ROIBIN-SZ: Fast and Science-Preserving Compression for Serial Crystallography

ROBERT UNDERWOOD,¹ CHUNHONG YOON,² ALI GOK,¹ SHENG DI,¹ AND FRANCK CAPPELLO¹
¹Argonne National Laboratory, 9700 S. Cass Avenue, Lemont, IL 60439; ²SLAC National Accelerator Center, 575 Sand Hill Road Menlo Park, CA 94025-7015

1. Introduction

Upcoming synchrotron and free-electron laser light source upgrades such as Argonne National Laboratory’s Advanced Photon Source Upgrade (APS-U) and SLAC National Accelerator Laboratory’s Linac Coherent Light Source II High Energy (LCLS-II-HE) facilities will provide greater insights into the fundamental structures of materials, chemistry, and biology than is possible with current systems. These facilities will have increased spatial/temporal resolution and increased data rates. Together applications like crystallography are expected to produce enormous volumes of data at line rates of approximately 1 TB/s, requiring the use of high-performance computing to process the data stream.

The corresponding parallel file system and network fabrics used to store the data generally have substantially lower capacity and data transfer bandwidth than needed. Even if 1,000 PB of storage were available—more than all storage at the Argonne Leadership Computing Facility combined—these light sources would exhaust the available capacity in less than 12 days of continuous operation. This situation presents critical bottlenecks for scientists planning to study fundamental structures using these light sources. Although non-hit rejection and lossless compression technology exist, these methods will be insufficient with the coming light sources.

Figure 1 shows that light source data contains substantial background noise, even after gain correction and preprocessing, so they are difficult to compress with lossless compressors that rely on identifying patterns in the data. Lossy compression has been recognized as a promising solution to this problem. However, even leading state-of-the-art lossy compressors such as SZ introduce too much data distortion in the critical regions of the data to accomplish important tasks such as constructing electron density models at expected compression ratios.

We propose a specialized, parallel lossy compression scheme, called ROIBIN-SZ (Region Of Interest BINning with SZ lossy compression), for data produced by these instruments that achieve high compression ratios and bandwidth to scale to the needs of these systems while ensuring the scientific integrity of the results from the decompressed data.

Several challenges exist for optimized lossy compression methods for datasets generated in crystallography. First, the diffraction images from crystallography are noisy, so it is nontrivial to obtain a high compression ratio even using the state-of-the-art lossy compressors such as...
SZ [1] and ZFP [2]. Second, investigating the impact of lossy compression on post hoc analysis in crystallography is nontrivial. Specifically, a comprehensive study may cover different datasets generated by different detectors on different crystal structures. This end-to-end verification of the science results also calls for a series of sophisticated tools [3,4] and analysis methods [5,6]. Third, many existing state-of-the-art lossy compression algorithms have been proposed, each with distinct design principles and thus potentially largely different compression performances and qualities.

In this work:

- We develop a flexible hardware and software co-design, ROIBIN-SZ, that can adapt automatically to new hardware and easily adapt to diverse compression methods.
- We develop a number of performance optimization strategies that enable processing images at scale.
- We perform quality assessments on a serial crystallography dataset collected at LCLS, based on our developed compression solution ROIBIN-SZ, and compared with multiple related state-of-the-arts. Experiments show no degradation of scientific outcomes based on standard crystallography metrics.
- With faithful/acceptable fidelity on reconstructing electron densities, our suggested approach achieves an improvement of up to 25.8x in compression ratio over the leading lossy compressors on selenobiotinyl-streptavidin.

2. Overview of the design

ROIBIN-SZ was designed for use in upcoming high-data-rate facilities such as LCLS-II-HE depicted in Figure 2. In this system, each portion of the detector has the ability to write directly to RAM on a preprocessing node. The processor can then access the data from the system RAM for processing. The proposed design of LCLS-II-HE will operate at 1 MHz beam rate (potentially collecting up to one million diffraction patterns) with the incoming data stream arriving at a rate of 1 TB/s.

Once data is loaded from the detector for processing, the processor will handle multiple tasks, including detector calibration (pedestal, common-mode, and gain correction), peak-finding, non-hit rejection (NHR), data compression, and other forms of preprocessing. First, each panel is calibrated to account for known noises in the detector. Such a process involves converting the raw 16-bit unsigned integer data into 32-bit IEEE floating-point data, effectively doubling the input data rate. This detail is important because when compression ratios are reported later in this work, they are reported relative to the 16-bit unsigned integer data rather than the 32-bit floating-point data that is passed to the compressor.

The peak-finding process then locates Bragg peaks within a detector panel to determine regions of interest. This peak-finding algorithm is performed separately and is needed for NHR performed earlier in the pipeline, and optimizing peak-finding further is out of scope for this paper. For our current work, we use the well-established peak-finding algorithm from [7]. If the peak-finding algorithm detects fewer than some number of peaks (set to 10 in our studies), the data from this event is discarded—NHR. Based on our observations as well as some published work on peak-finding [7], this process would typically discard on average 50% of the incoming events, leaving a stream of \( \approx 500 \text{ GB/s} \) that needs to be further reduced.

Regions of interest change per image because of the random orientation of the crystal. We employ a peak-finding algorithm called peak_finder_v3 [7]. The algorithm starts by identifying all local intensity maxima within a sliding window of size 7x7 pixels (set proportional to the typical size of a Bragg peak). Local maxima below 300 ADUs are rejected. All neighboring pixels above 0 ADUs are considered part of the peak. The total peak intensity must be greater than 600 ADUs, and...
The signal-to-noise ratio must be greater than 10. The number of neighboring pixels must be between 2 and 30 pixels. All these parameters are configurable by the user. Peak finding was performed by using MPI in psocake [8,9]. For a 2-megapixel CSPAD detector, it took an average of 65 ms for detector correction and 100 ms for peak finding per image on Intel Xeon CPU E5-2620 v3 @ 2.40 GHz.

This stream is then compressed with ROIBIN-SZ, as illustrated in Figure 3. We first bisect the incoming data stream into the region of interest and the background. For each peak located during peak finding, we save a rectangular region around the peak. We choose the region of interest size to be twice that of the peak size parameter of the peak finder + 1 (17x17). We choose this size to prevent excessive overlaps of regions for non-detected peaks from being treated as background information. We leave further refinement of the handling of regions of interest to future work.

We then apply lossless compression to these regions of interest. In our case, we found that the lossless compressor fpzip—a specialized compressor for floating-point values—achieves the greatest compression ratio for this data. We note that the maximum number of peaks in each event is small ≤ 2,048 relative to the size of the background of the detector, and in practice, a much smaller number of peaks is found in each event. This means that relative to the detector the region of interest is at most 5% and often less than 1% of the data to be compressed for each event and has a modest impact on the runtime (at most 3.4%—10 ms—in the worst case, 2.2% in the median case), and on the overall compression ratio.

After lossless preservation of the regions of interest around the peaks, we apply binning followed by lossy compression to the background. This background information is still important for weak Bragg peak integration; namely, peaks that were too weak to be detected by the peak-finding algorithm. This background information can be noisy, resulting in poor compression performance for lossless and lossy compressors alike. We found, however, that binning reduces the volume of the data substantially while smoothing the underlying data enabling lossy compressors to achieve higher compression ratios without impacting the scientific quality of the data.

Our implementation makes use of LibPressio—a generic interface for lossless and lossy compression of dense tensors—to compose the phases of our implementation [10]. This allows us to quickly experiment with many possible compressor configurations for each stage of our process and consider alternative approaches without changes to the underlying code. This also makes our implementation robust to improvements in the detector pipeline: application-specific integrated circuits, field programmable gate arrays (FPGAs), and GPU-based compressors.

3. Experimental setup
3.1 Hardware
We conduct all of our experiments on up to 10 identical nodes from Phase 18b of the Palmetto Supercomputer at Clemson University. Our evaluation code can be found on GitHub (https://github.com/robertu94/roibin-sz3-experiments).

3.2 Datasets
We conducted quality assessments on a selenobiotinyl-streptavidin dataset [11] from a CSPAD detector with a total of 4,326,979 images where 744,150 contained hits (17.2%). The compression ratio for only non-hit rejection is the inverse of the hit rate, CR = 5.81. This detector has a resolution (4096, 1024). The Se-SAD phasing technique is used for reconstructing streptavidin, which means that a weak anomalous signal from selenium atoms has to be detectable.
after decompression, making this an ideal dataset to test the sensitivity of our lossy algorithm.

For the experiments in quality assessment (Section 4), we use entire runs of the experiments because using the entire dataset is essential to the assessment of the quality of the approach. However, for experiments in the performance assessment (Section 5), we use only a subset of a few hundred images to quickly assess a variety of methods.

The datasets considered are limited by the fact that end-to-end evaluations consume enormous amounts of resources for time and domain expert labor. The raw data for Sc-SAD alone was 20TB and multiple passes over the data are required during peak finding, parameter grid-search for ROIBIN-SZ compression and decompression, indexing of decompressed data, merging into 3D diffraction volume, and phase retrieval; moving data between facilities and processing them in full for the quality analysis takes multiple days using many nodes. More work is needed to facilitate automated processing of this data.

3.3 Compressor configurations

To highlight the benefits of our approach, we consider a range of different compressor configurations to represent a wide array of possible compression approaches. We choose three leading lossless and three leading lossy compressors for the baseline of our comparison. We additionally consider six variants on our approach that measure the performance of just binning and region of interest selection, as well as different lossy compressors for compressing the background.

We also considered several methods from related work. NHR is a largely orthogonal topic that can be used in conjunction with our approach. ZFP is a leading lossy compressor for scientific data that we do consider in our work. SZ compression by itself—without region of interest protection—either failed to achieve a high compression ratio or failed to reproduce the electron densities. We also found techniques that required transferring the data to the GPU for deep-learning-based inference such as TEZIP [12] would be far too slow after accounting for just moving the data to the GPU without additional processing.

Note that we only consider the CPU versions of these compressors. The current design of the detectors as described above starts with the data in memory that is local to the CPU, not the GPU. This requires that the use of any GPU-based compressor begin and end with transfers to and from the CPU, which ends up being the bottleneck in these uses even though GPU-based compressors can get much higher throughput than do CPU ones if the data is resident on the GPU.

4. Quality assessment of ROIBIN-SZ

Figures 4 and 5 show the faithful reconstruction of the electron density from the original and decompressed dataset for ROIBIN-SZ. We additionally find that assessment metrics such as Rsplit, CC1/2, CCano, Rwork, Rfree, and Map-Model-CC are highly similar to the original dataset as shown in Table 1.

More details and an additional dataset on the tuning of these parameters for quality preservation can be found in our full paper [13].

5. Performance assessment

Next, we consider scaling to multiple nodes. For this experiment, we run the execution on an increasing number of tasks and cores that span multiple nodes.

As we scale from 30 to 300 tasks (40 to 400 cores), we find that the execution scales linearly from 7.56 GB/s to 70.69 GB/s. Dataset-to-dataset variation in compressor bandwidth is to be expected with compressors such as SZ. This indicates that ≈ 67 ∼ 84 to nodes would be required using this configuration to scale to the desired 500 GB/s bandwidth after NHR.

Figure 4: Original streptavidin electron density.
Next, we consider throughput and compression ratios at scale for the dataset in Table 2.

We find that ROIBIN-SZ is able to achieve very high compression ratios, up to 46.4 on Se-SAD relative to the uint16 raw data format from the detectors and able to meet the 500 GB/s bandwidth requirement with ≈82 nodes. This is a substantial improvement over lossless methods that, relative to the detector’s raw format, actually result in an increase in storage used.

Table 1: Crystallography Metrics. Metrics are calculated for resolution range 28Å–1.9Å.

| Metric               | Original | ROIBIN-SZ |
|----------------------|----------|-----------|
| Total compression ratio | 2.91     | 70.7      |
| Average compression ratio | .5       | 12.16     |
| NHR only compression ratio | 5.81     | 5.81      |
| Number of images     | 4,326,979| 4,326,979 |
| Number of hits       | 744,150  | 744,150   |
| Number indexed       | 255,065  | 255,918   |
| RSplit               | .758     | .708      |
| CC1/2                | .997     | .997      |
| CCano                | .087     | .104      |
| Rwork                | .206     | .199      |
| Rfree                | .231     | .223      |
| Map model CC         | .81      | .80       |

Table 2: Compression Ratio and bandwidth for various configurations.

| Configuration   | Compression ratio | Bandwidth (GB/s) for 400 cores |
|-----------------|-------------------|---------------------------------|
| BZIP2-9         | .6                | 2                               |
| BZIP2-6         | .6                | 2.2                             |
| BLOSC-ZSTD-3    | .61               | 25.6                            |
| BLOSC-ZSTD-6    | .63               | 6.68                            |
| BLOSC-ZSTD-9    | .64               | 1.1                             |
| ROIBIN-BZIP-6   | 2.2               | 6.9                             |
| ROIBIN-BZIP-9   | 2.2               | 6.6                             |
| ROIBIN-FPBZIP   | 2.5               | 35.8                            |
| ROIBIN-BLOSC-3  | 2.5               | 76.4                            |
| ROIBIN-BLOSC-6  | 2.5               | 24.9                            |
| ROIBIN-BLOSC-9  | 2.5               | 4.6                             |
| MGARD           | 1.4               | 1.9                             |
| ZFP             | 1.8               | 26.5                            |
| ROIBIN-MGARD    | 7.1               | 7.7                             |
| ROIBIN-ZFP      | 10.5              | 66.3                            |
| ROIBIN-SZ       | 46.4              | 50.61                           |
| ROIBIN-SZ3      | 39.1              | 60.27                           |

The best performing Compression Ratio and Bandwidth numbers for completely lossless, binning only, and binning-lossy have been bolded.
We also find that the variants of our method, such as ROIBIN-MGARD and ROIBIN-ZFP, outperform their non-ROIBIN counterparts. This result can be attributed to the relative speed of binning to these compressors algorithms and the comparative smoothness of the data after binning. ROIBIN-ZFP takes the position as the highest compression bandwidth for this dataset, although this comes at a large trade-off in compression ratios. With ROIBIN-ZFP, the 500 GB/s target could be met with ≈ 73 nodes.

6. Conclusions

In this work we have shown substantial improvements to the compression of serial crystallography data while performing science-preserving compression. We were able to achieve up to a 46.44× compression ratio (and up to 154.18× total when non-hit rejection is used additionally) respectively on selenobiotinyl-streptavidin while preserving the data sufficiently to reconstruct the structure at bandwidths and scales that are reasonably obtainable to match the compression bandwidth needs of the upcoming APS-U and LCLS-II-HE systems.

For future work, we would like to consider the application of this approach to other domains. Additionally, we would like to consider other forms of light source data that may benefit from our approach and experiment with FPGAs/GPUs. We consider additional aspects in our full paper [13].

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