Optimizing Python-Based Spectroscopic Data Processing on NERSC Supercomputers

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Abstract—We present a case study of optimizing a Python-based cosmology data processing pipeline designed to run in parallel on thousands of cores using supercomputers at the National Energy Research Scientific Computing Center (NERSC).

The goal of the Dark Energy Spectroscopic Instrument (DESI) experiment is to better understand dark energy by making the most detailed 3D map of the universe to date. Over a five-year period starting this year (2019), around 1000 CCD frames per night (30 per exposure) will be read out from the instrument and transferred to NERSC for processing and analysis on the Cori and Perlmutter supercomputers in near-real time. This fast turnaround helps DESI monitor survey progress and update the next night's observing schedule.

The DESI spectroscopic pipeline for processing these data is written almost exclusively in Python. Using Python allows DESI scientists to write very readable and maintainable scientific code in a relatively short amount of time, which is important due to limited DESI developer resources. However, the drawback is that Python can be substantially slower than more traditional high performance computing languages like C, C++, and Fortran.

The goal of this work is to improve the performance of DESI's spectroscopic data processing pipeline at NERSC while satisfying their productivity requirement that the software remain in Python. Within this space we have obtained specific (per node-hour) throughput improvements of over 5x and 6x on the Cori Haswell and Knights Landing partitions, respectively. Several profiling techniques were used to determine potential areas for improvement including Python's cProfile and line_profiler packages, and other tools like Intel VTune and Tau. Once we identified expensive kernels, we used the following techniques: 1) JIT-compiling hotspots using Numba and 2) restructuring the code to lessen the impact of calling expensive functions. Additionally, we seriously considered substituting MPI parallelism for Dask, a more flexible and robust alternative, but have found that once a code has been designed with MPI in mind, it is non-trivial to transition it to another kind of parallelism. We will also show initial considerations for transitioning DESI spectroscopic extraction to GPUs (coming in the next NERSC system, Perlmutter, in 2020).

Index Terms—NumPy, SciPy, Numba, JIT compile, spectroscopy, HPC, MPI, Dask

Introduction

DESI is the Dark Energy Spectroscopic Instrument [noae]. Though dark energy is estimated to comprise over 70 percent of our universe, it is not currently well-understood [PR03], [MWW13]. Many experiments, including DESI, are seeking to uncover more information about the nature of dark energy. The goal of the DESI experiment is, over 5 years, to map 30 million galaxies and use spectroscopically obtained redshift data to measure their distances. The statistical properties of this 3D galaxy map will help shed light on the physical nature of dark energy and its role in the evolution of the universe. An image of the Mayall telescope, on Kitt Peak, Arizona, where the DESI instrument is installed, is shown in Figure 1.

Fig. 1: A photograph of the Mayall telescope (large dome in the center of the image), where the DESI instrument has been installed, on Kitt Peak, Arizona.

In fall 2019 DESI will begin sending batches of CCD images nightly to the National Energy Research Scientific Computing Center (NERSC) for data processing. Each exposure contains the data from 5000 galaxies, quasars, stars, and reference calibrators, routed by fiber optic cables from the telescope to 10 spectrographs with 3 CCDs (red, blue, and infrared) and 500 spectra each. This means that each exposure contains 30 individual images (with each exposure totaling about 6 GB). DESI expects to collect over 30 exposures in a typical night, resulting in over 1000 images.

A small subset of example data are shown in Figure 2 with 21 spectra distributed horizontally and different wavelengths of light dispersed vertically. This image represents less than one millionth of the DESI data obtained per night. Most spectra look the same since all fibers see the same night sky. The slight excess in the middle of the leftmost fiber is the signal from a distant galaxy. Even though this is faint compared to the sky background, this example is in the brightest 15% of galaxies that DESI will observe.

Compared to prior galaxy redshift surveys, DESI will observe fainter, more distant objects at lower signal-to-noise, necessitating more sophisticated algorithms to optimally extract the signal from the data. This requires a full 2D modeling of the data,

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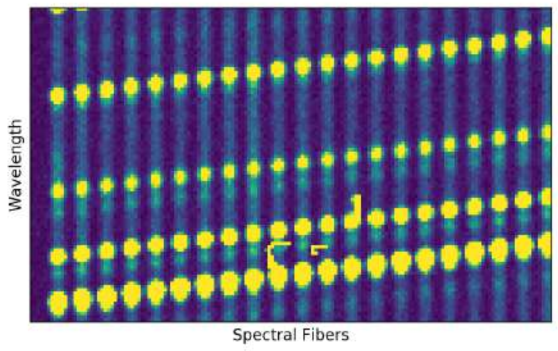


Fig. 2: *Example DESI data showing spectra from 21 of the 5000 fibers distributed horizontally, with wavelengths dispersed vertically. Most spectra look the same since they all see the same sky background light. The slight excess of light in the middle of the leftmost spectrum is the signal from a distant galaxy.*

fitting multiple spectra and wavelengths simultaneously using the "spectroperfectionism" algorithm [BS10], which is only computationally feasible due to a divide-and-conquer technique. This case study focuses on this spectral extraction part of the data processing pipeline since it is the algorithmically most expensive step; it includes eigenvalue decomposition, special function evaluation, and all the necessary bookkeeping required to manage the spectral data in each exposure.

The overarching goal of this work is to speed up the DESI experiment's Python spectroscopic data processing pipeline on the Cori supercomputer's KNL partition at NERSC. NERSC [noag] is the largest Department of Energy computing facility in terms of number of users (7000) and scientific output [noal]. Cori is NERSC's current flagship supercomputer, a Cray XC40 with a theoretical peak performance of 28 PF, comprised of approximately 20 percent Intel Haswell nodes and 80 percent manycore Intel Knights Landing (KNL) nodes.

Achieving good performance with the manycore KNL nodes has proven difficult for many science teams. Because the Haswell nodes are "easier" to use (i.e. applications often run faster on them out of the box), they are increasingly crowded. For this reason NERSC established a program called NESAP (NERSC Exascale Science Applications Program, [noah]) to help science teams transition successfully to the KNL nodes. NESAP provides technical expertise from NERSC staff and vendors like Intel and Cray to science teams to improve the performance of their application on the Cori KNL partition and prepare for the manycore future of high-performance computing (HPC). NESAP's goal is to help move a large fraction of the NERSC workload from the Haswell to the KNL partition; this will ease queue wait times and help increase job throughput for all users.

Achieving optimal Python performance on KNL is especially challenging due its slower clock speed and difficulty taking advantage of the KNL AVX-512 vector units (which is not possible in native Python). A more detailed discussion of the difficulties of extracting Python performance on KNL can be found in [RTD$^+$17]. This case study is borne out of DESI's participation in the NERSC NESAP program.

Despite these difficulties, DESI requested that their code should not be re-written in another language like C due to their own limited developer resources. They did consider both Cython [noad] and Numba [noai] as options for improving performance, but after some initial testing they found that both delivered approximately equivalent speedups for their specific test cases. Citing Numba's ease of use, automatic compilation, and ability to gracefully fall back to non-compiled code, they requested that NESAP proceed with Numba-based optimizations where necessary.

In what follows we will present a case study that describes how a Python image processing pipeline was optimized *without rewriting the code in another language like C* for increased throughput of 5-7x on a high-performance system. We will describe our workflow of using profiling tools to find candidate kernels for optimization and we will describe how we used just in time compiling to speed up these kernels. We will also describe our efforts to restructure the code to minimize the impact of calling expensive kernels. We will compare parallelization strategies using MPI and Dask, and finally, we will discuss a preliminary study for moving the DESI code to GPUs.

Profiling the Code

Our first step in this study was to use profiling tools to determine places in the DESI code where it was worthwhile to target our optimization efforts. We made heavy use of tools designed especially for Python. In general our process was to start with the simplest tools and then, when we knew what we were looking for, use the more complex tools.

We should note that we profiled the DESI code on both Cori Haswell and KNL nodes. There were some minor differences in the relative time spent in each kernel between the two architectures, but overall the same patterns were present on both Haswell and KNL.

cProfile

Python's built-in cProfile package [noaa] was the first tool we used for collecting profiling data. We found cProfile simple and quick to use because it didn't require any additions or changes to the DESI code. cProfile can write data to a human-readable file, but we found that using either Snakeviz [noaq] or gprof2dot [Fon19] to visualize the profiling data was substantially more clear and useful.

An example of data collected using cProfile and visualized with gprof2dot is shown in Figure 3. We prefer gprof2dot to Snakeviz visualizations because they are static images instead of browser-based. This makes them easier to store, share, quickly view, and embed in papers and talks. If you prefer accessing the cProfile data interactively, and clicking on a function to see all of its children, for example, Snakeviz can provide this functionality. However, we found the several extra steps required to use Snakeviz, and the difficulty storing and sharing the visualizations, made it less appealing than gprof2dot.

Examining the visualized cProfile data allowed us to identify expensive kernels in the DESI calculation. In Figure 3, the functions are color-coded according to how much total time is spent in each of them. In this example, the function `traceset` accounts for approximately 37 percent of the total runtime and was a good candidate for optimization efforts.

Information like that shown in Figure 3 is nevertheless incomplete in that it can only provide detail at the function level. From these data alone it was difficult to know what specifically in the

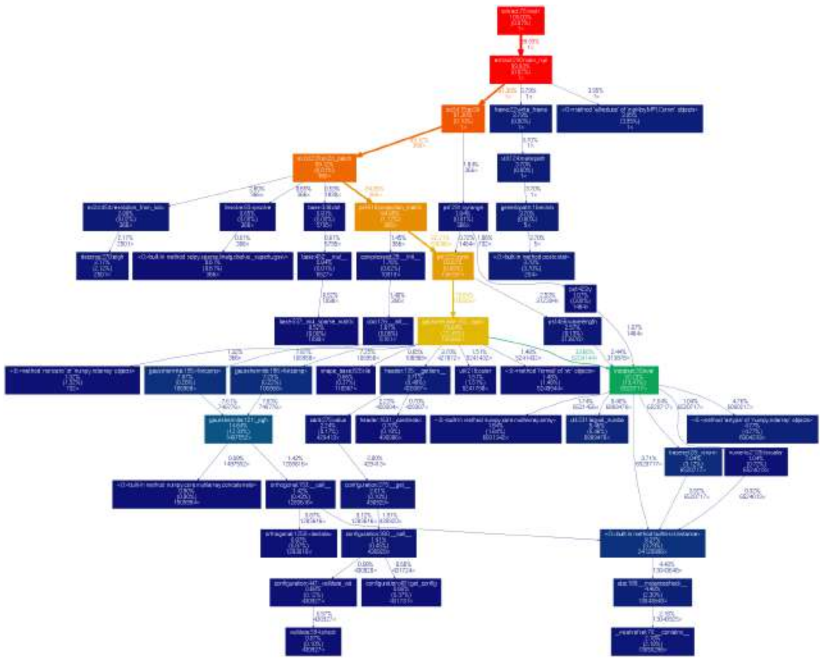


Fig. 3: This is an example image created from data collected using cProfile and visualized using gprof2dot [Fon19]. This profile was obtained from an early stage in the NESAP optimization effort.

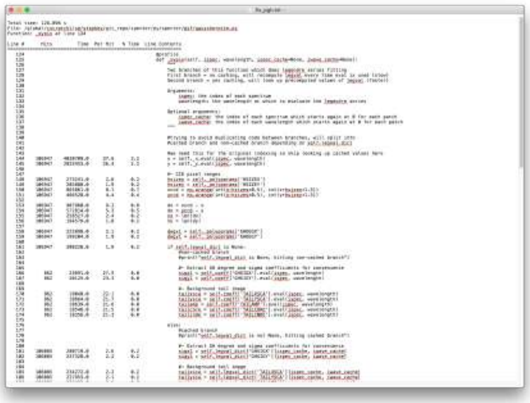
function "traceset" was so time-consuming. Once we had a list of expensive kernels from our cProfile/gprof2dot analysis, we started using the line_profiler tool.

line_profiler

line_profiler [Ker19] is an extremely useful tool which provides line-by-line profiling information for a Python function. However, this more detailed information comes at a cost: the user must manually decorate functions that he or she wishes to profile. For a small code this exercise might be trivial, but for the many thousand line DESI code 1) hand-decorating every function would have been extremely time-consuming and 2) searching through the line_profiler output data to find expensive functions would have also been cumbersome and potentially error-prone. For this reason we recommend starting with cProfile and then moving to line_profiler once the user has identified a few key functions of interest.

Once decorated, line_profiler provides a great deal of information for each line of the function, including how many times each line was invoked and the total amount of time spent on each line. An example of line_profiler output for the function `xypix` is shown in Figure 4. This information was vital to our optimization efforts because it could point to functions that were particularly expensive, such as numpy's `legval` or scipy's `erf`. Once we had this information, we could make decisions about how to reduce the time spent in these functions, either by speeding up the functions themselves through JIT compiling, or by restructuring the code to make the functions either less expensive or avoid calling them as often. We will describe these approaches in the sections that follow.

Together, cProfile and line_profiler were sufficient for almost all of the performance optimization work in this case study. However, because the DESI extraction code is an MPI code, these profiling tools do have some limitations. Both of these tools can be used to collect data for each MPI rank, but visualizing and using



```
[illegible]
```

Fig. 4: Here is a sample output window from line_profiler [Ker19] for the function "xypix". The clear, human-readable output files produced by line_profiler are a very nice feature.

the information in a meaningful way is challenging, especially when there are 68 outputs from a KNL chip, for example.

VTune and Tau

Once we reached the point where we wanted to investigate 1) each individual MPI rank and 2) whether all ranks were appropriately load-balanced, we needed more powerful profiling tools like Intel VTune [adm] and Tau [noar]. While VTune is a very powerful general tool for studying code, we found that it was difficult to get the information we wanted in a clear, understandable format. For example, VTune would often display extremely low-level information that obfuscated the higher-level Python calls we were trying to investigate. We found gprof2dot and Snakeviz visualizations easier to navigate than the VTune GUI. We ultimately found the Tau profiler more useful and well-suited for our application, although we should note that we required the help of the Tau

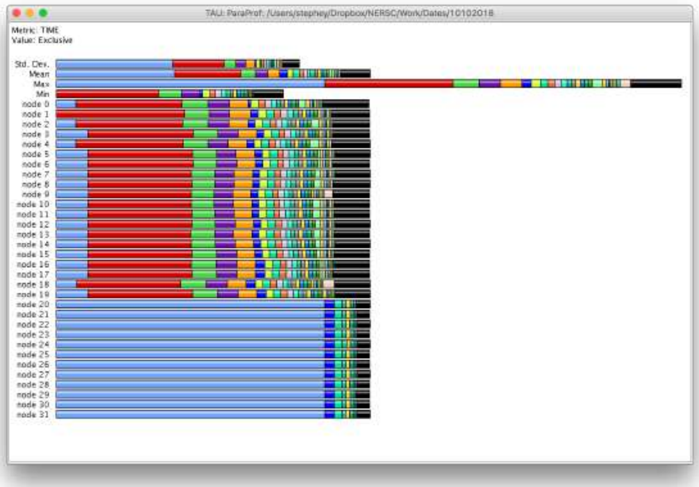


Fig. 5: *A sample Tau [noar] output for the DESI spectral extraction code on a Haswell processor (which has 32 ranks). It is clear from this output that only 20 of the ranks are being utilized. This motivated the restructure to allow parallelization of subbundles, rather than bundles, which could more flexibly utilize the whole processor's resources.*

developers to build it. (Tau works best when it is built for the type of application you will profile. In our case it was a Python MPI code running on a Cray system, all of which are configurations that Tau supports.) Though building a profiling tool from scratch was non-trivial, it was also very possible with the help of the Tau team. Once built, Tau provided clear information about how each MPI rank was occupied and how each rank compared to the others. A sample Tau output window is shown in Figure 5. These profiling data were obtained while the DESI frame was parallelized over bundles which left 12 of the 32 Haswell ranks unoccupied. It is clear from this Tau visualization that we were not making good use of processor resources.

Just-in-time (JIT) Compilation with Numba

The first major approach to achieve speedups in this work has been to focus on making expensive functions run more quickly. To achieve this, we have used Numba [LPS15], a just-in-time compiler for Python.

We used Numba for three functions that, through profiling, we identified as expensive. These functions were 1) `numpy.polynomial.legendre.legval` [noaj], 2) `scipy.special.erf` [noao], and 3) `scipy.special.hermitenorm` [noap], which henceforth we will refer to as `legval`, `erf`, and `hermitenorm`.

`legval` was perhaps the most straightforward of these three to JIT compile. Unlike Python, Numba requires that all variables and arrays cannot change type, nor can they change size (e.g. this information must be known prior at compile time). This necessitated several small changes to the `legval` algorithm to put it in the form required by Numba. Several other lines of the function that performed type checking were removed. This placed the onus on the developer to make sure the correct types are supplied, which was acceptable for us. The original and modified `legval` functions are shown in Figure 6.

The two scipy functions were also somewhat challenging to implement in Numba. At the time of this writing, Numba does not yet support directly compiling scipy functions. This meant that we needed to extract the core part of these scipy functions and mold them into a form that Numba would accept. For scipy `erf`, this meant translating the Fortran source code into Python. For scipy `hermitenorm`, which was fortunately already in Python, algorithmic changes similar to those we made in `legval` were necessary to ensure all variables were a constant type and size.

We should note that we tried to cache the compiled Numba functions with the `cache=True` option to save time, but with larger numbers of MPI ranks, we found that this sometimes caused a data race between the Numba caches written by each rank. To avoid this problem we considered using ahead of time (AOT) instead of JIT compiling but since implementing this change was somewhat awkward, for now we have removed the `cache=True` setting and will consider using AOT in the future.

Restructuring the Code

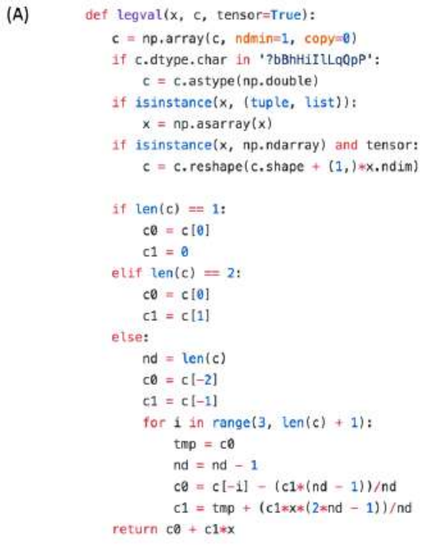
Restructuring the code was the second major optimization strategy we used. In the three subsections that follow, we will describe three types of restructuring efforts that we have completed or will soon complete. In the first restructure, we have altered the code to process smaller matrices at a time to reduce the performance hit we take in the `scipy.linalg.eigh` function. In the second restructure, we have changed the code to avoid calling an expensive function, `numpy.polynomial.legendre.legval`. In the third restructure, which is currently in progress, we are changing the structure of parallelism to divide the problem by subbundle rather than by bundle. This restructure doesn't itself provide a performance boost, but it does provide substantially increased flexibility for the DESI code.

Implement Subbundles

Profiling data indicated that when matrix sizes were large, `scipy.linalg.eigh`, a key part of the spectroperfectionism extraction, was extremely slow. This is not surprising because Jacobi eigenvalue algorithms scale as $O(n^3)$ [PTV+92]. One recommendation from an Intel Dungeon session (a collaborative hack session between NESAP teams and Intel engineers) was to reduce the number of fibers processed at a time. This meant dividing a single bundle of 25 fibers into 6 smaller groups known as subbundles. By computing the eigenvalues of more, but smaller, covariance matrices, DESI was able to reduce their computation time. It is important to mention that DESI can only use this type of approach because they have been careful to design their experiment so as to minimize crosstalk between individual fibers, which results in a sparse covariance matrix. We will also note that there was nothing magical about the number 6; anywhere from 2 to 10 subbundles provided a similar performance increase on both KNL and Haswell. While this strategy was successful on CPUs, we will revisit this strategy in the section "Does it Make Sense to Run DESI Code on GPUs".

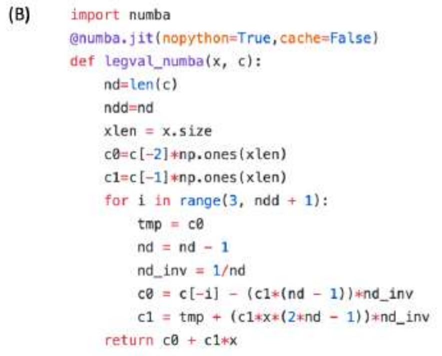
Add Cached `legval` Values

Another outcome from the Intel Dungeon session was the recommendation to restructure the code to avoid calling `legval`. The problem with `legval` wasn't just that it was an expensive function; rather, it was also contributing to a large fraction of the total runtime because it was called millions of times for each CCD image in the DESI spectral extraction calculation. Worse, `legval` was called with scalar values even though it was able to handle vector inputs.


(A)

```python
def legval(x, c, tensor=True):
    c = np.array(c, ndmin=1, copy=0)
    if c.dtype.char in '?bBhHiIlLqQpP':
        c = c.astype(np.double)
    if isinstance(x, (tuple, list)):
        x = np.asarray(x)
    if isinstance(x, np.ndarray) and tensor:
        c = c.reshape(c.shape + (1,)*x.ndim)

    if len(c) == 1:
        c0 = c[0]
        c1 = 0
    elif len(c) == 2:
        c0 = c[0]
        c1 = c[1]
    else:
        nd = len(c)
        c0 = c[-2]
        c1 = c[-1]
        for i in range(3, len(c) + 1):
            tmp = c0
            nd = nd - 1
            c0 = c[-i] - (c1*(nd - 1))/nd
            c1 = tmp + (c1*x*(2*nd - 1))/nd
    return c0 + c1*x
```


(B)

```python
import numba
@numba.jit(nopython=True,cache=False)
def legval_numba(x, c):
    nd=len(c)
    ndd=nd
    xlen = x.size
    c0=c[-2]*np.ones(xlen)
    c1=c[-1]*np.ones(xlen)
    for i in range(3, ndd + 1):
        tmp = c0
        nd = nd - 1
        nd_inv = 1/nd
        c0 = c[-i] - (c1*(nd - 1))*nd_inv
        c1 = tmp + (c1*x*(2*nd - 1))*nd_inv
    return c0 + c1*x
```

Fig. 6: *(A) The official* `numpy.polynomial.legendre.legval` *function. Profiling data indicated that this was an expensive function. To conserve space the docstring has been removed. (B) Our modified* `legval` *function that was much faster than its original numpy counterpart. Note the removal of the type checking and the addition of the* `np.ones` *array to instruct Numba about the sizes of each array (and prevent them from changing during every iteration.)*

This restructuring required us to modify several major functions and redefine some of the bookkeeping that keeps track of which data corresponds to which part of the image on the CCD. Prior to the restructure, profiling data indicated that `legval` was called approximately 7 million times per frame with scalar values.

The code was restructured so that `legval` was now called 800,000 times per frame. Of course this is still a large number, but it is almost an order of magnitude fewer times than the original implementation. The calculated values were stored as key-value pairs in a dictionary. We then modified the part of the code that previously calculated `legval` to instead look up the required values stored in the dictionary.

Parallelize over Subbundles Instead of Bundles

Desipte these optimizations, the DESI code still has several known issues: poor load-balancing and rigid requirements for job sizes (9 nodes for KNL and 19 Nodes for Haswell, for example). We are in the process of addressing these issues and thought that our efforts were worth mentioning.

The goal of parallelizing over subbundles, rather than bundles, is to restructure the code to divide the spectral extraction into smaller, more flexible pieces. This will relax the previous requirement that each frame be divided into 20 bundles, which is an awkward number for NERSC hardware (and a restrictive condition in general). When completed, the 500 spectra will be more evenly doled out to 32 processors (about 16 spectra each) or 68 processors (about 7 spectra each). This means that all processors can be used for any given job size, not just for a carefully chosen job size. However, like the other restructuring efforts, we have found that implementing this change is nontrivial.

Additionally, this refactor will help improve load balancing. Since the processing time differs for the three types of DESI frames (blue, red, and infrared), prior to the refactor, the processors assigned to the blue frames finished before the infrared frames, wasting both valuable processor resources and time. In this new design, frame types will be grouped together so processor time is not wasted.

Optimization Results

How effective were all these different optimization efforts we just described? The most straightforward benchmark is one in which raw runtime (and hopefully speedup) is measured. In this case, we measured the time to complete the processing of a single DESI frame on a single Edison, Cori Haswell, and Cori KNL node. In Figure 7 we show how each optimization affected the single frame runtime. The optimizations are plotted chronologically against the overall runtime of the frame on each architecture.

Figure 7 shows that the first few changes we made had the largest overall impact: the later optimizations exhibited some diminishing returns. Over the course of this work the runtime for a single frame was decreased from 4000 to 525 seconds for KNL, from 862 to 130 seconds for Haswell, and from 1146 to 116 seconds for Ivy Bridge (the processor architecture on NERSC's now retired Edison system). The overall increases in raw speed varied between 7-10x for each architecture. One major goal of the NESAP program was to reduce the DESI runtime on KNL to below the original Edison Ivy Bridge benchmark, which is indicated by the red dotted line. Once we implemented our `legval` cache fix, we achieved this goal.

A more informative benchmark for DESI is specific processing throughput, stated in frames processed per node-hour. Measuring this quantity makes it clear how much of DESI's computing allocation is needed to complete a given amount of processing. Higher specific throughput indicates more effective use of computing resources. We measure this benchmark using a full exposure (30 frames), instead of a single frame. We also measure on either 19 or 9 nodes for Haswell and KNL, respectively, due to the limitations we described earlier (in the Parallelize over Subbundles Instead of Bundles subsection). Though a single exposure is still a relatively small test because DESI expects to collect 30 or more exposures per night (approximately 1000 frames), it much more

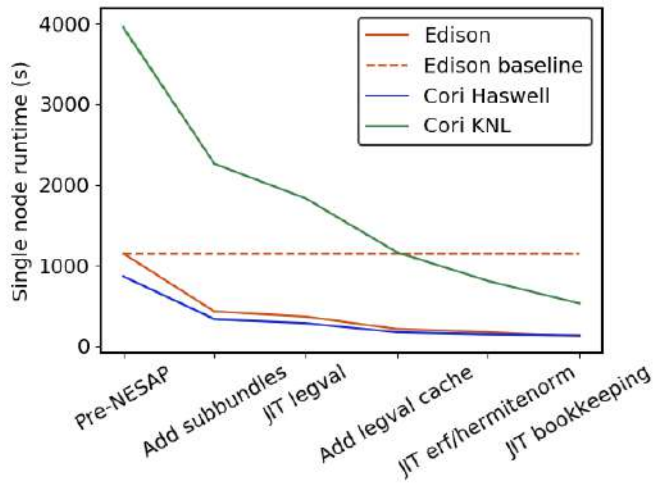


Fig. 7: The single-node speedup achieved on Intel Ivy Bridge, Haswell, and KNL architectures throughout the course of this study.

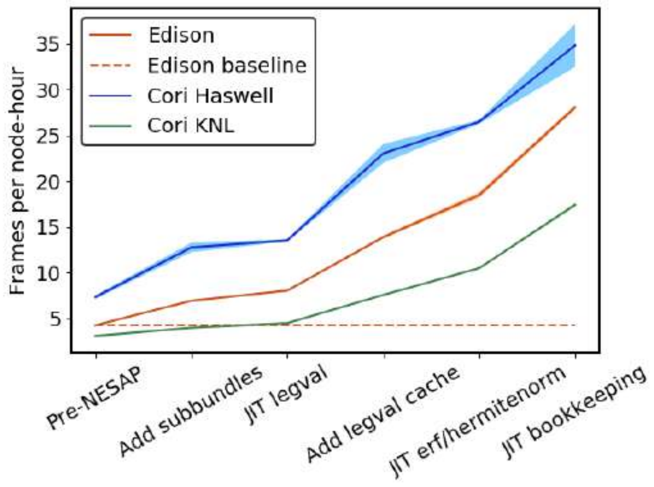


Fig. 8: This figure shows the improvement over the course of this study in the DESI spectral extraction specific throughput.

closely approaches the real DESI workload than the single frame benchmark. One feature encoded in this benchmark which is not captured in the speed benchmark is the increasingly important role that MPI overhead begins to play in multi-node jobs, which is a real factor with which DESI will have to contend during its large processing runs. The frames per node-hour results are plotted in Figure 8. While the increases in specific throughput we have obtained are more modest than the raw speedup, these values are a more accurate representation of the actual improvements in DESI's processing capability. For this reason we emphasize that we were able to achieve a 5-7x specific throughput increase instead of the (more exciting but less meaningful) 7-10x in raw processing speed.

It is worth mentioning that using Numba allowed us to make notable improvements specifically on KNL, which was of course the main goal of this study. For `legval` in particular, shown in Figure 6, we found that JIT compiling this function provided 15x speedup on KNL vs only 5x speedup on Haswell. This additional speedup on KNL was because Numba was able to target the KNL AVX-512 vector units. We therefore strongly recommend

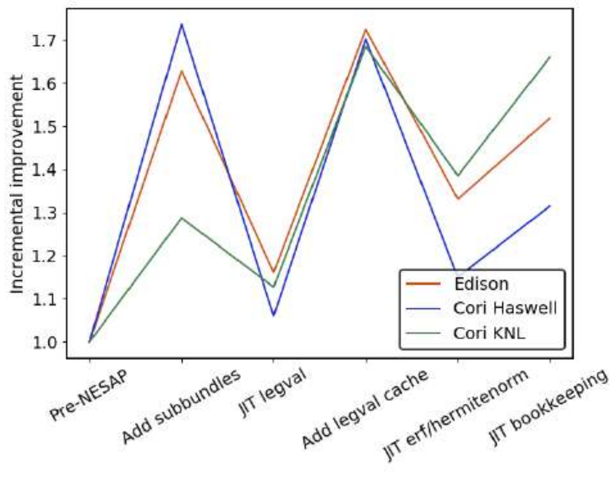


Fig. 9: Types of optimization efforts performed in this study and their resulting incremental specific throughput improvements on Intel Ivy Bridge, Haswell, and Knights Landing architectures. These optimizations are listed in chronological order.

investigating Numba to any developer trying to optimize Python code to run on a system with vectorization capabilities.

Finally, in Figure 9 we summarize the incremental specific throughput improvements we obtained throughout this study on Edison Ivy Bridge, Cori Haswell, and Cori KNL. The code optimizations are plotted in chronological order. Perhaps these results are the most generally instructive. First, they demonstrate that the restructuring-based optimizations were more valuable than the JIT-based optimizations. For example, the overall speedup of adding the `legval` cached values was approximately 1.7x, although this was also the most difficult of all the optimizations implemented in this study. In contrast, our relatively painless JIT compiled optimizations were not as effective in terms of speedup, averaging between a factor of 1.1-1.5x improvement. The takeaway from these results might be that if a developer has enough time, the larger, more complex restructuring optimizations may be extremely worthwhile. The flip side is that if the developer has limited time, small fixes like JIT compiling can still provide reasonable gains without a major time investment.

Alternatives to MPI?

A few problems with the current MPI implementation of the DESI spectral extraction code prompted us to take a step back and consider if newer frameworks like Dask [noaf] would be a better solution for parallelization within DESI. The reason we considered Dask, and not Apache Spark or similar frameworks, was 1) because converting to Dask would require a less extreme refactor and 2) the Dask adpatations would not preclude smaller-scale users from running DESI processing routines on their laptops, which would have been the case with Spark.

The first problem we hoped to address was the relative inflexibility of the division of work between bundles[1] . The second was the issue of resiliency: if a node goes down, it will take the entire MPI job with it[2] . An additional feature we liked about Dask is the ability to monitor Dask jobs in real time with their Bokeh status page. We thought Dask seemed promising enough that it was worth taking a careful look at what it would mean to replace the DESI MPI with Dask.

Dask is a task-based parallelization system for Python. It is comprised of a scheduler and some number of workers which communicate with each other via a client. Dask is more flexible than traditional MPI because it can start workers and collect their results via a concurrent futures API. It should be noted that this is also possible in MPI with dynamic process management, but since Cray does not yet support dynamic process management under the Slurm workload manager, we haven't been able to try it at NERSC.

During this process, we discovered that it is non-trivial to convert a code already written in MPI to Dask, and it would likely be difficult to convert from Dask to MPI as well. (It would likely be easier to convert from dynamic process management MPI to Dask, but the DESI spectral extraction code is not written with this API.)

One major difference between MPI and Dask is the point at which the decision of how to divide the problem occurs. In MPI since all ranks are generally passing over the code, dividing the data and performing some operation on it in parallel can be done on the fly. In Dask, however, the scheduler needs to know in advance which work to assign to workers. This means that the work must already be divided in sensible way. Collecting the information required for Dask-style parallelism in advance would have required a substantial restructuring on the order of what was performed for `legval`, if not more ambitious. At this point we decided that if the DESI code had been written from the start with Dask-type parallelism in mind using Dask would have been a good choice, but converting existing MPI code into Dask was unfortunately not a reasonable solution for us.

Does it Make Sense to Run DESI Code on GPUs?

Because HPC systems are becoming increasingly heterogeneous, it is important to consider how the DESI code will run on future architectures. The next NERSC system Perlmutter [noak] will include a CPU and GPU partition that will provide a large fraction of the system's overall FLOPS, so it is pertinent to examine if and how the DESI code could take advantage of these accelerated nodes.

Since GPUs are fundamentally different from CPUs, it may be necessary to rethink much of the way in which the DESI spectral extraction is performed. At the moment, each CCD frame is divided into 7200 overlapping subregions such that each matrix to solve is typically 400x400 elements. Though this division of a larger frame into smaller pieces makes sense for CPU architectures, it may not be optimal for GPU architectures. In fact for GPUs often the opposite is true: the programmer should give the GPU as much work as possible to keep it occupied; thus it may be beneficial to operate on a smaller number of larger matrices. Additionally, it may be necessary to change the code so that the matrices are both constructed and solved on the GPU to bypass inefficient subregion bookkeeping, which is currently interleaved between constructing and solving the matrices, and avoid expensive data transfer. This means that helping the DESI extraction code run efficiently on GPUs could require a major restructuring to better adapt the problem for the capabilities of the hardware.

1. Although this is currently being addressed in the subbundle division restructure.

2. This is not an issue in Dask, in which dead workers can be seamlessly revived while the calculation continues.

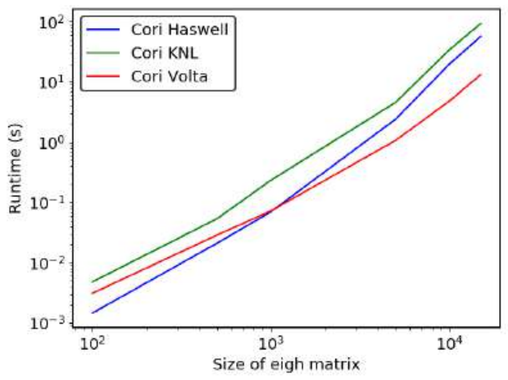


Fig. 10: *Data from performing an eigh matrix decomposition of various sizes on Edison Ivy Bridge, Cori Haswell, Cori KNL, and Cori Volta. We used CuPy to perform eigh on the Volta GPU.*

Preliminary testing is underway to give some indication of what we might expect from a major overhaul. From profiling information we expect that the `scipy.linalg.eigh` function will constitute a larger part of the workload as matrix sizes increase. We have measured the runtime of `scipy.lialg.eigh` and `cupy.linalg.eigh` [noac] as an initial test case on Cori Haswell, KNL, and the new Cori Volta GPUs. (We could not make these measurements on Edison Ivy Bridge because it has now been decommissioned.) Figure 10 shows the `eigh` runtime for various sizes of positive definite input matrices. These data show that for larger matrix sizes (above approximately 1000) the Volta begins to outperform the CPUs. However, these data do not include any possible gains from a divide-and-conquer approach (which has proven very successful for DESI). Investigating this strategy is near-term future work.

This `eigh` study is just the first of many planned GPU experiments. DESI has additional matrix preparation steps, bookkeeping, and special function evaluations (like `legval`) which also constitute a large part of their total workload. At this time it is unclear which of these might perform well on the GPU and make the relatively expensive host to device data transfer worthwhile. We will perform many experiments to evaluate how well each of these are suited to the GPU (or perhaps not suited to the GPU) as future work.

We should note that one of the major conclusions of this case study has been that large restructuring efforts have been worthwhile for DESI. If indeed we choose to embark upon another major restructure for GPUs, what is the best approach? As we have detailed above, we have had reasonably good success with Numba, which also supports GPU offloading. Other options are CuPy [noab], which aims to be a drop-in replacement for NumPy, pyCUDA [noam], and pyOpenCL [noan]. How best to support GPU offloading without having to fill the DESI code with distinct CPU and GPU blocks, and additionally to avoid being tied to a particular vendor, is still an open question for us.

Conclusions and Future Work

Over the course of this work, we have achieved our goal of speeding up the throughput of the DESI spectral extraction code on NERSC Cori Haswell and KNL processors by a factor of 5-7x without rewriting their Python code in another language.

DESI will process its data at NERSC both in semi-realtime and additionally, it will reprocess all of its data each year (at least) with the latest pipeline version. At the start of this work, the final data processing would have taken 33 million CPU hours. The work presented in this study has reduced that to 6.5 million hours, making much more efficient use of the resources available at NERSC, thus benefitting both the DESI project and also the many other users who share the NERSC systems. Additionally, this algorithm speedup lets DESI process a night's data in a matter of hours instead of days, enabling the ability to use one night of data as feedback to the survey operations the following night. This results in more efficient survey operations, reducing the time to completion.

Our strategy was as follows: we employed profiling tools, starting with the most simple tools (cProfile + gprof2dot) and progressing as necessary to more complex tools (line_profiler and Tau), to get an idea of which kernels are most expensive and what types of structural changes could help improve runtime and flexibility. We used Numba to JIT compile several expensive functions. This was a relatively quick way to obtain some speedup without changing many lines of code. We also made larger structural changes to avoid calling expensive functions and also to increase the flexibility and efficiency of the parallelism. In general these larger structural changes were more complex to implement, as well as more time consuming, but also resulted in the biggest payoff in terms of speedup.

We considered changing the parallelism strategy from MPI to Dask, but ultimately found that changing an existing code is non-trivial due to the fundamentally different strategies of dividing the workload, and decided to continue using MPI. Work is in progress to address two remaining issues: load-balancing and inflexible job size. Finally, we are now investigating how the DESI code could run effectively on GPUs by since the next NERSC system Perlmutter will include a large CPU and GPU partition. Exploratory studies for how the DESI code can be optimized are being performed using `scipy.linalg.eigh` and `cupy.linlg.eigh` as a test case now and will continue as future work.

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References

[adm] admin. Python* Code Analysis. URL: https://software.intel.com/en-us/vtune-amplifier-help-python-code-analysis.

[BS10] Adam S Bolton and David J Schlegel. Spectro-perfectionism: an algorithmic framework for photon noise-limited extraction of optical fiber spectroscopy. *Publications of the Astronomical Society of the Pacific*, 122(888):248, 2010. doi:10.1086/651008.

[Fon19] José Fonseca. Converts profiling output to a dot graph. Contribute to jrfonseca/gprof2dot development by creating an account on GitHub, April 2019. original-date: 2015-03-13T07:19:30Z. URL: https://github.com/jrfonseca/gprof2dot.

[Ker19] Robert Kern. Line-by-line profiling for Python. Contribute to rkern/line_profiler development by creating an account on GitHub, April 2019. original-date: 2014-08-31T11:45:05Z. URL: https://github.com/rkern/line_profiler.

[LPS15] Siu Kwan Lam, Antoine Pitrou, and Stanley Seibert. Numba: a LLVM-based Python JIT compiler. In *Proceedings of the Second Workshop on the LLVM Compiler Infrastructure in HPC - LLVM '15*, pages 1–6, Austin, Texas, 2015. ACM Press. URL: http://dl.acm.org/citation.cfm?doid=2833157.2833162, doi:10.1145/2833157.2833162.

[MWW13] Michael J Mortonson, David H Weinberg, and Martin White. Dark energy: a short review. *arXiv preprint arXiv:1401.0046*, 2013.

[noaa] 26.3. The Python Profilers — Python v3.2.6 documentation. URL: https://docs.python.org/3.2/library/profile.html.

[noab] CuPy. URL: https://cupy.chainer.org/.

[noac] cupy.linalg.eigh — CuPy 5.4.0 documentation. URL: https://docs-cupy.chainer.org/en/stable/reference/generated/cupy.linalg.eigh.html.

[noad] Cython: C-Extensions for Python. URL: https://cython.org/.

[noae] Dark Energy Spectroscopic Instrument (DESI). URL: https://www.desi.lbl.gov/.

[noaf] Dask: Scalable analytics in Python. URL: https://dask.org/.

[noag] National Energy Research Scientific Computing Center. URL: https://www.nersc.gov/.

[noah] NESAP. URL: https://www.nersc.gov/users/application-performance/nesap/.

[noai] Numba: A High Performance Python Compiler. URL: http://numba.pydata.org/.

[noaj] numpy.polynomial.legendre.legval — NumPy v1.16 Manual. URL: https://docs.scipy.org/doc/numpy/reference/generated/numpy.polynomial.legendre.legval.html.

[noak] Perlmutter. URL: https://www.nersc.gov/systems/perlmutter/.

[noal] Publications Resulting from the Use of NERSC Resources. URL: https://www.nersc.gov/news-publications/publications-reports/nersc-user-publications/.

[noam] PyCUDA. URL: https://mathema.tician.de/software/pycuda/.

[noan] PyOpenCL. URL: https://mathema.tician.de/software/pyopencl/.

[noao] scipy.special.erf — SciPy v0.14.0 Reference Guide. URL: https://docs.scipy.org/doc/scipy-0.14.0/reference/generated/scipy.special.erf.html.

[noap] scipy.special.hermitenorm — SciPy v1.2.1 Reference Guide. URL: https://docs.scipy.org/doc/scipy/reference/generated/scipy.special.hermitenorm.html.

[noaq] SnakeViz. URL: https://jiffyclub.github.io/snakeviz/.

[noar] TAU - Tuning and Analysis Utilities -. URL: https://www.cs.uoregon.edu/research/tau/home.php.

[PR03] P James E Peebles and Bharat Ratra. The cosmological constant and dark energy. *Reviews of modern physics*, 75(2):559, 2003. doi:10.1086/185100.

[PTV$^+$92] William H Press, Saul A Teukolsky, William T Vetterling, Brian P Flannery, and M Metcalf. Numerical recipes in Fortran 90. *The art of scientific computing,(Cambridge, 1996)*, 1992. doi:10.1109/MCC.1998.736436.

[RTD$^+$17] Zahra Ronaghi, Rollin Thomas, Jack Deslippe, Stephen Bailey, Doga Gursoy, Theodore Kisner, Reijo Keskitalo, and Julian Borrill. Python in the NERSC Exascale Science Applications Program for Data. In *Proceedings of the 7th Workshop on Python for High-Performance and Scientific Computing - PyHPC'17*, pages 1–10, Denver, CO, USA, 2017. ACM Press. URL: http://dl.acm.org/citation.cfm?doid=3149869.3149873, doi:10.1145/3149869.3149873.