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Jet Propulsion Laboratory
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Big Data Analytics Using Apache Spark

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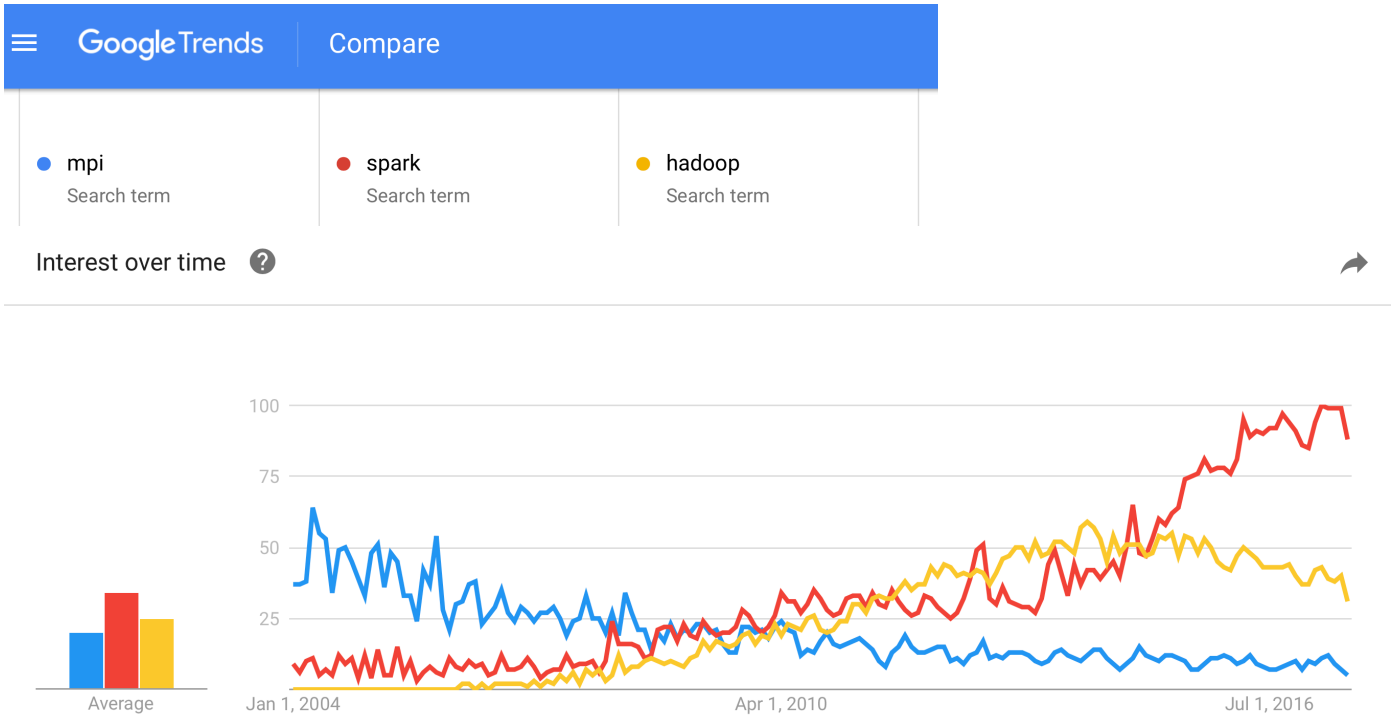
High Performance Computing: Alternative Approaches

- Dataflow / Workflow / Graph
  - Taverna
  - Pegasus
  - Spring XD
- Vector Computations
  - Vendor specific
- Message Passing
  - Parallel Virtual Machine (PVM)
  - Message Passing Interface (MPI)
- Shared Memory
  - OpenMP
  - Vendor-specific
- Hybrid OpenMPI / MPI
- Hardware-based approaches
  - VHDL, Verilog - Field Programmable Gate Array (FPGA)
  - CUDA – GPU
  - OpenCL – Heterogeneous platforms
- Master-Worker
  - Condor
  - Apache Spark
- Map-Reduce
  - Apache Hadoop
  - Apache Spark
- Grid Computing
  - Globus Toolkit
  - NASA Information Power Grid (IPG)
  - NSF TeraGrid
- Cloud Computing
  - Amazon Web Services (AWS)
  - Microsoft Azure
  - Google Cloud Platform
  - IBM Cloud

HPC Showdown: Spark vs MPI

- Jonathan Dursi's Blog [www.dursi.ca]: **"HPC is dying, and MPI is killing it"**
  - *"In [the modern era of internet-scale big data], one might expect that programmers with HPC experience – who have dealt routinely with terabytes and now petabytes of data, and have years or decades of experience with designing and optimizing distributed memory algorithms – would be in high demand. They are not."*
  - *"MPI is at the wrong level of abstraction for application writers [and] tool builders"*
  - *"MPI is more than you need for modest levels of parallelism [and] less than you need at extreme levels of parallelism."*



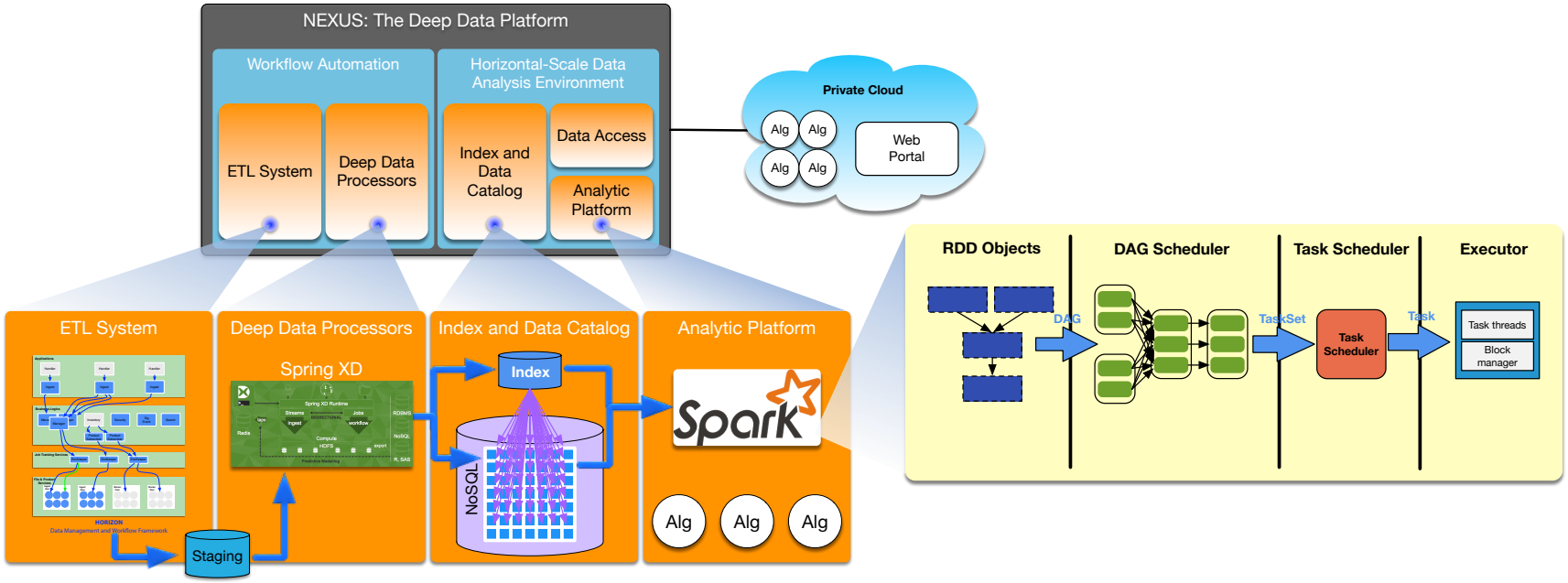
HPC Showdown: Spark vs MPI (cont.)

- J. L. Reyes-Ortiz, L. Oneto, D. Anguita, **"Big Data Analytics in the Cloud: Spark on Hadoop vs. MPI/OpenMP on Beowulf"**, 2015 INNS Conference on Big Data, Vol. 53, 2015, pp. 121-130.
  - *"the MPI/OpenMP implementation is much more powerful than the Spark on Hadoop alternative in terms of speed. [For KNN], it can be more than 10 times faster."*
  - *"MPI/OpenMP scales better than Spark."*
  - *"Nevertheless, Spark on Hadoop may be preferred because it also offers a distributed file system with failure and data replication management, allows the addition of new nodes at runtime, and provides a set of tools for data analysis and management that is easy to use, deploy and maintain."*

- MPI offers low level control and highly optimized communications
  - For applications that cannot be carved up into nice independent partitions, MPI performance can greatly exceed that of Spark, which was not designed for that use case.

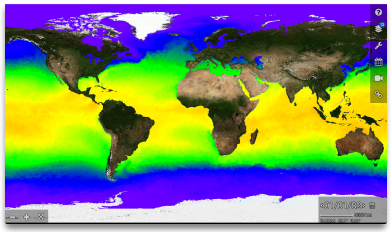
- Spark offers more than just computational speed
  - Excellent performance across clusters for algorithms that are "embarrassingly" parallel.
  - Easy to deploy and manage on a cluster computer
  - Excellent support by cloud vendors
  - Convenient API at a level of abstraction that frees application developers to focus on numerical operations rather than inter-process communications.
  - Automatic rescheduling of tasks hosted on failed or overloaded nodes.

The NEXUS Architecture

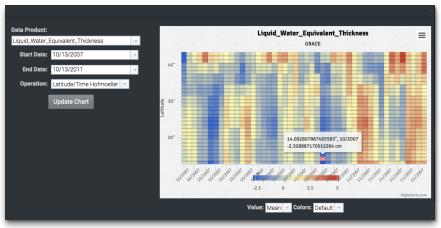


- Extract/Transform/Load (ETL) System – Ingest and stage data
- Deep Data Processors – metadata, statistics, and tiles
- Index and Data Catalog – horizontal-scale geospatial search (Solr) and tile retrieval (Cassandra)
- Analytic Platform – Spark- based domain-specific analytics
- Data Access – tile and collection-based data access
- Cloud Platform – portal and custom VMs

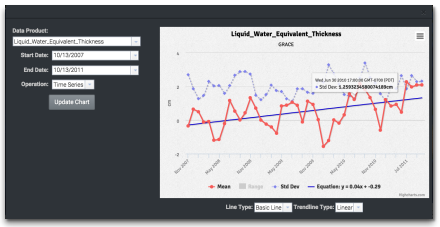
From Files to Tiles



Display Variables on Map



Latitude-Time Hovmoller



Plot Aggregate Statistics

Chunk Chunk Chunk
Chunk Chunk Chunk ...
Chunk Chunk Chunk

Cassandra DB Cluster &
Spark In-Memory
Parallel Compute!

Fast & Scalable

Solr DB Cluster

Meta Data | Meta Data | Meta Data | Meta Data ...

Metadata (JSON): Dataset and granule metadata, Spatial Bounding Box & Summary Statistics

Custom Analytics

Subset Variables & Chunk Spatially

Each file contains many high-resolution geolocated arrays

SMAP | MODIS | GRHSST | JASON

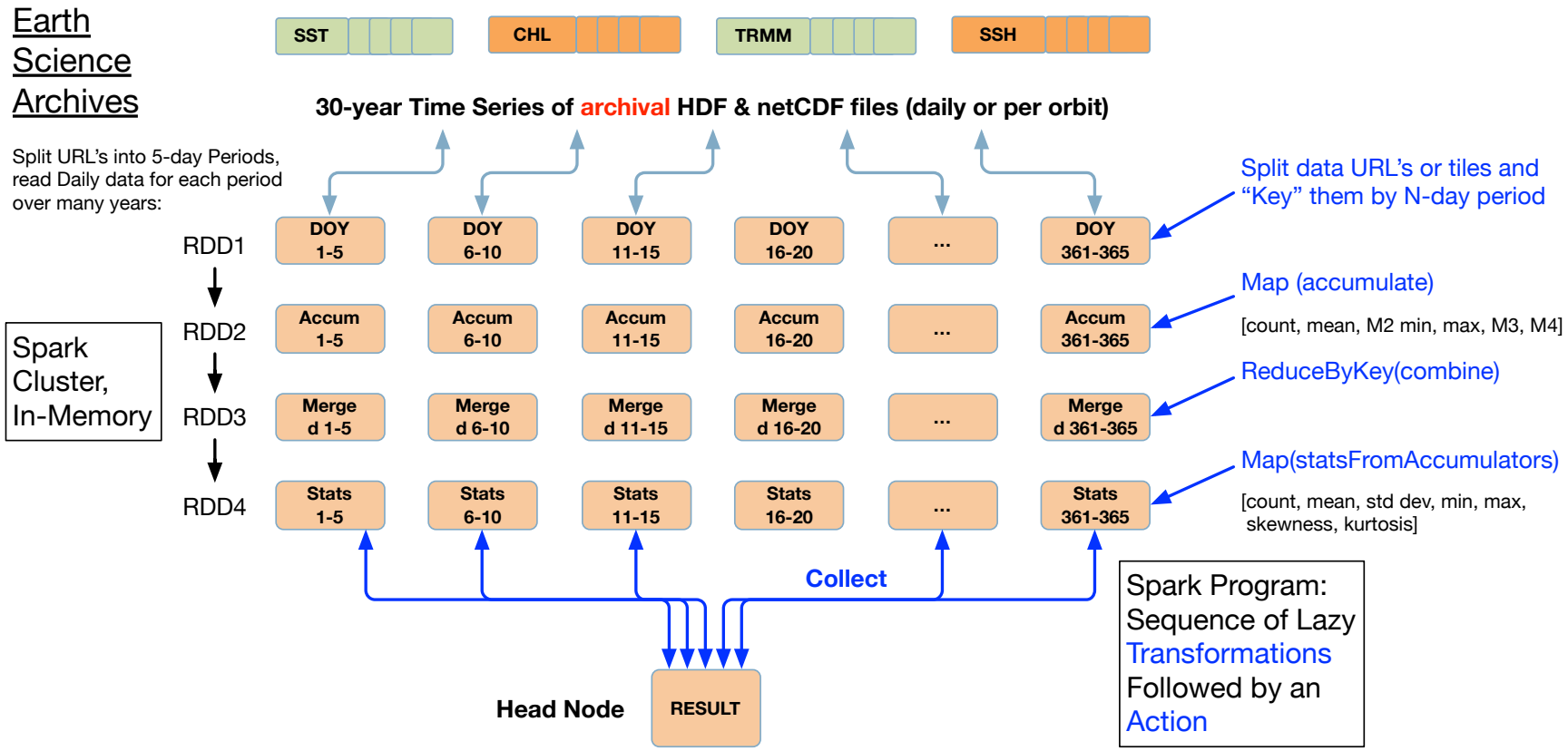
Slow File I/O

30-Year Time Series of archival HDF & netCDF files (daily or per orbit)

Map-Reduce Style Computation

Resilient Distributed Dataset (RDD)

- The RDD is Spark's abstraction of a dataset as a collection of elements that are partitioned across a cluster computer.
- Parallel computations can be applied to an RDD to produce a new RDD.
- Fault tolerant



NEXUS Spark Analytics Algorithms

Included with NEXUS:

- Area-Averaged Time Series
  - Compute statistics (e.g., mean, minimum, maximum, standard deviation) for each time step within a user-specified spatiotemporal bounding box.
  - Optionally apply seasonal or low-pass filters.
  - Return result in ascending time order in JSON format.
- Time-Averaged Map
  - Compute a geospatial map that averages gridded measurements over time at each grid coordinate within a user-defined spatiotemporal bounding box.
- Correlation Map
  - Computes the correlation coefficient at each grid coordinate within a user-specified spatiotemporal bounding box for two identically gridded datasets.
  - Automatically aligns the time stamps for the two datasets being compared.
- Climatological Map
  - Similar to Time-Averaged Map, but only includes measurements in the time average that are within a user specified month.

Application Specific Extension: Anomaly Detection (OceanXtremes)

- Climatology
  - For each day-of-year (1-366) or month (1-12), computes a ”typical value” for each coordinate grid location.
  - The ”typical value” may be the result of either (1) a standard pixel mean with optional smoothing over time (e.g. 5-day average), (2) Gaussian interpolation [Armstrong and Vazquez-Cuervo, 2001], or Empirical Orthogonal Function (EOF).
- Daily Difference Average
  - Subtract a dataset from its climatology, then, for each time stamp, average the differences within a user-specified spatiotemporal bounding box.
  - Product can be used to search for anomalies compared to the historical norm.

Application-Specific Extension: Distributed Oceanographic Match-up Service (DOMS)

- In Situ Match
  - Discover in situ measurements that correspond with a gridded satellite measurement.

The Spark Approach I

- Multiple Shells/API:
  - Java
  - Scala
  - **Python (PySpark)**
  - R (SparkR)
- Multiple deployment modes:
  - Standalone
  - Hadoop YARN
  - **Apache Mesos**

The Spark Approach I

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- Multiple deployment modes:
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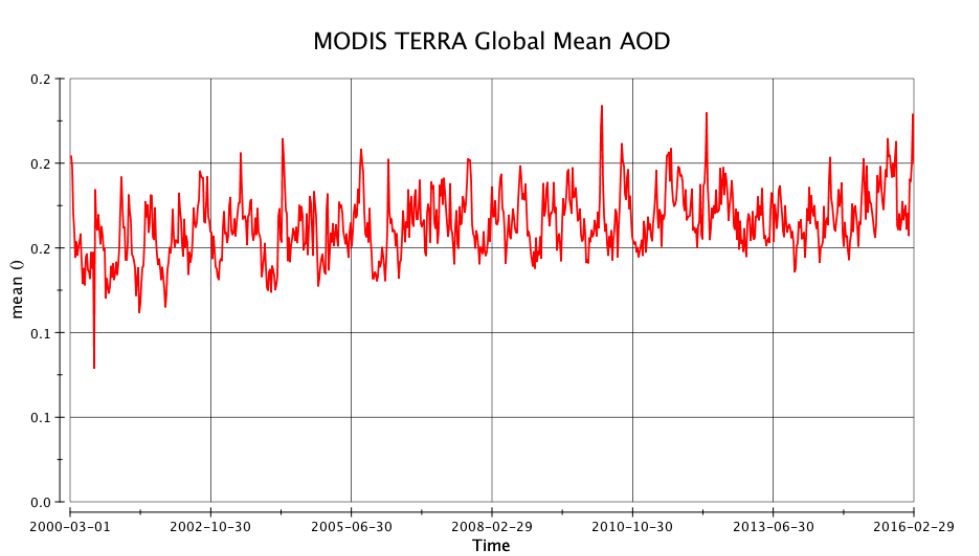
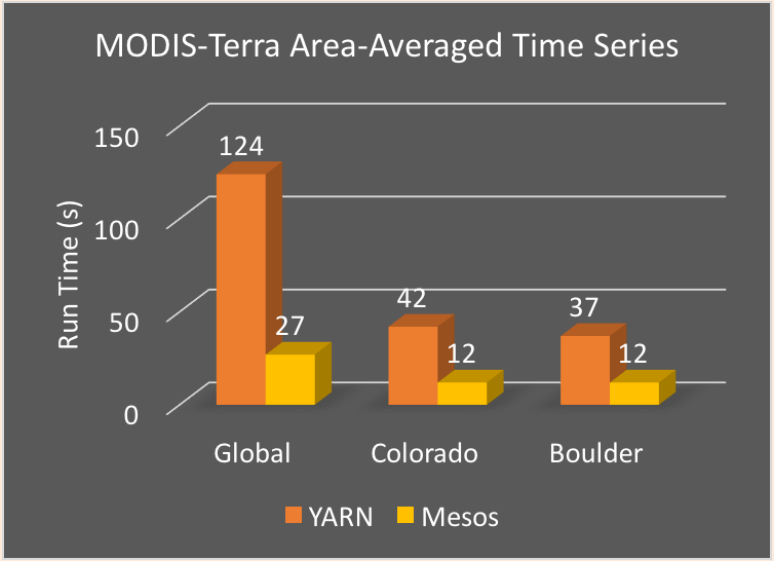


- NEXUS run on 8-node cluster computer at JPL running Solr, Cassandra, Spark 2.0, with the YARN or Mesos scheduler, as indicated in the plot.
- Area-Averaged Time Series over the indicated spatial subset (Global, State, City) run with 16-way parallelism.
- Variable plotted: MODIS-Terra Aerosol Optical Depth (AOD) 550 nm dark target
- 5,789 daily data granules covering the globe at 1 deg resolution with date range: 3/1/2000 – 2/29/2016 (3 GB input data volume).
- In our experiments, using Mesos consistently yields a speedup of 2 to 4 times over YARN.



The Spark Approach II

- Spark applications follow the master-worker paradigm:
  - Driver program creates the RDD and defines “map” and ”reduce” operations to be applied to the data.
  - Executors (Workers) collectively store the RDD in memory and in parallel perform the specified transformations on the data.

- Spark applications follow the map-reduce paradigm:
  - Spark API provides multiple “map” functions:
    - `map()` : operates on dataset elements
    - `mapPartitions()` : operates on entire data partitions
  - Spark API provides a variety of ways to collect the result of a computation back to the driver node, or perform reduction (summarization of the results)
    - collect() : merge all elements of the RDD into a single list
      - Use with care: the combined dataset must be small enough to fit in the driver node’s memory!
    - reduce()
    - reduceByKey()
    - foldByKey()
    - combineByKey()

PySpark Program Structure I

- This is a simple program structure for cases where:
  - All the data fits in memory on the head node.
  - The computation simply maps each element in the data array to an output
  - The results are simply collected back to the head node. There is no further reduction operation.

```
def map(x):
        # transform x and return a value
        return f(x)

def main():
        data = <an array of input data>
        ...
        # Configure Spark
        sp_conf = SparkConf()
        sp_conf.setAppName("MyApp")
        sp_conf.set("spark.executor.memory", "4g")
        ...
        sp_conf.set( < more settings >)

        # Create Spark Context and initial Spark RDD
        sc = SparkContext(conf=sp_conf)
        rdd = sc.parallelize(data, num_partitions)

        # Perform map computation and collect the results back to
        # this head node.
        results = rdd.map(map).collect()
        <print, save, or plot results>
```

PySpark Program Structure II

- This program structure is for cases where a map and reduce operation is required.
  - All the data fits in memory on the head node.
  - The computation maps each element in the data array to an output key-value pair
  - The results are added by key and collected back to the head node.

```
from operator import add

def map(x):
        # transform x and return a key-value pair (example: time, value)
        return create_key(x), create_value(x)

def main():
        data = <an array of input data>
        ...
        # Configure Spark
        sp_conf = SparkConf()
        sp_conf.setAppName("MyApp")
        sp_conf.set("spark.executor.memory", "4g")
        ...
        sp_conf.set( < more settings >)

        # Create Spark Context and initial Spark RDD
        sc = SparkContext(conf=sp_conf)
        rdd = sc.parallelize(data, num_partitions)

        # Perform map computation and collect the results back to
        # this head node.
        map_result = rdd.map(map)
        reduce_result = map_result.foldByKey(0, add).collect()

        <print, save, or plot results>
```

Practical Considerations I

- For big data, the map function might have to do the I/O.
  - The canonical Spark tutorial example application, word count, is not a good example of how a science algorithm would use Spark!
  - Insufficient memory on a single node.
  - Carefully consider size of the data being collected.
  - Single pass algorithms needed
  - Database query size must be considered
    - Very small queries are inefficient
    - Very large queries might time out, or result in excessive memory consumption.
- The map function must be static
  - Trying to use a class method as your map function will result in an exception.
  - Python decorator: @staticmethod
  - Other class variables or methods ("self") not available inside map function.
  - Can get a program working with python's built-in map() function first; small additional leap to make it work with Spark.
- The map function takes just one input argument
  - Use a tuple or list to pass in more information if needed. Unpack the tuple inside the map function.
  - If many necessary arguments don't change from one map call to the next, consider using the partial function in the Python functools module to create a new version of the function with only the arguments that change.

```
from functools import partial
def f(a, b, c):
   return a+b*c
f_part = partial(f,1,2)
x = 3
# The following returns the same
# result as f(1,2,x)
y = f_part(x)
```

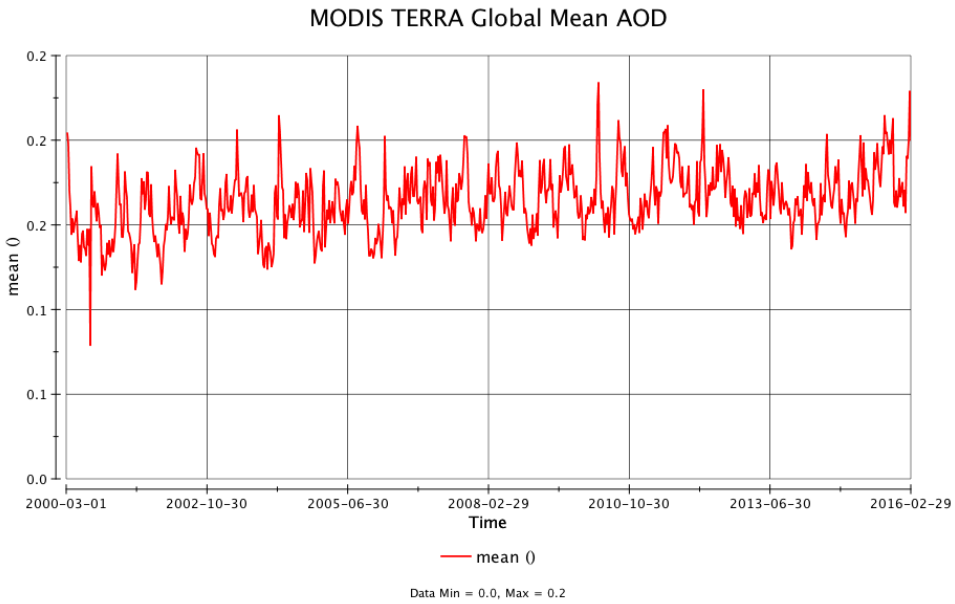
Practical Considerations II

- Control number of Spark executors and data partitions
  - Executors are the worker processes that are instantiated when the Spark cluster is initialized and last for the life of the Spark application.
  - A data partition represents a chunk of work that is scheduled for processing on an executor.
- Spark performance depends on configuration.
  - Number of executors, E
  - Cores per executor
  - Memory per executor
  - Number of data partitions, P
  - Recommended that 2 <= P/E <= 4
  - > 200 configuration parameters in Spark 2.2.0 documentation
  - Nontrivial to squeeze best performance out of Spark for complex applications.
- The Scheduler used can impact performance
  - Spark uses YARN by default
  - Mesos is available as a separate package
  - In our benchmarks, Mesos consistently yielded 2-4 times faster run times compared to YARN.
- The data partitioning scheme used can impact performance
  - Calculations on global data or very large subsets have best performance with a few large tiles.
  - Many small tiles are preferred for calculations on smaller subsets.

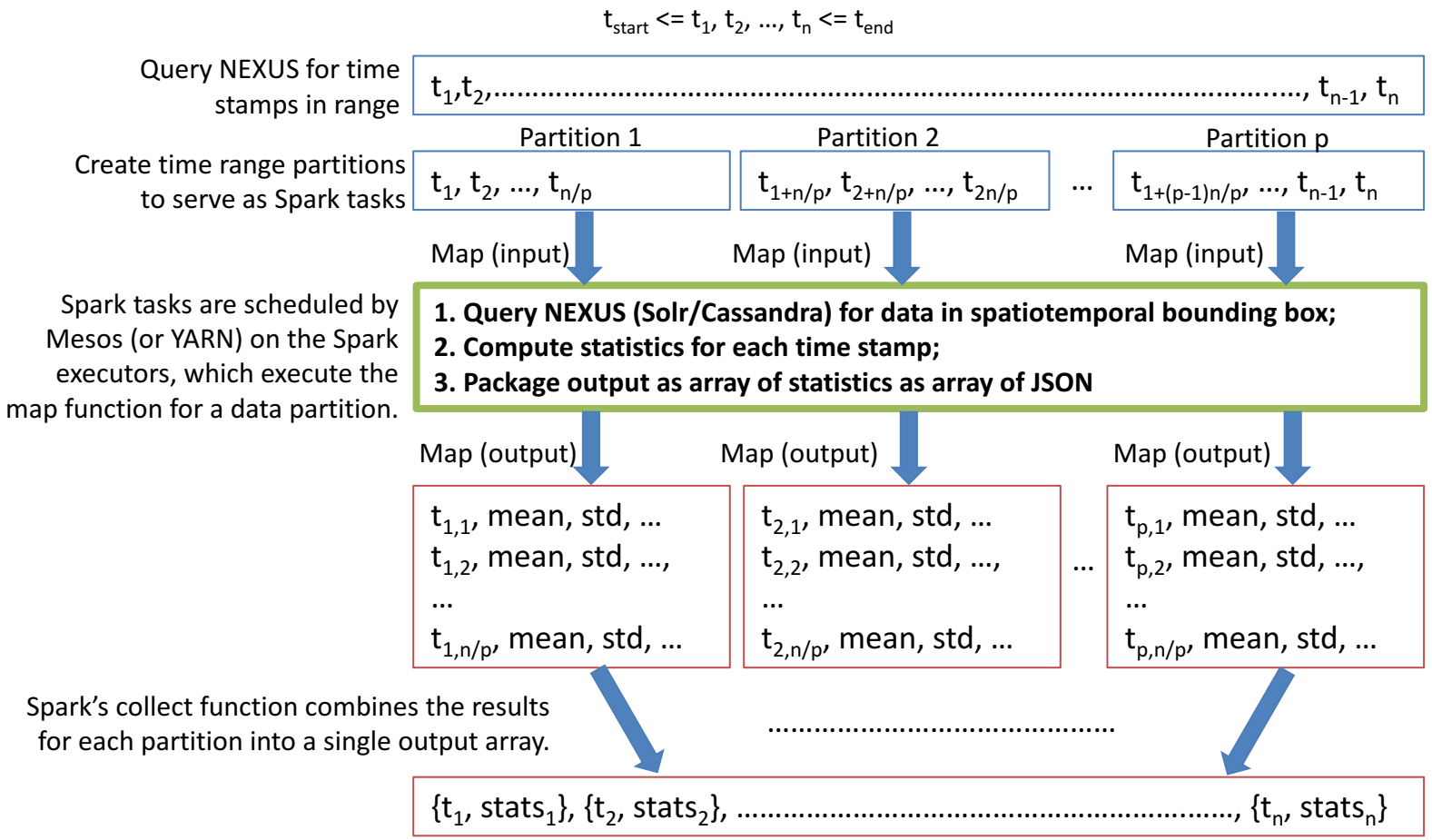
Time Series Analysis

- Compute statistics (e.g., mean, minimum, maximum, standard deviation) for each time step within a user-defined spatio-temporal bounding box.
  - Optionally apply seasonal or low-pass filters.
  - Return result in ascending time order in JSON format.


```
"data": [
  [
    {
      "std": 1.4744961225186004,
      "cnt": 2107,
      "minSeasonalLowPass": -1.3469589497685839,
      "minSeasonal": -1.3745376124526523,
      "maxLowPass": 15.435052751030272,
      "min": 9.32000732421875,
      "max": 15.44000244140625,
      "meanSeasonal": -1.9343310558434688,
      "ds": 0,
      "meanSeasonalLowPass": -1.9285414148993034,
      "maxSeasonalLowPass": -2.1962260569545178,
      "time": 1427846400,
      "maxSeasonal": -2.1875730572324805,
      "meanLowPass": 12.279365215634886,
      "minLowPass": 9.3507517896462442,
      "mean": 12.273533821105957
    }
  ], ...
```

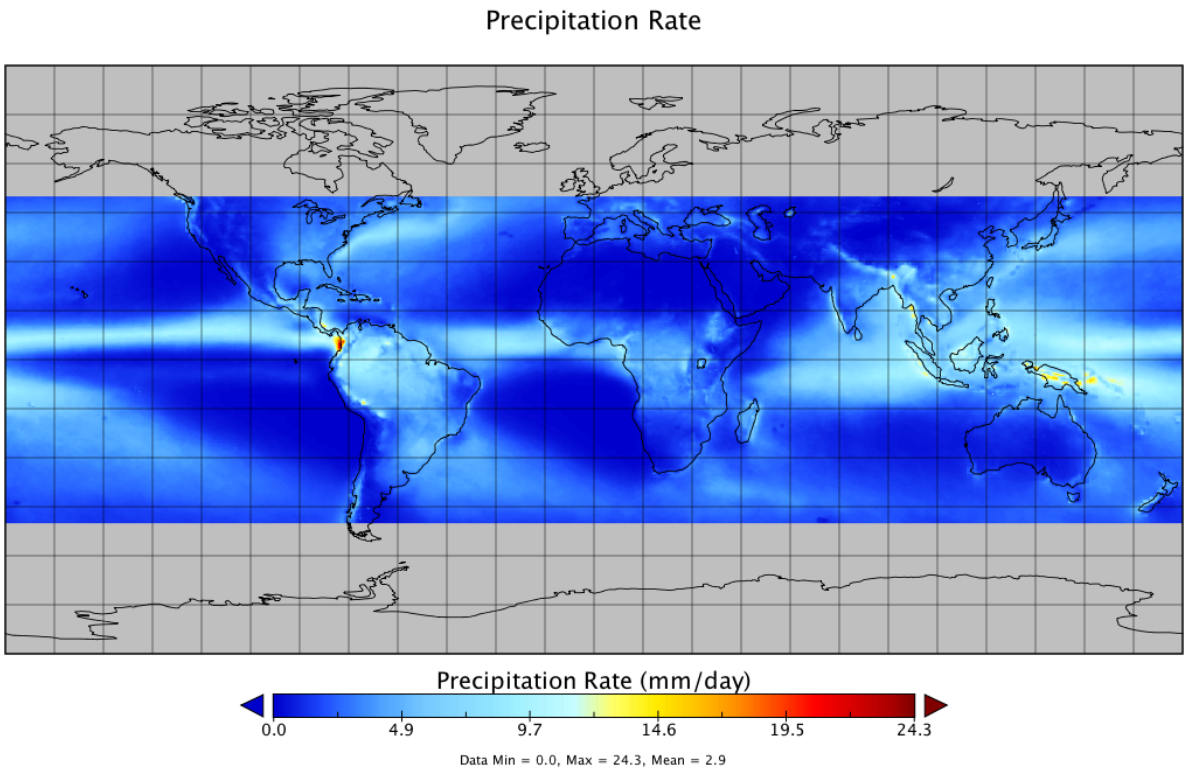



Time Series Spark Implementation

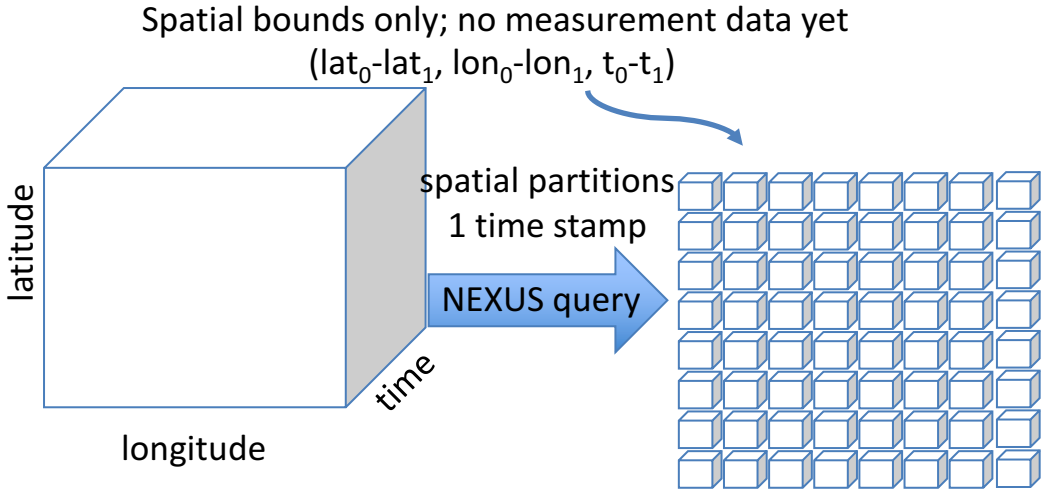


Time-Averaged Map

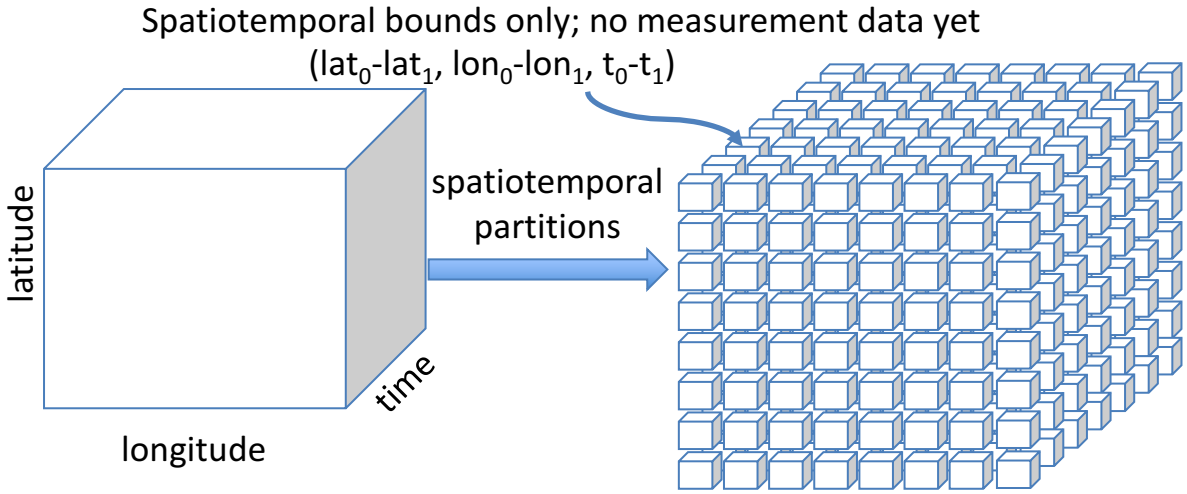
- Compute a geospatial map that averages gridded measurements over time at each grid coordinate within a user-defined spatiotemporal bounding box.
- Fill values are excluded from the calculation
- Result provided as in JSON format or NetCDF.



Time-Averaged Map Spark Implementation

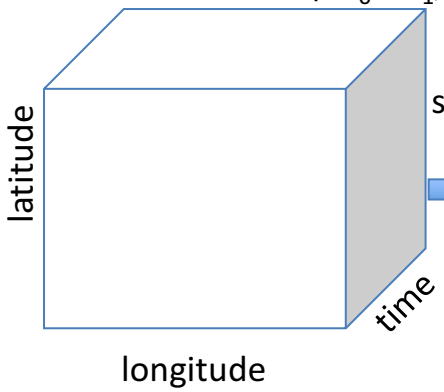


Time-Averaged Map Spark Implementation

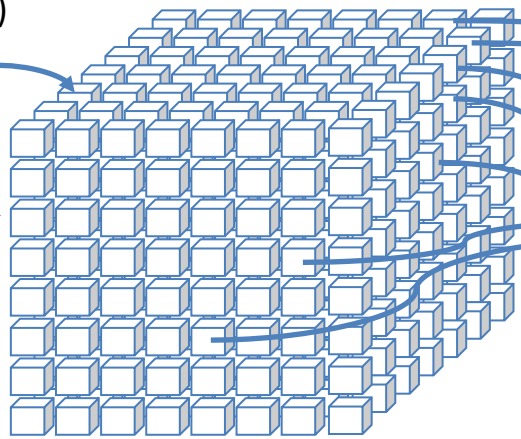


Time-Averaged Map Spark Implementation

Spatiotemporal bounds only; no measurement data yet
(lat_0-lat_1, lon_0-lon_1, t_0-t_1)



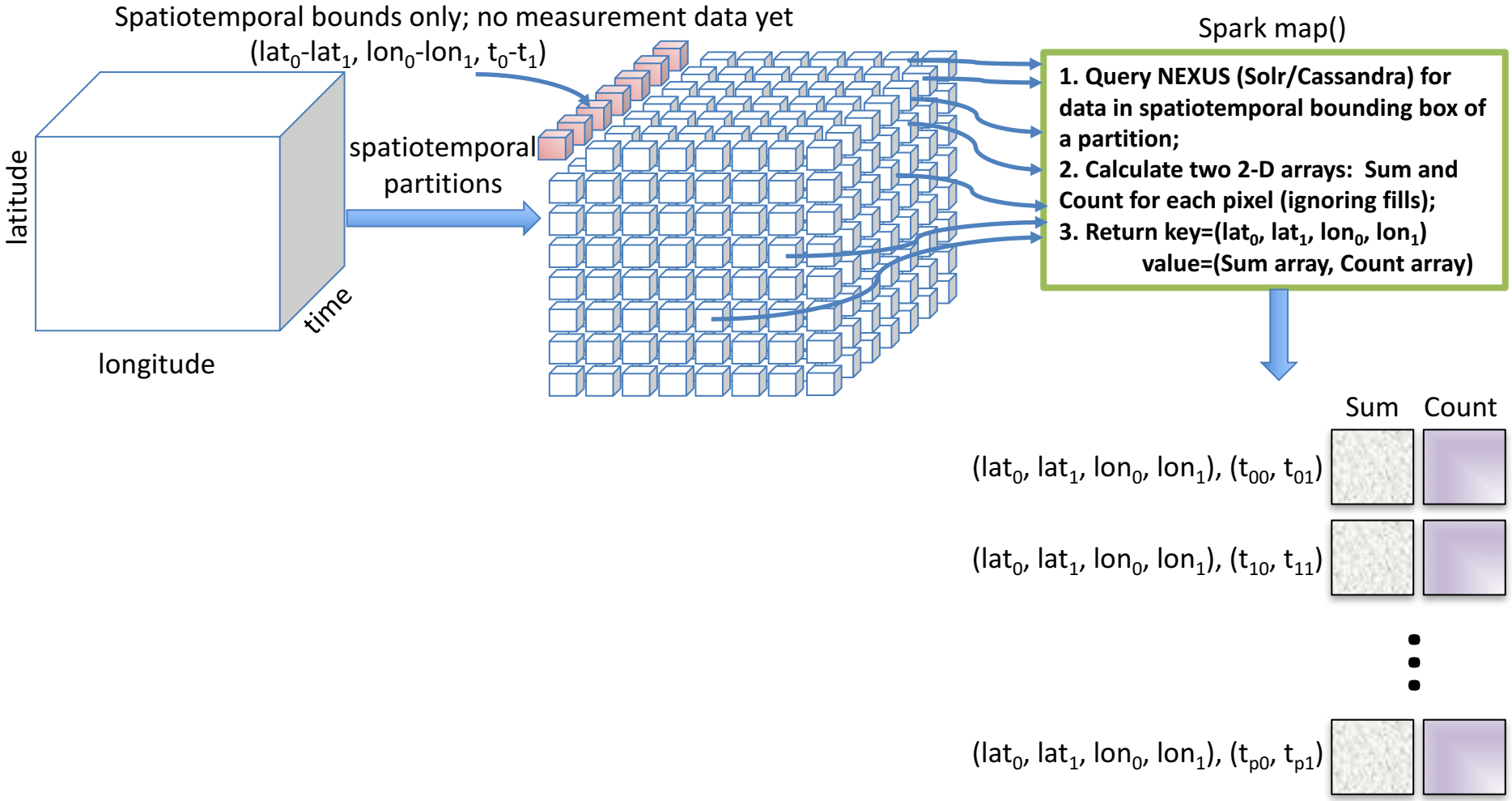
spatiotemporal partitions



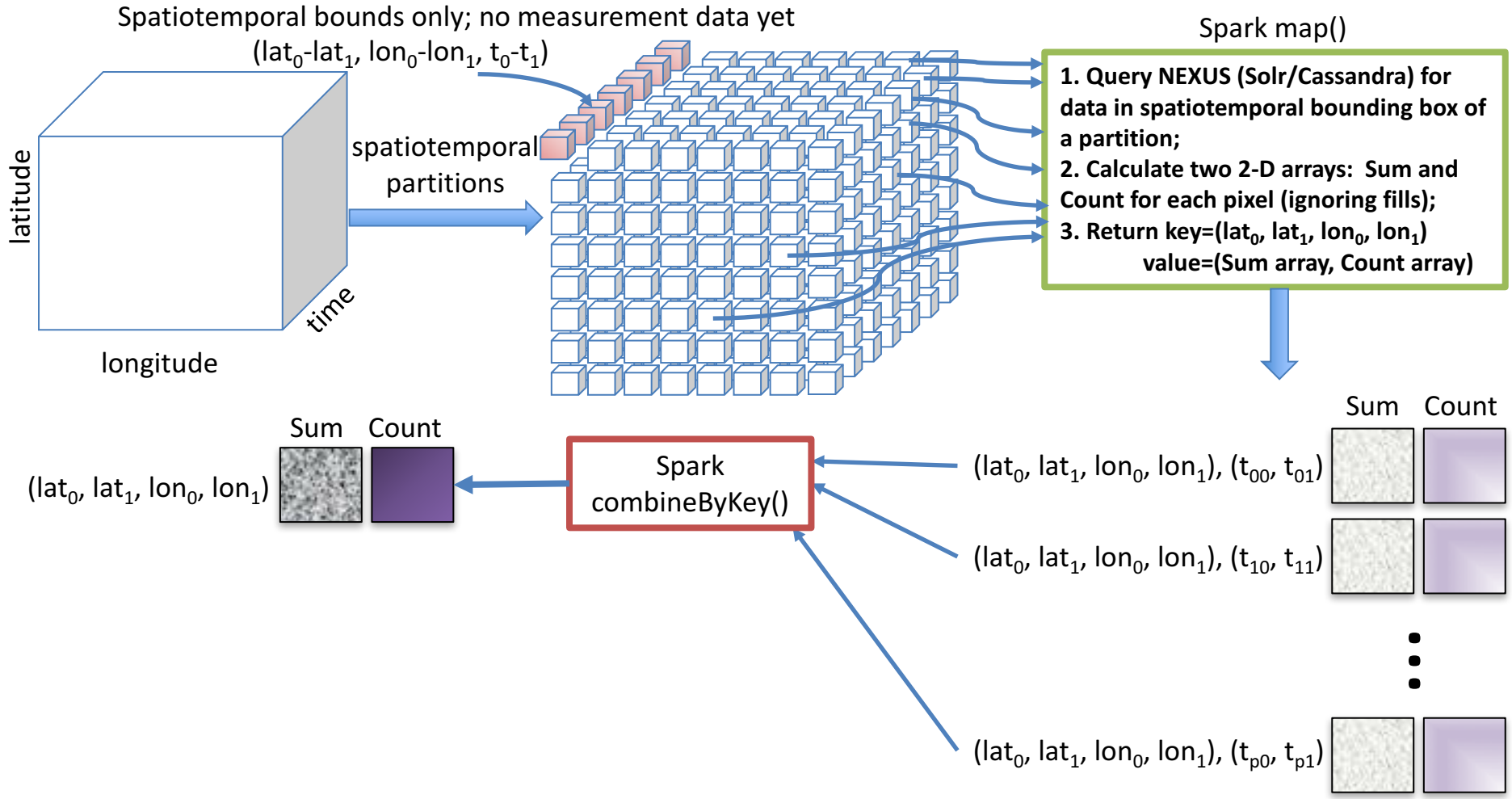
Spark map()

1. Query NEXUS (Solr/Cassandra) for data in spatiotemporal bounding box of a partition;
2. Calculate two 2-D arrays: Sum and Count for each pixel (ignoring fills);
3. Return key=(lat_0, lat_1, lon_0, lon_1)
value=(Sum array, Count array)

Time-Averaged Map Spark Implementation



Time-Averaged Map Spark Implementation



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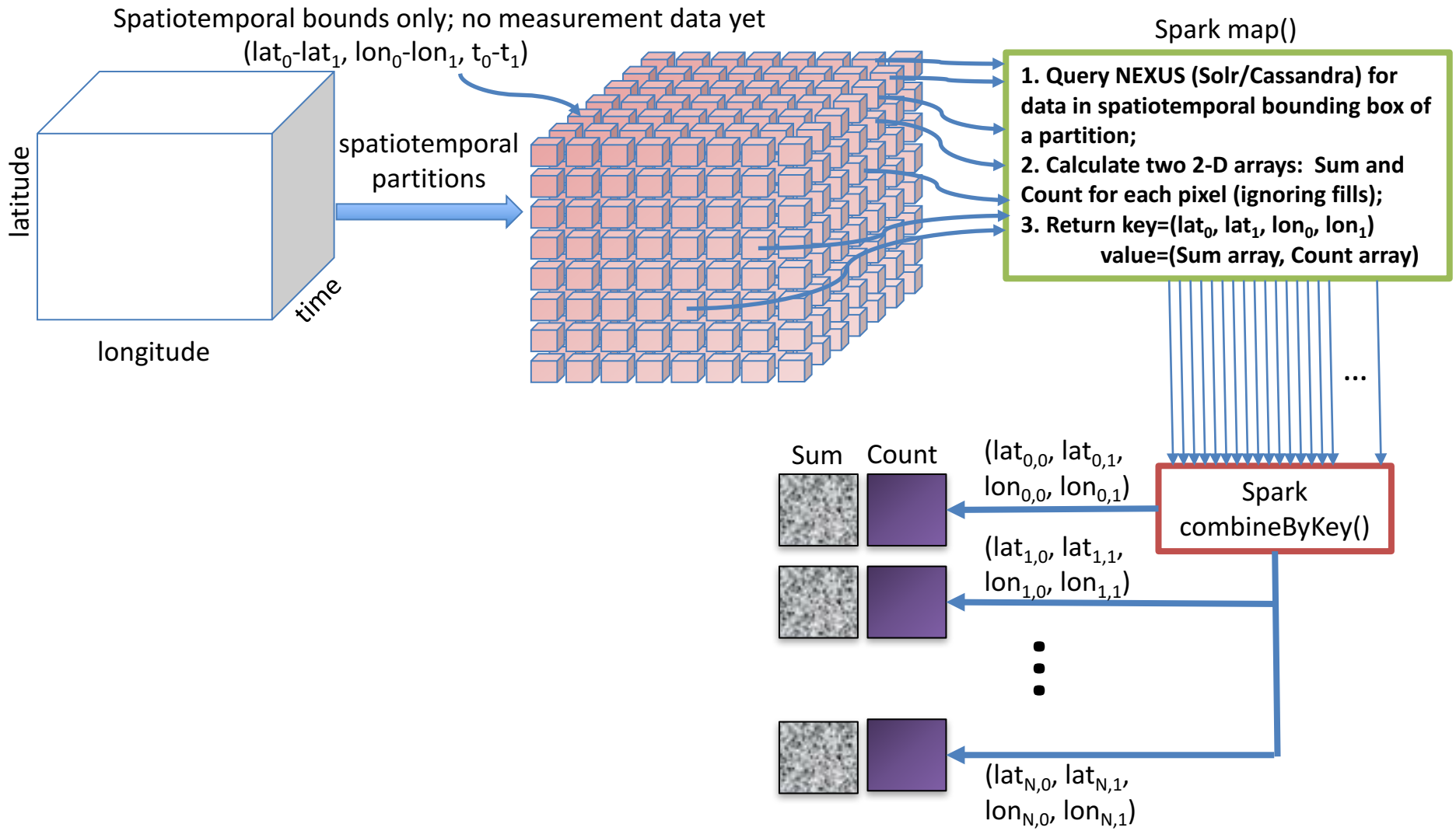

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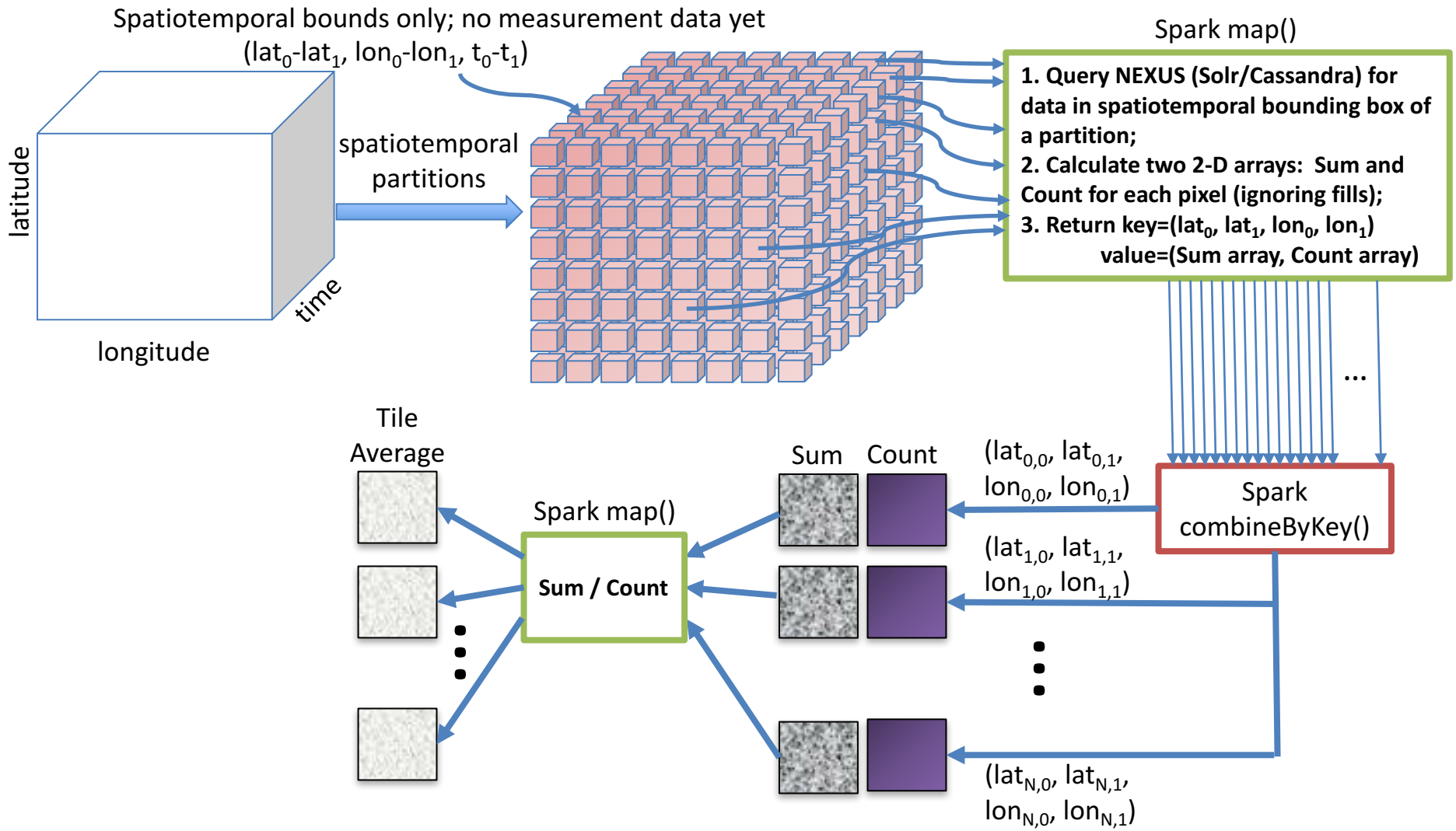

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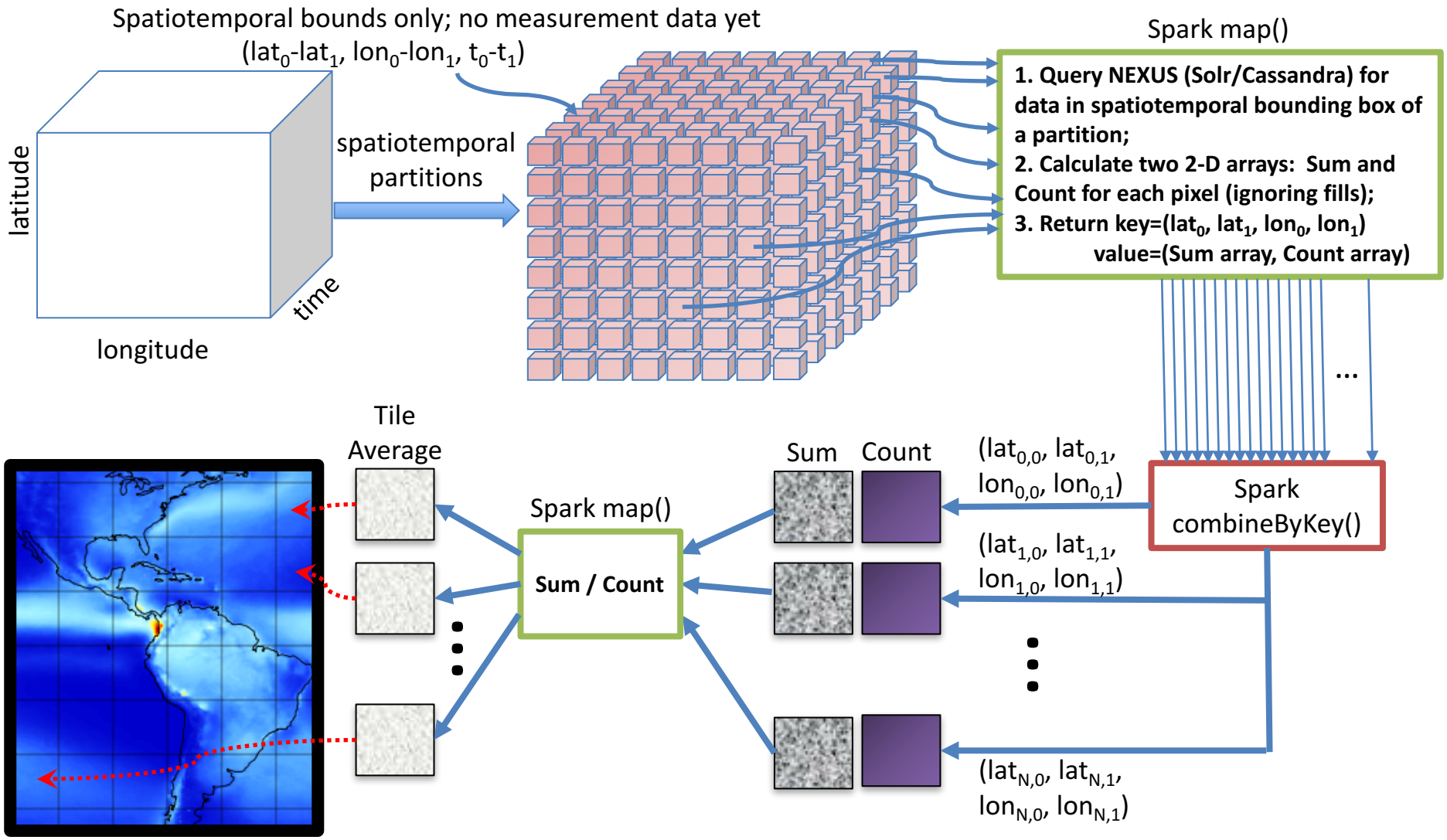


NEXUS Spark Analytics Algorithms

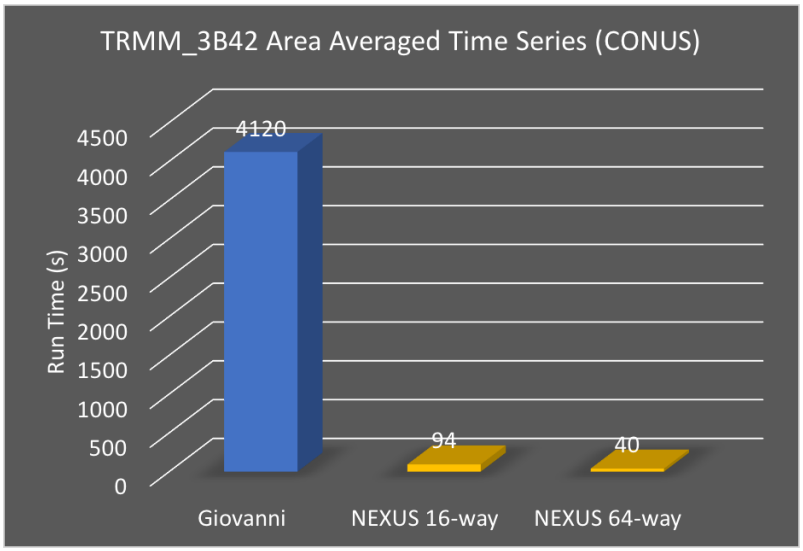
Compute statistics over time to produce a single value for each coordinate grid location.

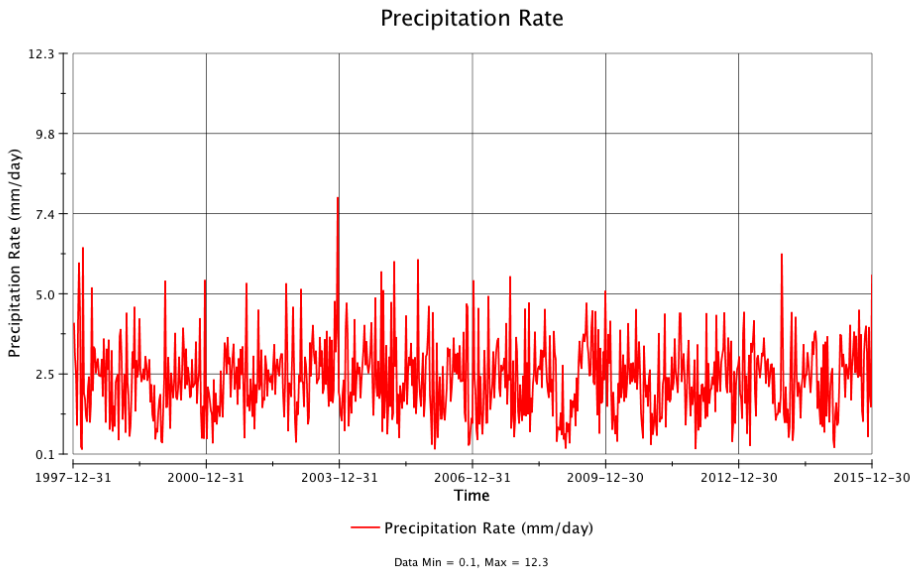
- Time-Averaged Map
  - Compute a geospatial map that averages gridded measurements over time at each grid coordinate within a user-defined spatiotemporal bounding box.
- Correlation Map
  - Computes the correlation coefficient at each grid coordinate within a user-specified spatiotemporal bounding box for two identically gridded datasets.
  - Automatically aligns the time stamps for the two datasets being compared.
- Climatological Map
  - Similar to Time-Averaged Map, but only includes measurements in the time average that are within a user specified month.
- Climatology
  - For each day-of-year (1-366) or month (1-12), computes a ”typical value” for each coordinate grid location.
  - The ”typical value” may be the result of either (1) a standard pixel mean with optional smoothing over time (e.g. 5-day average), (2) Gaussian interpolation [Armstrong and Vazquez-Cuervo, 2001], or Empirical Orthogonal Function (EOF).

Compute spatial statistics to produce a single value (or set of statistics) for each time stamp.

- Area-Averaged Time Series
  - Compute statistics (e.g., mean, minimum, maximum, standard deviation) for each time step within a user-specified spatiotemporal bounding box.
  - Optionally apply seasonal or low-pass filters.
  - Return result in ascending time order in JSON format.
- Daily Difference Average
  - Subtract a dataset from its climatology, then, for each time stamp, average the differences within a user-specified spatiotemporal bounding box.
  - Product can be used to search for anomalies compared to the historical norm.

Time Series: Comparison of Giovanni and NEXUS Performance





- NEXUS run on 8-node cluster computer at JPL running Solr, Cassandra, Spark 2.0, Mesos
- Area-Averaged Time Series over the continental United States
- Variable plotted: TRMM daily precipitation rate (TRMM_3B42_daily_precipitation_V7)
- 6,574 daily data granules covering the globe at 0.25 deg resolution with latitude +/- 50 deg and date range: 1/1/1998 – 12/31/2015 (26 GB input data volume).
- Giovanni implementation uses highly optimized compiled code based on NetCDF Operator (NCO) toolkit, but is single threaded. NEXUS is implemented in Python and parallelized with Apache Spark.
- Giovanni execution time is compared with NEXUS for 16-way and 64-way parallelism.

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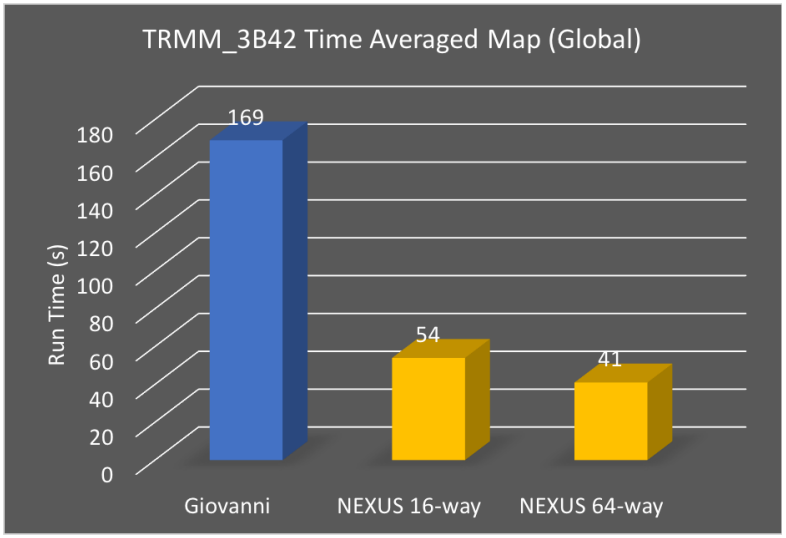
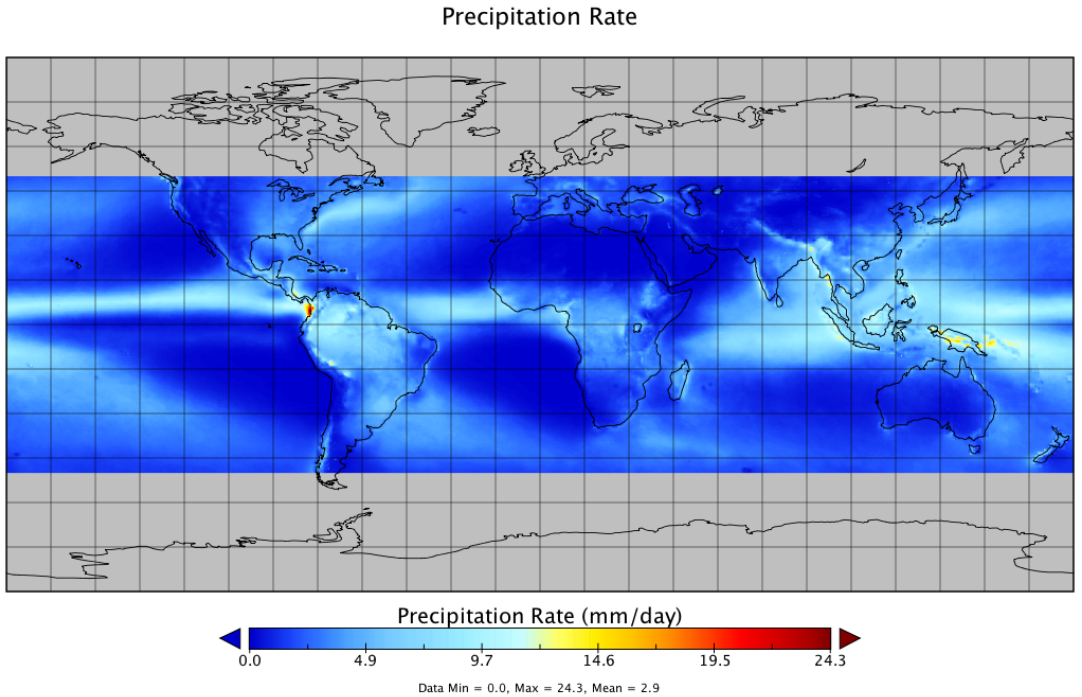
Time Averaged Map: Comparison of Giovanni and NEXUS Performance





- NEXUS run on 8-node cluster computer at JPL running Solr, Cassandra, Spark 2.0, Mesos
- Global Time-Averaged Map
- Variable plotted: TRMM daily precipitation rate (TRMM_3B42_daily_precipitation_V7)
- 6,574 daily data granules covering the globe with latitude +/- 50 deg and date range: 1/1/1998 – 12/31/2015 (26 GB input data volume).
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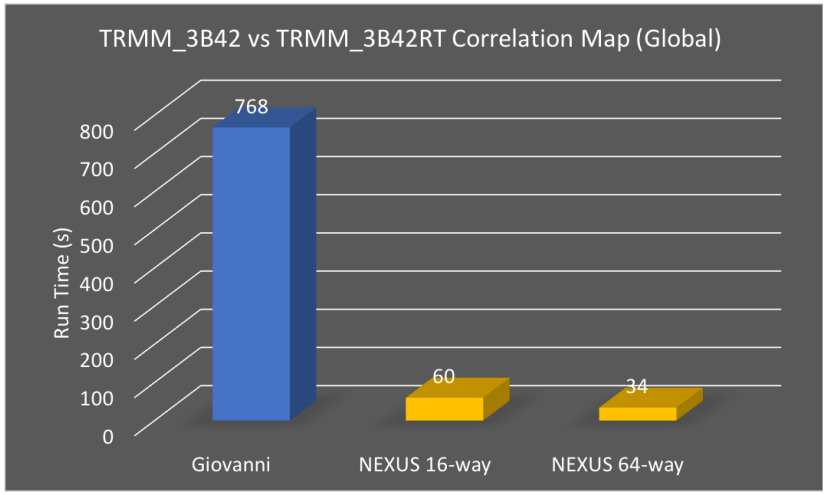
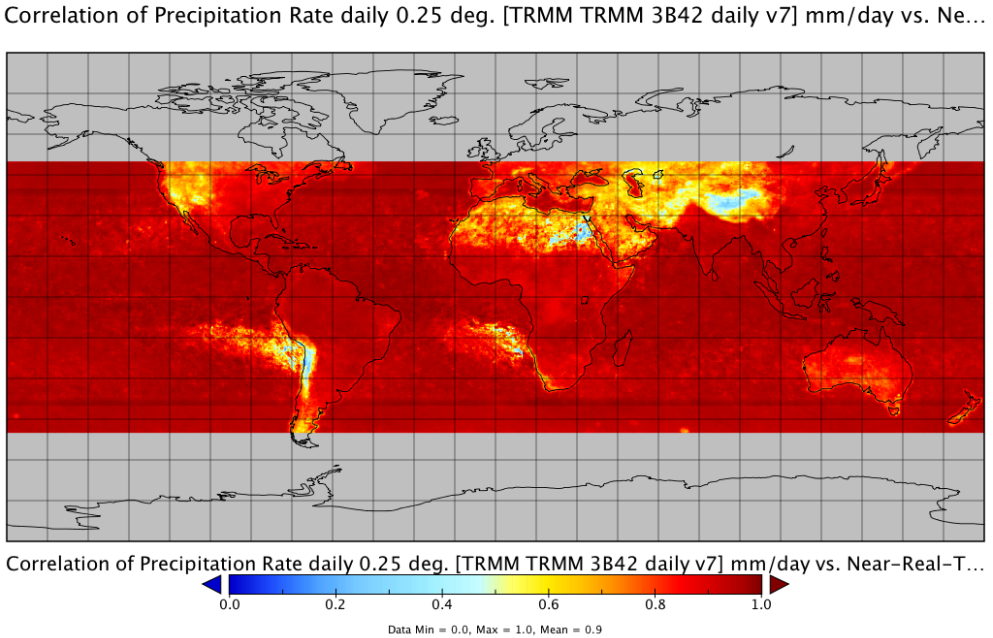
Correlation Map: Comparison of Giovanni and NEXUS Performance





- NEXUS run on 8-node cluster computer at JPL running Solr, Cassandra, Spark 2.0, Mesos
- Global Correlation Map
- Variable plotted: TRMM daily precipitation rate (TRMM_3B42_daily_precipitation_V7) vs TRMM real-time daily precipitation (TRMM_3B42RT_daily_precipitation_V7)
- 5,113 daily data granule pairs covering the globe with latitude +/- 50 deg and date range: 1/1/2001 – 12/31/2014 (40 GB input data volume).
- Giovanni implementation uses highly optimized compiled code based on NetCDF Operator (NCO) toolkit, but is single threaded. NEXUS is implemented in Python and parallelized with Apache Spark.
- Giovanni execution time is compared with NEXUS for 16-way and 64-way parallelism.

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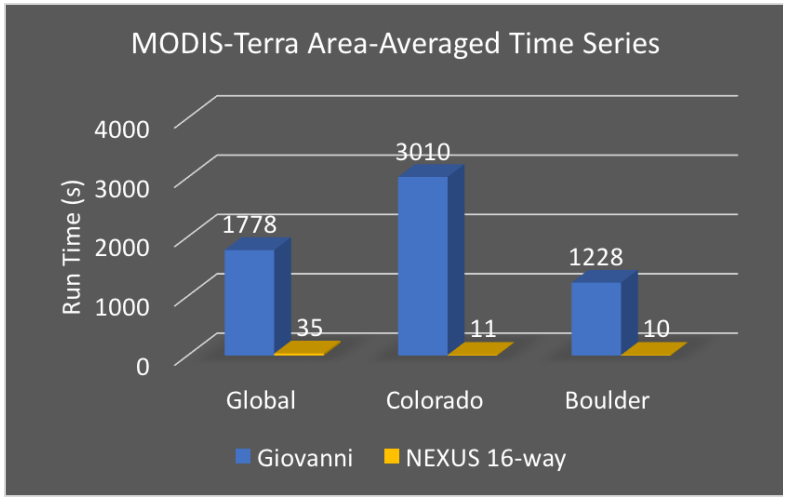
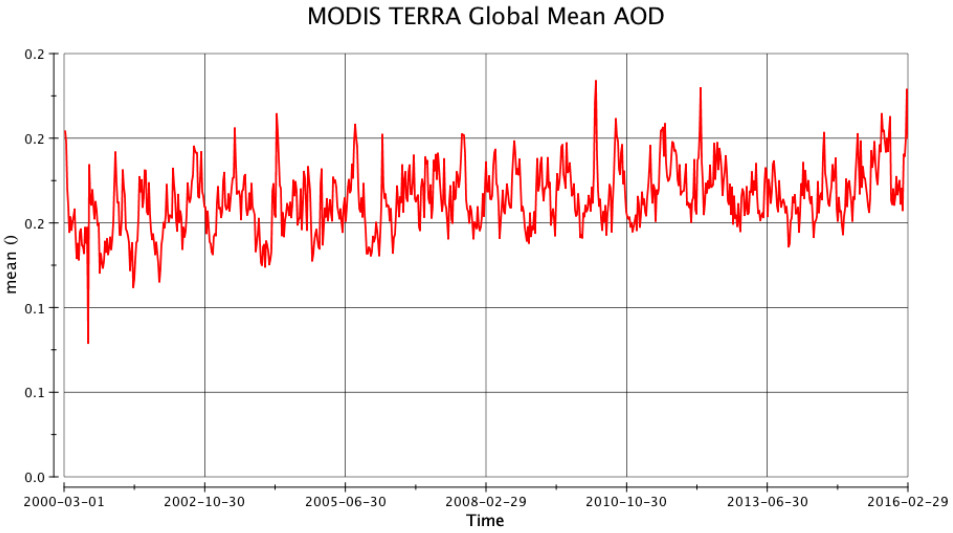
Time Series: Comparison of Global vs. Subset Performance of Giovanni and NEXUS





- NEXUS run on 6 Amazon Web Services (AWS) Cloud instances of type “i2.4xlarge” running Solr, Cassandra, Spark 2.0, Mesos
- Area-Averaged Time Series over the indicated spatial subset (Global, State, City)
- Variable plotted: MODIS-Terra Aerosol Optical Depth (AOD) 550 nm dark target
- 5,789 daily data granules covering the globe at 1 deg resolution with date range: 3/1/2000 – 2/29/2016 (3 GB input data volume).
- Giovanni implementation uses highly optimized compiled code based on NetCDF Operator (NCO) toolkit, but is single threaded. NEXUS is implemented in Python and parallelized with Apache Spark.
- Giovanni execution time is compared with NEXUS for 16-way parallelism.
- NEXUS has superior performance for subsetting operations, as indicated by the ~300x speedup for the Colorado subset.

Summary

- Spark is a good choice for many algorithms, but consider inter-process communication.

- Benchmark NEXUS speedup factors over Giovanni
  - ~300x speedup for 16-year area-averaged time series of Moderate Resolution Imaging Spectroradiometer (MODIS-Terra) Aerosol Optical Depth (AOD) at 1 degree resolution for Colorado with NEXUS running on 6 “i2.4xlarge” Amazon Web Services Cloud instances with Spark configured for 16-way parallelism.
  - ▪ ~100x speedup for area-averaged time series of daily precipitation rate for the Tropical Rainfall Measuring Mission (TRMM with 0.25 degree spatial resolution) for the Continental United States over 18 years (1998 - 2015) with 64-way parallelism on an 8-node cluster computer at JPL.
  - ▪ ~4x speedup for 18-year (1998 - 2015) TRMM daily precipitation global time averaged map (64-way parallel).
  - ▪ ~22x speedup for 14-year (2001 - 2014) global map of correlation between TRMM daily and real time precipitation rate (64-way parallel).
  - For small datasets, compiled, optimized, single- threaded executables like the NetCDF Operators (NCO) toolkit used in Giovanni work well.
  - For large data analytics, NEXUS significantly outperforms due to its ability to horizontally scale in a cloud computing environment.

- Data tiling recommendations
  - Tiling data into chunks yields significant performance benefits over monolithic global granule files, particularly for regional subsets.
  - For calculations on small subsets, use a small tile size.
  - For global or near-global calculations use larger tiles to optimize data read performance.

- Choose your scheduler carefully
  - In our benchmarks, Mesos consistently yielded 2-4 times faster run times compared to YARN.
  - YARN included with Spark distribution; Mesos is a separate package.

- JPL and NASA support open source development
  - NEXUS is an open-source big data analytics framework, available at: *https://github.com/dataplumber/nexus*