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Reviewer 1

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3.3 C Interface

It is also important to conduct garbage collection
(GC) in this C interface for every time step. This is because arr
and p_arr in the code snippet are allocated and then deallocated
in E3SM for every time step, and the Julia runtime is not aware of
this and hence needs explicit GC

This is not what the C code in code 2 is doing: as described in https://docs.julialang.org/en/v1/manual/embedding/#Memory-Management, the `JL_GC_PUSH3` macro "roots" the variables so they are *not* collected, and `JL_GC_POP` simply removes that root (so they can be cleaned up by the garbage collector). The Julia garbage collector runs automatically (unless it is disabled, but this is not described in the paper)

Response: We have corrected the code description of `JL_GC_PUSH3 and JL_GC_POP.`

3.5 Noninvasive Compilation

Some more details could be useful here: how did you load the Julia code? (e.g. did you make use of a precompiled system image?) How did you switch between (or switch off) the in situ analysis codes? Again, having the actual code available could make this easier.

Response: We have elaborated the Julia ocde loading and static module switching in section 3.5. We have also added the code and instructions to the repo.

4.1 Sudden Stratospheric Warming (SSW)

I'm not sure Algorithm 1 is correct: shouldn't it reset the counter to 0 if "global zonal mean zonal wind >= 0"? If it is negative for 20 days, does that count as 2 events?

Response: We have corrected the algorithm to reset the counter to 0. In addition, we edited text in Section 4.1, second paragraph, to read: "Based on the definition of SSW, this value needs to be negative for at least 10 consecutive days, so we maintain a global counter variable that keeps track of the number of consecutive days for which the value is negative. Once the value of that counter reaches 10, we record a SSW event for that simulation year (where the event continues until the mean zonal wind becomes non-negative again)."

There isn't much detail on the actual GEV fitting, and I found it difficult to understand. Is it fitting a different GEV distribution at every point? What is the prior distribution used for the GEV parameters? Some more details on this would be helpful (as well as linking to the code).

Response: In Section 4.1, final paragraph, we edited the text to state: "To characterize spatial patterns in surface temperature across CONUS following a detected SSW (compared to no detected SSW), we fit two separate GEV models, similar to~\cite{ssw_isav}. These models represent the distribution of the daily minimum temperatures separately at each spatial location. Specifically, we transform the surface temperature data by subtracting 300°K and multiplying by negative one, then fit GEV models. Briefly, we fit Gumbel models with probability density function $p(x; \mu, \beta) = \frac{1}{\beta}\exp \left\{ -\left[\frac{x-\mu}{\beta}+\exp\left(-\frac{x-\mu}{\beta}\right)\right] \right\}$ where the initial priors are $p(\mu) \sim \mathcal{N}(0, 10)$ and $\beta \sim \text{LogNormal}(0, 0,5)$. As described in~\cite{ssw_isav}, Algorithm 1, model parameters are updated periodically using a buffer of recent data, depending on whether or not an SSW event was recently detected; at each step, the approximate variational posterior distribution from the previous step is used as the prior when updating the model with the new data point to achieve approximate streaming Bayesian inference across time points."

4.2 TributaryPCA

While I understand the problem it is trying to solve, I found it difficult to understand algorithm, and the Code 4 block is somewhat unclear:

- What is X_par? Is it a matrix or a vector, and what are the dimensions?
- What is the initial value (and size) of alpha and V_par?
- Some lines are written using in-place allocation free functions (e.g. mul!), yet not others. There are several calls to copy which seem completely unnecessary.

(I don't have access to the TributaryPCA paper, so couldn't look it up there either).

I would suggest either having a mathematical exposition of the algorithm, and/or making the code a bit more readable.

Response: We agree that the original exposition was not clear especially without access to the TributaryPCA paper. We added to Section 4.2 so that it reads: "In streaming PCA, data $X_i \in \mathbb{R}^{d \times 1}, i=1,...,N$ arrives sequentially and the goal is to compute V using all N samples, where V is updated sequentially with the current estimate denoted as V_i. The AdaOja algorithm relies on an initial learning rate α which we initialize to $1e-5$. In TributaryPCA, we have the additional complication that data X_i is partitioned across B compute nodes. The key portion of the in situ code (that would be called at each time step during the simulation) is shown in the following listing, where \texttt{X_par} is the data on the current node (of shape $d_b \times 1$ where d_B is the dimension of the data on a single compute node indexed by b), \texttt{V_par} is the node's spatial subset of the current global estimate of the eigenvectors (of shape $d_B \times k)$, \texttt{comm} is the MPI communicator object, \texttt{master} denotes the root/master node, and \texttt{grad_par}, \texttt{abs2}, α are pre-initialized arrays. The code has three key steps: first, the gradient for the AdaOja streaming PCA update is computed; this quantity is $X_i X_i^T V_{i-1}$, which is computed with a local dot product at each node followed by an \texttt{Allreduce} to combine results across nodes, and another multiplication locally. The second step is to update the learning rate based on the norm of the gradient and take a gradient step to update V_{i-1} to V_i based on data X_i. Finally, the result must be projected to ensure V_i is orthogonal. This is accomplished by QR decomposition $V_i = Q_i R_i$ where V_i is updated to the orthogonal Q_i. For distributed QR decomposition, we use CholeskyTSQR~\cite{demmel2012communication}." We also added comments to the code block to identify the three key steps and removed the unnecessary copy statements.

Is the data centered (i.e. do you subtract the mean)? The lack of red in Fig 3, PC1 suggests that it isn't, but that isn't clear. If you aren't then the interpretation changes slightly.

Response: The data is not centered because the mean (across time steps, in this case) is not available during the execution of the streaming algorithm. We added to Section 5.3 so that when interpreting Figure 3, it reads “In particular, the first component indicates a temperature differential between equatorial and polar regions; because the mean was not removed, this component can be interpreted as the mean pattern across the time steps.”

5.2 In Situ SSW Detection and Characterization Results

I don't quite understand this: it doesn't actually analyse the SSW case? It just seems to be an illustration of how one might do an analysis.

Response: Your interpretation is correct. Our algorithm is intended to compare SSW and non-SSW cases through the estimated model parameters to determine quantities of interest (such as likelihood of extreme temperatures) based on the fitted models. However, the focus here is to demonstrate the in situ architecture, and the simulation run was only long enough to capture one SSW event, resulting in high variation in the parameter estimates and lack of interpretable structure. We added to Section 5.2: “for the purposes of this paper, we are interested in demonstrating the in situ, streaming modeling approach in general rather than drawing specific conclusions from the simulation in question. As a result, we will show the GEV modeling results for the non-SSW simulation periods because the models were updated more total times and therefore achieve lower parameter variance and greater interpretability.”

5.3 PCA Results

The details are a bit lacking. Was the data collected every time step? Or is it based on daily snapshots or averages? How long was the simulation?

Response: The simulation time duration was one year with 6-hour time steps; we updated the TributaryPCA model at each simulation time step. We now clarify this in Section 5.3: “”

I disagree with the interpretation of figure 3: you can't really assign "warmer vs colder" to principal components (the sign of eigenvectors doesn't matter). My interpretation of the figures is that:

- PC1: the lack of red suggests the data hasn't been centered (or is centered around the equatorial temperature?). As a results it is just explaining that "poles are colder than the equator"
- PC2 and PC3: these look to be roughly the first Fourier components by longitude, i.e. are some orthogonal variation of sin(long) and cos(long): my guess is that they're just capturing the daily temperature changes as the sun rotates around the earth? Can you plot the corresponding eigenvalues?

While it's useful that you can capture this, it's not particularly scientifically interesting.

Response: You are correct, thank you. Our original description fell into the trap of interpreting the sign, but was technically incorrect because the sign of the eigenvector can be reversed. We have updated the description of Figure 3 as follows: “In particular, the first component indicates a temperature differential between equatorial and polar regions; because the mean was not removed, this component can be interpreted as the mean pattern across the time steps. The second component indicates a temperature differential between much of the Eastern hemisphere and the Americas and parts of Africa. The third component indicates a temperature differential between Africa and Europe and other regions." Furthermore, the Figure 3 caption now reads: "First three spatial principal components obtained by in situ TributaryPCA method. Within each component, white color indicates no change to surface temperature, while blue and red indicate temperatures deviating in different directions from zero. The first principal component appears to indicate the overall difference between poles and equator. The second principal component indicates differences between the Eastern hemisphere and Africa/the Americas, while the third component indicates differences in Africa and Europe compared to other regions." We also modified the legend in Figure 3.

We agree that the results are not necessarily scientifically interesting. Our primary goal was to demonstrate the algorithm in situ and evaluate computational cost. Furthermore, our current implementation focuses on recovering the eigenvectors, but the eigenvalues are not stored as they would be the projections at time i onto V_i rather than of each time step onto the final estimated V_N; coming up with a streaming algorithm to update the eigenvalues is an extension we are interested in pursuing in future work.

5.4 Performance

The SSW seems to have negligible overhead (which is not surprising since it is evaluated infrequently), so there is not much to say about the analysis.

It could be helpful if you could add the number of MPI ranks to Table 1?

I'd be interested to know more about the performance bottlenecks of the PCA code? Which parts were the most expensive? Did the Julia garbage collector cause problems with scaling?

Response: We added more information to Table 1. We also added the answers to the questions in the Framework Performance subsection.

Minor comments

Should "in situ" be italicized? I don't know if there is a style guide.

Response: We have seen both nonitalicized and italicized usages, but most are nonitalicized. Therefore, we keep them nonitalicized.

The formatting of the references is somewhat messed up (e.g. many abbreviations are uncaptialized), and many DOIs are missing (e.g. the TributaryPCA one).

Response:

Since you make use of it, it would be nice if you could cite the MPI.jl paper (https://github.com/JuliaParallel/MPI.jl#citation) [disclaimer: I'm one of the authors, but it is the only software mentioned which is uncited]

Response: We cited the MPI.jl paper.

Slurm appears both capitalized and uncapitalized.

Response: We fixed the typo.

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Reviewer 2

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Major points:

1. Make the abstract more to the point for this work. Write in 250 words what was done for this paper and is unique. It reads more like an introduction. Please see your references for examples for self-contained abstracts

Response: We rewrote the abstract and were able to make it under 250 words.

2. The introduction needs fewer technical details as they can go in the background section. Instead, explain why the "challlenges" in the second paragraph are actual challenges. It needs a more high-level explanation of why Julia is chosen over current alternatives earlier in the introduction. Provide the motivation, hypothesis, etc. Also, describe the outline of the paper: Section 2 describes X, Section 3 introduces Y, etc. That way the reader has a good idea what to expect.

Response: We rewrote the introduction section for adding challenge description, motivation, hypothesis, and in situ alternatives. We also added one paragraph outlining the paper structure.

3. Explain the motivation for in-situ analysis: is it data bottlenecks? Is it the only way this could be achieved? What are the potential trade-offs? JIT, back end support, ecosystem maturity etc.

Response: We added the answers to these questions in both the introduction and background and related work sections.

4. Overhead in Figures 4 and 5 results is unclear or not noticeable, perhaps use a different scale or plot style

Response: We redrew Figures 4 and 5 and modified related discussion of the Figures.

5. Please mention efforts in SCORPIO, as it's been an effort to add more I/O backend to E3SM. It would be good to compare with existing in-situ methods.

Response: We mentioned and cited SCORPIO in both the Introduction and Background and Related Work sections. However, unfortunately, we don't have resources of conducting more SCORPIO experiments.

6. One major question is not described, does the current data consumption pattern is independent of the simulation output? Meaning there is some buffer (near real-time) or this is not required as the post-processing is almost negligible.

Response: We added the answers to these questions in the Overall Design subsection.

7. One thing it's not clear is what's the quantified advantage over just storing data and doing post-processing. Is this only possible using "in-situ"?

Response: We added the answers to these questions in the Overall Design subsection.

8. Also, add codes available for reproducibility purposes.

Response: We added the code and instructions to the repo.

9. The motivation for SSW is unclear. It's mostly "there is no overhead" type of case, but how does it compare with using disk directly and not in-situ?

Response: SSW events often lead to extreme cold temperatures across the United States, sometimes referred to as polar vortex events, which can have severe downstream impacts on energy systems (e.g., power grid) and on human lives. Unfortunately, we don't have the results of not in situ as modifying E3SM to support SSW with post-hoc is not straightforward. We added the SSW motivation in the SSW subsection.

Minor points:

1. Spell out acronyms on first use (e.g. R&D, EAM) starting in the introduction section.

Response: We added those missing spellings for the acronyms in their first use.

2. LLVM is no longer low-level virtual machine

Response: We corrected it.

3. The phrase: "Julia can couple with C/C+++/Fortran applications that are naturally supported by LLVM." I think it is not completely accurate. Julia can interoperate with C and Fortran libraries not necessarily compiled or "supported" by LLVM

Response: We agree with that this sentence could be misleading, so we deleted this sentence.

4. ADIOS2 is mentioned but the cited reference is for an earlier ADIOS work. Please cite the appropriate ADIOS2 reference.

Response: We changed the citation to the ADIOS2 reference.

5. Related to 4. I'd highly encourage citing papers related to packages used (e.g. MPI.jl)

Response: We added the MPI.jl reference.

6. If possible, add a table to describe the hardware characteristics

Response: We added a new table to describe the hardware characteristics.

7. Improve Table 1 caption PE Layout is also the 1st column, maybe add MPI information

Response: We added more information to Table 1.