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COMPSs Tutorial

February 9-10 2016, Valencia

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EXCELENCIA
SEVERO
OCHOA

Outline (Feb 9th 2016)

- Session 1 (15:00 – 16:30): Introduction to COMPSs
  - Programming model
    - Java Syntax
    - Demo: First Java example
    - Python syntax
    - Demo: First Python example
    - Other sample codes
- Coffee break (16:30 – 16:45)
- Session 2 (16:45 – 18:15):
  - COMPSs execution environments

Outline (Feb 9th 2016)

- Session 3 (18:15 - 19:45) Hands-on I
  - Virtual Machine Setup
  - Java Hands-on
    - Word-count taskified code
    - Configuration, monitoring, debugging
    - Graph generation
- Session 4 (19:45 – 21:00): Hands-on II
  - Python Hands-on
    - Word-count without annotations
    - Annotate tasks
    - Execution in MN 3
    - Overview of tracing, trace analysis
    - Code optimization (reduce in a tree)
- Final notes

Outline (Feb 10th 2016)

- Session 5 (10:00 - 12:00) Hands-on III – EGI
  - Virtual Machine Setup - Daniele
  - Java Hands-on – Daniele

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Introduction

Motivation

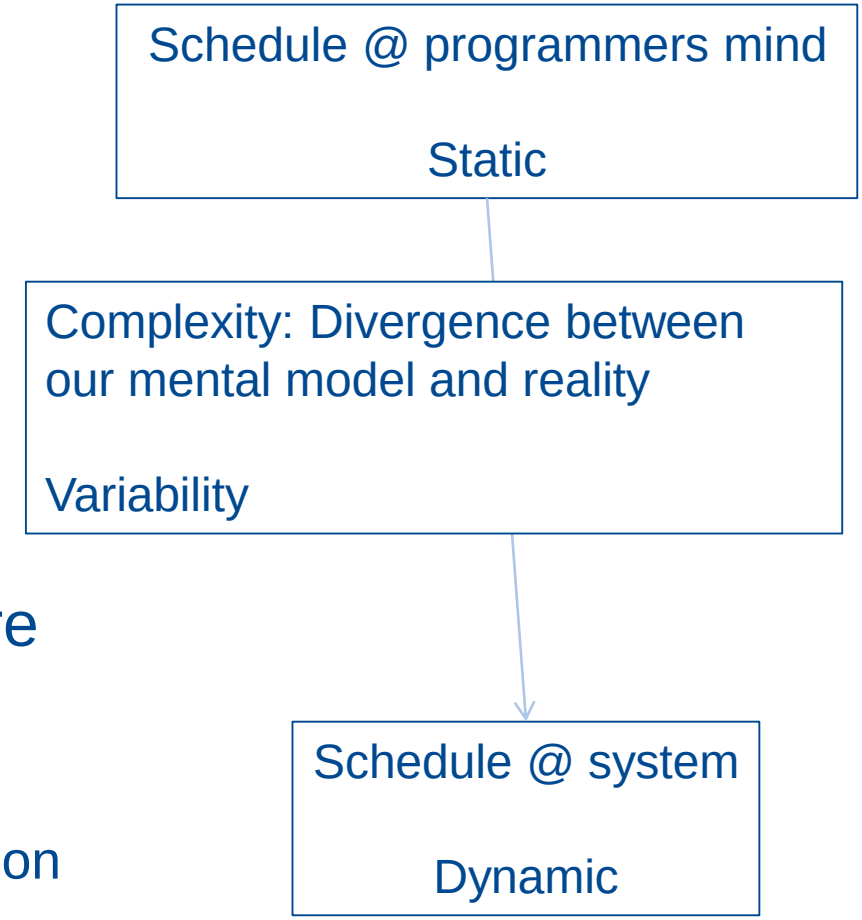
- New complex architectures constantly emerging
  - With their own way of programming them
    - Fine grain: e.g. APIs to run with GPUs, NVMs (Non-Volatile Memories)
    - Coarse grain: e.g. APIs to deploy in Clouds
  - **Difficult** for programmers
    - Higher learning curve / Time To Market (TTM)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

Motivation

- Create tools that make user's life **easier**
  - Intermediate layer: let the difficult parts to those tools
    - Act on behalf of the user
    - Distributing the work through resources
    - Dealing with architecture specifics
    - Automatically improving performance
  - Tools for visualization
    - Monitoring
    - Performance analysis

The parallel programming revolution

- Parallel programming in the past
  - Where to place data
  - What to run, where
  - How to communicate



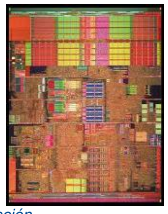
- Parallel programming in the future
  - What do I need to compute
  - What data do I need to use
  - Hints (not necessarily very precise) on potential concurrency, locality,…
  - YOU PROGRAM **SEQUENTIALLY**!!!

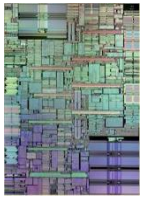
Living in the programming revolution

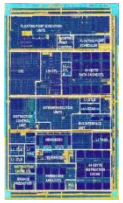
- At the beginning there was one language

Applications

ISA / API







Programs "decoupled" from hardware

Simple interface Sequential program

ILP

Living in the programming revolution

- Multicores made the interface to leak

Application logic
+
Platform specificities

Address spaces (hierarchy, transfer), control flows, …

BSC Vision in the programming revolution (StarSs)

- Need to decouple again

Applications

PM: High-level, clean, abstract interface

Power to the runtime

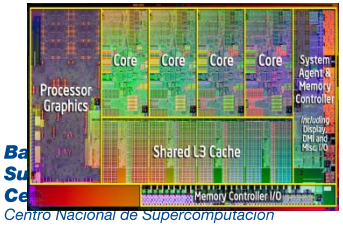
ISA / API

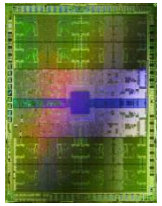
Application logic

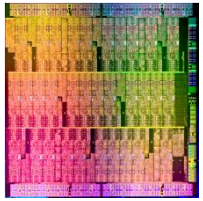
Arch. independent

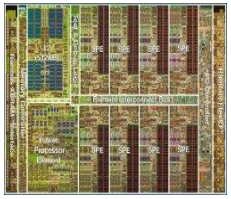
General purpose
Task based
Single address space

"Reuse"
architectural ideas
under
new constraints
(Out-Of-Order
execution)









BSC Vision in the programming revolution (StarSs)

Applications

DSL1

DSL2

DSL3

PM: High-level, clean, abstract interface

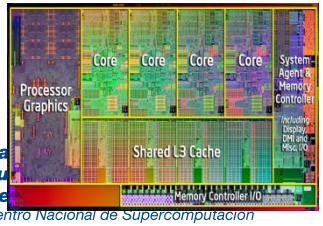
Power to the runtime

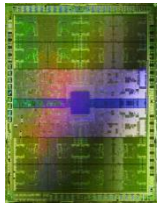
ISA / API

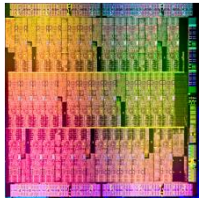
Fast prototyping

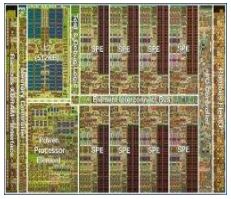
Special purpose

Must be easy to develop/maintain









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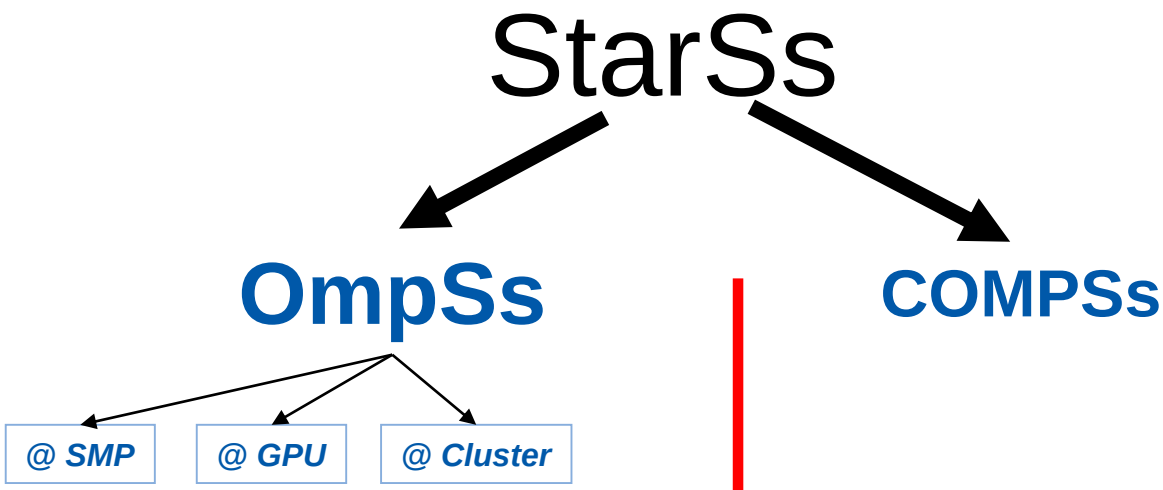
The StarSs "Granularities"



Average task Granularity:	
100 microseconds – 10 milliseconds	10 ms - 1 day
Address space to compute dependences:	
Memory	Files, Objects, NVMs
Language bindings:	
C, C++, FORTRAN	Java, C/C++, Python

SMPs, Clusters **Clusters, Clouds**

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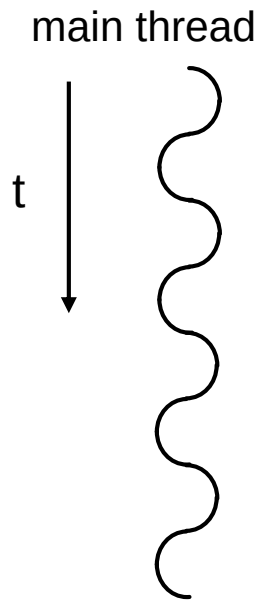
Let's narrow the StarSs idea…for Distributed Architectures

- Cluster / Cloud applications are complex to develop
  - Even more if you want to run things in parallel
  - **Goal 1: Keep a Sequential Programming Paradigm**
    - Writing an application for a computational distributed infrastructure should be as easy as writing a sequential application
  - **Goal 2: Exploit parallelism**
    - Run it as fast as possible
- Target applications: composed of tasks, most of them repetitive
  - Granularity of the tasks: enough to be distributed (simulators, …)
  - Data: files, objects, arrays and primitive types

Programming Model: Properties (I)

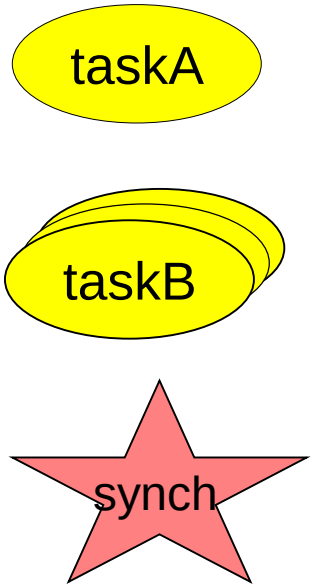
- Based on sequential programming
  - No APIs, no threading, no messaging
  - No parallel constructs, no pragmas
  - Sequential consistency




```
Main Program {
   taskA(data1);

   for (int i=0; i< N; i++)
     taskB(data1, data2);

   if (condition)
     process(data2);
}
```



Runtime System

Application

Task Selection Interface

Runtime System

Grid

Cluster

Cloud

Supported Features

- Basic Features:
  - Data dependency analysis
  - Data transfer
  - Task scheduling
  - Resource management
  - Results collection
  - Fault tolerance
  - Method and Web Service Tasks

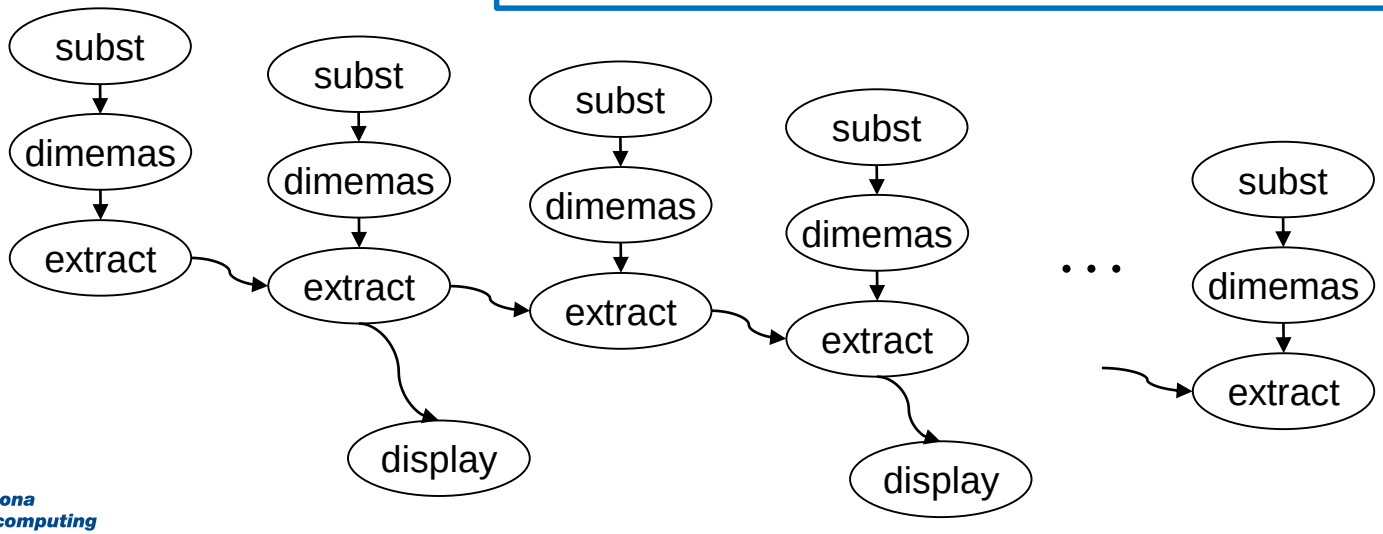
- Advanced Features:
  - Shared disks support
  - Constraints based scheduling
  - Task versioning support

Programming Model: Dependency detection

- Automatic on-the-fly creation of a task dependency graph

Main Program

```
for (int i = 0; i < N; i++) {
   newBWD = random();
   subst(refCFG, newBWD, newCFG);
   dimemas(newCFG, trace, dimOUT);
   extract(newBWD, dimOUT, finalOUT);
   if (i % 2 == 0) display(finalOUT);
}
```



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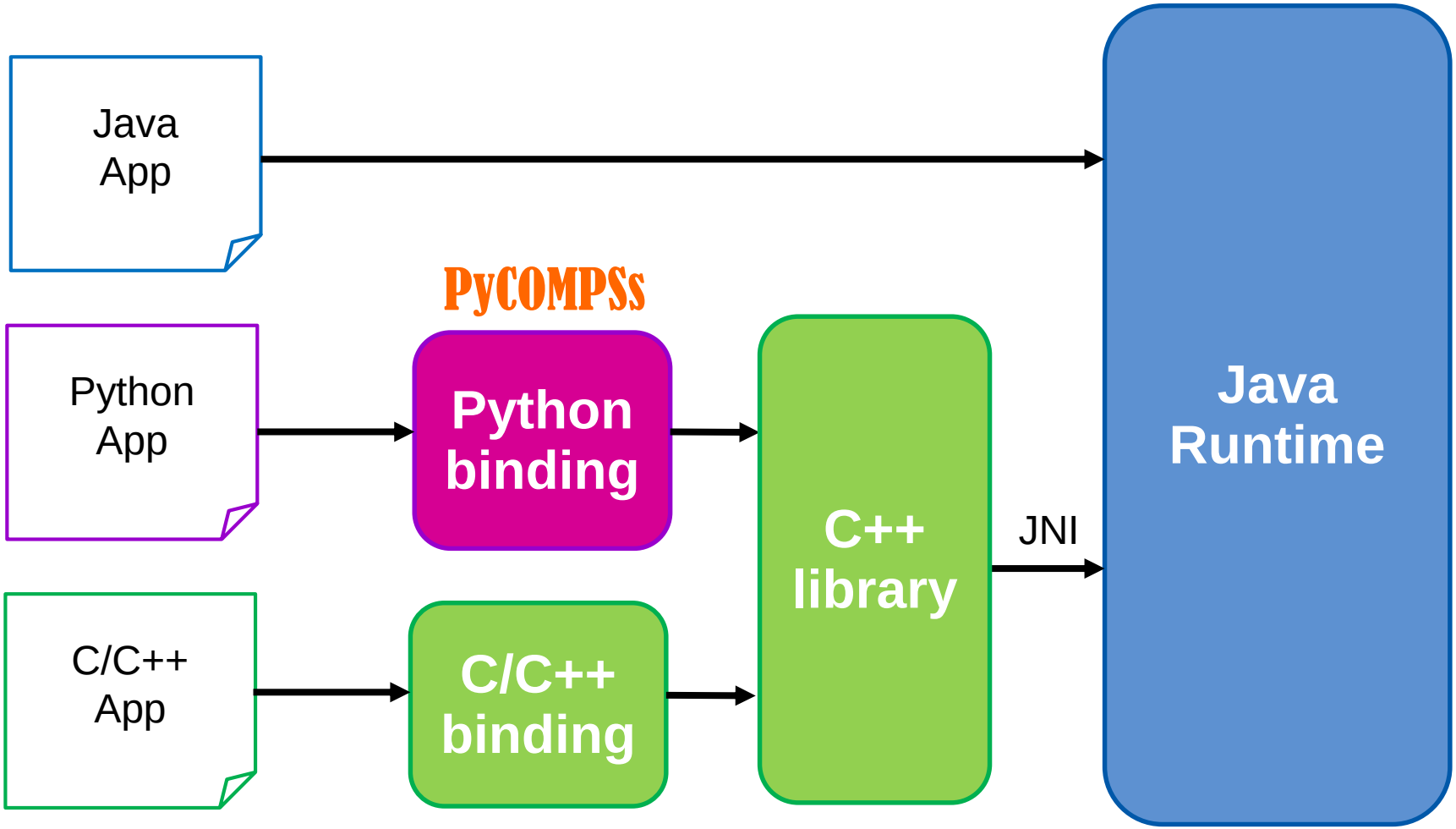
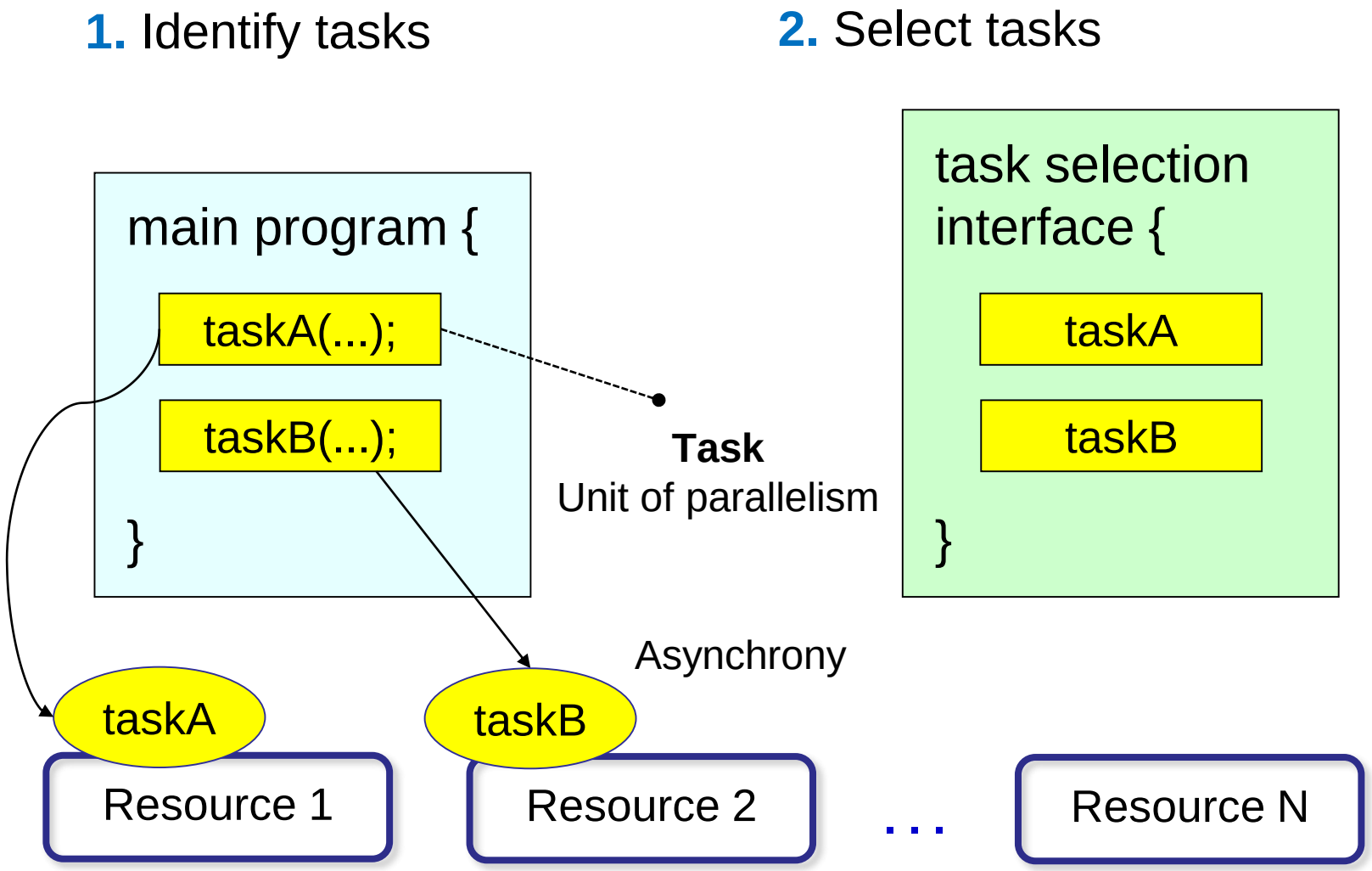
Java Syntax

COMPSs Bindings



Programming Model: Steps



Programming Model: Task selection interface

```
public interface SampleItf {
   @Constraints(processorCPUCount = 1, memoryPhysicalSize = 0.5f)
   @Method(declaringClass = "servicess.Example")
   void myMethod(
      @Parameter(direction = INOUT)
      Reply r
    );

   @Service(namespace = "http://servicess.es/example",
            name = "SampleService",
            port = "SamplePort")
   Reply myServiceOp(
      @Parameter(direction = IN)
      Query q
    );
}
```

Programming Model: Regular Main program

```
public class App {

   public static void main(String[] args) {
       Query query = new Query(…);
       Reply reply = myServiceOp(query);

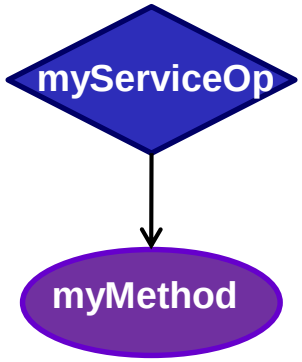
       myMethod(reply);

       reply.printToLog();
   }
}
```

Service task call

Method task call

Synchronization

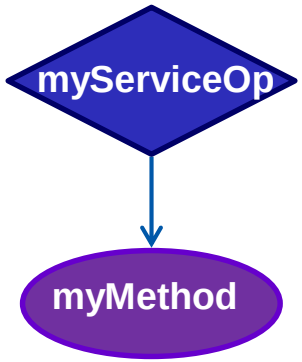


Programming Model: Service Operation

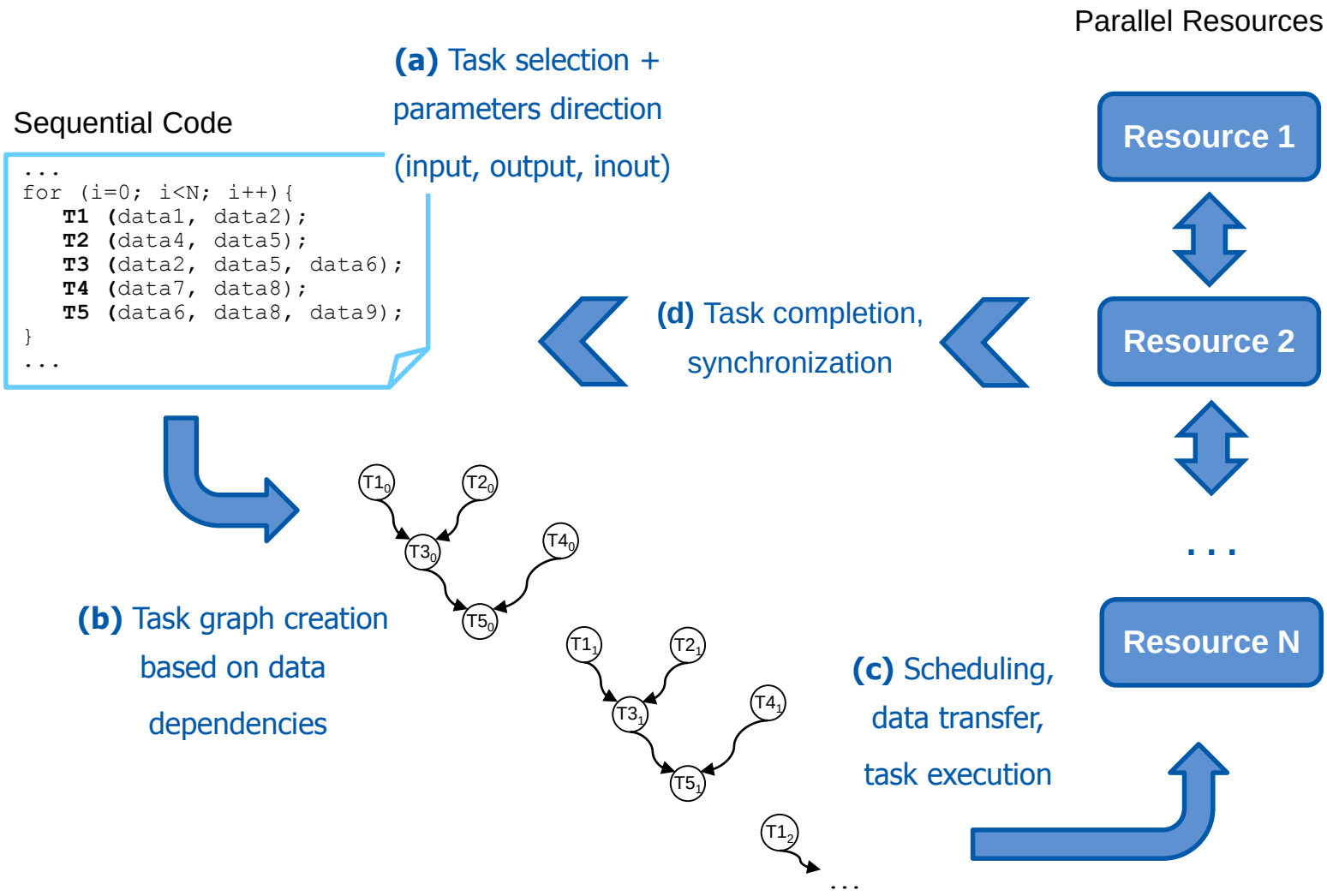
```
public class ServiceApp {
   @Orchestration
   public static void sampleComposite() {
       Query query = new Query(…);
       Reply reply = myServiceOp(query);

       myMethod(reply);

       reply.printToLog();
   }
}
```



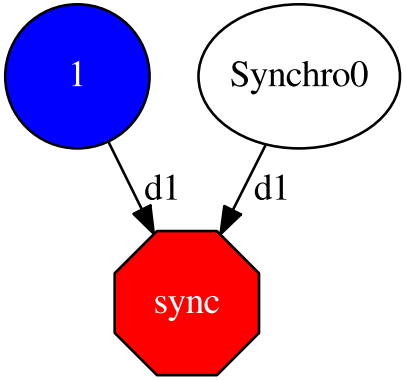
Programming Model: Summary



JAVA EXAMPLE

Java COMPSs applications

Simple counter




```
// Write value
FileOutputStream fos = new FileOutputStream(fileName);
                fos.write(initialValue);
                fos.close();                System.out.println("Initial counter value
is " + initialValue);

//Execute increment     SimpleImpl.increment(fileName);

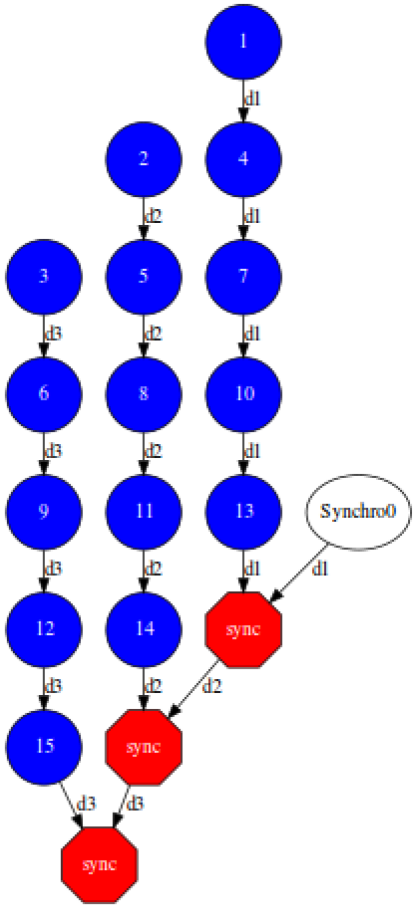

// Write new value
FileInputStream fis = new FileInputStream(fileName);
 int finalValue = fis.read();
                fis.close();
```

```
public interface SimpleItf {
                @Constraints(processorCoreCount = 1)
                @Method(declaringClass = "simple.SimpleImpl")

void increment(
        @Parameter(type = Type.FILE, direction = Direction.INOUT)
          String file          );}
```

Java COMPSs applications

- Counter++




```
int N = Integer.parseInt(args[0]);
int counter1 = Integer.parseInt(args[1]);
int counter2 = Integer.parseInt(args[2]);
int counter3 = Integer.parseInt(args[3]);

// Initialize counter files
System.out.println("Initial counter values:");
                initializeCounters(counter1, counter2, counter3);
                // Print initial counters state
                printCounterValues();

// Execute increment tasks
for (int i = 0; i < N; ++i) {
                IncrementImpl.increment(fileName1);
                IncrementImpl.increment(fileName2);
                IncrementImpl.increment(fileName3);
}

public static void increment(String counterFile) throws
FileNotFoundException, IOException {                    // Read value
                        FileInputStream fis = new
FileInputStream(counterFile);                   int count = fis.read();
                fis.close();                                    // Write new
value                   FileOutputStream fos = new
FileOutputStream(counterFile);                  fos.write(++count);
                fos.close(); }
```

Matrix multiply in Java

```
for (int i = 0; i < MSIZE; i++){
    for (int j = 0; j < MSIZE; j++){
        for (int k = 0; k < MSIZE; k++){
            MatmulImpl.multiplyAccumulative( _C[i][j], _A[i][k], _B[k][j] );
        }
    }
}
```

```
public static void multiplyAccumulative( String f3, String f1,
String f2 )
{
    Block a = new Block( f1 );
    Block b = new Block( f2 );
    Block c = new Block( f3 );
    c.multiplyAccum( a, b );
    try
        …
}

public void multiplyAccum ( Block a, Block b )
{
    for( int i = 0; i < this.bRows; i++ )          // rows
        for( int j = 0; j < this.bCols; j++ )      // cols
            for ( int k = 0; k < this.bCols; k++ )// cols
                this.data[i][j] += a.data[i][k] * b.data[k][j];
}
```

Matrix multiply in Java

```
package matmul;

import integratedtoolkit.types.annotations.Constraints;
import integratedtoolkit.types.annotations.Method;
import integratedtoolkit.types.annotations.Parameter;
import integratedtoolkit.types.annotations.Parameter.*;


public interface MatmulItf {
@Constraints(processorCoreCount = 4, memoryPhysicalSize = 1.5f)
@Method(declaringClass = "matmul.MatmulImpl")
void multiplyAccumulative(
    @Parameter(type = Type.FILE, direction = Direction.INOUT)
    String file1,

    @Parameter(type = Type.FILE, direction = Direction.IN)
    String file2,

    @Parameter(type = Type.FILE, direction = Direction.IN)
    String file3
);

}
```

Python Syntax

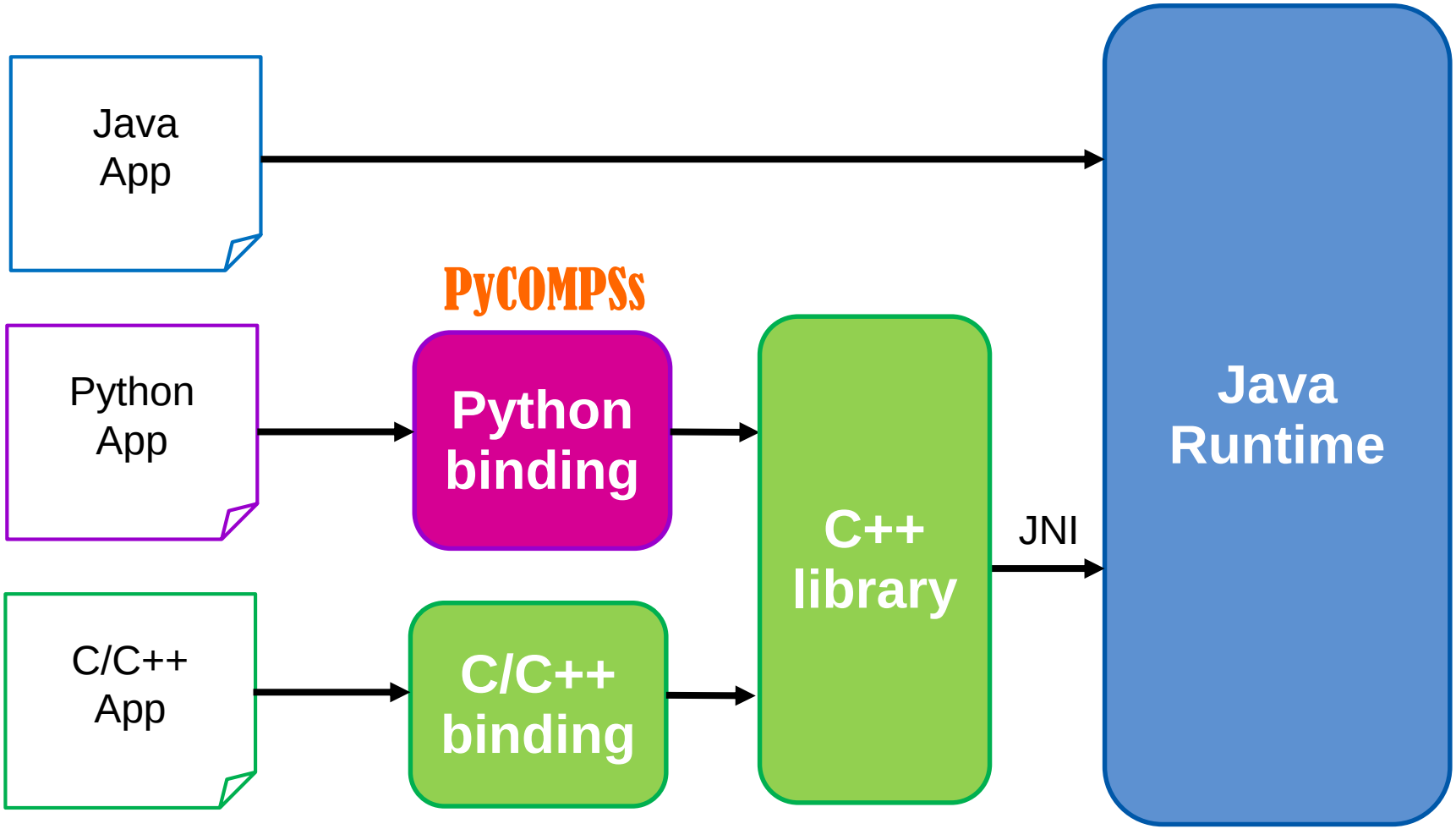
Why Python?

- Python is powerful... and fast;
  plays well with others;
  runs everywhere;
  is friendly & easy to learn;
  is Open. *

- Its design philosophy emphasizes code readability, and its syntax allows programmers to express concepts in fewer lines of code than would be possible in languages such as C
- Large community using it, including scientific and numeric
- Object-oriented programming and structured programming are fully supported
- Large number of software modules available (38,000 as of January 2014)

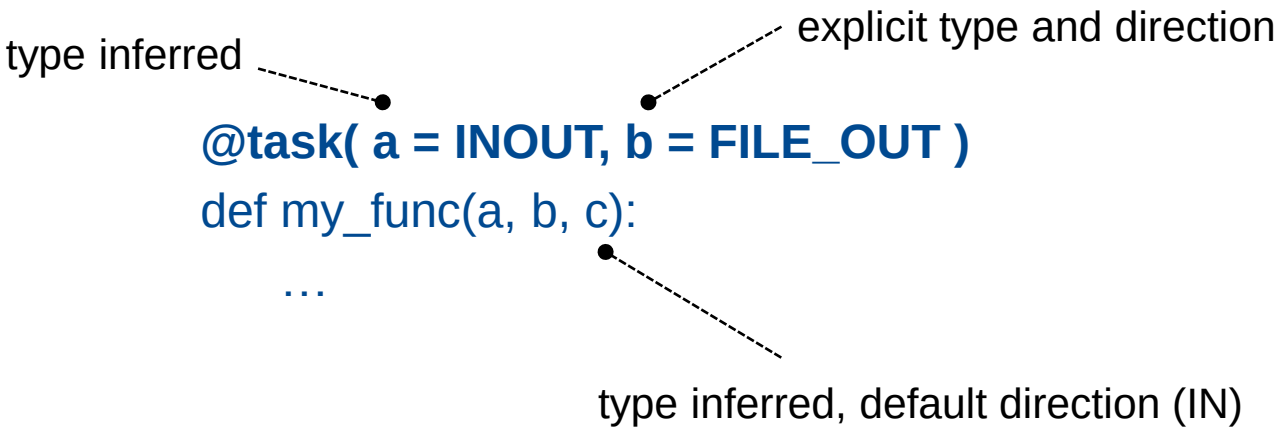
* From python.org

COMPSs Bindings



PyCOMPSs: Task definition

- Task definition with Python decorators
  - Provide information about task parameters (*TYPE_DIRECTION*):
    - Type
      - Only mandatory for files
      - Inferred for the rest of the types
    - Direction
      - Default IN (read-only)
      - Mandatory for INOUT (read-write) and OUT (write-only)



PyCOMPSs: Task definition (II)

- The @task decorator: special arguments
  - Type of the return value → mandatory if a value is returned

```
@task(returns = int)
def ret_func():
    return 1
```

  - Does the task modify the callee object? → default True

```
class MyClass(object):

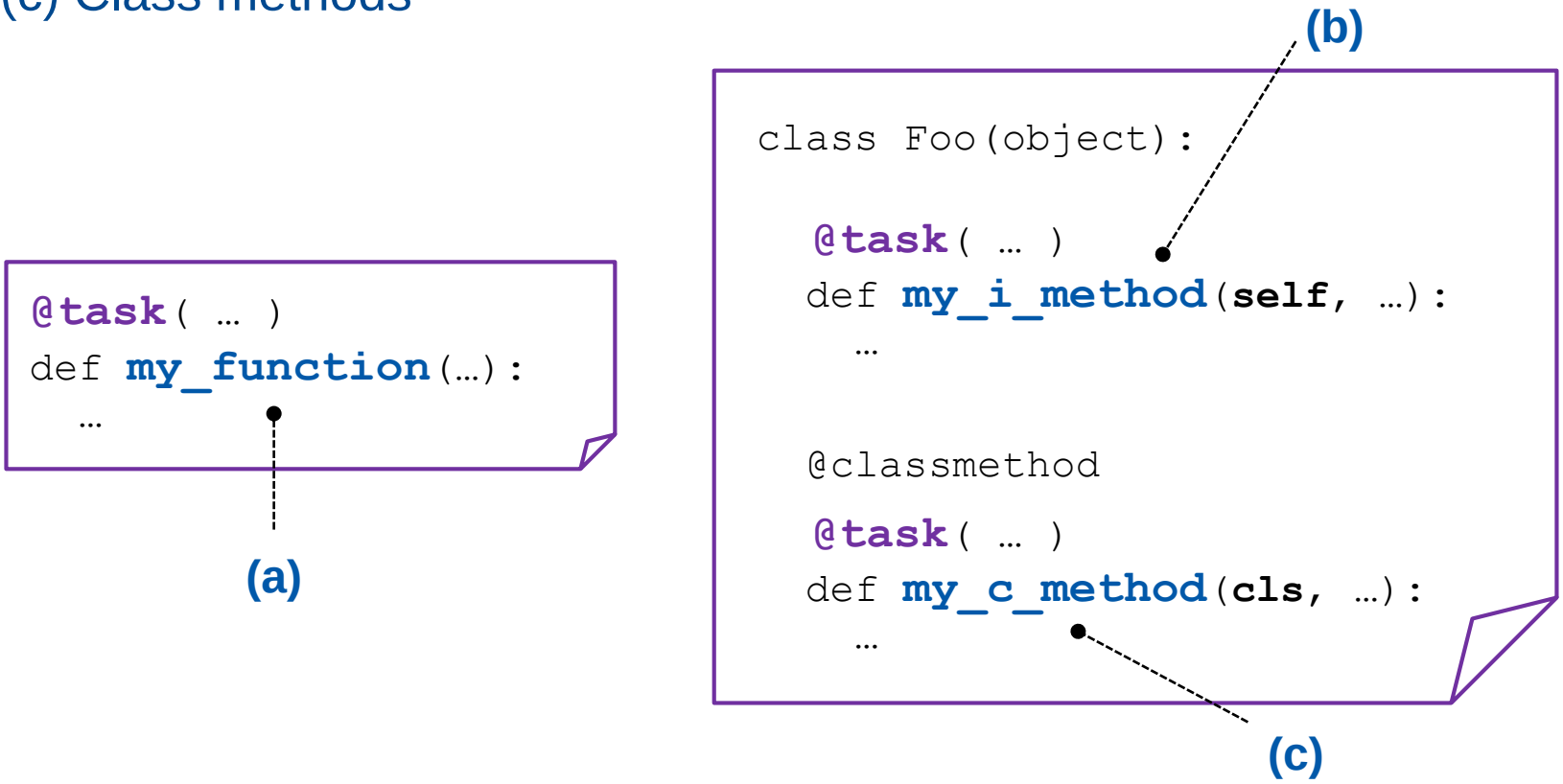
    @task(isModifier = False)
    def instance_method(self):
        …  # self is NOT modified here
```

  - Is it a priority task? → Default False

```
@task(priority = True)
    def prio_func():
        …
```

PyCOMPSs: Task types

- What can be selected as a task?
  - (a) Functions
  - (b) Instance methods
  - (c) Class methods



PyCOMPSs: Main program → Synchronization API

- Data created or updated by a task can be used in the main program of the application
  - But we need to synchronize first!

- Two API methods for synchronization
  - *compss_open* → files

```
my_file = 'file.txt'
func(my_file)
fd = compss_open(my_file)
…
```

func is a task that modifies *my_file*

  - *compss_wait_on* → objects

```
my_obj = MyClass()
my_obj.method()
my_obj = compss_wait_on(my_obj)
…
```

method is a task that modifies *my_obj*

PyCOMPSs: Main program → Future objects

- Mechanism to make asynchronous those tasks that return a value
  - Synchronization is only triggered when necessary
- The future object is a representative of the object yet to be generated

```
@task(returns = MyClass)
def ret_func():
    return MyClass(…)
…
```

future object

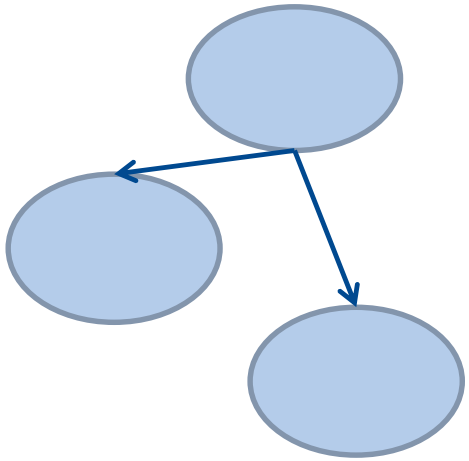
```
o = ret_func()
```

PyCOMPSs: Main program → Future objects (II)

- A future object can be involved in a subsequent task call
  - PyCOMPSs will automatically enforce the dependency

future object ----------•

```
o = ret_func()
…
another_task(o)
…
o.yet_another_task()
```



- Synchronization from main program (same as other objects):

```
o = ret_func()
…
o = compss_wait_on(o)
```

PyCOMPSs Constraints

- Enables definition of tasks' constraints
  - Resource to execute the task should meet the constraint
- Decorator definition:
  - @constraint(constraint1="value1", constraint2="value2, …)
- Examples of supported constratints:
  - ProcessorArch
  - ProcessorCoreCount
  - MemoryPhysicalSize
  - AppSoftware

PyCOMPSs: Wrap-up example

- Invoke tasks as Python functions/methods
- API for data synchronization

Main Program

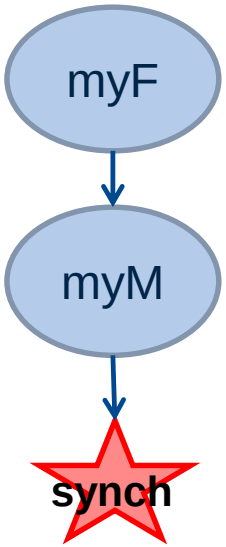
```
foo = Foo()
myFunction(foo)
foo.myMethod()
…
foo = compss_wait_on(foo)
foo.bar()
```

- Task selection in function definition (decorators)

Function definition

```
@task( par = INOUT )
def myFunction(par):
  …
```

```
class Foo(object):
  @task()
  def myMethod(self):
    …
```



Increment.py

Increment is an applic
that takes three differe
values and increases t
a number of given time

The purpose of this
application is to show
parallelism between th
different increments.

Counters stored
in files

```
def main_program():
    # Check and get parameters
    if len(sys.argv) != 5:
        usage()
        exit(-1)
    N = int(sys.argv[1])
    counter1 = int(sys.argv[2])
    counter2 = int(sys.argv[3])
    counter3 = int(sys.argv[4])

    # Initialize counter files
    initializeCounters(counter1, counter2, counter3)
    print "Initial counter values:"
    printCounterValues()

    # Execute increment
    for i in range(N):
        increment(FILENAME1)
        increment(FILENAME2)
        increment(FILENAME3)

    # Write final counters state (sync)
    print "Final counter values:"
    printCounterValues()
```

Increment.py

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        exit(-1)
    N = int(sys.argv[1])
    counter1 = int(sys.argv[2])
    counter2 = int(sys.argv[3])
    counter3 = int(sys.argv[4])

    # Initialize counter files
    initializeCounters(counter1, counter2, counter3)
                                                values:"
```

```
@task(filePath = FILE_INOUT)
def increment(filePath):
    # Read value
    fis = open(filePath, 'r')
    value = fis.read()
    fis.close()

    # Write value
    fos = open(filePath, 'w')
    fos.write(str(int(value) + 1))
    fos.close()
```

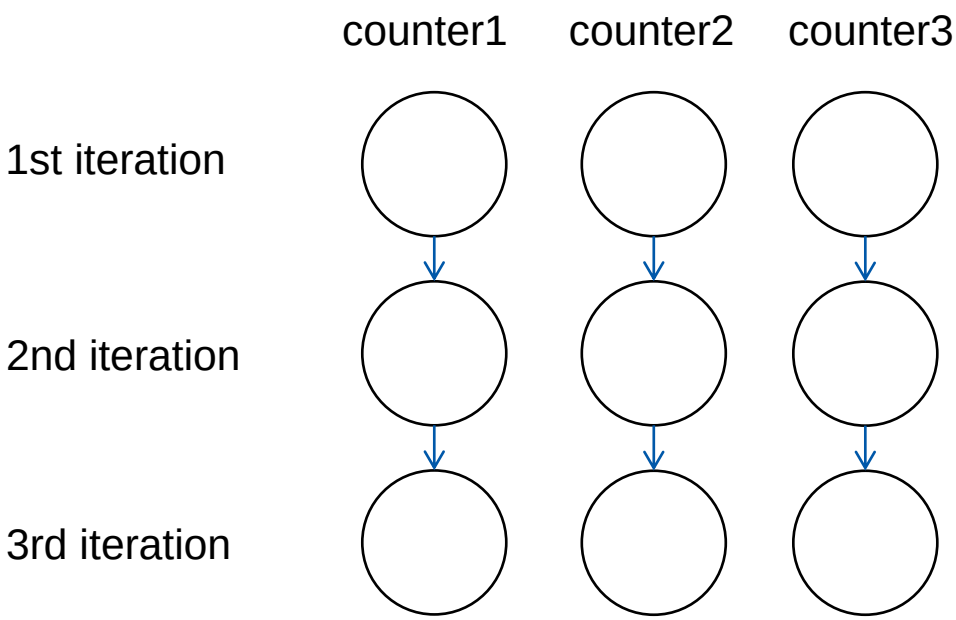
```
                                                )
                                                2)
                                                3)

                                                state (sync)
                                                alues:"
```

Increment.py

- Task graph identical to the Java case

Task Graph

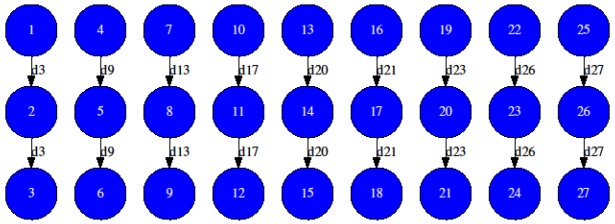


Other sample codes

Matrix multiply with constraints in Python

```
from pycompss.api.constraint import constraint
from pycompss.api.task import task
from pycompss.api.parameter import INOUT

@constraint(ProcessorCoreCount=8)
@task(c = INOUT)
def multiply(a, b, c):
    import numpy
    c += a*b
```




```
    args = sys.argv[1:]
    MSIZE = int(args[0])
    BSIZE = int(args[1])

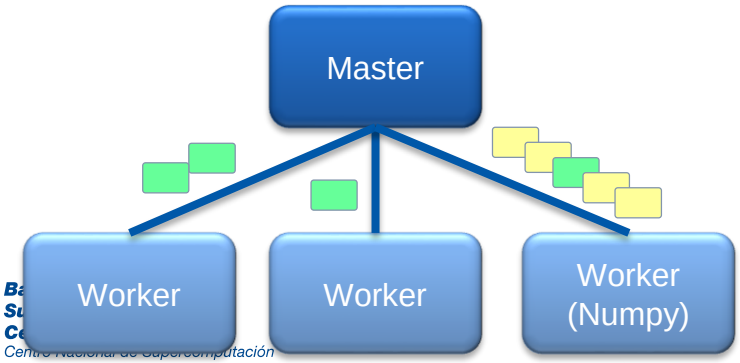
    A = B = C = []
    # Initialize A, B & C as np.array(BSIZE, BSIZE)
    initialize_variables()

    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])
```

PyCOMPSs constraints

```
@task(returns=str)
def mutate(source):
    charpos = random.randint(0, len(source) - 1)
    parts = list(source)
    parts[charpos] = chr(ord(parts[charpos]) +
                         random.randint(-1,1))
    return ''.join(parts)
```

```
@constraint(AppSoftware="Numpy")
@task(returns=int)
def fitness(source, target):
    import numpy
    fitval = 0
    a = numpy.array([ord(i) for i in source])
    b = numpy.array([ord(i) for i in target])
    fitval = numpy.linalg.norm(a-b)
    return fitval
```




```
fitval = fitness(source, target)
i = 0
while True:
    i += 1
    m = mutate(source)
    fitval_m = fitness(m, target)
    fitval_m = compss_wait_on(fitval_m)
    if fitval_m < fitval:
        fitval = fitval_m
m = compss_wait_on(source)
```

Sample code: Kmeans @ PyCOMPSs

```
from pycompss.api.api import compss_wait_on
size = int(numV / numFrag)

X = [genFragment(size, dim) for _ in range(numFrag)]
mu = init_random(dim, k)
oldmu = []
n = 0
startTime = time.time()
while not has_converged(mu, oldmu, epsilon, n, maxIterations):
    oldmu = mu
    clusters = [cluster_points_partial(X[f], mu, f * size) for f in range(numFrag)]
    partialResult = [partial_sum(X[f], clusters[f], f * size) for f in range(numFrag)]

    mu = merge_reduce(reduceCentersTask, partialResult)
    mu = compss_wait_on(mu)
    mu = [mu[c][1] / mu[c][0] for c in mu]
    n += 1
return (n, mu)
```

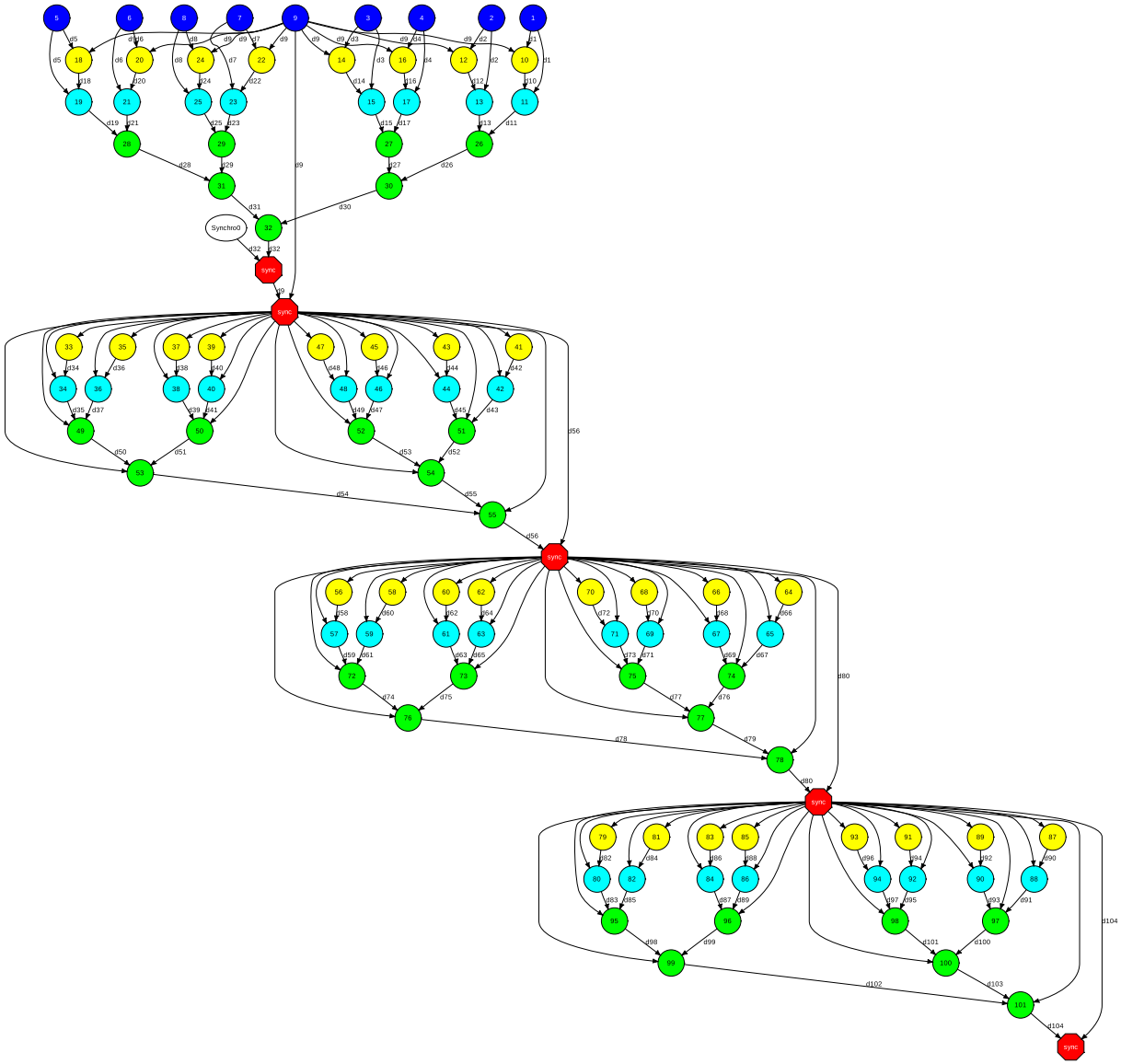
```
@task(returns=dict, priority=True)
def reduceCentersTask(a, b):
    for key in b:
        if key not in a:
            a[key] = b[key]
        else:
            a[key] = (a[key][0] + b[key][0],
                      a[key][1] + b[key][1])
    return a
```

```
@task(returns=dict)
def partial_sum(XP, clusters, ind):
    import numpy as np
    XP = np.array(XP)
    p = [(i, [(XP[j - ind]) for j in clusters[i]]) for i in clusters]
    dic = {}
    for i, l in p:
        dic[i] = (len(l), np.sum(l, axis=0))
    return dic
```

```
@task(returns=dict)
def cluster_points_partial(XP, mu, ind):
    import numpy as np
    dic = {}
    XP = np.array(XP)
    for x in enumerate(XP):
        bestmukey = min([(i[0], np.linalg.norm(x[1] - mu[i[0]]))
                         for i in enumerate(mu)], key=lambda t: t[1])[0]
        if bestmukey not in dic:
            dic[bestmukey] = [x[0] + ind]
        else:
            dic[bestmukey].append(x[0] + ind)
    return dic
```

Sample code: Kmeans @ PyCOMPSs

- Task graph:
  - 8 fragments
  - 4 iterations



- Computation of mutual cross-correlations between all pairs of a set of spike data
- Also computes the cross-correlations for surrogate data sets for each neuron pair

Sequential code

```
f = open('./spikes.dat', 'r')
spikes = pickle.load(f)
f.close()
#preallocate result variables
num_ccs = (num_neurons**2 - num_neurons)/2
cc_orig = zeros((num_ccs,2*maxlag+1))
cc_surrs = zeros((num_ccs,2*maxlag+1,num_surrs))
idxrange = range(num_bins-maxlag,num_bins+maxlag+1)
row = 0

#for all pairs ni,nj such that nj > ni
for ni in range(num_neurons-1):
  for nj in range(ni+1,num_neurons):
                cc_orig[row,:] = correlate(spikes[ni,:],spikes[nj,:],…
                num_spikes_i = sum(spikes[ni,:])
                num_spikes_j = sum(spikes[nj,:])
                for surrogate in range(num_surrs):
                  surr_i = zeros(num_bins)
                  surr_i[random.random_integers(0,num_bins-1,num_spikes_i)] = 1
                  surr_j = zeros(num_bins)
                  surr_j[random.random_integers(0,num_bins-1,num_spikes_j)] = 1
                  cc_surrs[row,:,surrogate] = correlate(surr_i,surr_j,"full")[idxrange]
                row = row +1
#save results
f = open('./result_cc_originals.dat','w')
pickle.dump(cc_orig,f)
f.close()
f = open('./result_cc_surrogates.dat','w')
pickle.dump(cc_surrs,f)
f.close()
```

Neuroscience Data Processing @ Parallel Python

Main program

```
…
# tuple of all parallel python servers to connect with
ppservers = ('comp1.my-network', 'comp2.my-network' …

if len(sys.argv) > 1:
    ncpus = int(sys.argv[1])
    #creates jobserver with ncpus workers
    job_server = pp.Server(ncpus, …
else:
    #creates jobserver with workers automatically detected
    job_server = pp.Server(ppservers=ppservers,  …

#wait for servers to come up
time.sleep(5)

#calculate number of nodes in total
nlocalworkers = job_server.get_ncpus()
activenodes = job_server.get_active_nodes()
workerids = activenodes.keys()
nworkers=sum( [activenodes[workerids[i]] for i in
range(len(workerids))] ) + nlocalworkers
num_ccs = (num_neurons**2 - num_neurons)/2

#calculate number of pairs each worker should process
step = ceil(float(num_ccs)/nworkers)
start_idx = 0
end_idx = 0
starts = zeros((nworkers+1,))
…
```

Explicit resources declaration

Function definition

```
def cc_surrogate_range(start_idx, end_idx, seed, num_neurons,
num_surrs, num_bins, maxlag):
  …
```

Main program (cont)

```
for worker in range(nworkers):
    start_idx = end_idx
    end_idx = int(min((worker+1)*step,num_ccs))
    …
    depfuncs = ()
    depmodules = "numpy","pickle",
    jobs.append(job_server.submit(cc_surrogate_range,…
    …
cc_original = zeros((num_ccs,2*maxlag+1))
cc_surrs = zeros((num_ccs,2*maxlag+1,2))
for worker in arange(nworkers):
    start = starts[worker]
    end = starts[worker + 1]
    result = jobs[worker]()
    cc_original[start:end,:] = result[0]
    cc_surrs[start:end,:,:] = result[1]

f = open('./result_cc_originals.dat','w')
pickle.dump(cc_original,f)
f.close()
f = open('./result_cc_surrogates_conf.dat','w')
pickle.dump(cc_surrs,f)
f.close()
```

Explicit fork join

Data back

Neuroscience Data Processing @ PyCOMPSs

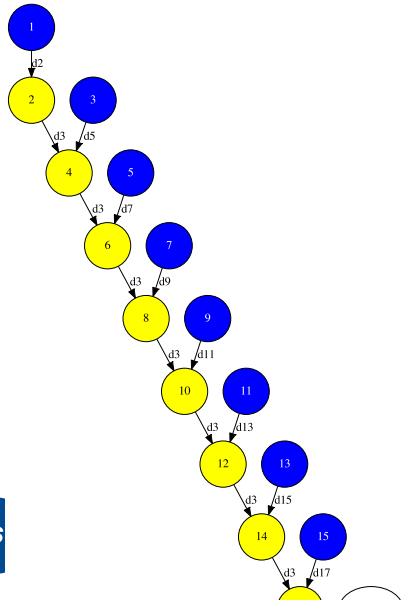
Main program

```
Import sys
from pycompss.api.api import compss_wait_on

num_frags = int(sys.argv[1])

#calculate number of pairs per fragment
num_ccs = (num_neurons**2 - num_neurons)/2
step = ceil(float(num_ccs)/num_frags)
start_idx = 0
end_idx = 0

seed = 2398645
delta = 1782324
```



Tasks definition

```
@task(cc_original = INOUT, cc_surrs = INOUT, priority = True)
def gather(result, cc_original, cc_surrs, start, end):
    cc_original[start:end,:] = result[0]
    cc_surrs[start:end,:,:] = result[1]

@task(returns = list)
def cc_surrogate_range(start_idx, end_idx, seed, num_neurons,
num_surrs, num_bins, maxlag):
    …
```

Main program (cont)

```
cc_original = zeros((num_ccs,2*maxlag+1))
cc_surrs = zeros((num_ccs,2*maxlag+1,2))
for frag in range(num_frags):
    start_idx = end_idx
    end_idx = int(min((frag+1)*step,num_ccs))
    result = cc_surrogate_range(start_idx, end_idx, seed, …
    gather(result, cc_original, cc_surrs, start_idx, end_idx)
    seed = seed + delta

f = open('./result_cc_originals.dat','w')
cc_original = compss_wait_on(cc_original)
pickle.dump(cc_original,f)
f.close()

f = open('./result_cc_surrogates_conf.dat','w')
cc_surrs = compss_wait_on(cc_surrs)
pickle.dump(cc_surrs,f)
f.close()
```

COMPSs execution environment examples

Runtime System

Application

Task Selection Interface

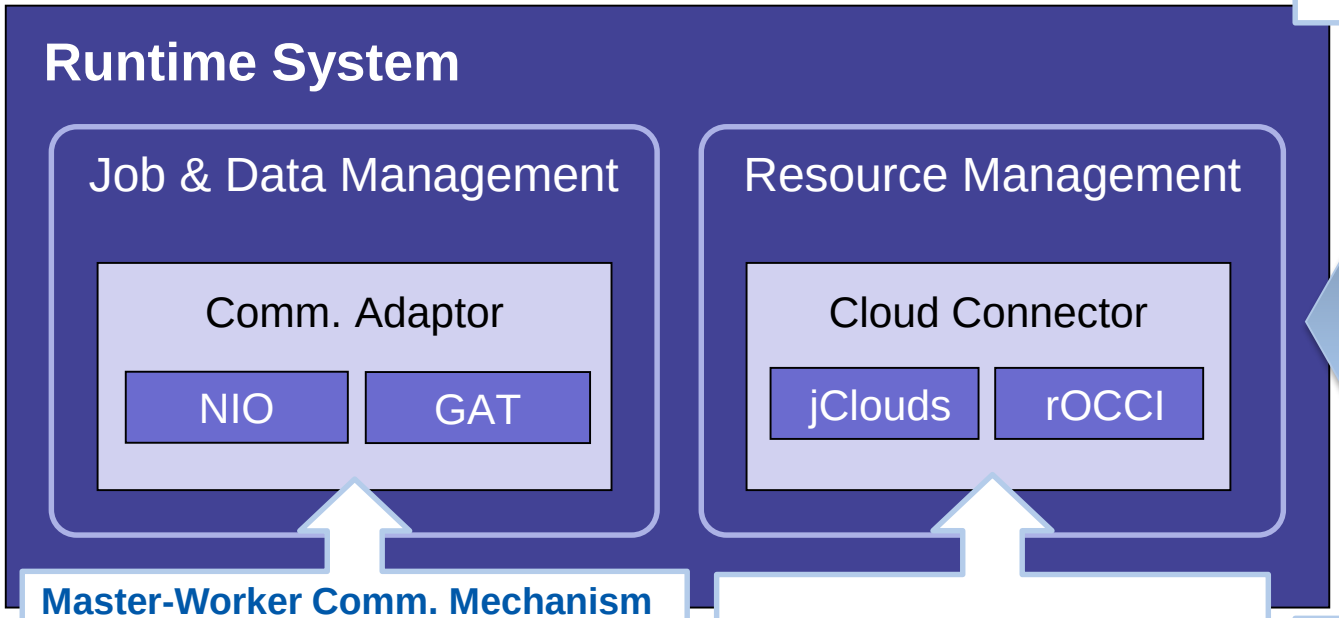
How can I select the execution platform?

Grid

Cluster

Cloud

Execution Environment Configuration Overview



Infrastructure Description
- Describe the available resource in the infrastructure
- Describe Cloud Providers: Images and VM Templates

resources.xml

project.xml

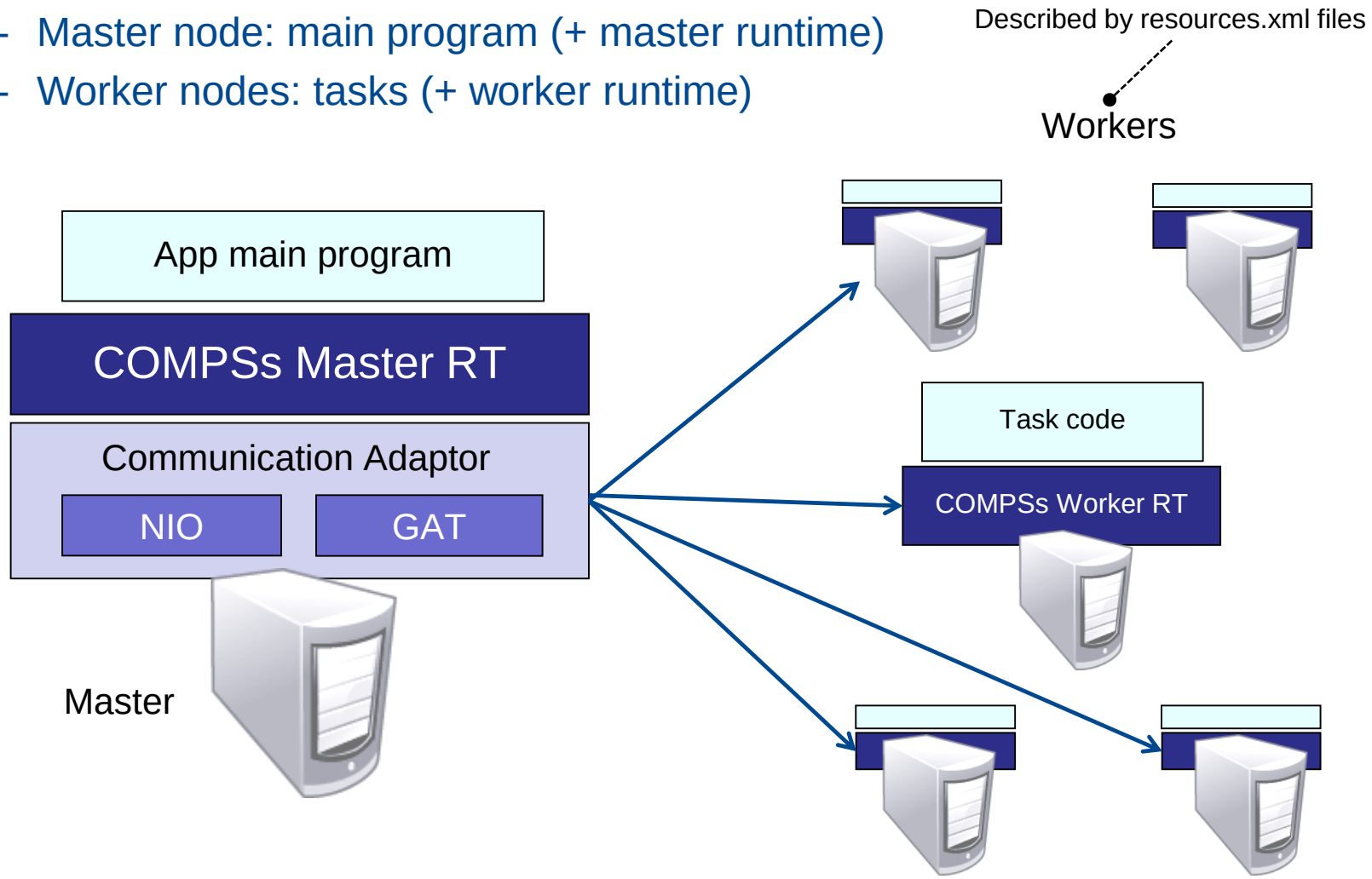
Master-Worker Comm. Mechanism
- GAT: Restrictred environments (only ssh access) and Grid Middleware
- NIO: Efficient Persistent workers implementation
- Controlled and secured environments
- Provided as execution command argument

Resource Scalability
- jClouds: access to most of commercial public clouds
- rOCCI: OGF standard
- Extensible (support others..)
- Described in the resources and project files

Application Exec. Description
- Selection of resources
- Application Code Location
- Working directory
- Provided as execution command argument

COMPSs in remote hosts (interactive)

- Typical setup:
  - Master node: main program (+ master runtime)
  - Worker nodes: tasks (+ worker runtime)



Configuration: Resources Specification

Resources.xml

```
<?xml version="1.0" encoding="UTF-8"?>
<ResourceList>
    <!--Description for any physical node-->
    <Resource Name="172.20.200.18">
        <Capabilities>
            <Host>
                <TaskCount>0</TaskCount>
                <Queue>short</Queue>
                <Queue/>
            </Host>
            <Processor>
                <Architecture>x86</Architecture>
                <Speed>3.0</Speed>
                <CoreCount>2</CoreCount>
            </Processor>
            <OS>
                <OSType>Linux</OSType>
                <MaxProcessesPerUser>32</MaxProcessesPerUser>
            </OS>
            <StorageElement>
                <Size>30</Size>
            </StorageElement>
            …
            <Memory>
                <PhysicalSize>1</PhysicalSize>
                <VirtualSize>8</VirtualSize>
            </Memory>
            <ApplicationSoftware>
                <Software>Java</Software>
            </ApplicationSoftware>
            <Service/>
            <VO/>
            <Cluster/>
            <FileSystem/>
            <NetworkAdaptor/>
            <JobPolicy/>
            <AccessControlPolicy/>
        </Capabilities>
        <Requirements/>
    </Resource>
    <Resource Name="172.20.200.19">
        ...
    </Resource>
</ResourceList>
```

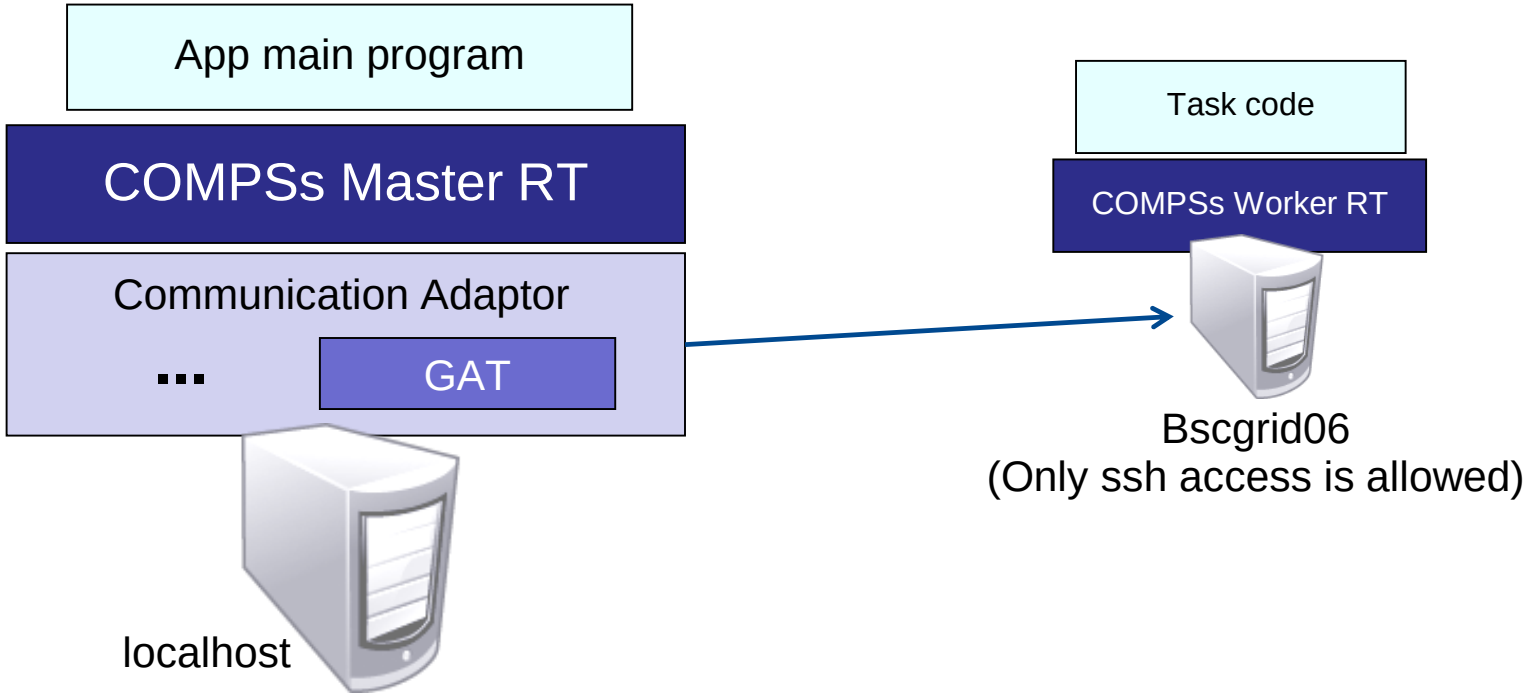
Configuration: Project Specification

Project.xml

```
<?xml version="1.0" encoding="UTF-8"?>
<Project>
        <!--Description for any physical node-->
        <Worker Name="172.20.200.18">
                <InstallDir>/opt/COMPSs/Runtime/scripts/</InstallDir>
                <WorkingDir>/tmp/</WorkingDir>
                <User>user</User>
                <LimitOfTasks>1</LimitOfTasks>
        </Worker>

        <Worker Name="172.20.200.19">
           …
        </Worker>
        ….
</Project>
```

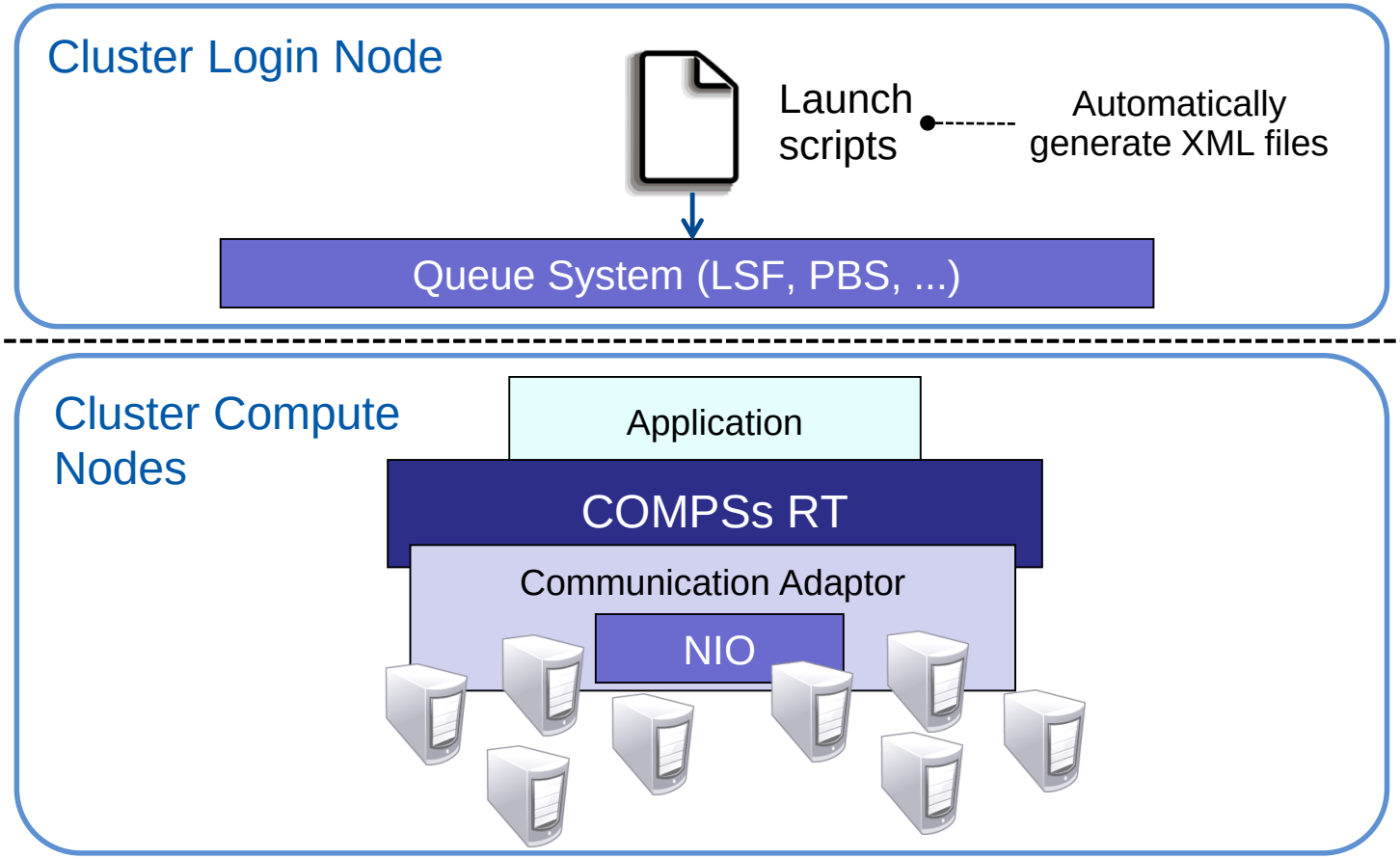
Example: COMPSs using Remote hosts (interactive)



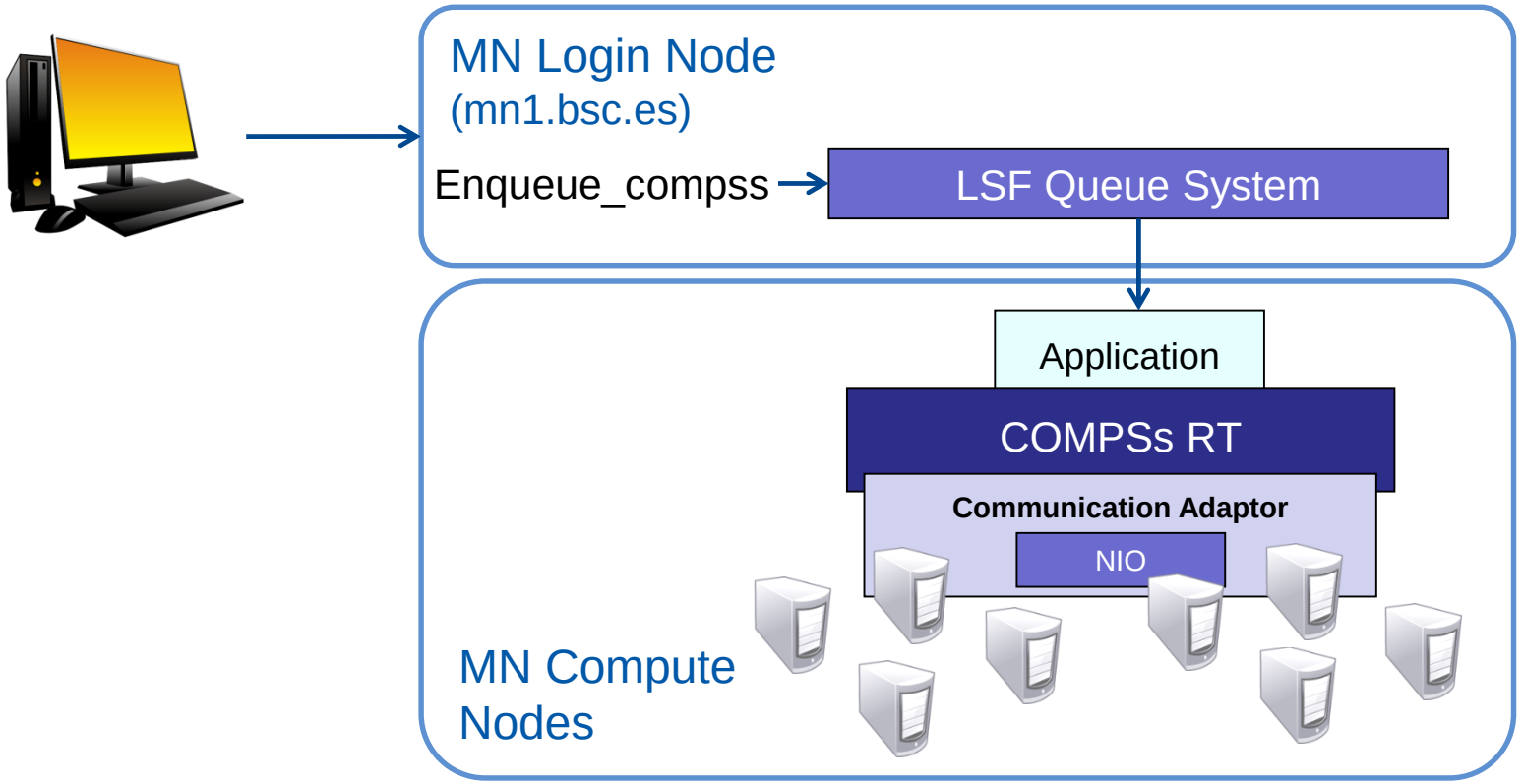
- Steps:
  - Deploy code in worker
  - Run the application with specific resources and project.xml and GAT the adaptor

COMPSs in a Cluster (queue system)

- Execution divided in two phases
  - Launch scripts queue a whole COMPSs app execution
  - Actual execution starts when reservation is obtained



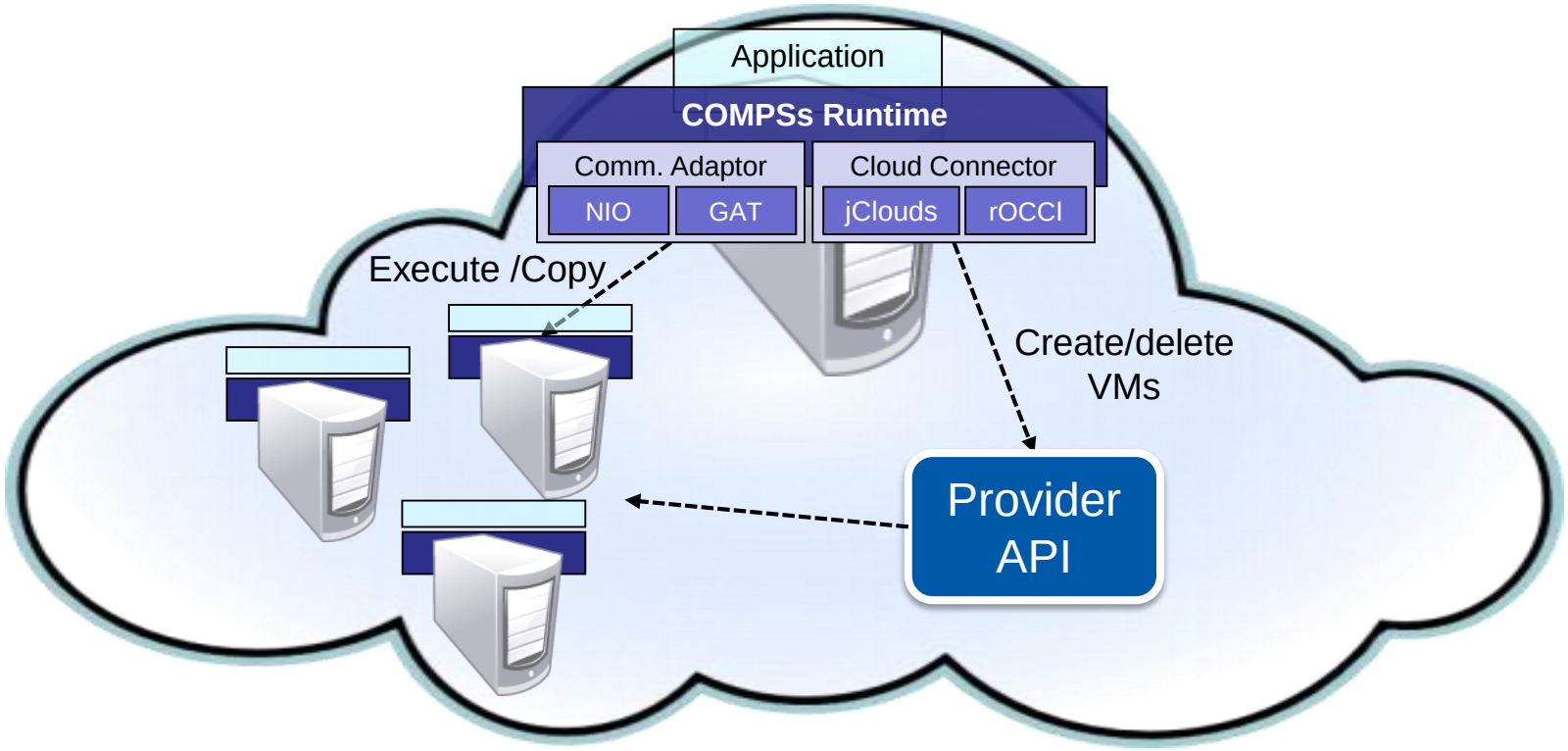
COMPSs in a Cluster (queue system)



- Steps:
  - Deploy app in MN
  - Connect login node
  - Launch “enqueue_compss” script requesting the number of nodes

COMPSs in Clouds

- Execution of COMPSs applications in Clouds
  - Select theconnector to interact with the Cloud provider
  - Adaptor to communicate VMs (NIO if provider supports firewall management, GAT if only ssh)



Cloud Configuration: Resources Specification

Resources.xml

```
<ResourceList>
   <CloudProvider name="BSCCloud">
            <Server>https://bscgrid20.bsc.es:11443</Server>
            <Connector>integratedtoolkit.connectors.rocci.ROCCI</Connector>
            <ImageList>
                  <Image name="debianbase"/>
            </ImageList>
            <CreationTime>120</CreationTime>
            <InstanceTypes>
                  <Resource Name="bsc.small">
                        <Capabilities>
                              <Processor>
                                    <CoreCount>1</CoreCount>
                              </Processor>
                              <StorageElement>
                                    <Size>10.0</Size><!– GB -->
                              </StorageElement>
                              <Memory>
                                    <PhysicalSize>1</PhysicalSize> ><!– GB -->
                              </Memory>
                        </Capabilities>
                  </Resource>
                  <Resource Name="bsc.medium">
                     …
                  </Resource>
               </InstanceTypes>
   </CloudProvider>
</ResourceList>
```

Cloud Configuration: Project Specification

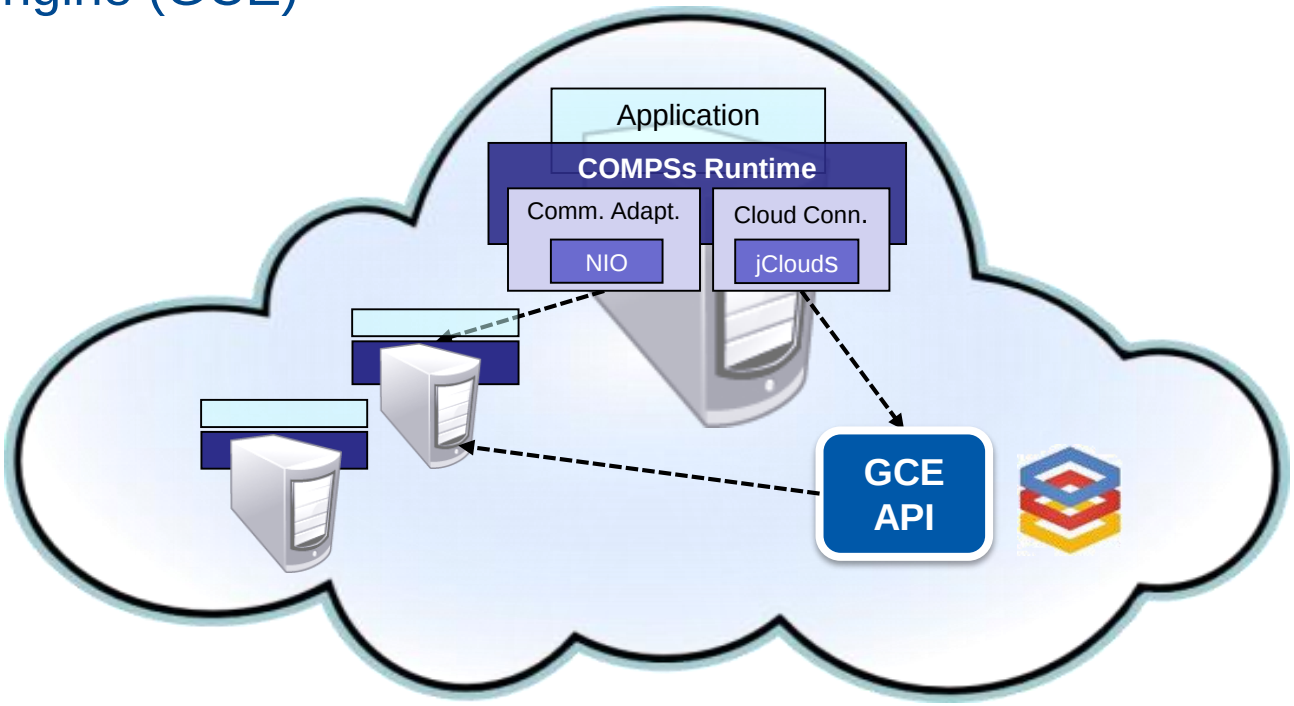
Project.xml

```
<Project>
 <Cloud>
        <InitialVMs>0</InitialVMs>
        <minVMCount>2</minVMCount>
        <maxVMCount>5</maxVMCount>
        <Provider name="BSCCloud">
            <LimitOfVMs>5</LimitOfVMs>
            <Property>
                <Name>user-cred</Name>
                <Value>/home/.../cert.pem</Value>
            </Property>
            <Property>
                <Name>user</Name>
                <Value>userbsc</Value>
            </Property>
    ...
```

```
...
                <ImageList>
                    <Image name="debianbase">
                        <InstallDir>/opt/COMPSs/Runtime/scripts</InstallDir>
                        <WorkingDir>/tmp/</WorkingDir>
                        <User>user</User>
                        <Package>
                            <Source>/home/.../AppName.tar.gz</Source>
                            <Target>/home/user</Target>
                        </Package>
                    </Image>
                </ImageList>
                …
                <InstanceTypes>
                    <Resource name="bsc.small"/>
                </InstanceTypes>
            </Provider>
        </Cloud>
</Project>
```

DEMO: COMPSs in Clouds

- Execution of COMPSs applications in Google Compute Engine (GCE)



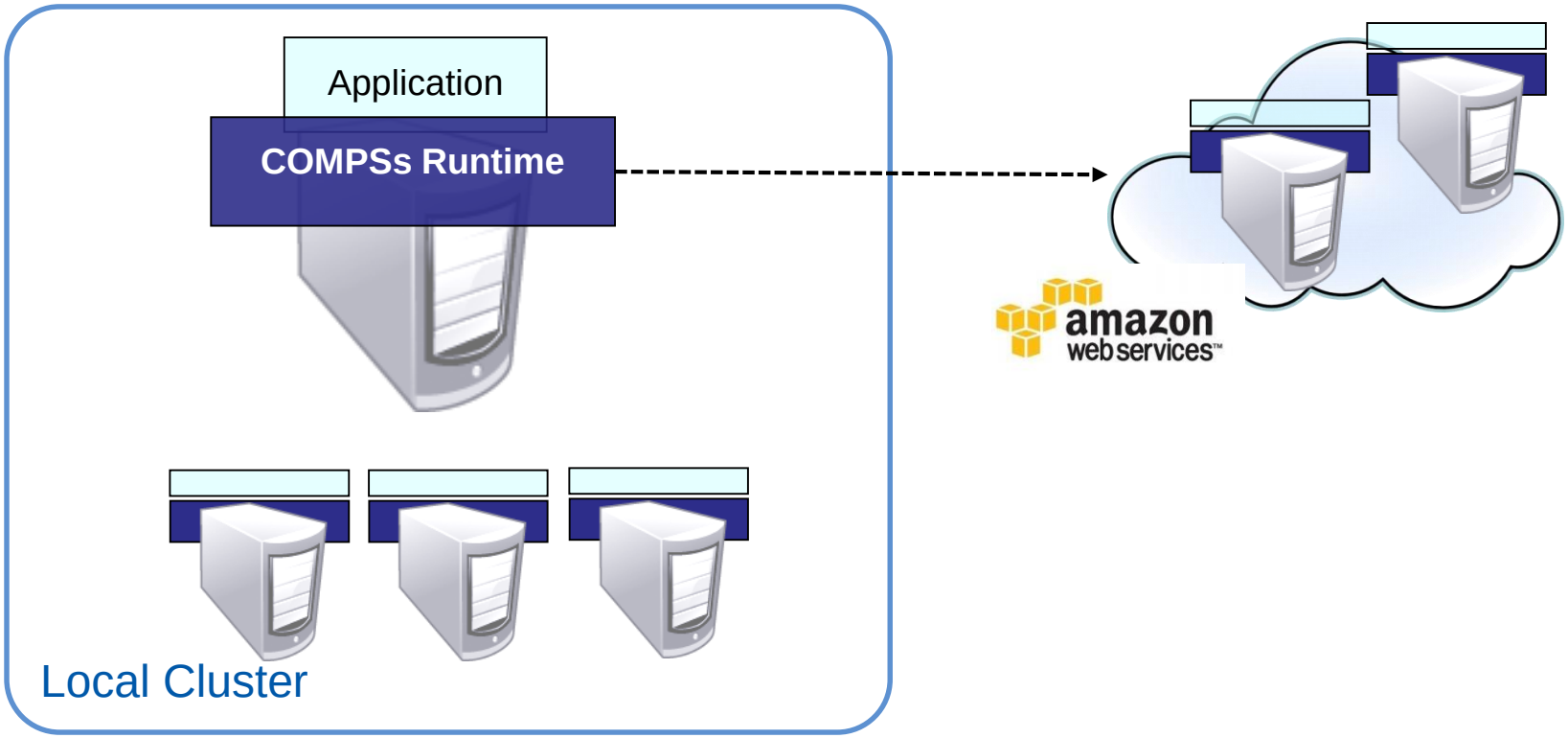
https://www.youtube.com/watch?v=XGaqUje_2zY

Advanced Usage Examples

- Combine Different Environment
  - Cloud Bursting
  - Multiple Grids
- COMPSs for scaling Web Service
- Real Applications implemented with COMPSs

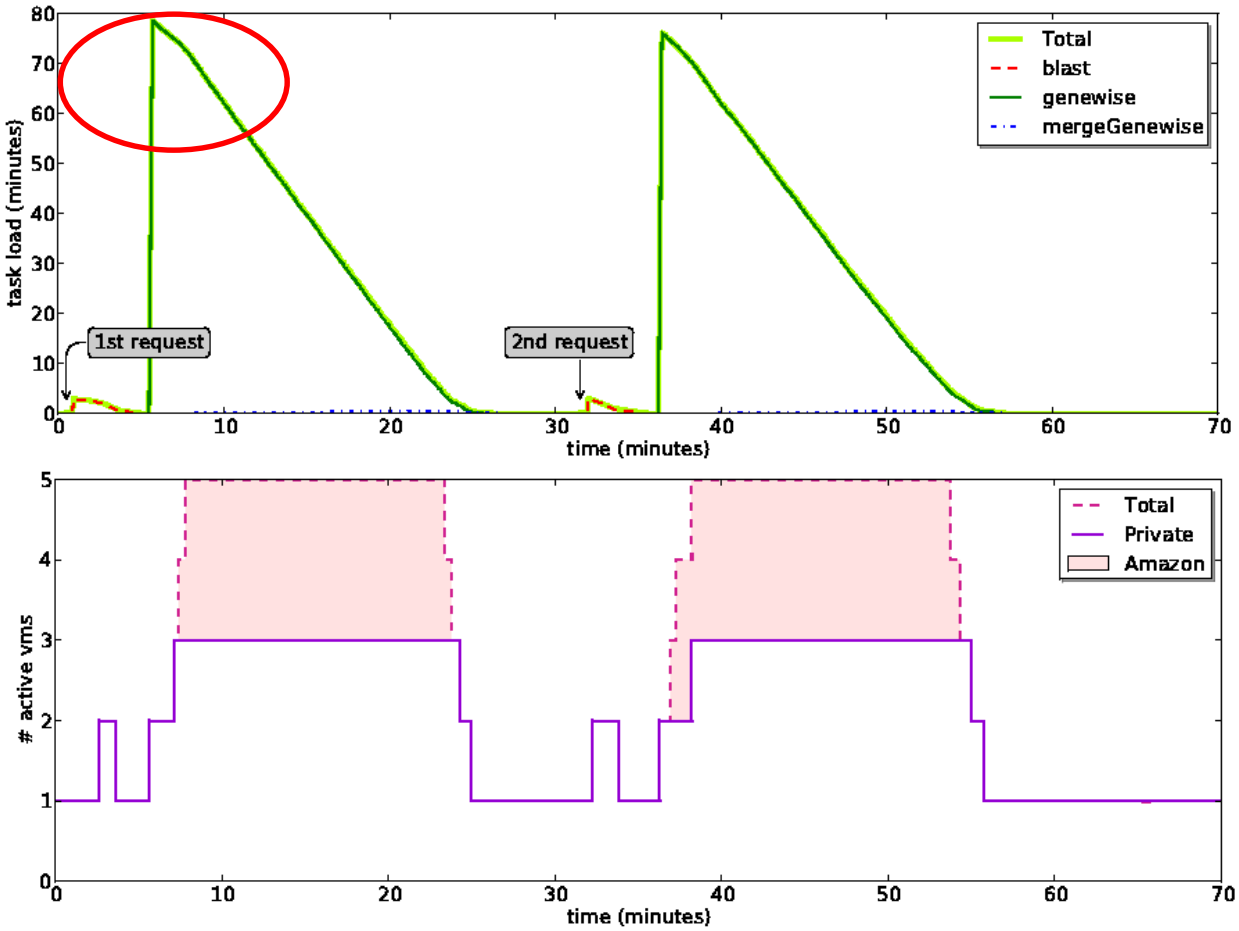
Cloud Bursting

- Execution of COMPSs applications in Clouds
  - Select de connector to interact Cloud providers connectors, SSH

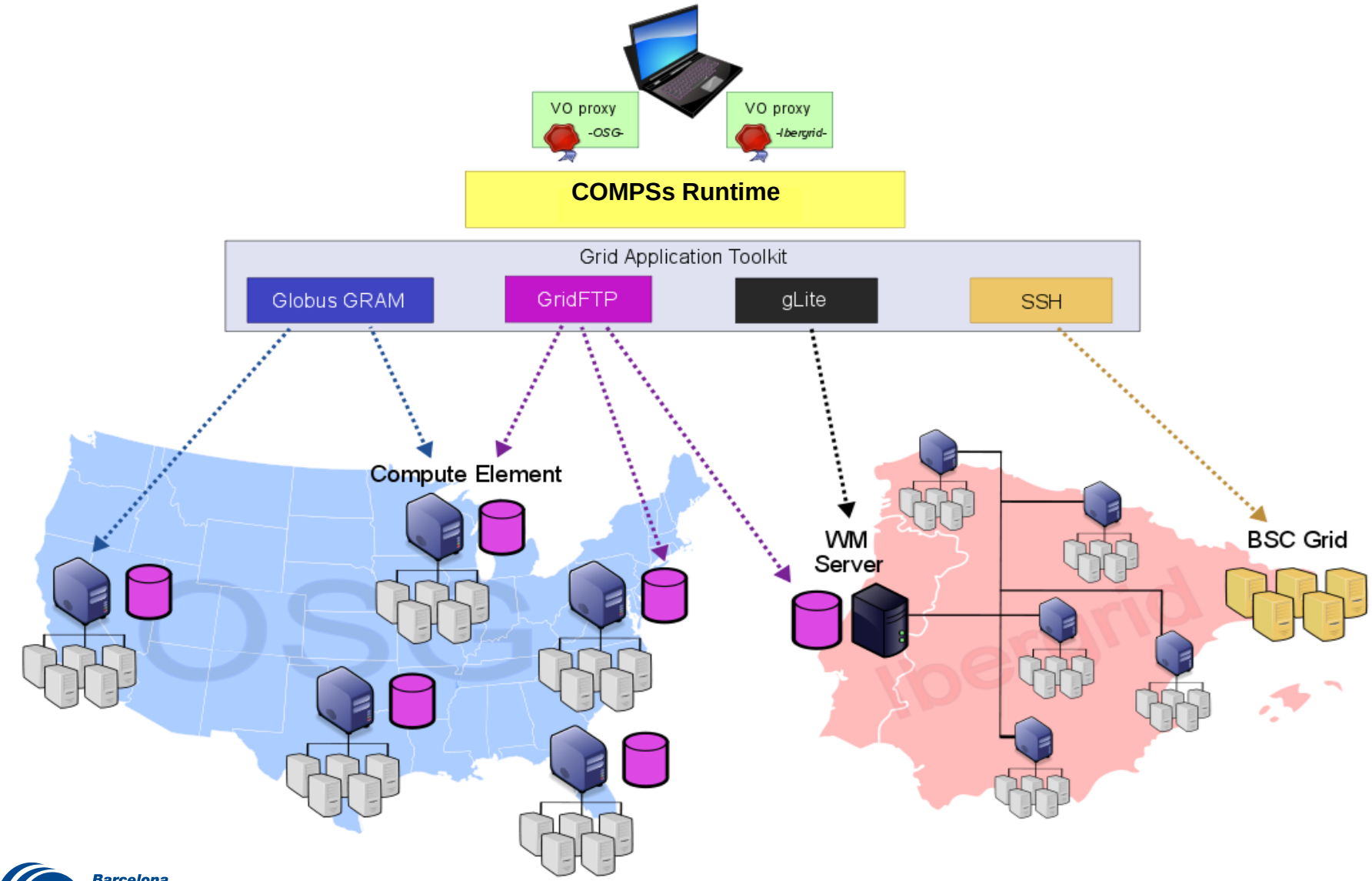


Cloud Bursting

- Increase/decrease number of VMs depending on task load
- Bursting to Amazon EC2 to face peak load

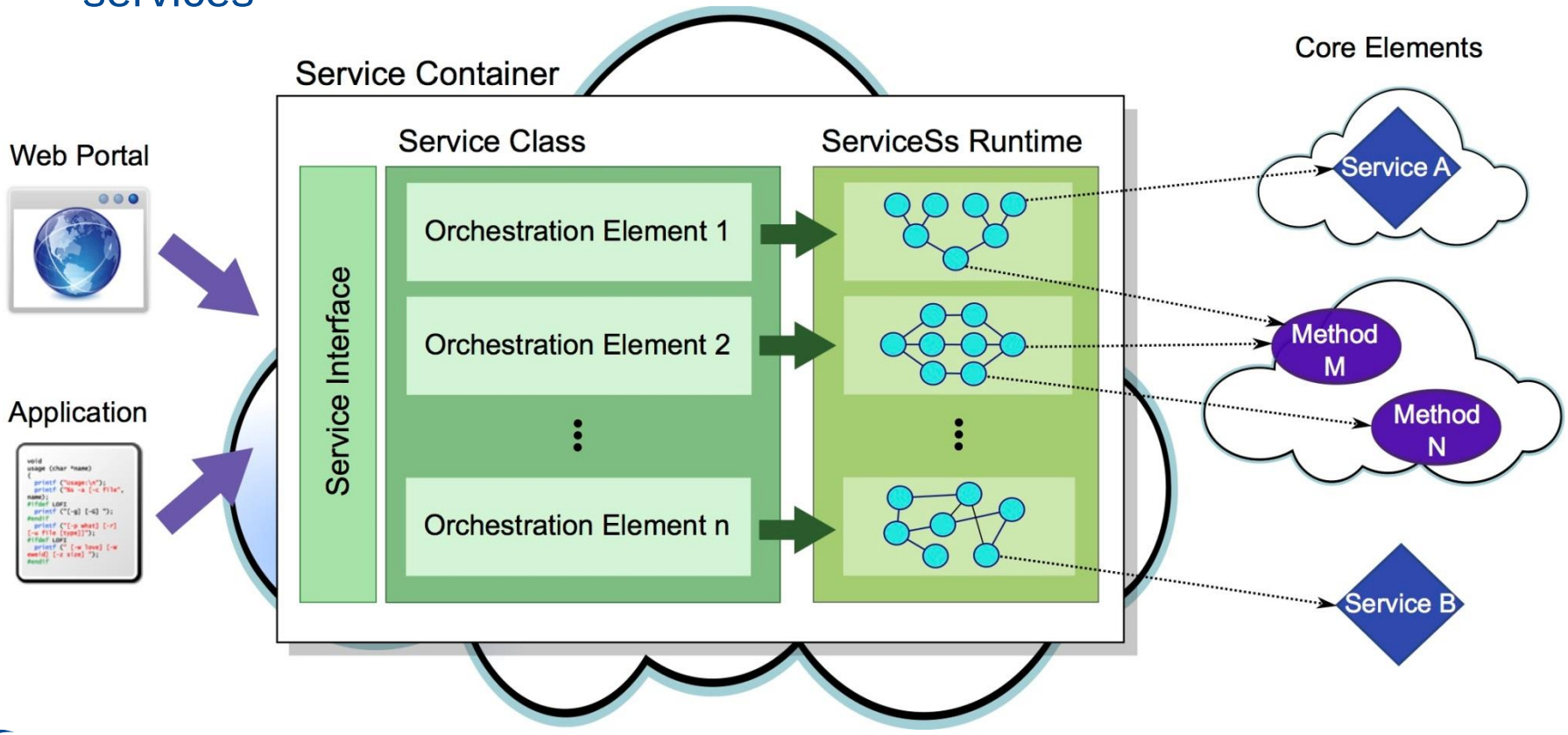


COMPSs in a Grid



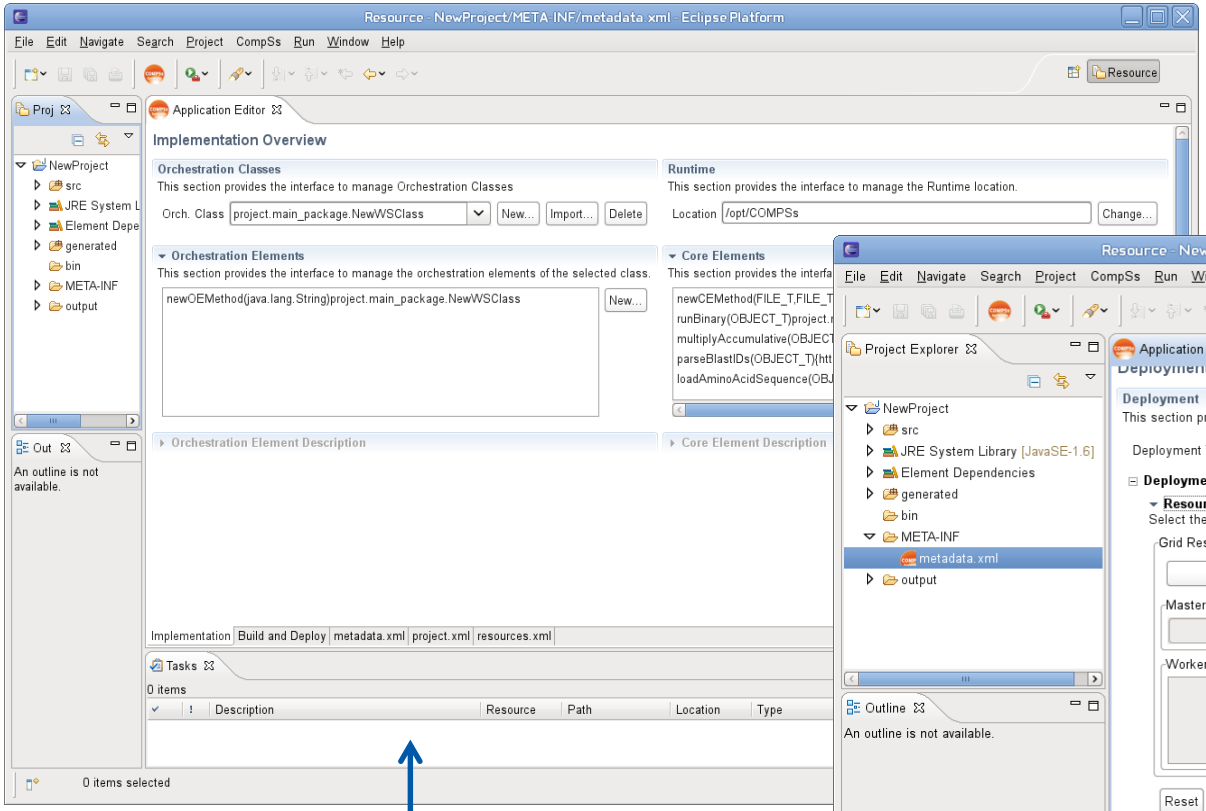
Web service implementations with COMPSs

- A WS method implements a worklfow of tasks
- Different invocations generate different tasks
- Runtime manages the execution of the different calls in the available services



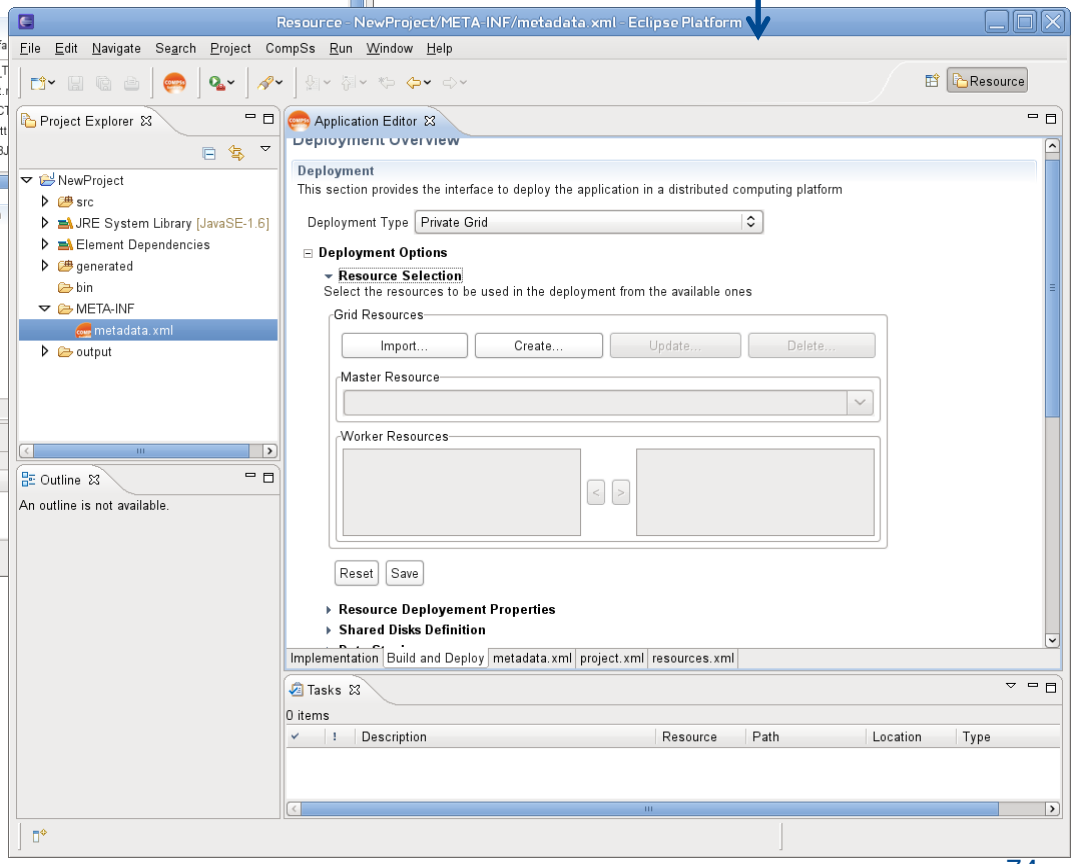
IDE for COMPSs applications

IDE for implementing and deploying applications



Building & Deployment:

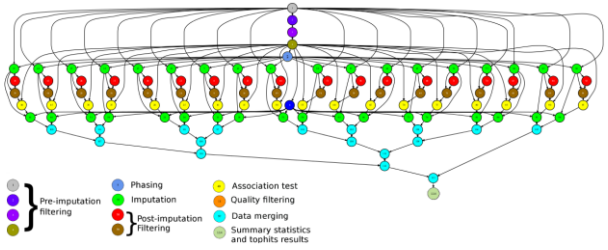
- Generate Packages
- Define hosts & Deploy



Tasks Definition:

- Service Operations (Orchestration
- Tasks (Core Element)

COMPSs Framework



Application repository

- AlyaADAN
- Gipsy/LOFAR
- BioVeL
- transPLANT

EGI AppDB

Enactment Service (PMES)

Programmatic interface to execute COMPSs applications

- OGSA-BES SOAP API
- Support to OCCI and CDMI
- Multiple cloud providers

Web Dashboard

- Management of applications, jobs, storage and users in the PMES
- Monitoring of execution

Programming Model

- Sequential programming model
- General purpose programming languages + annotations/hints
- Exploitation of implicit parallelism

- Automatic on-the-fly creation of a task dependency graph
- COMPSs workflows portable to HPC and Cloud without change

Runtime

- Parallelization of task execution
- Hybrid executions (Private+Public))
- Elastic management of resources
- Interoperability through standards
- Automatic selection of VM templates depending on the task.

Applications using COMPSs

- Personalized medicine
  - eIMRT: planning radiotherapy treatments
- Earth Science
  - HRT: modeling global ocean-atmosphere circulation
- 3D render
  - LuxRender: renderize architectural designs
- Civil Engineering
  - EnergyPlus: modeling airflows in buildings
  - Architrave: force-effects on buildings

Applications using COMPSs

- BioInformatics
  - Discrete: simulate molecular dynamics for proteins
  - Blast: alignments of protein sequences
  - Hmmer: alignment of protein sequences
  - GeneDetect: genetics algorithm
  - QSAR: drug design


BSC
Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación
HANDS-ON

Hands-On: Overview

- COMPSs Virtual Machine Set-up
- Java Hands-on
  - Compilation & Execution
  - Configuration
  - Monitoring, debugging, graph generation
- Python Hands-on
  - Annotate tasks
  - Execution in VM
  - Overview of tracing, trace analysis
  - Code optimization

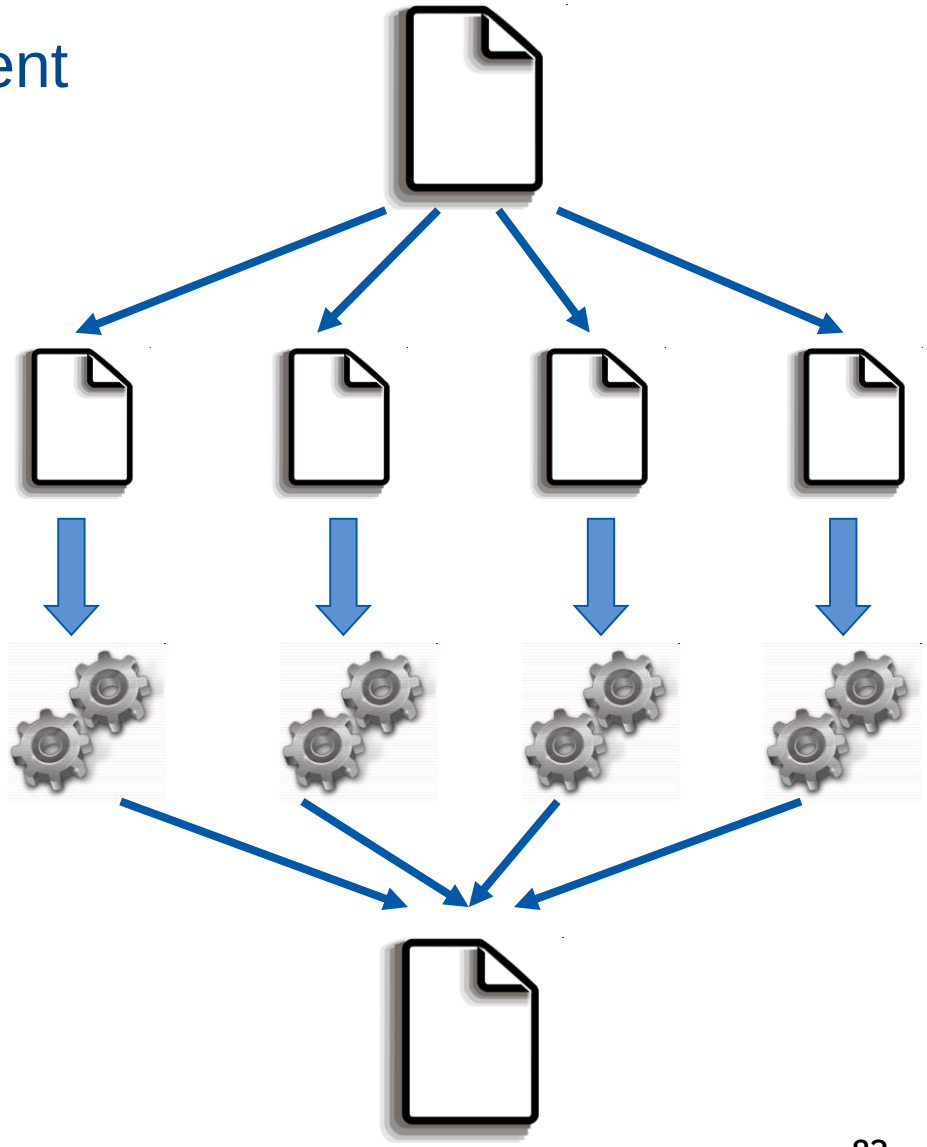
COMPSs development VM Installation

- COMPSs Virtual Appliance
  - Available from website
    - http://compss.bsc.es/releases/vms/COMPSs-1.3-VM.ova
- VirtualBox: Import Virtual Appliance…
  - user: compss, password: compss2016

Java Hands-on

Word Count

- Counting words of a document
- Parallelization
  - Split documents in blocks
  - Count words of Blocks
  - Merge results



Java Hands On: Exercise

- Complete the Word Count parallelization with COMPSs
  - Level 0: No Java background
    - Look the implementation (wordcount project)
  - Level 1: Basic Java background
    - Define methods in the interface (wordcount_sequential)
  - Level 2: Java background
    - Define methods in the interface and complete the part of the main code with helper methods (wordcount_blanks)

Java Hands On: Exercise Solution

Main Code

```
private static void computeWordCount() {
        HashMap<String, Integer> result  = new HashMap<String, Integer>();
        int start = 0;
        for (int i = 0; i < NUM_BLOCKS; ++i) {
                HashMap<String, Integer> partialResult = wordCountBlock(DATA_FILE, start, BLOCK_SIZE);
                start = start + BLOCK_SIZE;
                result = mergeResults(result, partialResult);
        }
        System.out.println("[LOG] Counted Words is : " + result.keySet().size());
}
```

Interface

```
public interface WordcountItf {
        @Method(declaringClass = "wordcount.uniqueFile.Wordcount")
        public HashMap<String, Integer> mergeResults(
                @Parameter HashMap<String, Integer> m1,
                @Parameter HashMap<String, Integer> m2
        );

        @Method(declaringClass = "wordcount.uniqueFile.Wordcount")
        HashMap<String, Integer> wordCountBlock(
                @Parameter(type = Type.FILE, direction = Direction.IN) String filePath,
                @Parameter int start,
                @Parameter int bsize
        );
}
```

Java Hands-on: Compilation and Simple Execution

- Compilation (Eclipse IDE)
  - Package Explorer -> Project (wordcount) -> Export… (Solution)
- Use runcompss command to run the application
  - runcompss [options] < FQDN app. classname> <application args>

- ***Exercise:*** Simple wordcount execution
  - Usage:

    wordcount.uniqueFile.Wordcount <data_file> <block_size>


```
$compss@bsc:~/> cd ~/workspace_java/wordcount/jar
$compss@bsc:~/workspace_java/wordcount/jar/> runcompss wordcount.uniqueFile.Wordcount
    /home/compss/workspace_java/wordcount/data/file_short.txt 650
```

Java Hands-on: Result

```
$compss@bsc:~/workspace_java/wordcount/jar/> runcompss wordcount.uniqueFile.Wordcount
    /workspace_java/wordcount/data/file_short.txt 500

Using default location for project file:
    /opt/COMPSs/Runtime/scripts/user/../../configuration/xml/projects/project.xml
Using default location for resources file:
    /opt/COMPSs/Runtime/scripts/user/../../configuration/xml/resources/resources.xml

----------------- Executing wordcount.uniqueFile.Wordcount -------------------------

WARNING: IT Properties file is null. Setting default values
[   API]  -  Deploying COMPSs Runtime v1.3 (build xxxx)
[   API]  -  Starting COMPSs Runtime v1.3 (build xxxx)
DATA_FILE parameter value = /home/compss/workspace_java/wordcount/data/file_short.txt
BLOCK_SIZE parameter value = 650
[LOG] Computing word count result
[LOG] Counted Words is : 250
[   API]  -  No more tasks for app 1
[   API]  -  Getting Result Files 1
[   API]  -  Execution Finished

------------------------------------------------------------
```

Java Hands-on: Configuration

- Project.xml: /opt/COMPSs/Runtime/configuration/xml/projects/project.xml

```
<?xml version="1.0" encoding="UTF-8"?>
<Project>
        <!--Description for any physical node-->
        <Worker Name="localhost">
                <InstallDir>/opt/COMPSs/Runtime/scripts/system</InstallDir>
                <WorkingDir>/tmp/localhost</WorkingDir>
        </Worker>
</Project>
```

  - Other optional parameters
    - User, AppDir, LibraryPath

Java Hands-On: Configuration

- Resources.xml: /opt/COMPSs/Runtime/configuration/xml/resources/resources.xml

```
<?xml version="1.0" encoding="UTF-8"?>
<ResourceList>
    <!--Description for any physical node-->
    <Resource Name="localhost">
        <Capabilities>
            <Host>
                <TaskCount>0</TaskCount>
                <Queue>short</Queue>
                <Queue/>
            </Host>
            <Processor>
                <Architecture>IA32</Architecture>
                <Speed>3.0</Speed>
                <CoreCount>4</CoreCount>
            </Processor>
            <OS>
                <OSType>Linux</OSType>
                <MaxProcessesPerUser>32</MaxProcessesP
            </OS>
            <StorageElement>
                <Size>8</Size>
            </StorageElement>
            …
            …
            <Memory>
                <PhysicalSize>2</PhysicalSize>
                <VirtualSize>8</VirtualSize>
            </Memory>
            <ApplicationSoftware>
                <Software>Java</Software>
            </ApplicationSoftware>
            <Service/>
            <VO/>
            <Cluster/>
            <FileSystem/>
            <NetworkAdaptor/>
            <JobPolicy/>
            <AccessControlPolicy/>
        </Capabilities>
        <Requirements/>
        <Adaptors>
            <Adaptor
            name="integratedtoolkit.nio.master.NIOAdaptor">
                <MinPort>43001</MinPort>
                <MaxPort>43002</MaxPort>
            </Adaptor>
        </Adaptors>
    </Resource>

<ResourceList>
```

Affects to application parallelism

Java Hands-On: Monitoring

- The runtime of COMPSs provides real-time monitoring
  - http://localhost:8080/compss-monitor/
  - If not started run as root:
    - /etc/init.d/compss-monitor start
- The user can log-in and follow the progress of the executions
  - Running tasks, resources usage, execution time per task, real-time execution graph, etc.
- Activate monitoring with a runcompss flag
  - Setting a monitoring interval
    - runcompss **--monitoring=<int>**
  - With a default monitoring interval
    - runcompss **–m** (or) runcompss **--monitoring**
- ***Exercise:*** run wordcount enabling monitoring


```
$compss@bsc:~/> cd ~/workspace_java/wordcount/jar
$compss@bsc:~/workspace_java/wordcount/jar/> runcompss –m wordcount.uniqueFile.Wordcount
    /home/compss/workspace_java/wordcount/data/file_long.txt 250000
```

Java Hands-on: Debugging

- Different log levels activated as runcompss options
  - runcompss **--log_level**=<level>
    (**off**: for performance | **info**: basic logging | **debug**: detect errors)
  - runcompss **–debug** or runcompss **-d**
- The output/errors of the main code of the application are shown in the console
- Other logging files are stored in:
  - $HOME/.COMPSs/<APP_NAME>_XX
- Inside this folder, the user can check the following:
  - The output/error of a task # N : ***/jobs/jobN.[out|err]***
  - Messages from the COMPSs : ***runtime.log***
  - Task to resources allocation: ***resources.log***
- ***Exercise:*** run wordcount with debugging


```
$compss@bsc:~/> cd ~/workspace_java/wordcount/jar
$compss@bsc:~/workspace_java/wordcount/jar/> runcompss –d wordcount.uniqueFile.Wordcount
    /home/compss/workspace_java/wordcount/data/file_short.txt 650
```

Java Hands-on: Graph generation

- To generate the graph of an application, it must be run with the monitor or graph flags activated
  - runcompss **-m** (or) runcompss **–graph** (or) runcompss **-g**
- The graph will be stored in:
  - $HOME/.COMPSs/<APP_NAME>_XX/monitor/complete_graph.dot
- To convert the graph to a PDF format use gengraph command
  - Usage: gengraph <dot_file>
- **Exercise:** generate the graph for the wordcount application


```
$compss@bsc:~/> cd ~/workspace_java/wordcount/jar
$compss@bsc:~/workspace_java/wordcount/jar/> runcompss –g wordcount.uniqueFile.Wordcount
     /home/compss/workspace_java/wordcount/data/file_short.txt 650

… application execution …

$compss@bsc:~/workspace_java/wordcount/jar/> cd ~/.COMPSs/wordcount.uniqueFile.Wordcount_04/monitor
$~/.COMPSs/wordcount.uniqueFile.Wordcount_04/monitor> gengraph complete_graph.dot
Output file: complete_graph.pdf
$~/.COMPSs/wordcount.uniqueFile.Wordcount_04/monitor> evince complete_graph.pdf
```

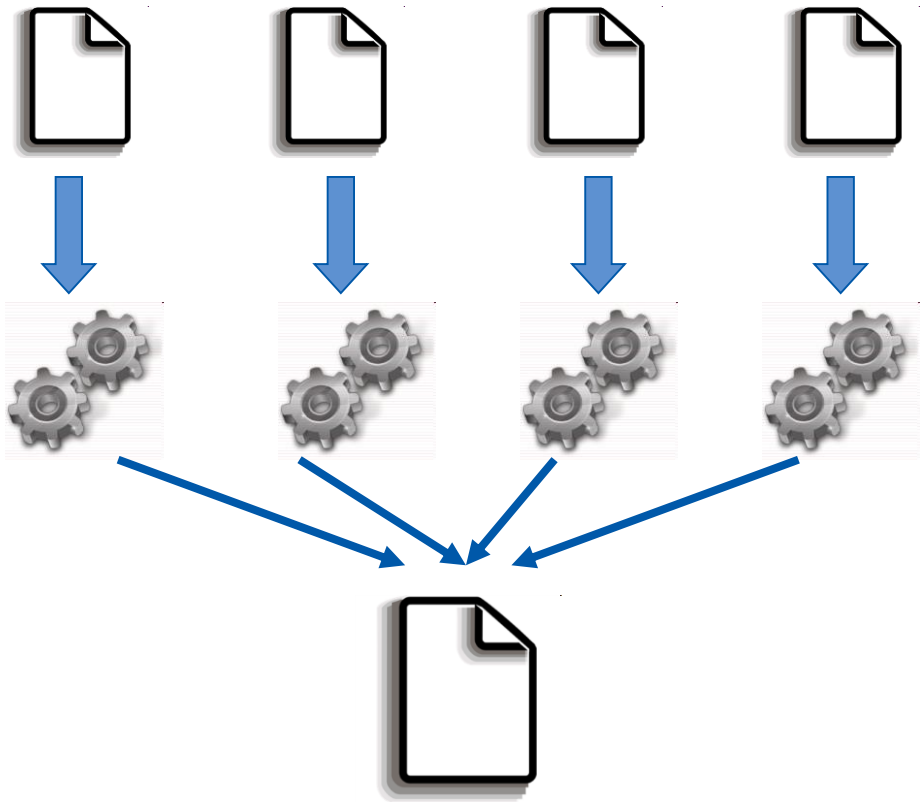
Python Hands-on

PyCOMPSs Hands On: Exercise

- Complete the WordCount parallelization with PyCOMPSs
  - Task definition with python decorators
  - Execution in MareNostrum III
  - Optimize the reduce method

Word Count

- Counting words of a set of documents
- Parallelization
  - Phase 1: Count words of a set of document
  - Phase 2 : Merge results



First step - Connecting to MareNostrum III

- How to connect to MN3?
  - > ssh -X nct01XXX@mn3.bsc.es
  - Password: COMPSS-0216.0XX

- Update .bashrc
  - Edit: **.bashrc**
  - Add: "**module load COMPSs/1.3**" at the end
  - Execute: **source .bashrc**

- Where is the source code?
  - **cd**
  - **cp /gpfs/projects/nct01/nct01001/source/* .**

launch_pycompss.sh
wordcount.py

- Where is the dataset?
  - **cp -r /gpfs/projects/nct01/nct01001/dataset/ .**

- Available editors
  - vi
  - emacs

WordCount @ Sequential (wordcount.py)

```
def read_file(file_path):
    data = []
    with open(file_path, 'r') as f:
        for line in f:
            data += line.split()
    return data
```

```
def wordCount(data):
    partialResult = {}
    for entry in data:
        if entry in partialResult:
            partialResult[entry] += 1
        else:
            partialResult[entry] = 1
    return partialResult
```

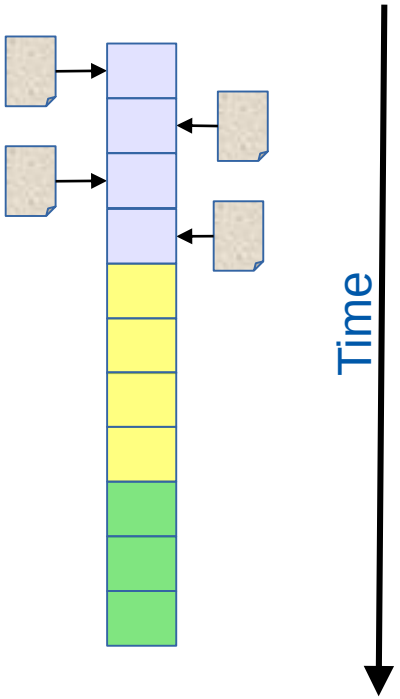
```
def merge_two_dicts(dic1, dic2):
    for k in dic2:
        if k in dic1:
            dic1[k] += dic2[k]
        else:
            dic1[k] = dic2[k]
    return dic1
```

```
if __name__ == "__main__":
    pathDataset = sys.argv[1]
    # Construct a list with the file's paths from the dataset
    paths = []
    for fileName in os.listdir(pathDataset):
        paths.append(os.path.join(pathDataset, fileName))

    # Read file's content
    data = map(read_file, paths)

    # From all file's data execute a wordcount on it
    partialResult = map(wordCount, data)

    # Accumulate the partial results to get the final result.
    result = reduce(merge_two_dicts, partialResult)
```

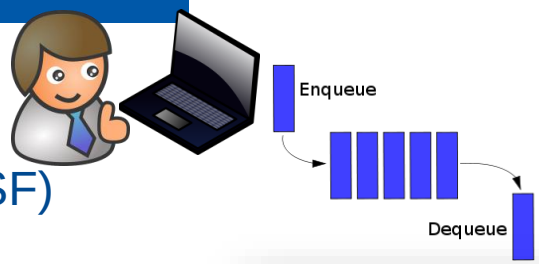


WordCount @ Sequential

- Remember the dataset path
- How to launch with python sequentialy?
  - > **python wordcount.py /home/nct01/nct01XXX/dataset/4files/**

  Results:

```
user@login3:~> python wordcount.py /path/to/dataset/
Ellapsed Time (s)
0.959941864014
Words: 2545211
```



- Submit jobs to MareNostrum III
  - All jobs should be submited to the queuing system (LSF)
  - We will use a launcher script: **launch_pycompss.sh**
  - Useful commands:
    - bjobs – This command shows the status of the job.
    - bkill jobId – This command kills a job with id ‘jobId’.

PyCOMPSs Hands On: Exercise

- Complete the WordCount parallelization with PyCOMPSs
  - **Task definition with python decorators**
    - **Modify the wordcount.py**
  - **Execution in MareNostrum III**
    - **Use launch_pycompss.sh**
  - Optimize the reduce method

Execution in MareNostrum III - HandsOn

launch_pycompss.sh

```
#/bin/bash


enqueue_compss \
  --exec_time=10 \
  --num_nodes=2 \
  --tasks_per_node=8 \
  --lang=python \
  --classpath=/gpfs/home/nct01/nct01XXX/ \
  --tracing=true \
  --graph=true \
  /home/nct01/nct01XXX/wordcount.py /gpfs/home/nct01/nct01XXX/dataset/64files
```

Parameters:

- num_nodes: amount of nodes where to execute (1 master + 1 worker).
- tasks_per_node: amount of tasks that can be processed in parallel (1-16).
- Dataset path: **/gpfs/home/nct01/nct01XXX/dataset/64files**

How to execute with PyCOMPSs?

- **./launch_pycompss.sh**

WordCount @ PyCOMPSs (option1)

```
def read_file(file_path):
    data = []
    with open(file_path, 'r') as f:
        for line in f:
            data += line.split()
    return data
```

```
@task(returns=dict)
def wordCount(data):
    partialResult = {}
    for entry in data:
        if entry in partialResult:
            partialResult[entry] += 1
        else:
            partialResult[entry] = 1
    return partialResult
```

```
@task(returns=dict, priority=True)
def merge_two_dicts(dic1, dic2):
    for k in dic2:
        if k in dic1:
            dic1[k] += dic2[k]
        else:
            dic1[k] = dic2[k]
    return dic1
```

```
from pycompss.api.task import task
from pycompss.api.parameter import *

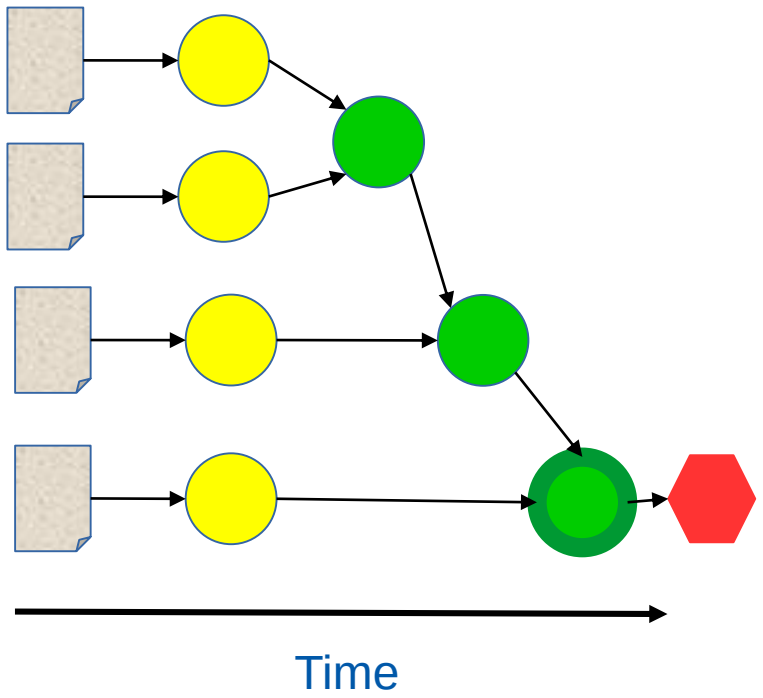
if __name__ == "__main__":
    from pycompss.api.api import compss_wait_on
    pathDataset = sys.argv[1]
    # Construct a list with the file's paths from the dataset
    paths = []
    for fileName in os.listdir(pathDataset):
        paths.append(os.path.join(pathDataset, fileName))

    # Read file's content
    data = map(read_file, paths)

    # From all file's data execute a wordcount on it
    partialResult = map(wordCount, data)

    # Accumulate the partial results to get the final result.
    result = reduce(merge_two_dicts, partialResult)

    # Wait for result
    result = compss_wait_on(result)
```



WordCount @ PyCOMPSs (option 2)

```
@task(returns=list,
      file_path=FILE_in)
def read_file(file_path):
    data = []
    with open(file_path, 'r') as f:
        for line in f:
            data += line.split()
    return data
```

```
@task(returns=dict)
def wordCount(data):
    partialResult = {}
    for entry in data:
        if entry in partialResult:
            partialResult[entry] += 1
        else:
            partialResult[entry] = 1
    return partialResult
```

```
@task(returns=dict, priority=True)
def merge_two_dicts(dic1, dic2):
    for k in dic2:
        if k in dic1:
            dic1[k] += dic2[k]
        else:
            dic1[k] = dic2[k]
    return dic1
```

```
from pycompss.api.task import task
from pycompss.api.parameter import *

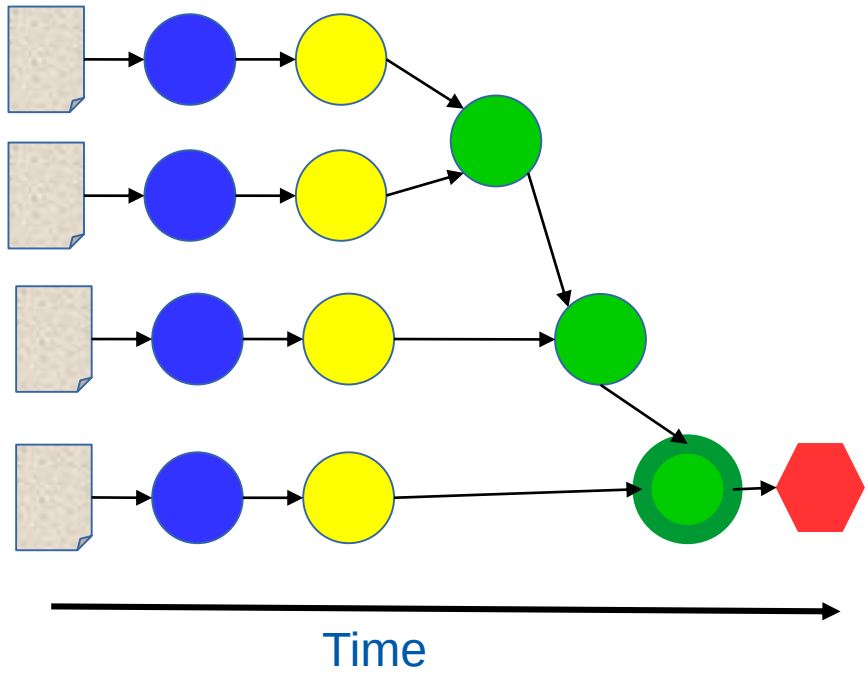
if __name__ == "__main__":
    from pycompss.api.api import compss_wait_on
    pathDataset = sys.argv[1]
    # Construct a list with the file's paths from the dataset
    paths = []
    for fileName in os.listdir(pathDataset):
        paths.append(os.path.join(pathDataset, fileName))

    # Read file's content
    data = map(read_file, paths)

    # From all file's data execute a wordcount on it
    partialResult = map(wordCount, data)

    # Accumulate the partial results to get the final result.
    result = reduce(merge_two_dicts, partialResult)

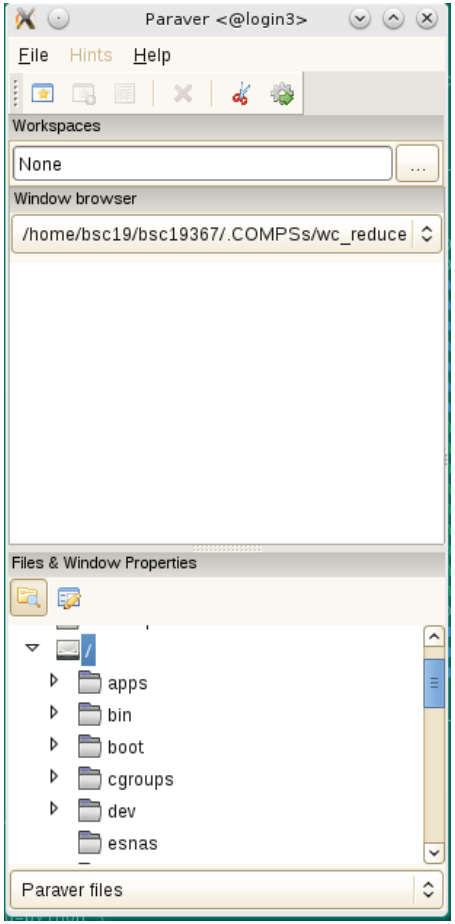
    # Wait for result
    result = compss_wait_on(result)
```

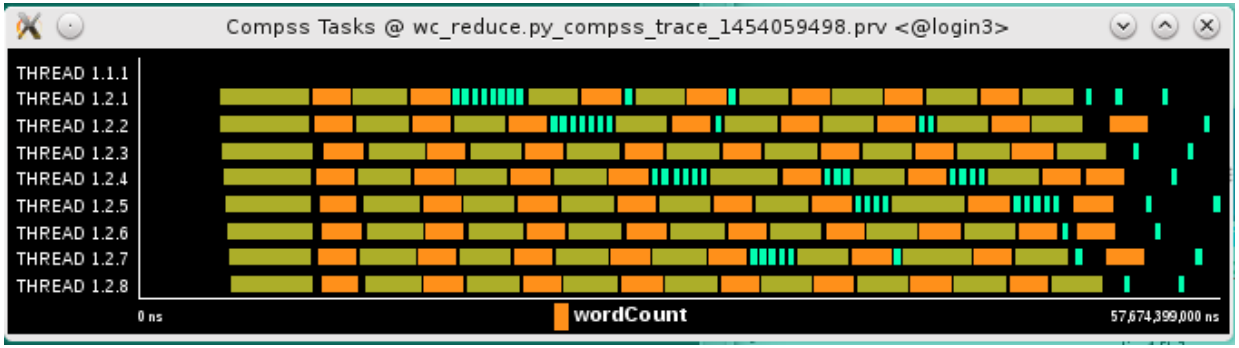


Wordcount @ Performance Analysis

- Paraver is the BSC tool for trace visualization
  - Trace events are encoding in Paraver (.prv) format by Extrae
  - Paraver is a powerful tool for trace visualization.
  - An experimented user could obtain many different views of the trace events.

- For more information about Paraver visit:
  - http://www.bsc.es/computer-sciences/performance-tools/paraver





Wordcount @ Performance Analysis

- COMPSs can generate post-execution traces of the distributed execution of the application
  - Useful for performance analysis and diagnosis
- How it works?
  - Task execution and file transfers are application events
  - An XML file is created at workers to keep track of these events
  - At the end of the execution all the XML files are merged to get the final trace file
  - COMPSs uses Extrae tool to dynamically instrument the application
    - In a worker:
      - Extrae keeps track of the events in an intermediate file
    - In the master:
      - Extrae merges the intermediate files to get the final trace file

Wordcount @ Performance Analysis

```
---------- Executing wc_reduce.py -------------------------

Welcome to Extrae 3.1.1rc (revision 3360 based on extrae/trunk)
Extrae: Generating intermediate files for Paraver traces.
Extrae: Intermediate files will be stored in /.statelite/tmpfs/gpfs/home/bsc19/bsc19000/Apps/WC/src/tutorial
Extrae: Tracing buffer can hold 500000 events
Extrae: Tracing mode is set to: Detail.
Extrae: Successfully initiated with 1 tasks

[   API]  -  Deploying COMPSs Runtime v1.3 (build 20151211-1532)
[   API]  -  Starting COMPSs Runtime v1.3 (build 20151211-1532)
...
[   API]  -  No more tasks for app 0
[   API]  -  Getting Result Files 0
[   API]  -  Execution Finished
...

Extrae: Application has ended. Tracing has been terminated.

merger: Output trace format is: Paraver
merger: Extrae 3.1.1rc (revision 3360 based on extrae/trunk)

mpi2prv: Selected output trace format is Paraver
mpi2prv: Parsing intermediate files
mpi2prv: Generating tracefile (intermediate buffers of 745642 events)

mpi2prv: Congratulations! ./trace/wc_reduce.py_compss_trace_1453885329.prv has been generated.
```

Extrae starts before the user application execution

COMPSs runtime starts

The application finishes and the tracing process ends

COMPSs runtime ends

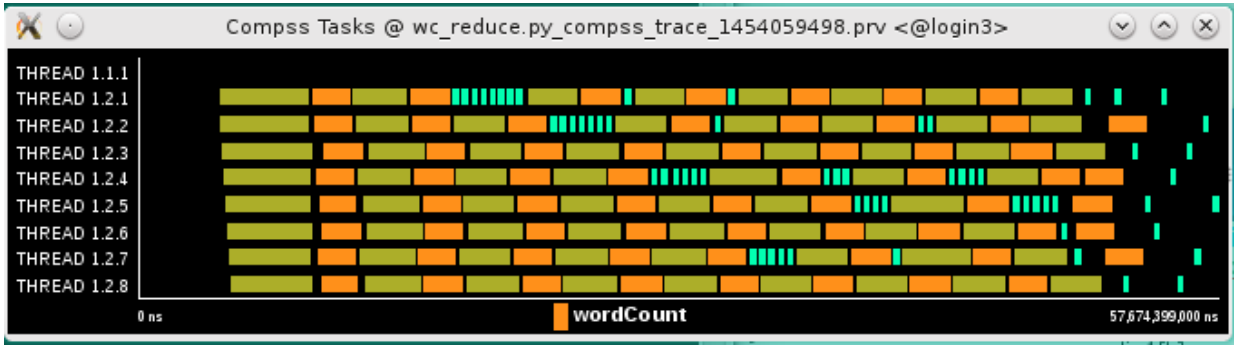
The merge process starts

Intermediate trace files are processed

The final trace file is generated

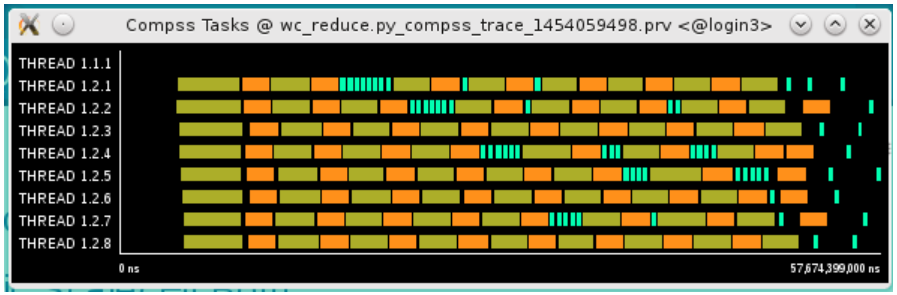
WordCount @ Performance Analysis

- Open Paraver
  - > module load paraver
  - > cd $HOME/.COMPSs/wordcount.py_01
  - > wxparaver trace/*.prv
- COMPSs provides some configuration files to automatically obtain the view of the trace
  - File/Load Configuration: (/gpfs/apps/MN3/COMPSs/1.3/Dependencies/paraver/cfgs/compss_tasks.cfg)

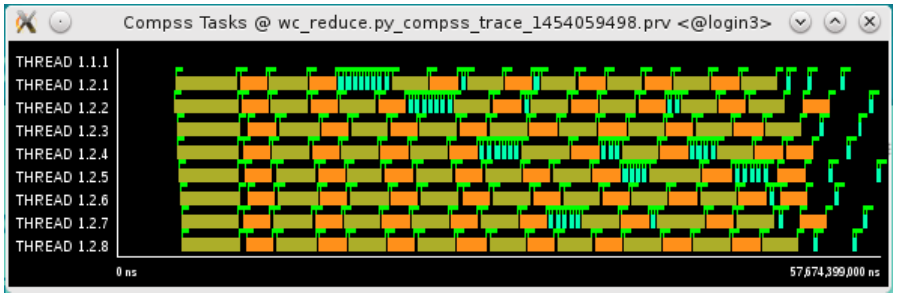


Wordcount @ Performance Analysis

- Fit window
  - Right click on the trace window
  - Fit Semantic Scale/ Fit Both



- View Event flags
  - Right click on the trace window
  - View / Event Flags



Wordcount @ Performance Analysis

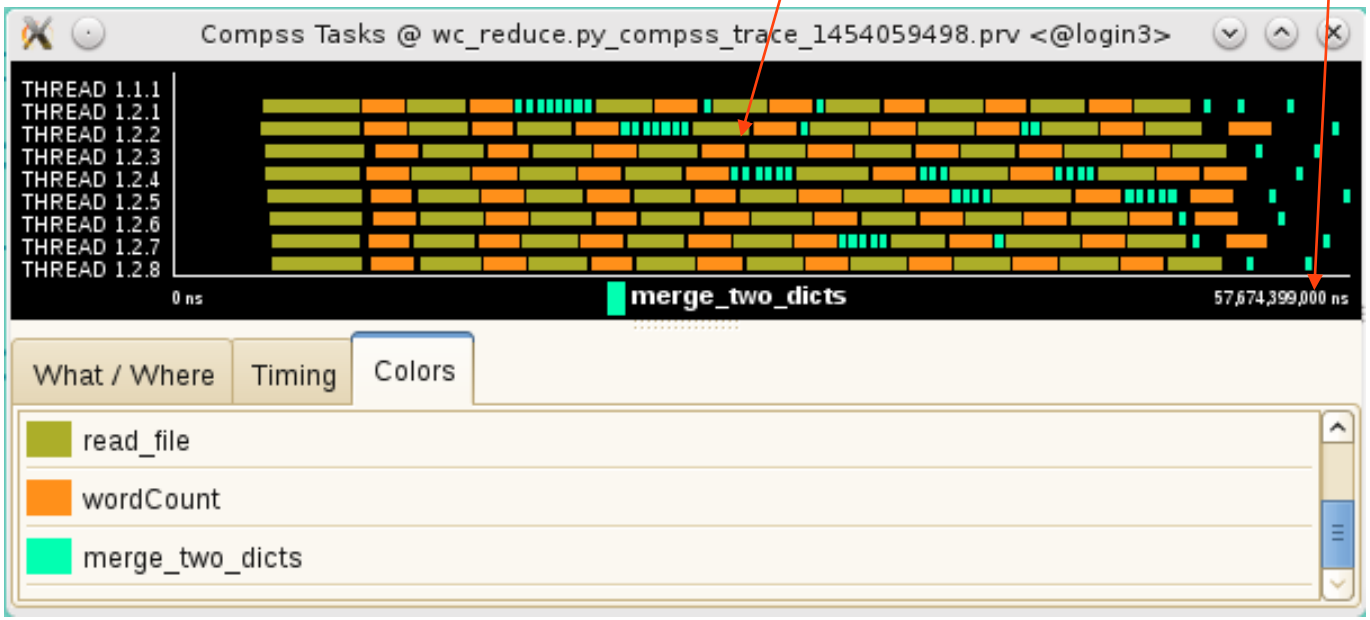
Show info Panel

- Right click on the trace window
- Check info panel option
- Select Colors tab of the panel

Tasks

Execution time

Threads

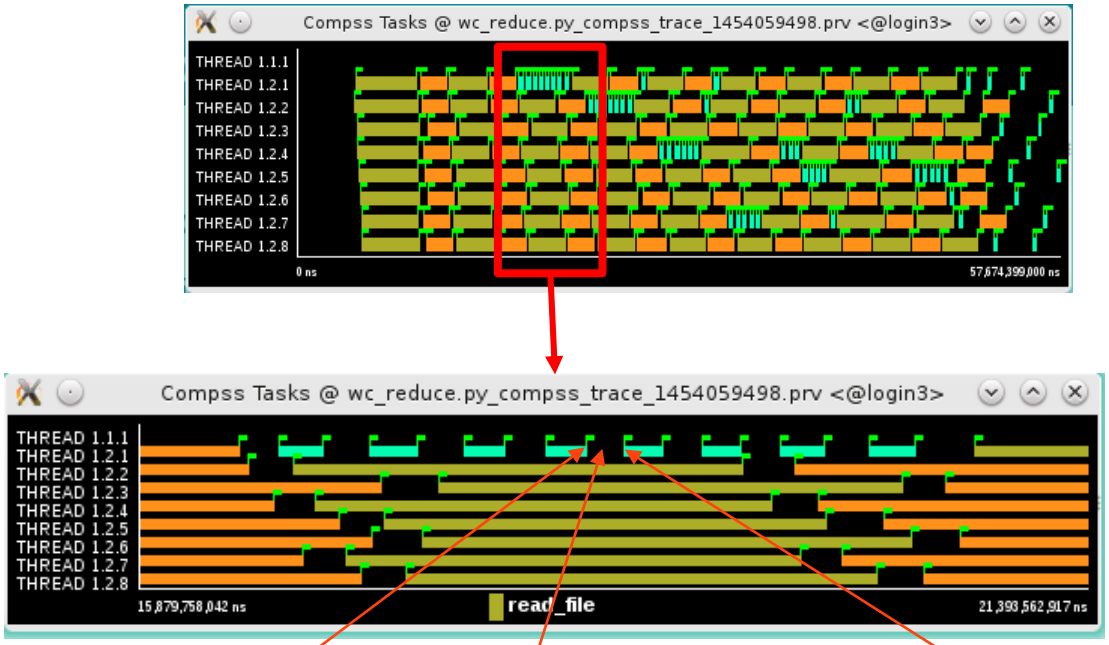


Legend with task names

Wordcount @ Performance Analysis

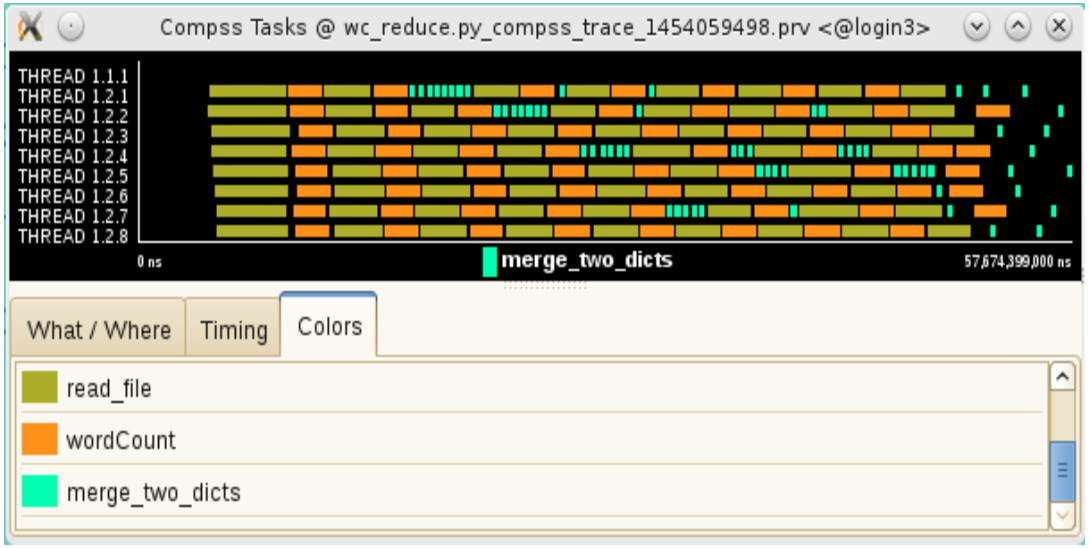
Zoom to see details

- Select a region in the trace window to see in detail
- And repeat the process until the needed zoom level
- The undo zoom option is in the right click panel



Wordcount @ Performance Analysis

- Summarizing:
  - Lines in the trace:
    - One line for the master
    - N lines for the workers
- Meaning of the colours:
  - Black: idle
  - Other colors: task running
    - see the color legend
- Flags (events):
  - Start / end of task



PyCOMPSs Hands On: Exercise

- Complete the WordCount parallelization with PyCOMPSs
  - ~~Task definition with python decorators~~
  - ~~Execution in MareNostrum III~~
  - **Optimize the reduce method**

WordCount @ PyCOMPSs (option 2)

```
@task(returns=list,
      file_path=FILE_in)
def read_file(file_path):
    data = []
    with open(file_path, 'r') as f:
        for line in f:
            data += line.split()
    return data
```

```
@task(returns=dict)
def wordCount(data):
    partialResult = {}
    for entry in data:
        if entry in partialResult:
            partialResult[entry] += 1
        else:
            partialResult[entry] = 1
    return partialResult
```

```
@task(returns=dict, priority=True)
def merge_two_dicts(dic1, dic2):
    for k in dic2:
        if k in dic1:
            dic1[k] += dic2[k]
        else:
            dic1[k] = dic2[k]
    return dic1
```

```
from pycompss.api.task import task
from pycompss.api.parameter import *

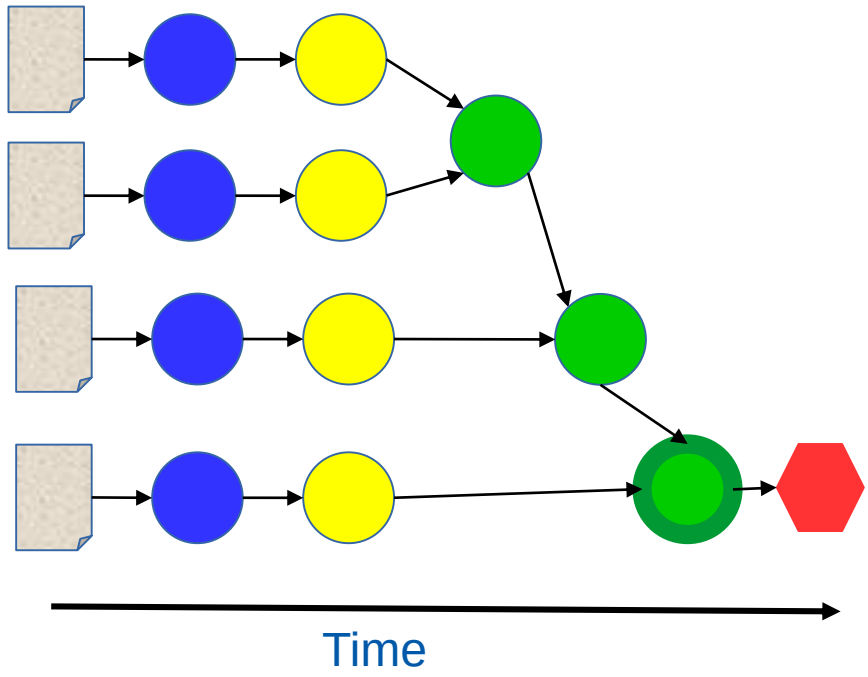
if __name__ == "__main__":
    from pycompss.api.api import compss_wait_on
    pathDataset = sys.argv[1]
    # Construct a list with the file's paths from the dataset
    paths = []
    for fileName in os.listdir(pathDataset):
        paths.append(os.path.join(pathDataset, fileName))

    # Read file's content
    data = map(read_file, paths)

    # From all file's data execute a wordcount on it
    partialResult = map(wordCount, data)

    # Accumulate the partial results to get the final result.
    result = reduce(merge_two_dicts, partialResult)

    # Wait for result
    result = compss_wait_on(result)
```



WordCount @ PyCOMPSs (Optimization)

```
@task(returns=list ,
      file_path=FILE_IN)
def read_file(file_path):
    data = []
    with open(file_path, 'r') as f:
        for line in f:
            data += line.split()
    return data
```

```
@task(returns=dict)
def wordCount(data):
    partialResult = {}
    for entry in data:
        if entry in partialResult:
            partialResult[entry] += 1
        else:
            partialResult[entry] = 1
    return partialResult
```

```
@task(returns=dict, priority=True)
def merge_two_dicts(dic1, dic2):
    for k in dic2:
        if k in dic1:
            dic1[k] += dic2[k]
        else:
            dic1[k] = dic2[k]
    return dic1
```

```
from pycompss.api.task import task
from pycompss.api.parameter import *

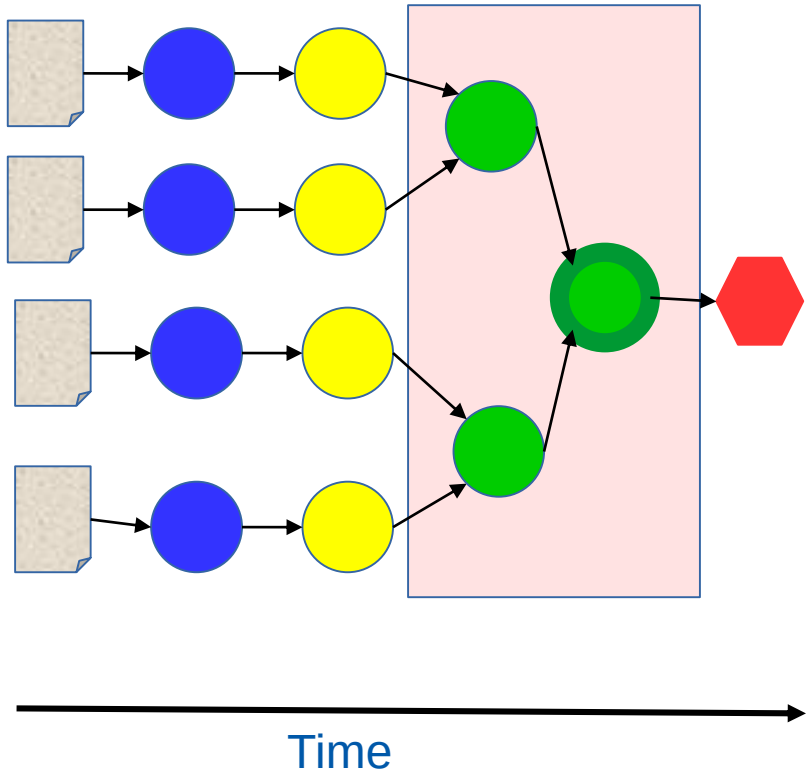
if __name__ == "__main__":
    from pycompss.api.api import compss_wait_on
    pathDataset = sys.argv[1]
    # Construct a list with the file's paths from the dataset
    paths = []
    for fileName in os.listdir(pathDataset):
        paths.append(os.path.join(pathDataset, fileName))

    # Read file's content
    data = map(read_file, paths)

    # From all file's data execute a wordcount on it
    partialResult = map(wordCount, data)

    # Accumulate the partial results to get the final result.
    result = mergeReduce(merge_two_dicts, partialResult)

    # Wait for result
    result = compss_wait_on(result)
```



Execution in MareNostrum III - HandsOn

launch_pycompss.sh

```
#/bin/bash


enqueue_compss \
  --exec_time=10 \
  --num_nodes=2 \
  --tasks_per_node=8 \
  --lang=python \
  --classpath=/gpfs/home/nct01/nct01XXX/ \
  --tracing=true \
  --graph=true \
  /home/nct01/nct01XXX/wordcount_optimized.py /gpfs/home/nct01/nct01XXX/dataset/64files
```

Parameters:

- num_nodes: amount of nodes where to execute (1 master + 1 worker).
- tasks_per_node: amount of tasks that can be processed in parallel (1-16).
- Dataset path: **/gpfs/home/nct01/nct01XXX/dataset/64files**

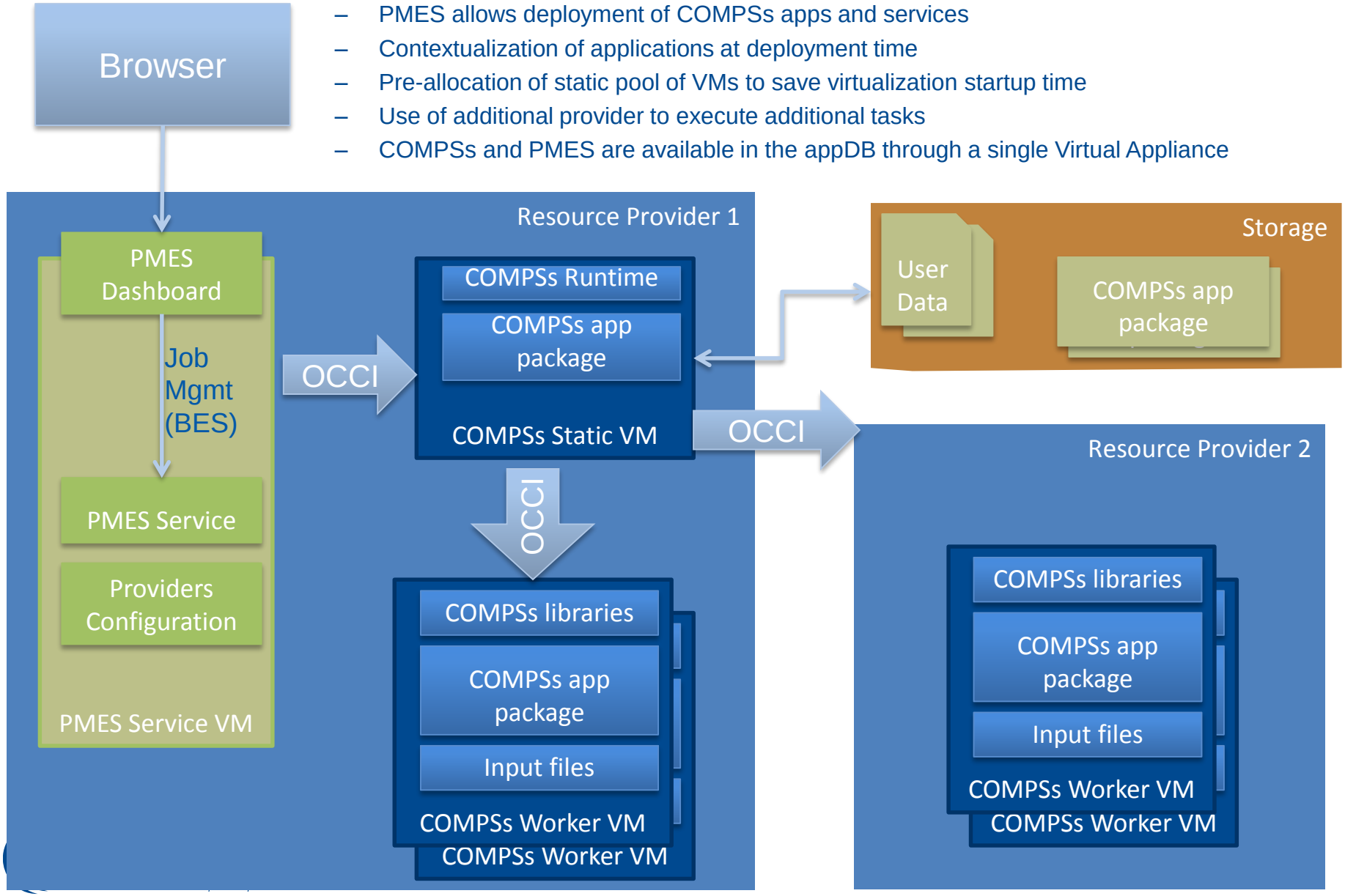
How to execute with PyCOMPSs?

- **./launch_pycompss.sh**

COMPSs and EGI
HANDS-ON

Deployment of COMPSs and PMES on EGI

- PMES allows deployment of COMPSs apps and services
- Contextualization of applications at deployment time
- Pre-allocation of static pool of VMs to save virtualization startup time
- Use of additional provider to execute additional tasks
- COMPSs and PMES are available in the appDB through a single Virtual Appliance



Configuration

- Choose the fedcloud.egi.eu VO
  - UPV Provider: https://fc-one.i3m.upv.es:11443
  - Pre Instantiated VMs
- EGI AppDB Image
  - uuid_image_for_compss_pmes_ubuntu1504kv_im153_128
  - User: compss Password: compss2015
- COMPSs configuration
  - Configuration files for local and cloud execution available at:
    - http://bscgrid05.bsc.es/~lezzi/local.tgz
    - http://bscgrid05.bsc.es/~lezzi/cloud.tgz
- Prepare the COMPSs package
  - Blast application in Java workspace
- Monitoring
  - http://158.42.105.X:8080/compss-monitor

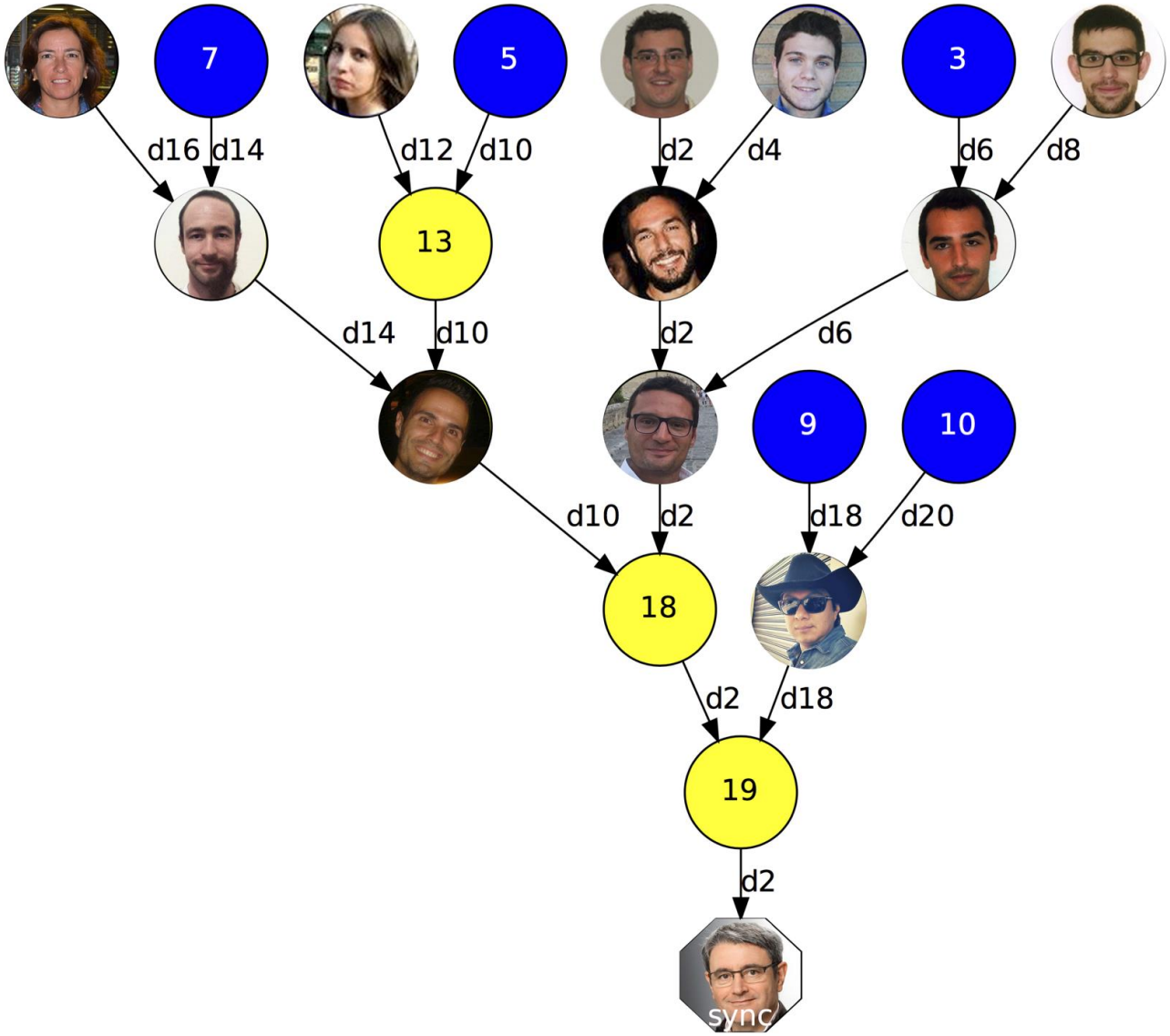
Final Notes

- Sequential programming approach
- Parallelization at task level
- Transparent data management and remote execution
- Can operate on different infrastructures:
  - Cluster
  - Grid
  - Cloud (Public/Private)
    - PaaS
    - IaaS
  - Web services

Final Notes

- Project page:
  - http://www.bsc.es/compss
- Direct downloads page:
  - http://www.bsc.es/computer-sciences/grid-computing/comp-superscalar/download
    - Virtual Appliance for testing & sample applications
    - Tutorials
    - Red-Hat & Debian based installation packages
    - Source Code
- Application Repository
  - http://compss.bsc.es/projects/bar/wiki/Applications
    - Several examples of applications developed with COMPSs

COMPSs Group



www.bsc.es

Barcelona Supercomputing Center

Centro Nacional de Supercomputación

Thank you!

For further information please contact

support-compss@bsc.es