VELaSSCo overview : Big Data for Computational Engineering

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Goal of VELaSSCo

Visual Analysis

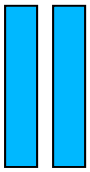
for **E**xtremely **La**rge-**S**cale

Scientific **Co**mputing

The Research leading to these results has received funding from the European Community's Seventh Framework Programme (FP7/2007-2013)

Goal of VELaSSCo

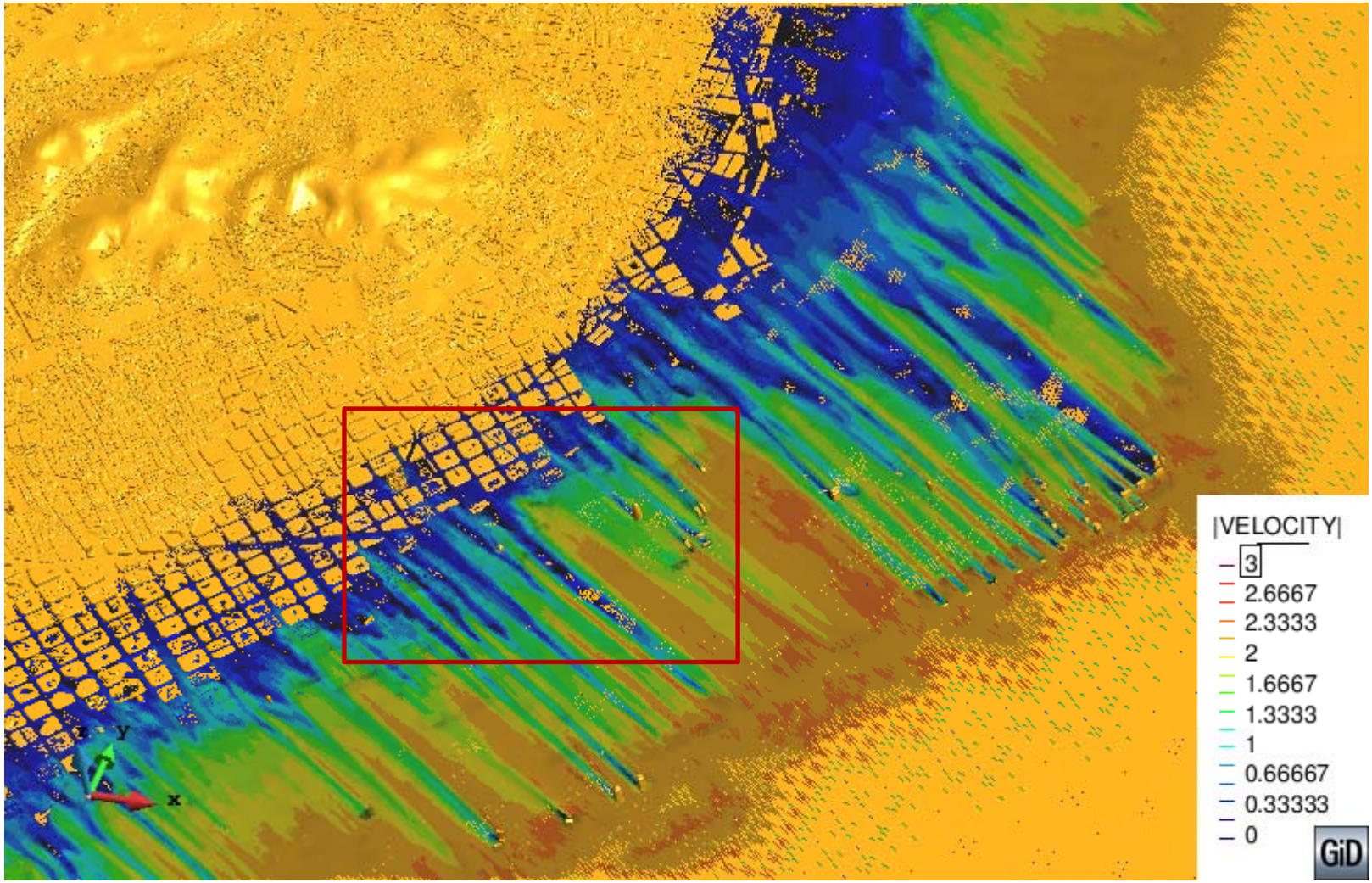
*The **Vision** of **VeLASSCo** is to provide new visual analysis methods for large-scale simulations serving the petabyte era and preparing the exabyte era by adopting Big Data tools/architectures for the engineering and scientific community leveraging new ways of in-situ processing for data analytics and hardware accelerated interactive visualization.*



- Integrate post-process analytics in a Big data framework embedded in the HPC, where the data is being calculated or stored.

Wind flow around buildings @ 40 m

- 8m resolution: 100 M tetrahedrons



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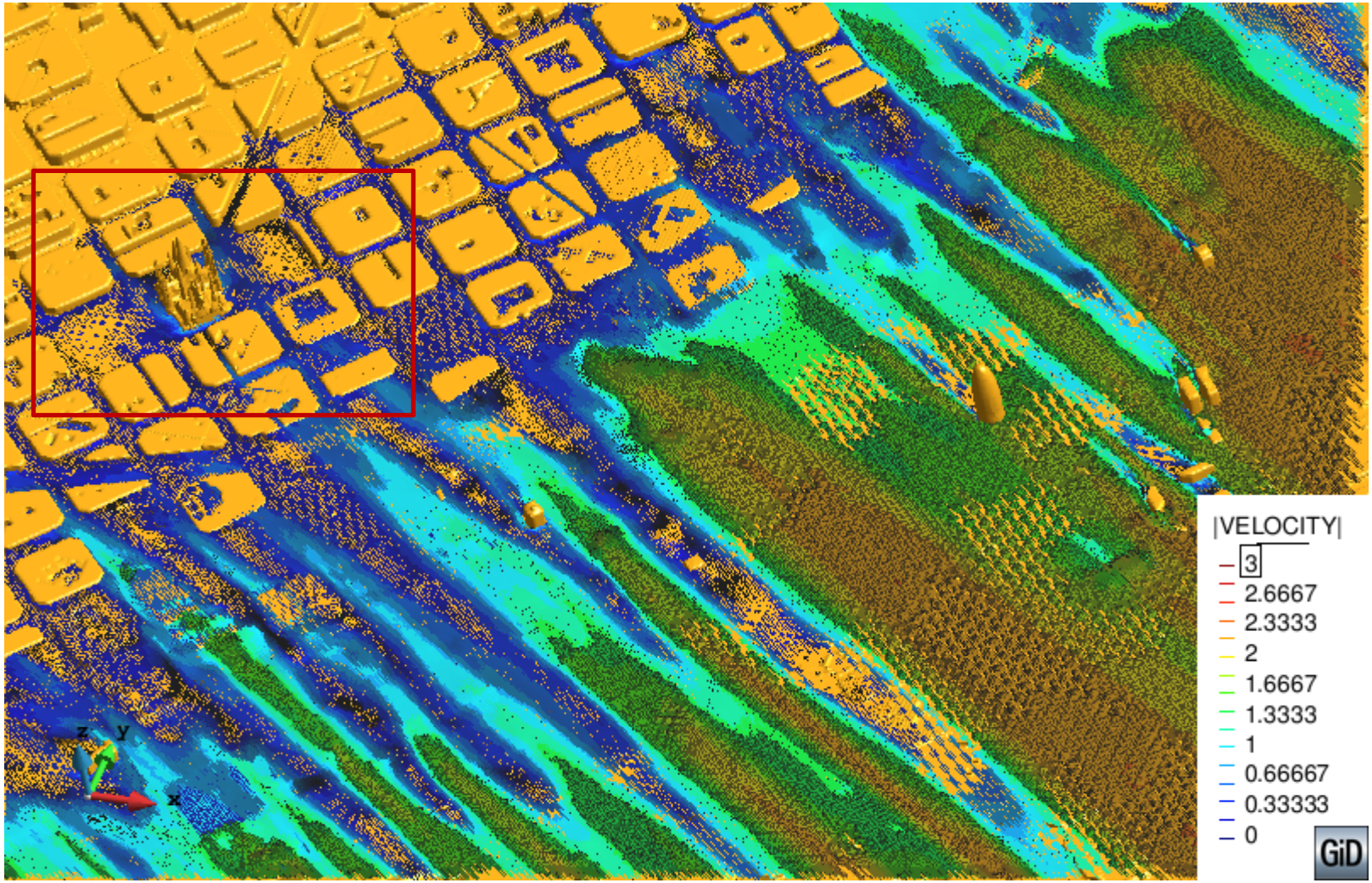

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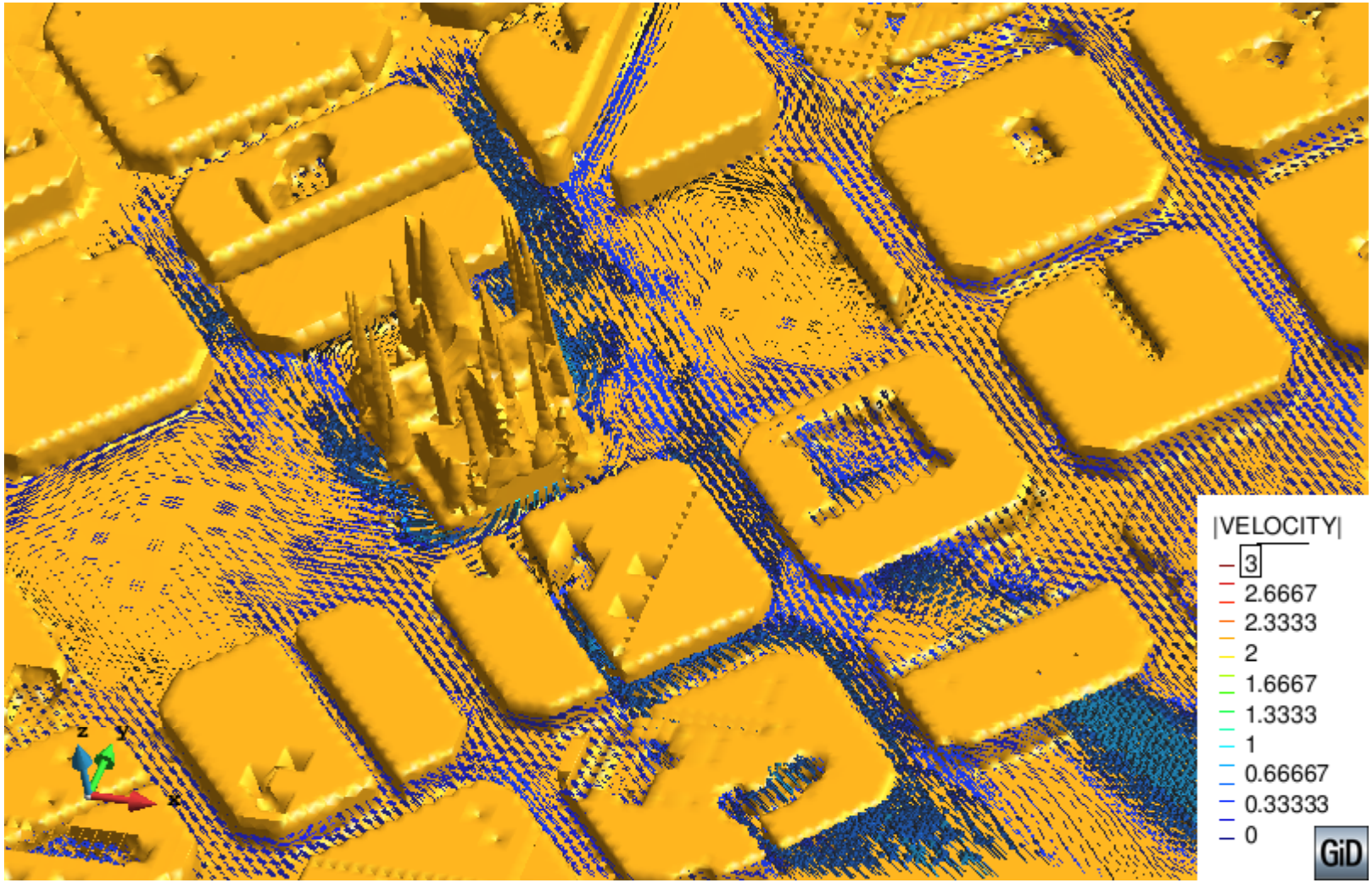

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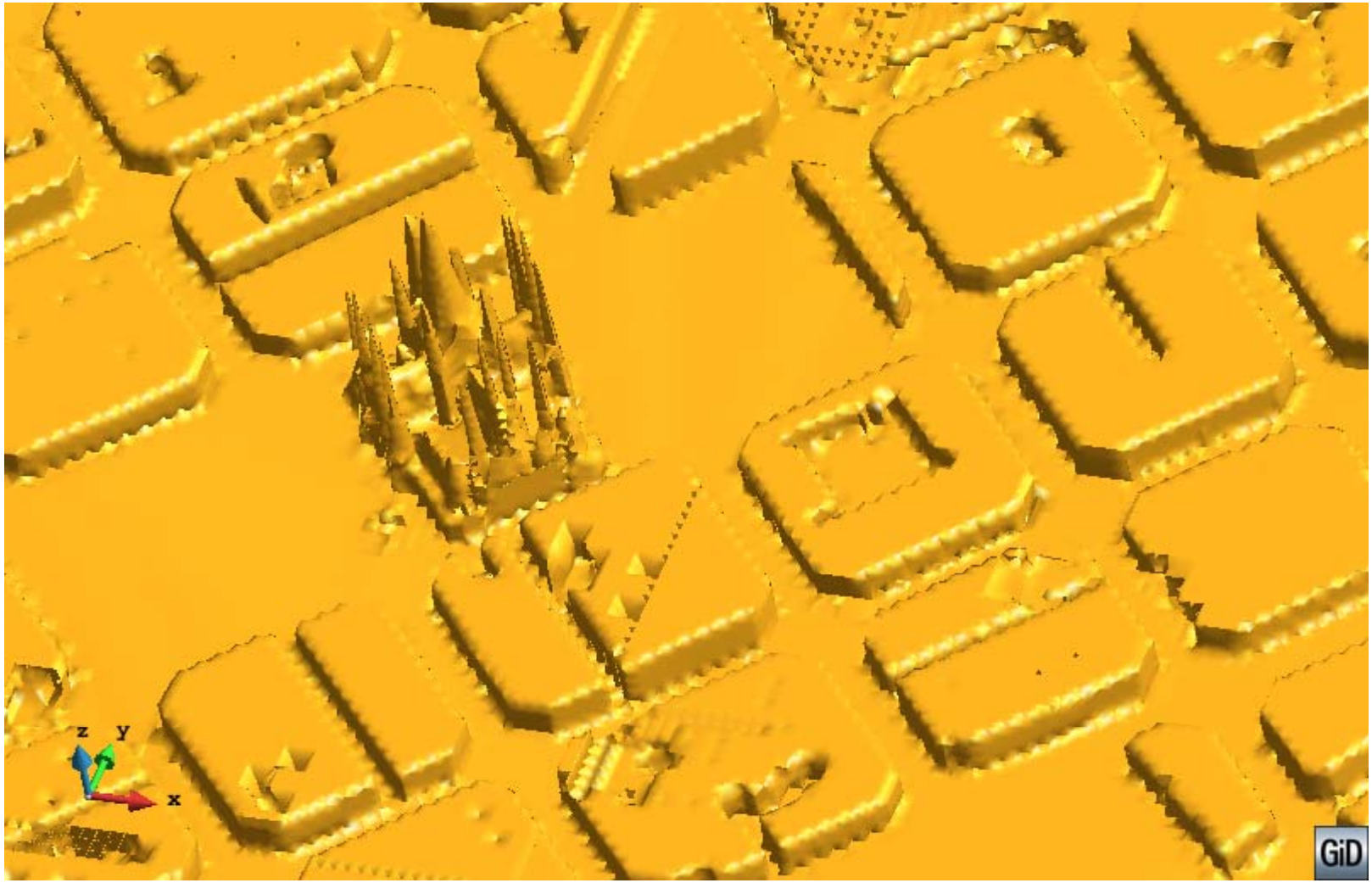
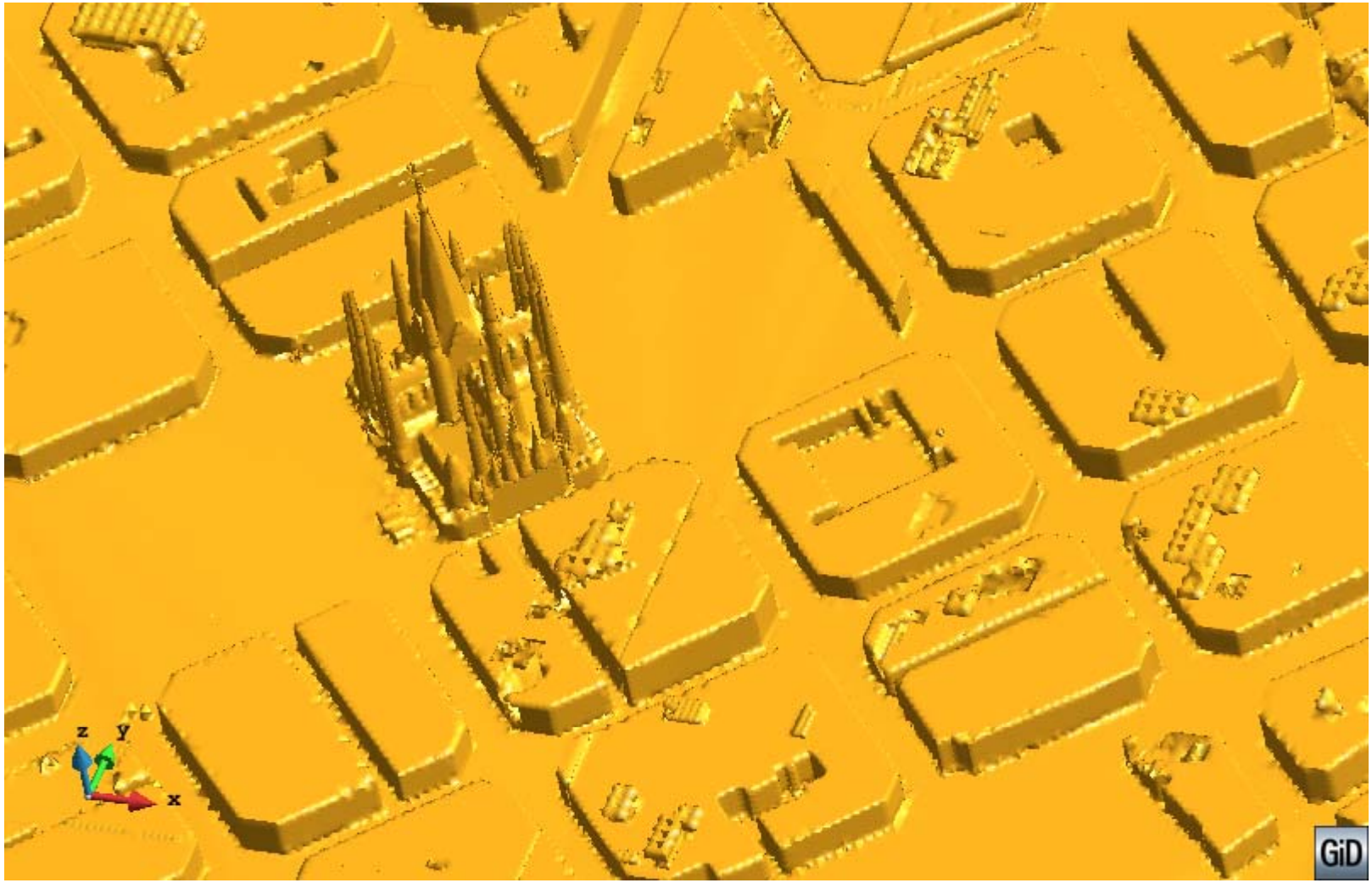


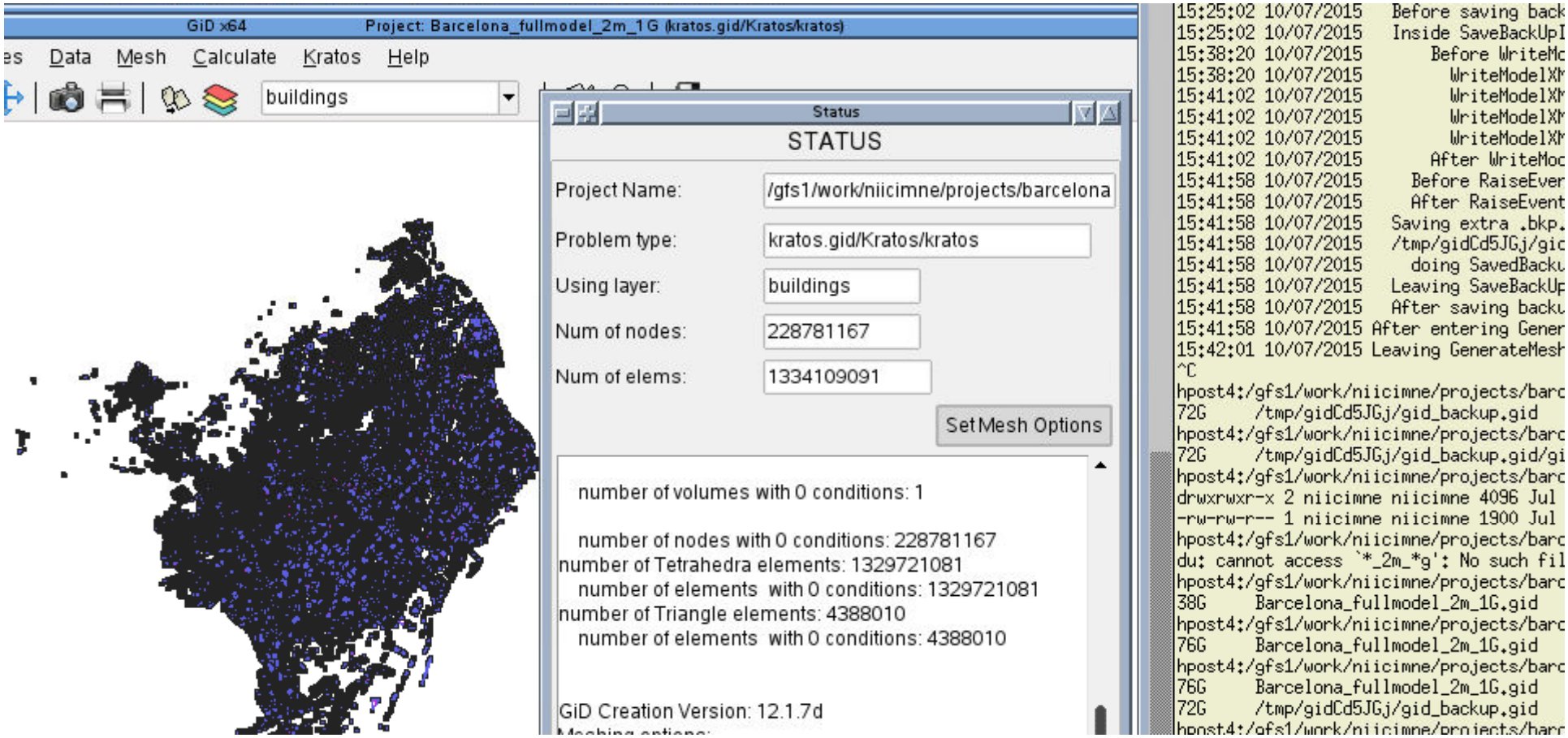
Wind flow: traditional post-process limits

- 4m resolution: 340 M tetrahedrons



1.3 billion tetrahedrons

- 2m resolution: several difficulties

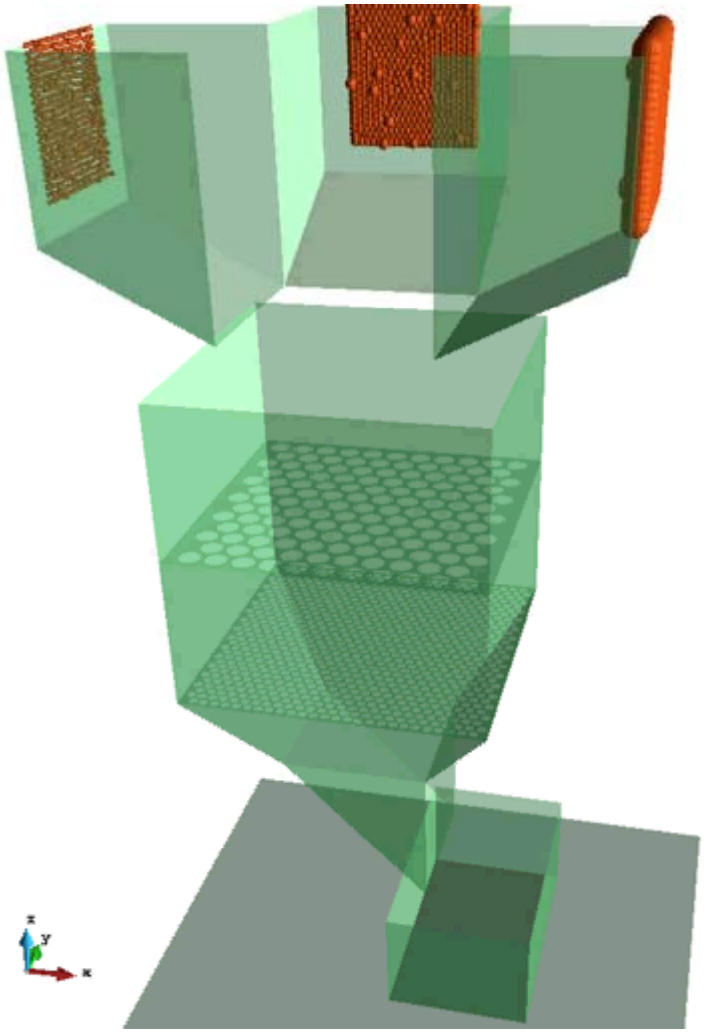


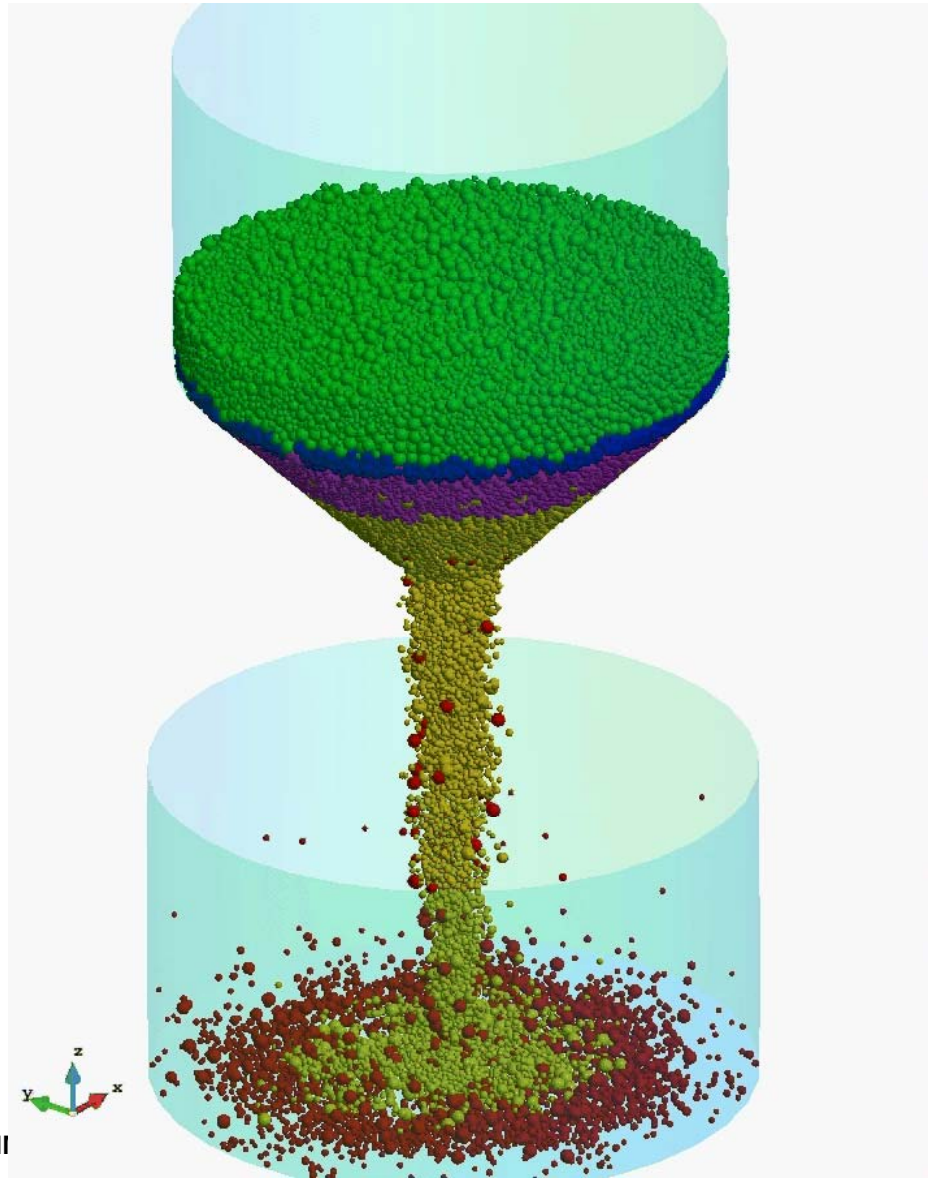
Remote cluster

- Barcelona 2m resolution: 1.3 billion tetrahedrons (2015)
  - 72 GB mesh only
  - 1 time-step (pressure, velocity) ~ 9 GB
  - 100 time-steps = 972 GB = 55 h @ 5MB/s
  - 1 time-step (distance, partition index, pressure, reaction, velocity) ~ 22 GB
-

Motivation

- Particle methods





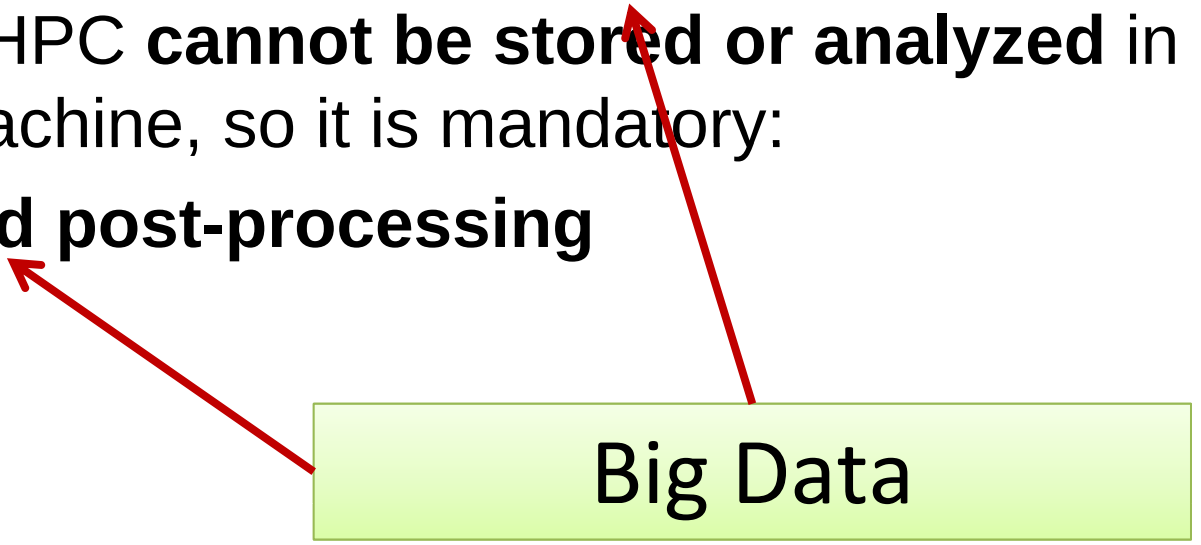
Target data

- Estimated data size in a couple of years

	DEM	FEM
Total size	**50 GB → 1 PB**	**30 GB → 50 TB**
Partitions		1 → 10,000
Particles / elements	10 million	8 million → 1 billion
Time-steps	1 billion	40 → 25,000
Variables per node	10 variables	2-8 scalars, 1-2 vectors, ?1 tensor?

VELaSSCo approach

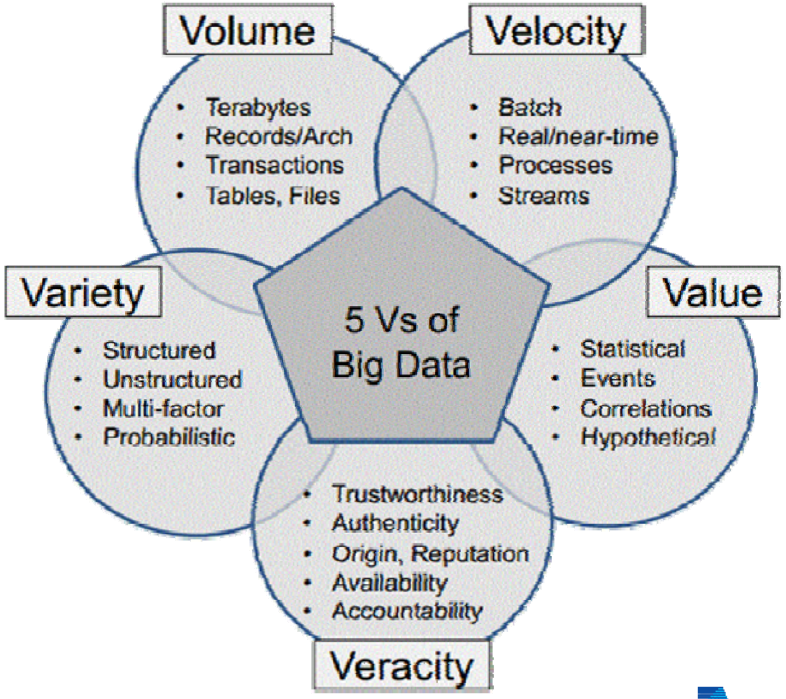
- Nowadays the **huge amount of data** provided by the solver in HPC **cannot be stored or analyzed** in one single machine, so it is mandatory:
  - **Distributed post-processing**



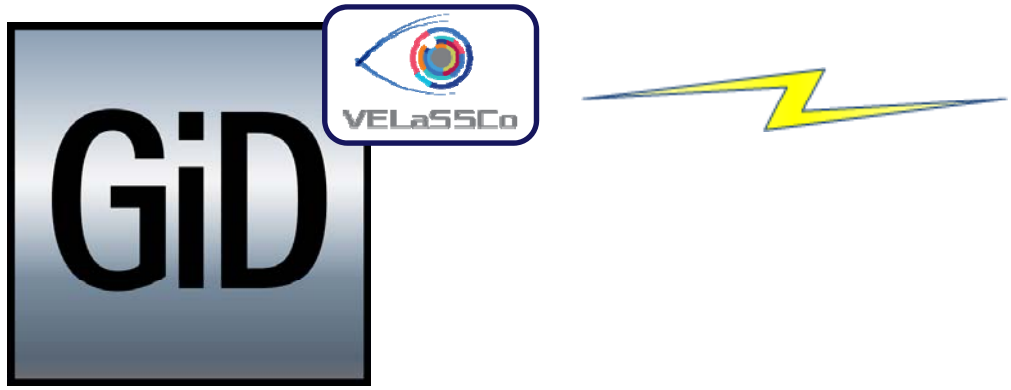
- Integrate post-process analytics in a Big Data framework embedded in the HPC, where the data is being calculated.

Big Data for what

- Store data in a distributed way: robust, redundancy
- Perform analytics in a distributed way:
  - Post-process = extract information + visualize
- High scalability



GiD point of view



- User will:
  - Launch GiD
  - Connect to VELaSSCo platform
  - Select model
  - Interact with a (simplified) version
  - Request results view: get a (simplified) view, while full-detailed view is received

Solver's point of view

- Output the results to the platform
- Using GiDpost:
  - GiD_PostInit(VELaSSCo, username, pass)
  - GiD_fOpen(…)
  - GiD_fWrite(…) // write mesh & results
  - GiD_fClose()
  - GiD_PostDone()

Contents

- VELaSSCo architecture
- Hadoop framework
- Current development status

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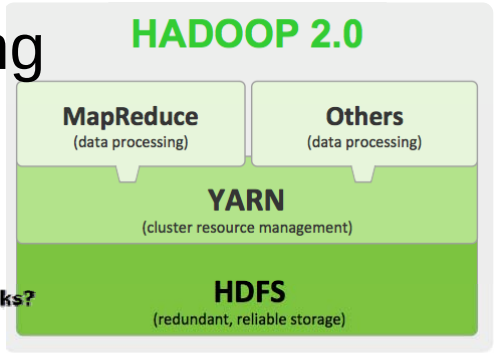
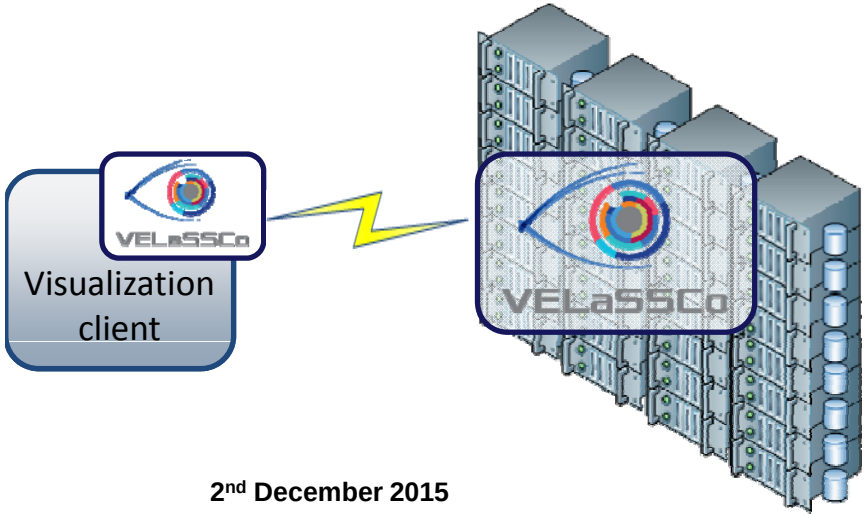
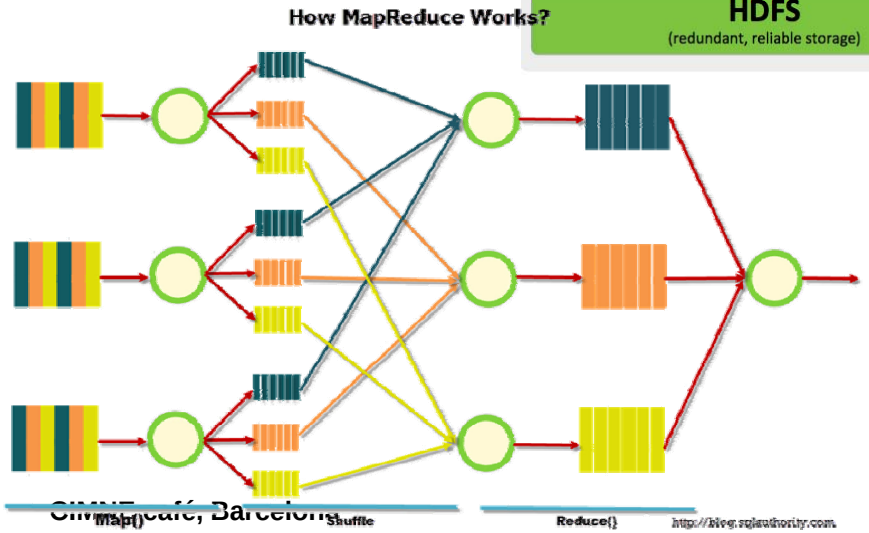
VELaSSCo key-points

- Based on open source Hadoop
  - and also on Jotne's EDM
- Analyze the data where they are: in the HPC
- Post-process algorithms are distributed using Yarn and MapReduce
- Visualize on local machine







VELaSSCo architectures

- Two versions:
  - OpenSource: using Hadoop, HDFS, Hbase, YARN
  - CloseSource: using JOTNE's EDM
- Visualization client communication using Thrift
- Data ingestion using Apache flume:
  - From files or running simulation
- Runs on an HPC with:
  - Local storage on some nodes: Vnodes
  - Dedicated queue for Vnodes
  - Vnodes can also be used to calculate when idle

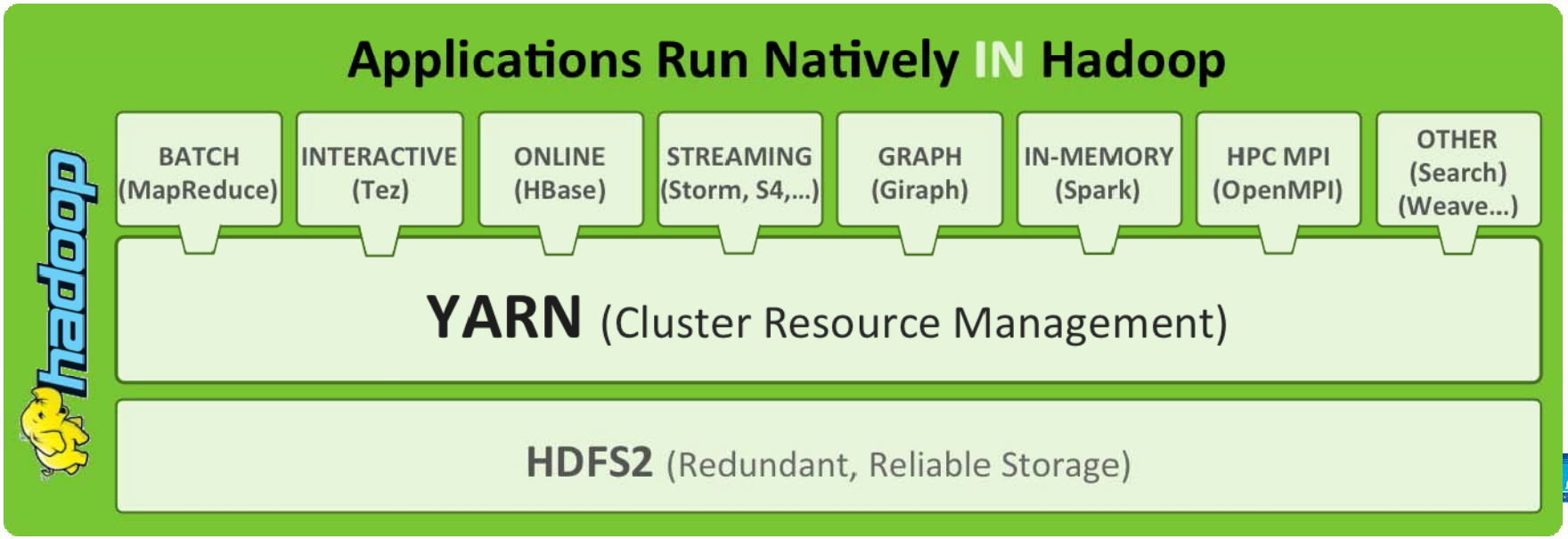
Hadoop

- “Apache Hadoop is an **open-source** software framework written in **Java** for **distributed storage** and distributed **processing** of very large data sets on computer clusters built from commodity hardware.” (Wikipedia)

- Core blocks:
  - HDFS: Hadoop Distributed File System
  - YARN: Yet Another (computing) Resource Manager, application scheduler
  - MapReduce: programming model
  - Common: tool-set, scripts for extensions

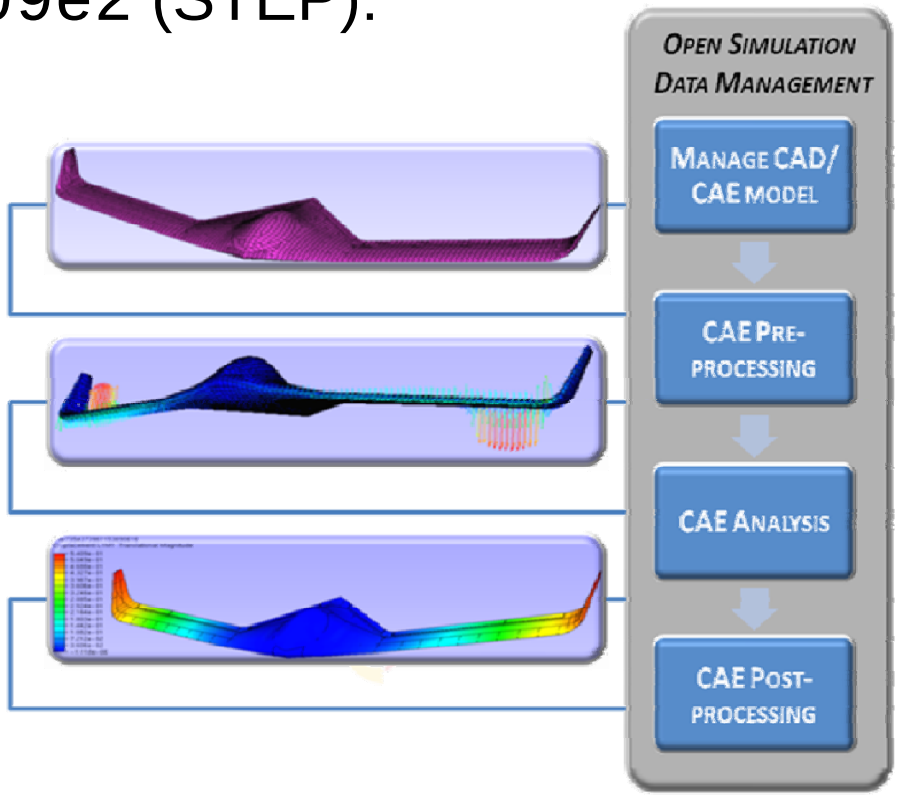
Hadoop

- Extensions:
  - Hbase: distributed (table) database
  - Hive: data access, query and analysis language over Hbase / HDFS, SQL-like
  - Spark: in-memory MapReduce engine also over YARN/HDFS



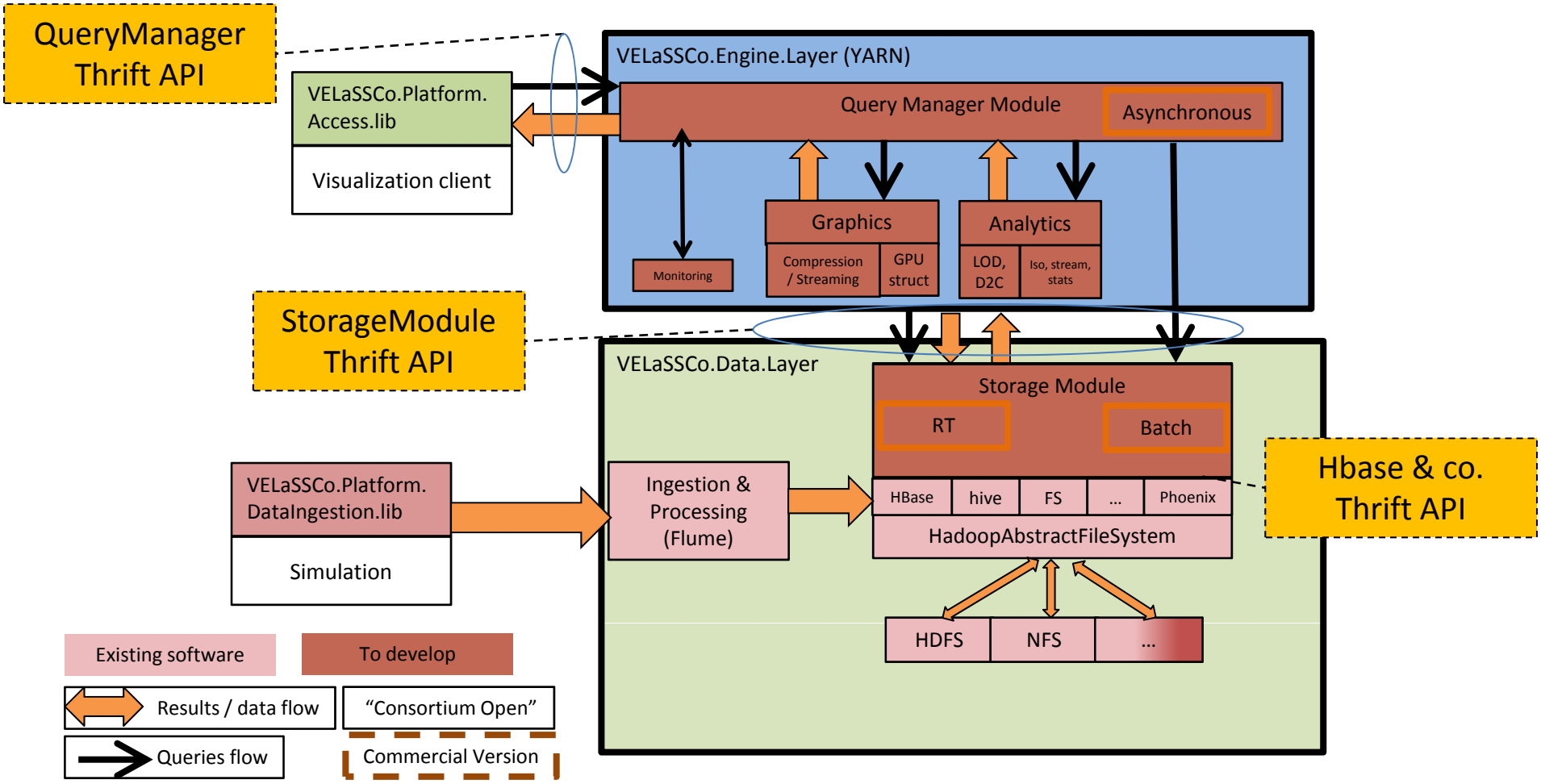
JOTNE's EDM

- Express Data Manager
- Open Simulation Data Management (SDM) using ISO standards, ISO 10303-209e2 (STEP):
  - Object Oriented DB
  - Conceptual models



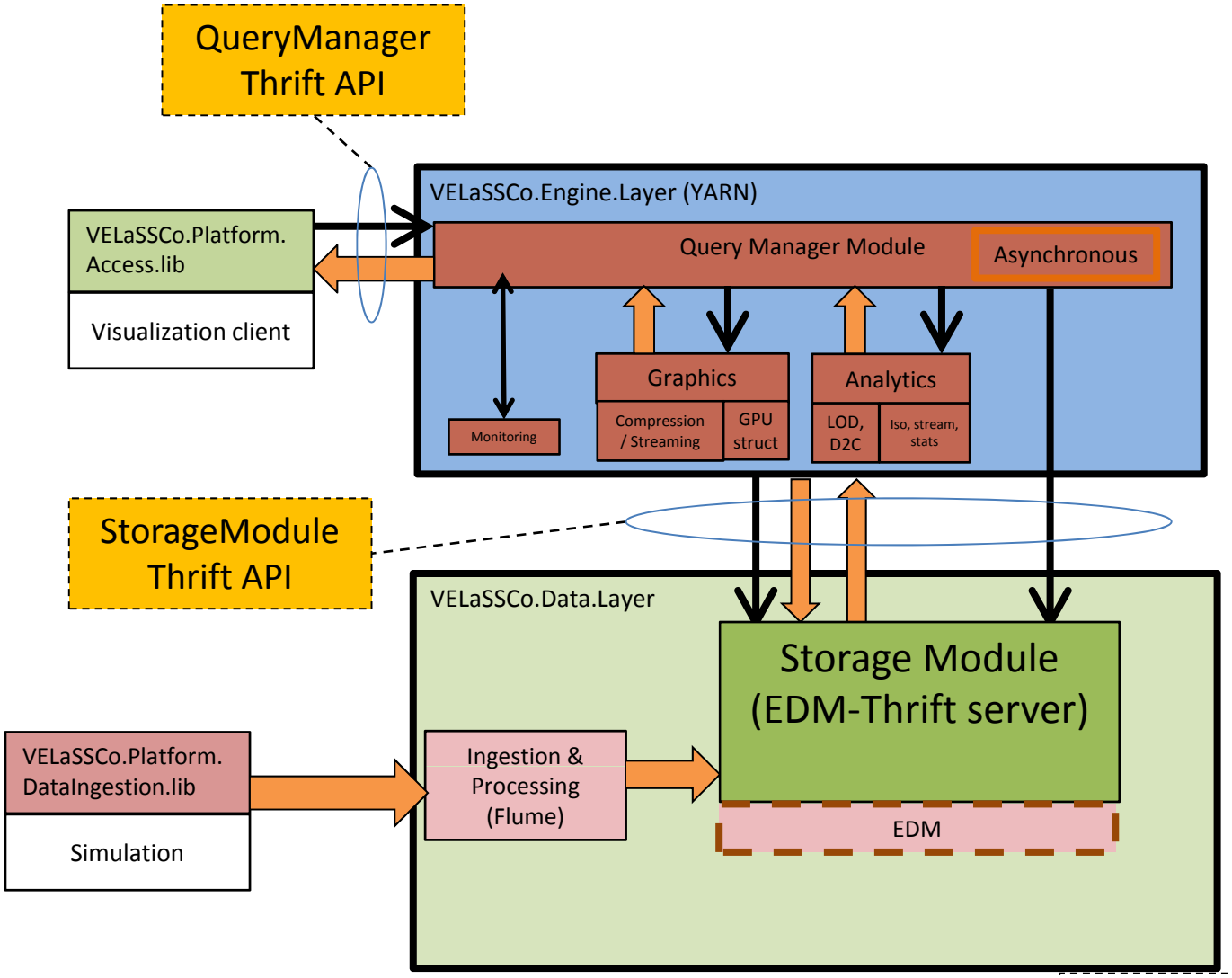
EXPRESS Data Manager
OpenSimDM™

VELaSSCo OpenSource architecture



Oslo 2015.06.16-19

VELaSSCo CloseSource architecture

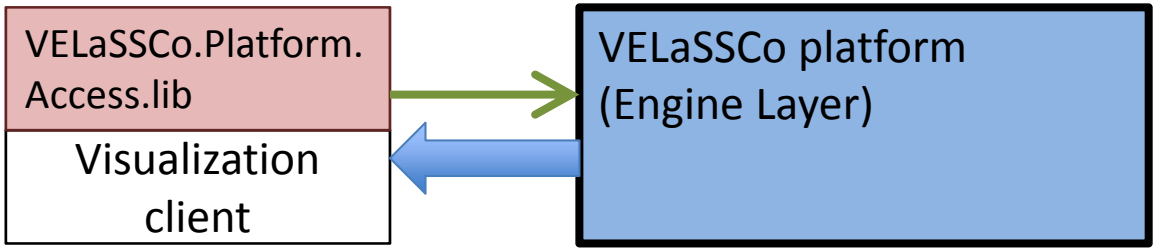


2015.11.18

VELaSSCo platform

- Engine Layer a stand-alone application with:
  - The Query Manager Module as thrift server
  - Graphics as CLI program and later as library
  - Analytics using: Hive, YARN MapReduce/… later eventually with Spark
  - Communicates with CLI and Thrift with Data Layer (Storage module)
- Data Layer:
  - Storage Module as thrift server
  - Will connect to Hbase (using CURL or Thrift) or EDM thrift server

User interaction: Vqueries



- User interaction generates VELaSSCo-queries
  - Show me the model
    → getBoundaryMesh() + RenderBoundaryMesh()
  - Visualize sea surface with velocity vectors
    → getIsoSurface() + interpolateResult(velocity) + RenderData()
  - Traveling from point A to B (*streaming version*)
    → loop of getMeshData(BoundingBox/UserView)
  - For costly queries:
    →doQuery(simplified model) + doQuery(full model)

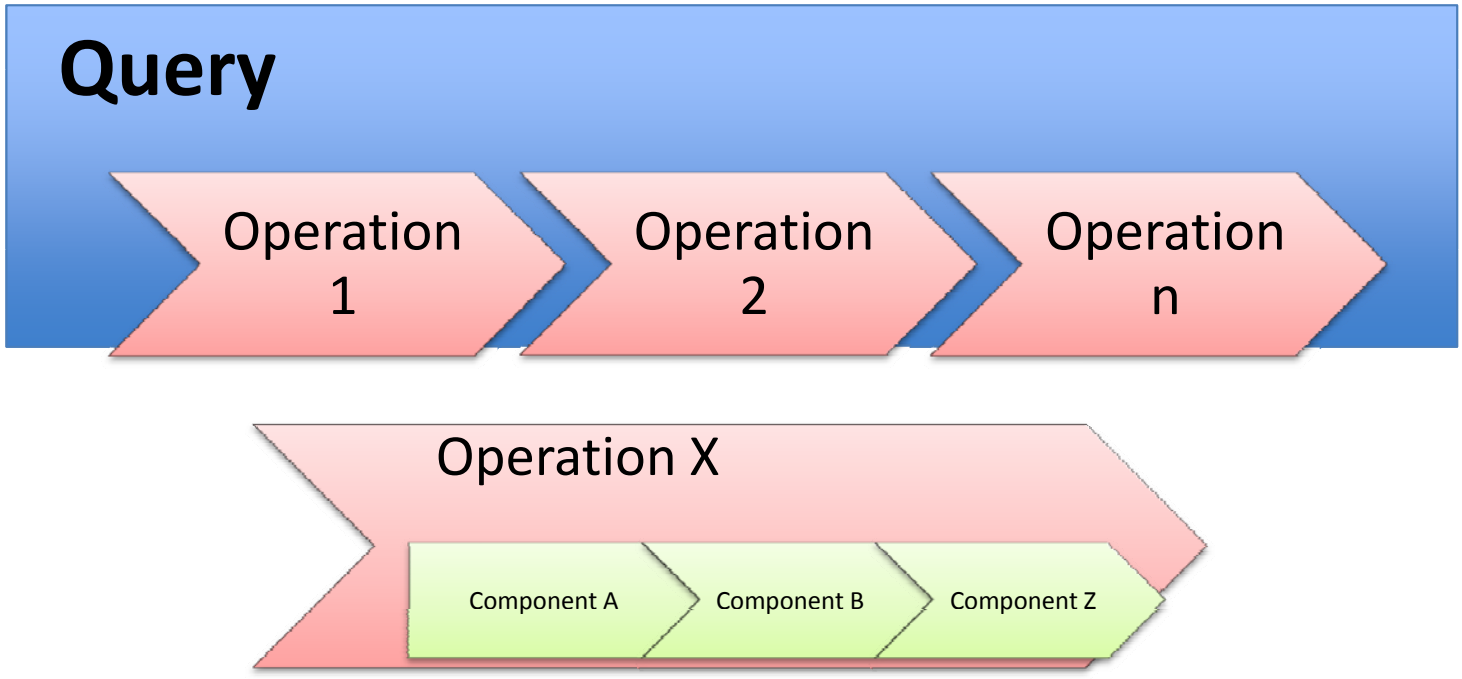
→ Communication using Thrift

VELaSSCo-queries families

- **Session Queries (SQ):** User connection, model selection, thumbnails and validation status
- **Direct Result Queries (DRQ):** Get mesh and results information from the data without analytics, such as: get result of node or element number n
- **Result Analysis Queries (RAQ):** Postprocess operations on data (data analytics), such as: calculate skin mesh, streamlines, isosurface or cut
- **Data Ingestion Queries (DIQ):** Insert data in the Data Layer, and merge into a Hbase data table

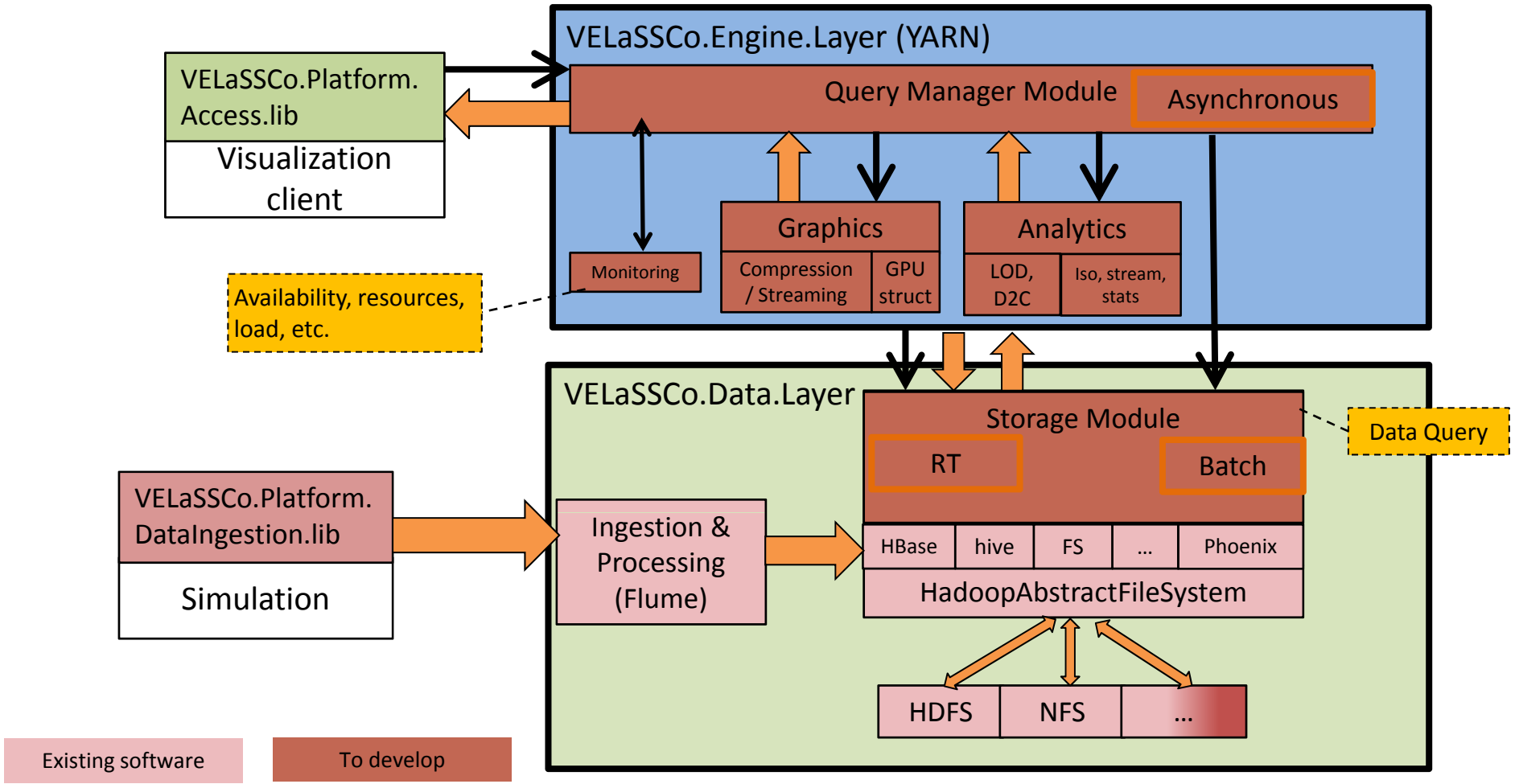
Development: Vqueries

- VQuery decomposition into operation and components:



- Allows to monitor the progress of the platform

VELaSSCo OpenSource architecture



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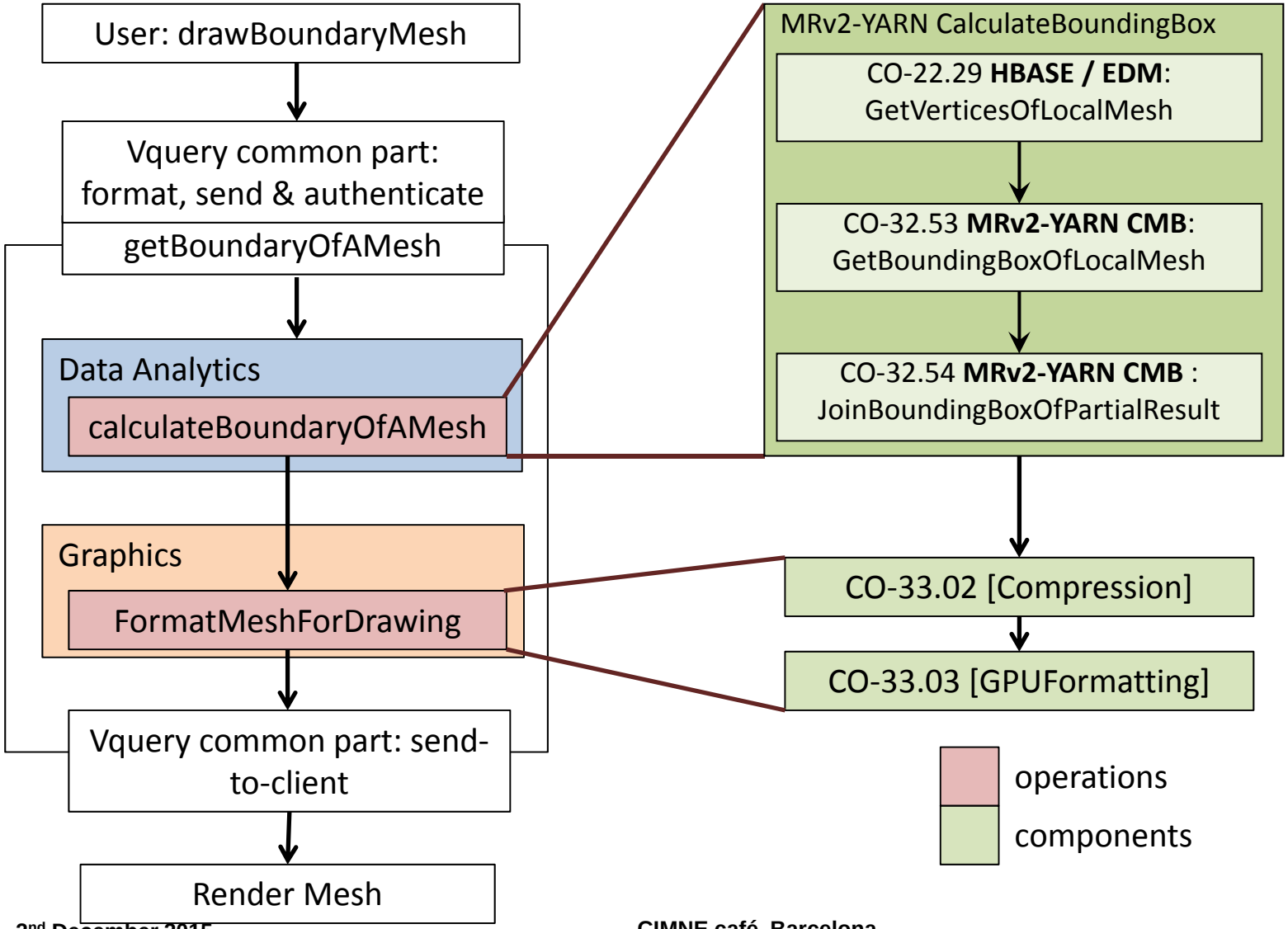
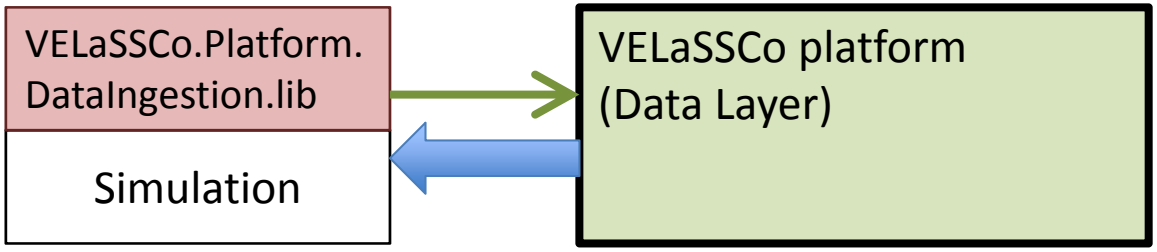
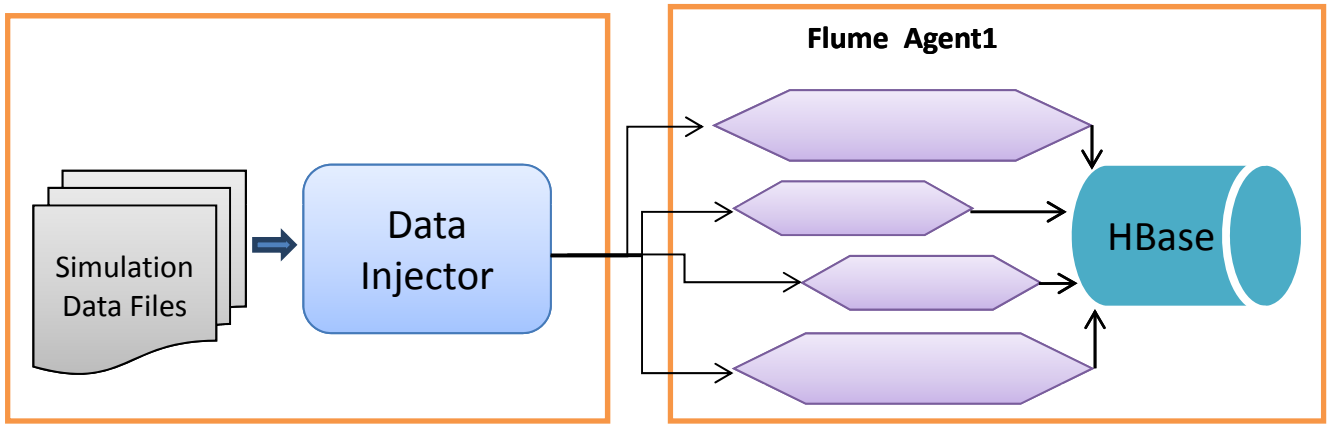
Vquery example: getBoundaryOfAMesh()



Data Ingestion



- Through Flume agents, as RESTfull service
- Injector applications using Hbase-thrift
- From already existing data
- From a running simulation: using GiDpost



Development plan

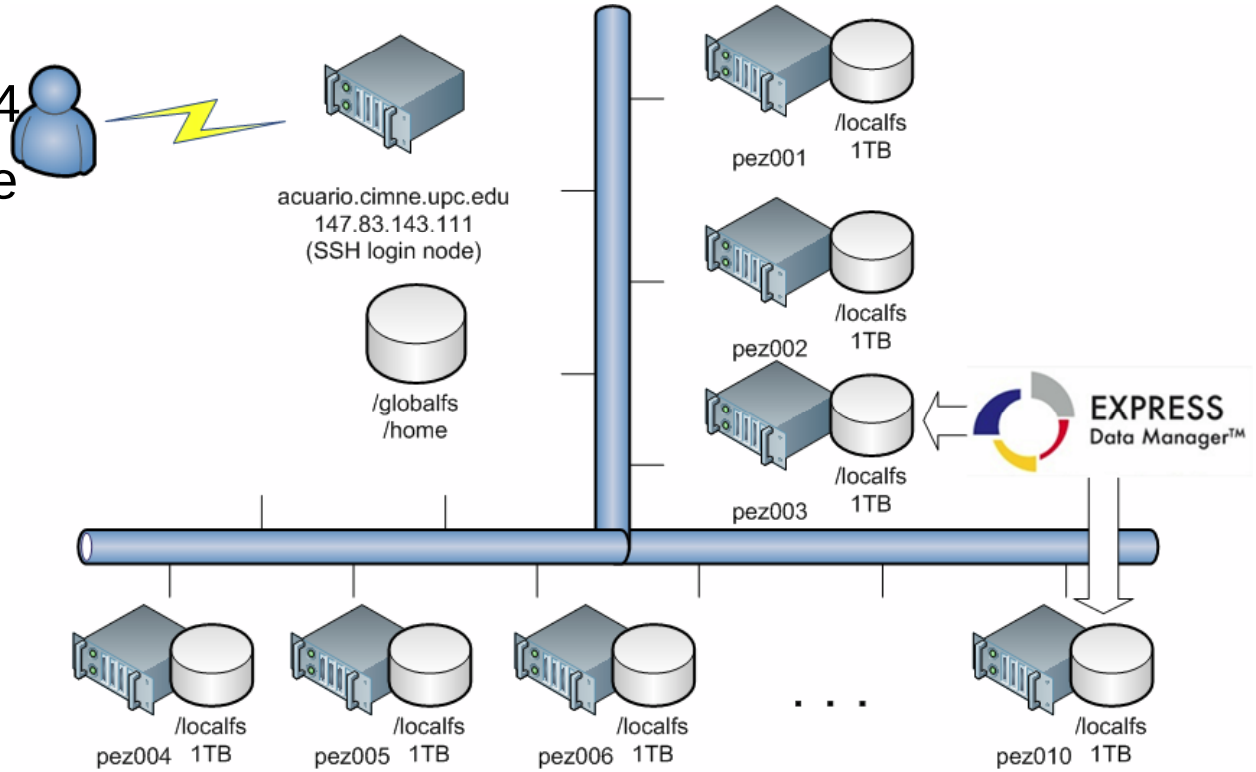
- First prototype with simple queries:
  - User login, model information, summaries,
  - Mesh view: surfaces, skins,
  - Results views: results on nodes,
  - Analytics:
    - Bounding box, boundary/skin, point interpolation, discrete 2 continuum transformation, Coarser model
    - Cut planes with interpolation (segments),
    - (Isosurfaces with interpolation)
  - Visualization:
    - On demand
    - 1-LOD

Development plan

- Final prototype with complex queries:
  - Analytics:
    - Isosurfaces with interpolation
    - Results statistics, stream lines,
    - Bspline representation for lines, surfaces, ?volumes?
  - Pre-computed queries: detection of most used ones
  - Visualization:
    - Navigation, streaming
    - Several LOD

Done so far

- Ingestion: almost done
- Few data information retrieval and analytics queries
- Deployed in acuario: 8 + 2 nodes
  - 2 x QuadCores E5410 @ 2.33 GHz
  - RAM: 16 GB
  - Infiniband DDRx4
  - 1TB local storage



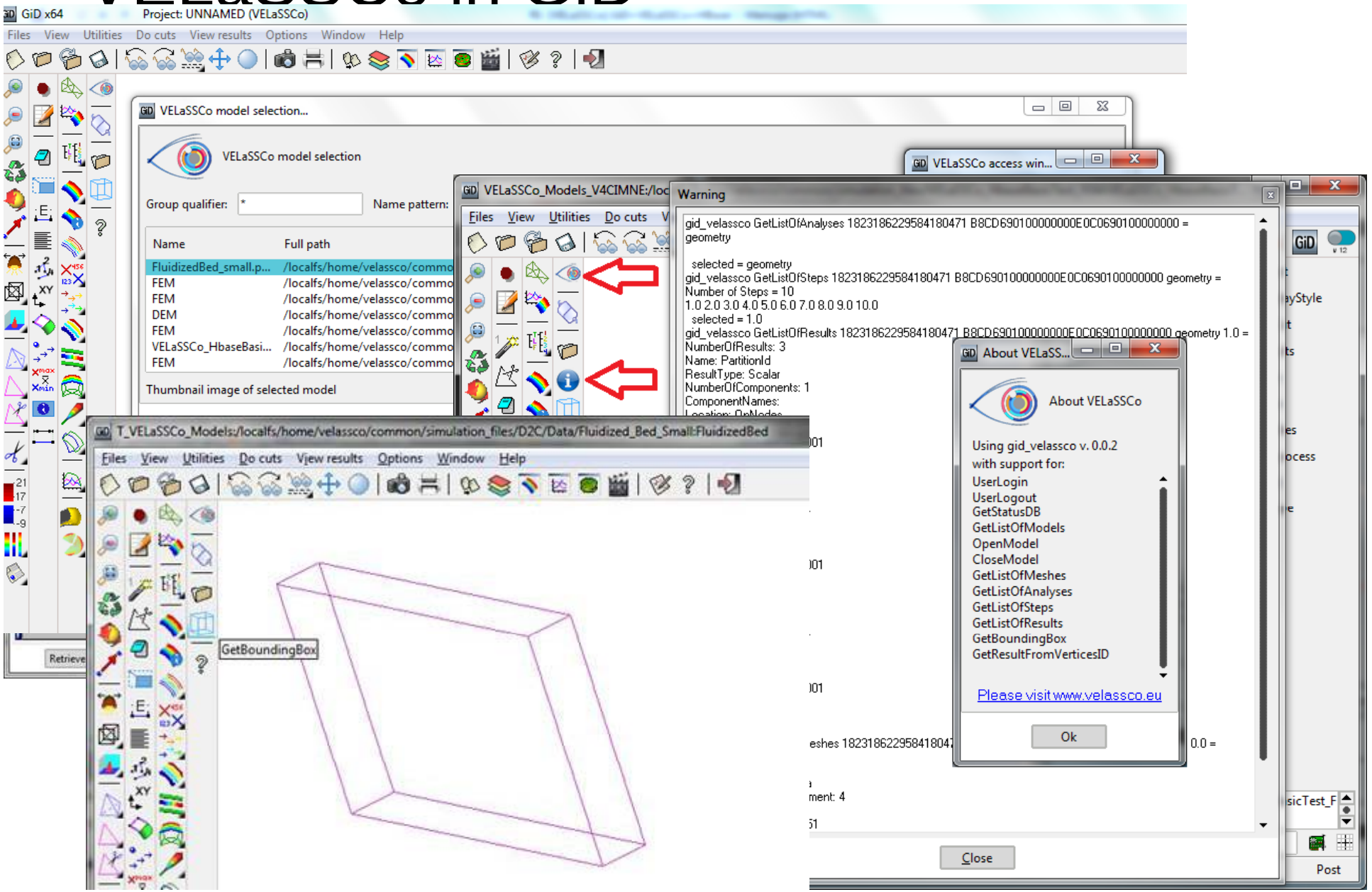
Some preliminary numbers (Hadoop)

- Ingestion:
  - Current speed is 1.4 MB/s (Hbase-thrift), 2.6 MB/s (EDM-thrift)
  - Initial speed is 122 KB/s, 523 KB/s (Hbase-REST)
- Information:
  - Getting model information: 34,406 rows in 3.7 s.
- GetBoundingBox (MapReduce):
  - 24 M tetrahedra in 128 sub-domains:
    - Job time: 38 s. / wall clock: 63 s.
  - 485 M particles in 40,801 steps:
    - Job time: 334 s. / wall clock: 346 s.

Development status

- First prototype:
  - ready by December / January
  - deployed in UEDIN's cluster using 20 nodes with:
    - 2 x Xeon E5-2630v3 2.4 GHz = 16 cores
    - 64 GB RAM
    - 700 GB local storage = 14 TB → Project goal 200 TB
  - Evaluation event at mid January
- Revision of design and architecture
- Final prototype September 2016

VELaSSCo in GiD



Visual Analysis for Extremely Large-Scale Scientific Computing

Thanks for your attention

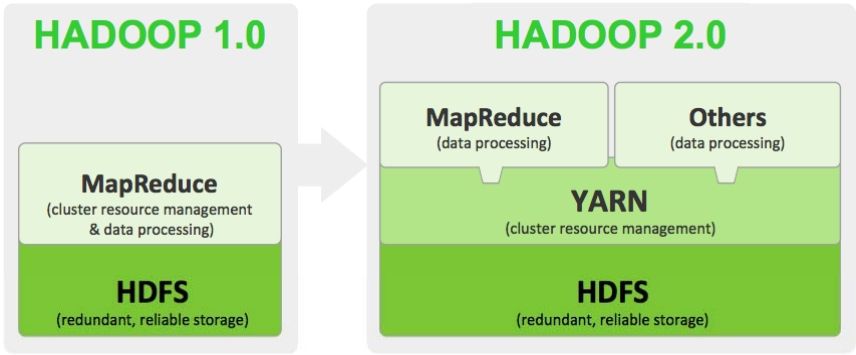
Questions or comments ?

Contents

- VELaSSCo architecture
- Hadoop framework
- Current development status

Hadoop eco-system

- A wide variety of plug-ins
  - Support of SQL
  - Storage (columns, files, …)
  - File System
  - Computational model
  - Query model
  - Management
  - Deployment ….
- A main evolution with YARN
  - Up to 10.000 nodes per cluster
  - Efficient cluster usage with Yarn
  - HDFS 2
  - Compatible with existing extensions
- Hadoop distributions: Cloudera, Ambari, Intel's hadoop, Apache Hadoop, Hortonworks (HDP), …



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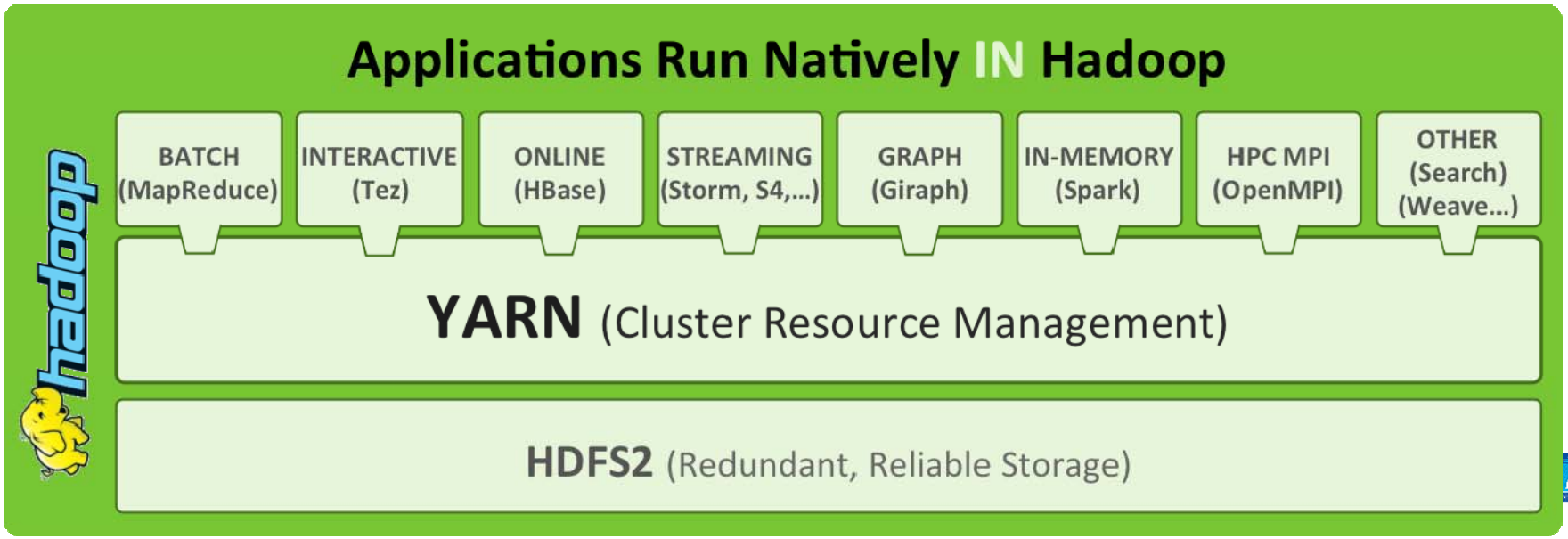
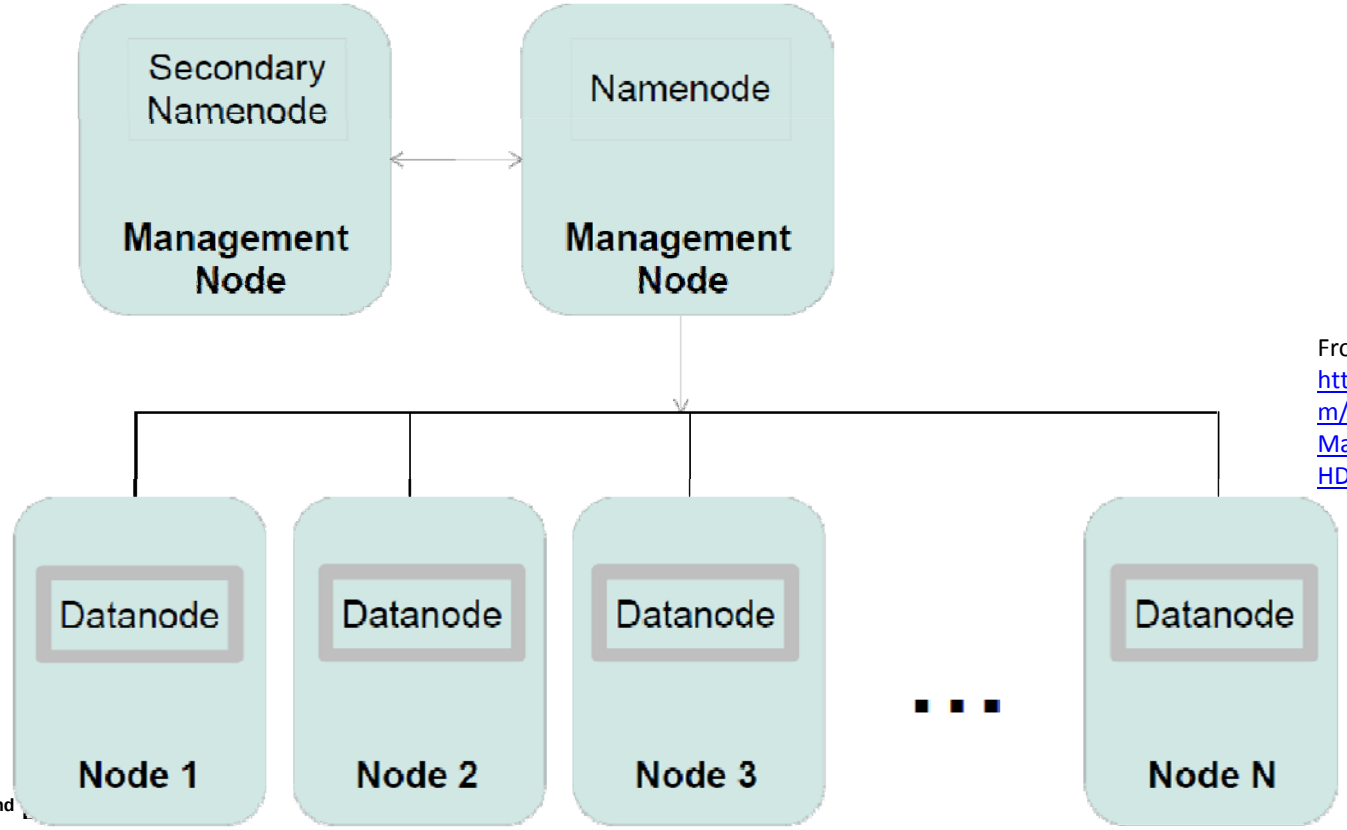


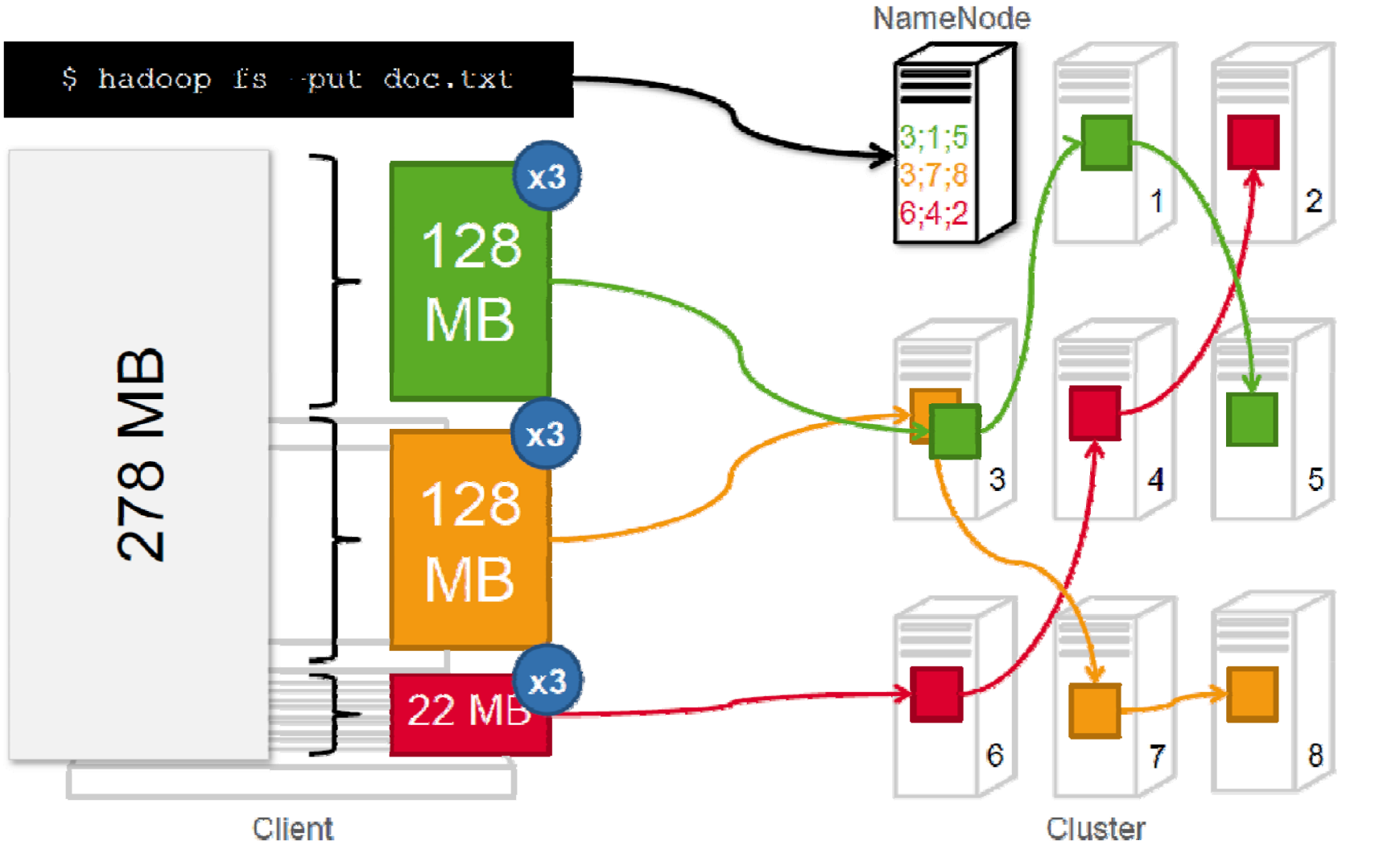
HDFS

- Store files in a distributed, split and redundant way.
- Default chunk size = 64/128 MB, redundancy level = 3
- 1 Name node = metadata (Files → Blocks → Nodes)



From "HDFS overview" http://courses.coreservlets.com/Course-Materials/pdf/hadoop/02-HDFS_1-Overview.pdf

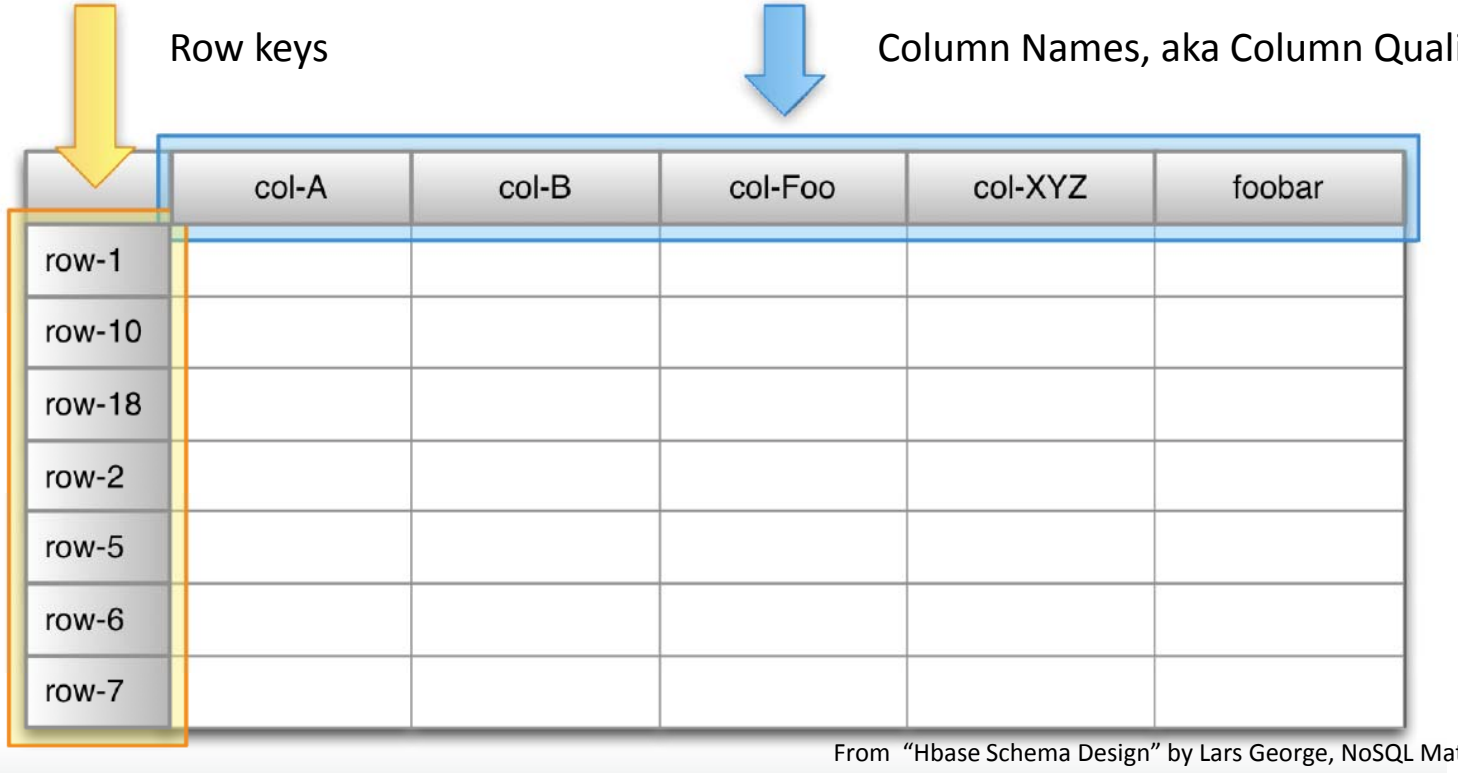
HDFS



From "Hadoop in a Nutshell"
http://www.metafinanz.de/sites/default/files/Hadoop_in_a_Nutshell.pdf

HBase

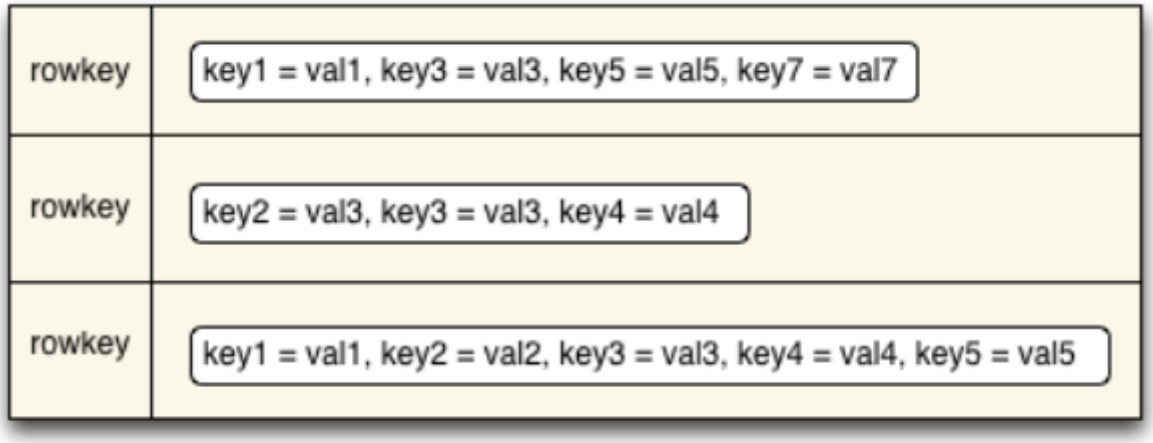
- Table (column) oriented distributed data store, over HDFS
- In Java providing thrift, rest, … services
- Integrated in MapReduce



From "Hbase Schema Design" by Lars George, NoSQL Matters, 2013

Hbase basic

- **Table**: design-time namespace, has many rows.
- **Row**: atomic key/value container, with one row key
- **Column**: a key in the k/v container inside a row
- **Value**: a value in the k/v container inside a row



From "Hbase Schema Design" by Ian Varley, HBaseCon 2012

Hbase column families

- **Table**: design-time namespace, has many rows.
- **Row**: atomic key/value container, with one row key
- **Column Family**: groups ‘related columns’ / divide rows into physical files.
- **Column-qualifiers**: a key in the k/v container inside a row

- **Value**: a value in the k/v container inside a row

- → Row is atomic: flushed periodically
  - Colum-Families: groups of columns with ‘related’ data:
    - to store in separate files, do compression, in-memory options, …
- → Family definitions are static, limited to small number of families
- → Column-qualifiers may vary from row to row.

From “Hbase Schema Design” by Ian Varley, HBaseCon 2012

Hbase time-stamp

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- **Row**: atomic key/value container, with one row key
- **Column Family**: groups ‘related columns’ / divide rows into physical files.
- **Column-qualifiers**: a key in the k/v container inside a row
- **Timestamp**: long milliseconds, sorted descending
- **Value**: a time-versioned value in the k/v container inside a row

- → Row is atomic: flushed periodically
  - Colum-Families: groups of columns with ‘related’ data:
    - to store in separate files, do compression, in-memory options, …
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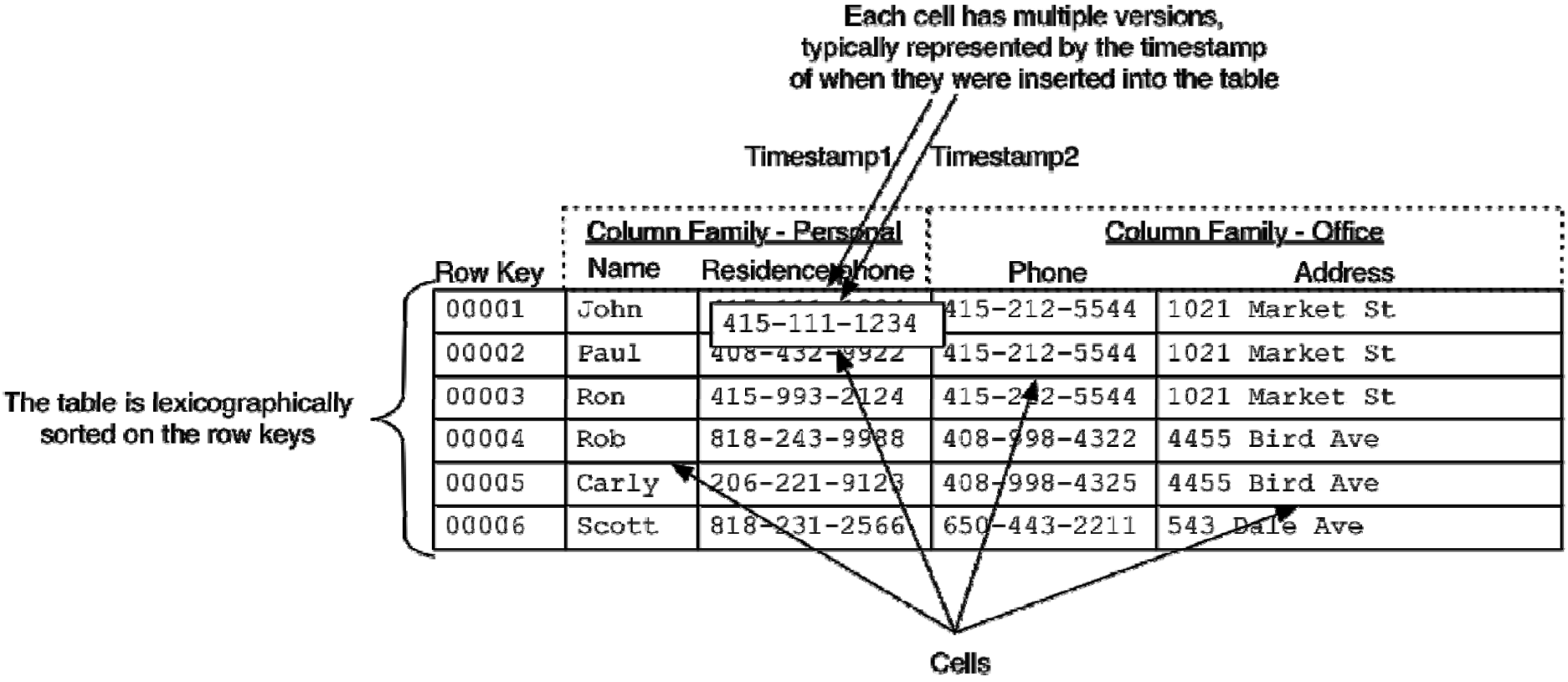
From “Hbase Schema Design” by Ian Varley, HBaseCon 2012

Hbase sumary



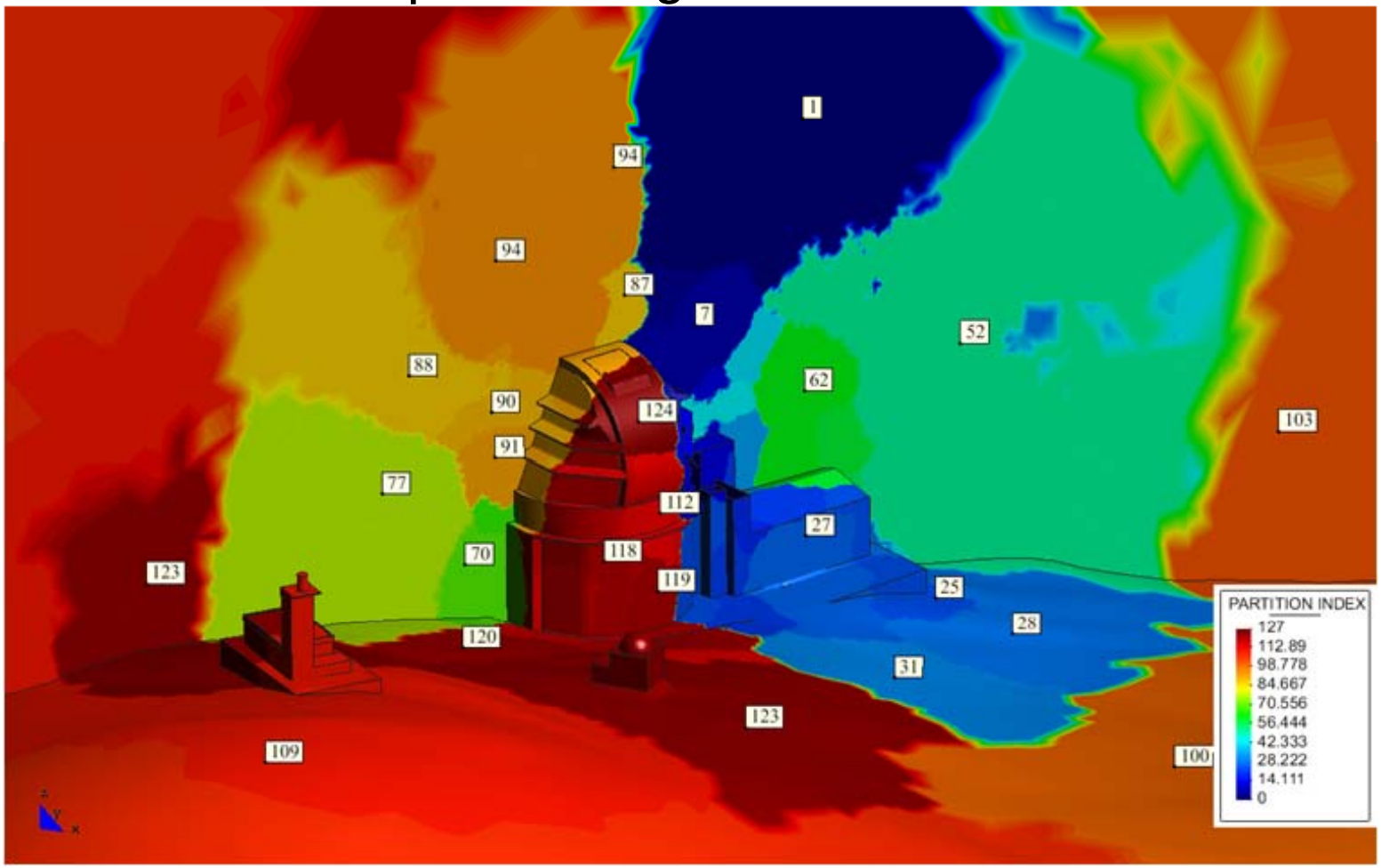
From "Introduction to Hbase Schema Design" by Amandeep Khurana

Hbase summary

Row Key	CF: Personal	CF: Office
00001	Name:t1 = John Residence_phone:t1 = 415-111-1224 Residence_phone:t2 = 415-111-1234	Phone:t1 = 415-212-5544 Address:t1 = 1012 Market St
00002	Name:t10 = Paul Residence_phone:t10 = 408-432-9922	Phone:t11 = 415-212-5544 Address:t11 = 1012 Market St
…	…	…
…	…	…
0000N	Name:t1234 = Eventually Residence_phone:t1234 = 555-111-111 Residence_phone_alternative:t1234 = 666-666-666	

Hbase in VELasSCo

- Solver: Domain partitioning for distributed calculation

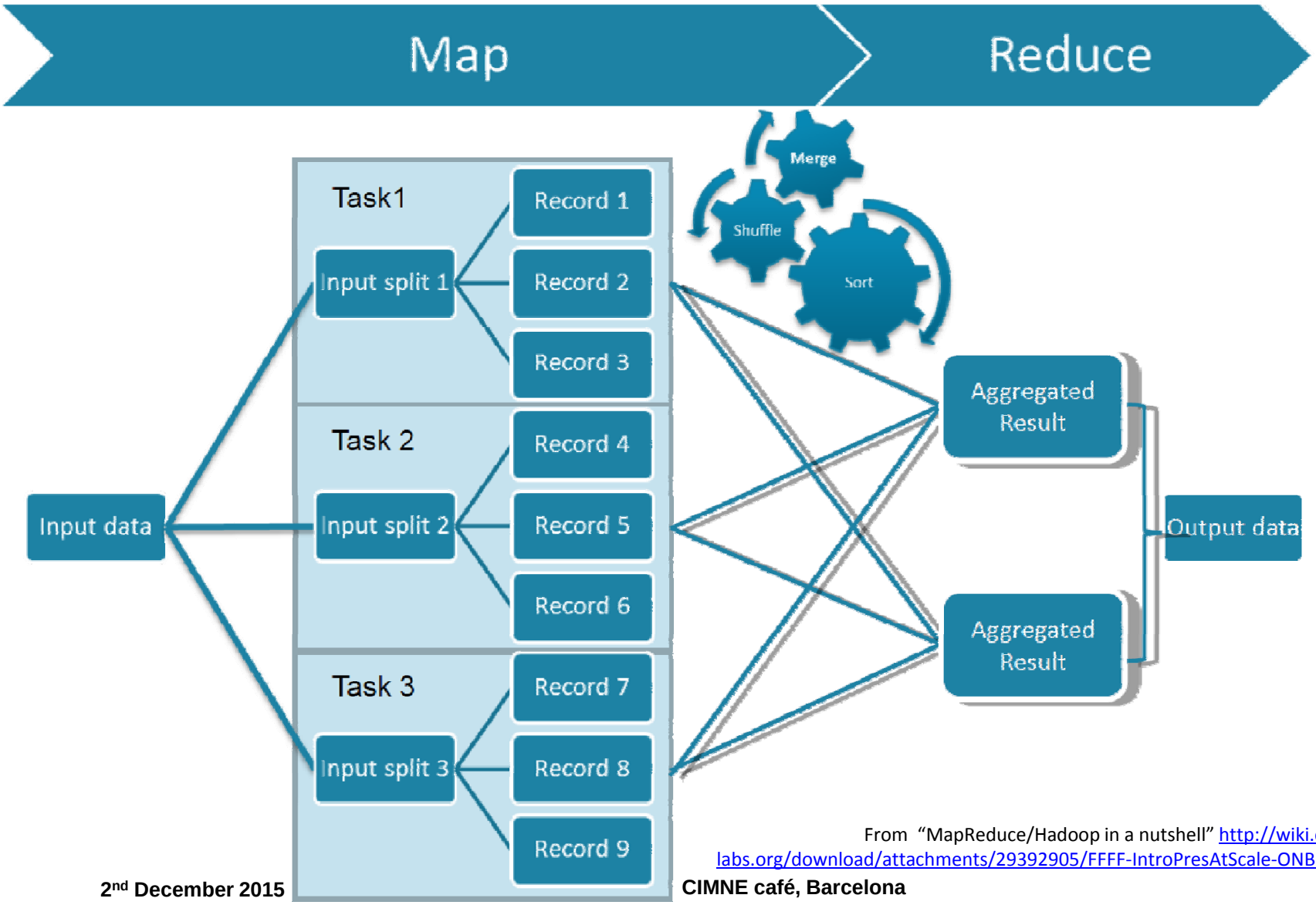


Hbase in VELaSSCo

- 3 tables: model list, metadata and data
- Simulation_Data:
  - Results for 1 time-step and 1 partition in one row
  - 2 column families: M(esh) and R(esults)
  - Each coordinate or result value in one column qualifier

Key: SimulationId + *Analysis* + *Step* + *PartitionID*	CF: *M*	CF: *R*
0x0001 + 0 + "" + 0.0 + 0	c000001_0 = (0.0, 0.0, 0.0), c000001_339185 = (1.0, 1.0, 1.0), m000001cn_0 = (1, 2, 3, 4), m000001gr_0 = (1), m000001cn_717793 = (339184, 339183, 339182, 339181), m000001gr_717793 = (2), m000002cn_717794 = (1, 2, 3) m000002cn_739513 = (7,66, 8)	(empty)
0x0001 + 6 + "RANSOL" + 91.5 + 0	(empty)	r000001vl_1 = (4), r000001vl_339184 = (324), r000002vl_1 = (1.1, 2.2, 3.3), r000002vl_339184 = (10.0, 10.0, 9.1), …
0x0001 + 6 +"RANSON" + 200.0 + 127	(empty)	…

MapReduce



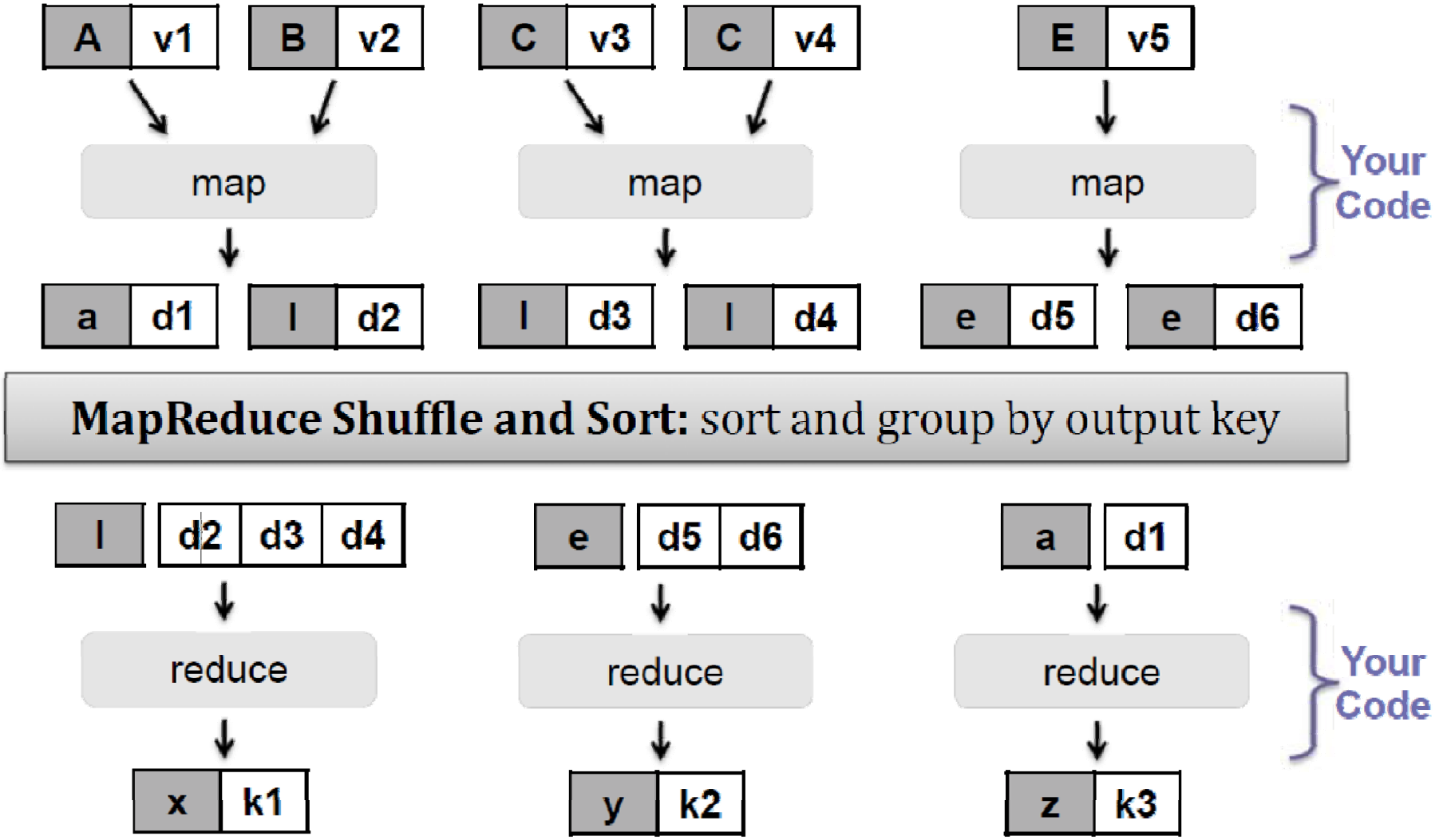
From "MapReduce/Hadoop in a nutshell" http://wiki.opf-labs.org/download/attachments/29392905/FFFF-IntroPresAtScale-ONB.pdf

MapReduce

- Key-value Input/Output
- Uses map and reduce functions:
  - Map: (k1, v1) → list (k2, v2)
  - Reduce: (k2, list(v2)) → list(k3, v3)
  - Map function applied to every input k-v pair
  - Map function generates intermediate k2-v2 pairs
  - Intermediate results are sorted and grouped by key
  - Reduce applied to sorted and grouped intermediate results
  - Reduce emits result key-value s

From "MapReduce overview" http://courses.coreservlets.com/Course-Materials/pdf/hadoop/04-MapRed-1-OverviewAndInstall.pdf

MapReduce



From "MapReduce overview" http://courses.coreservlets.com/Course-Materials/pdf/hadoop/04-MapRed-1-OverviewAndInstall.pdf

MapReduce: color count with Java API

```java
package de.inovex.academy.hadoop.candy;
import org.apache.hadoop...;

public class ColorMapper // extends Mapper< k_i, v_i, k_t, v_t>
       extends Mapper<LongWritable, Text, Text, IntWritable> {
       private static IntWritable one = new IntWritable( 1 );
       /**
        * in: ( byte-pos, "color flavor size batch bag" )
        * out: ( color, 1 )
        */
       @Override
       protected void map( LongWritable key_in, Text va_in,
                           Context context )
                     throws IOException, InterruptedException {
              String[] fields = va_in.toString().split( "\\t" );
              context.write( new Text( fields[0] ), one );
       }
}

public class IntSumReducer // ext. Reducer< k_t, v_t, k_o, v_o>
       extends Reducer<Text, IntWritable, Text, IntWritable> {

       @Override
       protected void reduce( Text key_in, Iterable<IntWritable>
                                  values_in, Context context )
                     throws IOException, InterruptedException {
              int sum = 0;
              for ( IntWritable partialCount : values_in ) {
                     sum += partialCount.get();
              }
              context.write( key_in, new IntWritable( sum ));
       }
}
```

```java
package de.inovex.academy.hadoop.candy;
import org.apache.hadoop...;

public class ColorCount
       extends Configured implements Tool {
       @Override
       public int run(String[] args) throws Exception {
              Job job = new Job();
              job.setJarByClass( ColorCount.class );
              job.setJobName( "color-count" );

              FileInputFormat.addInputPath( job,
                                           new Path( args[0] ));
              FileOutputFormat.setOutputPath( job,
                                           new Path( args[1] ));

              job.setMapperClass( ColorMapper.class );
              job.setReducerClass( IntSumReducer.class );
              job.setNumReduceTasks( 6 ); // 6 different colors

              job.setOutputKeyClass( Text.class );
              job.setOutputValueClass( IntWritable.class );

              return job.waitForCompletion( true ) ? 0 : 1;
       }

       public static void main( String[] args )
                     throws Exception {
              int exitCode = ToolRunner.run( new ColorCount(),
                                                  args);
              System.exit(exitCode);
       }
}
```

YARN

- Thrift API

Others

- Hive, FLUME, …

Distributed post-processing: VELaSSCo

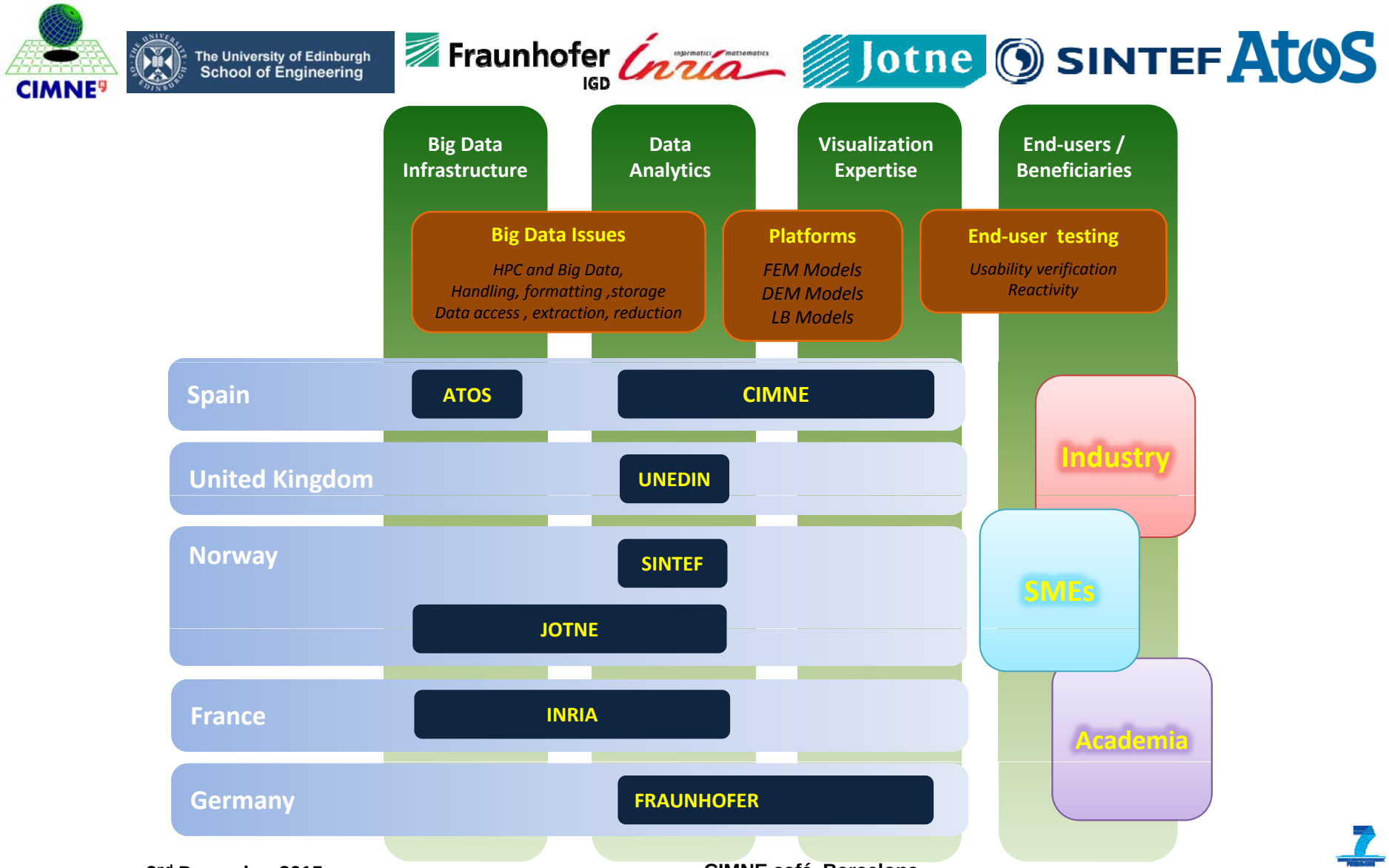
- **V**isual Analysis for **E**xtremely **La**rge-**S**cale **S**cientific **Co**mputing
  - grant agreement # 619439 (FP7/2007-2013)
  - 3 Years: January 2014 – December 2016
  - collaborates with HPC projects: **NUMEXAS**, **Fortissimo** and **CloudFlow**
- Integrate post-process analytics in a Big Data framework embedded in the HPC, where the data is being calculated.
- http://www.velassco.eu

VELaSSCo

European Union

SEVENTH FRAMEWORK PROGRAMME

Partners


Big Data Infrastructure
Data Analytics
Visualization Expertise
End-users / Beneficiaries
Big Data Issues
HPC and Big Data,
Handling, formatting ,storage
Data access , extraction, reduction
Platforms
FEM Models
DEM Models
LB Models
End-user testing
Usability verification
Reactivity
Spain
ATOS
CIMNE
United Kingdom
UNEDIN
Norway
SINTEF
JOTNE
France
INRIA
Germany
FRAUNHOFER
Industry
SMEs
Academia

Partners

- CIMNE: FEM data analytics
- UEDIN: DEM data analytics
- SINTEF: high degree spline representation
- FRAUNHOFER: GPU leverage
- INRIA: Big Data framework
- JOTNE: Big Data framework + STEP format
- ATOS: Big Data framework, user efectiveness

VELaSSCo

Thanks for your attention

… questions & comments …