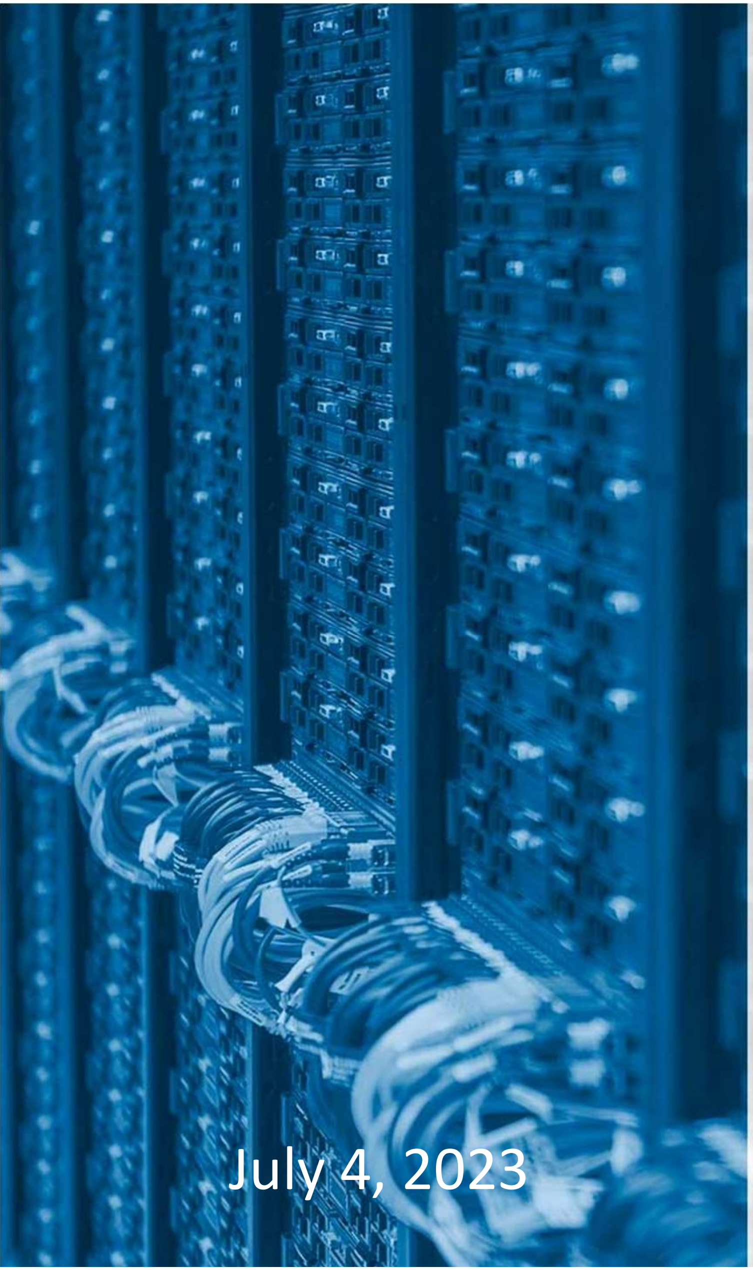

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EXCELENCIA SEVERO OCHOA

Leveraging HPC techniques for data analytics

Anna Queralt, Francesc Lordan, Alex Barceló

Workflows and Distributed Computing Group

eBISS 2023

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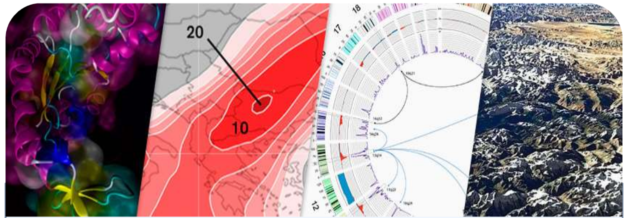
BSC-CNS objectives

Supercomputing services
to Spanish and EU researchers



R&D in Computer, Life, Earth and
Engineering Sciences

PhD programme, technology
transfer, public engagement

BSC-CNS is a consortium that includes

Spanish Government	60%	Gobierno de España, Ministerio de Ciencia, Innovación y Universidades
Catalan Government	30%	Generalitat de Catalunya Departament d'Empresa i Coneixement
Univ. Politècnica de Catalunya (UPC)	10%	Universitat Politècnica de Catalunya BarcelonaTech

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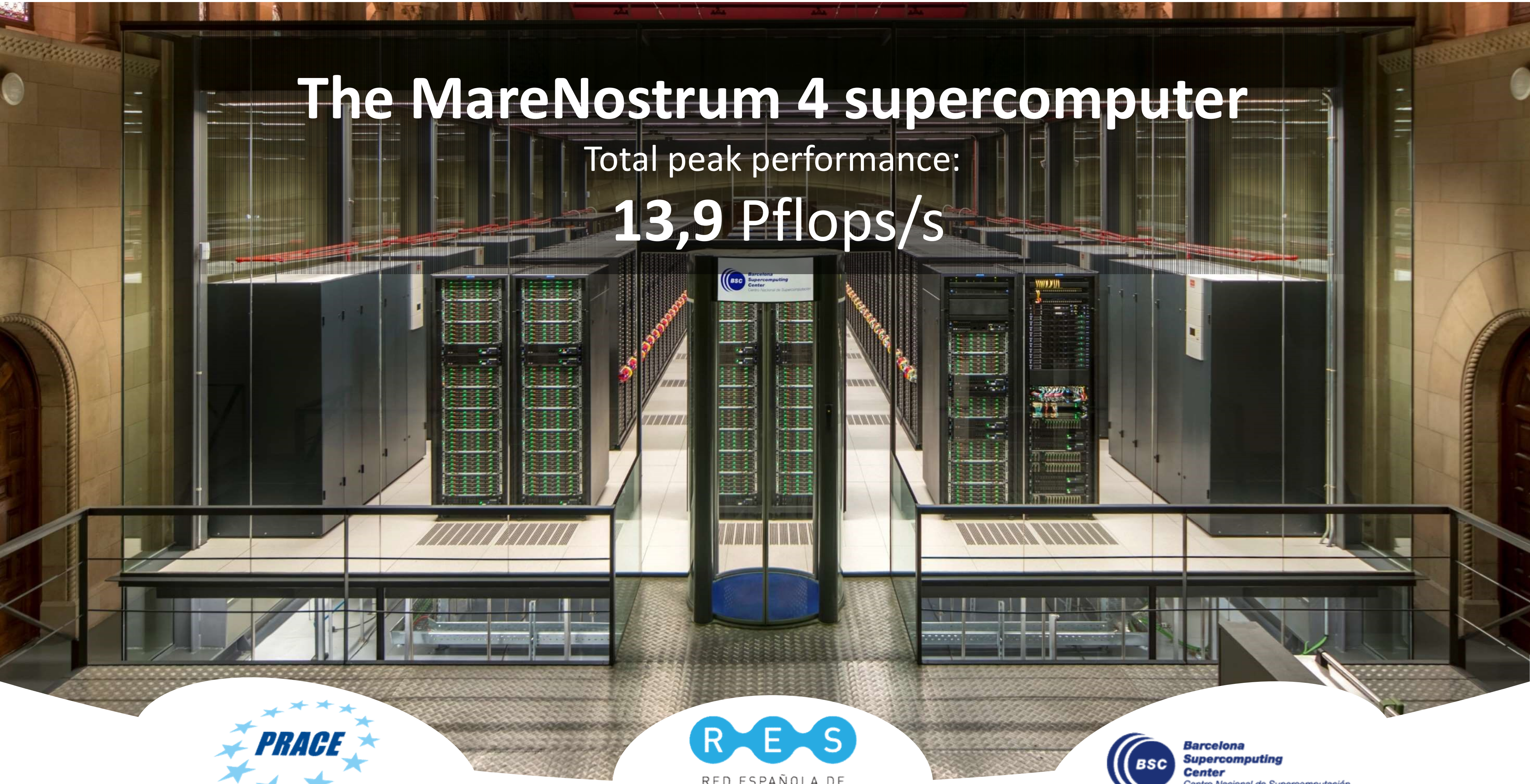
The MareNostrum 4 supercomputer

Total peak performance:

13,9 Pflops/s



PRACE

Access: prace-ri.eu/hpc-access

RES

RED ESPAÑOLA DE SUPERCOMPUTACIÓN

Access: bsc.es/res-intranet

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Computer Sciences

Influence the way machines are

- **BUILT** → **Holistic Computer Architecture Research**
- **PROGRAMMED** → **20 years innovating in Programming Models**
- **USED** → **Performance Analytics Tools: From Data to Insight**

In the context of

- Race towards Exascale
- HPC and Big Data convergence
- Artificial Intelligence era
- Multiple architectures for different applications domains

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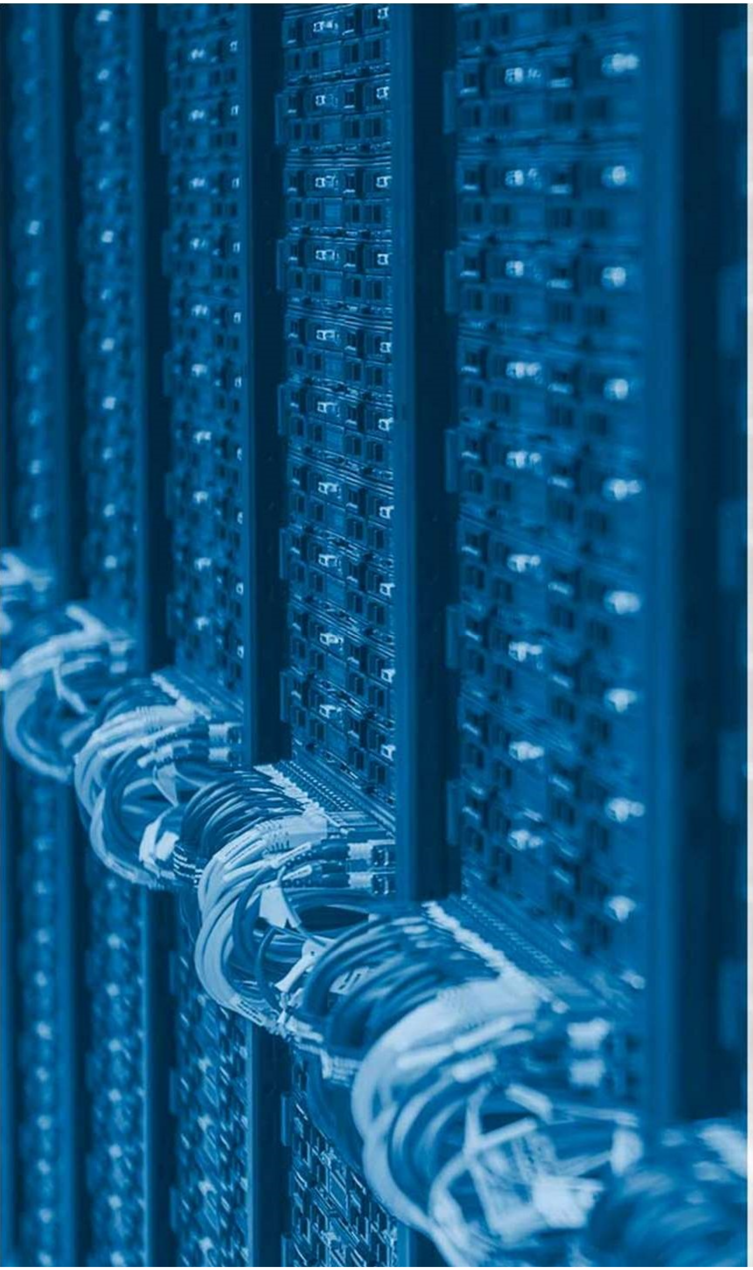

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EXCELENCIA SEVERO OCHOA

Leveraging HPC techniques for data analytics

Outline

- **Motivation**
  - BSC vision on data analytics
- **Distributed computing platform: COMPSs**
  - COMPSs overview
  - Demo

Coffee Break

- **Distributed data management platform: dataClay**
  - dataClay overview
  - Demo
- **COMPSs and dataClay for data analytics**
  - ML application
  - DL application

Until mid 2000's…

Relational databases and data warehouses

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Then…

- 2005: Facebook, Youtube
- 2006: Twitter, Amazon Web Services
- 2007: Netflix, iPhone
- 2008: Spotify
- 2009: Whatsapp, Instagram
- …

New data processing and management solutions are required:

- Complex analytics workflows including ML/DL
- More flexible (and efficient) data models
- Distribution and parallelism (clusters)

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Photo by Sara Kurfeß in Unsplash

Now…

- Some platforms have been widely adopted in the data analytics community

hadoop · APACHE Spark · cassandra · MongoDB

- In the meantime, in HPC…

MPI · dask · IBM GPFS · daos

- Main differences/disadvantages:
  - Data analytics: “requires” memory, data movements
  - HPC: steep learning curve


Photo by Alexander Schimmeck in Unsplash

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The best of both worlds

- From data analytics
  - Programmability
  - Abstraction of the infrastructure

- From HPC
  - Performance and scalability
  - Flexibility

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Photo by Ahtziri Lagarde in Unsplash

Achieving flexibility

…And programmability at the same time

	Spark	COMPSs
Algorithms	MLlib	dislib
Operators	Spark operators	DDS
Parallelism	Pre-defined tasks	Arbitrary tasks
Scheduling	Spark runtime	COMPSs runtime
Data types	RDD/DataFrame	Arbitrary types

dataClay


Photo by Tim Mossholder in Unsplash

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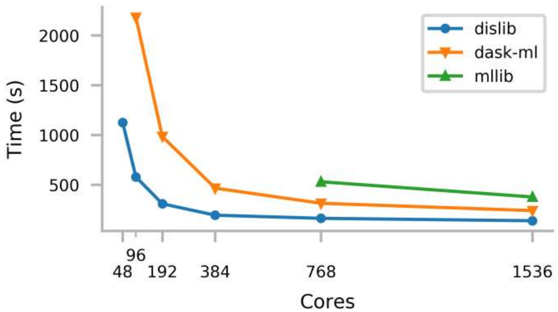
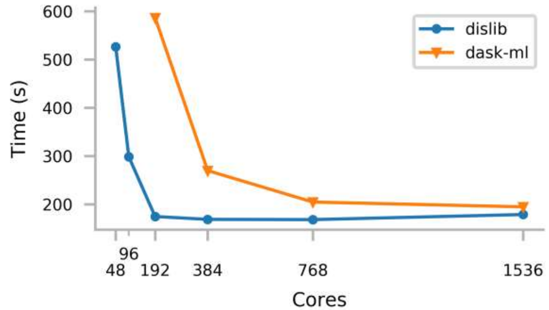
… and performance and scalability

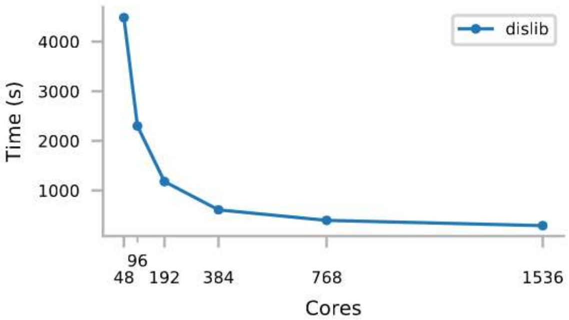
- K-means clustering
  - For very large sizes, MLlib and Dask-ML fail to finish the execution



500 million samples, 100 features



1 billion samples, 50 features



2 billion samples, 100 features

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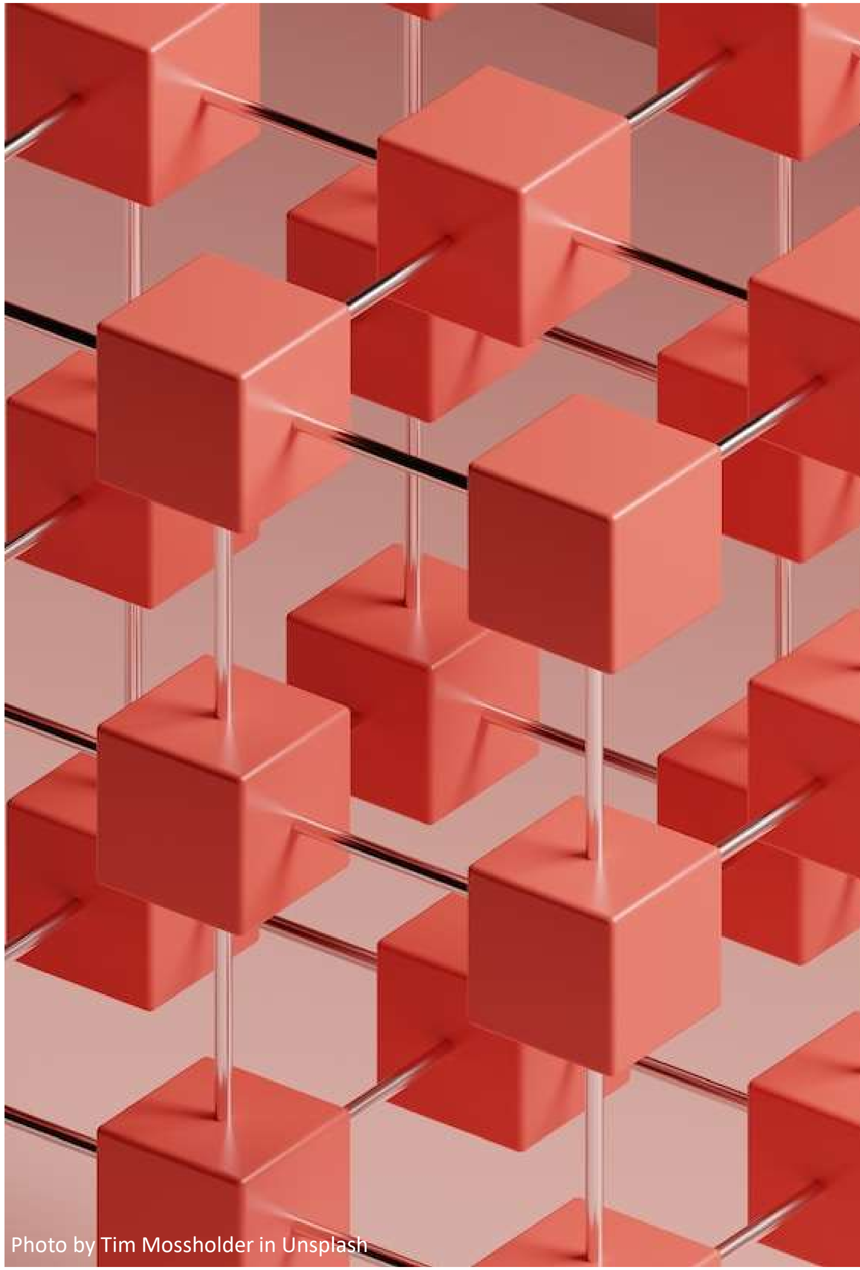

… even beyond the datacenter

For different reasons than in HPC, in edge computing you also want to:

Distribute the processing

- Due to limited resource capabilities

Minimize data transfers

- To avoid network and privacy issues

Avoid disk accesses

- Many devices don't have them

Abstraction of the infrastructure for programmability

- Very complex and unstable

Edge-to-cloud environments can be seen as "a single" data processing platform

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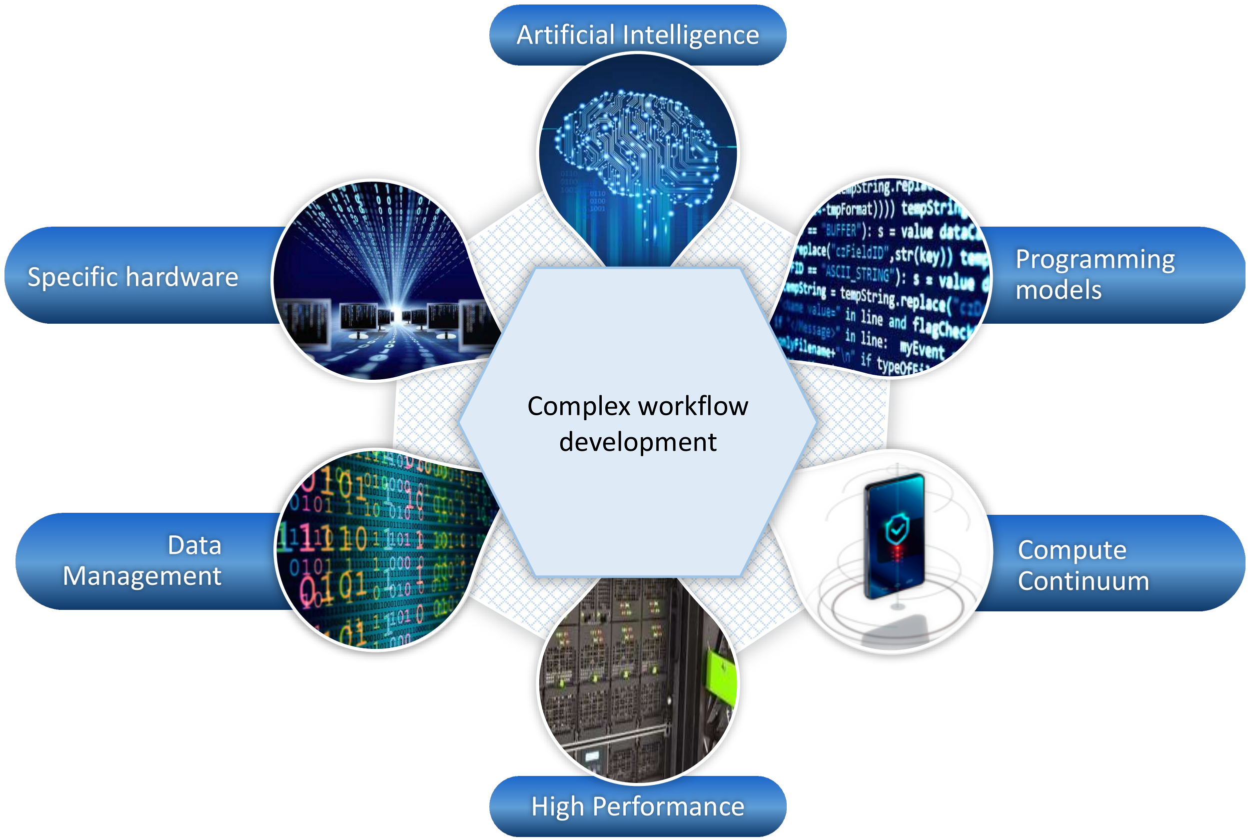
The Workflows and Distributed Computing group

- **Different** methodologies and software stacks are available
  - HPC simulation and modeling
  - Big Data
  - Artificial Intelligence
- There is a need for **integration** into a single application workflow
  - Facilitates complex workflow development
  - Enables global optimizations



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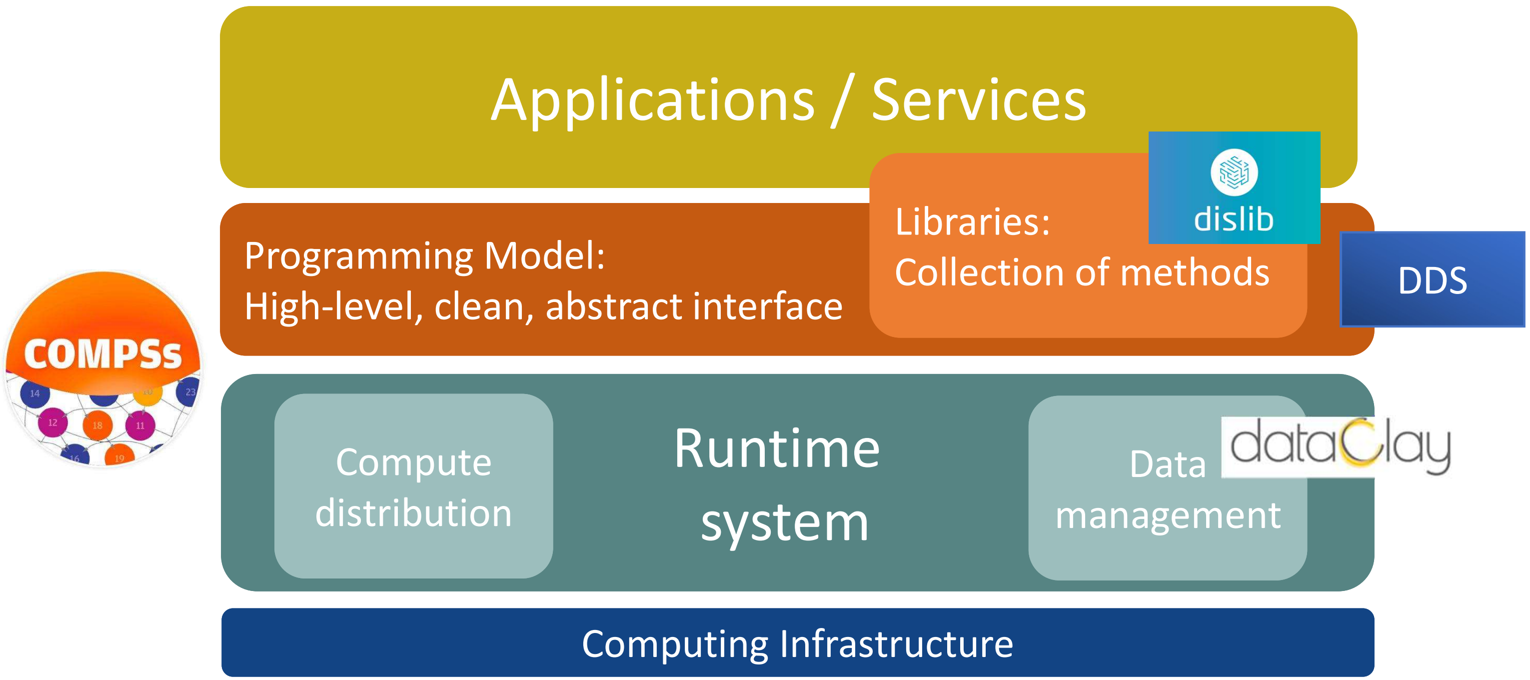
Software stack



PyCOMPSs ecosystem

Francesc Lordan

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Motivation

New complex architectures constantly emerging

- Hardware Heterogeneity
  - Different HW characteristics (performance, memory, etc)
  - Different architectures -> compilation issues
- Network
  - Different types of networks
  - Instability
- Dynamicity
  - How to dynamically add/remove nodes to the infrastructure
- Trust and Security
- Power constraints from the devices in the edge

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Motivation

New complex architectures constantly emerging

- With their own way of programming them
  - Fine grain: e.g. Programming models and APIs to run with GPUs, NVMs (Non-Volatile Memories)
  - Coarse grain: e.g. APIs to deploy in Clouds
- **Difficulty** to develop applications
  - Higher learning curve / Time To Market (TTM)
  - What about non computer scientists???
- **Difficulty** to understand what is going on during execution (**Efficiency**)
  - Was it fast? Could it be even faster?
  - Am I paying more than I should?
- Tune your application for each architecture (or cluster)
  - E.g. partitioning data among nodes

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Motivation

- Create tools that make developers' life **easier**

  - Allow developers to focus on their problem
    - Integration of computational workloads (PyCOMPSs)
    - with machine learning and data analytics (dislib / DDS)

  - Intermediate layer: let the difficult parts to those tools
    - Act on behalf of the user
    - Distribute the work through resources
    - Deal with architecture specifics
    - Automatically improve performance

  - Tools for visualization
    - Monitoring
    - Performance analysis

Applications

High-level, clean, abstract interface

Power to the runtime

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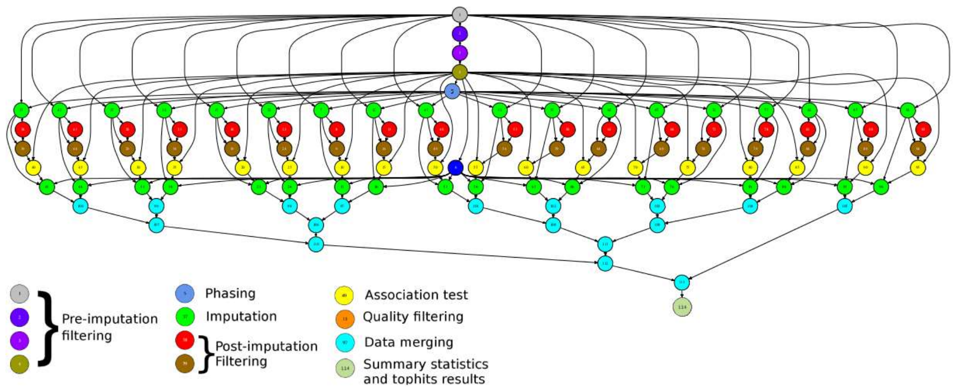
Motivation

- Programming
  - Sequential programming
  - Agnostic of the target computing platform
  - Standard programming languages: Java, Python, C/C++
    - annotations/hints
  - Task based: task is the unit of work

- Runtime
  - Builds a task graph at runtime that express potential concurrency (workflow)
  - Exploitation of parallelism
  - Resource Management and Workload distribution



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PyCOMPSs ecosystem overview

Applications

DDS

dislib

PyCOMPSs

COMPSs
Runtime

Skeletons to operate on large datasets

Library of ML algorithms

General-purpose task-based programming model

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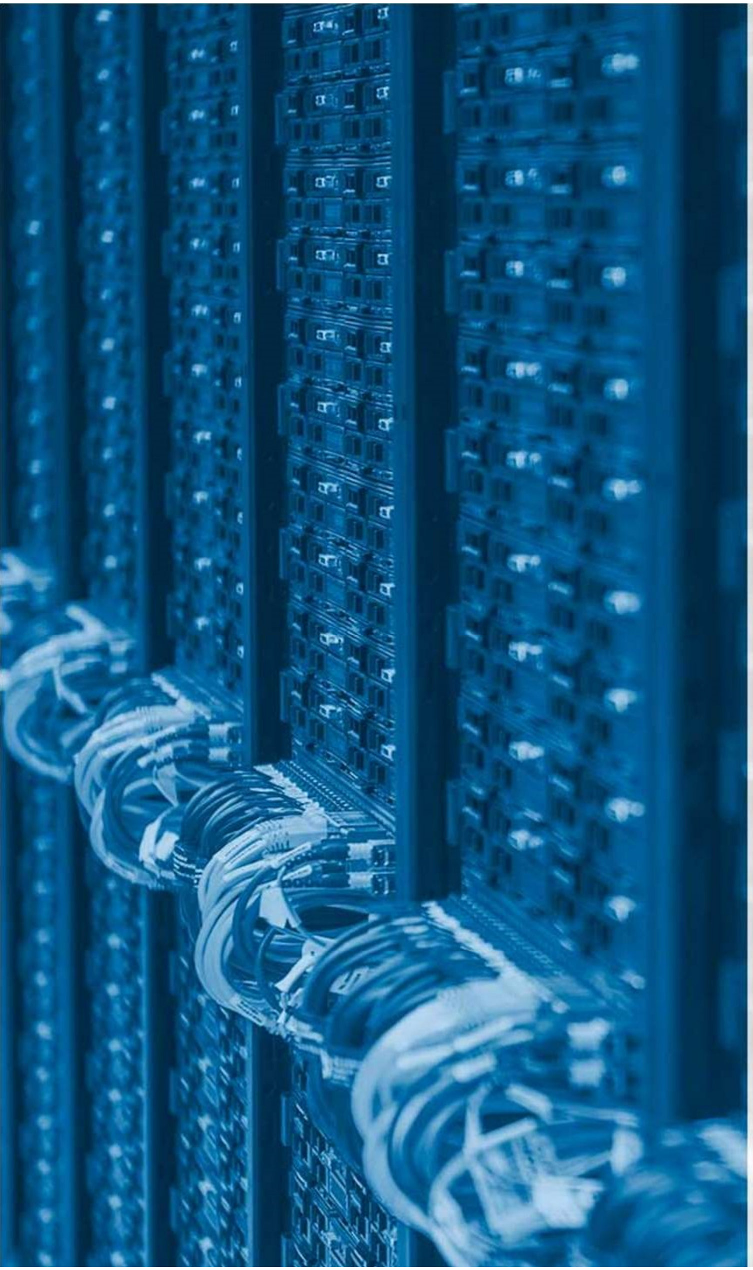

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SEVERO
OCHOA

dislib

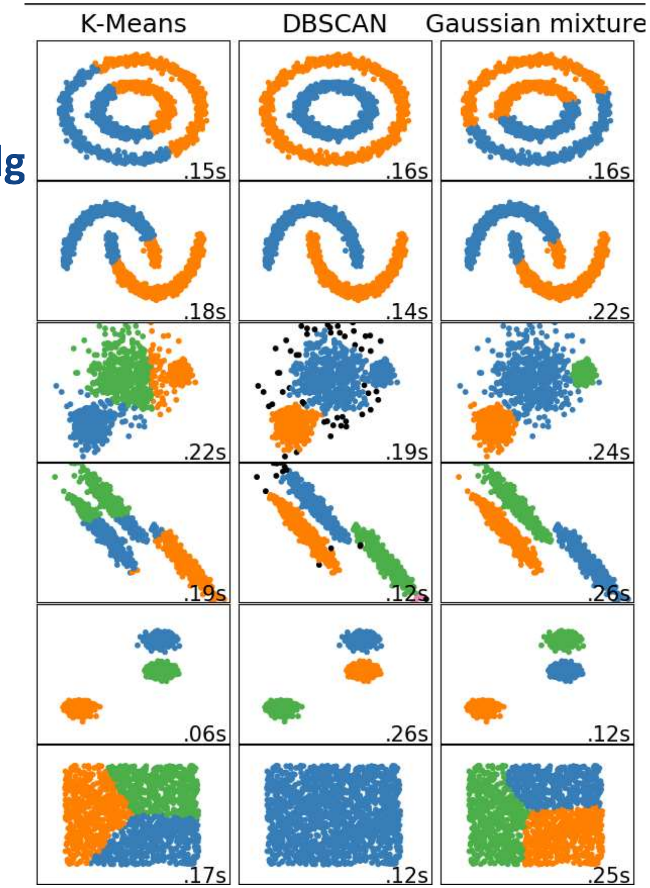
dislib: parallel machine learning

dislib: Collection of machine learning alg

- Unified interface, inspired in scikit-learn (fit-predict)
- Based on a distributed data structure (ds-array)
- Unified data acquisition methods
- Parallelism transparent to the user – PyCOMPSs parallelism hidden
- Open source, available to the community

Provides multiple methods:

- data initialization
- Clustering
- Classification
- Model selection, ...



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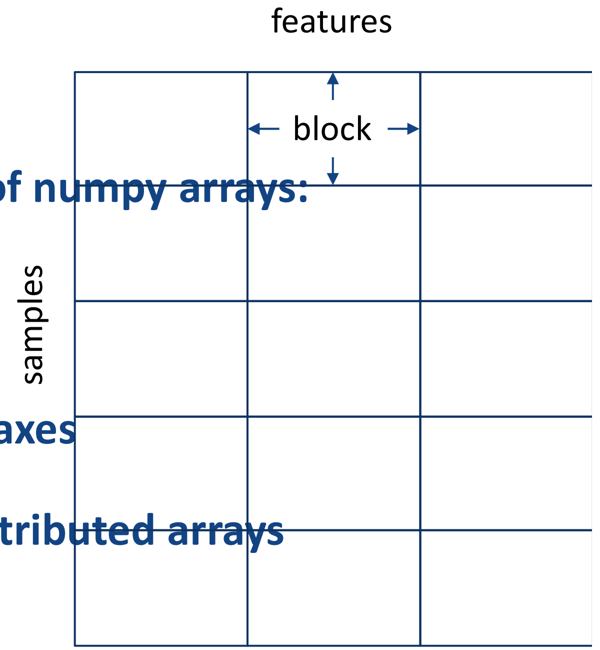
Distributed array (ds-array)

- **2-dimensional structure (i.e., matrix)**
  - Divided in blocks (NumPy arrays)
- **Works as a regular Python object**
  - But not always stored in local memory!
- **Methods for instantiation and slicing with the same syntax of numpy arrays:**
  - Loading data (e.g., from a text file)
  - Indexing (e.g., x[3], x[5:10])
  - Operators (e.g., x.min(), x.transpose())
- **ds-arrays can be iterated efficiently along both axes**
- **Samples and labels can be represented by independent distributed arrays**
- **Data not always in memory:**
  - Inherent support for out-of-core operations, enabling large data-sets



Supported Methods

- **Array creation routines**
  - random,
  - existing data
  - files
- **Matrix decomposition:**
  - Principal Component Analysis (PCA)
  - QR
  - TSQR
  - SVD
- **Clustering**
  - DBSCAN
  - K-Means
  - Gaussian Mixture
  - Daura (Gromos)
- **Neighbour queries**
  - K-nearest neighbours (KNN)
- **Classification**
  - CascadeSVM
  - RandomForest classifier
  - DecisionTree classifier
- **Recommendation:**
  - Alternating least squares (ALS)
- **Regression**
  - Linear regression
  - LASSO
  - RandomForest regressor
  - DecisionTree regressor
- **Model Selection**
  - GridSearch
  - RandomizedSearch
  - K-fold

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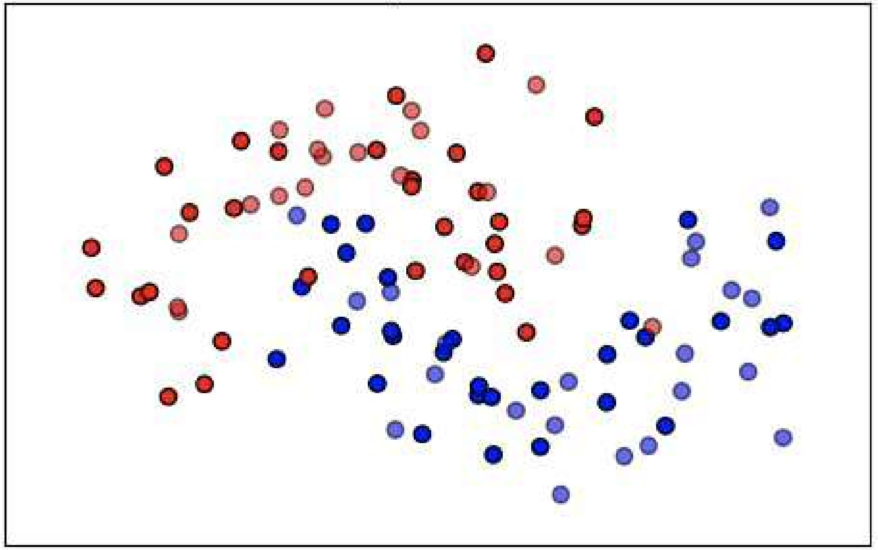
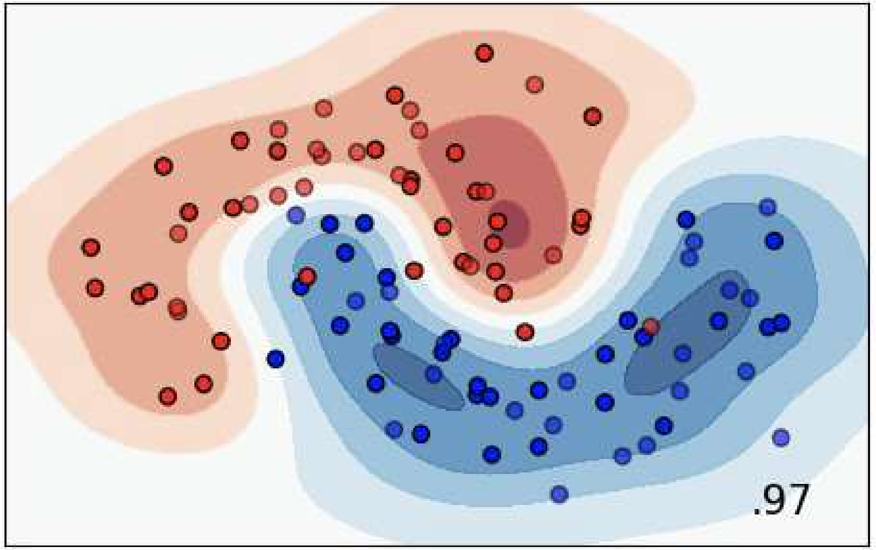
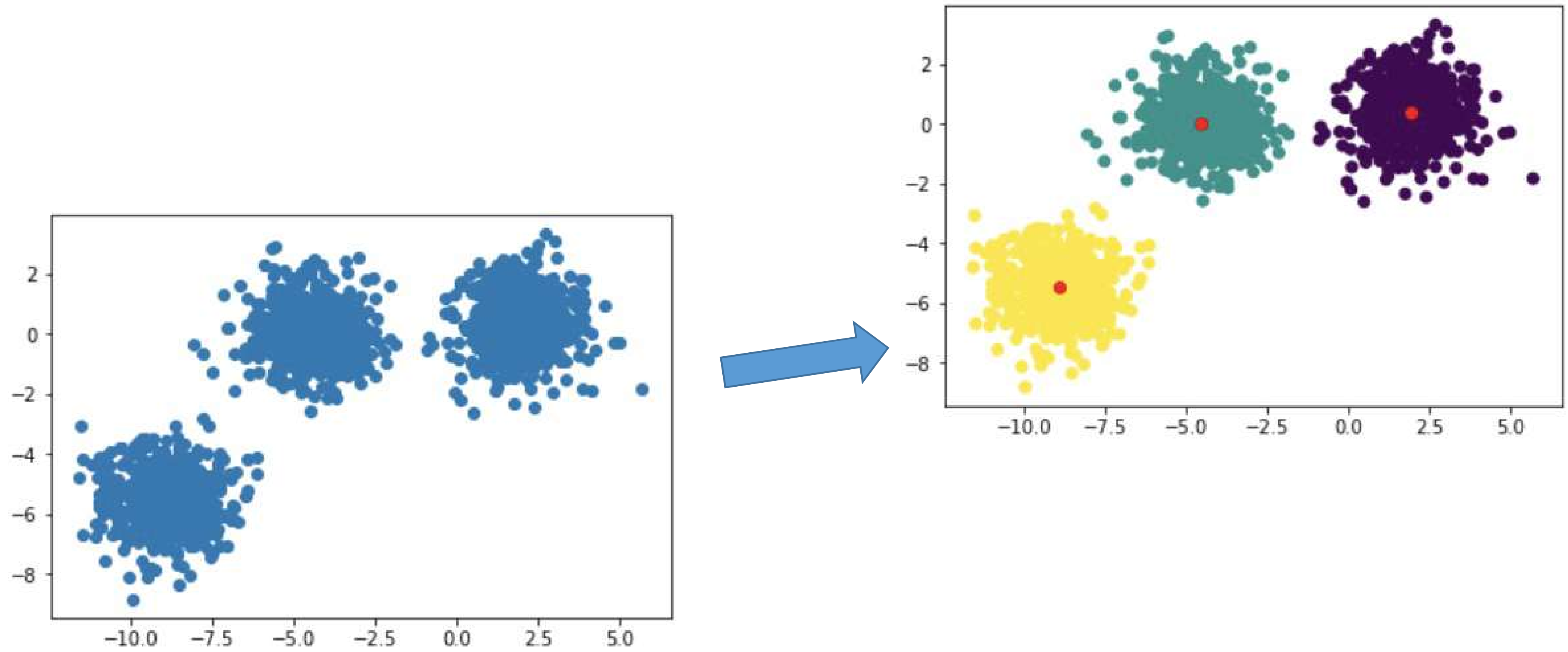
Classification – Labeled data





Clustering – Unlabeled data



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Typical program using dislib

Block size

1. Read input data from file/s

2. Instantiate estimator with parameters

3. Fit estimator with training data

4. Make predictions on test data

```
x = load_txt_file("train.csv", (10, 780))
x_test = load_txt_file("test.csv", (10, 780))

kmeans = KMeans(n_clusters=10)

kmeans.fit(x)

kmeans.predict(x_test)
```

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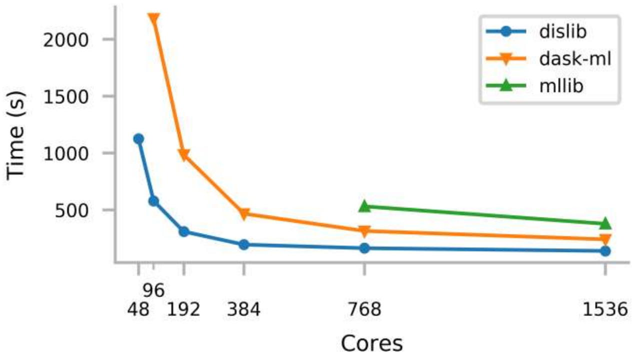
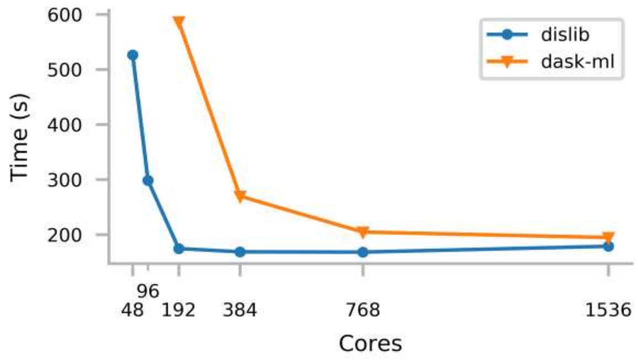
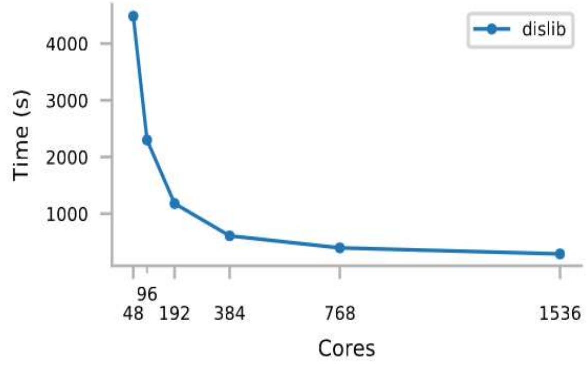
Performance evaluation



500 million samples
100 features



1 billion samples
50 features



2 billion samples
100 features

For very large sizes, dislib can obtain results while MLlib and dask fail to finish the execution

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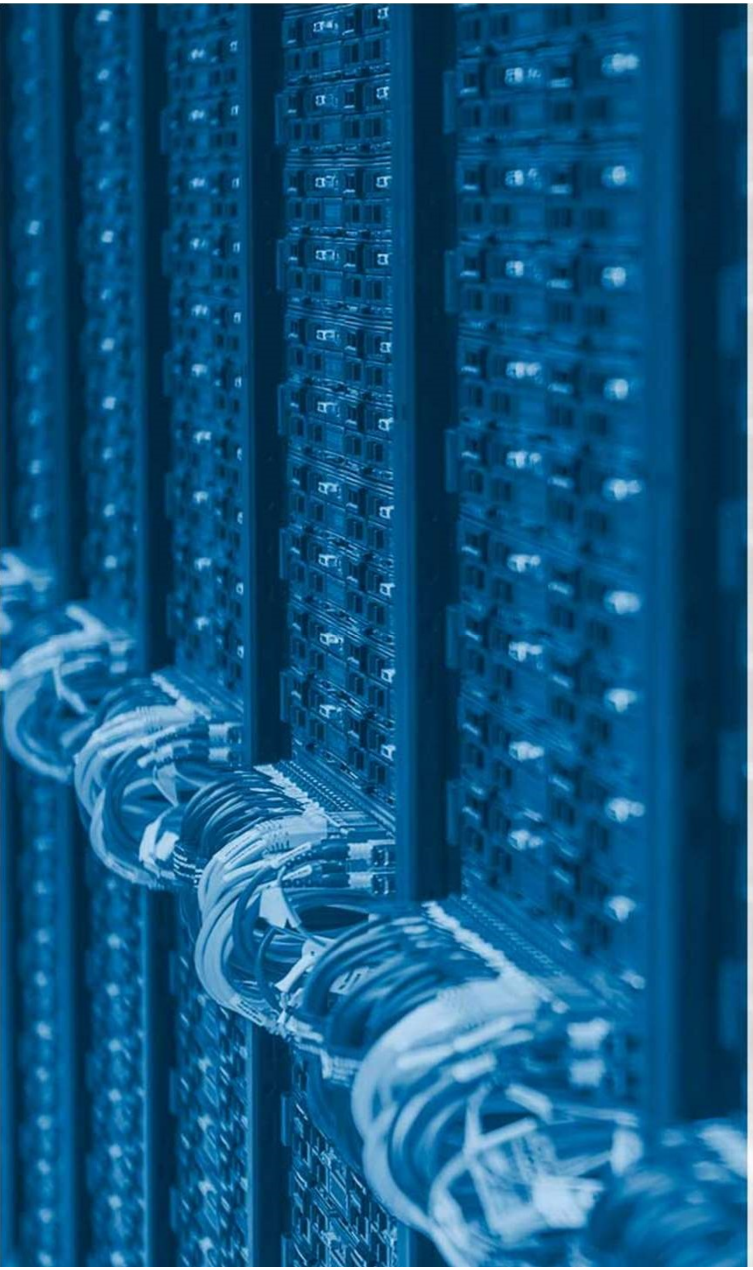

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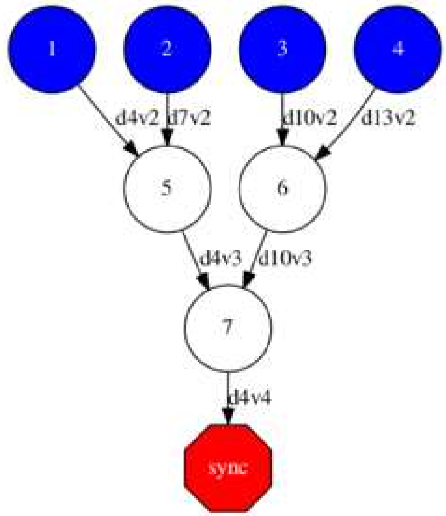
DDS

DDS

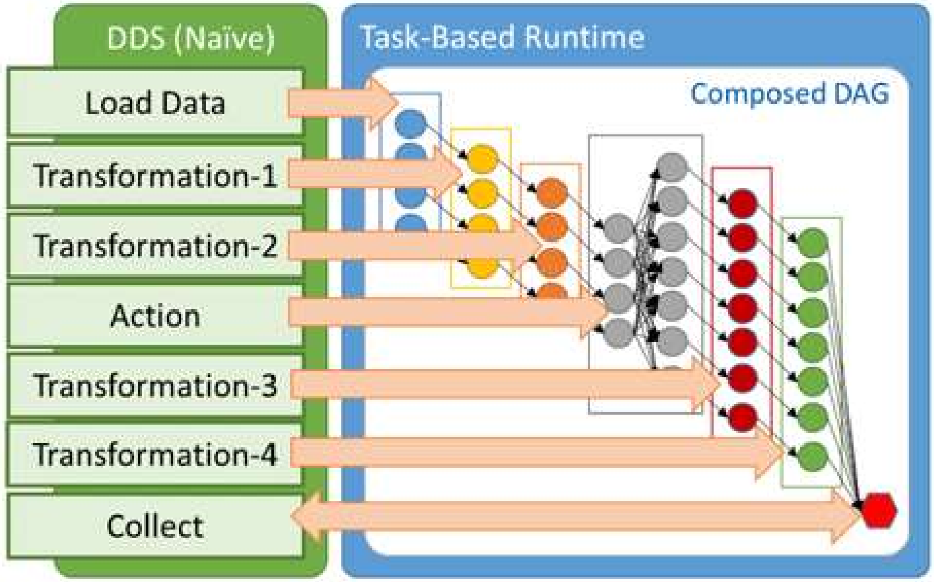
```python
# DDS implementation
from dds import DDS
wc_dds = DDS().load_files("<dir_path>")\
  .flat_map(lambda x: x[1].split()) \
  .map(lambda x: ''.join(e for e in x if e.isalnum())) \
  .count_by_value()

# RDD implementation
from pyspark import SparkContext
wc_rdd = SparkContext().wholeTextFiles("<dir_path>") \
  .flatMap(lambda pair: pair[1].split()) \
  .map(lambda x: ''.join(e for e in x if e.isalnum())) \
  .countByValue()
```

(a) Code comparison

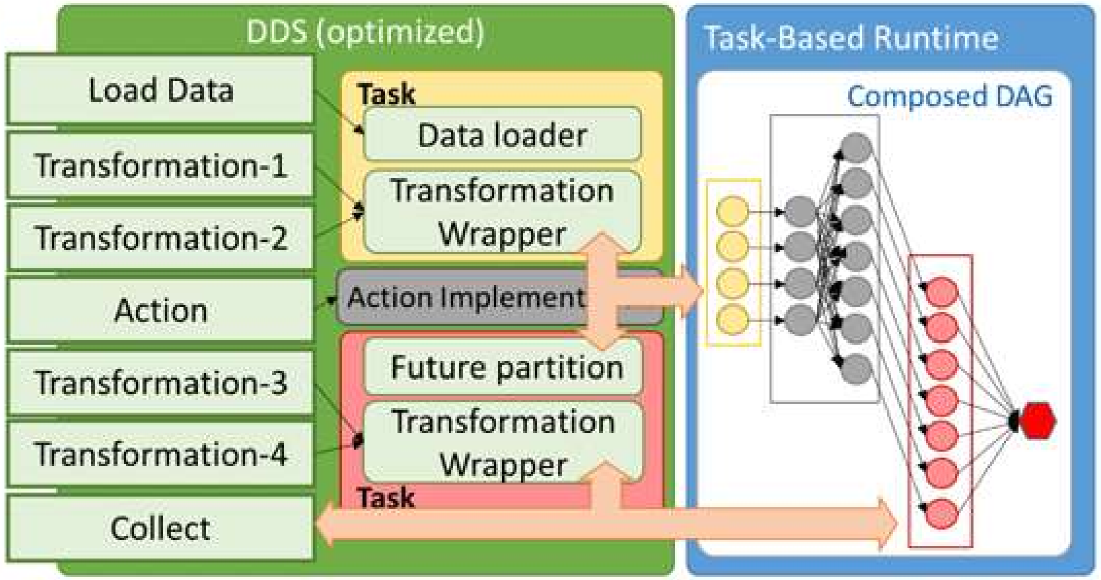


(b) Task Graph

DDS: Optimizations



(a) Naive solution for DDS



(b) Optimized solution for DDS

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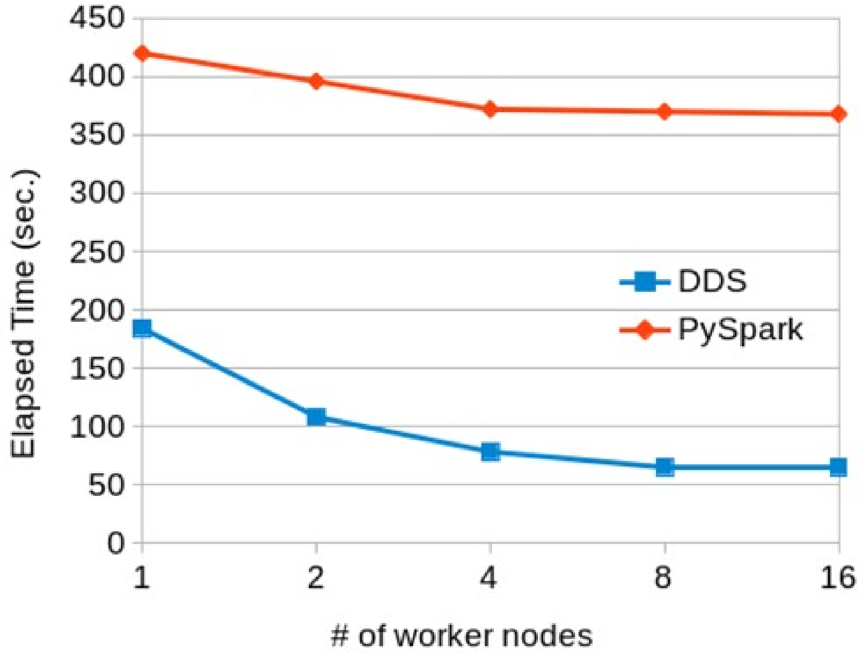
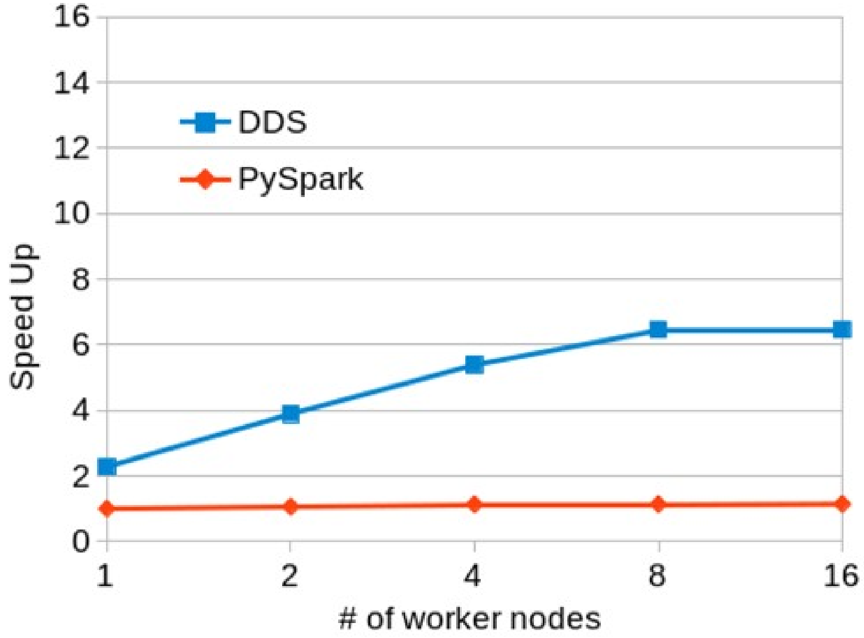
Performance

Wordcount Gutenberg dataset (80GB)





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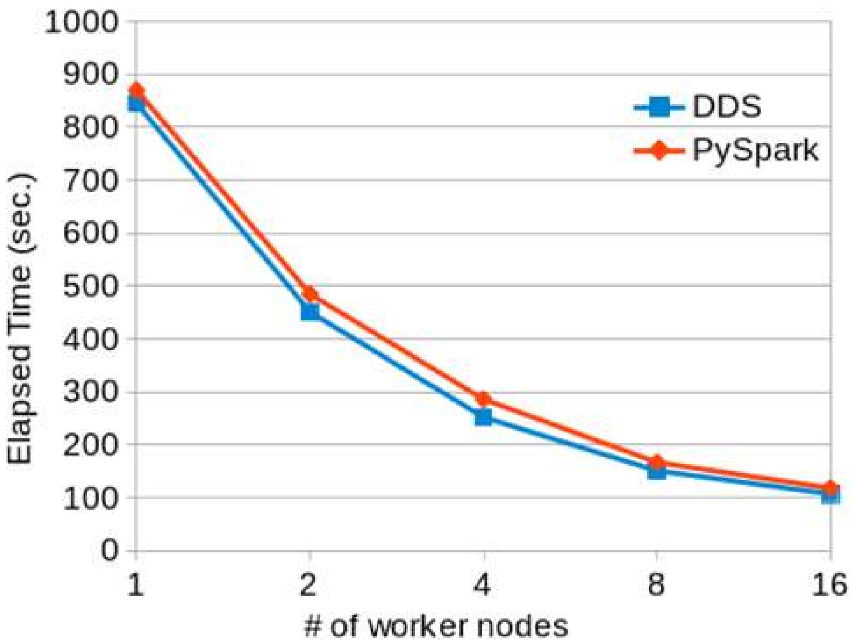
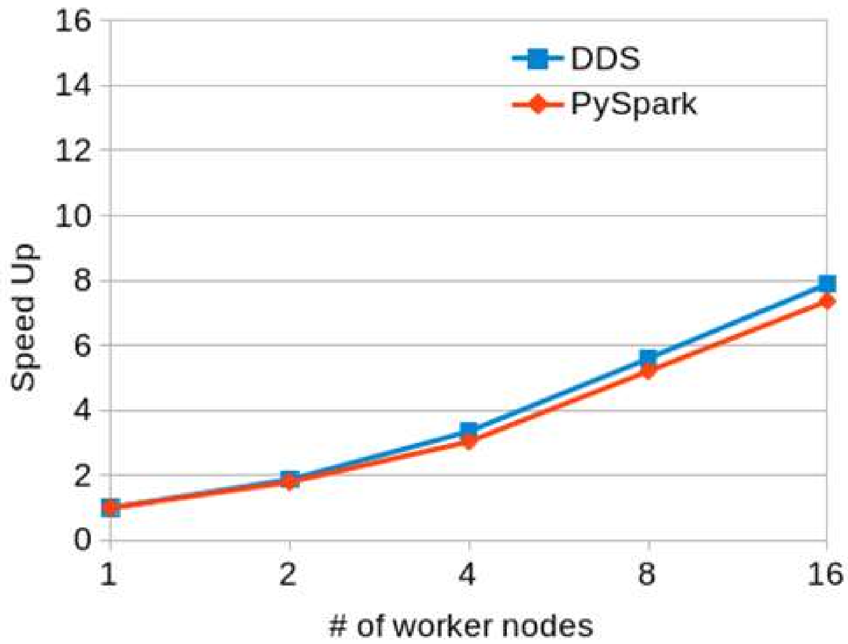
Performance

Wordcount Lorem Ipsum dataset (100GB)





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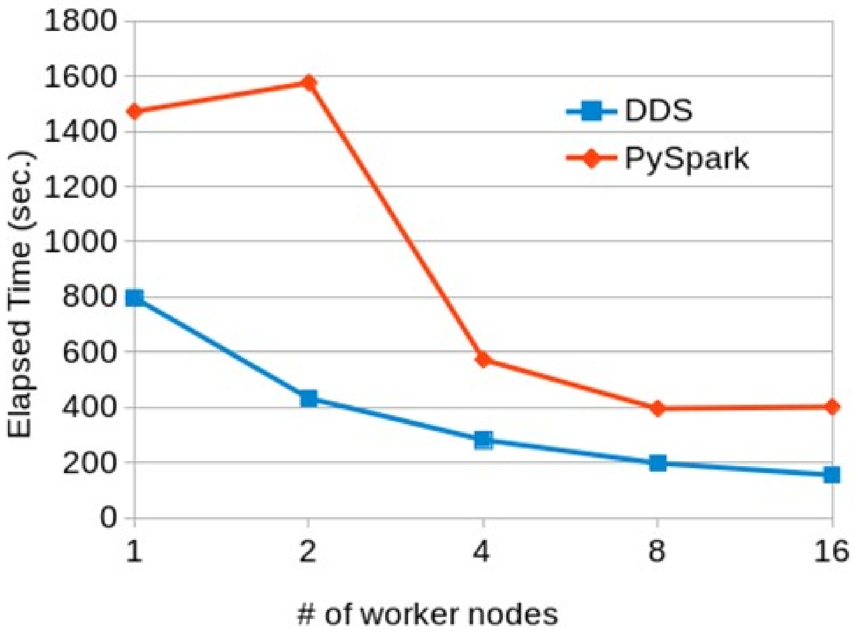
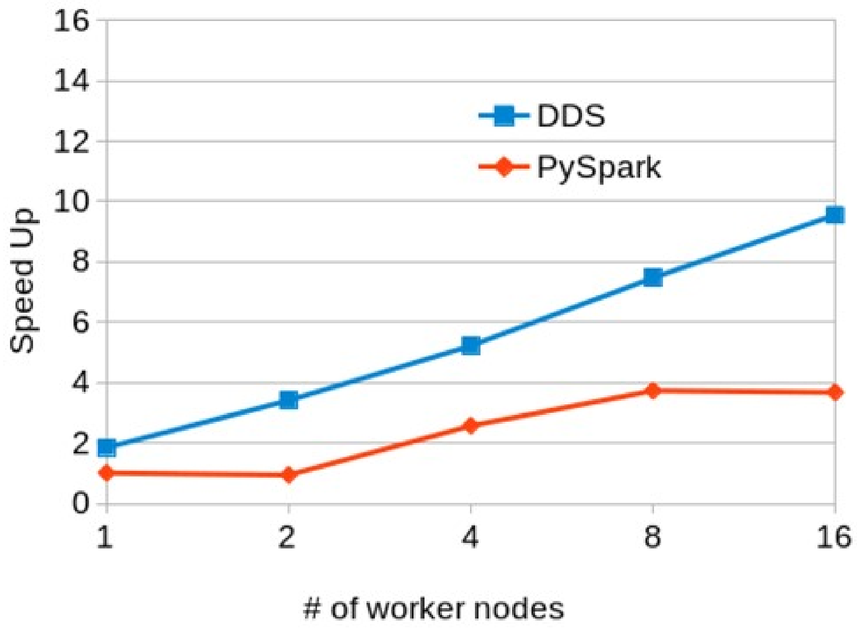
Performance

Terasort (200GB dataset)





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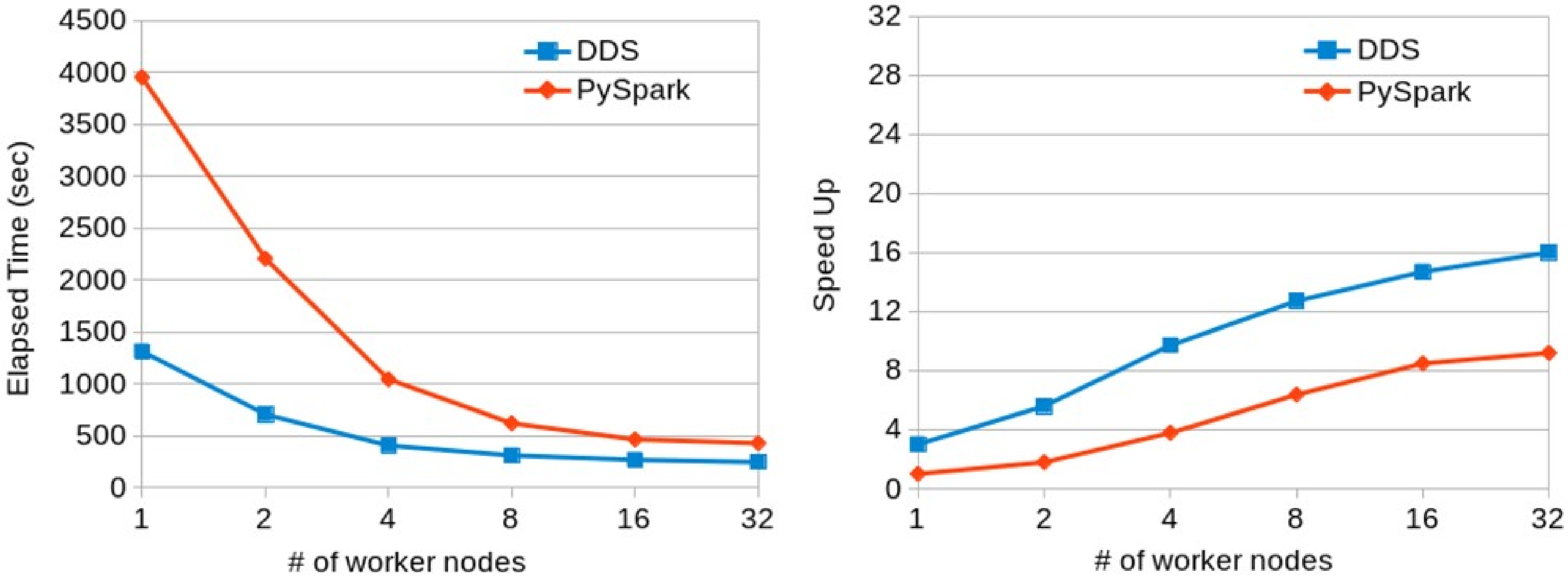
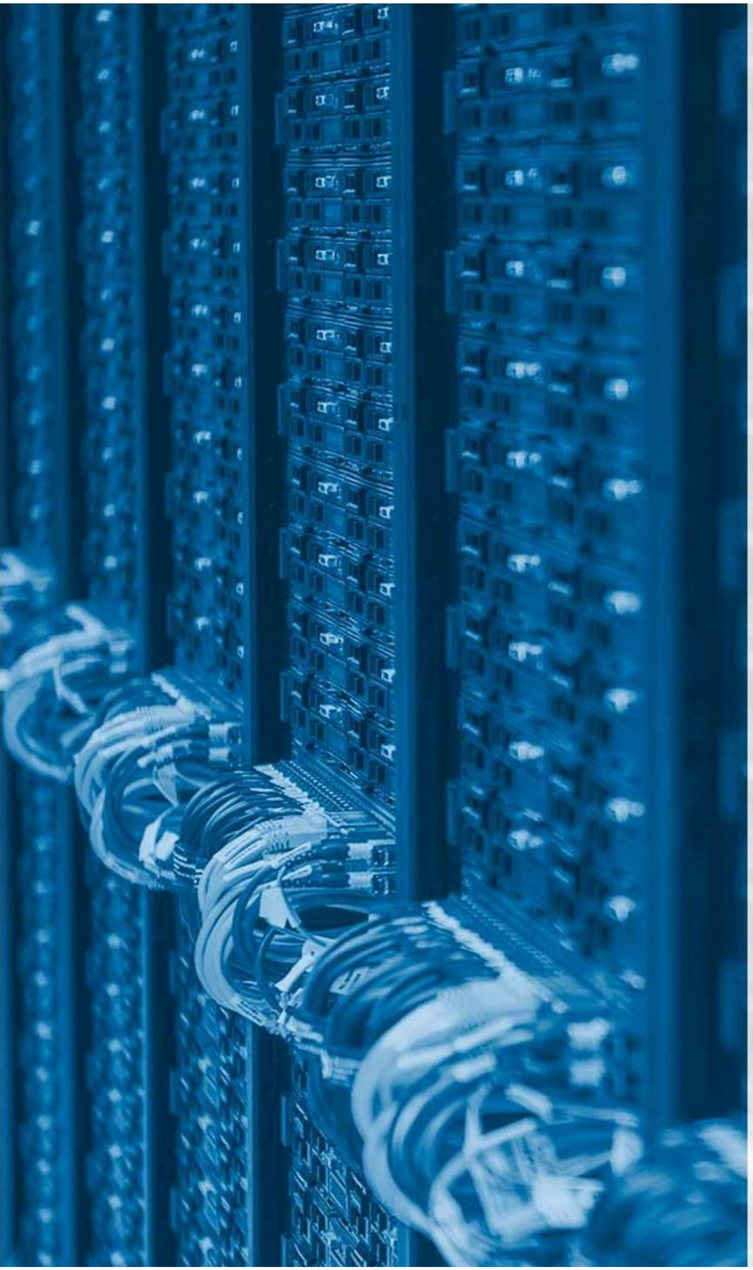
Performance

Transitive Closure (15GB dataset)





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pyCOMPSs

COMPSs Documentation

- Official Website:
  - http://compss.bsc.es
- Github repository
  - https://github.com/bsc-wdc/compss
- Documentation
  - https://compss-doc.readthedocs.io/en/stable/
- Tutorials
  - https://compss-doc.readthedocs.io/en/stable/Sections/10_Tutorial.html

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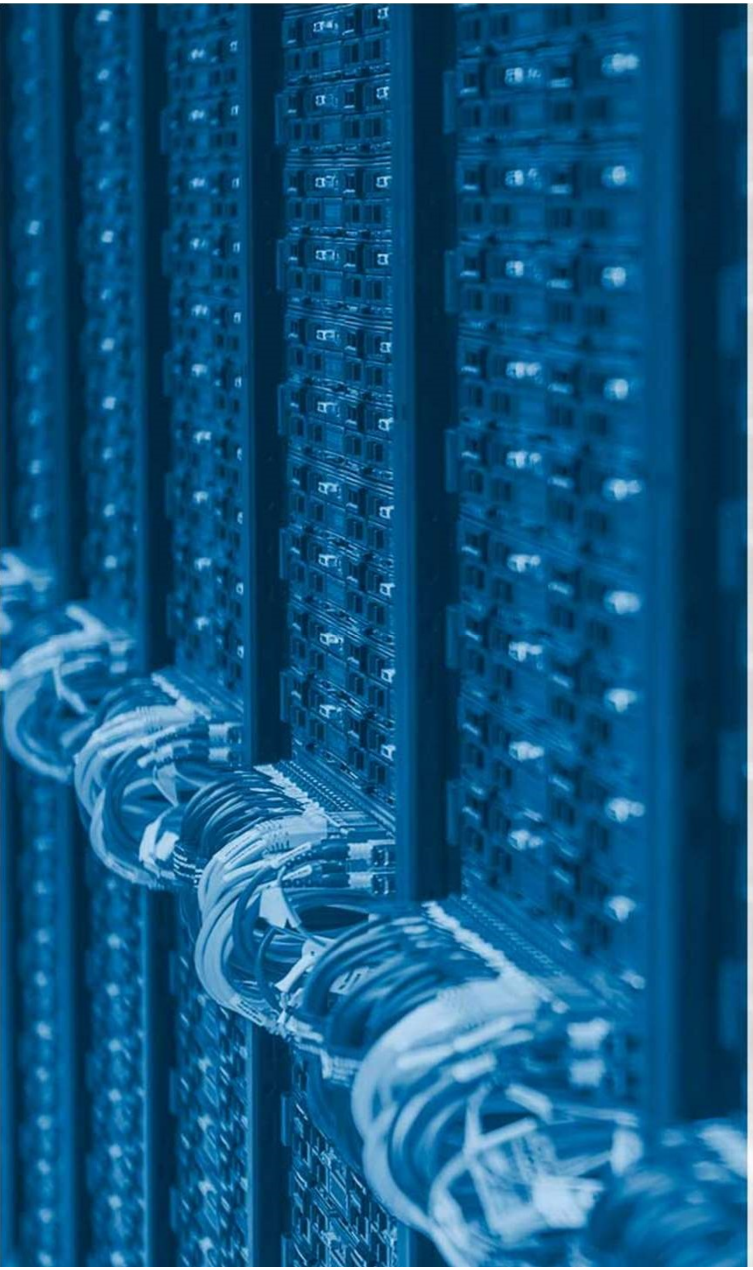

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dataClay

Active objects across the network

Anna Queralt, Alex Barceló

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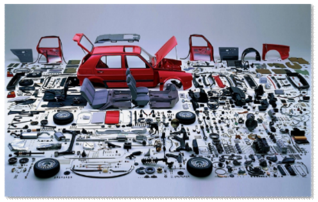
alex.barcelo@bsc.es

From the application point of view

- There is still a gap between computation and data
- Physical separation → Communications
  - Serialization/deserialization is the main cost in data analytics applications [NSDI15]

- Different data models → Transformations
  - Overcoming the *impedance mismatch* amounts to up to 30% of the code [ICSE14]



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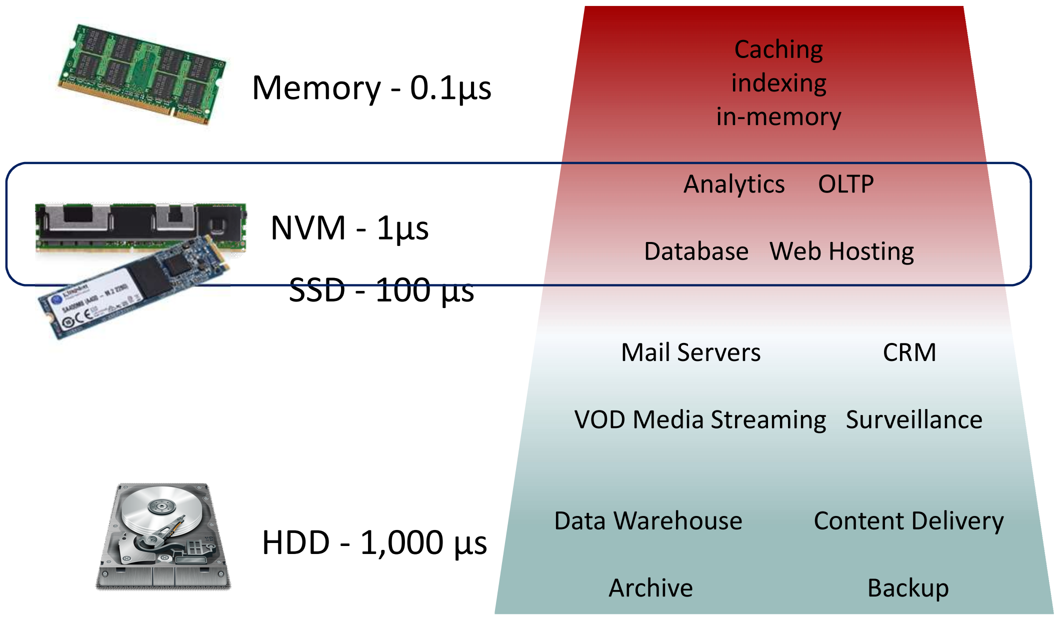
[NSDI15] K.Ousterhout et al. Making sense of performance in Data Analytics Frameworks. USENIX Symposium on Networked Systems Design and Implementation, 2015)
[ICSE14] T.H.Chen et al. Detecting performance anti-patterns for applications using object-relational mapping. Intl. Conf. Software Enginneering 2014

From the hardware point of view

- New storage devices, called Non-Volatile Memories or Persistent Memories, are becoming available
- Performance similar to memory, capacity similar to disk
- Byte-addressable: can store objects, not files



Computation can be done directly on stored data, without moving it to RAM

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Goal

- Building a distributed data management solution that:
- Maximizes performance and scalability
  - Bringing computation close to data by design
    - Enabling the execution of arbitrary code within the data store
  - Providing mechanism without imposing policy
    - Enabling customization (replication, placement, consistency guarantees…) according to application semantics
  - Can take advantage of new storage devices
- Lets the programmer focus on the domain
  - Supporting the data structures needed by the application
    - All data accessed in the same way, regardless if it's local or remote, persistent or volatile
  - Providing the illusion of infinite memory

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Approach

- Taking object stores as a starting point
  - Provides scalability
- Adding semantics to objects
  - Enables managing data at fine granularity
- Associating behavior to stored objects
  - Avoids data movements

Implementation using object-oriented abstractions

- Natural way of joining data and computation → performance
- Structure and behavior customizable per type → scalability
- Arbitrary data structures → representation of the domain

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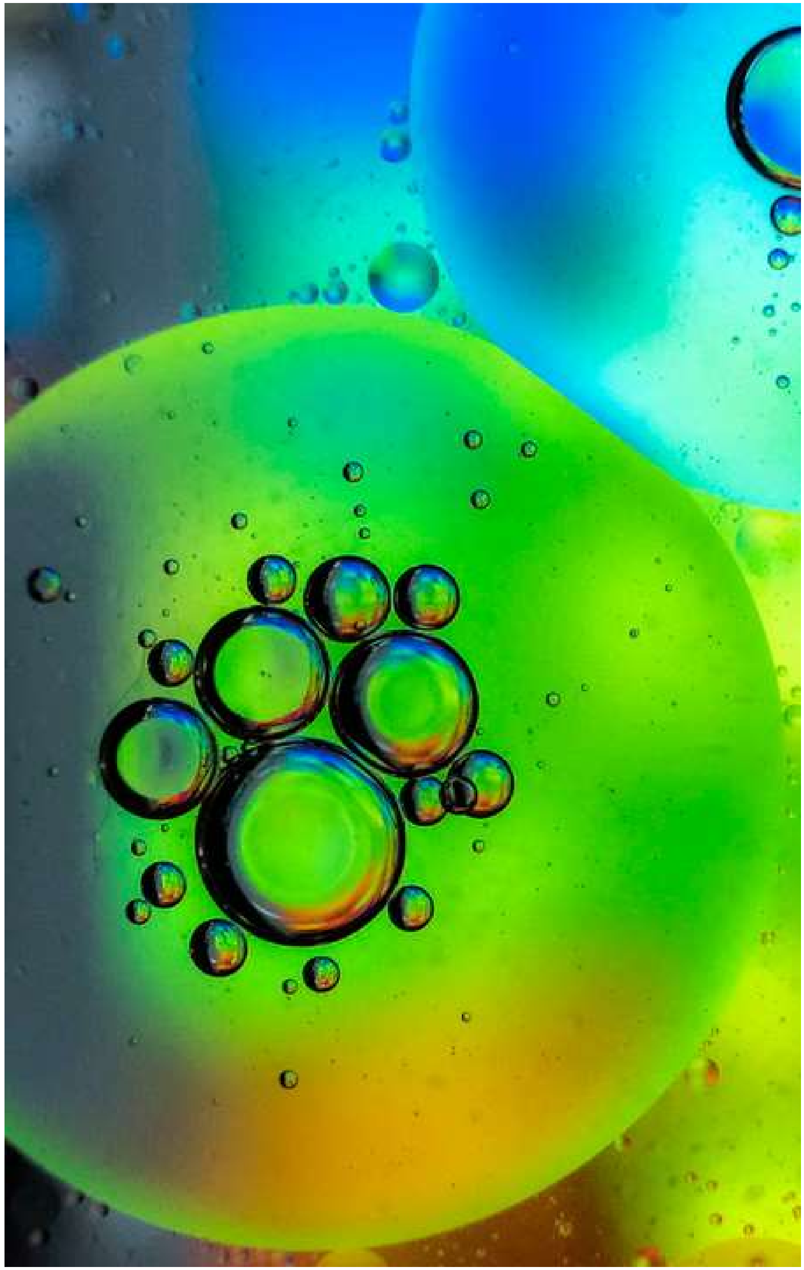
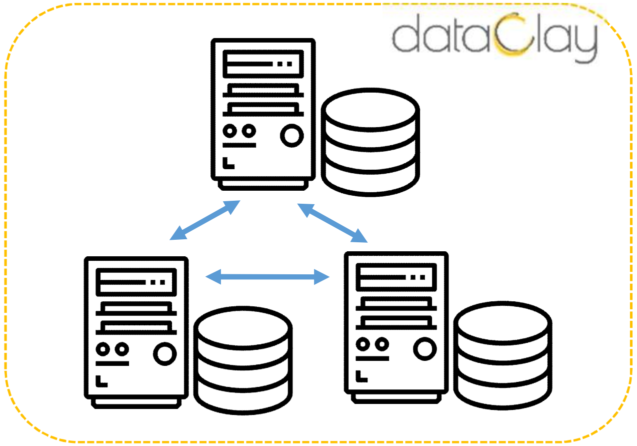


dataClay in a nutshell

- Distributed *active object store* for HPC and data analytics applications
  - Facilitates the development
  - Optimizes execution
- A single data model to manage transparently:
  - Persistent and volatile data
  - Local and remote data
- Inherently exploits data locality
  - Objects = data + methods
- In-memory
  - Objects ready to be used
  - No transformations or serializations



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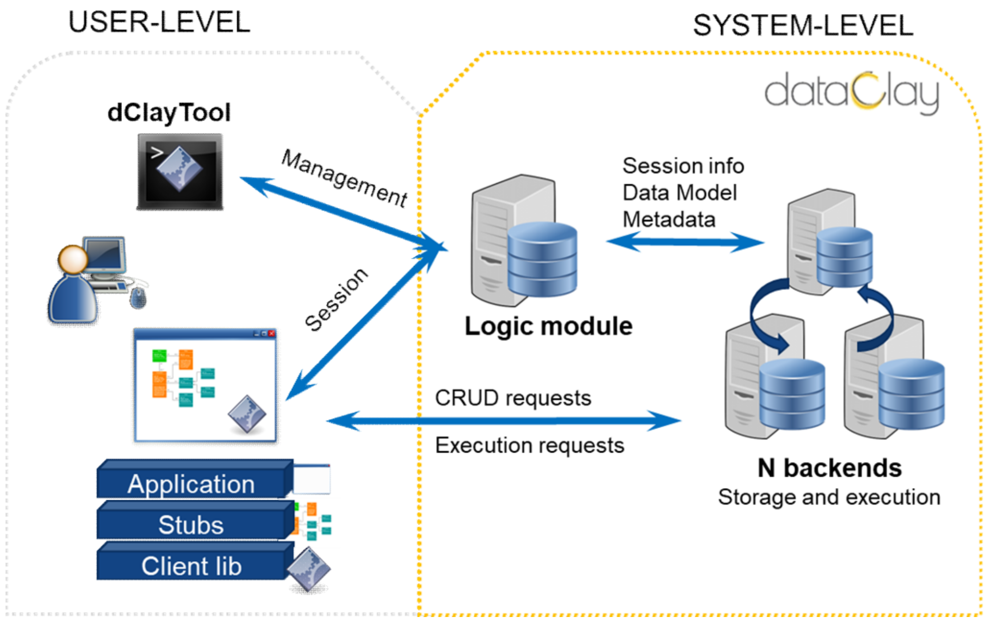
dataClay architecture

- Several backends for storage and execution of methods
- Logic module as entry point
- Persistent classes are registered in dataClay
  - Remote method execution
  - Fast serialization
- dataClay transparently forwards method execution to the backends



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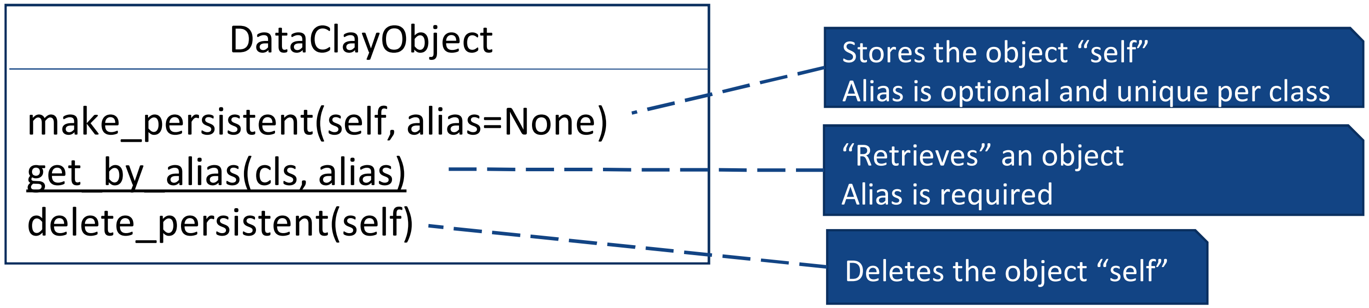
DataClayObject

- A class that enriches Python objects with generic data storage and access functionalities



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Example: a simple persistent class

```
from dataclay import DataClayObject, activemethod


class SampleClass(DataClayObject):
     number: int
     mean: float
     another_object: B
     a_list: list[B]
     a_dict: dict[str, tuple[float, float]]


     @activemethod
     def func(self, incr: int) -> int:
          return self.number + incr
```

- **Derive class from *DataClayObject***
- Specify properties and their types
- Annotate methods with *@activemethod*
- Specify types of parameters

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- Specify properties and their types
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Example: an application with persistent objects

```
class SampleClass(DataClayObject):
      number: int
      mean: float
      another_object: B
      a_list: list[B]

      def func(self, incr: int)...
```

```
from my_classes.simple import SampleClass

...

a = SampleClass()
a.number = 24
a.make_persistent()

a.another_object = B()
b = a.another_object

c = SampleClass()
c.make_persistent("sample36")
c.a_list = [b]

c = SampleClass.get_by_alias("sample35")
d = c.func(e)
```

- **Code application using the classes**
- To store an object, call its *make_persistent* method
    - Related objects will be made persistent recursively
- To update a persistent object, just use the assignment instruction
    - Changes will be persistent, too
- To access a persistent object, either:
    - Retrieve it by alias
    - Navigate through relationships

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Example: an application with persistent objects

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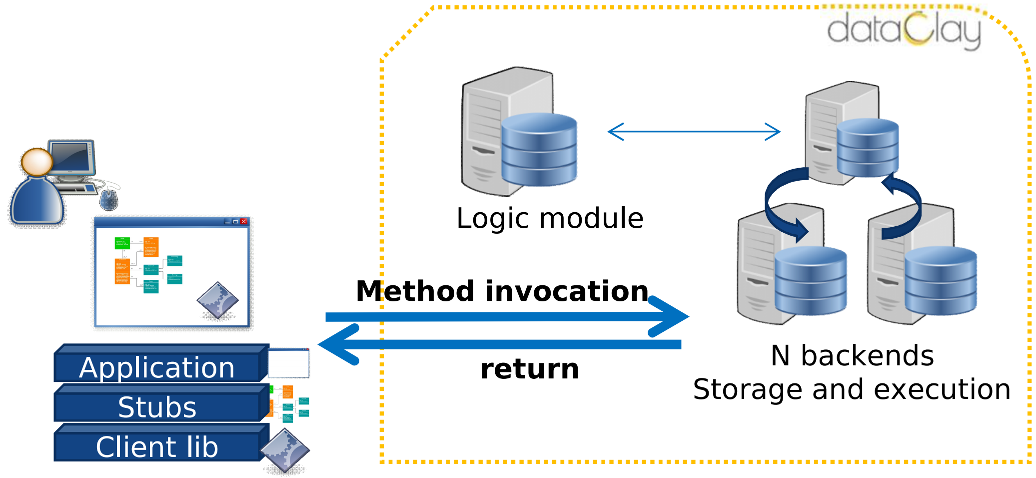
Active storage



Application

```python
from my_classes.simple import SampleClass

...

a = SampleClass()
a.make_persistent()
print(a.func(4))

...
```

Registered class

```python
class SampleClass(DataClayObject):
      number: int
      mean: float
      another_object: B
      a_list: list[B]

     @activemethod
      def func(self, incr: int) -> int:
           return self.number + incr
```

Why is this useful?

Without using active storage features

```
from my_classes.sim import Observations

temps = Observations.get_by_alias("temps")

n = 0
avg = 0
for value in temps.values:
    avg += value
    n += 1
avg /= n

print(avg)
```

The whole content of “temps” is transferred from dataClay to the application to find the average

Using active storage features

```
from my_classes.sim import Observations

temps = Observations.get_by_alias("temps")

avg = temps.get_average()

print(avg)
```

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```
from dataclay import DataClayObject, activemethod

class Observations(DataClayObject):
    values: list[int]

    @activemethod
    def get_average(self) -> float:
        n = 0
        avg = 0
        for value in temps.values:
            avg += value
            n += 1
        avg /= n
```

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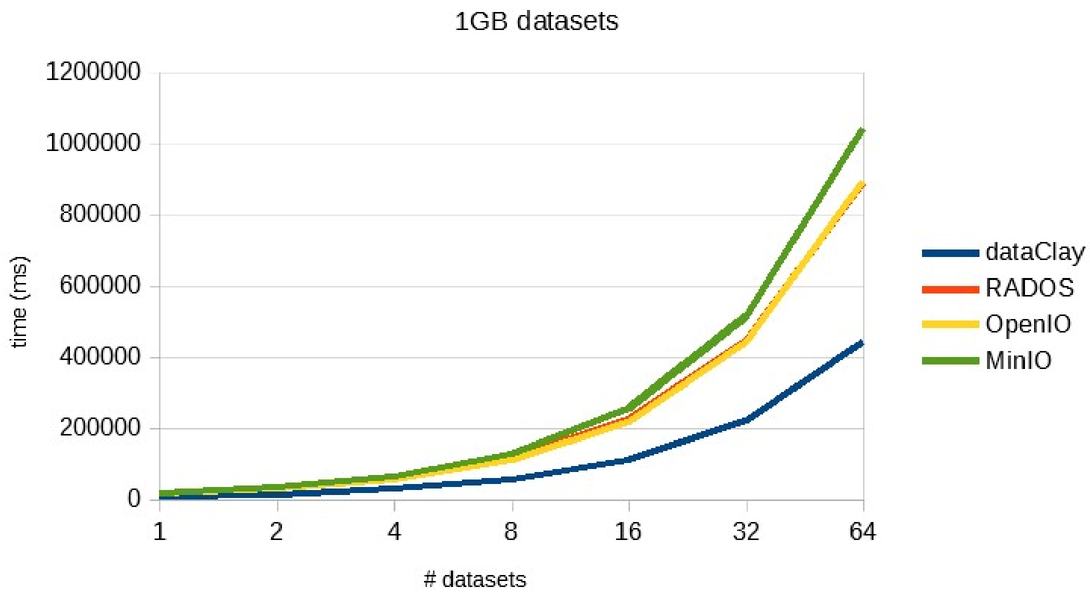
Performance improvement

- Processing a dataset (an int array) and returning 50% of its elements as a result
  - 1GB per dataset
- Executed in Grid5000, 4 nodes
  - 128 GB RAM, 48 cores
- Comparison with other object stores
  - With RADOS, OpenIO and MinIO the datasets are returned to the application, where the processing is applied
  - As the amount of data grows, performance gains with dataClay increase
  - Same happens as the size of the result decreases (not shown)
- The difference is even higher when using Non-Volatile Memories instead of disk



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dataClay
Active objects across the network

dataClay demo

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Links of interest

- eBISS 2023 demos: https://github.com/bsc-dom/eBISS-2023

- dataClay site: http://www.bsc.es/dataClay
- Documentation: https://dataclay.readthedocs.io
- Repository: https://github.com/bsc-dom
  - Source code
  - Examples
  - Demos

- Contact and support: support-dataclay@bsc.es

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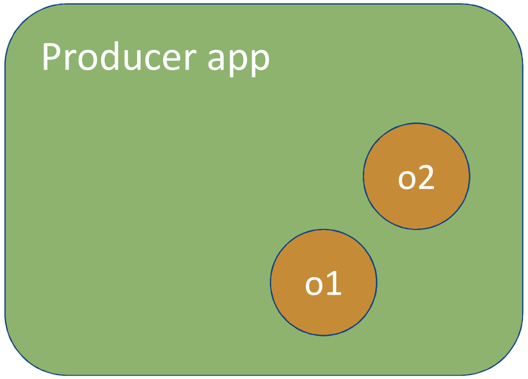
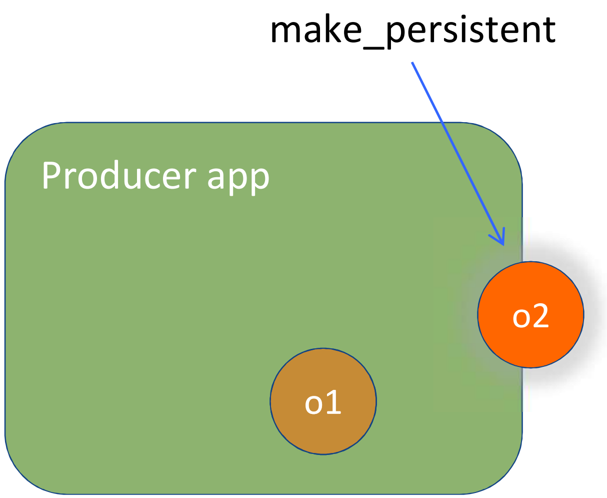
An integrated demo

dataClay within a workflow



- Applications can operate on persistent and in-memory objects seamlessly
- Producer-consumer workflows can easily share objects
- Flat object space shared across nodes
- Data transfers are avoided (in-situ processing)

dataClay within a workflow



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dataClay within a workflow

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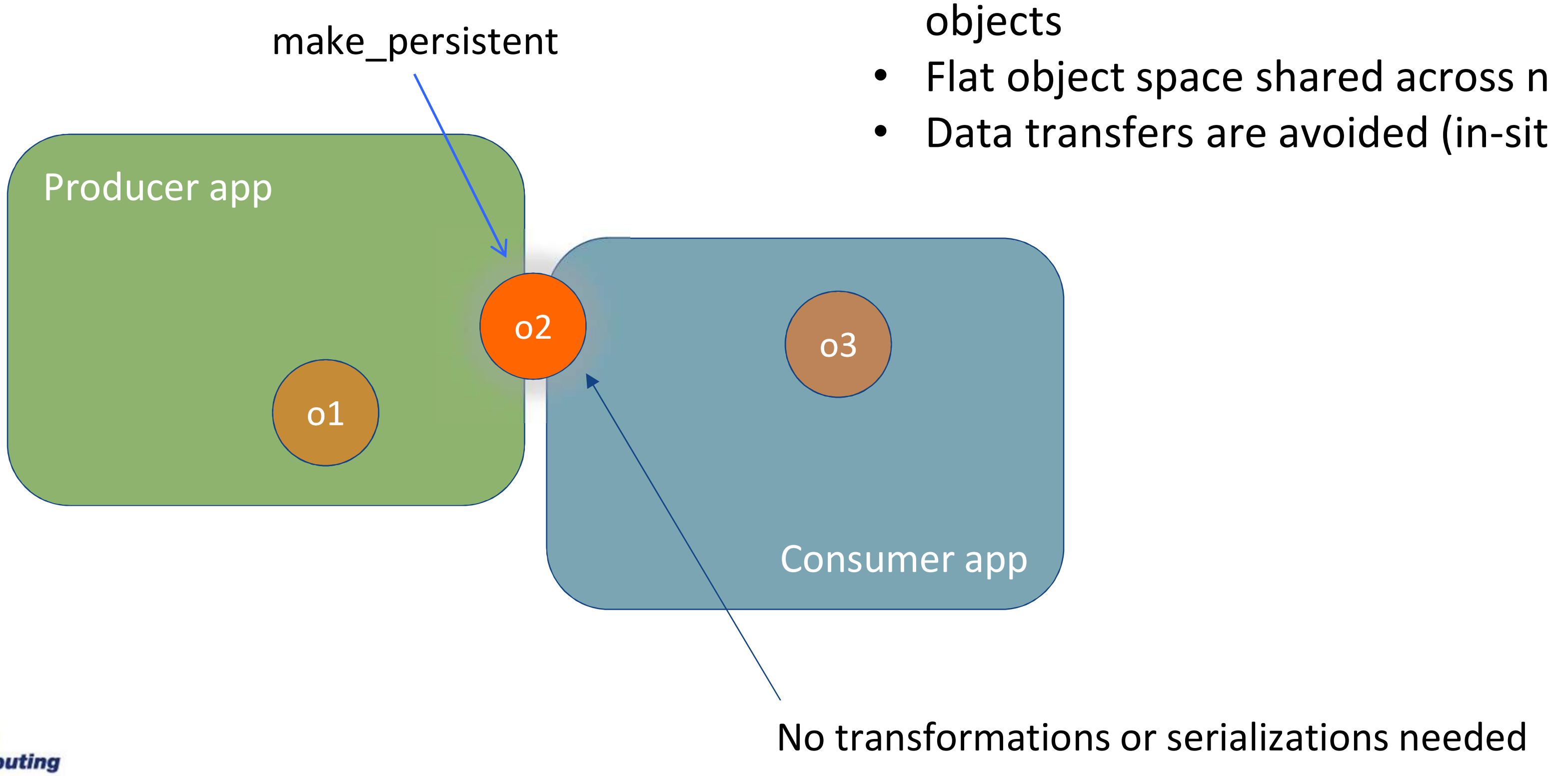

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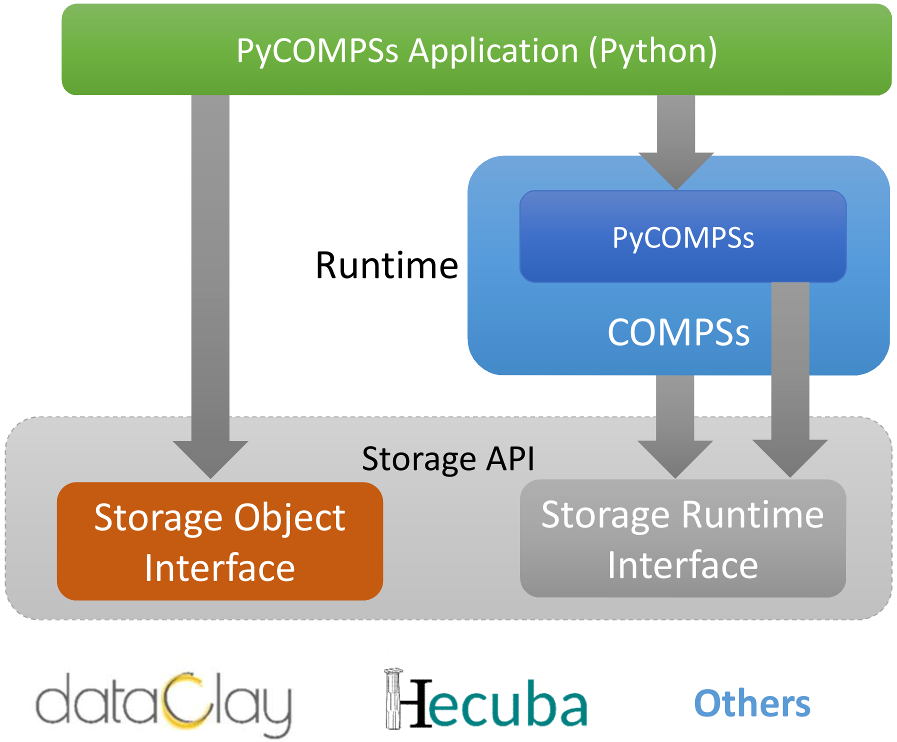
Integration with COMPSs

- Abstract *Storage Object Interface*
- Two types of functionalities:
  - For the application developer
    - *Storage Object Interface*
  - For the programming model runtime
    - *Storage Runtime Interface*



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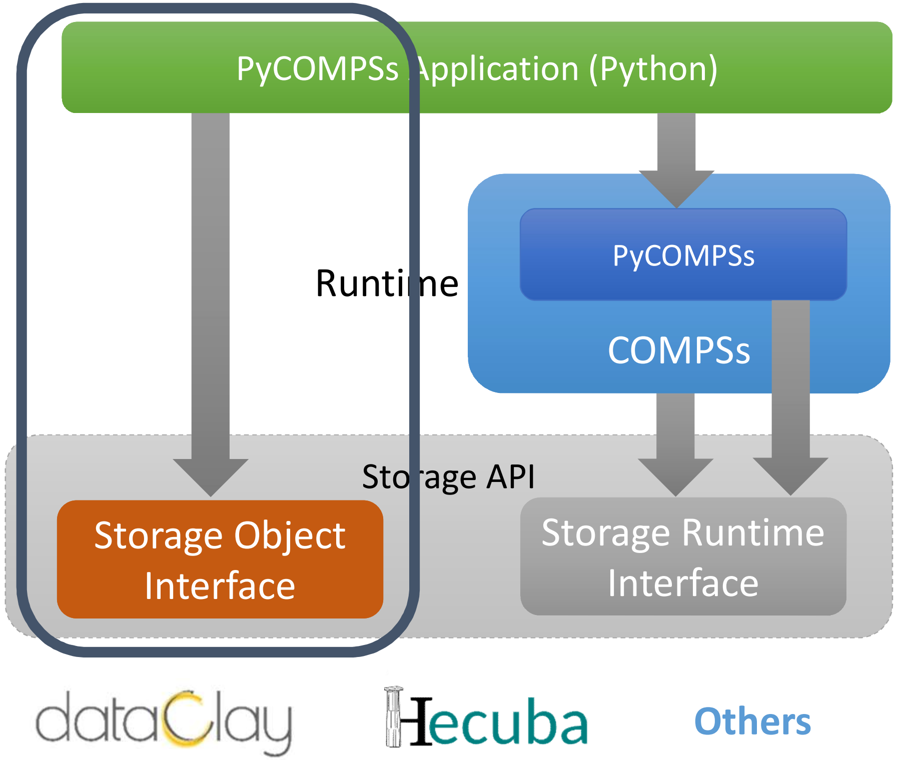

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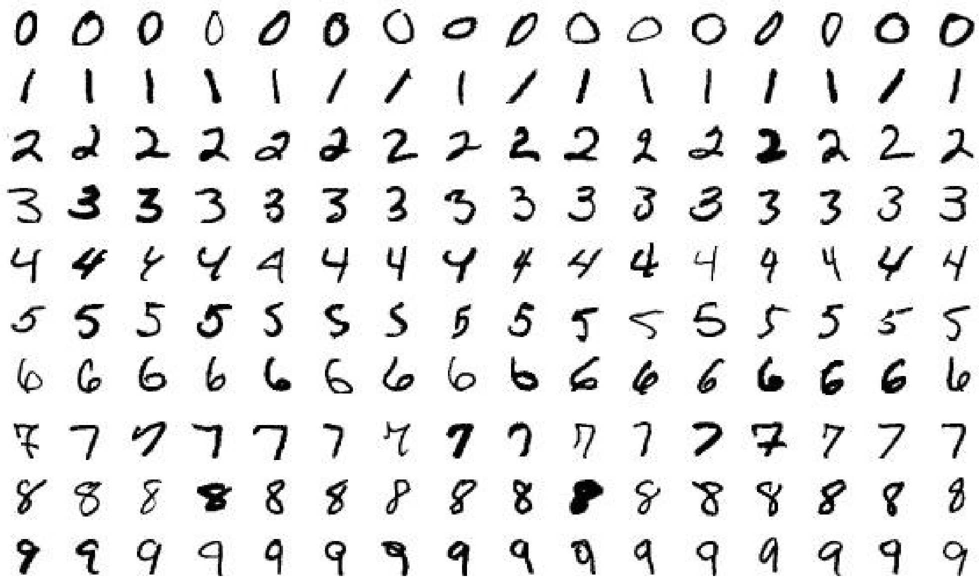
Demo

- Handwritten digits recognition
- 2 alternatives
  - Machine Learning version
    - K-nearest neighbors
    - Implemented using COMPSs (and dislib) and dataClay
  - Deep Learning version
    - CNN
    - Implemented using PyTorch and dataClay



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Thank you

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