Understanding I/O Behavior in Scientific Workflows on High Performance Computing Systems

Fahim Chowdhury[1], Francesco Di Natale[2], Adam Moody[2], Elsa Gonsiorowski[2], Kathryn Mohror[2], Weikuan Yu[1]

[1] Florida State University, [2] Lawrence Livermore National Laboratory

Overview

- ❑ Leadership high performance computing (HPC) infrastructures empower scientific, research or industry applications
- ❑ Heterogeneous storage stack is common in supercomputing clusters
- ❑ **Project goals**
  - To extract the I/O characteristics of various HPC workflows
  - To develop strategies to optimize overall application performance by improving the I/O behavior
  - To leverage heterogeneous storage stack
- ❑ **Initial steps**
  - To understand I/O behavior in scientific application workflow on HPC
  - To perform systematic characterization and evaluation

I/O Workloads on HPC Workflow

- ❑ What is HPC Workflow?
  - Pre-defined or random ordered execution of set of tasks
  - Tasks performed by inter-dependent or independent applications
- ❑ Data transfer or dataflow in HPC Workflows can create bottleneck
- ❑ **Dataflow examples**
  - Huge **metadata overhead** on parallel file systems (PFS) by random tiny read requests in deep learning (DL) training workflow [1]
  - **Sequential write-intensive** applications, e.g., CM1
  - **In-situ and in-transit analysis** in applications, e.g., Montage
  - **Checkpoints and update-intensive** applications, e.g., Hardware Accelerated Cosmology Code (HACC) [2]

Heterogeneous Storage Stack

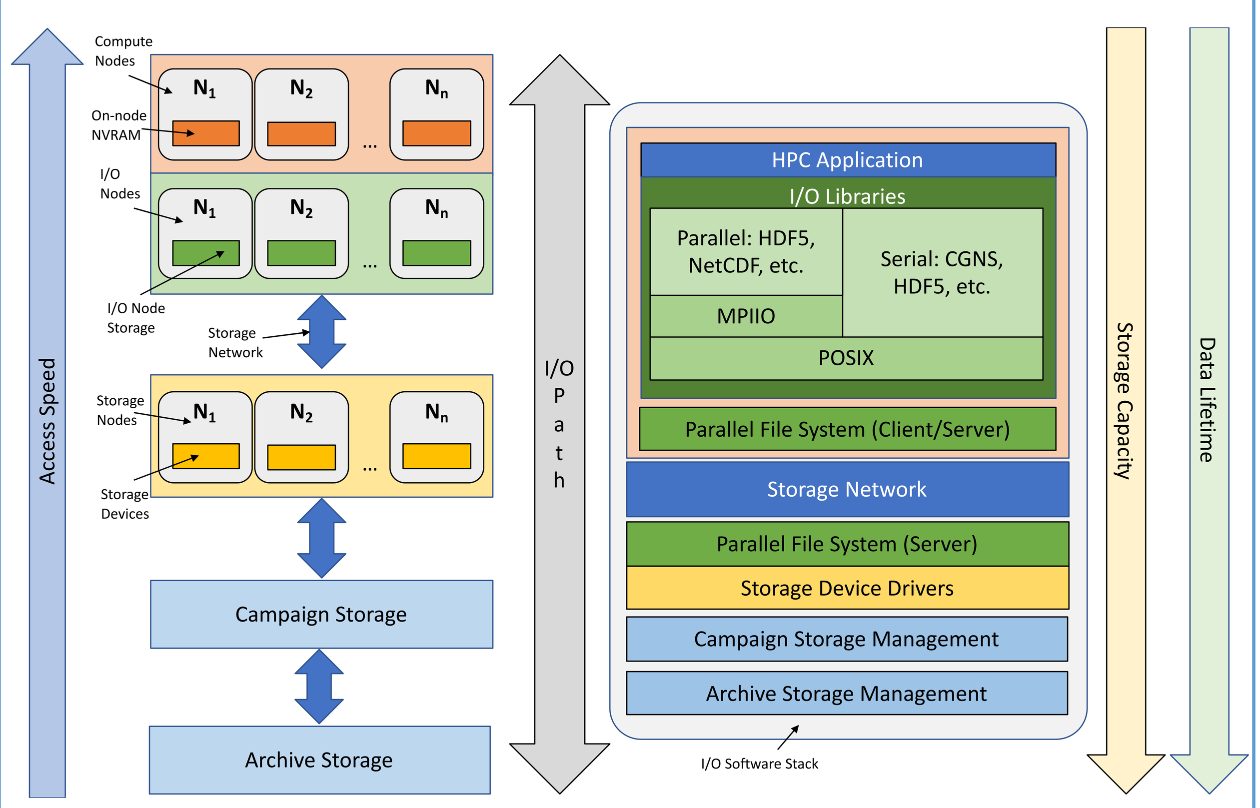


Fig. 1: Typical HPC I/O system architecture

Emulating Different Types of HPC I/O Patterns

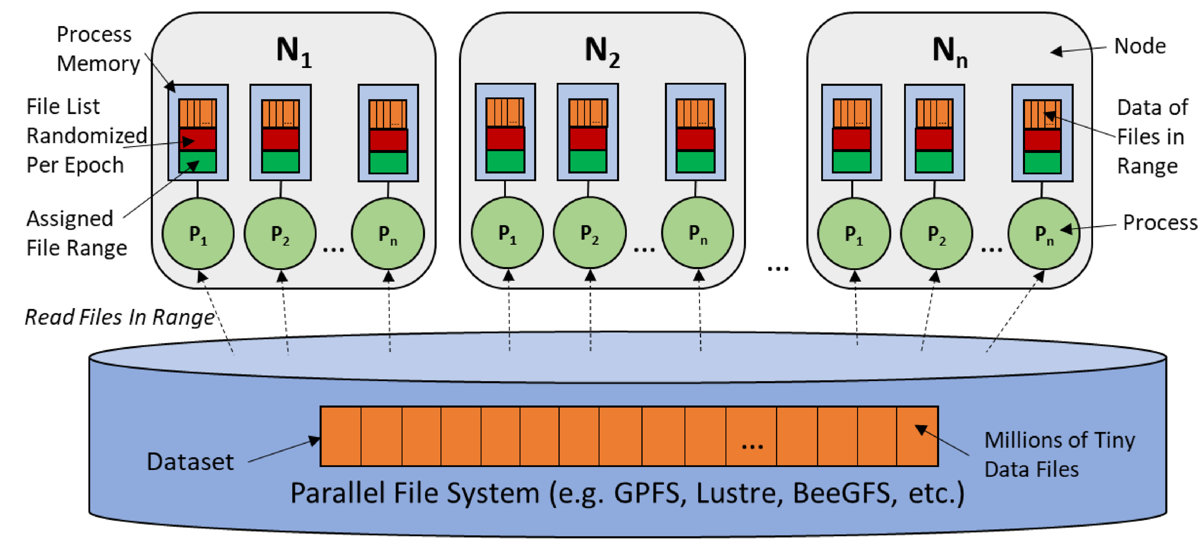


Fig. 2: Deep Learning Training I/O Pattern

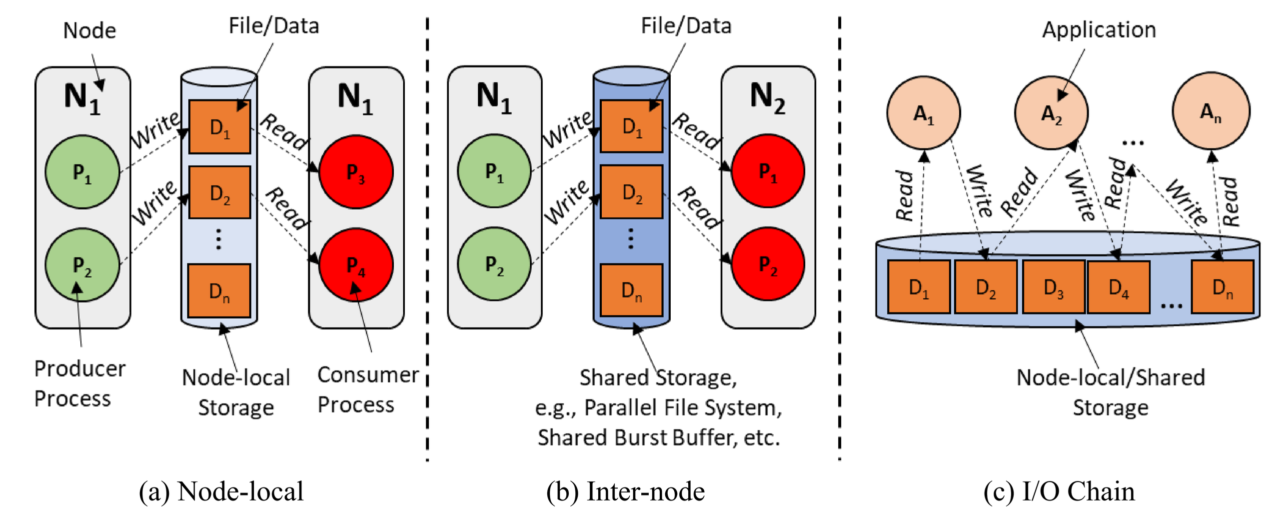


Fig. 3: Producer-Consumer I/O Pattern

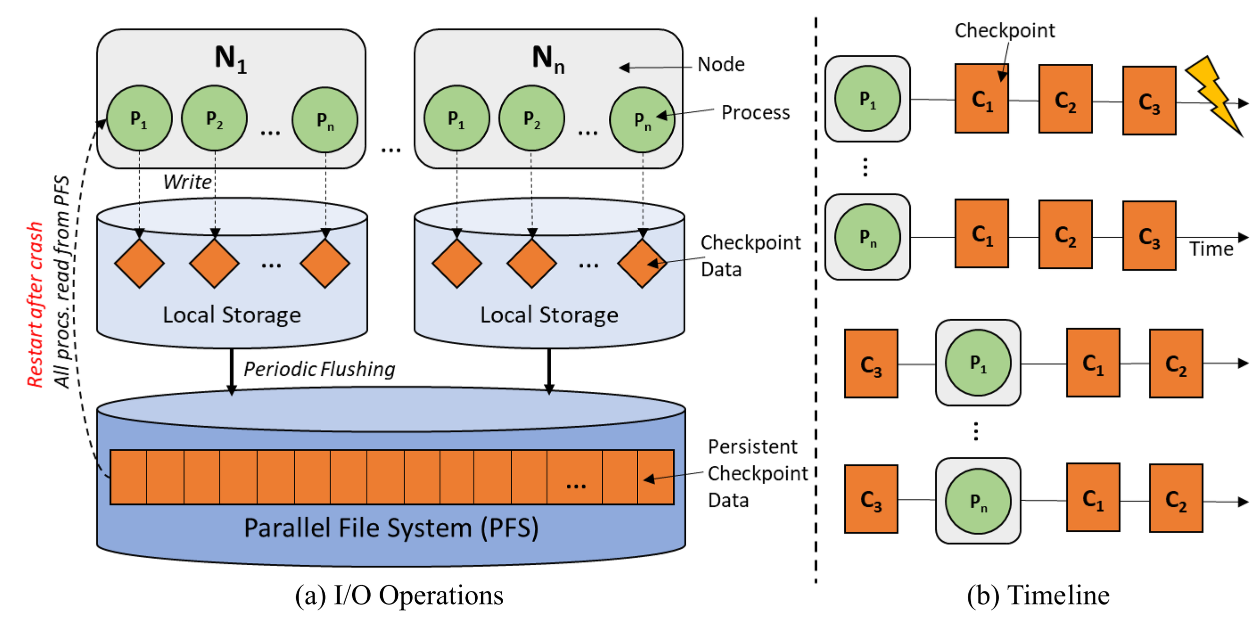


Fig. 4: Checkpoint/Restart I/O Pattern

✓ MPI enabled C++ Application to Emulate HPC I/O

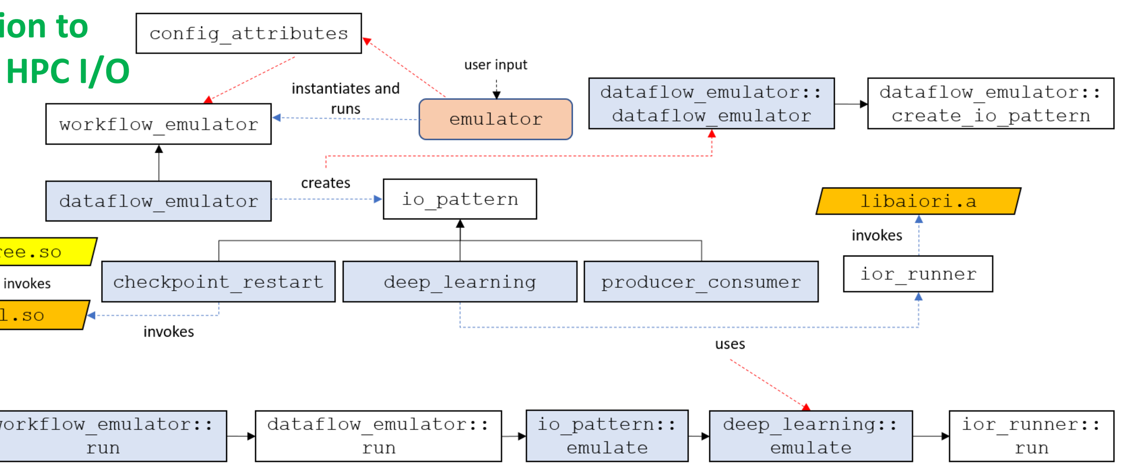


Fig. 5: Class Diagram of Dataflow Emulator

- ✓ Usage: *./emulator --type data --subtype dl --input_dir <dataset_dir>*
- ➢ Currently under active development

Experimental Results from Emulator

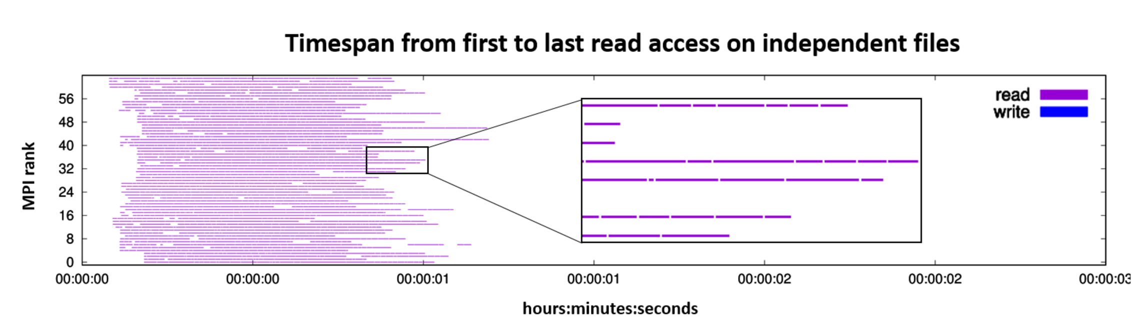


Fig. 6: Deep Learning Training I/O Timeline

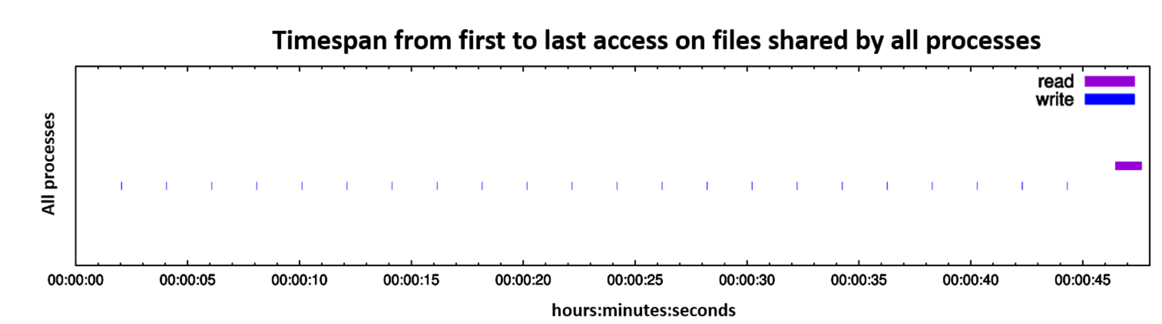
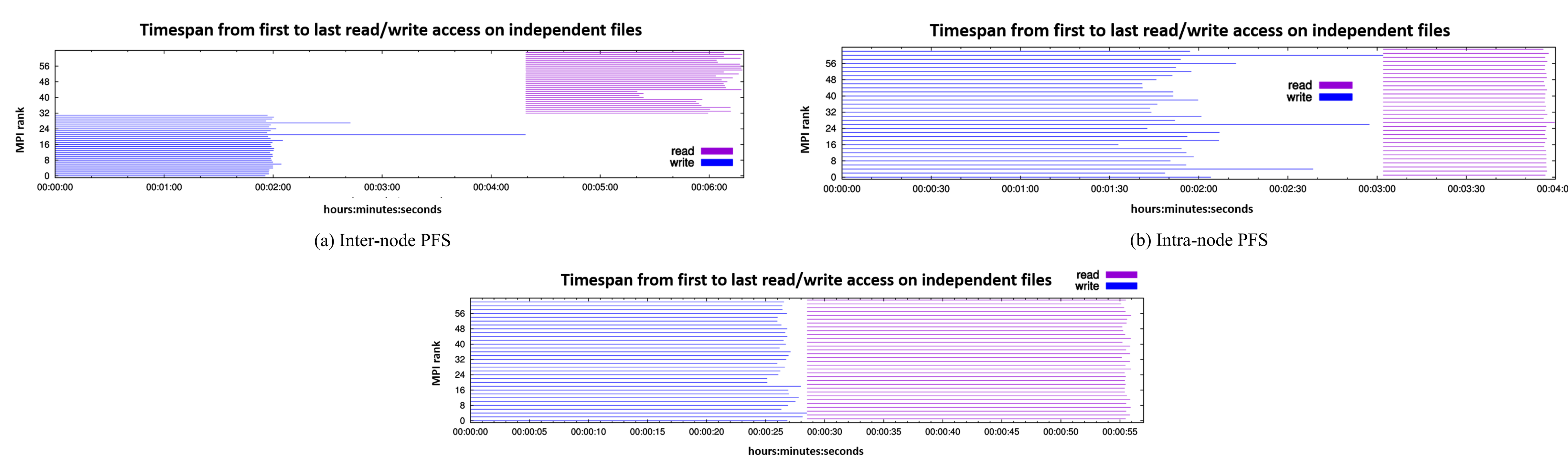


Fig. 7: Checkpoint/Restart I/O Timeline



(a) Inter-node PFS

(b) Intra-node PFS

(b) Intra-node Burst Buffer

Fig. 8: Producer-Consumer I/O Timeline

I/O Demands of Cancer Moonshot Pilot-2

- ❑ Cancer Moonshot Pilot2 (CMP2) [3] project
  - Aims at using HPC for cancer research
  - Seeks to simulate RAS protein and cell membrane interaction
- ❑ I/O behavior in CMP2
  - Producer-consumer pattern between different submodules

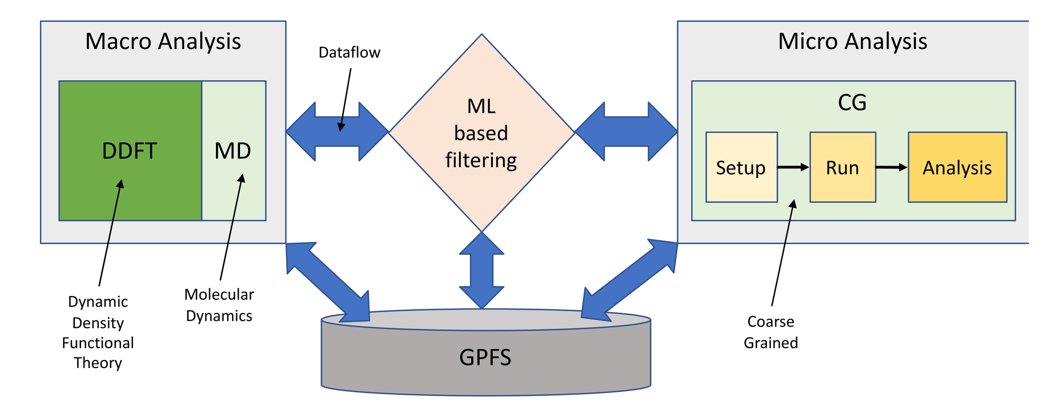


Fig. 9: Dataflow in CMP2 HPC implementation

Conclusion and Future Plans

- ❑ Handling dataflow in scientific applications' workflows is critical
- ❑ Effective I/O management system is necessary in workflow manager like MaestroWF [4]
- ❑ Intelligent data transfer among different units of heterogeneous storage resources in leadership supercomputers can improve performance
  - Third party API libraries like Asynchronous Transfer Library (AXL) [5] can be leveraged
- ❑ **Current Efforts**
  - ✓ Developing a Dataflow Emulator to generate different types of HPC I/O workloads
  - ✓ Analyzing the CMP2 project to detect possible I/O vulnerabilities
- ❑ **Future Plans**
  - ➢ To detect I/O behavior and dataflow by profiling CMP2 workflow
  - ➢ To develop data management strategies to properly handle the dataflow in complicated and composite HPC workflows like CMP2

References

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[3] D. H. Ahn et al., "Flux: Overcoming Scheduling Challenges for Exascale Workflows," 2018 IEEE/ACM Workflows in Support of Large-Scale Science (WORKS), Dallas, TX, USA, 2018.

[4] MaestroWF. https://github.com/LLNL/maestrowf

[5] Asynchronous Transfer Library. https://github.com/ECP-VeloC/AXL

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Contact Information

Email: fchowdhu@cs.fsu.edu; ftc17@my.fsu.edu; **Phone:** (786) 406-2617