Response to reviewers

We first wish to thank reviewer #2 for reading our manuscript so carefully and for raising so many interesting questions. Below we have numbered the reviewer questions from 1 to 37 and detailed our response and actions taken in regard to each question.

The author compares high-order integral formulations for the numerical solution of 2D Helmholtz transmission problem (arising eg in z-invariant time-harmonic Maxwell) with arbitrary complex wavenumber ratios, and sometimes corners. The main issues studied are accuracy (focusing on high accuracies close to machine precision), and robustness (existence of spurious solutions or eigenwavenumbers). The accuracy addressed includes that of evaluation of the potential and its gradient close to the surface, an important issue common to all integral equation methods. The author’s RCIP scheme for refined panels at corners is used. Errors are assessed by convergence, apart from the disc case.

Response: Thanks for an excellent summary of the paper.

The paper is of high quality, addresses a tricky problem using powerful tools, and is useful for the numerical PDE and optics/EM community. The techniques demonstrated require careful analytic work (Sec. 4) but are essentially unbeatable in terms of accuracy (close to machine precision), using small numbers of unknowns. The novelties include a new split for the hypersingular operator, and using difference kernels and the null-field method for accurate evaluation of the grad near the surface. There is not room to present all numerical details; hence I hope the author will include a URL to codes that others can try.

Response: Thanks for appreciating what we have done. And, in particular, thanks for understanding that there is not room to present all numerical details (most of which have already been explained in the various references). Actually, the program which produces Figure 20 has been available via an URL for about half a year. See:

http://www.maths.lth.se/na/staff/helsing/Tutor/demo19.txt

The other programs are similar, but of course we can make more programs available should there be a demand.

1) The writing and math is generally very clear. The paper has useful reviews on surface plasmons and their absorption at corners (Sec 6-7). Numerical results focus on eigenwavenumbers ($k_1$ values, for a fixed eps; maybe the introduction could emphasize this EVP as much as it does the scattering BVP?).

Response: Thanks for the suggestion to emphasize the eigenvalue problem aspect of our work more.
When we started this project, the intention was to write a short note where we summarized the most common integral equations for this scattering problem (the 2D Helmholtz transmission problem) in a unified notation and investigated them numerically for an inclusion with a corner, using the RCIP-accelerated Nyström discretization, under **plasmonic conditions**. With this we mean that $k_1$ is real and positive and $\varepsilon$ is real and negative.

The first point – to present the most common integral equations in a unified notation – felt important for a particular reason: when talking to colleagues at conferences etc., we have found that there often is a big confusion of what names like “the Müller-Rokhlin equation” exactly refer to. As the project progressed we found “forgotten” integral equations with good spectral properties and we decided to add some sections where the physics behind our problem was briefly discussed. There was also a need to analyze the kernels of various integral operators and the paper grew longer.

Eigenvalues, and in particular, false resonances and false near-resonances are important when analyzing the differences between various integral equation formulations for the transmission problem. Eigenvalue computations are also important when verifying programs for correctness (that the system matrix and it discretization is correct), since eigenvalues (for inclusions in the shapes of disks) can be obtained using semi-analytic methods.

But our numerical scheme is a scheme intended primarily for scattering problems. And the main topic of the paper is scattering under plasmonic conditions. It is true that, in our first few numerical examples, we do compute eigenvalues/resonances very accurately for reasons mentioned in the previous paragraph, but we do not have any new fast schemes for eigenvalue search. We simply use a combination of brute force and Broyden’s method as we have done before. See Section VI B of


In order maintain the focus of the paper we prefer not to further promote eigenvalue aspects of our algorithm, if that is OK.

although they also study absorption cross-sections. There are other minor confusions and mathematical issues to fix, and some vagueness about the take-home message for the various schemes. These are listed below along with various optional suggestions. If most of these are addressed I am very happy to recommend publication.

**Response:** OK. We will do our best to fix these issues.

2) In the intro, the author might want to cite Vico, Greengard and Ferrando, arxiv 1704.06741, who also address a large range of complex $\mu$ and $\varepsilon$ parameters.

**Response:** Yes, we are well aware of this paper on an integral equation for time harmonic Maxwell in 3D that is free of false resonances and we have read it many times (the DFIE). The scope of the paper is broader than
that of our paper in that the authors vary both $\varepsilon$ and $\mu$. Our plasmonic conditions correspond to $\mu = 1$ and $\varepsilon$ real and negative.

A problem with this paper, from our point of view, is that in its abstract it says that the DFIE is false-resonance-free for negative permittivities, while in equation (6) and in the text afterwards it says that negative permittivities are not included.

This is confusing, and we have asked one of the authors of the paper about it. The response we got was that the issue was unclear. So that is why we did not cite the paper. We simply did not know what to say about the properties of the DFIE under our plasmonic conditions. What should we say?

3) p.2: "An incorrect choice of integral equations or an inadmissible choice of eps inevitably leads to spurious resonances, or to no solution at all." Could this be split into two clear statements? Does it mean: for some eps, there is no solution to the BVP? Moreover, for the eps where there is a solution, a bad IE rep choice leads to spurious resonances? (numerical failure for a discrete set of eps?)

4) p.3: please state here if $k_1$ is real or complex.

5) When $k_1$ is not real, such as for an eigenwavenumber with $\text{Im}(k_1) \neq 0$, (8) no longer applies since $U^{sc}$ grows exponentially with $r$! This should be explained and if possible the correct mathematical radiation conditions given.

6) (9)-(10) look peculiar to physicists/engineers, who expect $\exp(i.\omega.\tau)$ Maybe write $\phi$, a general phase, instead of t?

7) (14) is twice the usual definition (in eg Colton and Kress works); this should be commented on.

Response: Thanks for pointing this out. We like the present definition because of its simpler appearance. In particular, it is clearer what the kernel of the operator is. But we agree that it could also be confusing. Action: We have now added a remark in Section 3.2 where we comment on the original appearance of these expressions in the Colton and Kress book.

8) Although (17), (18) are standard, it would be good to clarify that $\partial/\partial'_\nu$ means with respect to variation of $r'$ in the $\nu'$ direction.

9) p.5: unlike the KM1 system which arose from substituting the ansatz into the transmission conditions, the derivation of (32) is not obvious; the reader has to discover that doing the direct substitution gives a 1st-kind hypersingular system. I suggest adding a sentence to explain that particular null-fields must be added to give a 2nd kind system. Otherwise also the final sentence of Sec 5.3 is mysterious.
10) p.6: "by adding the null fields" & referring to equations the reader has to look up in KM might be more simply explained as: using the Greens representation formulae [eg cite Colton-Kress] in the complementary domain cases where they generate the zero field.

11) Maybe stating the two null field equations would allow the paper to clarify both the above issues?

12) Sec. 3.6: Since (36)-(37) are equivalent to (5)-(6) with a rescaling of $U$ in $\Omega_2$, it might be clearer to not mention (36)-(37) and instead simply rewrite the KR and MR representations for the case (5)-(6). The point seems to be that KR won’t be studied, and MR is equiv to KM1. So, I’m not sure why sec 3.6 is needed at all; maybe just cut?

Response: Well, the MR system is the same as the KM1 system with $c = 1$, but the boundary conditions and the right hand side are different as is the field representation. It is precisely these kinds of fine details that, in our experience, cause great confusion when talking to colleagues. So we rather not cut these equations out. See, further, the response to 1).

13) (65) I’m not sure what $|\epsilon| \neq \infty$ means - I think it’s unnecessary. Isn’t eps already given as a number, and therefore finite?

14) Sec 5.3: refers to "conditions of Sec 5.2", but I find this unclear. Does this mean (65), in which referring to that equation is clearer?

15) p.11 Sec 5.3: "null fields" means identically zero? State this more clearly (since "null field" is previously used to mean a Green’s representation formula that vanishes).

16) p.12 after (671): Sobolev-Besov - does this mean a usual Sobolev space? (I am not used to the Besov naming).

Response: Thanks for pointing this out. The Sobolev–Besov space is a generalization of the regular Sobolev space. Action: We have now changed from “Sobolev–Besov space” to “fractional Sobolev space”, which should be easier to understand, and added reference.

17) Sec 6 is a useful review, but for (72) a reference (Jackson’s book?) would be useful.

18) p.13 middle: it should be clarified that the condition (eps j -1) and transverse wavenumbers discussed only hold for planar surface Gamma. Somehow the opening sentence doesn’t state that the

19) For Sec 7.1-7.2 it might also be worth citing Greiser’s mathematical review on plasmonic eigenvalues (although it may not deal with corners): https://doi.org/10.1142/S0129055X14500056
20) (80) is for the case of $\Omega_2$ an infinite wedge, both inside and out? (ie same set of $r$ as (77)?)

21) After (84) it might be clearer to add that power is flowing as surface plasmons towards the corner, where it is absorbed. (Is the physical reason that the linear BVP physically breaks down at the corner? Otherwise corner rounding at the atomic scale would prevent power absorption for $\varepsilon$ negative real?)

22a) After Sec 6-8 I am left a bit confused if $\sigma_{abs}$ can be positive in the case of $\varepsilon$ negative and real, if the limit $\varepsilon + i\delta$ is taken.

22b) Is it correct to say that the order of limits between making a corner sharper vs taking $\delta \to 0^+$ matters?

Response: The referee is absolutely correct here. The order of limits matters enormously. We only consider infinitely sharp corners and let $\delta \to 0^+$. Should one take limits in the opposite order, that is, start with $\delta = 0$ and a rounded corner, and then increase the sharpness of the rounded corner, there would be no (pointwise) convergence of quantities like $\sigma_{abs}$ (when $\varepsilon$ is such that (71) holds). This phenomenon is discussed and illustrated (in the Laplace setting) in Section 10 of former Ref. [12]:

https://doi.org/10.1016/j.acha.2012.07.006

23) In Sec 8 all makes sense apart from (89), although it appears to be the "optical theorem" which is standard in physics books but I cannot find in Colton-Kress’s book. A more standard math reference than [18] would be useful.

24) Sec 9.1: it’s curious why the 2nd Calderon relation demands quite a large number of nodes for such a low $k$.

Response: We totally agree and wish we understood this phenomenon better. We have done extensive testing and the pattern is always the same on the “star geometry”: The 1st Calderon identity converges quickly with at least 16th order convergence while the 2nd identity has delayed and slightly more irregular convergence of order (perhaps) 14. The achievable accuracy for the two identities, however, is about the same and very high. Both identities are also very stable under increased overresolution. Maybe the slower convergence of the 2nd identity has something to do with $S_k$ being a smoothing operator while $T_k$ is a two times differentiating operator? Since we start with a smooth function $f(r)$, it is better for the final result to first “differentiate” and then “smooth”, rather than to do it in the opposite order. The most important thing, however, in the present paper is that the identity holds to high precision as the mesh is refined. Since we do not fully understand the difference in convergence between the two identities we refrain from commenting upon them in the text.
25) p.17: "As it turns out, the eigenwavenumbers of the KM1/GL system and those of the KM2 system are the same." Please clarify if this is a heuristic or analytic statement. Also to me this seems inconsistent with the statement that KM1/GL cannot have false eigenwavenumbers (Sec 5.3), yet Table 1 has false ones. I am confused.

26) Sec 9: how are eigenwavenumbers found in the complex $k_1$ plane? Since they play such a role in the examples, the method seems important to mention.

Response: OK. The eigenwavenumbers are found using a combination of brute-force random search and Broyden’s method: we choose a “search box” in the complex $k_1$-plane and measure the smallest eigenvalue of the discretized system matrix at an extremely large number of randomly placed $k_1$-points in that box. If we detect a particularly small eigenvalue we activate Broyden’s method and see if there is a zero of the smallest eigenvalue nearby. MATLAB’s built-in function `eigs` is used for finding eigenvalues. There may be more time-efficient methods, but this was the best we could think of. Action: We add a reference in Section 9.2 to one of our papers where we have used this “method” before and where a few more details of the method are explained.

27) Sec 9.2 - it might be worth mentioning that eps=2.25 corresponds to refractive index of 1.5, typical for glass at optical frequencies.

28) p.18 bottom and Figure 2: refer back to (67) for choice of c. If GL is a special case of KM1, how can GL have false eigenwavenumbers? It also needs to be stated what KM2 does here - is it the same as either GL or KM1?

Response: Yes, we agree that things could be clarified in Section 9.2. GL (now renamed KM0) is a special case of KM1. More precisely, KM0 corresponds to KM1 with the fixed choice $c = 1$, as stated in Section 3.5. Furthermore, the choice $c = 1$ guarantees that KM1 has no false eigenwavenumbers on the positive real $k_1$-axis when $\varepsilon$ is positive (according to (67)). So KM0 has no false eigenwavenumbers on the positive real $k_1$-axis when $\varepsilon$ is positive.

Now, in Figure 2, $\varepsilon$ is negative. Then $c = -i$ in KM1, according to (67), and KM0 and KM1 are no longer the same (KM0 always has $c = 1$). KM1 is still guaranteed to be free of false resonances on the positive real $k_1$-axis (from the theory of Kleinman–Martin and as confirmed by the numerical experiment) while KM0 now exhibits eight false resonances on the positive real $k_1$-axis for $k_1 \in [0, 10]$ (and only numerically demonstrated – there seems to be no theory for false resonances in KM0 under plasmonic conditions).

Neither for KM2 there is any theory for false resonances under plasmonic conditions. The behaviour of KM2, in this example, is very similar to that
of KM0 (that is why we forgot to mention it). The condition numbers of the system matrices in KM2 are similar to, but slightly lower than, those of KM0 and we found five false resonances for $k_1 \in [0, 10]$.

**Action:** New text is added in Section 9.2 that tells what KM2 does here and reminds the reader that KM0 and KM1 are not the same unless $\varepsilon$ and $k_1$ are positive. Two references back to (67) are added. Furthermore, an error is corrected in the first two paragraphs of Section 9.2: Figure 1 shows results for KM0 and KM2. This was not clear in the previous text and we apologize for that mistake, which may have caused confusion.

29) Sec 9: 16 digits seem to be quoted in all eigenwavenumbers. Are all such digits believed correct? If so, this should be stated.

**Response:** This is a good point. No, all digits are not always believed to be correct. In the numerical experiments presented, we typically get convergence to plus/minus one in the last digit. The results reported are our best guess (with regard to the last digit). Furthermore, even when we get very stable convergence also in the last digit, that is not a rigorous proof that the last digit is correct. Comparison with semi-analytic solutions on the unit circle confirms our numerical results (for the unit circle) with a relative precision of $4 \cdot 10^{-16}$. But these semianalytic solutions also involve non-trivial computations and it is unclear if they are more accurate than the estimates produced by our integral equation based codes. In conclusion, we only feel sure about the fifteen first digits in the eigenwavenumbers. Still, it could be useful to present our best guess for the last digit if someone is to repeat our experiments. **Action:** “eigenwavenumber” is replaced by “estimated eigenwavenumber” on 5 occasions. We also add a sentence in Section 9.2 where we state that the relative error estimate $4 \cdot 10^{-16}$ is indicative of the error in all presented eigenwavenumbers.

30) In the corner examples, quoting the number of panel refinement levels before RCIP might be useful.

31) Figure subplots are not labeled with (a), (b), etc... but are referred to in captions and text - please label. Also font sizes, especially for the log10 colorbar, should be bigger, since they communicate error level.

32) p.20: dynamics $\rightarrow$ dynamic range.

**Response:** Thanks for pointing this out. **Action:** “full color dynamics” has been replaced with “full dynamic color range”.

33) p.20 last line: accurate $\rightarrow$ relative (?)

**Response:** Yes, “ten accurate digits” is maybe not correct language. But “ten relative digits” also sounds strange. **Action:** We changed to “ten digit accuracy”.

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34) Fig.8(b): the color of points are hard to distinguish - make larger or use different symbols?

35) Could it be commented how RCIP (which uses geometric panel refinement) handles the plasmon waves which are also geometrically shrinking towards the corner? In the limit of approaching eps negative real, surely the waves do not die towards the corner (since they are carrying power towards the corner)? Does this prevent RCIP from converging?

36) In Sec 9, a couple of datapoints on solution and field evaluation times should be given. The reader doesn’t know if it is seconds or days.

37) The Conclusion needs a summary statement on which formulation, and which choice of c, should be used. The reader is confused, since KM1 seems best for robustness of the eigenproblem, but KM2 is best for accuracy of field evaluation close to the boundary. Should one be used and then the other if found to be robust? What is the big picture for users of the methods?