Comment on gmd-2021-138
Peter Baumann (Referee)

Referee comment on "A Parquet Cube alternative to store gridded data for data analytics and modeling" by Jean-Michel Zigna et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2021-138-RC2, 2021

The authors perform a comparison of several systems on 3D and 4D gridded data, with a particular view on parallelization. Tools addressed are THREDDS/NetCDF on standard file system and an object store, pangeo/Dask, and Hadoop/Spark/Parquet. The conceptual model is a 4D cube where the vertical dimension is "nullable" in case of 3D data. This resembles the model of the Barrodale engine on top of Informix, for example.

In Section 2, I get puzzled about the experimental setup description:
- the "criteria identified to stress" are not justified and sometimes surprising: why is it relevant for storage (!) whether a pixel is ocean or land? why is complex processing, heterogeneous data fusion, etc. not considered?
- "enrichment of CSV locations": CSV = comma-separated values? if so, why is that format choice important over, e.g., JSON? what does enrichment mean, and what is the scenario? why is it relevant?
- "parallelized processing" (check language use!) is not a user scenario, but an implementation detail. What would be interesting is what operations exactly to parallelize - for example, an edge filter or matrix operations are harder to parallelize than the trivial pixel operations such as NDVI or subsetting.

Generally there seems to be a lack in concise description of the relevant choices, impacts, and measures. Just one example (p 11): "We repeated the tests several times to obtain the most reliable metrics." A rigorous approach might "run all tests 5 times on a [hot|cold] setup, discarding the maximum and minimum value and averaging the 3 remaining measurements". The algorithms used for the scenarios, such as extracting significant continuous areas and enrichment, are only given cursorily, without a rigorous pseudo code or mathematical description.

In 3.3, it is claimed that datacubes need reprojection which should be avoided. However,
for join/fusion of datasets in different projections there needs to be a reprojection. And rescaling (which likewise involves resampling) is performed routinely by the approach. So I do not see the substantial difference. In fact, substantial preprocessing takes place at datacube creation time, massaging data to make them suitable for the processing lateron. For example, all cubes are forced into the same space/time resolution - a brute-force method, and certainly more dangerous from a scientist perspective than reprojection. Other datacube approaches work on the original data and perform dynamic recombination.

The Parquet format does not seem efficient for cubes. By materializing the coordinates for each point the data volume is blown up immensely, and processing (including data bus transport between RAM and CPU) get slowed down. Combine this with the 3x explosion contributed by HDFS (not to speak about its inflexible page size), it is not clear how this approach can be efficient in comparison to others published. Certainly not a "green computing"!

Partitioning, a well-known technique for gridded data, is applied here as well. The parameters chosen are not justified, though: why regular partitioning? why partition length 1 day along time? We just learn "the partitioning-per-day makes sense", probably because the demonstration scenarios have been pre-trimmed to that. This will be problematic in a general-purpose operational deployment.

Sadly, the performance comparison of the different implementations was done on rather different infrastructure, so comparison of the results is problematic.

In Table 3, performance results for single-file conversion are reported. There is a breathtaking span from 1 to 12816 seconds per file. Unfortunately, it is not explained sufficiently.

Performance results (Figure 8) are a little hard to follow due to nonlinearity - eg, time axis extraction starts with 1D (incidentally the stored grid resolution) and then scales with a factor 30 (?), 3, 2, 2. Equidistant spacing would help understanding the results. Surprisingly, performance degrades quadratic with increasing data volume returned, whereas other tools in the field commonly show a linear behavior. Parallelization does not seem to help much.

Also surprising (and unexplained) is the non-monotonicity in Fig 11 for THREDDS / North Sea while THREDDS / global shows reasonable monotonicity. Further, in Fig 13 there is a huge outlier for THREDDS / hourly / 1M - is this a measurement issue, or a real result? Unfortunately, no explanation is attempted.

On p 18 I would like to understand how "significant" data are determined algorithmically - as it stands, the system load generated cannot be estimated. Further, as "continuous" areas are retrieved there is likely some kernel operation involved. How does kernel computation work at partition boundaries, is it still correct (ie, fetches values from neighboring partitions where necessary)?
Looking at the results on p 19: Performing a simple subsetting returning an estimated 5 MB of data using 10 cores in 30 seconds is breathtakingly slow - other systems can do that in less than 1 second.

Overall, seeing the data set in the conclusion is described as having 2 TB and Spark/Dask were used on 50/40 cores: that means about 40 GB per node - loading that into RAM of each node and using just numpy etc. should be faster by orders of magnitude. Shouldn't the test go well beyond the cumulated RAM?

Bottom line, what I take home is
- THREDDS is not really scalable (which is confirmed by other studies)
- Parquet works well in situations where data and scenarios are carefully aligned
- benchmark deployments have so many special tweaks and differences that a comparison is difficult
- both Spark-Parquet and Pangeo-Zarr fall significantly behind the performance of other tools around
- dynamic partitioning (as studied by Paula Furtado, for example) has not yet found wide recognition

editorial comments:
- p 3: URLs in the make the text ugly to read, better make it a reference.
- p 3: "N variables" - what does that want to tell us? Unknown, variable, or...?
- maybe recheck for typos, such as p 4 "librairies"
- best use uniform nomenclature, not "4G" and "4 go" for 4 GB
- p 5: "The number of cores is increased for the Pangeo-Zarr and the Spark-Parquet environments." ...why? what is the number of cores there? Best motivate such decisions.
- Figure 9: as the diagram lines are greyscale they are not easy to distinguish. If color is not possible consider dashed lines etc.
- check for French words occurring, such as "Novembre"