MSc Degree Project Proposal
Computer Science

Name: Casper Ove Kristiansson
Email: Casperkr@kth.se

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1 Background and Literature Review

Modern synchrotron and neutron facilities face issues with data handling where experiments can produce terabytes of data per day, which has overwhelmed traditional storage and analysis methods [1]. Over the last decade, numerous strategies have emerged to optimize data storage, management, and access for these large-scale scientific datasets. This thesis will investigate and prototype certain cloud-based solutions (particularly on AWS) to handle large volumes of experimental data. Below is a review of the relevant literature and approaches from approximately the past ten years.

1.1 Automated Data Archiving & Management Systems

A common approach involves platforms that automatically capture raw data, metadata, and even preliminary results, ensuring minimal data loss and efficient sharing. For example, the Australian Synchrotron developed *Store.Synchrotron*, a cloud-based archive for X-ray diffraction data [2]. In its first 9 months, it archived about 22.4 TB (about 1.7 million images) of beamline data, providing researchers with real-time online access to a fully redundant, secure storage system [2]. Additionally, a key theme in such systems is *cost-aware storage policies*. Storing petascale datasets fully online in commercial clouds (e.g., Amazon AWS) can become expensive for *actively accessed* data.

1.2 Cloud-Based Solutions (AWS) for Large-Scale Experiments

As cloud technologies have matured, many facilities began integrating public clouds to help or replace on-premises resources.

- **AWS for Remote Data Portals:** The Materials & Life Science Facility (MLF) at J-PARC (Japan) leverages AWS to allow users to remotely monitor and analyze neutron scattering data without physically transporting terabytes of raw files [3]. Their system uses Amazon S3 for storage and AWS Lambda for serverless triggers [3].

- **Hybrid HPC & Cloud Archival:** KEK, a research organization in Japan, adopted a hybrid approach to extend on-premises HPC resources into AWS. This enables "burst" capacity for beamtime while lowering costs in the off-season [4]. When experiments are not running, the cloud resources can be turned off, avoiding ongoing charges.

1.3 Scalable Storage Architecture and Performance Optimizations

Data volume alone does not capture the challenge; performance for reading, writing, and retrieving partial datasets is often the true bottleneck.

- **Tiered and Distributed Storage:** Large facilities typically adopt tiered storage architectures (fast parallel file systems for immediate processing, tape or high-capacity disk arrays for archival), sometimes also integrated with a cloud backend [2].

- **High-Performance I/O and Data Reduction:** Oak Ridge National Lab's neutron sources (SNS and HFIR) handle around 1.2 TB of raw data per day, employing new I/O optimization strategies that can reduce processing time by 11–30% [5]. Techniques like in-memory metadata indexing, chunked file formats, or streaming data pipelines (e.g., ADIOS2) are highly relevant to modern HPC scenarios.

1.4 Synthesis for This Project

The last decade of work highlights the need for:

1. Automated ingestion and management platforms to ensure data is captured seamlessly with rich metadata.

2. Hierarchical or hybrid storage solutions to balance cost, performance, and scalability, often combining disk, tape, and cloud.

3. Software-level optimizations (e.g., chunked storage, advanced data formats) to handle partial reads efficiently.

This thesis intends to *compare* multiple AWS-oriented storage approaches (HDF5, Zarr, Parquet, and DynamoDB) using real-world synchrotron/neutron datasets. The goal is to characterize performance (latency, throughput), cost, and ease-of-integration for partial retrieval or queries—key operations in beamline and scattering experiments.

2 Thesis Title

From Experiment to Insight: A Comparative Study of Storage Approaches for Large-Scale Synchrotron and Neutron Scattering Data on AWS

3 Research Question

How do HDF5, Zarr, Parquet, and a NoSQL store compare in terms of performance, scalability, and cost when storing large-scale synchrotron and neutron scattering data on AWS, particularly for partial row or column retrieval?

4 Hypothesis

1. **Columnar Advantage (Parquet):** Columnar storage (Parquet) should excel for queries involving partial-column reads, reducing I/O overhead.

2. **Chunked Object Storage (Zarr):** Zarr's chunk-based design may outperform HDF5 for parallel reads/writes in a purely cloud-native (object store) environment.

3. **HDF5 Familiarity:** HDF5 may remain favorable for certain multidimensional access patterns or for legacy HPC-style workflows.

4. **NoSQL (DynamoDB) Trade-offs:** DynamoDB may be beneficial for extremely high concurrency, but less suitable for large-scale partial scans (e.g., retrieving entire columns or slices of data).

5 Method

1. **Requirements & Literature Review:** Collect typical data requirements for scattering experiments, referencing the approaches in [1]–[5] and other HPC data management projects.

2. **Prototype Implementation:**
   - Create a consistent dataset in HDF5, Zarr, Parquet, and DynamoDB (using AWS S3 or AWS native services).
   - Apply consistent chunking/partitioning logic, so each approach handles partial reads comparably.

3. **Testing and Metrics:**

- *Dataset Volume:* Terabytes of realistic scattering data.
- *Performance Metrics:* Read/write latency, throughput under parallel access, storage cost (S3 usage, DynamoDB R/W units, data egress), partial retrieval overhead.
- *Scalability Testing:* Evaluate each approach as the dataset size and number of concurrent users grows.

4. **Analysis:**

- Compare trade-offs in cost, performance, and complexity.
- Provide recommendations on when each approach (HDF5, Zarr, Parquet, DynamoDB) is most appropriate for large-scale facility data.

6 Relevance / Who Cares?

- **Scientific Facilities:** Synchrotrons, neutron sources, and other big-science labs need robust, future-proof strategies.

- **Industrial Partners:** Companies analyzing materials data at scale can adopt more efficient workflows, reducing time-to-insight and costs.

- **Data Management Community:** Expands best-practices on HPC-cloud integration, partial reads, and cost-optimized big-data solutions.

7 Background of the Student

I am completing an MSc in Computer Science at KTH with coursework in *Data-Intensive Computing, Data Storage Paradigms, Advanced Algorithms*, and significant experience (2,000+ hours) as a Full Stack Developer at Scatterin AB building AWS-based platforms for scientific data. My prior Bachelor's thesis on cloud computing pricing complements the cost analysis in this project.

8 Supervision & Resources

- **Scatterin AB:** Hosting the project, providing real experimental data and existing AWS infrastructure.

- **Supervisor:** Dr. Ahmet Bahadır Yıldız, KTH Royal Institute of Technology (SwedNess).

- **Additional Expertise:** Prof. Peter Hedström (Scatterin AB, KTH).

- **Location:** Work carried out primarily at Scatterin AB's KTH campus office, with daily supervision opportunities.

9 Eligibility

I have verified that I'm eligible to start my degree project, that I fulfill the basic requirements of starting the project and that all relevant courses are already completed for the project.

10 Study Planning

Currently, the only remaining course I need to complete for my Master of Science in Computer Science is the Program Integrating Course in Computer Science (DD2300), which will run in parallel with the degree project. Additionally, I was enrolled in Scalable Software Development with Functional Programming (DD2489) during the most recent period, which ended one week ago. I have completed a substantial portion of the course requirements and am currently in discussion with the instructor to finalize the remaining components.

References

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[2] G. R. Meyer, D. Thompson, J. M. Guss, *et al.*, "Operation of the Australian Store.Synchrotron for macromolecular crystallography," *Journal of Applied Crystallography*, vol. 47, no. 4, pp. 1548–1560, 2014. DOI: 10.1107/S1600576714012410. [Online]. Available: https://pmc.ncbi.nlm.nih.gov/articles/PMC4187999/.

[3] T. Moriyama, T. Watanabe, H. Tominaga, T. Shoji, M. Ito, and K. Tamura, "Public Cloud-based Remote Access Infrastructure for Neutron Scattering Experiments at MLF, J-PARC," in *Proceedings of the 17th International Conference on Accelerator and Large Experimental Physics Control Systems (ICALEPCS)*, 2019. [Online]. Available: https://accelconf.web.cern.ch/icalepcs2019/papers/tubpl04.pdf.

[4] *KEK Creates HPC Environment and Reduces TCO with AWS*, Amazon Web Services Case Study, 2021. [Online]. Available: https://aws.amazon.com/solutions/case-studies/kek/.

[5] W. F. Godoy, N. Podhorszki, D. Pugmire, S. Klasky, *et al.*, "Efficient Data Management in Neutron Scattering Workflows," in *2021 IEEE International Conference on Big Data (Big Data)*, 2021. arXiv: 2101.02591. [Online]. Available: https://arxiv.org/pdf/2101.02591.