Dask IO for sequentially splitting, merging and resplitting multidimensional arrays

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Abstract—Todo.

Index Terms—multidimensional, array, split, merge, resplit, IO, processing, Dask, Python

I. INTRODUCTION

With the improvement of acquisition methods in several scientific domains such as health sciences, geology and astrophysics, new big data challenges have emerged. Such challenges includes processing big amounts of data and manipulating heavy files like ultra high resolution images. Big Brain, a brain model providing microscopic data (20 micrometers) for modeling and simulation [1] is an example of ultra high resolution images in the neuroscience field.

A. Multidimensional array chunking

On the one hand, scientific applications often model problems as multidimensional arrays that must be stored in chunks for later processing and analysis. Chunking allows for efficient queries and great flexibility in adding new data, among other things. On the other hand, block algorithms are necessary when data cannot be entirely loaded in memory and to parallelize computations.

Multidimensional array chunking raises the need for tools to efficiently split, merge and "resplit" or "rechunk" data files. Previous work in [2] show that naive algorithms to split an array into several files and merge back those files into one output file perform very poorly due to millions of seeks occuring on disk.

B. The occurrence of seeks

For this study we manipulate multidimensional arrays stored in hdf5 files, that is why we assume that files are written in row-major order (a.k.a "C" ordering), where the fastest moving dimension in the file is the last dimension in the array and the slowest moving dimension in the file is the first dimension in the array. For example a 3D array with dimensions i, j and k would be written on disk by writing the complete columns in the k dimension first (see Figure ??). As in previous work [2], we assume that the storage layout can be arbitrary as long as it is known to the algorithm.

Retrieving subarrays from an array stored on disk incurs seeks. When accessing a multi-dimensional array, seeks occur in two situations: (1) when an array block is opened for reading or writing, and (2) when the reading or writing process moves within the block to write at different places. While reading the data of interest, one needs to seek to the beginning of each

contiguous piece of data constituting the subarray. For a 3D cuboid of shape C, stored in row-major order, each column of data in the k dimension is contiguously stored. They are therefore Cj * Ci data columns for which a seek is required on disk. Although the seek time depends on various parameters such as the distance in bytes between two data columns, we assume all seeks to incur the same time overhead for the sake of simplicity. We further assume that reducing the number of seeks is representative of reducing the processing speed.

C. The multiple and clustered strategies

Two strategies have been introduced in [2] for the split and merge tasks. To illustrate these strategies we shall apply it to the split task (R = I) as it is considered a dual operation of the merge task. The naive strategy to split an array is to repetedly loading one subarray of shape O and writing it down into an output file [2].

The clustered strategy consists in loading contiguous blocks of data of shape O from the input array in order to write it in one seek in each output file which data has been loaded. This strategy loads data blocks one by one, block columns by block columns or blocks slices by block slices. Using this strategy for resplitting would imply reading multiple input files that are contiguous in the reconstructed image or reading the data of contiguous output files by seeking into input files. In either case one can easily find bad cases in which the algorithm seeks in all dimensions.

The multiple strategy aims at not doing any seek while reading and writing. For example, one would read the input file slice by slice and write this slices contiguously in the output files. The tradeoff lies in switching between files at each buffer loading. Using this strategy for the resplit task would imply reading contiguous columns or slices of data from the input files and writing it contiguously in the output files. This would result in even more switches between input and output files and one can easily find worst cases when using small I and O shapes for example where a smarter strategy would be appreciated.

To the best of our knowedge however, no algorithm has been proposed for the resplit task.

D. Problem definition

We focus on 3D arrays for simplicity. Consider a 3D array of shape $R = (R_i, R_j, R_k)$, stored as input blocks of uniform shape $I = (I_i, I_j, I_k)$. Our goal is to resplit the

input blocks into output blocks of uniform but different shape $O = (O_i, O_j, O_k)$.

A resplit algorithm (Algorithm 1) takes as input a list of input blocks inblocks of shape I, a list of output blocks outblocks of shape O, the amount of available memory m, and a list of buffers buffersList defining a partition of array R. The algorithm successively loads the image regions defined by the buffers, and writes them to the output blocks.

For simplicity, we require that all buffers in buffersList have the same shape. Our problem is to find the partition bufferList that minimizes the number of seeks done by Algorithm 1 given I and O, subject to the amount m of available memory.

Algorithm 1 General resplit algorithm

Inputs: inFiles, outFiles, buffersList
for buffer in buffersList do
 read(inFiles, buffer)
 write(outFiles, buffer)

end for

E. Baseline solution

A naive, baseline algorithm for the resplit task is to load one input file at a time into memory and write it in the appropriate output files. We can compute the amount of seeks produced by this algorithm with the algorithm described in Algorithm??. As one can see from the algorithm, unless the dimensions of the input and output files matches a considerable amount of seeks will occur. Also, an overlap in the k dimension is more costly than one in the j dimension. Finally, if the output file shape is greater than the input file shape it also incurs the maximum amount of seeks.

F. Considerations on shape mismatch

If Ix != Ox in a given dimension x, we call it a shape mismatch. As it has been shown in the paragraph on the baseline algorithm, if Ix; Ox and we read one file at a time, we are condamned to seek in the output files at write time. If, however, Ix; Ox, then we get remainders. Finally, if we just read what we need from the input files to write in output files contiguously, we seek while reading and writing. A solution to reduce the number of seeks seems to be to read more than Ox and to elaborate a strategy to keep the remainders in memory instead of writing it down directly until we get enough data to write it with a reduced amount of seeks. Such a strategy is presented in the section keep algorithm.

G. Contributions

This paper makes the following contributions:

- We define the resplit problem
- We propose a first sequential algorithm to efficiently resplit multidimensional arrays
- We give a public implementation of such algorithm in the Python library dask
- We enable the use of the clustered strategy for splitting and merging multidimensional arrays in dask

II. THE "KEEP" ALGORITHM

III. A MEMORY ANALYSIS OF THE KEEP STRATEGY

This section covers how we estimate the amount of memory required by the keep strategy to know how much the buffer can be stretched in a given direction

IV. METHODS

V. IMPLEMENTATION DETAILS

VI. RESULTS

VII. DISCUSSION

Future work: - the split and merge tasks are special cases of the resplit task, which gives an opportunity to solve the three problems at once.

VIII. CONCLUSION

IX. ACKNOWLEDGMENTS

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