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 Lagrangian*Local* flow maps for three data sets and compare to the ground truth FTLE generated using the full spatial resolution and every cycle of the time interval.

**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 heatmap 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 font.**

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**Reviewer 1**  
  
    - 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.

    - 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 FTLE visualizations enabling a comparison and visualization of the possible impacts of using a communication-free model.

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**Reviewer 2**  
  
Still, interested parties in adopting this technique should be aware of the tradeoffs between reconstruction accuracy of discarded particle trajectories and full pathlines.

Thank you for your comments. We hope the newly added figures aid readers in further accessing the tradeoffs involved. Additionally, we have added text to the manuscript in Section 7 to discuss situations where the technique would be useful and where it requires improvement for broader application.

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**Reviewer 3**  
  
    - 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 desired analysis can be performed using these flow maps, then 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. We introduce a paragraph in section 7 to discuss where we believe the technique can be used well.

    "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.

Thank you for your comment. Detailed derivations of these equations can be found in prior works. We add a statement for (3) indicating the same. For (4), we add that it follows from the mean value theorem. Additionally, in the manuscript we add a new statement regarding global truncation error. We hope these changes can help readers.

    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.

Thank you for this feedback. We did consider that spatial patterns exist as well. Exploring this more extensively would certainly be interesting from an uncertainty visualization perspective. Unfortunately, due to space limitations we did not pursue this idea for this manuscript. We hope that the FTLE visualizations show how reconstruction accuracy can be impacted by losing information near boundaries.

    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.  
  
  
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**Reviewer 4**

Before addressing the individual points, we wanted to make a general statement. First, thank you for sharing your concerns in the review, and we also acknowledge that there are situations where the technique has shortcomings. We did our best to highlight these limitations in our manuscript. That said, we do believe in our method. Unfortunately, visualization of large time-varying vector fields is challenging and currently involves choosing between many bad options. An Eulerian approach with heavy temporal sub-sampling is prone to significantly more error. While a Lagrangian approach using the Agranovsky approach (communication-based) addresses issues with temporal sub-sampling, it introduces a larger in situ encumbrance and poor scalability. Our approach introduces another option. Further, we feel that the results show errors occur at a lower-than-expected rate. Our violin plots, and newly added FTLE images show this is the case for many configurations. In many cases, particles of the flow map are reconstructed within a single grid cell side. Even in situations where the distance is greater, it remains relatively close considering the total number of cells. That said, propagation of error can be problematic and could result in undesirable outcomes. For Lagrangian analysis to be broadly applicable and widely adopted there are many steps required in future work – both on the in situ processing and post hoc reconstruction phases. In recent years, there has been increased interest in researching Lagrangian analysis. Notably, we believe extensions of existing in situ extraction works such as [SCB19] and [RPD19] --- which are designed for a single node (and our approach enables sampling techniques that themselves don’t scale well) --- could address some of the limitations of our proposed communication-free model. Further, most recently machine learning has been employed to improve up-sampling of flow maps compared to cubic up-sampling (we used a bilinear interpolation scheme in our work). Overall, we feel there are many efforts in this space to advance Lagrangian analysis and we strongly believe our work contributes an important piece to make Lagrangian analysis viable at scale.   
  
    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.

Thank you for bringing this to our notice. The format of some bibtex entries did not match the requirements of the algorithm in the .bst file. We have manually corrected these entries for consistency. We also note that [C\*20] has over 50 authors, and we chose to use this format due to space limitations.

    - Table captions should be above the table.

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 heatmap figures in Section 6, retaining only a subset.

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. 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.

Enabling exploratory time-varying flow visualization for large-scale simulation is indeed very challenging. In a recent paper, Leigh Orf referred to the use of ZFP to compress a time-varying vector field as “unfortunate but necessary.” We aren’t saying this to target ZFP, but to make the general statement that any data reduction/approximation technique likely introduces some form of uncertainty to a time-varying flow field. Often these impacts are difficult to observe due to the difficulty in performing uncertain flow visualization in practical settings. Further, any introduced uncertainty in this setting propagates due to the integration-based nature of most flow visualization algorithms. Although our study evaluated multiple data sets and focused a large part of our analysis on only the reconstruction of the discarded trajectories, there are certainly cases where a flow field might be misrepresented. The current literature lacks a closer investigation of how various data reduction techniques for time-varying vector fields (Eulerian sub-sampling, Lagrangian representations, ZFP, etc.) impact the reconstruction of specific flow features. We think such research would be invaluable to the flow visualization community and will consider it very seriously for future work (this topic is of importance to the authors). That said, we feel the errors we observed are generally good, at least in the context of how difficult it is to achieve fast and accurate time-varying flow visualization. Further, to reflect your concern in the manuscript, we include a discussion in Section 7 that focuses on how we believe our technique would be best used in a time-varying visualization setting where interpolation is limited to individual intervals, and error propagation can be reduced/eliminated.

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.

Thank you for your comment. We do believe there is a need for future work on adaptively deciding various parameters. In particular, the choice of time interval can greatly impact Lagrangian analysis (not limited to the communication-free model, but Agranovsky approach as well). In this context, we believe future work should decide the right “time interval” on a per particle basis to best capture the flow field behavior and produce the best data reduction. In our manuscript, we discuss this as future work in Section 7.

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.

Thank you for your comment. We agree that deciding parameters for configurations beforehand presents a challenge. However, it presents a challenge for all Lagrangian representations in general. Currently, we view this as something that is determined by total data storage budget, length of the simulation, and total number of grid points per rank. We hope that our FTLE visualizations for the ABC, Nyx and Jet data sets help the assessment.

    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.

As the MPI ranks increased, the change in encumbrance got to 4X. Since Lagrangian techniques need to run every cycle, savings like this are significant. One of our target applications has a 0.5s cycle time, meaning 0.04 puts us within 10% overhead (a common rule of thumb for acceptable in situ encumbrance), while 0.16 is 30% overhead (often viewed as too much).

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.

We provide FTLE visualizations for the ABC, Nyx and Jet data sets.

    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.

Thank you for concluding your review with this perspective, and we found these comments heartening. In all, it is our view that we have done a more thorough analysis of in situ costs than has been done previously, and we are showing a proposition that was not previously available. Your comments about the failure modes are well taken, but resolving them will take additional analysis. While we stand by our work, we understand if some interpret this as a “step” / “first step” towards increased Lagrangian understanding. In particular, we felt your comments about bifurcation were interesting --- some sub-classes of features may be particularly important to preserve, and these features should be analyzed separately since they may get lost in global statistics. That said, we do view this as future work -- with this study, we have done more analysis than what has been done previously and are having to remove results to meet the page limit.

**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 Figure showing Cloverleaf3D data set reconstruction error for all the intervals of test T8.

Chart, bar chart

Description automatically generated

The following Figure showing Nyx data set reconstruction error for all the intervals of test T1.

Graphical user interface, application

Description automatically generated with medium confidence

The following paragraph from Section 3.2.

Text

Description automatically generated