



# Machine Learning for CUDA+MPI Design Rules

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## Automatic Discovery of Implementation Rules for Fast GPU + MPI Operations



- Fast libraries for heterogeneous architectures
  - Mapping computation onto processors
  - Choosing communication strategy
  - Unpredictable performance interaction
- Prototype automatic tooling for discovering important design decisions
  - Reduced developer effort for performance on new systems
  - Maintain human provenance of library design
  - e.g. Modernize Tpetra MPI+GPU distributed linear algebra operations

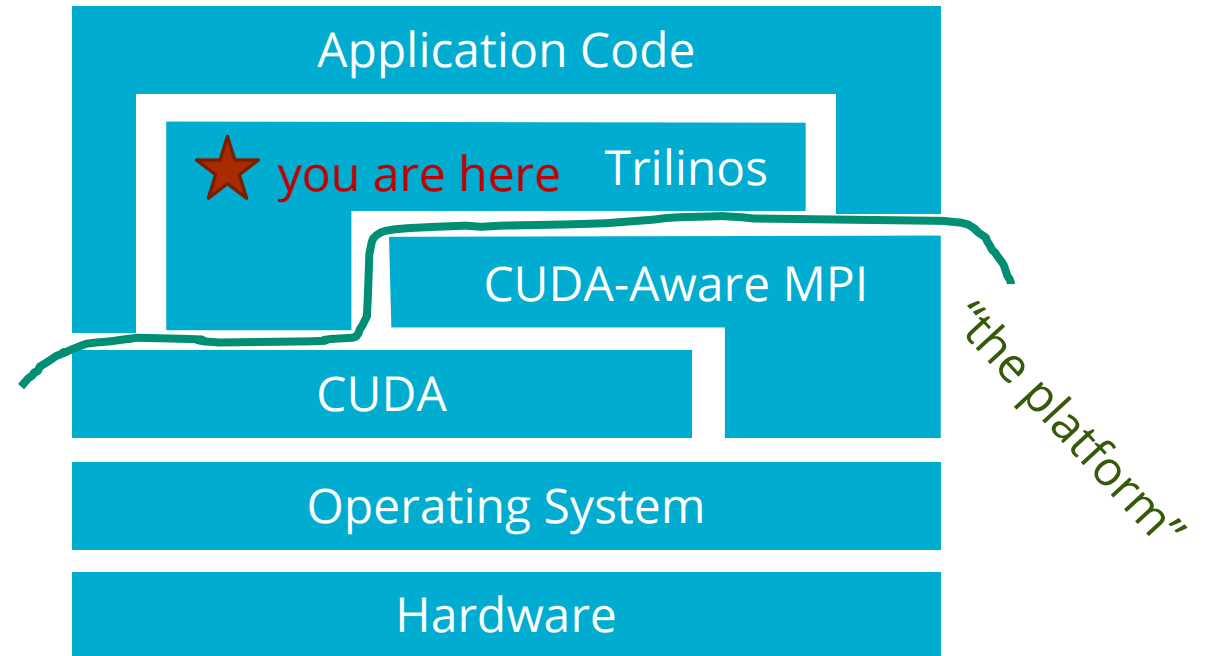
Key Challenge	How it's Done
Large Design Space	<ul style="list-style-type: none"><li>• Express operation as a directed acyclic graph (DAG) of operations</li><li>• Monte-Carlo Tree Search (MCTS) to identify and explore regions of interest</li></ul>
Extract performance insight	<ul style="list-style-type: none"><li>• Empirical benchmarking</li><li>• Feature vector for each implementation</li><li>• Decision tree training for design rules</li></ul>

Initial results pass “sniff test,” working on broader experiments and quantitative evaluation

# Libraries are built on existing lower-level primitives



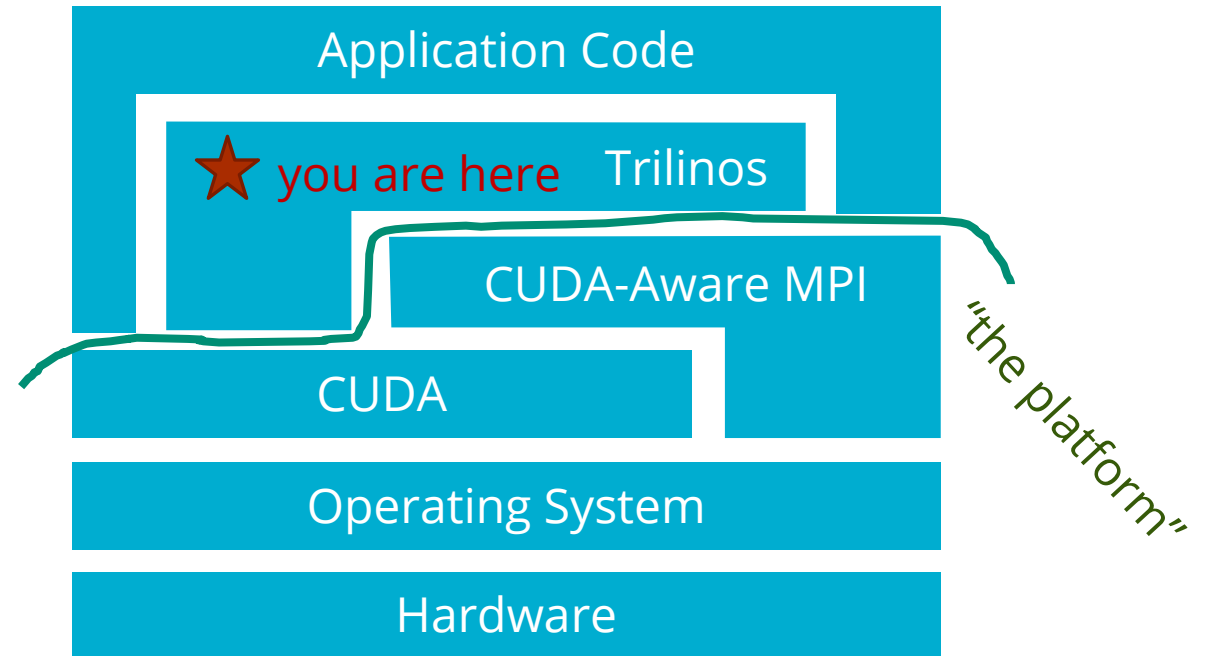
- Our libraries (and applications) are combinations of existing library and vendor operations
  - and code to coordinate them
  - and code to implement custom behavior



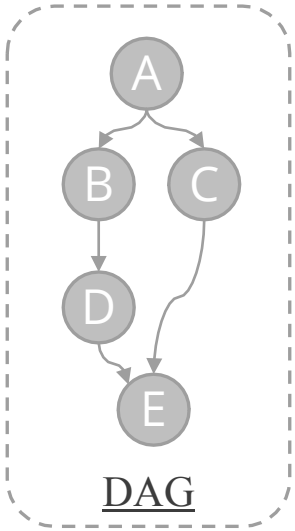
# Libraries are built on existing lower-level primitives



- Our libraries (and applications) are combinations of existing library and vendor operations
  - and code to coordinate them
  - and code to implement custom behavior
- Performance changes at many layers for new platforms
  - new hardware,
  - new CUDA version,
  - new OS version,
  - etc.



# Prototype Implementation in C++ and Python



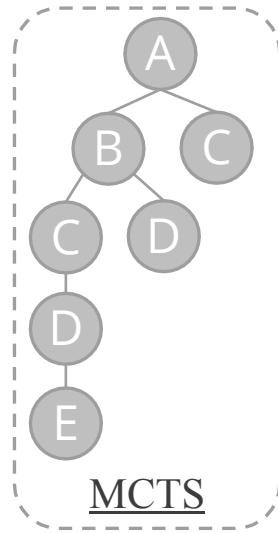
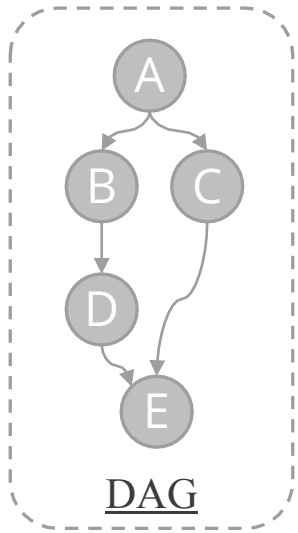
DAG

DAG of  
operations  
describes design  
space

C++ / CUDA / MPI

Python / scikit-learn

# Prototype Implementation in C++ and Python



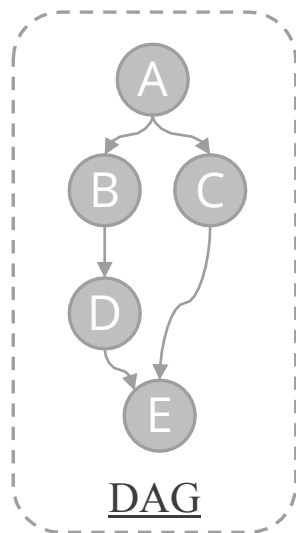
DAG of  
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MCTS searches  
order of operations  
and resource  
assignment

C++ / CUDA / MPI

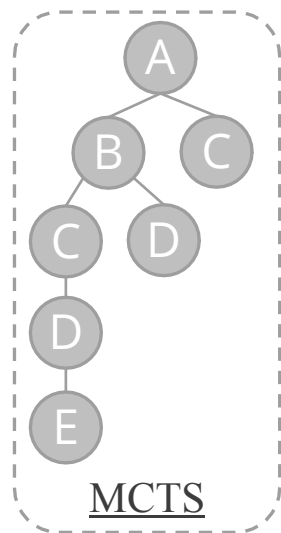
Python / scikit-learn

# Prototype Implementation in C++ and Python

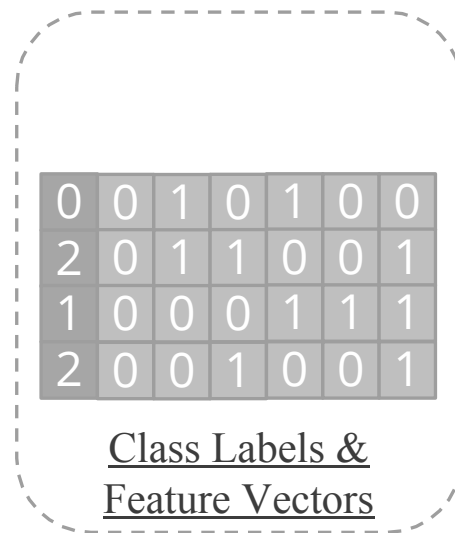


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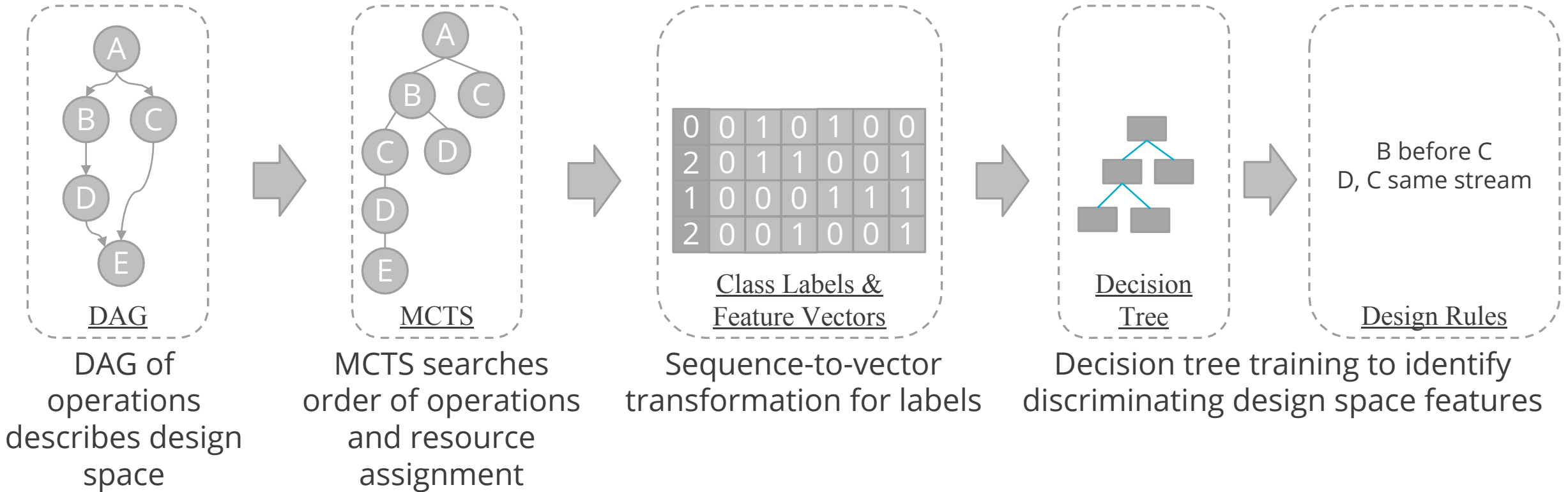
MCTS searches  
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Sequence-to-vector  
transformation for labels

Python / scikit-learn

# Prototype Implementation in C++ and Python



C++ / CUDA / MPI

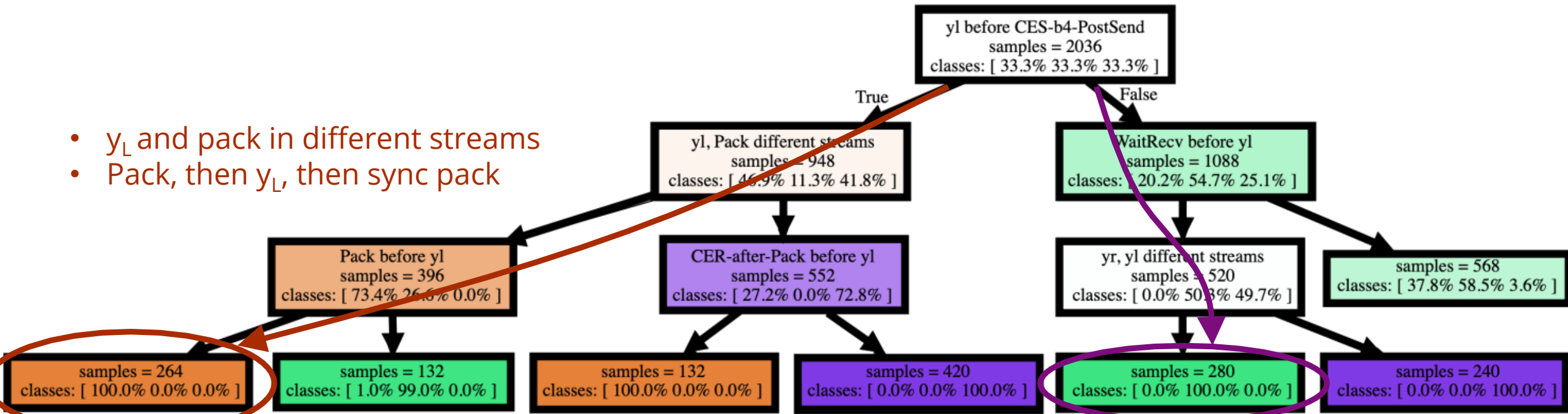
Python / scikit-learn



# Decision Tree Training to Determine which Rules Discriminate between Classes



- $y_L$  and pack in different streams
- Pack, then  $y_L$ , then sync pack



- sync pack before  $y_L$
- WaitRecv before  $y_L$
- $y_L, y_R$  in same stream

Each path through the tree is a set of design rules that define a performance class

# Vision for this work



- Current
  - C++ MCTS implementation for MPI/CUDA codes with multiple streams
  - Prototype feature-vector and decision tree training using SciKit in Python
  - Available at [github.com/sandialabs/tenzing](https://github.com/sandialabs/tenzing)
- Upcoming
  - Applying initial results to Tpetra distributed linear algebra package in Trilinos
- Future Explorations
  - Identify unexpected performance effects on target platforms (“performance bugs”)
  - What to do as communication / computation are more tightly integrated
- Summary
  - Represent CUDA+MPI operation as DAG
  - Automatically generate human-interpretable rules for library design
  - Maintain human provenance of implementation (no “black boxes”)