Dear Reviewers,

Thank you for your conscientious reviews and helpful feedback for how to improve the manuscript. This report contains a summary of the changes we have made in response. Further, as requested by the Papers Chairs, changed text in the new manuscript has been colored red.

The coordinator summary indicated we should address the following issues:

**1. Provide visualizations for comparison**

What was suggested: Visualizations that help assess error during reconstruction.

What we did: We prepare FTLE visualizations derived from both Lagrangian*Dist* and Lagrangian*Local* flow maps for each data set.

**2. Provide source code**

What was suggested: Publish a sample or source code under an open-source license.

What we did: In situ Lagrangian analysis capabilities for integration with a simulation code can be accessed via Ascent: <https://github.com/Alpine-DAV/ascent.git>

Single-node shared-memory implementation is available via VTK-m: https://gitlab.kitware.com/vtk/vtk-m/-/blob/master/vtkm/filter/Lagrangian.h

**3. Address additional issues raised by reviewers**

What was suggested: Reviewing individual reviews and implementing suggestions for improving the manuscript.

What we did: We address the reviewer points in the remainder of this document. That said, the reviewers caught several typos, and each of these were fixed. Such changes are not marked red. Finally, we received comments about improving captions. Each of these captions were improved and marked red in the new manuscript. That said, they are not discussed further below.

Of note, we had to remove some sub-figures and one paragraph, to meet the 10-page limit. Those removals are described at the end of this document. Finally, we also did a full grammar review (including issues with verb tense) and we have not highlighted such changes in red.

Best regards,

Authors of Scalable In Situ Computation of Lagrangian Representations via Local Flow Maps

**EGPGV 2021 Revision Report – Submission 1005**

**We use blue font to mark statements we viewed as revision comments from the reviewers. Our responses follow these comments in red.**

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**Reviewer 1**  
  
  Overall Rating [Early Submission]  
  
    Probably accept: I would argue for accepting this paper.  
  
  Expertise [Early Submission]  
  
    Passing Knowledge  
  
  Summary [Early Submission]  
  
    The paper proposes a communication-free model to compute flow maps in situ and compares that to the approach proposed in [ACG\*] that does require communication. The approach is based on computing only local flow maps and just ignoring particles crossing domain boundaries. The respective trajectories are instead interpolated from valid trajectories on adjacent processors during post-hoc analysis. The error from that is analyzed theoretically and in practice by comparing (amongst others) to ground-truth trajectories obtained using the approach from [ACG\*].  
  
  Contribution [Early Submission]  
  
    The authors present a very simple strategy to increase scalability of particle advection with Lagrangian flow maps on distributed memory systems, namely, by just discarding particles that cross domain boundaries. During post hoc analysis, this is accounted for by interpolating adjacent trajectories from neighboring compute ranks. This is obviously a very simple optimization; the authors very thoroughly evaluate the error from that wrt. to storage interval, grid resolution, different data sets, comparisons to both Eulerian and Lagrangian-with-communication ground truth methods, etc. and show that the approach is viable for a wide variety of configurations.  
  
  Clarity of Exposition [Early Submission]  
  
    The paper is well written. The following are only some minor remarks.  
  
    - Figure 1 I found a bit hard to comprehend; specifically, because of the description in the text that the flow maps are denoted FX->Y, and X and Y customarily not used for time / storage intervals. F presumably means snapshot file? The figure seems to be based off of Figure 2 in [ACG\*], where the concepts are explained in more detail. The figure and its description should be edited for clarity.

Thank you for your feedback. We address this confusion by updating the figure. We note a second reviewer also found this figure could be improved. Thus, we revised the figure completely. We hope the new presentation along with the caption is more readable and provides an idea of the baseline approach taken for Lagrangian analysis.

    - Figure 3 (a)-(d) are never referenced in the text. (b) and (d) presumably depict the Delaunay triangulations mentioned in Section 3.4, but this is not mentioned in the caption.

Thank you for bringing the lack of a reference to our attention. We now reference the subfigures in Section 3 and connect figures (b) and (d) to Section 3.4 in the caption of the figure itself.

     - In general, please provide more informative figure captions. When devising those, imagine a reader skimming through only the figures and captions; in the best case, the gist of the paper should be comprehensible to them from just the captions.

Thank you for this constructive feedback. We address this by improving our captions for several Figures across the manuscript. We mark these captions with red text in the manuscript.

    - Section 5.3: Typo: Lagrangian\_{D}ist

We have addressed this typo.  
  
    - Figure 3 (b) and (d): do the triangulations really reach across boundaries? The text in Section 5.3 suggests otherwise ("a Delaunay triangulation is per- formed using CGAL [CGA20] on a local cluster"). Please define what you mean by "local cluster" and clarify in the text / caption.

Thank you for pointing this issue out. We believe the confusion arises from the node boundaries in (b) and (d) of the notional example. We address this issue by correcting the figures (we remove the boundaries) and mention using a global Delaunay triangulation in the caption. Further, we change our “local cluster” to “single-node workstation” for clarity.

  Quality of References [Early Submission]  
  
    I can't identify any missing references, but I only have passing knowledge in this area and am not too familiar with the complete state of the art.  
  
  Reproducibility [Early Submission]  
  
    The methods should be reproducible, possibly by also referring to [ACG\*].  
  
  Evaluation [Early Submission]  
  
    Yes, the method is very thoroughly evaluated. My only critique is that the evaluation only presents statistics, w/o giving a sense of the visual error that can be observed. I understand that the error will not manifest as artifacts in the visualization but rather trajectories just being "wrong" or missing when for example the velocity is very high. Nevertheless, a visual comparison based on a post hoc analysis and pointing out where the visualizations differ (e.g., for a case where the method works well, and for a case where it doesn't, like the Jet Flow data set) would be highly appreciated.  
  
  Explanation of Recommendation [Early Submission]  
  
    The paper presents a very simple optimization to improve scalability of in situ flow map communication, namely just performing no communication whatsoever across ranks assigned to the spatial domain composition.  
  
    Pros:  
    - The authors provide a comprehensive study of the error resulting from that, and the increase in scalability observed; the error and scalability studies are very thorough, take different types of configurations into account.  
    - The evaluation stresses configurations that result in large error (e.g., large storage intervals or data sets with high velocity) and thereby uncover the (obvious) limitations of the method; it is shown that for a wide variety of data sets the error is acceptable.  
  
    Cons:  
    - Figures and captions are a bit hard to read; in the best case, the gist of the paper should be comprehensible from just the figures and captions.  
    - Apart from the measured error, I'm missing a 3D visualization showing the impact in terms of a ground truth comparison and using post hoc analysis.

Thank you for the feedback. We address the first issue by improving our descriptions in the captions. This is valuable feedback that we will carry forward to future works as well. We address the second issue by performing post hoc analysis using the extracted Lagrangian flow maps to produce 3D FTLE visualizations enabling a comparison and visualization of the possible impacts of using a communication-free model.

    I understand that this optimization is really a very simple one; nevertheless, I feel that the study is interesting, contributes to the state of the art, and is well suited for EGPGV. Generally, the pros outweigh the cons for me. The latter (figures and captions, 3D visualization to show the error for some assorted data sets and configurations) should be addressable in a revision  
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**Reviewer 2**  
  
  Overall Rating [Early Submission]  
  
    Borderline: The strengths and weaknesses balance for this paper.  
  
  Expertise [Early Submission]  
  
    Knowledgeable  
  
  Summary [Early Submission]  
  
    The authors presented a variation of the technique introduced in Agranovsky et al. The more significant change was the elimination of the intercommunication step to calculate flow maps. Removing communication improved the scalability of the technique as the results showed, while some tradeoffs between reconstruction accuracy of discarded particle trajectories and full pathlines, should be considered.  
  
  Contribution [Early Submission]  
  
    Improved scalability while maintaining some acceptable error while reconstruction  
    the flow maps.  
  
  Clarity of Exposition [Early Submission]  
  
    Yes, paper well organized and easy to follow.  
  
  Technical Soundness [Early Submission]  
  
    Yes, the paper also report  some detailed results.  
  
  Quality of References [Early Submission]  
  
    No  
  
  Reproducibility [Early Submission]  
  
    Yes  
  
  Evaluation [Early Submission]  
  
    Yes, it includes four different use cases were the technique is verified in different contexts, i.e. performance evaluation (in-situ) and  post-processing.  
  
  Explanation of Recommendation [Early Submission]  
  
    Removing communication improved the scalability of the technique as the results showed. Still, interested parties in adopting this technique should be aware of the tradeoffs between reconstruction accuracy of discarded particle trajectories and full pathlines.

TODO: No concrete suggestions made by the reviewer.

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 **Reviewer 3**  
  
  Overall Rating [Early Submission]  
  
    Probably accept: I would argue for accepting this paper.  
  
  Expertise [Early Submission]  
  
    Knowledgeable  
  
  Summary [Early Submission]  
  
    This paper proposes a communication free algorithm for computing in situ flow representation based on lagrangian flow maps. The original algorithm was introduced by AGRANOVSKY et al. in 2014. The main idea is to compute in situ short flow maps from uniformly spread particles and save these short trajectories. And then build long trajectories post-hoc from the particles chosen by the user using the short trajectories computed in situ. This algorithm enables to significantly reduce the amount of data to save compared to a traditional approach for an equivalent quality of results. This also enables to speed-up the post-hoc computation as the amount of data to handle is reduced (less I/O costs) and part of the computations have already been done in situ (so less computation load post hoc).  
  
  Contribution [Early Submission]  
  
    The original algorithm required communication steps during the in situ phase to move the particles from one cell to another if reaching the cell boundary before the end of the particle transport time. Here the authors propose to simply drop this communication phase and discard the particles that reach cell boundaries before the end time.  This leads to significant performance gains during the in situ phase of course.  The authors present extensive experimental results, comparing the original algorithm with their version, but also with the traditional Eulerian approach. Their results shows that the amount of dropped particles is often reduced to a few percents and that the reconstruction error during the post hoc phase is also small. Notice that they clearly compute the error only for the particles that are concerned with discarded trajectories, as other trajectories are not affected. Obviously as the cell size decreases the percentage of discarded particles tend to increase.  
  
  Clarity of Exposition [Early Submission]  
  
    Could be improved (see below)  
  
  Technical Soundness [Early Submission]  
  
    ok  
  
  Quality of References [Early Submission]  
  
    Probably ok  
  
  Reproducibility [Early Submission]  
  
    Probably but making code available would be much better.  
  
  Evaluation [Early Submission]  
  
    Yes  
  
  Explanation of Recommendation [Early Submission]  
  
    First I remember ready the original AGRANOVSKY et al. in 2014 paper with enthusiasm as seeing there on of the first true in situ algorithm (this paper got LDAV best paper).  And I agree with the authors that this original paper was short on experiments (not even 100% sure they actually ran any real in situ experiment). So the current paper is welcome in the sense that it comes with extensive experimental results of this approach. And the results confirm the quality of AGRANOVSKY algorithm in term of I/O savings and quality of final results. Then the improvement they propose, though simple, is effective.  
  
    Where I would be more critical about this paper is:  
    - Writing:  not well organized/structured, making it difficult to read. Bellow  
    the bar of what we usually expect from a scientific paper.

We hope our revisions – particularly improving the descriptions in the captions and additional editing – helps readability.

    - The authors kind of stay in the middle with the evaluation of their approach. Is the proposed algorithm usable as the entailed errors can stay under control or the user can be warned that some of the data may be subject to some errors, or the algorithm requires further work as suggested through the proposed future direction of investigation.

Thank you for your comment. We believe this is an application-specific problem. The errors are dependent on the specific configuration parameters and the underlying time-varying vector field. We believe for many cases, if there is a prior understanding of the vector field or if storage interval can be kept short, the technique can be employed. In more complex scenarios, future work would benefit the use of local flow maps particularly via adaptive sampling and flexible post hoc reconstruction schemes. TODO: In terms of manuscript,

    - They should make the code available and present their work as a benchmark suite (but this is still doable for the final version).  
  
    "In this paper, we do not analyze the parallel I/O times, and consider I/O optimization methods to be beyond the scope of this work." I think this is a mistake as one of the main motivation of in situ processing is I/O savings. The saving intervals has clearly an impact on the performance. And one way to limit the amount of discarded particles is to keep this interval small. It would not be complicated to report on the in situ phase exec time, including the I/O time (or this is really not well done and you prefer to "hide" it :-) Does fig 4 includes I/O time or not?

Figure 4 does not include I/O write times. We had three primary reasons. First, parallel I/O is highly variable, which can make interpretation difficult. Second, we found that write times on Summit were very fast for the size of files written by individual ranks in our experiments. Overall, for the file sizes we considered, write times are faster than a single cycle of corresponding in situ Lagrangian computation. We do not expect that this rate of I/O would continue on a full machine run, or on read. Third, our approach always results in less data, and so it will take less I/O. In terms of the manuscript, we expanded the discussion in section 5.3 to better explain why we did not consider parallel I/O times in our studies.

    I miss in this paper one, even short, clear presentation of the algorithm. Fig 1. gives some elements in the introduction and the next elements are kind of spread in the paper.  I understand that the authors assume that it was already published in AGRANOVSKY et al., but for completeness and as the current algorithm differs from the original one, a clean presentation would help the reader.

We revise Figure 1 to show the intervals, uniform seeding used in the Agranovsky algorithm more clearly. We hope this presentation and descriptive caption is more tuned to what the reviewers believe would be useful for readers.   
  
    I am not convinced by the Theoretical analysis that is detailed for the easy part (eq. 2) while it goes quite fast for the difficult part (3, 4). This can be improved. As it is I would not guarantee this analysis is fully relevant.

TODO: I have emailed Roxana if she has any specific suggestions. I’m hoping we can add a sentence to say we’ve attempted improving clarity.   
  
    Fig 5: Put in the caption that left is for the dist algo and the right for the local algo. Would be better to actually have the exec time for both algos and split this exec time in com/advection/I-O

Thank you for your feedback. We improve the description in the caption to distinguish the two more clearly. Our objective with presenting these separately is to highlight the increased cost of weak scaling for particle advection on a single node – where the number of GPUs used, or co-located ranks increases. Resulting in contrasting impacts, communication benefits from weak scaling on a single node whereas the use of shared memory by an increased number of GPUs results in a slowdown of particle advection.

    Even if the authors made the efforts to detail the error distribution, they do not analyze if there is a spatial impact. I would expect that for the cells where the flow is faster, the percentage of discarded particle be significantly higher than for others, and so the error. But it is unclear if this happens in some critical areas. For instance, plotting a histogram with the amount of dropped trajectories per cell could be one way in that direction.  Something that could probably be easy to do is to attach to post hoc reconstructed trajectories the portions that have been reconstructed from a degraded density of short trajectories. This may be sufficient to warn users that in some areas the data must be taken more carefully.

TODO: Thank you for this feedback. We did consider that spatial patterns exist as well. This could be something interesting to do. This is more complicated considering the time-varying nature of this behavior – perhaps accumulated over time is one solution to that problem.

    Reproducibility. I did not find mention of code availability in the paper. That a point that could significantly boost the impact of this paper. As the author did a significant work in setting-up these implementations and experiments, that would be very valuable to make them available to the community as it could become a benchmark.

Thank you for this suggestion. We provide source code that can be used as a benchmark in future works.   
  
    2 typos page 7:  
    - number of CNs increaseS  
    - accurately (under 100 ....)

We address these typos.  
  
  
----------------------------------------------------------------  
 **Reviewer 4**  
  
  Overall Rating [Early Submission]  
  
    Probably reject: I would argue for rejecting this paper.  
  
  Expertise [Early Submission]  
  
    Knowledgeable  
  
  Summary [Early Submission]  
  
    The paper proposes an optimization for the in situ computation of flow maps. To avoid communication and thus to improve scalability, the flow map is limited to a local region. The authors study the introduced error and scalability of the flow map computation.  
  
  Contribution [Early Submission]  
  
    An optimized flow map computation is introduced, which speeds up the in situ analysis performed during a simulation. The scalability of this method is evaluated extensively.  
  
  Clarity of Exposition [Early Submission]  
  
    The paper is well written.  
  
    There are some minor points:  
    - The citation abbreviations are inconsistent. Often, the year is missing, e.g. [ACG\*].  
    - In the references [C\*20], has missing author names.

TODO: I need to figure out how to correct all the references – I’m not sure about the reason for inconsistency. EGPGV allows a maximum of 1 page of references. So I’ll need to reduce the overall length of the document through edits. C\*20 has many many names (ISTP).

    - Table captions should be above the table.

TODO: The instructions indicate the same treatment for tables and figures. I could not verify that captions need to be above the table. I can make this change if needed.

    - Some figures in  Sec. 6 are barely, if at all, discussed in the paper. Maybe some figures can be moved to a supplementary document or even left out?

Thank you for this suggestion. We reduce the number of subfigures in Section 6, retaining results from only the extremes of the parameter selection.

  Technical Soundness [Early Submission]  
  
    The optimization is simple and straightforward. The authors acknowledge some limitations in Sec. 7. However, I feel that the theoretical limitations are far greater than described in the paper. Most concerning, the method is inherently biased since it simply drops sampled trajectories that leave the local region. This implies that it can systematically misrepresent a flow. Indeed, it is quite trivial to construct a theoretical, but not unrealistic, flow that is not well represented by local flow maps. Note that this is not limited to flows/regions of high velocity but might also be caused by bifurcations and other non-linear flow behavior. Due to the inherent sensitivity to small perturbations in most time-varying flows, this is deeply concerning to me.

Thank you for sharing your concerns, and we also acknowledge that this is a significant concern. That said, we strongly believe in our method. In particular, it is our view that time-varying flow is choosing between many bad options. An Eulerian approach with heavy temporal sub-sampling is prone to significantly more error. A Lagrangian approach using the Agranovsky approach (crossing boundaries) introduces a large in situ encumbrance. This approach introduces another option. Further, we feel that the results show that this concern (while legitimate) occurs at a lower-than-expected rate. One piece of evidence is the newly added FTLE plots, which do not show significant errors. That said, we feel an even stronger piece of error are the violin plots (figures 6, 10, 12, and 14). These plots consider only particles that cross the block boundaries. For Figure 6, most particles end up quite “close” to the correct outcome (i.e., <25% of a cell width away). For the other figures, the distance is larger, but still quite close when considering the total number of cells. In all, we felt your concern and how our results respond to this concern were an important point that was not properly represented in the manuscript. To address this, we added several sentences in Section <X>.

TODO: Add statements. These could be pointed to do address the previous reviewer’s comments as well.

    As shown in Sec. 4, the error is bounded by the time interval, velocities, and spatial extent of the region. Although this is a good result, it also implies that these parameters have to be set carefully and preferably adaptively. This is noted as future work by the authors. In my opinion, this is far from trivial and would ultimately decide how useful local flow maps can be in practice.  
  
  Quality of References [Early Submission]  
  
    To my knowledge, all important references are included and are well discussed. The related work section outlines a clear need for research in this direction.  
  
  Reproducibility [Early Submission]  
  
    The method is straightforward and is discussed in detail. The evaluation is well described.  
  
  Evaluation [Early Submission]  
  
    The quantitative study is well done. Although it does not convince me of the usefulness of the method, it does convey interesting insights into implementing scalable in situ Lagrangian analysis.  
  
  Explanation of Recommendation [Early Submission]  
  
    The paper is well written and the study is insightful. Although I like the method for its simplicity, I have a lot of concerns regarding its correctness and thus usefulness.  
  
    The Cloverleaf3D results are promising, especially the comparison to the Eulerian representation. Results of the ABC flow look good, but the error seems quite extreme for the Nyx and Jet flows. I would like to see more comparisons between the two Lagrangian methods regarding the error on the ABC, Nyx, and Jet flows. Currently, the improved scalability of local flow maps (less than one order of magnitude) does not justify the high error, in my opinion. Although some configurations with a lower error exist, it seems difficult to select such a configuration beforehand and the error can grow quite large. I fear that addressing this will require the adaptive method that has been noted as future work.  
  
    Distributed particle tracing is well studied and not significantly (i.e. orders of magnitude) slower - this makes the method seem impractical to me. I was not convinced otherwise by the paper, but the authors might be able to address this.

TODO: The nature of interfacing with the simulation, resource allocation and location, and overall scale impact the overhead of distributed memory particle advection. Thus as the scale increases it is possible that it can be an order of magnitude higher.   
  
    The distribution of errors is nicely visualized by the violin plots. However, it is difficult to tell the impact of the error on post hoc flow analysis and visualization methods. Studying visualizations such as the finite-time Lyapunov exponent (FTLE) that operate on the flow map would give a different perspective on the introduced error and how much impact it has on the flow behavior.  
  
    In conclusion, I have strong doubts regarding the correctness and thus usefulness of local flow maps. I could be persuaded to accept the paper on the grounds that this study can serve as a first step for future research. I do believe that this is an interesting research direction.

**The following content has been omitted from the revised manuscript.**

Subfigure (b) of the following Figure.

Graphical user interface, application

Description automatically generated with medium confidence

Subfigures (b) and (c) of the following Figure.

Application, PowerPoint

Description automatically generated with medium confidence

The following paragraph from Section 3.2.

Text

Description automatically generated