Porting IDL programs into Python for GPU-Accelerated In-situ Analysis

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Motivation

• As computation is optimized, I/O and post processing becomes the next major bottleneck in MURaM workflow.
• After I/O challenges are addressed, the post processing analysis scripts written in IDL need to be ported and optimized to take advantage of GPUs.
• IDL is proprietary and has a small community of programmers (mostly astrophysics researchers).
• Python is an alternative worth exploring for analysis: open source, large community, can be optimized for different hardware.

Goals

• Port analysis IDL programs into Python.
• Optimize Python code.
• Explore parallelization of Python program for both CPUs and GPUs.

Porting

• Porting done with Numpy, Scipy and Xarray.
• Automatically extracted and converted data from MURaM into Zarr.
• Zarr is format for storing compressed, chunked N-dimensional arrays.

Parallelism

There are two potential routines that could be parallelized: tracing and interpolation. These were both explored through the use of several libraries.

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<th>Explanation</th>
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<td>Tracing</td>
<td>Dask</td>
<td>Algorithm too complex for Dask to parallelize</td>
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<td>Interpolation</td>
<td>CuPy</td>
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Plots

Fig. 1: Proposed workflow to address the I/O issues by GPU-to-GPU communication with the help of DataSpaces framework. The analysis is shown in the lower square.

Fig. 2: Proposed workflow to address the I/O issues by GPU-to-GPU communication with the help of DataSpaces framework. The analysis is shown in the lower square.

Fig. 3: Top view plot of results produced by IDL.

Fig. 4: Top view plot of results produced by Python.

Benchmarks

Fig. 5: Benchmark of two implementations of the same algorithm.

Figure 7 shows the benchmarking information extracted for both IDL and Python programs. The data represents ten runs on Casper for each IDL and Python implementations. The runs are aggregated with mean and error bars. Lower and upper whiskers show standard deviation of runs for each implementation. IDL is almost 10 times faster than Python because IDL’s interpolation is parallel by default.

Future Work

• Investigate the use of alternative Python implementations (Jython, IronPython, etc.) due to CPython’s limitations.
• Implement interpolation in C++.
• Investigating the use of transcompilers.
• Extend idlwrap Python library which provides IDL-like interface for Python

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References