Alchemist

An Apache Spark ⇔ MPI Interface

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In collaboration with UC Berkeley riselab UC Berkeley

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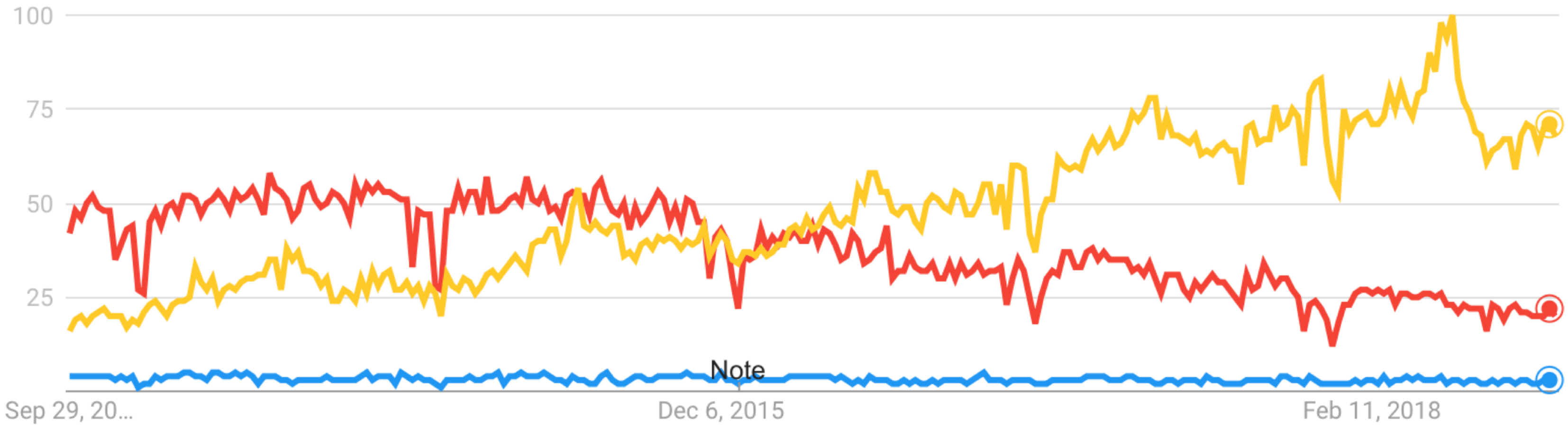
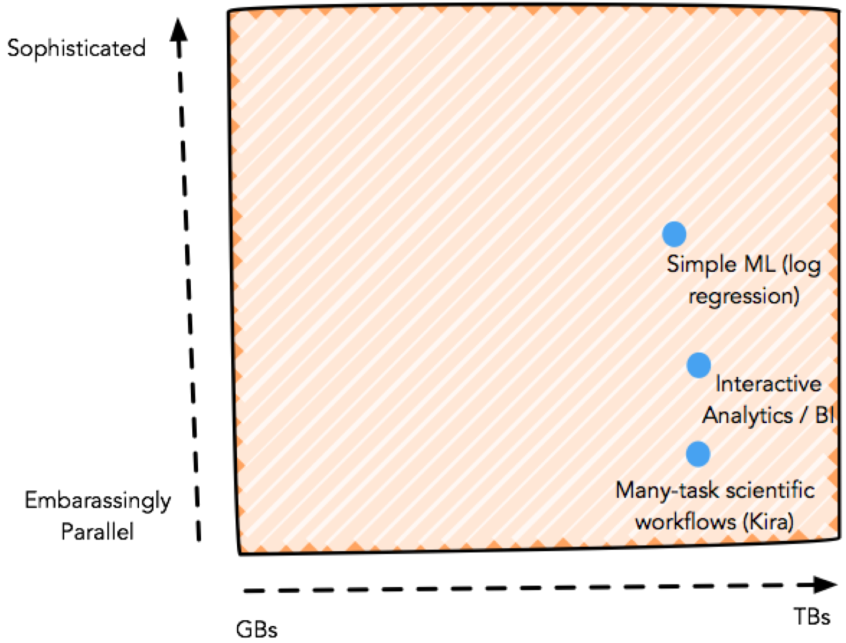
Why should MPI codes interface with Spark?



Google trends popularity: MPI vs Hadoop vs Spark

Spark Use Cases



Q: What about less embarrassingly parallel computations?
A: Use Spark and MPI

Example: linear algebra in Spark

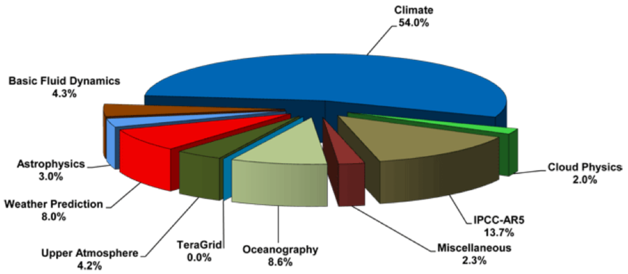
Pros for Spark:

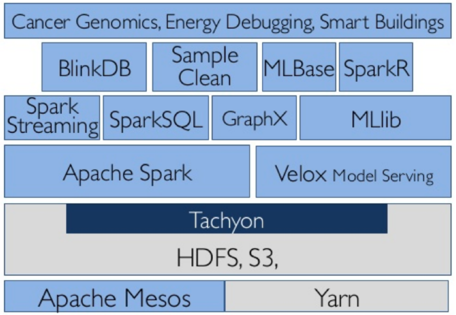
- Faster development, easier reuse
- One abstract uniform interface (RDD)
- An entire ecosystem that can be used before and after the NLA computations
- Spark can take advantage of available local linear algebra codes
- Automatic fault-tolerance, out-of-core support

Pros for MPI: Classical MPI-based linear algebra implementations will be faster and more efficient

Motivation

- **NERSC**: Spark for data-centric workloads and scientific analytics
- **RISELab**: characterization of linear algebra in Spark (MLlib, MLMatrix)
- **Cray**: users asking for Spark; understand performance concerns





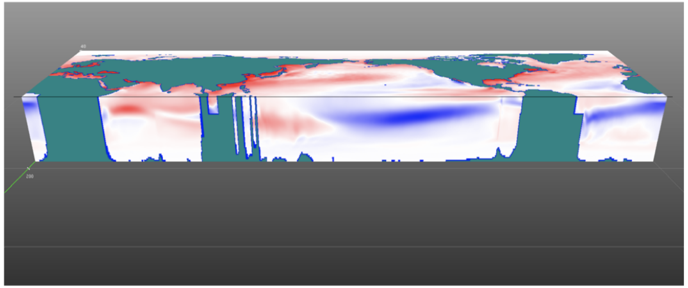
Case Study: Spark vs. MPI

- **Numerical linear algebra (NLA)** using Spark vs. MPI
- Computations performed on NERSC supercomputer **Cori** Phase 1, a Cray XC40
  - 2,388 compute nodes
  - 128 GB RAM/node, 32 2.3GHz Haswell cores/node
  - Lustre storage system, Cray Aries interconnect

A. Gittens et al. "Matrix factorizations at scale: A comparison of scientific data analytics in Spark and C+MPI using three case studies", 2016 IEEE International Conference on Big Data (Big Data), pages 204–213, Dec 2016.

Case Study: Spark vs. MPI

- **Numerical linear algebra (NLA)** using Spark vs. MPI
- Matrix factorizations considered include *truncated Singular Value Decomposition (SVD)*
- Data sets include
  - Ocean temperature data - 2.2 TB
  - Atmospheric data - 16 TB



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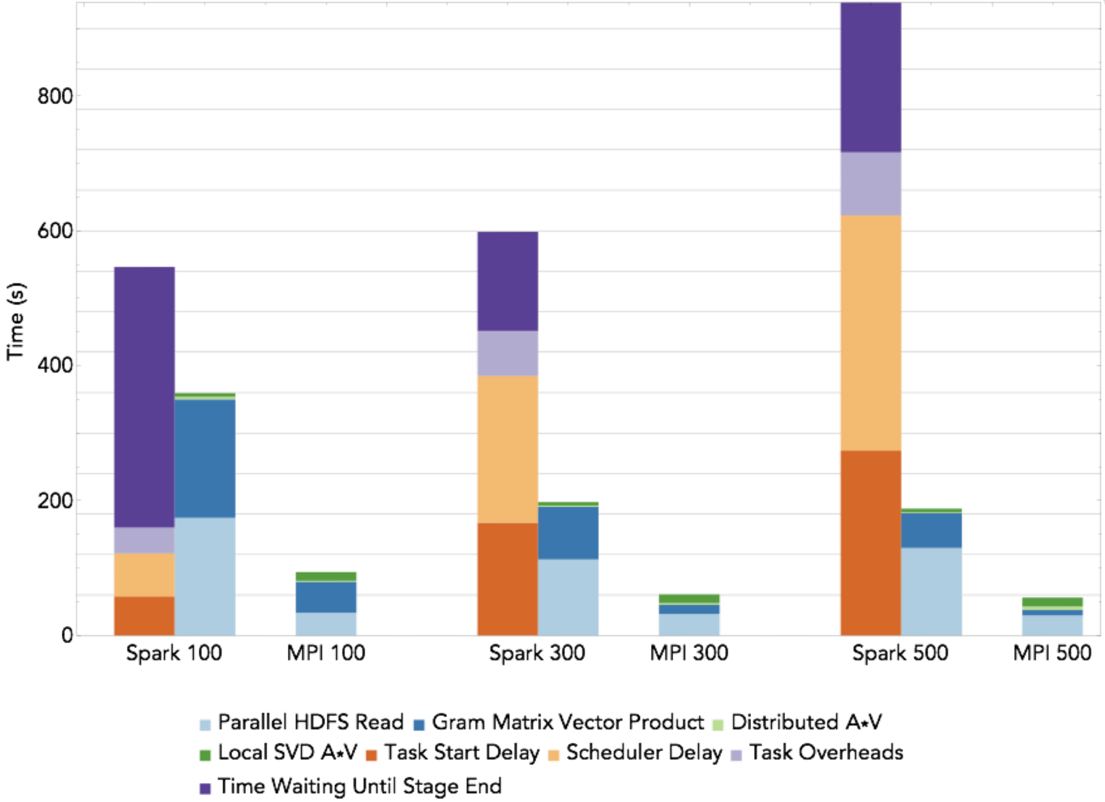
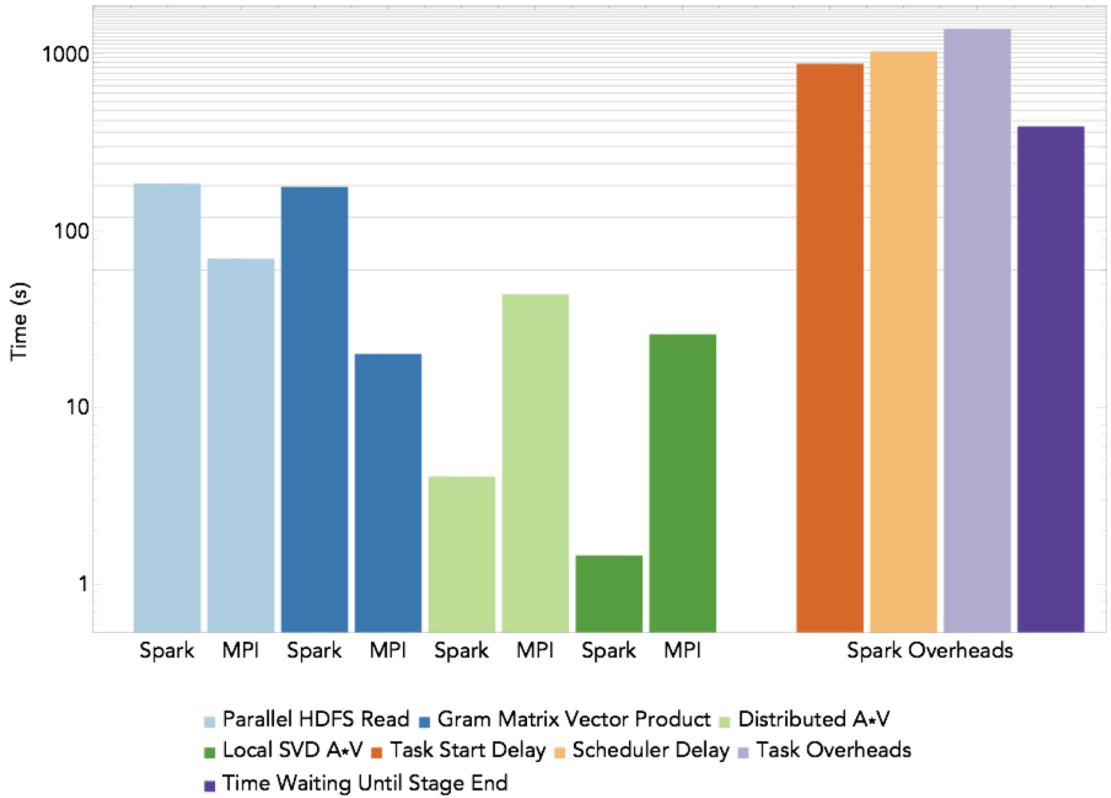
Case Study: Spark vs. MPI

Rank 20 SVD of 2.2TB ocean temperature data



Case Study: Spark vs. MPI

Rank 20 SVD of 16TB atmospheric data using 48K+ cores



Case Study: Spark vs. MPI

Lessons learned:

- With favorable data (tall and skinny) and well-adapted algorithms, linear algebra in Spark is 2x-26x slower than MPI when I/O is included
- Spark's overheads:
  - Can be order of magnitude higher than the actual computation times
  - Anti-scale
- **The gaps in performance suggest it may be better to interface with MPI-based codes from Spark**

- **Alchemist** interfaces between Apache Spark and *existing* or *custom* MPI-based libraries for **large-scale** linear algebra, machine learning, *etc.*
- ***Idea***:
  - Use Spark for regular data analysis workflow
  - When computationally intensive calculations are required, call relevant MPI-based codes from Spark using Alchemist, send results to Spark
- **Combine *high productivity* of Spark with *high performance* of MPI**

Alchemist

Target users:

- ***Scientific community:*** Use Spark for analysis of large scientific datasets by calling existing MPI-based libraries where appropriate
- ***Machine learning practitioners*** and ***data analysts***:
  - Better performance of a wide range of large-scale, computationally intensive ML and data analysis algorithms
  - For instance, SVD for principal component analysis, recommender systems, leverage scores, etc.

Basic Framework

- **Alchemist**: Acts as bridge between Spark and MPI-based libraries
- **Alchemist-Client Interface:** API for user, communicates with Alchemist via TCP/IP sockets
- **Alchemist-Library Interface:** Shared object, imports MPI library, provides generic interface for Alchemist to communicate with library

Basic Framework

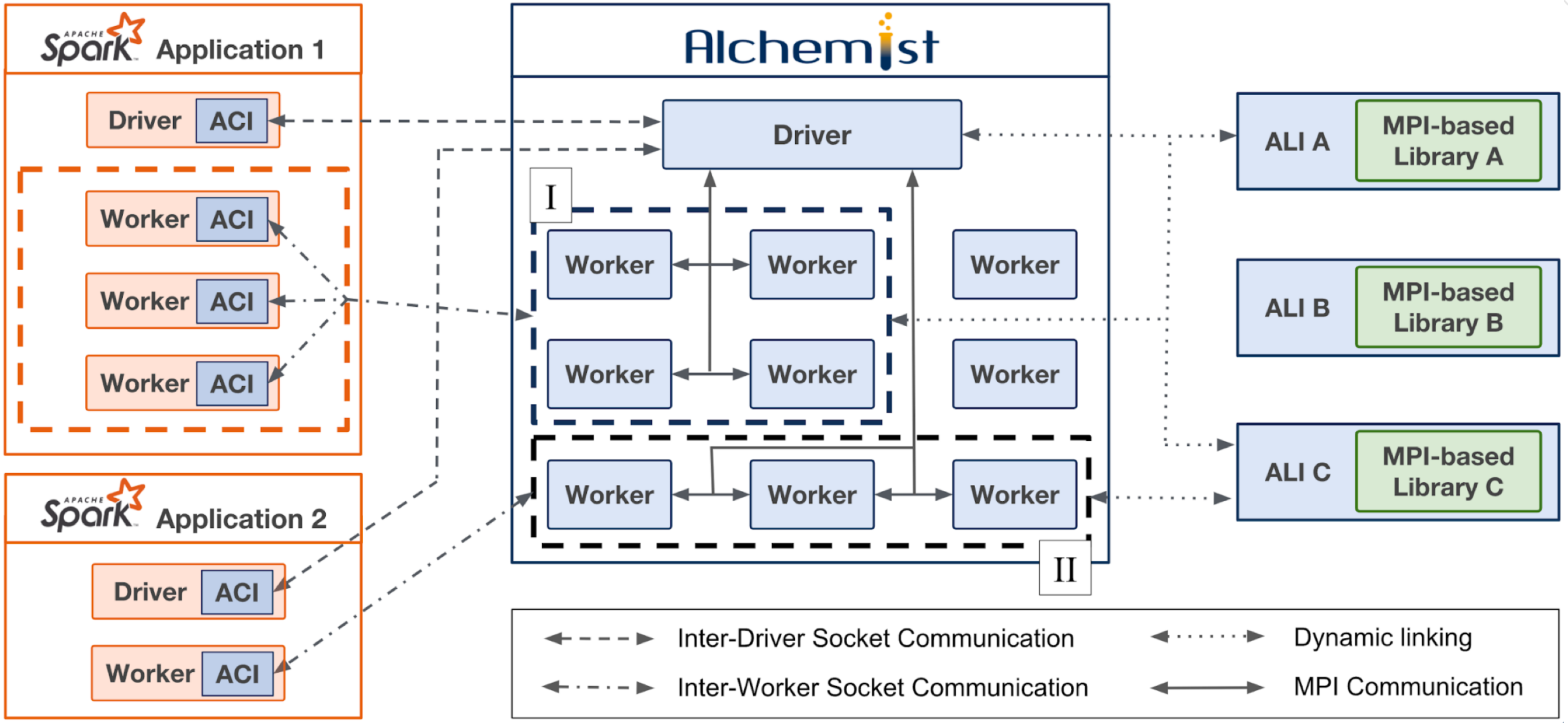
Basic workflow:

- Spark application:
  - Sends distributed dataset from RDD (`IndexedRowMatrix`) to Alchemist
  - Tells Alchemist what MPI-based code should be called
- Alchemist loads relevant MPI-based library, calls function, sends results to Spark

Basic Framework

- Alchemist can also load data from file
- Alchemist needs to store distributed data in appropriate format that can be used by MPI-based libraries:
    - Candidates: ***ScaLAPACK***, ***Elemental***, ***PLAPACK***
    - Alchemist currently uses Elemental, support for ScaLAPACK under development

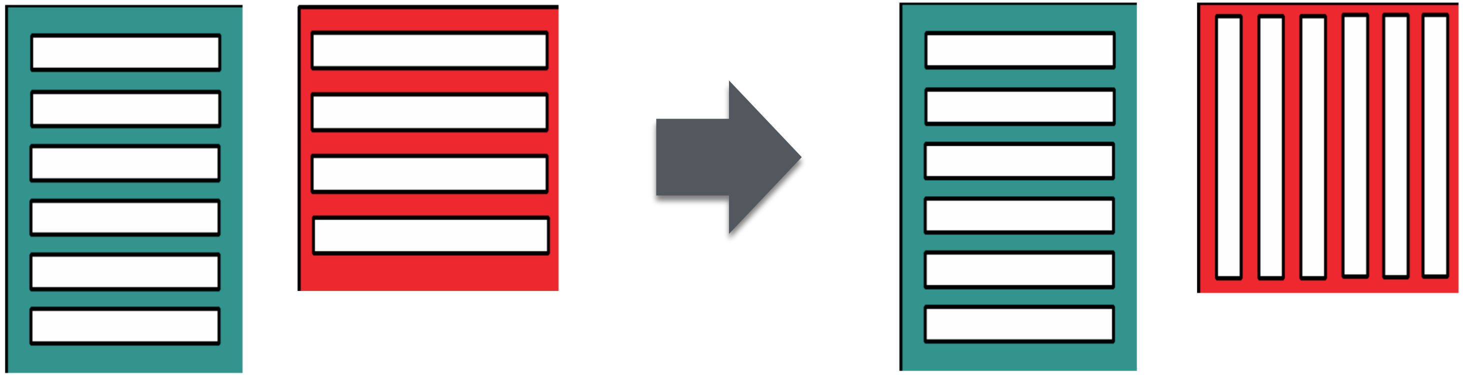
Alchemist Architecture



Sample API

```
import alchemist.{Alchemist, AlMatrix}
import alchemist.libA.QRDecomposition       // libA is sample MPI lib

// other code here ...

// sc is instance of SparkContext
val ac = new Alchemist.AlchemistContext(sc, numWorkers)
ac.registerLibrary("libA", ALIlibALocation)

// maybe other code here ...

val alA = AlMatrix(A)                        // A is IndexedRowMatrix

// routine returns QR factors of A as AlMatrix objects
val (alQ, alR) = QRDecomposition(alA)

// send data from Alchemist to Spark once ready
val Q = alQ.toIndexedRowMatrix()             // convert AlMatrix alQ to RDD
val R = alR.toIndexedRowMatrix()             // convert AlMatrix alR to RDD

// maybe other code here ...

ac.stop()                                    // release resources once no longer required
```

Example: Matrix Multiplication



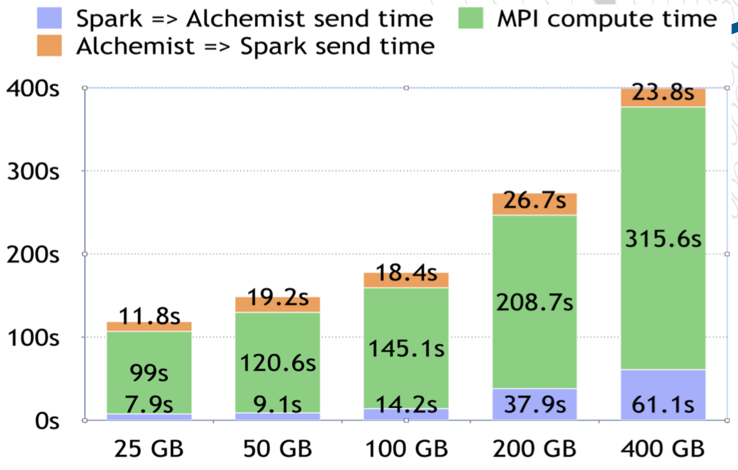
- Requires expensive shuffles in Spark, which is impractical:
  - Matrices/RDDs are row-partitioned
  - One matrix must be converted to be column-partitioned
  - *Requires an all-to-all shuffle that often fails* once the matrix is distributed

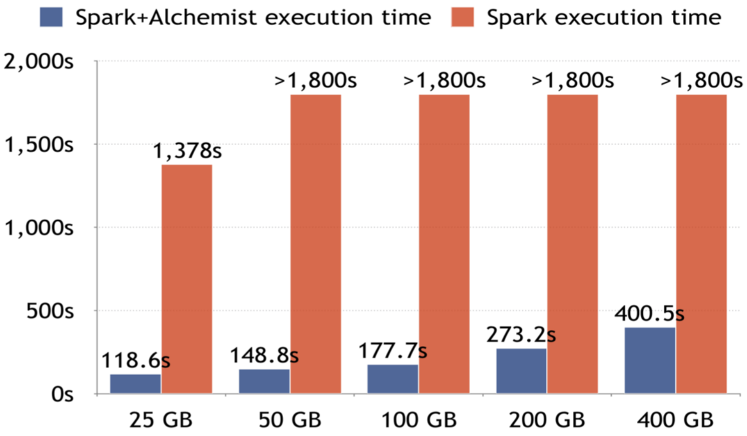
Example: Truncated SVD

Use Alchemist and MLlib to get rank 20 truncated SVD

Experiment Setup

- Spark: 22 nodes; Alchemist: 8 nodes
- A: m-by-10K, where m = 5M, 2.5M, 1.25M, 625K, 312.5K
- Ran jobs for at most 30 minutes (1800 s)

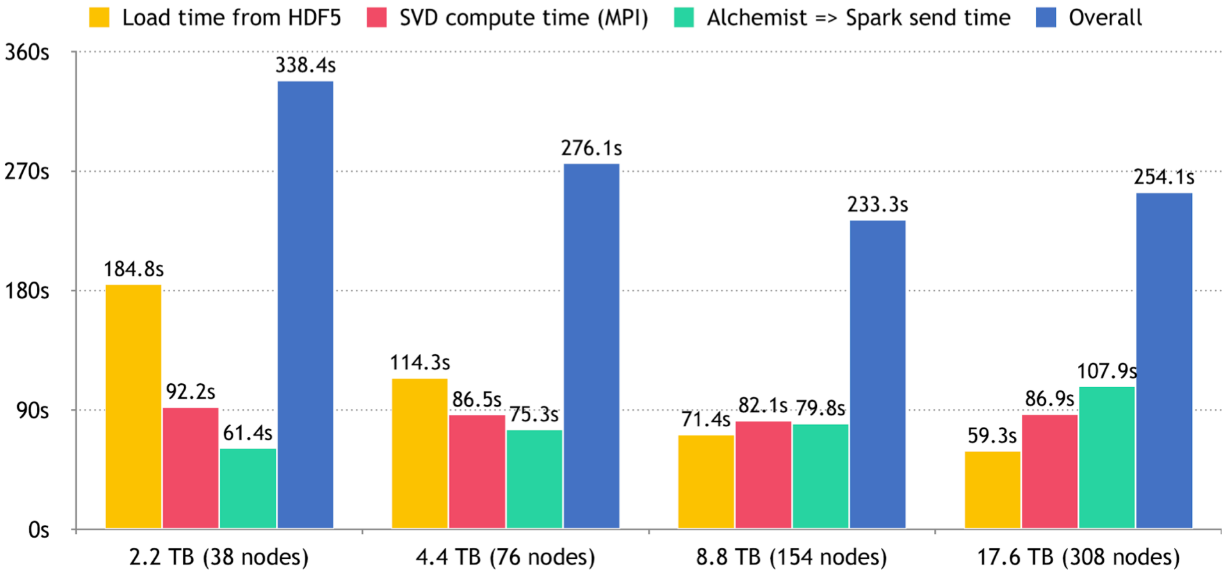




Example: Truncated SVD

Experiment Setup

- 2.2TB (6,177,583-by-46,752) ocean temperature data read in from HDF5 file
- Data replicated column-wise



Upcoming Features

- **PySpark, SparkR ⇔ MPI Interface**
    - Interface for Python => PySpark support
    - Future work: Interface for R
- **Direct Python interface, potential Dask integration**
- **More Functionality**
    - Support for sparse matrices
    - Support for MPI-based libraries built on ScaLAPACK
- **Alchemist and Containers**
    - Alchemist running in Docker and Kubernetes
    - Will enable Alchemist on clusters and the cloud

Limitations and Constraints

- **Two copies of data in memory**
- **Data transfer overhead** between Spark and Alchemist when data on different nodes
  - Subject to network disruptions and overload
- **MPI is not fault tolerant or elastic**
- **Lack of MPI-based libraries for machine learning**
  - No equivalent to MLlib currently available, closest is MaTEx
- Currently, **need to run Alchemist and Spark on separate nodes** -> more data transfer over interconnects -> larger overheads

Future Work

- **Apache Spark ⇔ X Interface**
  - Interest in connecting Spark with other libraries for distributed computing (e.g. Chapel)
- **Reduce communication costs**
  - Exploit locality
  - Reduce number of messages
  - Use communication protocols designed for underlying network infrastructure
- **Run as network service**
- **MPI computations with (basic) fault tolerance and elasticity**

github.com/project-alchemist/

References

- A. Gittens, K. Rothauge, M. W. Mahoney, *et al.*, "Alchemist: Accelerating Large-Scale Data Analysis by offloading to High-Performance Computing Libraries", 2018, *Proceedings of the 24th ACM SIGKDD International Conference,* Aug 2018, to appear
- A. Gittens, K. Rothauge, M. W. Mahoney, *et al.*, "Alchemist: An Apache Spark ⇔ MPI Interface", 2018, to appear in *CCPE Special Issue on Cray User Group Conference 2018*

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