nature portfolio

Peer Review File

Computation of eigenfrequency sensitivities using Riesz projections for efficient optimization of nanophotonic resonators

Reviewers' comments:

Reviewer #1 (Remarks to the Author):

I appreciate this opportunity to give my comments on the manuscript entitled "Computation of eigenfrequency sensitivities using Riesz projections for efficient optimization of nanophotonic resonators". This is indeed a useful technique that can be widely applied to designing photonic resonators for various applications. In order to obtain eigenfrequency sensitivities, the authors proposed an alternative approach to direct evaluation of resonances by taking advantage of a Riesz projection for Maxwell's equation. Therefore, a significant boost in efficiency is expected, as is claimed. In the manuscript, a theoretical background, simulation protocols and examples with comparison with previous methods and publications have been presented. In addition, an improved Q-factor was found using the proposed approach. I would like to recommend this work, but after critical considerations of several points listed herein.

First of all, I think Eigen value problems applied to photonic systems are widely studied using various approaches. I agree the majorities would use commercial solvers like FEM or FDTD packages to solve for Eigen frequencies, which is time consuming. There are, to the best of my knowledge, other approaches that are based on a surface integral approach of Maxwell's equations, which considerably reduces computational time consumption. I would be interested to read discussion from the authors that also includes those approaches in the comparison. This would contribute to a more comprehensive overview of solving Eigen frequency problems in photonics.

Secondly, to make a more significant impact, Eigen frequency sensitives are useful especially for nanofabrication; to lower sensitivities to geometries of Eigen frequencies etc. could help better control of qualities of nanophotonic devices. I would encourage the authors to search for a few challenging high-Q resonator projects in literature and evaluate the value of this current methods in their design and fabrication stages. Although, I also realize that this current research has been targeted on a concreate example from a publication on Science, which is a relatively simple structure aiming for nonlinear optical applications. Other more interesting examples involve but not limited to high-Q resonators for active polarization synthesis, active phase modulation etc. that would have a much wider potential in applications.

Thirdly, the comparison is presented in figure 3. An intuitive understanding is that the boost in computation efficiency is gained through the reusing of LU decomposition of matrix A in the manuscript. Indeed, it would need to inverse A in a FEM solver for multiple times, in order to obtain partial differentials of a quantity with respect to all parameters. Does the authors mean a direct inverse of A or A can also be solved iteratively sometimes, which is both time efficient and RAM efficient. Although, I notice a gigantic 1.5TB RAM was used in the paper, would the authors comment if RAM is in general a limitation for large photonic system in the proposed approach? And how does it scale in computation time with respect to problem size.

In addition, I would appreciate a detailed splitting of computation time scaling for each stage during computation of Eigen frequency sensitivities, depending on problem size, for example.

Technically, the numerical method depends on a contour integral. How is the stability of this approach depending on integral partition?

Eq.5 reuses LU decomposition of A. If I understand correctly, this is an assumption that a perturbation is used for parameters. Is A being perturbed also an assumption? On the other hand, what happens if A changes quickly even if parameters are perturbed.

How does it compare with classical perturbation approaches in estimating resonance frequencies in computation efficiencies? In my experience using the perturbation method, often an overlap integral is

sufficient, although more often finding the right integral is challenging when model profiles are needed once or twice, which can also be analytically implemented in very simple cases.

In the end, I think it would make this work more popular if source codes and tutorials are provided with the manuscript in some form of supplementary documents, if not presented already.

Thanks,

Reviewer #2 (Remarks to the Author):

In this work, the authors presented a method to compute the eigenfrequency sensitivity of resonances in non-Hermitian systems. The theory is based on Riesz projections, which has been proposed by the authors several years ago to compute the decay rate of a resonance. This work expands the existing work, and provides a theatrical framework for computing the sensitivity of the resonances. The method is argued to be much more efficient than finite-difference methods and can be used to optimize the Q factors of a resonator.

1. My major concern about the work is that, since the authors have previous work on a related topic, PHYSICAL REVIEW A 98, 043806 (2018), it seems that one can simply follow the published work and compute the sensitivity of the decay rate of a resonance, and thus obtain the eigenfrequency sensitivity. It should be valuable to at least comment on the connections between these two works.
2. It seems that the initial guess of the eigenfrequency needs to be provided by other methods. Therefore, is it true that the method only provides a way to optimize around a certain resonance, but not a global optimization?
3. It would be very interesting if the author can add a comparison between this analytical approach with the gradient descent method, which can also be used to optimize the structural performance in high dimensional parameter space.

Reviewer #3 (Remarks to the Author):

In this manuscript the authors report a new approach for computation of sensitivities of nanophotonic resonances. Their procedure, which essentially combines Riesz projections and direct differentiation, does not require solving the resonance problem directly. Its performance has been compared to the finite differences approach for a chosen nanophotonic application, and shown to be superior, in particular for calculation of large number of calculated sensitivities. Lastly, their method is shown to be useful for Q-factor optimization.

I find the work presented in the manuscript to be relevant, the paper is clearly written, and the results presented seem to be done correctly and sound. However, I would like to make one comment. I believe that properly addressing it would improve the quality of the paper.

The authors have developed the method for sensitivity calculations with special emphasis on nanophotonic applications. However, the approach seems to be more general and not restricted to a specific eigenproblem, which authors note only very briefly in the last paragraph of their manuscript. I would appreciate if the authors could be more elaborate and try to give some broader context on this issue.

To summarize, I think the manuscript does present relevant results in the field and should be published after responding to the comment above.

Computation of eigenfrequency sensitivities using Riesz projections for efficient optimization of nanophotonic resonators

Point-by-Point Response to Reviewers Communications Physics

June 9, 2022

Manuscript: COMMSPHYS-22-0308-T

Authors: Felix Binkowski, Fridtjof Betz, Martin Hammerschmidt,
Philipp-Immanuel Schneider, Lin Zschiedrich, Sven Burger

We would like to thank all reviewers for reviewing our manuscript and for their positive feedback with helpful points of critics, remarks and questions.

Reviewer 1 recommends the manuscript for publication in Communications Physics when their raised points of critics and questions are considered. The reviewer points out that the presented approach is a useful technique which can be widely applied in nanophotonics.
The major concern of Reviewer 2 is that the connection between the presented approach for

computing eigenfrequency sensitivities and previous works of the authors on the topic Riesz projections is not commented sufficiently in the manuscript. We agree with the reviewer that this connection should be more clearly stated in the manuscript.
Reviewer 3 finds the work to be relevant and that the paper is clearly written. The reviewer indicates that the presented approach is more general and can be also applied to eigenproblems other than those in nanophotonics. Reviewer 3 believes that this issue should be discussed in more detail and that the manuscript should be published afterwards.

In the following, we have addressed all reviewer concerns, remarks, and questions. Reviewer comments are in black, answers are in blue, and manuscript text changes are in red color. We further attached a version of the manuscript where all changes are marked and new text is indicated with red color. The references in this response letter correspond to the references in the new manuscript.

Response to Reviewer 1

Reviewer 1: I appreciate this opportunity to give my comments on the manuscript entitled "Computation of eigenfrequency sensitivities using Riesz projections for efficient optimization of nanophotonic resonators". This is indeed a useful technique that can be widely applied to designing photonic resonators for various applications. In order to obtain eigenfrequency sensitivities, the authors proposed an alternative approach to direct evaluation of resonances by taking advantage of a Riesz projection for Maxwell's equation. Therefore, a significant boost in efficiency is expected, as is claimed. In the manuscript, a theoretical background, simulation protocols and examples with comparison with previous methods and publications have been presented. In addition, an improved Q-factor was found using the proposed approach. I would like to recommend this work, but after critical considerations of several points listed herein.

Answer 1.0: We thank the reviewer very much for their positive feedback and for pointing out that our presented approach is a useful technique. In the following, we have addressed all points and questions.

Reviewer 1: First of all, I think Eigen value problems applied to photonic systems are widely studied using various approaches. I agree the majorities would use commercial solvers like FEM or FDTD packages to solve for Eigen frequencies, which is time consuming. There are, to the best of my knowledge, other approaches that are based on a surface integral approach of Maxwell's equations, which considerably reduces computational time consumption. I would be interested to read discussion from the authors that also includes those approaches in the comparison. This would contribute to a more comprehensive overview of solving Eigen frequency problems in photonics.

Answer 1.1: The reviewer is correct, there are also approaches for solving eigenproblems based on using boundary integrals, which can be also very efficient with respect to computation time. In our manuscript, the focus is not on computing eigenfrequencies and eigenvectors, but on computing eigenfrequency sensitivities. For this reason, we have omitted a discussion of general eigensolvers. However, we agree with the reviewer that a comment on numerical discretization techniques would be of interest for readers and have therefore included text on this topic in the first paragraph of Section II.C: "Note that also other methods can be used for numerical discretization. In the field of nanophotonics, common approaches are, e.g., the finite-difference time-domain method, the Fourier modal method, or the boundary element method [12,28]." We have added the reference [Comput. Phys. Commun. 183, 370 (2012)] to the manuscript, where an introduction on the boundary element method, including theory, and details on its numerical implementation can be found.

Reviewer 1: Secondly, to make a more significant impact, Eigen frequency sensitives are useful especially for nanofabrication; to lower sensitivities to geometries of Eigen frequencies etc. could help better control of qualities of nanophotonic devices. I would encourage the

authors to search for a few challenging high-Q resonator projects in literature and evaluate the value of this current methods in their design and fabrication stages. Although, I also realize that this current research has been targeted on a concrete example from a publication on Science, which is a relatively simple structure aiming for nonlinear optical applications. Other more interesting examples involve but not limited to high-Q resonators for active polarization synthesis, active phase modulation etc. that would have a much wider potential in applications.

Answer 1.2: We would like to thank the reviewer for their recommendation for the text. We have added a reference to a high-Q resonator review [B. Wang et al., High-Q Plasmonic Resonances: Fundamentals and Applications, Adv. Opt. Mater. 9, 2001520 (2021)] and text in the introduction: "For example, high-Q resonators can boost the brightness of quantum emitters, the sensitivity of sensors, or the emission processes in plasmonic lasers [11]." And, a second text in the next paragraph: "Nanoresonators with high Q-factors have been theoretically presented, but fabrication of these resonators is a limiting task [11]. The sensitivity analysis of eigenfrequencies can show a way to reduce the sensitivities of the Q-factors. This can support the nanofabrication processes."

Regarding the second remark of the reviewer: We have taken a relatively simple example from the literature for presenting our method, since the focus of our manuscript is on the introudction of the numerical method of an eigenvalue solver which allows to also compute partial derivatives. A simple example thereby allows the reader to easily understand the method. Nevertheless, the investigated nanoresonator is also very interesting from a physical point of view. The Q-factor of the original structure from [Science 367, 288 (2020)] is based on a bound-state-in-the-continuum (BIC) and such phenomena are currently much discussed in the literature; see, e.g., [Bound states in the continuum, C. W. Hsu et al., Nat. Rev. Mater. 1, 16048 (2016)].

Reviewer 1: Thirdly, the comparison is presented in figure 3. An intuitive understanding is that the boost in computation efficiency is gained through the reusing of LU decomposition of

matrix A in the manuscript. Indeed, it would need to inverse A in a FEM solver for multiple times, in order to obtain partial differentials of a quantity with respect to all parameters. Does the authors mean a direct inverse of A or A can also be solved iteratively sometimes, which is both time efficient and RAM efficient. Although, I notice a gigantic 1.5TB RAM was used in the paper, would the authors comment if RAM is in general a limitation for large photonic system in the proposed approach? And how does it scale in computation time with respect to problem size.

Answer 1.3: We thank the reviewer very much for their remarks and questions. The reviewer is correct, in the manuscript, the computation efficiency is gained due to reusing the LU-decomposition of the FEM system matrix $A(\omega_k)$: We compute, for all integration points ω_k, which lie in the complex frequency plane, an LU-decomposition of $A(\omega_k)$. With these LU-decompositions, the sensitivities $\partial E/\partial p_i$ with respect to several parameters can be computed by using Eq. (5) for the different parameters p_i,

$$LU\frac{\partial E}{\partial p_i} = \left(\frac{\partial f}{\partial p_i} - \frac{\partial A}{\partial p_i}E\right),$$

which is equivalent to

$$\frac{\partial E}{\partial p_i} = A^{-1}\left(\frac{\partial f}{\partial p_i} - \frac{\partial A}{\partial p_i}E\right).$$

This approach can only be used when a right hand side f is present, i.e., typically in light scattering problems. For resonance problems, no source term is present, and therefore this approach may not be applicable. However, when contour integral methods are exploited, then resonances (and their sensitivities) can also be computed by solving linear systems. This very powerful connection of the direct differentiation approach given by Eq. (5) and contour integration (in form of Riesz projections) is the main idea of the manuscript.

In principle, the linear system $AE = f$ could also be solved using iterative methods. However, to the best of our knowledge, this is typically inefficient because a suitable preconditioner is

required for iterative methods and multigrid methods for obtaining such a preconditioner are often difficult to realize (e.g., for Maxwell's equations in frequency ranges where the computational domain includes several or many wavelengths in each dimension). The reviewer is correct: For the case that one would apply iterative solvers, the RAM requirements would decrease compared to an LU-decompostion. In order to explain the approach with more detail and to answer this question also for the reader, we have extended the description in Section II.C; please see also Answer 1.6.

Furthermore, we agree with the reviewer that RAM is a general limitation for large photonic systems. However, also the CPU time for solving the large linear systems is a limitation, where the CPU time needed for the LU-decomposition is significant compared to the time spent for matrix assembly. The reason that we used a system with 1.5 TB RAM is that we performed computations in parallel. In this study, we have investigated various computation settings: rotational symmetric cases on a 2D discretization mesh, and full 3D cases (Fig. 3), on different accuracy levels (convergence study in Fig. 2(d,e), and for many parameter combinations in the optimization run (Fig. 4). Each of these settings leads to a different memory consumption, e.g., in the rotational symmetric cases between 1 GB and 30 GB, depending on accuracy, and in the 3D cases sometimes more than 100 GB. The reviewers' question has indicated to us that our previous statement on the total memory of the used computer was rather misleading, especially as this RAM of 1.5 TB has never fully been used by a single computation. We have therefore omitted this statement from the caption of Fig. 3. We thank the reviewer for the remark. We further note that we have now also included the reference [35], which shows the source code for performing the simulations in order to recompute the results of the manuscript. Memory requirements for the specific chosen accuracy settings can then also be obtained by the interested reader.

We note that, when solving resonance problems with material dispersion (nonlinear eigenproblems) without contour integration, an Arnoldi method with auxiliary fields is usually used; see, e.g., [Phys. Rev. B 97, 205422 (2018)]. The auxiliary fields increase the dimen-

sion of the problems and thus also the memory requirements. When using contour integral approaches, as in our manuscript, auxiliary fields are not needed because linear systems for certain complex frequencies are solved (see also discussion in Ref. [24]).

Reviewer 1: In addition, I would appreciate a detailed splitting of computation time scaling for each stage during computation of Eigen frequency sensitivities, depending on problem size, for example.

Answer 1.4: We have added information on the splitting of the computation time in the second paragraph of Section III.B: "For $N = 5$, the CPU time required to solve the linear system of equations, which includes the LU-decomposition, takes 81 % of the accumulated CPU time. In the rotational symmetric case, the time for solving the linear system is negligible."

Reviewer 1: Technically, the numerical method depends on a contour integral. How is the stability of this approach depending on integral partition?

Answer 1.5: We use a trapezoidal rule on circular contours with equidistant partition for the numerical realization of the contour integrals. This leads to exponential convergence, which we have noted in the last paragraph of Section II.C. This numerical quadrature rule is well known and often used for contour integration on circles or ellipses. It is stable and convergence tests have been performed in other works, e.g., in Ref. [24] or in [Linear Algebra Its Appl. 436, 3839 (2012)].

Reviewer 1: Eq. 5 reuses LU decomposition of A. If I understand correctly, this is an assumption that a perturbation is used for parameters. Is A being perturbed also an assumption? On the other hand, what happens if A changes quickly even if parameters are perturbed.

Answer 1.6: We thank the Reviewer for pointing out that the description of this critical point in the manuscript was not precise enough. We have therefore modified the text, in the second paragraph of Section II.C. The method we use for computing the partial derivatives is not a perturbation approach, but it relies on direct computation of the partial derivatives. In order

to make this more clear to the reader introduce LU decomposition in the text: "In a first step, instead of directly computing A^{-1}, an LU-decomposition of A, which can be seen as the matrix variant of Gaussian elimination, is computed to efficiently solve the linear system $AE = f$. In the FEM context, this step is usually a computationally expensive step in solving scattering problems, so reusing an LU-decomposition can significantly reduce computational costs. In a second step, the partial derivatives of the system matrix, $\partial A/\partial p_i$, and of the source term, $\partial f/\partial p_i$, are obtained quasi analytically, i.e., with negligible computational effort. Then, $A = LU$, E, $\partial A/\partial p_i$, and $\partial f/\partial p_i$ are used to compute $\partial E/\partial p_i$ in Eq. (5). The LU-decomposition can be used to obtain both E and $\partial E/\partial p_i$."

Reviewer 1: How does it compare with classical perturbation approaches in estimating resonance frequencies in computation efficiencies? In my experience using the perturbation method, often an overlap integral is sufficient, although more often finding the right integral is challenging when model profiles are needed once or twice, which can also be analytically implemented in very simple cases.

Answer 1.7: If we would like to apply classical perturbation theory, then we would compute the left and right eigenmodes of the eigenproblem. This can be a computationally expensive task since they are generally not identical for non-Hermitian problems. In addition, the eigenmodes must be appropriately normalized, which can also increase the computational cost. On the other hand, the computation of the left and right eigenmodes is not necessary in the case of the Riesz projection approach. This means that the Riesz projection approach is very different from the classical perturbation theory approach.

However, we did not benchmark between these two methods. We believe that each approach may have advantages for certain problems.

Reviewer 1: In the end, I think it would make this work more popular if source codes and tutorials are provided with the manuscript in some form of supplementary documents, if not presented already.

Answer 1.8: We thank the reviewer very much for this feedback improving our manuscript.

According to their suggestion, we have prepared source code and simulation results and will publish it on the open repository Zenodo. This publication comprises a basic example and a script for a Q-factor optimization. We have added the corresponding reference to the manuscript, at the end of Section III.A: "Exemplary source code for the Riesz projection DD method and simulation results are presented in Ref. [35]."

Response to Reviewer 2

Reviewer 2: In this work, the authors presented a method to compute the eigenfrequency sensitivity of resonances in non-Hermitian systems. The theory is based on Riesz projections, which has been proposed by the authors several years ago to compute the decay rate of a resonance. This work expands the existing work, and provides a theatrical framework for computing the sensitivity of the resonances. The method is argued to be much more efficient than finite-difference methods and can be used to optimize the Q factors of a resonator.

1. My major concern about the work is that, since the authors have previous work on a related topic, PHYSICAL REVIEW A 98, 043806 (2018), it seems that one can simply follow the published work and compute the sensitivity of the decay rate of a resonance, and thus obtain the eigenfrequency sensitivity. It should be valuable to at least comment on the connections between these two works.

Answer 2.0: We thank the reviewer very much for this suggestion for the manuscript. We agree with the reviewer, there is a connection between this manuscript and the method presented in [Phys. Rev. A 98, 043806 (2018)]. In [Phys. Rev. A 98, 043806 (2018)], Riesz projection have been introduced to compute modal expansions. It has been shown that contour integration can be used to obtain the expansion terms (including the expansion coefficients). On the other hand, the present manuscript is not about modal expansions, but it is about calculating the eigenfrequencies and their sensitivities. By simply following [Phys. Rev. A 98, 043806 (2018)], it is not clear how to compute the sensitivities with Riesz

projections. Furthermore, [Phys. Rev. A 98, 043806 (2018)] shows nothing about the direct differentiation approach shown in Eq. (5) in the present manuscript. The connection between Riesz projections, where essentially scattering solutions are computed, and the direct differentiation approach is the main idea of the present manuscript.

In order to make this point more clear to the reader of the manuscript, we have added text to the manuscript, at the end of Section II.B, where we have commented the connection of the present work and previous works: "Note that Riesz projections can also be used to compute modal expansions of physical observables, where scattering solutions are expanded into weighted sums of eigenmodes [26]."

And, at the end of and Section II.C: "Equation (4) and its numerical implementation exploiting Eq. (5) are the main results of this work and represent the difference from previous works on Riesz projections; cf. Ref. [26]."

Reviewer 2: 2. It seems that the initial guess of the eigenfrequency needs to be provided by other methods. Therefore, is it true that the method only provides a way to optimize around a certain resonance, but not a global optimization?

Answer 2.1: We thank the reviewer for this interesting question. The here presented approach can be extended to the case where several eigenfrequencies are inside a contour in the complex plane. Then, no a-priori knowledge on the position of a certain eigenfrequency is required. Riesz projections can be used to compute all eigenfrequencies lying inside the contour and their sensitivities. There is a note on that at the end of Section II.B.

Reviewer 2: 3. It would be very interesting if the author can add a comparison between this analytical approach with the gradient descent method, which can also be used to optimize the structural performance in high dimensional parameter space.

Answer 2.2: We have indeed also implemented and tested a gradient descent method. The result was that this approach performed much worse than the Bayesian optimization approach used in the manuscript. The problem was that gradient descent optimization leads to being stuck in local minima. Bayesian optimization is a global optimization approach

where local minima can also be left and it is possible to explore other regions for the target quantity.

We believe that including a comparison between a gradient descent optimization and a Bayesian optimization into the manuscript is out of the scope of the manuscript. In principle, the Riesz projection DD method (which is the main result of our manuscript) can be used for any optimization approach which is based on using sensitivity information. We have added a note regarding this issue to the manuscript, at the beginning of Section II.C: "However, other optimization approaches could be used as well."

Note that, in addition, we have also implemented the finite difference method, which can also be used for gradient descent optimization and Bayesian optimization. However, computing sensitivities with finite differences requires much more computational time than computing sensitivities using the Riesz projection DD method. This is shown in Fig. 3.

Response to Reviewer 3

Reviewer 3: In this manuscript the authors report a new approach for computation of sensitivities of nanophotonic resonances. Their procedure, which essentially combines Riesz projections and direct differentiation, does not require solving the resonance problem directly. Its performance has been compared to the finite differences approach for a chosen nanophotonic application, and shown to be superior, in particular for calculation of large number of calculated sensitivities. Lastly, their method is shown to be useful for Q-factor optimization.

I find the work presented in the manuscript to be relevant, the paper is clearly written, and the results presented seem to be done correctly and sound. However, I would like to make one comment. I believe that properly addressing it would improve the quality of the paper. The authors have developed the method for sensitivity calculations with special emphasis

on nanophotonic applications. However, the approach seems to be more general and not restricted to a specific eigenproblem, which authors note only very briefly in the last paragraph of their manuscript. I would appreciate if the authors could be more elaborate and try to give some broader context on this issue.

To summarize, I think the manuscript does present relevant results in the field and should be published after responding to the comment above.

Answer 3.0: We thank the reviewer very much for stating that our work is relevant and that the manuscript is clearly written. We also thank the reviewer for their comment regarding the generality of the approach presented. We agree with the reviewer and think that a comment on this can improve the manuscript. Accordingly, we have added, at two important positions, new text.

In the abstract: "The theory is based on Riesz projections and the approach can be applied to compute partial derivatives of the complex eigenfrequencies of any resonance problem. Here, the method is derived for Maxwell's equations.". At the end of Section II.C: "Note that the Riesz projection DD method is not limited to the field of nanophotonics, but can be applied to other eigenproblems as well. Maxwell's equations can be replaced by another partial differential equation, and then instead of the analytical continuation of the electric field **E**, the analytical continuation of another quantity is evaluated for the contour integration.".

Conclusion

We would like to thank the reviewers again for their helpful comments and questions. We believe that with the modifications, with the answers to the reviewers, and with the additional data and software the manuscript has been improved, and we hope that it is now suitable for being accepted for publication in Communications Physics.

REVIEWERS' COMMENTS:

Reviewer #1 (Remarks to the Author):

Dear Authors,

I appreciate the efforts that significantly improved the clarity of the paper. I think it is ready after minor revisions where necessary. Also, please allow one last follow-up comment regarding the computational efforts of figure 3. It showed linear trends in all three computations with respect to the problem size N. According to my personal experience, this is not quite linear for the finite difference method, especially when size of a problem grows into an a-hundred-Gigabyte-memory problem. Would you please leave a comment on that as well?

Many thanks,

Reviewer #2 (Remarks to the Author):

I appreciate the authors' response. The manuscript is satisfactory and can be accepted.

Reviewer #3 (Remarks to the Author):

The authors have responded to my comments, and I recommend their manuscript for publication in Communications Physics.

Computation of eigenfrequency sensitivities using Riesz projections for efficient optimization of nanophotonic resonators

Point-by-Point Response to Reviewers Communications Physics

July 8, 2022

Manuscript: COMMSPHYS-22-0308A

Authors: Felix Binkowski, Fridtjof Betz, Martin Hammerschmidt,
Philipp-Immanuel Schneider, Lin Zschiedrich, Sven Burger

We would like to thank all reviewers for their efforts and for recommending publication of our manuscript.

Reviewer 1 states that the last revision has significantly improved the clarity of the manuscript. The reviewer has one additional question, which we consider in the next part of this answer letter. **Reviewer 2** and **Reviewer 3** recommend publication of the revised manuscript.

In the following, the reviewer comment is in black, our answer is in blue, and the manuscript text change is in red color.

Response to Reviewer 1

Reviewer 1: I appreciate the efforts that significantly improved the clarity of the paper. I think it is ready after minor revisions where necessary. Also, please allow one last follow-up comment regarding the computational efforts of figure 3. It showed linear trends in all three computations with respect to the problem size N. According to my personal experience, this is not quite linear for the finite difference method, especially when size of a problem grows into an a-hundred-Gigabyte-memory problem. Would you please leave a comment on that as well?

Answer 1.0: We thank the reviewer for this follow-up comment. In the numerical experiments corresponding to the computational effort, we have sequentially added partial derivatives (this is N in our manuscript). In the case of the (central) finite difference method, this means that for each additional partial derivative we have to solve two additional problems around the unperturbed problem. The problem size of these perturbed problems is usually the same as that of the unperturbed problem because the step size for the finite difference method is small. This leads to a slope of 200 % for the finite difference method with a linear trend.

We thank the reviewer for this question and we have included a sentence to the manuscript for clarification, in the Section "Performance Benchmark": "In the case of using finite differences, the computational effort has a slope of about 200 % because for each sensitivity two additional problems with typically the same dimension as the unperturbed problem have to be solved."

Conclusion

We would like to thank the reviewers again for their very helpful comments that improved our manuscript.