, the entire passage describing the rotations was reviewed as detailed in our answers to RC1.

Also, Fig. 6 (p.11) has been updated. The new version now also indicates the midpoints used for the third rotation: The caption could be shortened by "The letters denote the GOME-2 pixel corners and centre, respectively." because this information is now in the legend of Figure 6(b).

p11, l 15: The constraint that the HR pixels are square and equidistant seems harsh in this respect. A simple global stretching in x-direction (so a varying delta-x) may be an idea; this will not make the remainder of the text/method more difficult.

We agree with the Referee that the HR pixels could be defined more generally. We therefore appended the following statement(p.11, l.10):

It needs to be noted that the choice of the HR grid is somewhat arbitrary, also irregular grid sizes are possible, but the resolution is constrained by original HR resolution and storage capacity. In this study, quadratic grids are mostly chosen for the sake of simplicity.

p12, eqs 2,3,4: the meaning of h changes two times. Confusing.

As also mentioned in our answers to RC1, we applied considerable modifications to this part of the manuscript. The step-by-step approach has been replaced by a more direct formulation in order to improve clarity. Naming conventions (k changed to j) are furthermore adapted to the Appendix. The changes are detailed in the latexdiff-document.

p12, l 19: linear independent refers to the rows in the matrix. In what way does it translate to the similarity of two or more HR measurements? This seems difficult, and only a brute force approach of defining a massive overdetermined system (more measurements) will ensure that the rank of the matrix will be at least n+1. See also general comment.

We agree with the reviewer. As pointed out in our answer to the previous question, we changed the entire mathematical formulation for the sake of clarity. This includes now also a statement on the rank of H.

The inversion of Eq. (4), however, is only successful if all input quantities were not significantly affected by measurement errors and rank H=n+1.

p13, l 13: Nothing is said about the expected behavior at the boundary. Is it enforced that the c_ij at the boundary approach zero or noise? From the remainder of the text I see that the grid is chosen large enough and that the noise is a good proxy for an empirical standard deviation.

The approach does not require any boundary conditions for c_ij. However, we now state the missing prerequisite of a domain including the entire FOV at p.12, l.10:

It is required that the HR image contains the entire LR FOV.

p15, fig 7: Here, and in other figures, it becomes clear that the grid has been chosen sufficiently large. In what sense does this extent influence the needed number of measurements?

This is an interesting question, which is investigated in the Appendix (see p.32, Fig. A2). This reference is now added to the manuscript for the sake of clarity (p.15., l.1), where

The influence of the LR spectral convolution kernels is further investigated in Sect. A1 in the Appendix.

is changed to

The influence of the LR spectral convolution kernel and the number of measurements is further investigated in Appendix A.

Related remark: If the number of coefficients c_ij becomes too large, it may be an idea to group the c_ij near the boundaries, thereby effectively grouping the square pixels (which are expected to be zero anyway).

Thank you for the remark. However, we decided to apply an unconstrained model. It is, however, possible in future implementations to regroup grid cells based on a-priori knowledge of the actual FOV.

[p19, l 8: The question about large m and having an underdetermined system as in the general comment refers to this OMI case.]

Yes, that is true. As mentioned in our answer above, the entire IFR method description has been cleaned up. We believe that the observation stated at the specified location is now easier to understand.

p19, l 21: The skewed FOVs (as in OMI) cannot be described by the super-Gaussian. Is that suggested here? Note that only a small extension (a mapping of x and y) is sufficient to have skewed super-gaussians.

We thank the Referee for this valuable suggestion. It is, of course, possible to extend the 2D super-Gaussian FOV model by an additional skewness parameter. Furthermore, also tilted and elliptical parameterisations exist in contrast to the rectangular superposition applied here and they must be chosen depending on the application. In this context, we decided to apply a simple FOV model to demonstrate the exceptional quantitative coherence between our results and the OMPIXCOR-product (p. 23, Fig. 17).

We doubt that introducing a skew to the Super-Gaussian model would improve the fit results (p.21, Fig. 14) because the IFR results (Figs. 13&16) do not unambiguously reveal a skewed FOV.

Two changes are applied to the manuscript following this suggestion

Add paragraph after p.14, l.5:

It is noted that there are several possibilities to formulate a 2D superposition of 2 super-Gaussians. Equation (9) models a rectangular FOV, but it is also possible to simultaneously model skewness and tilt using linear coordinate transformations. Also elliptical FOVs can be realised.

Changes to the discussion of the OMI results (p.27, l.6):

Therefore, the proposed 2D super-Gaussian appears to be a sufficient approximation, which could be implemented into standard gridding routines for OMI.

is replaced by

In principle, the OMPIXCOR pixel edges suggest a skewed 2D super-Gaussian. However, the IFR results obtained for OMI are not significantly skewed. The proposed 2D super-Gaussian therefore appears to be a sufficient approximation in this study, which could be implemented into standard gridding routines for OMI.

p27, l 26: possible explanations: The FOV can be re-computed with another grid size. Does it also occur in that case? If not, it seems a numerical artifact.

The mentioned preceding IFR experiments were also conducted at different grid sizes up to the MODIS swath width. The described behaviour was found essentially independent from the grid size and resolution.

This information is now included in the manuscript. The sentence (p.27, l.26)

Consequently, strong interferences for pixels affected by the row anomaly, which appeared later during the mission, were observed in preceding IFR experiments.

now reads

Consequently, strong interferences for pixels affected by the row anomaly, which appeared later during the mission, were observed in preceding IFR experiments conducted at various grid sizes and resolutions.

p29, l 6: Is the wind speed threshold robust? If the threshold is lower, then m decreases. The 15 m/s is a maximum; is that representative (instead of using a median)? Maybe the trade-off can become a bit better.

The choice of wind-speed threshold was found robust in that sense that changes did not have a strong influence on the results. We suspect that applying the median instead of the maximum is minor since we apply a meteorology model where vertical gradients may be assumed smooth enough.

See also answers to RC3.

p30, l 8 : Again, the $m < n$ case is confusing.

The error estimation in the appendix applies for the least-squares IFR solution only. Therefore, this is not applicable to the under-determined case.

Accordingly, the introductory paragraph of the appendix is changed (p.30 .l1):

The measurement errors of the input data applied in this study are not known a-priori. It is, however, still possible to estimate the goodness of the standard least-squares solution c from the reduced χ^2 , which is defined as the weighted sum of squared errors divided by the degrees of freedom.

The measurement errors of the input data applied in this study are not known a-priori. In case of the standard least-squares solution, it is, however, still possible to estimate the goodness of the fit result c from the reduced χ^2, which is defined as the weighted sum of squared errors divided by the degrees of freedom.

p32, fig A2: The lower boundary of the lines is expected at 1200 (30x40), which seems not the case in the graph. Further, pairs of filtered and all have the same m, which seems incorrect.

It is true that n is 1200 for the GOME-2 MSC IFR retrievals. The x-axis of Fig. A2, however, denotes the number of HR/LR measurement pairs m. The maximum possible m is 10^5 defining the lower boundary of lines for “all” data. “Filtered” data are significantly less, as indicated by the left-most blue squares and orange circles.

The ensembles of measurements used for calculating the standard deviation for less than maximum m are random selections of the basic populations. Therefore, same m for “all” and “filtered” are possible.

In order to clarify, the following statement is added to p.31, l. 7 (Figure A2 illustrates the results.):

Figure A2 illustrates the results using random selections of the basic populations of all data and data collected over ocean only.

Technical and minor corrections

p5, l 9: channel 2 -> 4 ?

Done. GOME-2 channel 4 is correct.

p7, fig 3: sake [of] clarity.

Done. of is now inserted

p13, l 27: three additional parameters

Done.

p13, l 27: two-dimensional

Done.

p14, l 5: seven parameters

Done.

p14, l 5: c_k is now described as one-dimensional, while c0 is discarded?

We understand the Referee's confusion about dimension of c_k. As mentioned above, the IFR formalism has been replaced. The new formulation provides only one definition of IFR coefficients. Furthermore, the super-Gaussian FOV parameterisation assumes an offset-corrected input and c0 is therefore discarded.

Changes applied to the manuscript (p.12, l.5):

which are derived from 2D IFR results c_k (j=1...n)

which are derived from IFR results c_j (j=1...n, c_0 is discarded)

p14 l 14
Energy: Then I would have expected a z_bˆ2 to be integrated. Unless it is a common expression.

We are confident that the Equations are correct. In order to reduce the risk of confusion, we replaced the term energy by radiance in the manuscript.

p15, fig 7: the color scales in a and b are different. The 1D-graphs with magenta lines have no vertical scale.

Done. The colorscales in a and b are now the same. The 1D-graphs now have scales and units.

p15, l 10: in a slightly

Done.

p20,l 9: approximates at?

The FOV maximum approximates at → The FOV maximum in Fig. 16(b) is approximately at

See also answer to specific comment above.

p21, l 2: An effect found ...: not a good sentence.

An effect found more frequently towards the swath edges (cf. Supplement). This behaviour is discussed in Sect. 4.2.

This behaviour becomes increasingly visible towards the swath edges (cf. Supplement) and is discussed in Sect. 4.2.

p30 l 11: are now equal the

are now equal the → are now equal to the

p31, l 7: ocean filer. Line 7 repeats sentence line 6.

sample number m and ocean filer was investigated. This study was performed using AVHRR channel 1 and the 630 nm LR convolution kernel. Figure A2 illustrates the results.

is changed to

sample number m and ocean filter was investigated. Figure A2 illustrates the results.