Subject: revised version of the manuscript amt-2022-82: “Synergistic retrieval and Complete Data Fusion methods applied to FORUM and IASI-NG simulated measurements”, by Ridolfi et al.

Dear Editor,

with reference to the manuscript under subject, please find below Author responses (in red) to the original reviewer comments (in black). Further Author notes to the Editor are included (in green).

We are submitting to AMT a revised version of the manuscript as well as a note with some supplemental material to be attached to the paper (see details below). A pdf file with marked changes with respect to the original version of the text is also supplied.

The revised manuscript should address all the major issues raised by the reviewers.

Thanks again for your kind support,
Best regards,

Marco Ridolfi & Co-Authors.

RC1: Comment on amt-2022-82, Anonymous Referee #2, 24 Jun 2022

Review of "Synergistic retrieval and Complete Data Fusion methods applied to FORUM and IASI-NG simulated measurements" by Ridolfi et al.

General comments
In this new study, Ridolfi et al. explore and compare the synergistic retrieval (SR) and complete data fusion (CDF) techniques for the upcoming European FORUM and IASI-NG infrared sounders. The authors discuss retrieval experiments for temperature, humidity, and surface temperature and emissivity for a clear-sky Antarctic atmosphere. Retrieval experiments are conducted for the cases of i) perfectly matching nadir observations of FORUM and IASI-NG and ii) potential mismatch or co-location errors of both instruments. It is demonstrated that the retrieval results of both, the SR and CDF techniques, provide good performance and agree well within the measurement noise errors of the FORUM and IASI instruments for both test cases.

Overall, this is a very carefully designed study with convincing results. The manuscript is well written, clear, and concise. It will be of interest to the retrieval community and I would like to recommend considering it for publication in AMT, subject to a few specific comments and corrections as listed below.

We thank the anonymous reviewer for the constructive comments. According to the reviewer's main comment, we have now run two additional test experiments: one based at Mid-Latitudes and one based at the Tropics. In the revised manuscript, we will summarize also the results of these two additional experiments, which, actually, do not change the conclusions of the paper, though, as expected, we find surface emissivity errors much larger than in the dry Antarctic conditions. We plan to supply as "supplemental material" (or to upload to Zenodo) the plots relating to the new experiments. We believe that, with this integration, the results presented are more robust and consolidated than before.

Results of test experiments based at mid- and tropical- latitudes were included in a small note provided as supplemental material to the paper.

Specific comments
l34-38: A number of references on the CDF technique is given below, but it seems this paragraph is lacking references on the SR technique.

We agree, in the revised manuscript we will cite a few papers on the SR technique also at this instance. Namely, we plan to cite Cuesta et al. 2013, 2018; Fu et al. 2013, 2016; Kuai et al. 2013; Landgraf, J. and Hasekamp, 2007 and Natraj et al. 2011.

Done.

l52-59: I remember seeing a few new papers on FORUM being submitted or published during the last 1-2 years. As FORUM is a new instrument, perhaps it might be good to add a few more references to this paper to provide a bit more background information for the reader? Same for IASI-NG.

In the revised version of the manuscript, for FORUM we will cite also Carnicero et al. 2020, Pachot et al. 2020, Di Natale et al. 2020, Ben Yami et al. 2022, Di Natale and Palchetti, 2022, and Sgheri et al. 2022. For IASI-NG, we plan to cite Bermudo et al. 2014, Clerbaux and Crevoisier 2013 and

Andrès et al. 2018. We are open to include further references that the reviewers may wish to suggest.

Done.

l64-66: The retrieval test cases presented here refer to a perfect situation due to the transparency and sensitivity to surface emissions of the Antarctic winter clear-sky atmosphere. The reader might ask, though, how large are the degradations for non-optimal atmospheric conditions at mid-latitudes or in the tropics?

This is correct. At latitudes different from Polar, when the atmosphere is not so dry, surface parameters can be hardly retrieved. Particularly, the sensitivity of the FIR spectral radiance to FIR surface spectral emissivity vanishes as soon as the atmosphere becomes opaque in this region, due to the water vapour absorption. A detailed study of the FIR emissivity retrieval performance for varying latitude and season is still missing, though it may be part of our future activities. So far, some results on this issue are presented in Oetjen at al. 2019, in Ridolfi et al. 2020 and in Ben Yami et al. 2022. Roughly, the outcome of these investigations is that FIR emissivity can be retrieved from FORUM with useful accuracy (absolute error in the range 0.01 – 0.02) only in dry Polar atmospheres. On the other hand, Polar Regions are the most interesting for the study of FIR surface emissivity, as the latter has an impact on the Outgoing Longwave Radiation, thus it influences the capability of our planet to loose heat to space.
Regarding temperature and water vapour profiles, as shown in Ridolfi et al. 2020, their retrieval error depends less critically on latitude / atmospheric conditions, as the retrieval extracts information on these parameters from the whole spectral interval measured.
In the revised paper, we will further extend the explanations in lines 64 – 66, and will include a summary of the results of the two additional experiments we have run for Mid- and Tropical latitudes (see also the general answer given above).

Text modified as specified above in the related paragraph.

How often are perfect conditions in the atmosphere being found so that the SR and CDF techniques can be applied ?

The SR and CDF techniques can always be applied, as the retrieval is based on optimal estimation, thus the inversion is always possible, even in the unlucky scenarios in which the measurements are not sensitive to the target parameters. Of course, in the latter case the retrieval and the CDF return the a priori state, thus the solution does not provide (or provides only little) extra information as compared to the a priori. In this case, the solution has an error equal (or similar) to the a priori error and its number of degrees of freedom approaches zero.

To which extent do the findings on the good agreement between SR and CDF still hold for non-optimal conditions?

This is an important point, thus in the mean time we carried out two additional test experiments at mid- and tropical- latitudes. In the revised version of the paper, we will report also the outcome of these new tests. The agreement between SR and CDF is linked to the degree of linearity of the forward model for variations of the state $\mathbf{x}$ in the range of the solutions $\mathbf{x}_1$ and $\mathbf{x}_2$ of the individual retrievals. Since the individual retrievals are constrained with the same a priori estimate, with a reasonably “small” error, we do not observe an important degradation of the agreement between SR and CDF for different atmospheric conditions.

See the note provided as supplemental material. In the revised paper, the paragraph at lines 64-66 has been modified.

l76: I would like to suggest to introduce a new subsection directly at the beginning of Sect. 2. For example, "2.1 SR and CDF retrieval theory", or similar.

OK, this can be done.

Finally we decided to keep unchanged the sub-sectioning of sect. 2. This is because the theory reported at the beginning of Sect. 2 actually applies to both the SR and the CDF approaches, that are discussed later, in Sub-sect's 2.1.and 2.2.

l309-313: This might be another place in the paper suitable to discuss and motivate why only a single (perfect) scenario was selected for the retrieval experiments.

Yes, in the revised version of the manuscript, we will include a paragraph to further explain the rationale of this choice and we will complement the discussion with the results of the new test experiments mentioned above.

At the end of the paragraph we now mention the further tests based at mid- and tropical- latitudes included as supplemental material.

l320 and l374: Introduce a new subsection 5.1 ("Results for perfectly matching measurements") at the beginning of Sect. 5?

OK, this can be done.

Done.

l377-380: I may have missed it earlier in the paper, but when considering the horizontal mismatch of up to 26 km, did you also consider horizontal smoothing effects related to the IFOV of the FORUM and IASI-NG instruments?

No, the smoothing effect of the finite aperture of the IFOV (15 and 12 km for FORUM and IASI-NG, respectively) is not considered here, neither in the forward, nor in the inverse simulations. This choice is motivated by the fact that: a) we do not have a very high resolution (~1km) atmosphere / surface model to simulate realistic IFOV inhomogeneities and b) so far a detailed instrument model with the capability to predict the effect of IFOV inhomogeneities onto the measured spectral radiance is not available. In the revised paper, we will mention explicitly this choice.

Done, inserted a small paragraph thereafter.

l381-383 and l391-392: Why are different surface emissivity models for snow applied for FORUM and IASI-NG?

This is to emulate the mismatch between the measurements, i.e., the two instruments may not sample exactly the same surface area, thus the sounded snow may be different.

l416: Maybe clarify "For a specific test scenario _with perfect/most suitable atmospheric conditions_ ..."?

Yes, in the revised manuscript, this sentence will be modified, also considering the outcome of the new test experiments we carried out in the meantime.

Done, the conclusions were modified accordingly.

Technical corrections
l331: fix sentence ("...is the reference a coarse snow..."?)
l399-400: merge dangling sentence with previous or next paragraph
l402: "this latter" -> "the latter"

All the technical corrections will be implemented in the revised manuscript.

Done.

Thanks again for your kind support.

RC2: Comment on amt-2022-82, Joern Ungermann, 28 Jun 2022

GENERAL COMMENTS

The paper compares two different methods of fusing the measurements of the IASI-NG and FORUM satellites to derive atmospheric states. One operating on level 1 data, one operating on level 2 data. It is found that both methods deliver (under reasonable assumptions) equivalent results. Such, the method simpler to implement can be chosen.

The topic fits the journal well.

The paper is concise and well written. I recommend publication after addressing the comments below.

We thank Joern Ungermann for revising the manuscript and for the constructive comments. We decided to change our test experiment setup to address the reviewer's main comment reported here below. With this modification and with the integration of the results of two new test experiments at mid- and tropical- latitudes, we believe that now the results presented are more robust and consolidated than before.

MAJOR COMMENTS
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lines 327ff
The test profiles for the perfectly co-located measurements are generated using a (fixed) a priori profile perturbed by random vectors according to the CM 0.5 S_m. This is strange as the matrix S_m was designed to represent the typical differences between two mis-aligned FORUM and IASI-NG profiles, not to represent the typical variability of Antarctic profiles in general in this seasons. I would assume that such neighboring profiles exhibit - on average - only small differences whereas Antarctic profiles exhibit a large variety of shapes.
I would have expected a much larger variety of profiles here based on a different CM matrix. Such more diverse profiles could then be perturbed using 0.5 S_m to generate the two differing profiles for the second part of the study. Please adapt the study or elaborate why the current choice sufficiently captures the required variability of atmospheric states. I do not expect a different outcome, but the examination of 900 probably very similar profiles seems questionable.

We agree with this comment. Originally, we designed the test experiments as if the atmosphere was "ideally" sounded for 900 times in a very short time interval, thus the reference atmosphere was varying only within 0.5 $\mathbf{S}_m$ (i.e., the sounded atmosphere was considered almost constant). In the revised version of the work, we changed this approach and the reference atmosphere changes from sounding-to-sounding by a much larger amount, consistently with a covariance matrix $\mathbf{S}_s$ (computed from ERA5 profiles) that represents the seasonal variability of the Antarctic atmosphere throughout the whole Antarctic winter. As anticipated by the reviewer, the conclusions of the work do not change; however, with the new approach, the results rely on a more solid basis.

In the revised paper we adjusted the paragraph describing the new test approach. Fig's 2 and 5 now show also the variability of the profiles used for the generation of synthetic measurements. All tests were re-run and all the figures were updated with the new data.

SPECIFIC COMMENTS

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line 94: It would be interesting to note how exactly the modification is performed. I would assume by an additional factor in front of the a priori precision matrix as described by Rodgers or with, e.g., a factor and an identity matrix as is often used in numerical libraries?

We multiply the diagonal elements of the Hessian of the cost function (2), i.e., the inverse of matrix $\mathbf{S}_i$ of Eq.(5), by $(1+\lambda)$, where λ is the Marquardt damping factor. We will specify this detail in the revised version of the manuscript.

Done.

Line 285: Is the emissivity linearly interpolated between the grid points? Please specify.

Yes, spectral emissivity is linearly interpolated between the retrieval grid points. In the revised text, we will specify this detail.

Done.

Line 293ff: This paragraph sounds as if there are different S_a matrices being used depending on the use case, if only w.r.t. to the surface emissivity. This should be taken up in the mathematical notation (e.g. with an i index).

Actually, the same $\mathbf{S}_a$ is used for all test cases and for both the SR and the individual retrievals, so we do not think that an additional index is required. Like $\mathbf{S}_M$ (see eq. 21), $\mathbf{S}_a$ is a block-diagonal matrix, each block referring to a specific section of the state vector: T(z), Ts, H2O(z), O3(z), e(v). In the revised version of the paper, we will include this additional note.

We realize now that at line 296 we promise to show the a priori errors in the subsequent figures, while they are not actually shown… We apologize for this inconvenience, in the revised version of the paper we will include also a priori errors in the plots.

Probably we initially misunderstood this comment of the reviewer. While the method used to build the a priori error CM is the same for all the retrievals, the actual numerical values of the errors in $\mathbf{S}_a$ change from retrieval to retrieval for several reasons. First, as explained in the text, the error on the a priori emissivity depends on the retrieval type: FORUM-only, IASI-NG-only or Sinergystic Retrieval. Secondly, the absolute a priori errors of the H2O and O3 profiles are computed as a percentage value of their a priori estimate $\mathbf{x}_a$, thus, rigorously speaking, the values in $\mathbf{S}_a$ change at every test retrieval. We revised the whole text to resolve the inconsistency of the symbols $\mathbf{x}_a$ and $\mathbf{S}_a$.

Line 345ff: It is surprising that the nadir sounders seem to replicate the true profile near-perfectly (on average). Due to the spatial smoothing of the true profile, I would have expected, e.g., systematic discrepancies close to the local extrema of the temperature and water vapour profiles. I.e. there should be a difference between true and retrieved profiles, simply due to the lower spatial resolution of the retrieval result. Or was the true profile folded with an averaging kernel as well to compared within the same spaces? Is there another explanation for the excellent performance?

There are several factors contributing to the excellent performance of the average of 900 profiles:

- The reference, a priori and retrieved profiles are all represented on the same 61 pressure levels grid, thus there is no smoothing error owing to profile interpolations.
- Therefore, the smoothing error is uniquely originated by the use of optimal estimation with an a priori profile $\mathbf{x}_a$. Both $\mathbf{x}_a$ (lines 333 – 334) and the true profile $\mathbf{x}_{t1}$ (lines 327 – 330) are obtained by applying to $\mathbf{x}_0$ a "zero-mean" random perturbation that changes from a test retrieval to the next. Therefore, the average difference (or bias) between $\mathbf{x}_a$ and $\mathbf{x}_{t1}$ is very close to zero. This implies also a "zero-mean" random smoothing error that produces no bias on the retrieved profiles. Being random, the smoothing error is then damped in the averaging process.

These conditions will not be fulfilled in the case of real measurements, where the a priori atmosphere is usually taken from a model that may be represented on levels different from the retrieval grid and may include also small biases. However, this setup is functional in our study to investigate the small differences between the SR and CDF solutions.

Data Availability
Is the test data set too big (or restricted by licenses) to be placed on, e.g., Zenodo?

OK, we will upload the final data set to Zenodo: although rather large (~15Gb) the dataset does not exceed the max allowed dataset size for Zenodo (50Gb / dataset).

We have uploaded to Zenodo the reference atmospheres, the surface states and their variability, the mismatch error variance data and the noise error covariance matrices associated with the FORUM and IASI-NG measurements. Moreover, we have included all the relevant instrument characteristics and retrieval setup assumed in the test experiments presented in the paper. These data, if used as described in the paper, with forward, retrieval and CDF codes implementing the equations presented in Sect. 2, will generate results with the statistics illustrated in the plots of the paper. We did not include the inputs and the outputs of the individual retrieval / CDF runs because the data volume would have been rather large: we now have 900 runs (of retrievals from FORUM-only, IASI-NG-only and FORUM+IASI-NG measurements and the CDF product) repeated for the two cases with and without measurement mismatch and for three atmospheric scenarios (Antartica, Mid-latitude, Tropical). We doubt that such a huge dataset could be useful to potential users.

MINOR REMARKS
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line 23: errors -> error
line 97: It'd be helpful to associate the terms with the mathematical notation in the text. I.e. CMs S_i and AKMs A_i.
line 101: convergence -> x^hat_i
line 279: This notation does not express properly, that T(p_k) expresses a subvector T(p_1) to T(p_n). Perhaps {T(p_k)}_k=1..61 ? Why T and not consistently x_T ?

The minor corrections will be all included in the revised text.

The revised text includes all the above minor suggestions. To comply with the reviewer's last suggestion, we also changed the notation in Eq.(22) and adjusted accordingly the text thereafter.

Thanks again for your kind support.