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EXCELENCIA SEVERO OCHOA

Task-based parallel programming model in Python

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Intel-BSC Exascale Lab

Collaboration between Intel and the Barcelona Supercomputing Center

10-13/09/2017

PPAM 2017, Lublin

The MareNostrum 4 Supercomputer

In operation since July 2017

Total peak performance

13.7 Pflops/s, 390TB

12 times more powerful than MareNostrum 3

Compute

General Purpose, for current BSC workload

More than 11 Pflops/s

3,456 nodes of Intel Xeon v5 processors

Emerging Technologies, for evaluation of 2020 Exascale systems

3 systems, each of more than 0.5 Pflops/s with KNL/KNH, Power9+NVIDIA, ARMv8

Storage

14 PB of GPFS

Storage System

Network

IB EDR/OPA

Ethernet

Operating System: SuSE

13th in TOP500

3rd in Europe

80% PRACE users

16% Spanish researchers

4% BSC researchers

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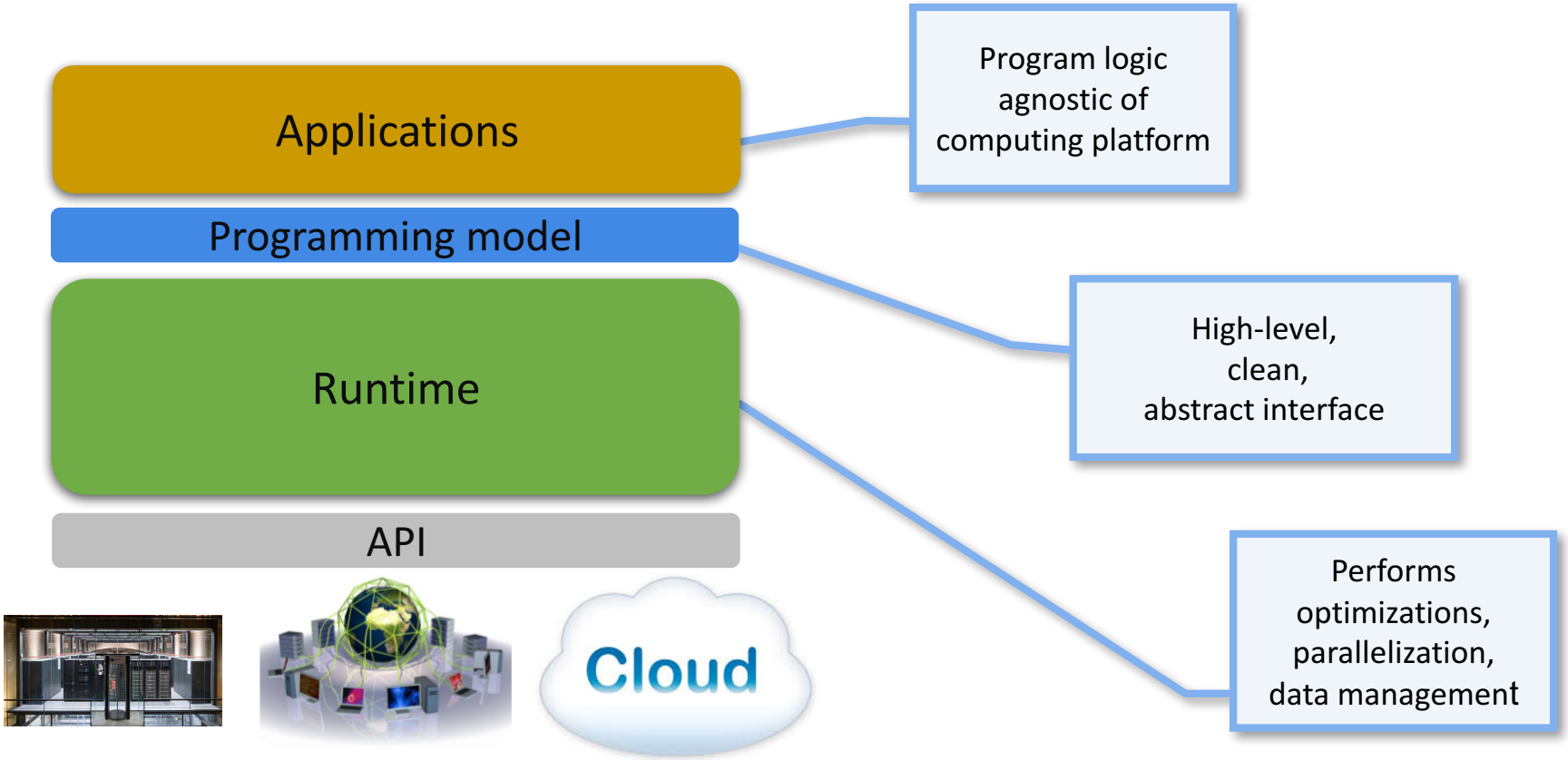
Challenges

- New architectures and organization of processors
  - Multicore
    - Including vector units
  - GPU/accelerators
  - FPGAs
- Shift on programming paradigms:
  - From sequential to parallel
  - New instructions/languages
- Storage systems
  - New storage technologies
  - Shift on storage paradigm

BSC vision on programming models



Outline

- PyCOMPSs overview
- Integration with new storage technologies
- Applying to linear algebra kernels
- Performance results in several architectures
- Conclusions

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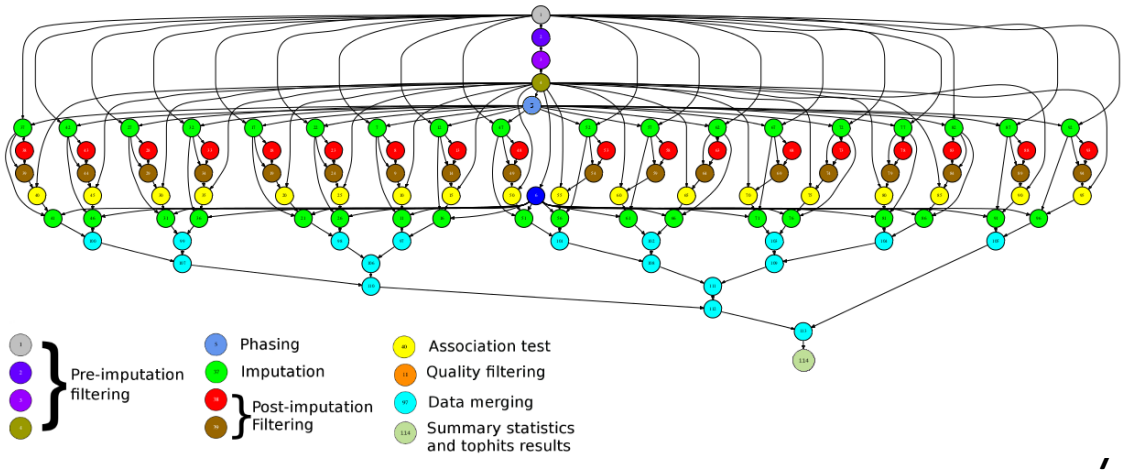
PyCOMPSs/COMPSs overview

Programming with PyCOMPSs/COMPSs

- Sequential programming
- General purpose programming language + annotations/hints
  - To identify tasks and directionality of data
- Task based: task is the unit of work
- Simple linear address space
- Builds a task graph at runtime that express potential concurrency
  - Implicit workflow
- Exploitation of parallelism
  - … and of distant parallelism
- Agnostic of computing platform
  - Enabled by the runtime for clusters, clouds and grids



PyCOMPSs

- Based on regular/sequential Python code
- Use of decorators to annotate tasks and indicate arguments directionality
- Other annotations: constraints
- Small API for data synchronization

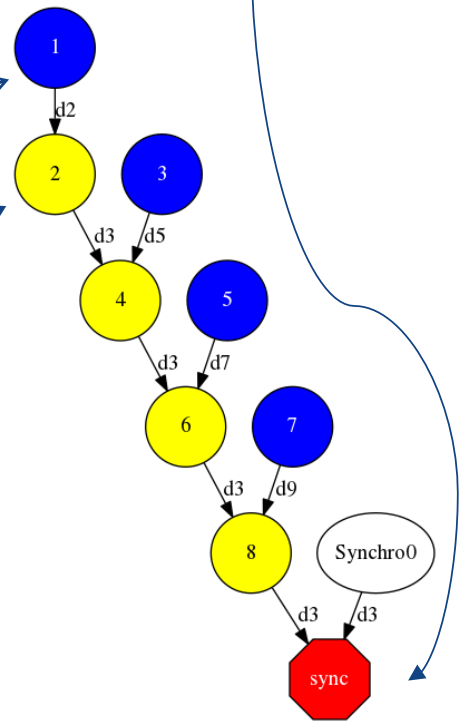
Main Program

```
Data = [block1, block2, …, blockN]
result=defaultdict(int)
for block in Data:
    presult = word_count(block)
    reduce_count(result, presult)
finalResult = compss_wait_on(result)
```

Tasks definition

```
@task(returns=dict)
def word_count(collection):
    ...
```

```
@task(dict_1=INOUT)
def reduce_count(dict_1, dict_2):
    ...
```



Tasks' contraints and versions

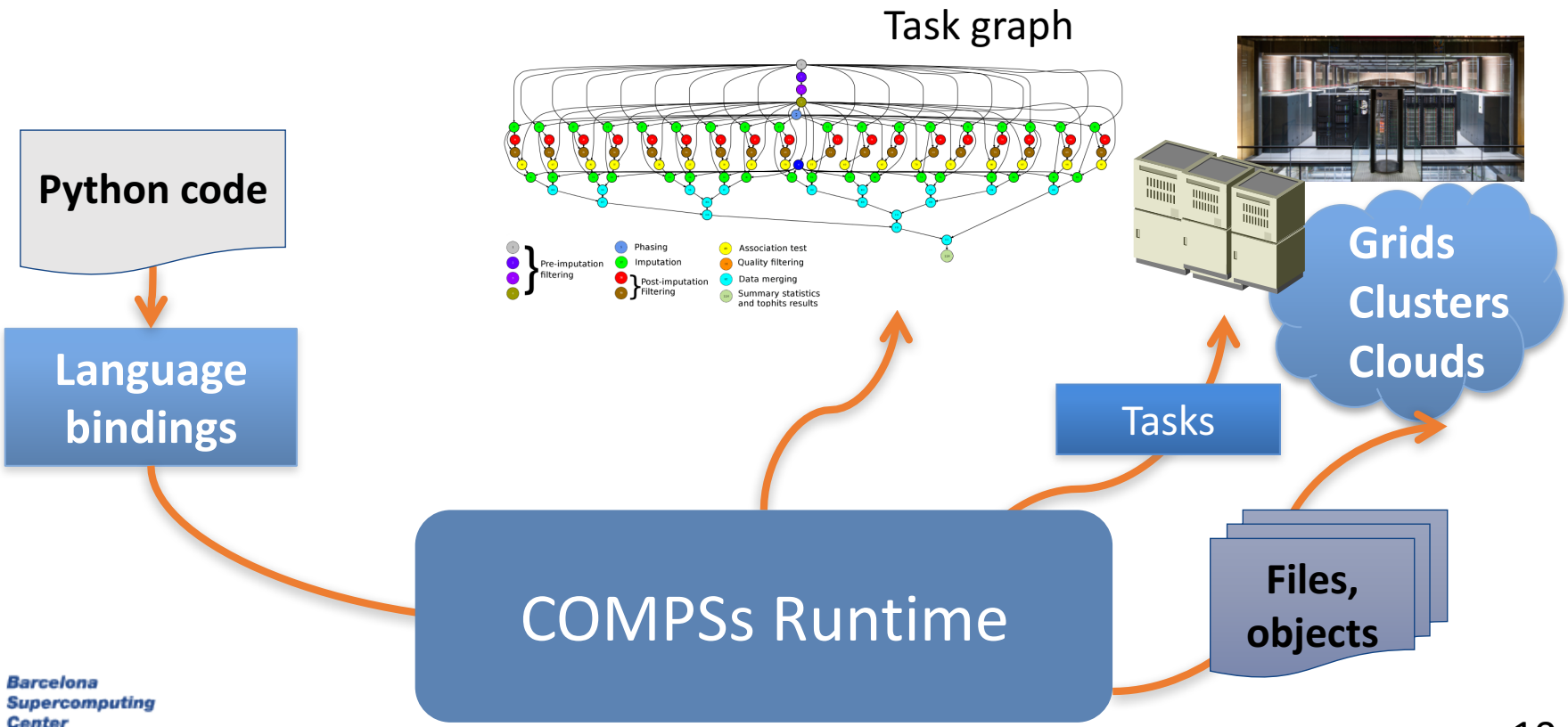
- Contraints enable to define the resource characteristics where to execute the task
- Versions. Mechanism to support multiple implementations of a single behavior
  - Combined with constraints to select different architectures
- Runtime selects more adequate version – depends on actual scheduling policy

```
@implement (source class="matmul objects MKL", method="multiply")
@constraint (ComputingUnits="$ComputingUnitsKNL", ProcessorName="KNL")
@task (c=INOUT)
def multiplyKNL(a, b, c, MKLProcXeon, MKLProcKNL):
os.environ["KMP AFFINITY"]="disabled"
os.environ["MKL NUM THREADS"]=str(MKLProcKNL)
c += a * b
```

```
@constraint (ComputingUnits="$ComputingUnitsXEON", ProcessorName="XEON")
@task (c=INOUT)
def multiply(a, b, c, MKLProcXeon, MKLProcKNL):
os.environ["MKL NUM THREADS"]=str(MKLProcXeon)
c += a * b
```

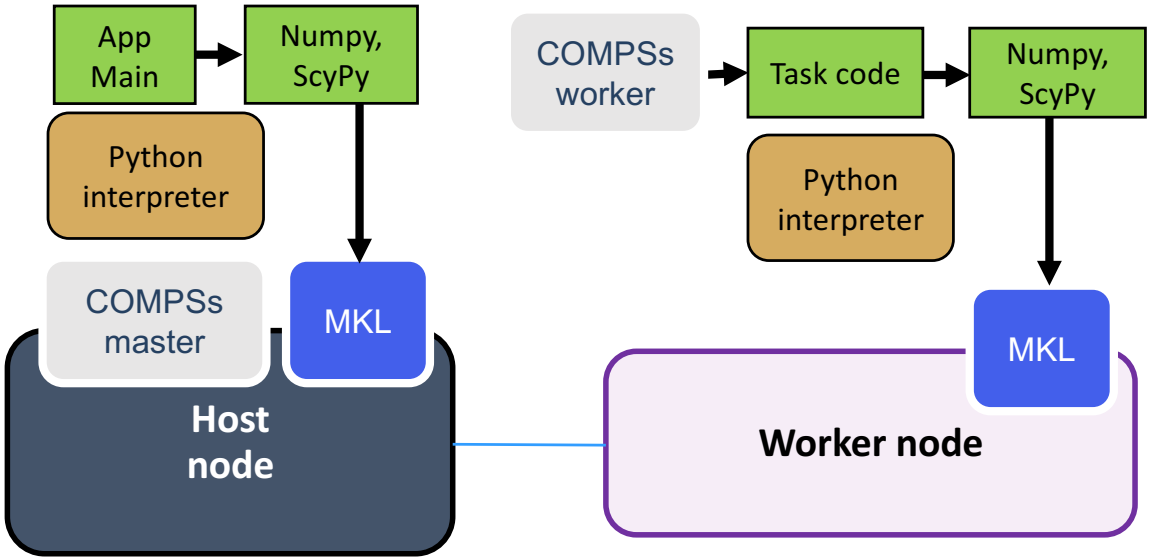
PyCOMPSs runtime

- Sequential execution starts in master node
- Tasks are offloaded to worker nodes
- All data scheduling decisions and data transfers performed by runtime



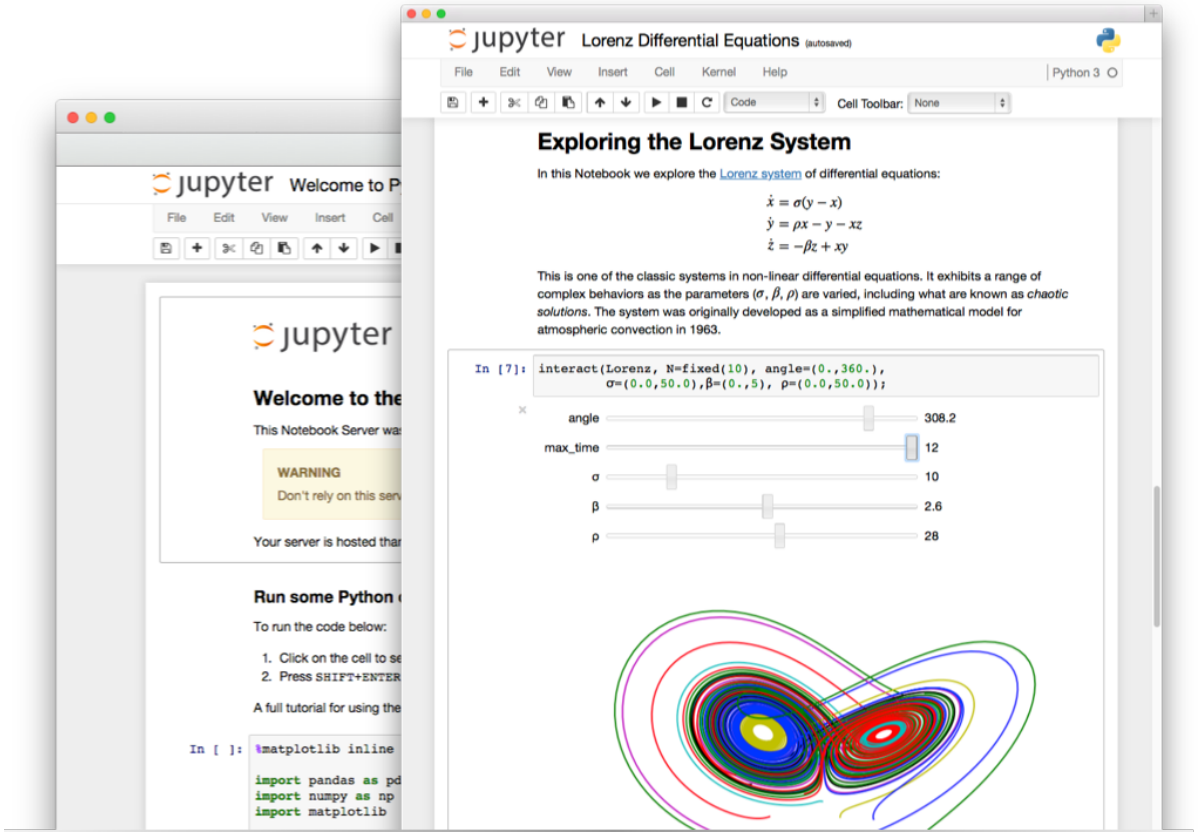
PyCOMPSs stack + Numpy and MKL

- Use of two level parallelism: task level and thread level (MKL)
- PyCOMPSs runtime binds MKL threads to single socket
- Programmer responsible of defining block size and threads to be used



Integration with Jupyter notebook

- The Jupyter Notebook is a web application that allows you to create and share documents that contain live code, equations, visualizations and explanatory text.
- Uses include: data cleaning and transformation, numerical simulation, statistical modeling, machine learning and much more.
- Runs Python – sequential
- Prototype of PyCOMPSs integrated with Jupyter notebook
  - Runs in parallel in local node and can offload tasks to external nodes



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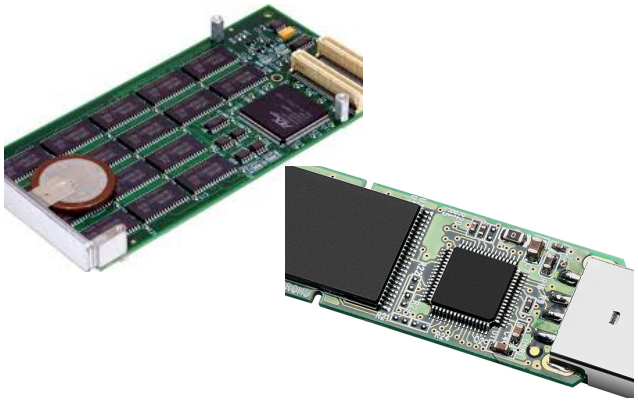
Integration with new storage technologies

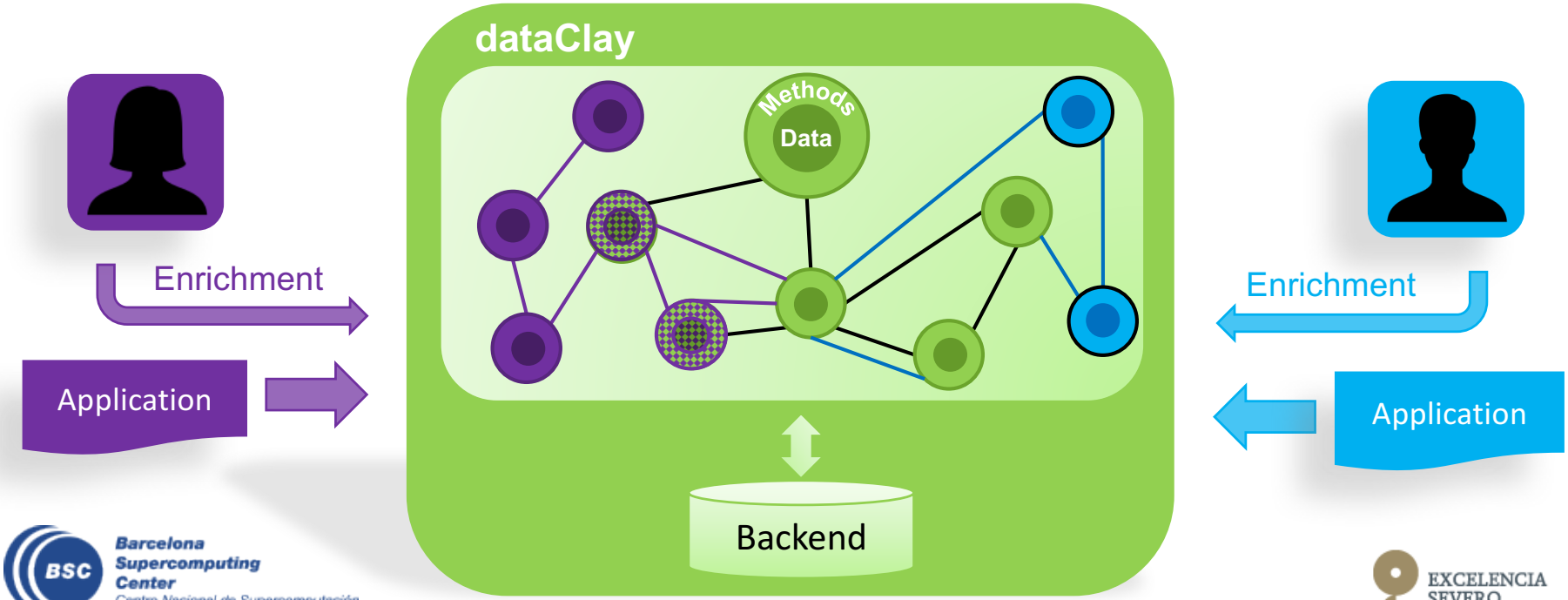
Revolution in the storage technologies



- New storage hardware
  - Non-Volatile RAM
  - Storage Class Memories
- Resemble more memory than storage
  - Low latency, high bandwidth
  - Byte-addressable interface
  - Using them as block devices for a file system does not seem to be the best option
- New storage methodologies are required
  - May imply a disruption on how data is accessed
  - There is no reason to access persistent data in a different way of how non-persistent data is
- New requirements from applications with regard (Big) Data management
  - Large amounts of data generated by simulations and applications in general
  - Moving data is expensive (time, power): in-situ processing

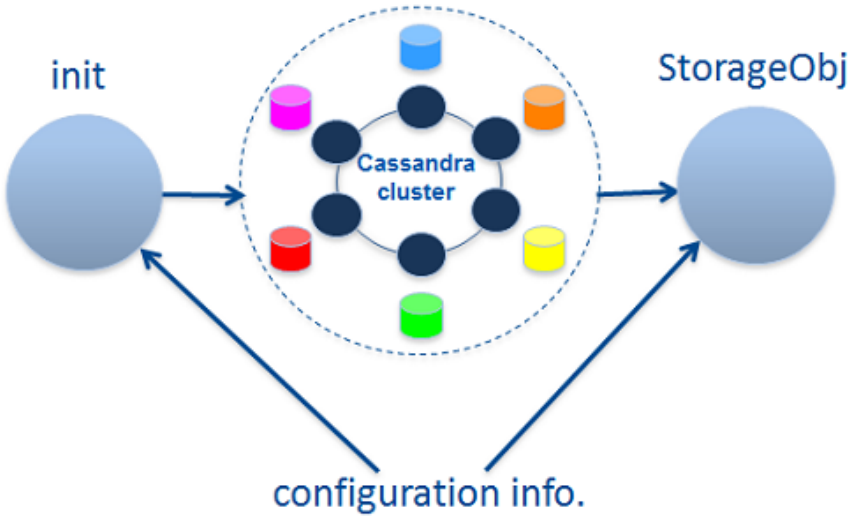
dataClay

- dataCLay: platform that manages **Self-Contained Objects** (data and code)
- Platform features:
  - Store and retrieve objects as seen by applications
  - Remote execution of methods
  - Add new classes
  - Enrich existing classes: With new methods and with new fields



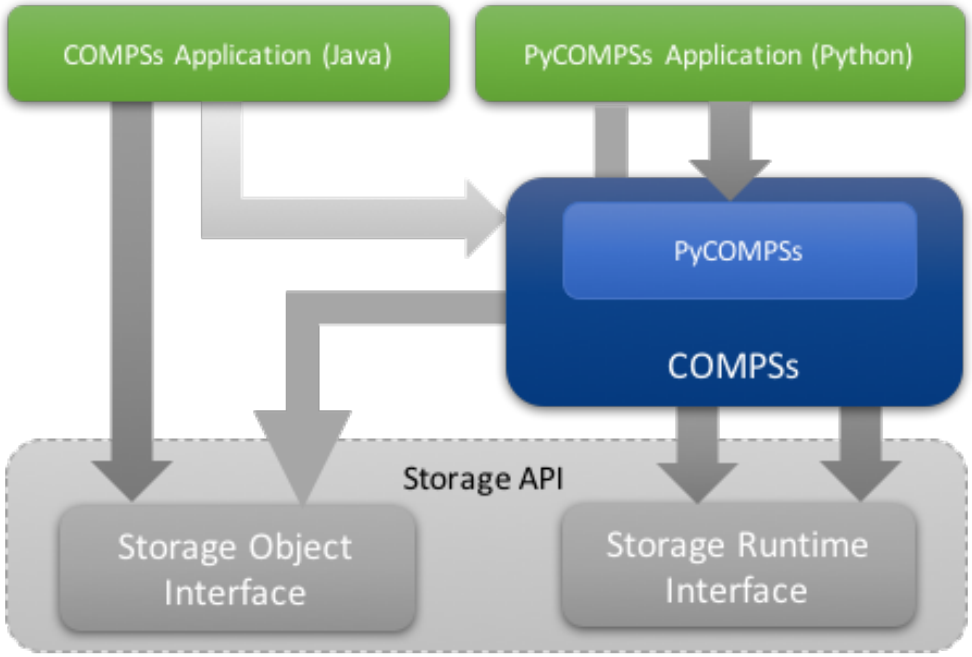
Hecuba

- Set of tools and interfaces that aim to facilitate an efficient and easy interaction with non-relational data-bases
- Currently implemented on Apache Cassandra database
  - However, easy to port to any non-relational key-value data store
- Mapping of Python dictionaries into Cassandra tables
  - Both consist on values indexed by keys
  - Only Python data type supported right now
- Redefinition of Python iterators
  - Accessing blocks of keys
  - Exploiting locality



Integration with Storage: Storage API

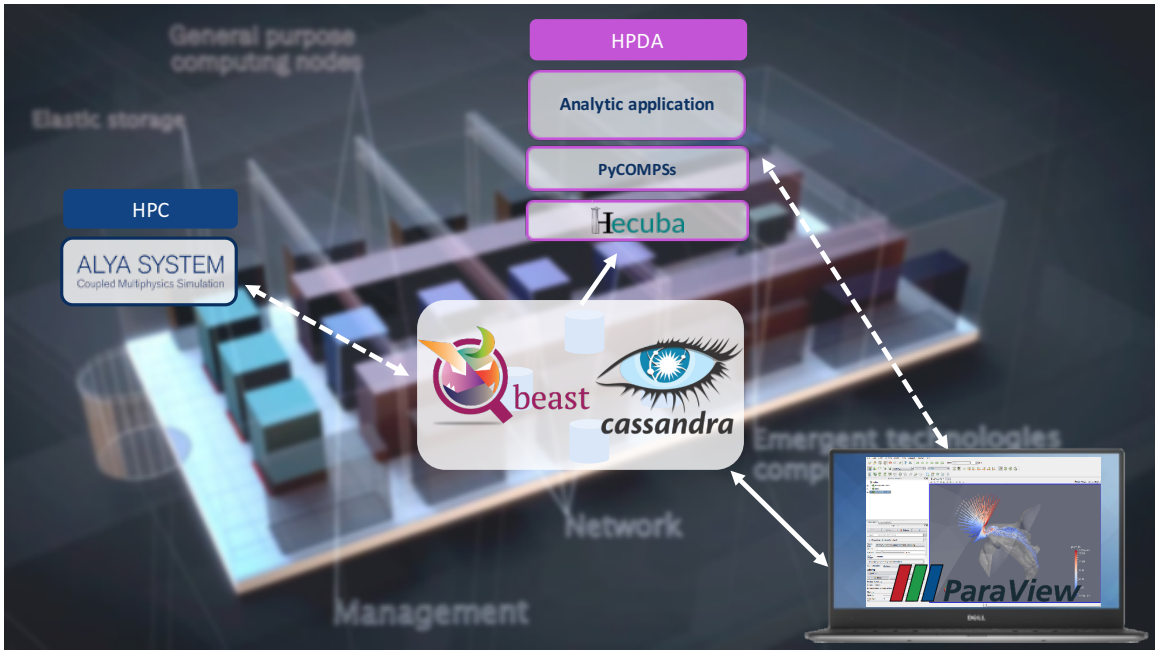
- Integration of programming model with new storage management platforms
- Data made persistent, application agnostic of this persistency
- Producer-consumer
- In-situ




```
...
for i in range(n_points // self.points_per_
    np.random.seed(base_seed + i)
    fragment = Fragment(dim=self.dim,
                        points=np.random.random([self.points_per_fragment, self.dim]),
                        base_index=i * self.points_per_fragment)
    fragment.make_persistent(dest_stloc_id=storage_locations.next())
    self.fragments.append(fragment)
```

Case of study with Hecuba: Respiratory system simulator

- Alya simulation of air flows through the respiratory system.
- Prototype demo implemented on top on key-value data store:
  - Particles generated by simulation stored in Cassandra
  - Managed by Hecuba
- Qbeast: D8-tree index distributed engine
  - Data access with linear scalability
- Queries parallelized with PyCOMPSs
- Visualization and queries simultaneous to simulation
- Demos 7



ISC High Performance
The HPC Event.

SC17

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Applying to linear algebra examples

Matrix multiply

- Blocked matrix
- Tasks operates on blocks of the matrices
- Blocks are NumPy arrays and operate on NumPy operations

```
@constraint (ComputingUnits="$ComputingUnits")
@task(c=INOUT)
def multiply(a, b, c, MKLProc):
    os.environ["MKL_NUM_THREADS"]=str(MKLProc)
    c += a*b
```

main

```
startTime = time.time()
initialize_variables()
barrier()
initTime = time.time() - startTime92
startMulTime = time.time()
for i in range(MSIZE):
   for j in range(MSIZE):
      for k in range(MSIZE):
         multiply (A[i][k], B[k][j], C[i][j], MKLProc)
barrier()
mulTime = time.time() - startMulTime
totalTime = time.time() - startTime
```

Matrix multiply

- Initialization performed with tasks
  - Memory is allocated in the node where the task is executed
- Scheduling will try to place tasks using the same blocks in the same node, reducing transfers and other overheads

```
@constraint(ComputingUnits="$ComputingUnits")
@task(returns=list)
def createBlock(BSIZE, res, MKLProc):
    os.environ["MKL_NUM_THREADS"]=str(MKLProc)
    if res:
        block = np.array(np.zeros((BSIZE, BSIZE)), dtype=np.double, copy=False)
    else:
        block = np.array(np.random.random((BSIZE, BSIZE)), dtype=np.double,copy=False)
    mb = np.matrix(block, dtype=np.double, copy=False)
    return mb
```

Initialization

```
def initialize_variables(MKLProc):
    for matrix in [A, B]:
        for i in range(MSIZE):
          matrix.append([])
          for j in range(MSIZE):
                mb = createBlock (BSIZE, False, MKLProc)
                matrix[i].append(mb)
    for i in range(MSIZE):
       C.append([])
        for j in range(MSIZE):
            mb = createBlock (BSIZE, True, MKLProc)
            C[i].append(mb)
```

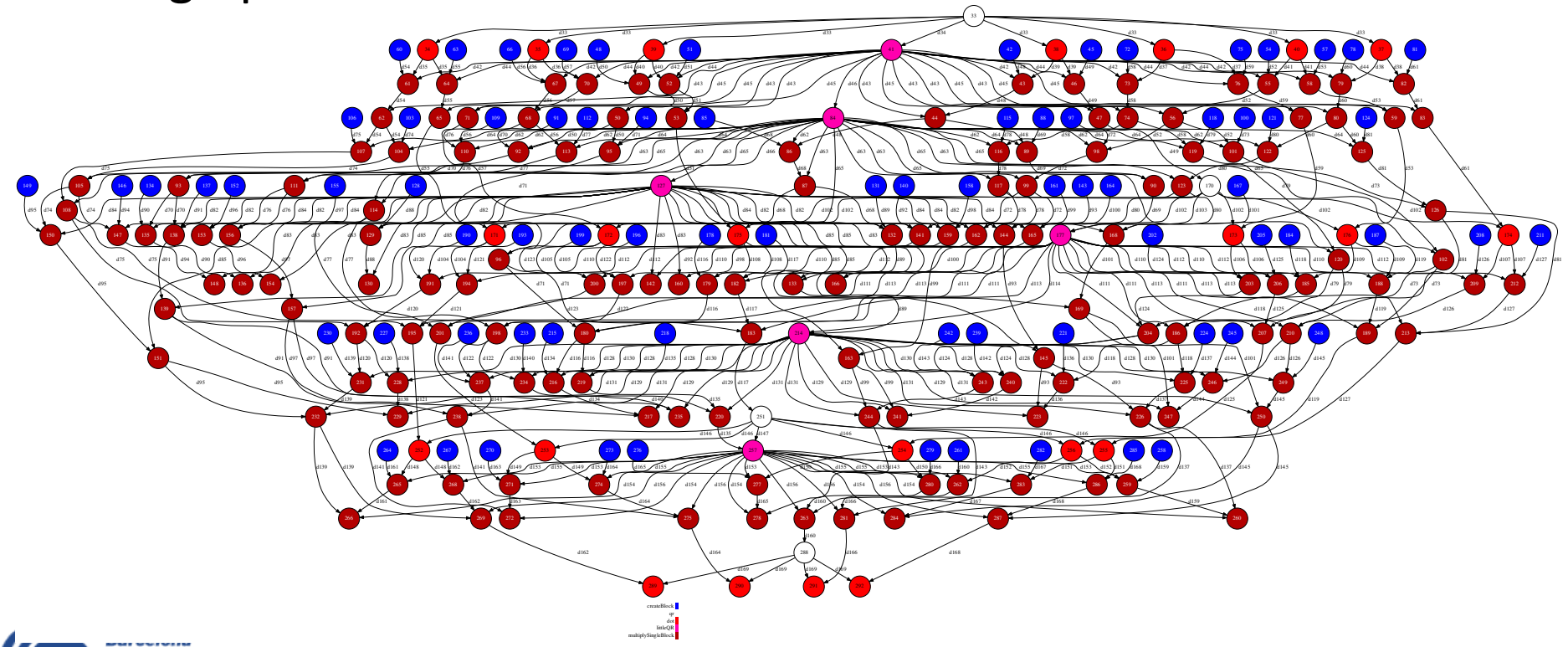
QR factorization

- QR based on Givens rotations, which access the data in the matrices by blocks
- Makes use of an auxiliary matrix
- Blocks are NumPy arrays and operate on NumPy operations

```
def qr_blocked(R):
    Q = genIdentity(MSIZE,BSIZE)
    for i in range(MSIZE):
        actQ, R[i][i] = qr(R[i][i], transpose=True)
        for j in range(MSIZE):
            Q[j][i] = dot(Q[j][i], actQ, transposeB=True)
        for j in range(i+1,MSIZE):
            R[i][j] = dot(actQ,R[i][j])
        #Update values of the respective column
        for j in range(i+1,MSIZE):
            subQ = [[np.matrix(np.array([0])),np.matrix(np.array([0]))],
                    [np.matrix(np.array([0])),np.matrix(np.array([0]))]]
            subQ[0][0],subQ[0][1],subQ[1][0],subQ[1][1],R[i][i],R[j][i] =
                    littleQR(R[i][i],R[j][i], BSIZE, transpose=True)
            #Update values of the row for the value updated in the column
            for k in range(i + 1,MSIZE):
                [[R[i][k]],[R[j][k]]] = multiplyBlocked(subQ, [[R[i][k]],[R[j][k]]],
                    BSIZE)
            for k in range(MSIZE):
                [[Q[k][i], Q[k][j]]] = multiplyBlocked([[Q[k][i], Q[k][j]]], subQ,
                    BSIZE, transposeB=True)
    return Q,R
```

QR factorization

- QR based on Givens rotations, which access the data in the matrices by blocks
- Makes use of an auxiliary matrix
- Task graph for a 4 x 4 blocks matrix



QR factorization: Memory save

- Auxiliary matrix: only those blocks different to identity or zero are allocated
- Main code remains the same

```
@constraint (ComputingUnits="${ComputingUnits}")
@task (returns=list)
def createBlockTask(BSIZE):
    setMKLNumThreads(mkl_threads)
    return np.matrix(np.random.random((BSIZE, BSIZE)), dtype=np.double,copy=False)
```

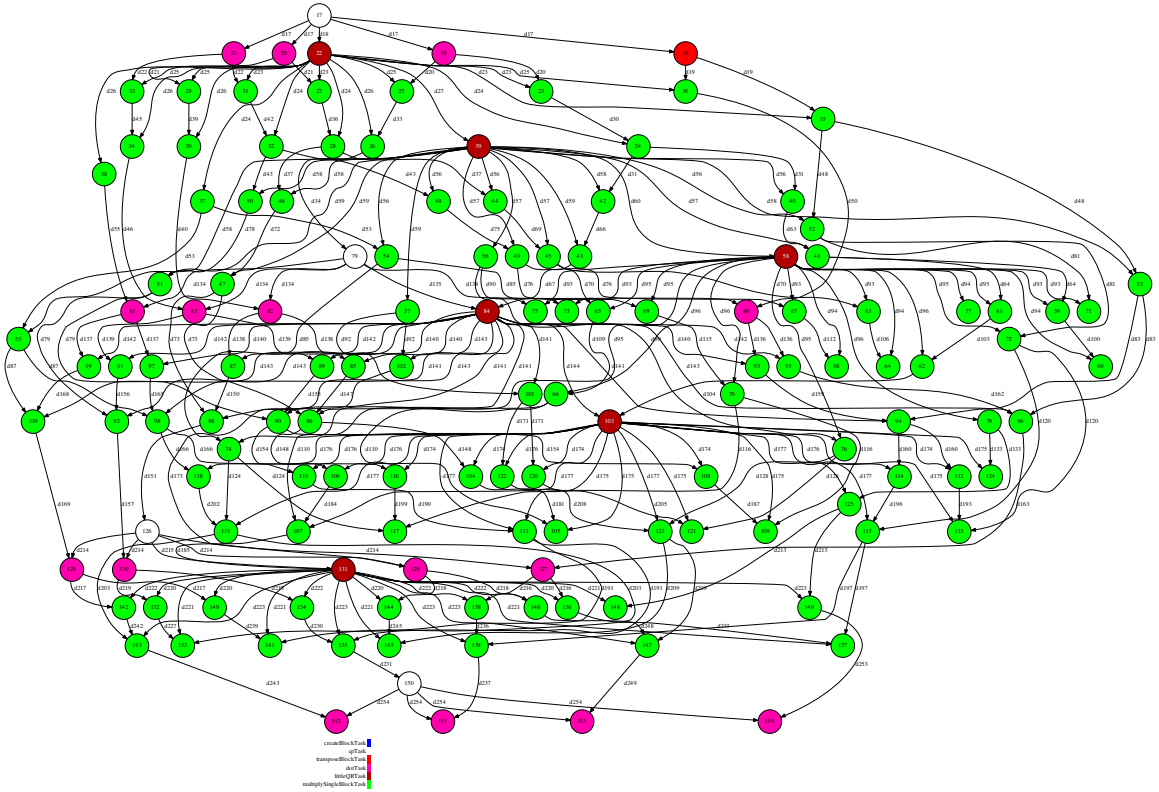
```
def createBlock(BSIZE, type='random'):
    if type == 'zeros':
        block = []
    elif type == 'identity':
        block = []
    else:
        block = createBlockTask(BSIZE)
    return [type,block]
```

```
@constraint (ComputingUnits="${ComputingUnits}")
@task (returns=list)
def transposeBlockTask(A):
    return np.transpose(A
```

```
def transposeBlock(A):
    if A[0] == 'zeros' or A[0] == 'identity':
        return A
    return ['random', transposeBlockTask(A[1])]
```

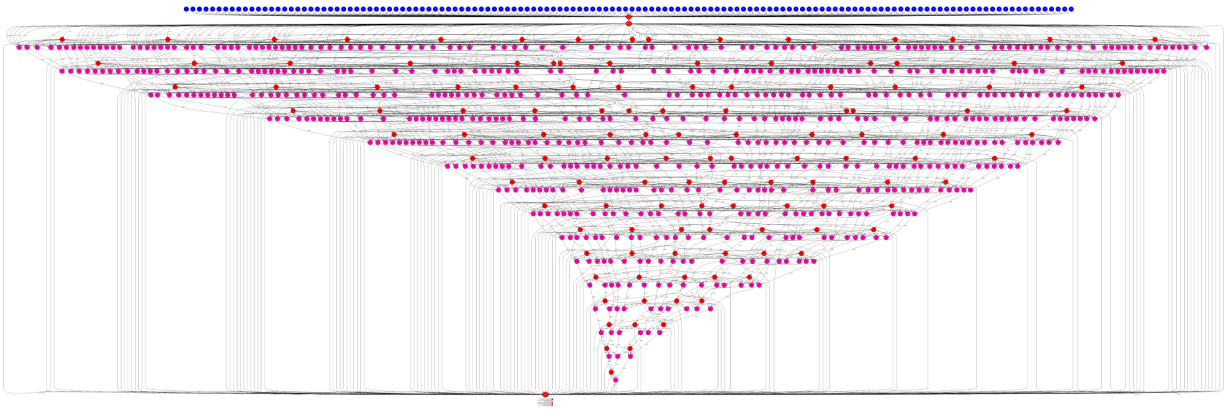
QR factorization: Memory save

- Auxiliary matrix: only those blocks different to identity or zero are allocated
- Main code remains the same
- Task graph for a 4 x 4 blocks matrix

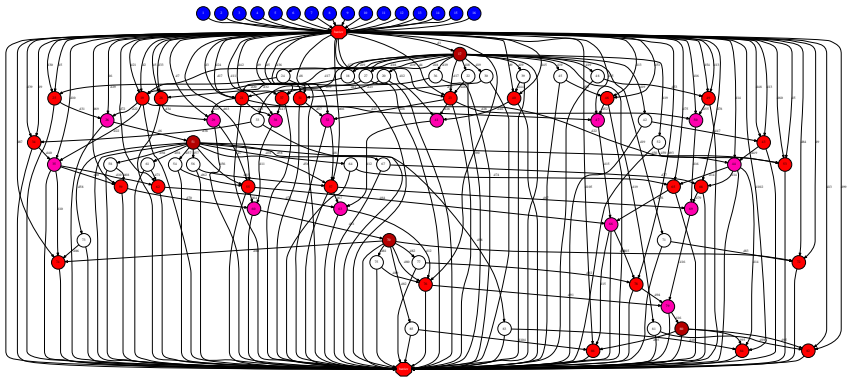


Other examples

- Cholesky – implementation based on right looking approach
  - Task graph for a 16 x 16 blocks factorization



- LU - Initial implementation with partial pivoting at block level
  - Task graph for a 4 x 4 blocks factorization



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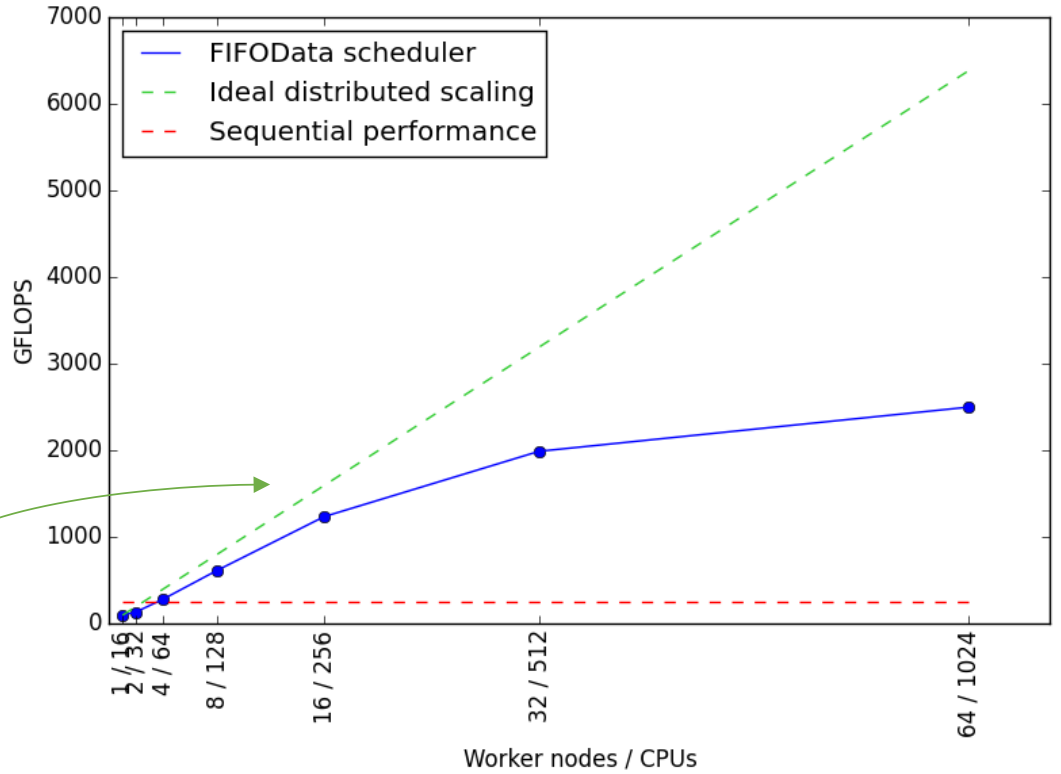
Performance results in several architectures

Matmul evaluation

- Sequential annotated code runs in MareNostrum III, distributed through several nodes
  - 2x Intel SandyBridge-EP E5-2670, 8 cores/socket
  - 32/128 GB per node
  - Infiniband network

Matrix size: 64K x 64 K doubles
Block size: 4096x4096 each block
4 tasks per node
16 MKL threads / task
oversubscription = 4

Baseline: PyCOMPSs execution with one worker node (whole matrix)



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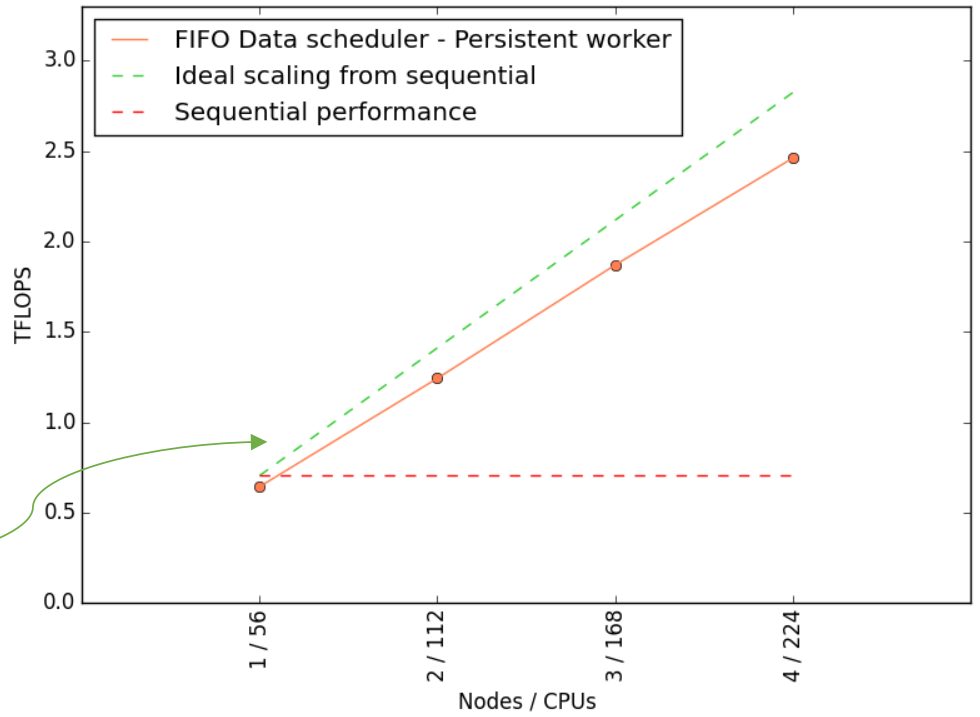
Matmul evaluation

- Results in SSF cluster, distributed through several nodes
  - Lustre as shared file system
  - 2 x Xeon E52690 – V4, 14 cores/socket, 2-threads/core
  - 110 GB/node

Matrix size: 128K x 128K doubles
Block size: 8192x8192 each block
8 tasks per node
7 MKL threads / task
No oversubscription
Master in first worker node

Baseline: Maximum performance
Obtained with multi-threaded
MKL in a single node
with a block of size 16384 x 16384



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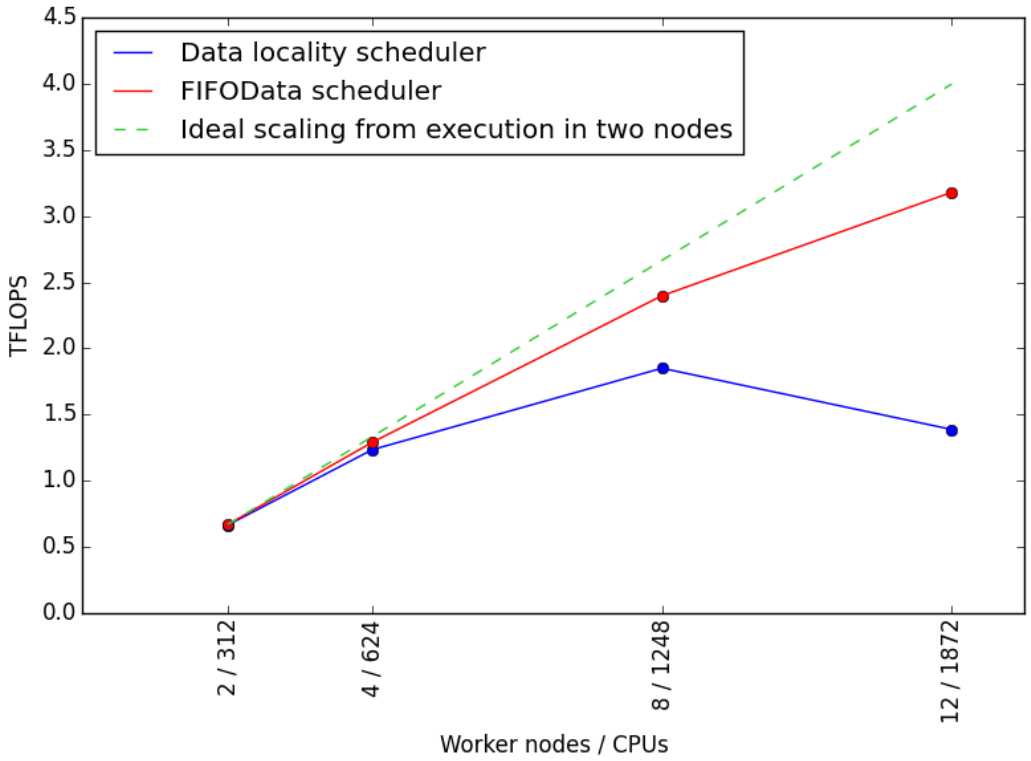
Matmul evaluation - heterogeneous nodes

- Results in SSF cluster, distributed through several heterogeneous nodes
  - Xeon E52690 – V4
    - 2 sockets/node, 14 cores/socket, 2-threads/core
  - KNL Nodes, Intel Xeon Phi 7210
    - 64 cores, 4 threads per core
- Performance using different schedulers



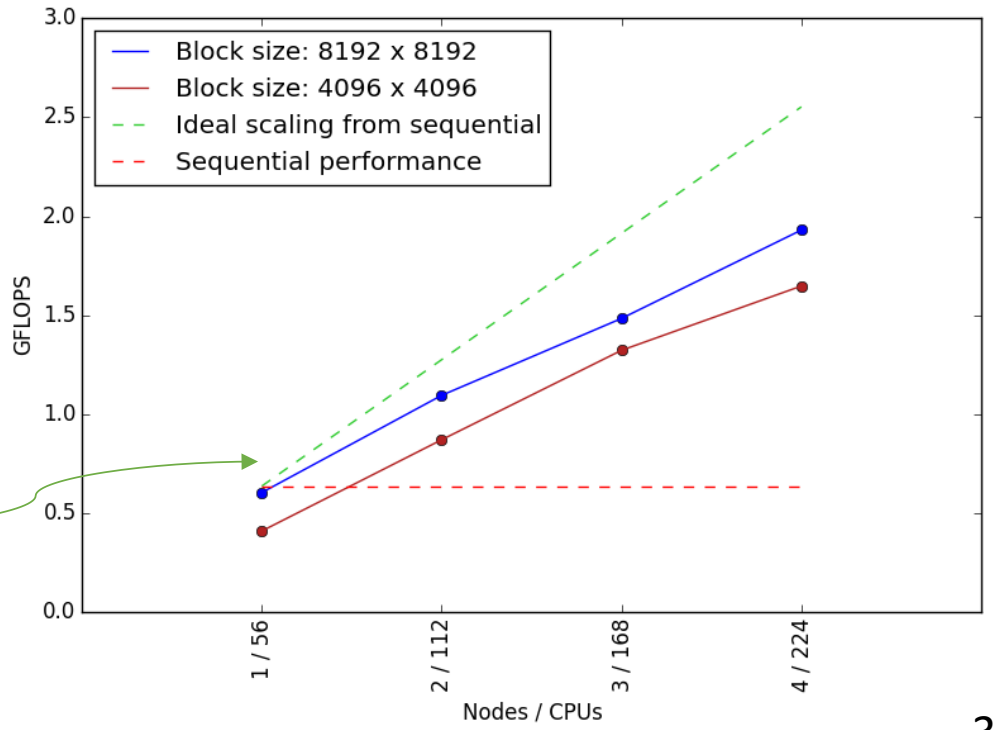
Matrix = 131 K X 131K doubles
Xeons: 8 tasks per node, 7 threads per task
KNL: 4 tasks per node, 64 threads per task
IntelPython 2.7.13
Block size: 4096 x 4096

Cholesky evaluation

- Results in SSF cluster, distributed through several nodes
  - Xeon E52690 – V4 with lustre as shared file system
  - 2 sockets/node
  - 14 cores/socket, 2-threads/core
- Evaluation of different block sizes

Matrix = 128K X 128K doubles
8 tasks per node
7 threads per task (oversubscription = 1)
IntelPython 2.7.13

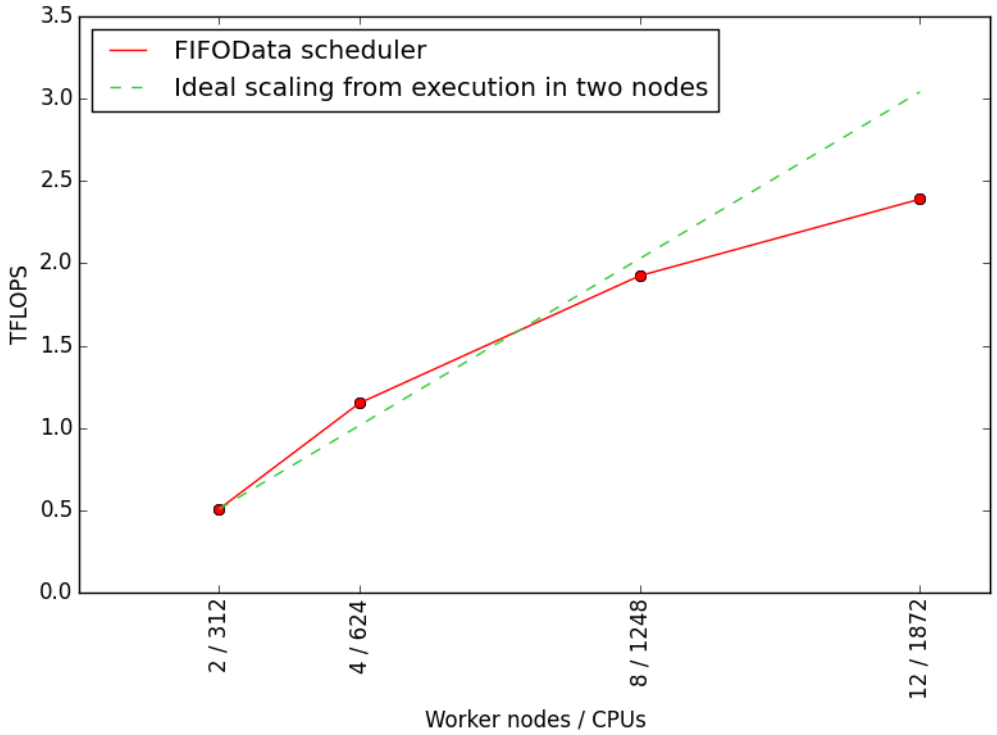
Baseline: Maximum performance obtained with multi-threaded MKL in a single node for a block of size 8192 x 8192



Cholesky evaluation– heterogeneous nodes

- Results in SSF cluster, distributed through several heterogeneous nodes
  - Xeon E52690 – V4
    - 2 sockets/node, 14 cores/socket, 2-threads/core
  - KNL Nodes, Intel Xeon Phi 7210
    - 64 cores, 4 threads per core

Matrix = 128K X 128K doubles
Xeons: 8 tasks per node, 7 threads per task
KNL: 4 tasks per node, 64 threads per task
IntelPython 2.7.13
Block size: 4096 x 4096



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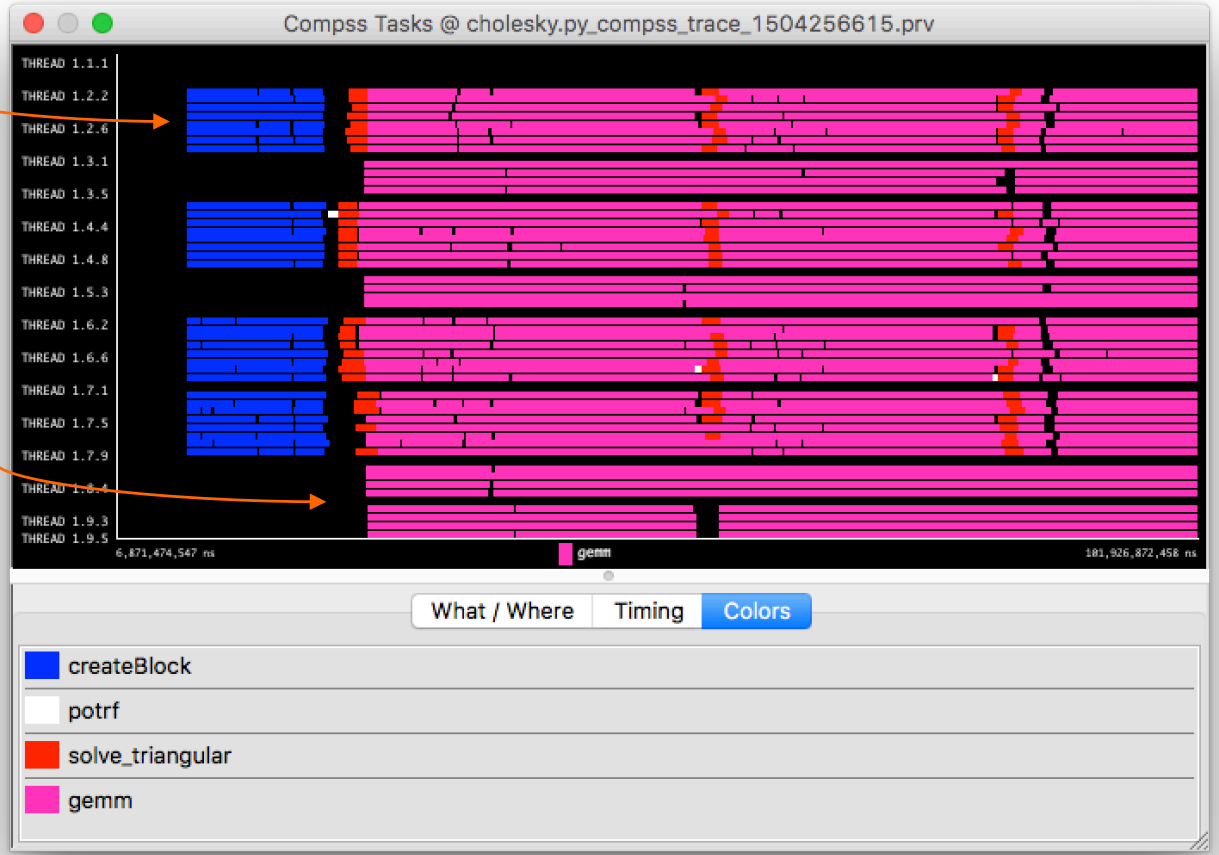
Cholesky evaluation– heterogeneous nodes

- Timeline of tasks
- KNL nodes only execute dgemms
  - Selected with constraints decorator

Xeon node

KNL node

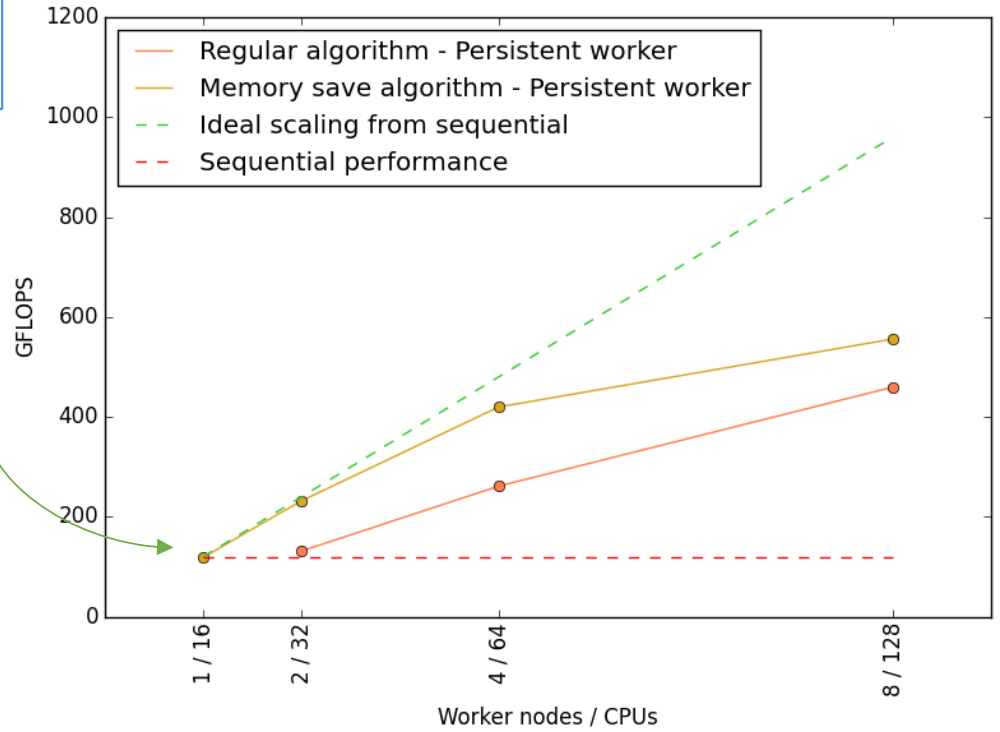


QR results: comparing algorithms

- Results in MareNostrum III, distributed through several nodes
  - Intel SandyBridge-EP E5-2670

Matrix = 32K X 32K doubles
Block size = 4096 x 4096 doubles
4 tasks per node
16 MKL threads per task (oversubscribing = 4)
IntelPython 2.7.13

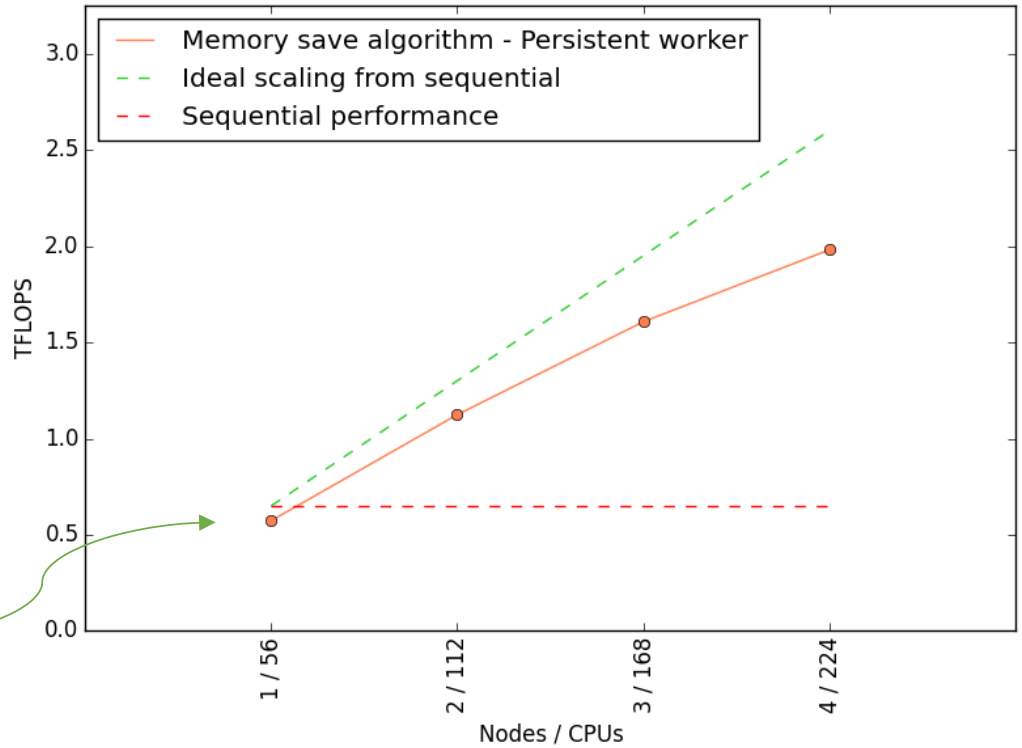
Baseline: one MKL QR
one block with 16 threads



QR memory-save results

- Results in SSF cluster, distributed through several nodes
  - Lustre as shared file system
  - 2 x Xeon E52690 – V4, 14 cores/socket, 2-threads/core
  - 110 GB/node

Matrix = 56K X 56K doubles
Block size = 4096 x 4096 doubles
8 tasks per node
7 MKL threads per task (oversubscribing = 1)
IntelPython 2.7.13



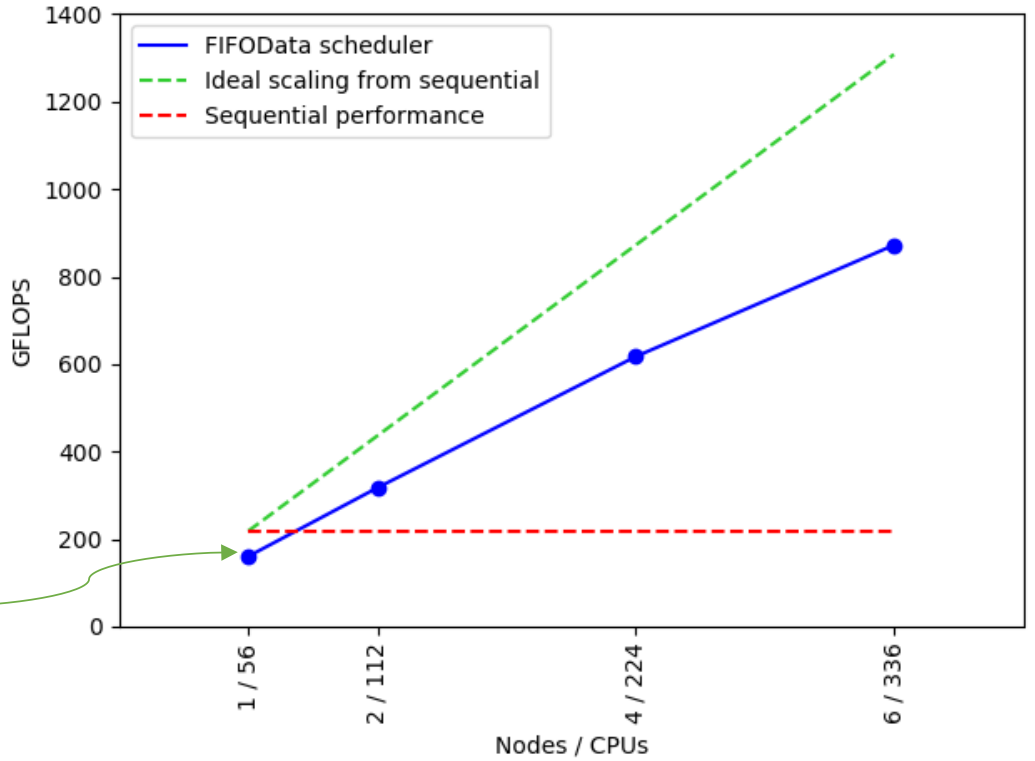
Baseline: Maximum performance attained with multi-threaded MKL in a single node
a block of size 32768 x 32768

LU evaluation

- Results in SSF cluster, distributed through several nodes
  - Lustre as shared file system
  - 2 x Xeon E52690 – V4, 14 cores/socket, 2-threads/core
  - 110 GB/node

Matrix = 82K X 82K doubles
Block size = 4096 x 4096 doubles
8 tasks per node
7 MKL threads per task (oversubscribing = 1)
IntelPython 2.7.13

Baseline: Maximum performance attained with multi-threaded MKL in a single node
a block of size 32K x 32K



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Conclusions and future work

Conclusions and future work

- Task-based programming models provide a friendly interface that enables the parallelization of sequential applications
- PyCOMPSs provides a high level, easy interface to develop parallel linear algebra codes
  - Sequential Python scripts
  - Two level of parallelism: Parallelisation at task level and thread parallelization (MKL)
  - Agnostic of the platform
  - Possibility to run Python sequential codes in distributed platforms with small effort
    - Performance reasonable
    - Use of distributed memory
- Tradeoff between scalability and performance
  - Performance analysis with Paraver helps significantly
    - PyCOMPSs traces with hardware counters
- Future work:
  - Enhacenments in scheduling policies
  - Develop reduction schemes
  - New codes and try new architectures
  - Implement data analytics algorithms on top of PyCOMPSs, using linear algebra parallelized kernels as basis

Workflows and distributed computing group (COMPSs)

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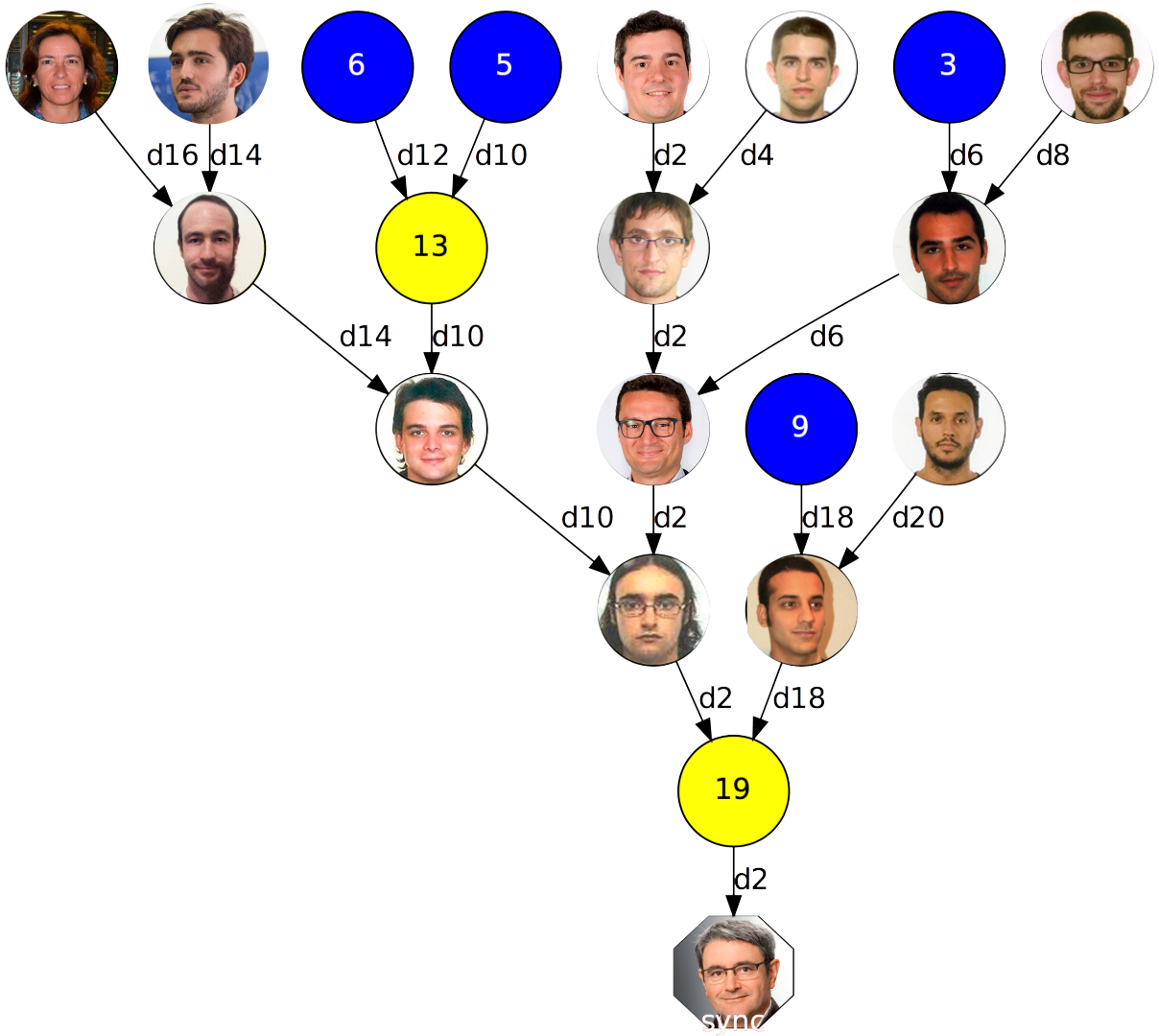

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Thanks!

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Intel-BSC Exascale Lab

Collaboration between Intel and the Barcelona Supercomputing Center