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Barcelona Supercomputing Center
Centro Nacional de Supercomputación

COMPSs Tutorial

February 20th 2014, Barcelona

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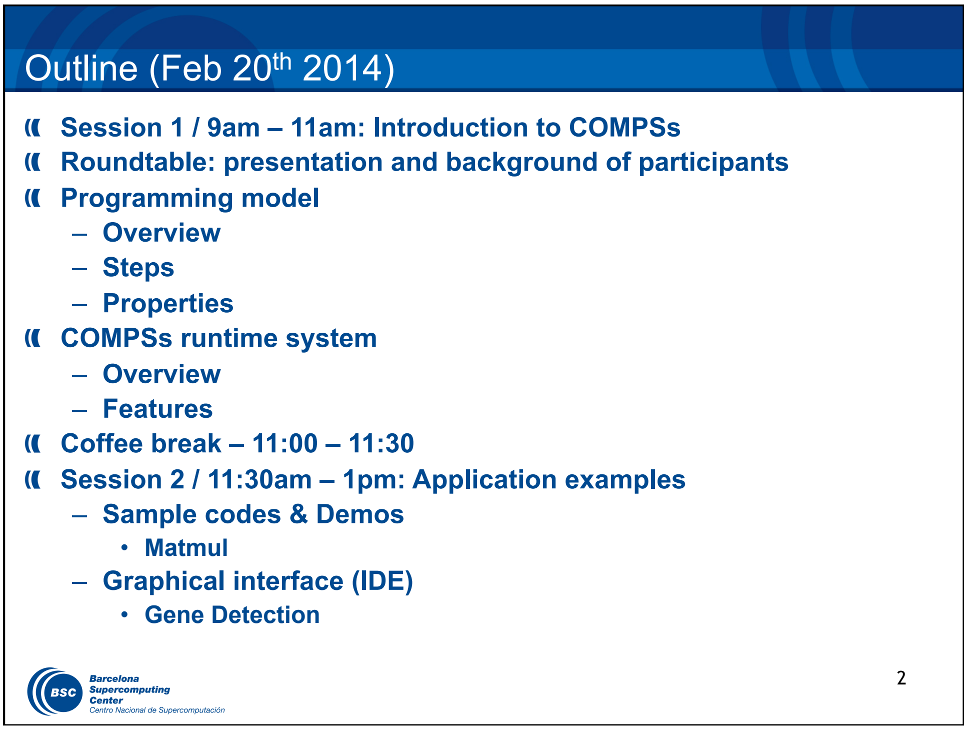
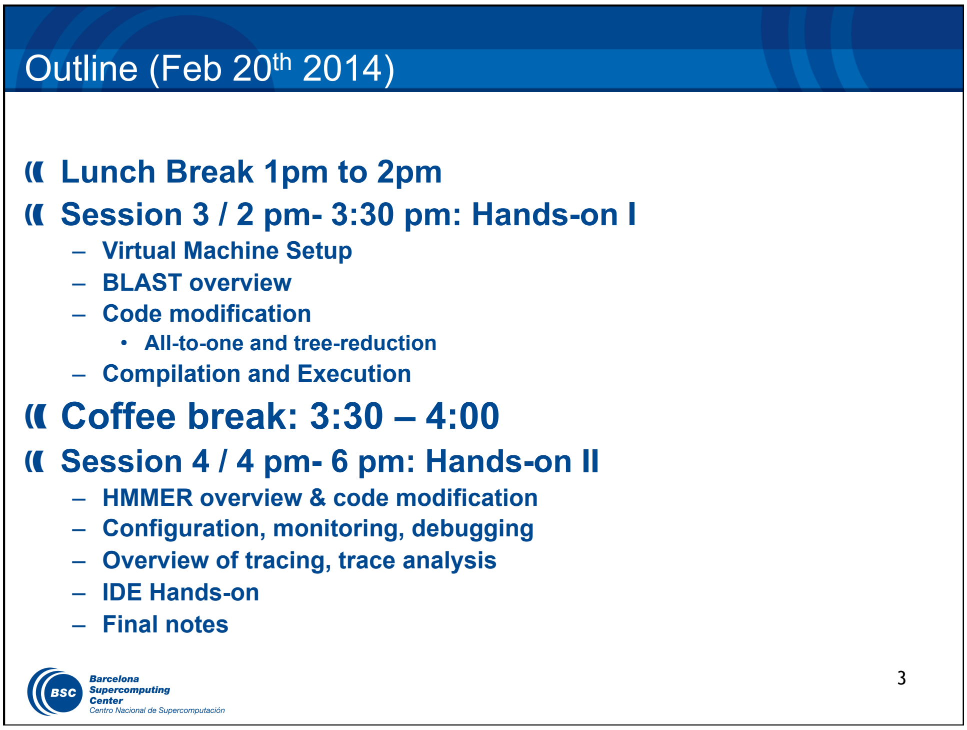


Outline (Feb 20th 2014)

- Session 1 / 9am – 11am: Introduction to COMPSs
- Roundtable: presentation and background of participants
- Programming model
  - Overview
  - Steps
  - Properties
- COMPSs runtime system
  - Overview
  - Features
- Coffee break – 11:00 – 11:30
- Session 2 / 11:30am – 1pm: Application examples
  - Sample codes & Demos
    - Matmul
  - Graphical interface (IDE)
    - Gene Detection



Outline (Feb 20th 2014)

- Lunch Break 1pm to 2pm
- Session 3 / 2 pm- 3:30 pm: Hands-on I
  - Virtual Machine Setup
  - BLAST overview
  - Code modification
    - All-to-one and tree-reduction
  - Compilation and Execution
- Coffee break: 3:30 – 4:00
- Session 4 / 4 pm- 6 pm: Hands-on II
  - HMMER overview & code modification
  - Configuration, monitoring, debugging
  - Overview of tracing, trace analysis
  - IDE Hands-on
  - Final notes

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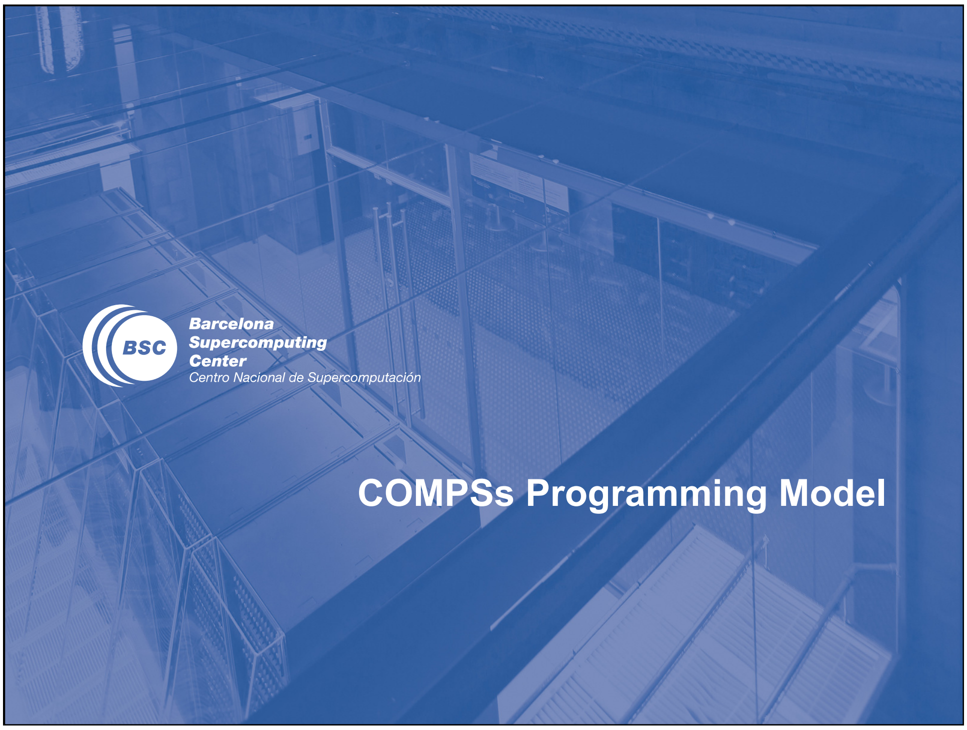

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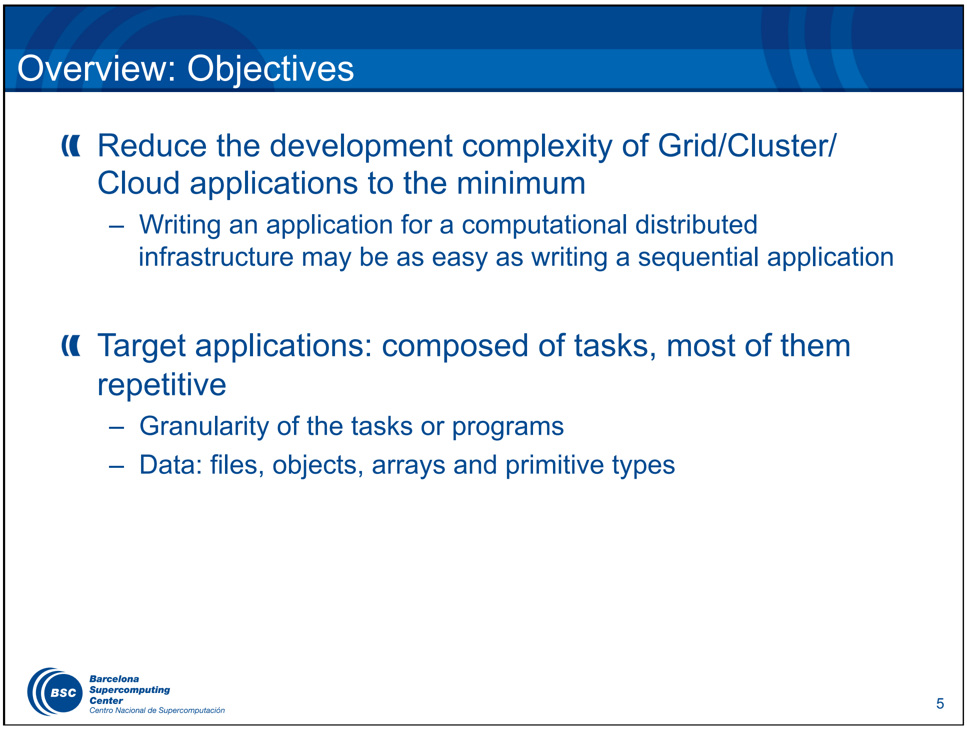
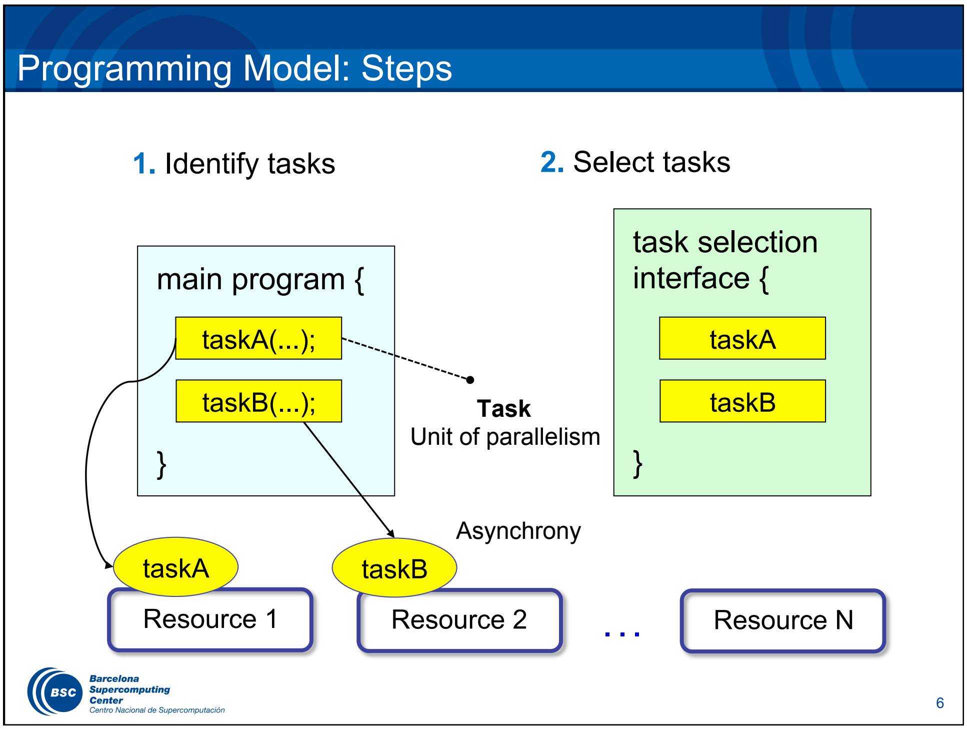
COMPSs Programming Model



Overview: Objectives

- Reduce the development complexity of Grid/Cluster/Cloud applications to the minimum
  - Writing an application for a computational distributed infrastructure may be as easy as writing a sequential application
- Target applications: composed of tasks, most of them repetitive
  - Granularity of the tasks or programs
  - Data: files, objects, arrays and primitive types



Programming Model: Steps

1. Identify tasks

2. Select tasks

main program {
taskA(...);
taskB(...);
}

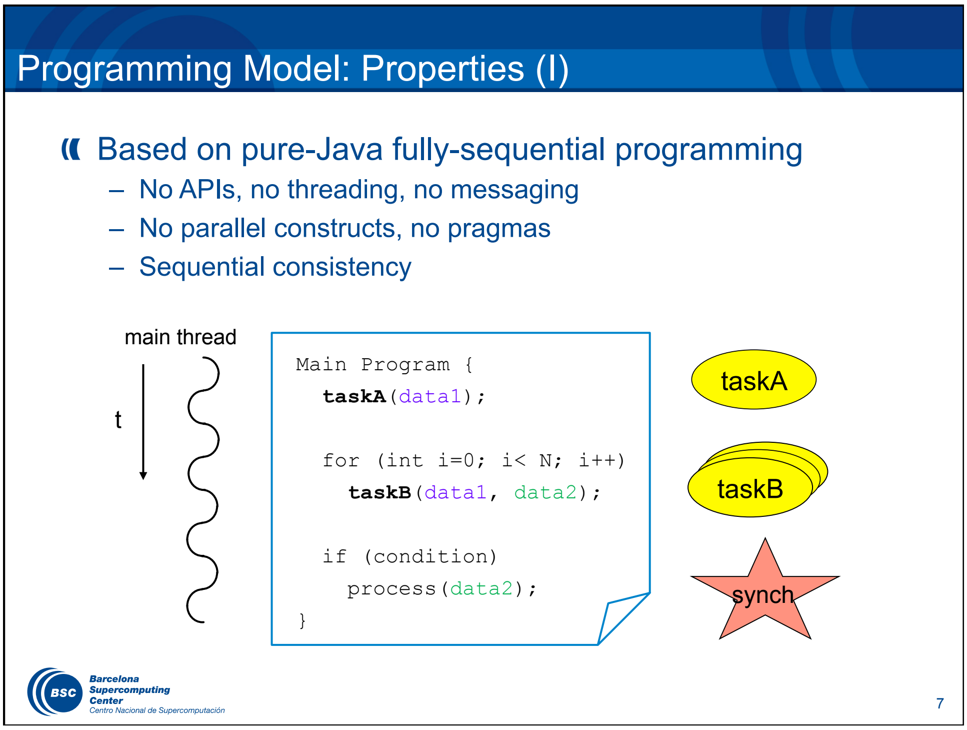
Task
Unit of parallelism

task selection interface {
taskA
taskB
}

Asynchrony

taskA
taskB

Resource 1
Resource 2
. . .
Resource N



Programming Model: Properties (I)

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

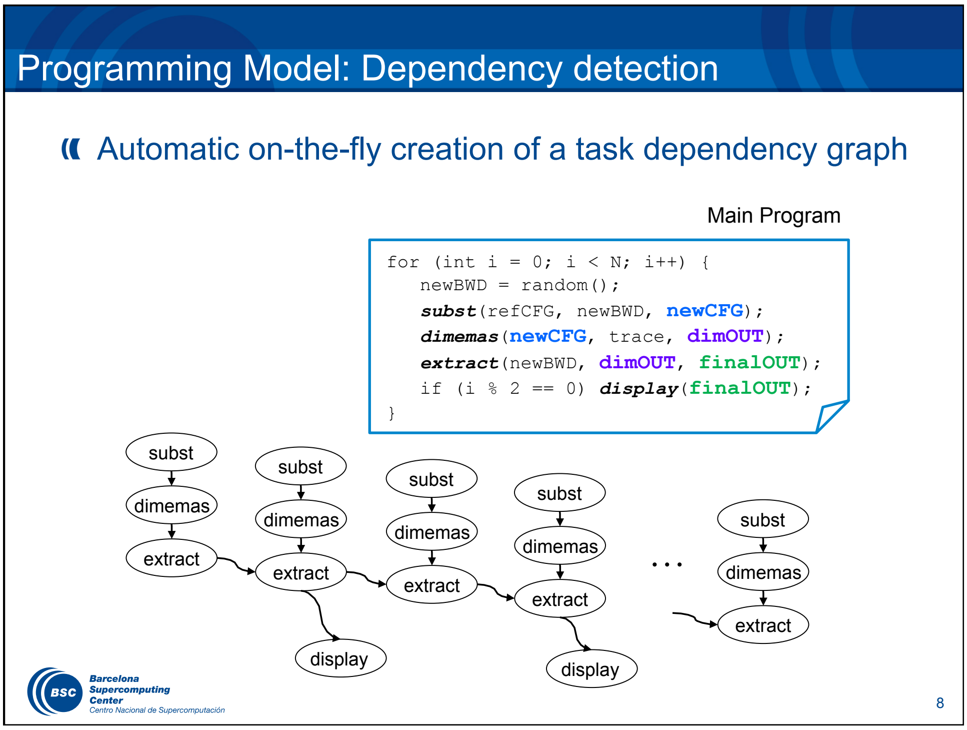
main thread
t

```
Main Program {
  taskA(data1);

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

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

taskA
taskB
synch



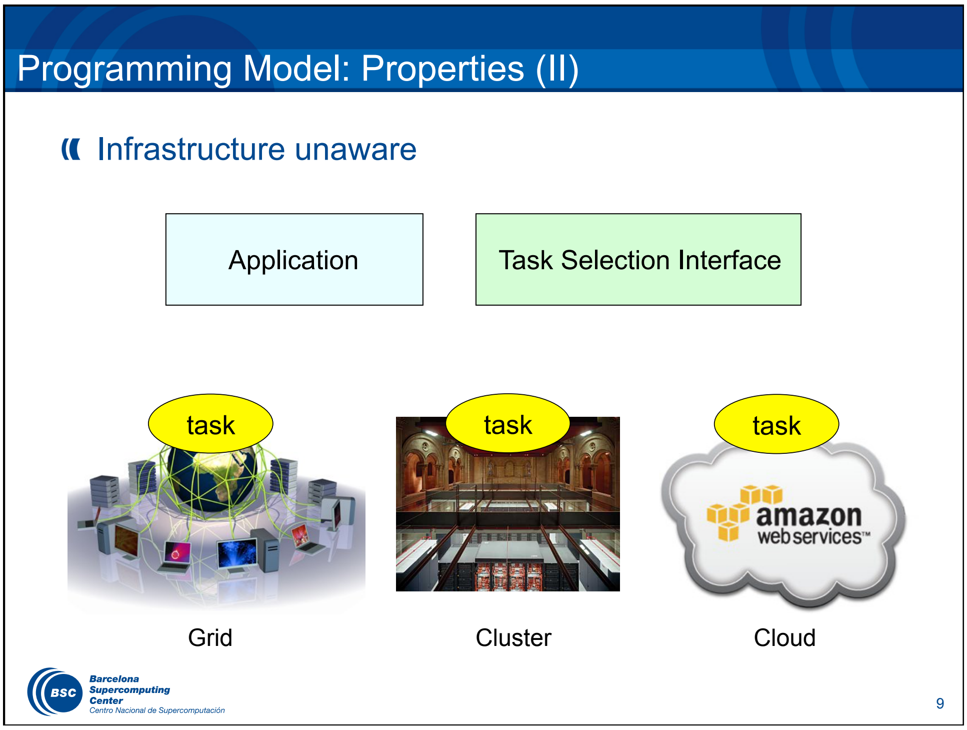
Programming Model: Dependency detection

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

Main Program

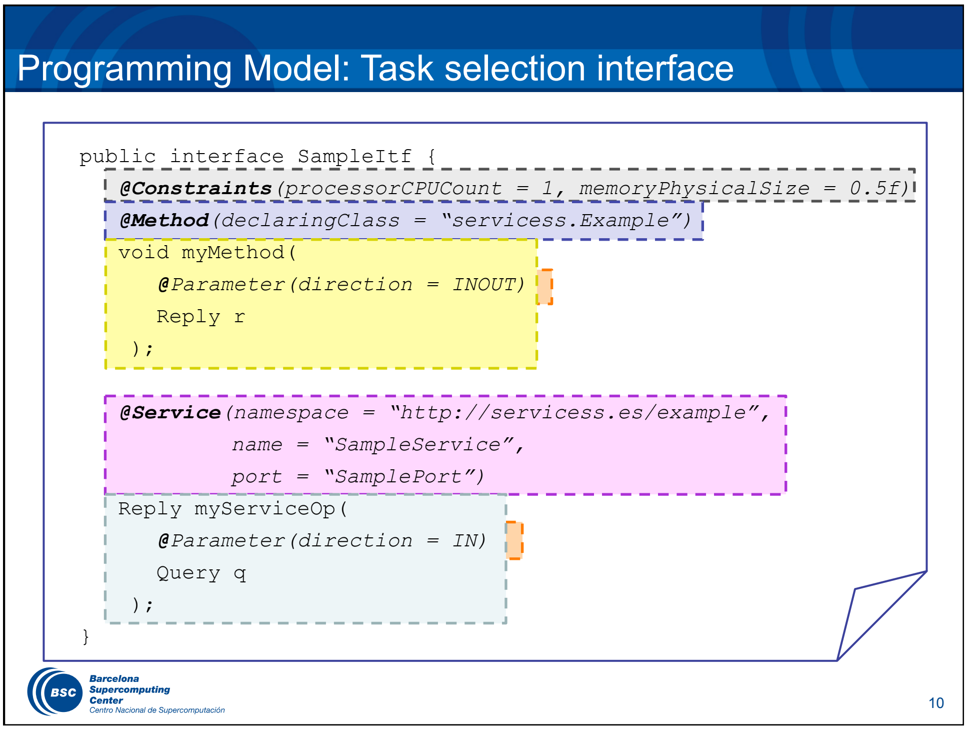
```
for (int i = 0; i < N; i++) {
   newBWD = random();
   subst(refCFG, newBWD, newCFG);
   dimemas(newCFG, trace, dimOUT);
   extract(newBWD, dimOUT, finalOUT);
   if (i % 2 == 0) display(finalOUT);
}
```

subst
dimemas
extract
subst
dimemas
extract
display
subst
dimemas
extract
subst
dimemas
extract
display
…
subst
dimemas
extract



Programming Model: Properties (II)

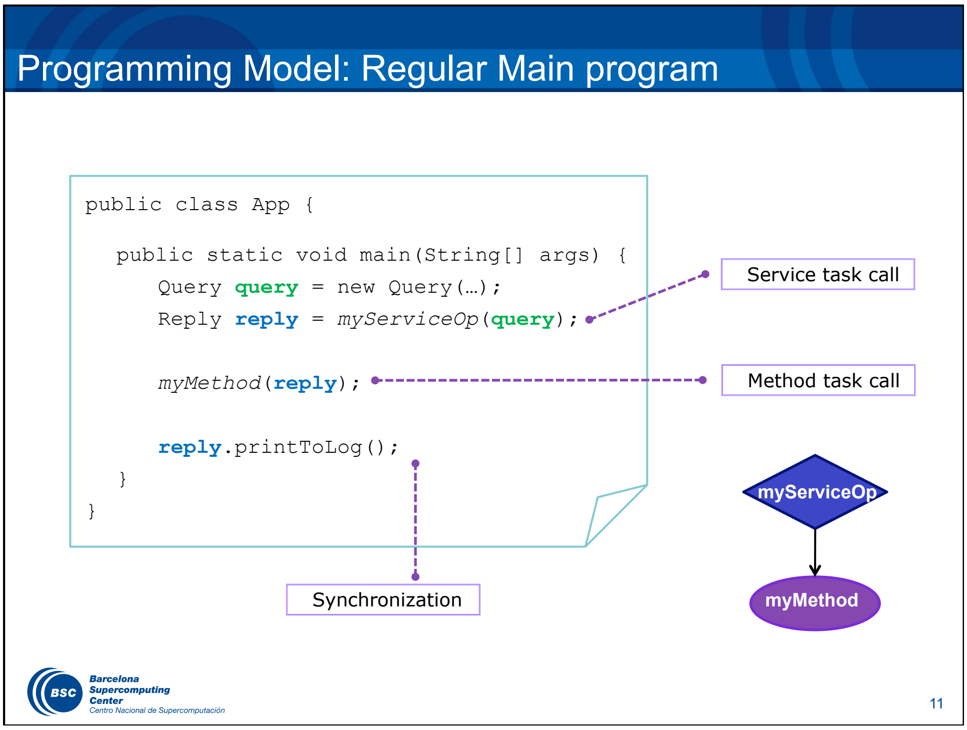
- Infrastructure unaware



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

myServiceOp
myMethod

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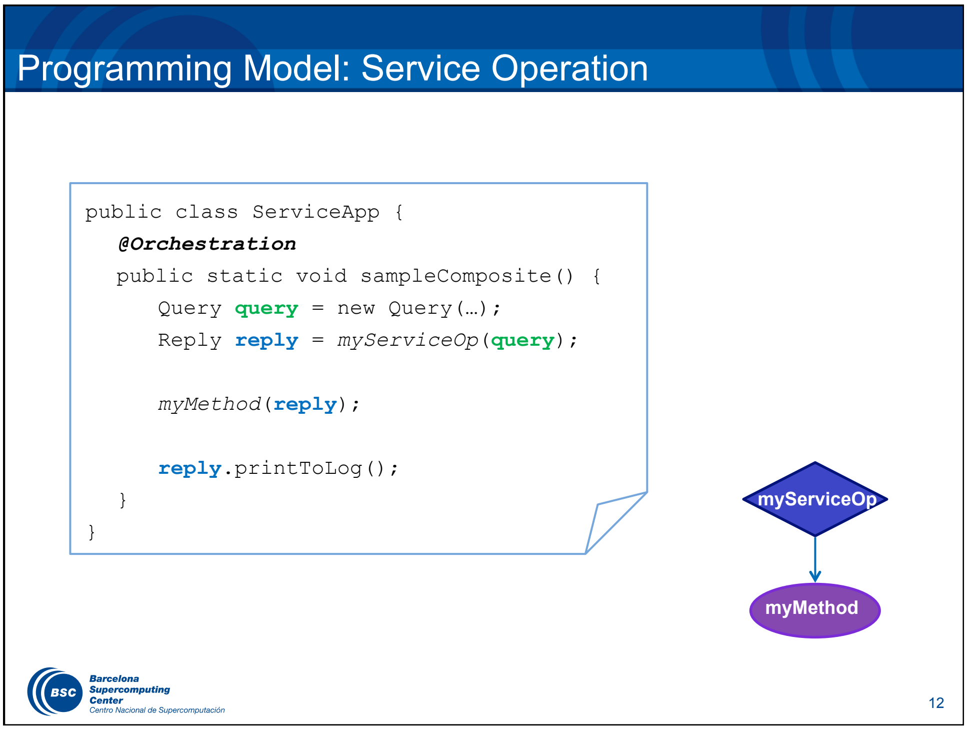

Programming Model: Service Operation

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

      myMethod(reply);

      reply.printToLog();
   }
}
```

myServiceOp
myMethod

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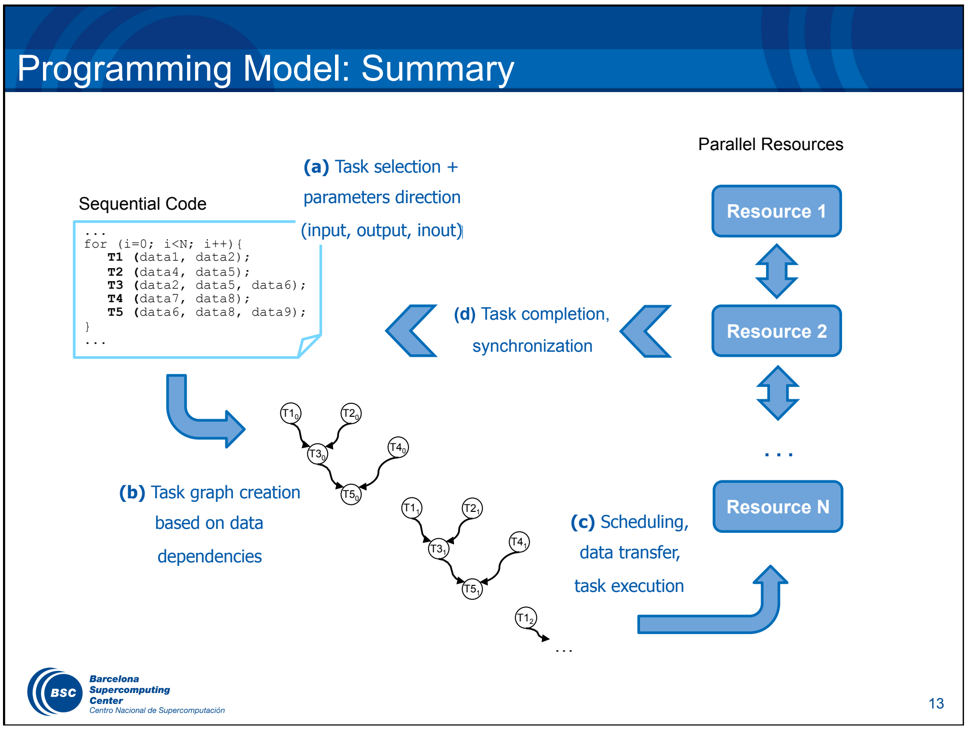

Programming Model: Summary

Sequential Code

```
...
for (i=0; i<N; i++){
   T1 (data1, data2);
   T2 (data4, data5);
   T3 (data2, data5, data6);
   T4 (data7, data8);
   T5 (data6, data8, data9);
}
...
```

(a) Task selection + parameters direction (input, output, inout)

(b) Task graph creation based on data dependencies

(c) Scheduling, data transfer, task execution

(d) Task completion, synchronization

Parallel Resources

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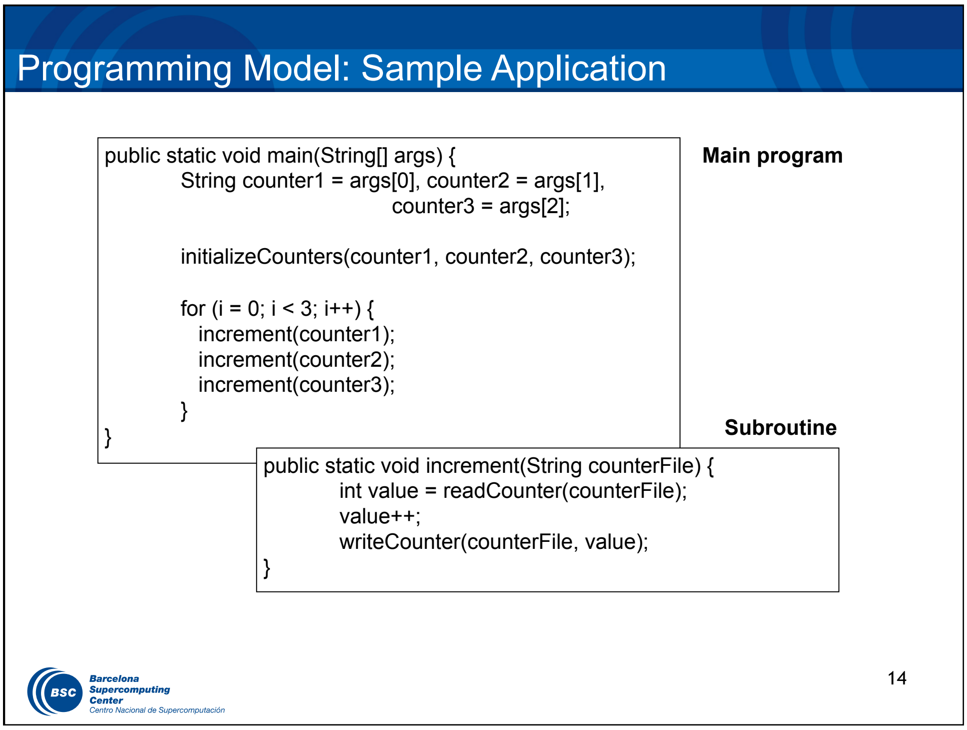

Programming Model: Sample Application

Main program

```
public static void main(String[] args) {
        String counter1 = args[0], counter2 = args[1],
                                 counter3 = args[2];

        initializeCounters(counter1, counter2, counter3);

        for (i = 0; i < 3; i++) {
          increment(counter1);
          increment(counter2);
          increment(counter3);
        }
}
```

Subroutine

```
public static void increment(String counterFile) {
        int value = readCounter(counterFile);
        value++;
        writeCounter(counterFile, value);
}
```

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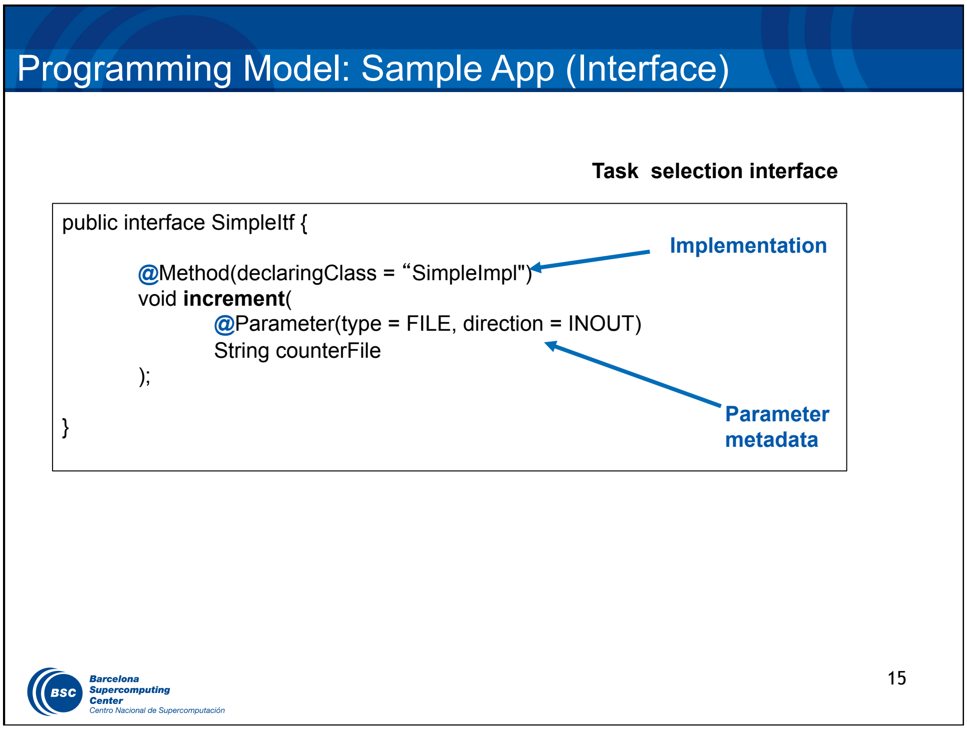

Programming Model: Sample App (Interface)

Task selection interface

```
public interface SimpleItf {

        @Method(declaringClass = “SimpleImpl")
        void increment(
                @Parameter(type = FILE, direction = INOUT)
                String counterFile
        );

}
```

Implementation

Parameter metadata

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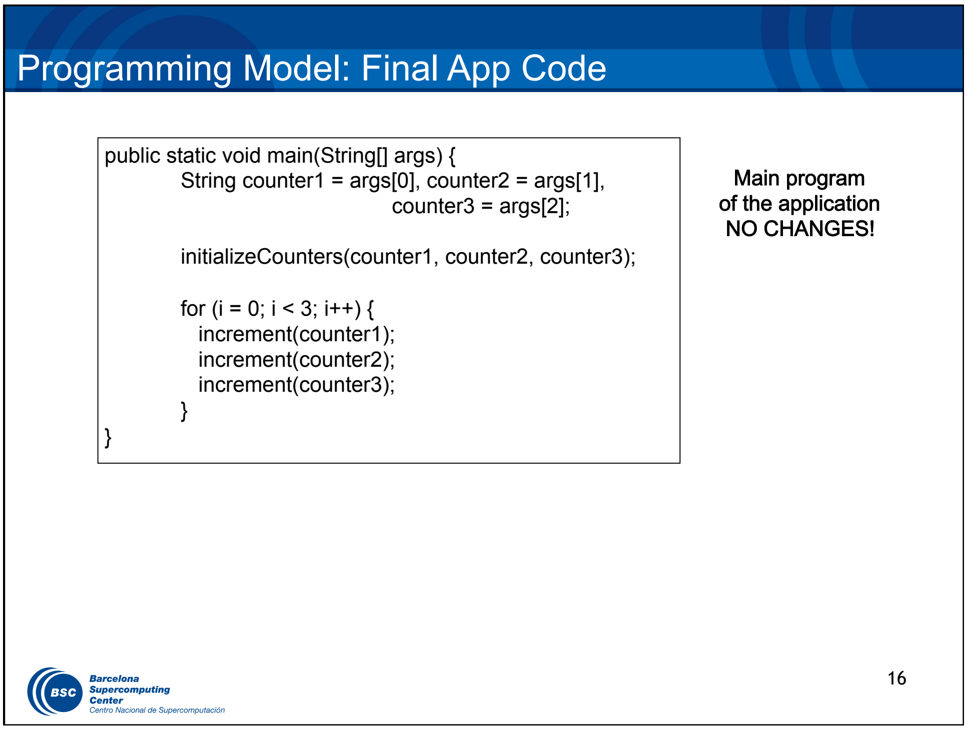

Programming Model: Final App Code

```
public static void main(String[] args) {
        String counter1 = args[0], counter2 = args[1],
                        counter3 = args[2];

        initializeCounters(counter1, counter2, counter3);

        for (i = 0; i < 3; i++) {
          increment(counter1);
          increment(counter2);
          increment(counter3);
        }
}
```

Main program
of the application
NO CHANGES!

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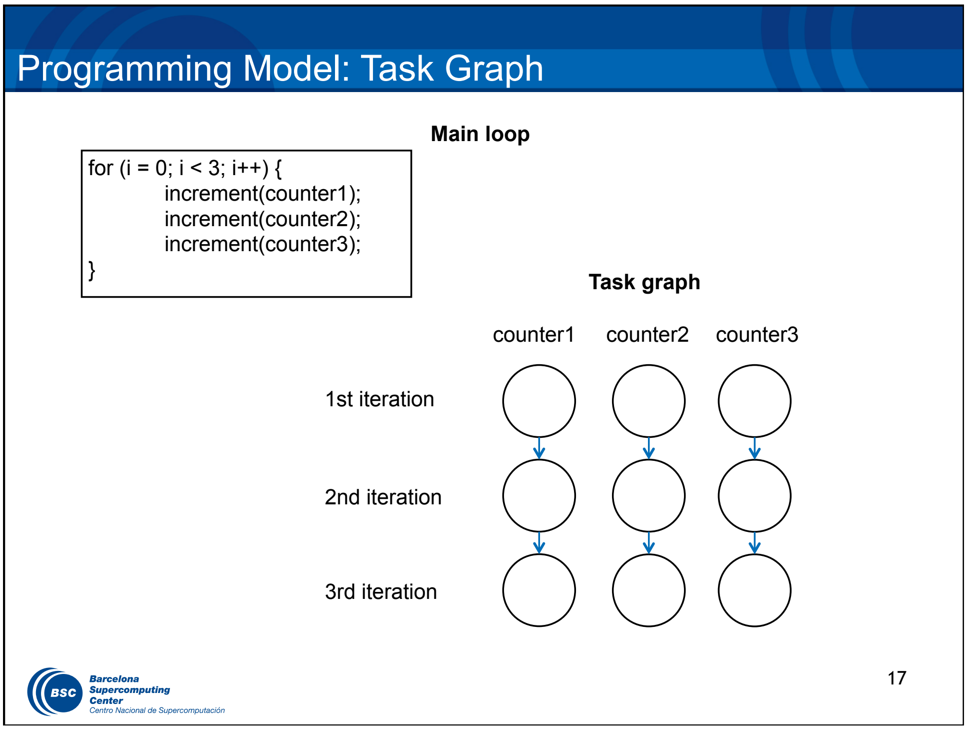

Programming Model: Task Graph

Main loop

```
for (i = 0; i < 3; i++) {
            increment(counter1);
            increment(counter2);
            increment(counter3);
}
```

Task graph

counter1 counter2 counter3

1st iteration

2nd iteration

3rd iteration

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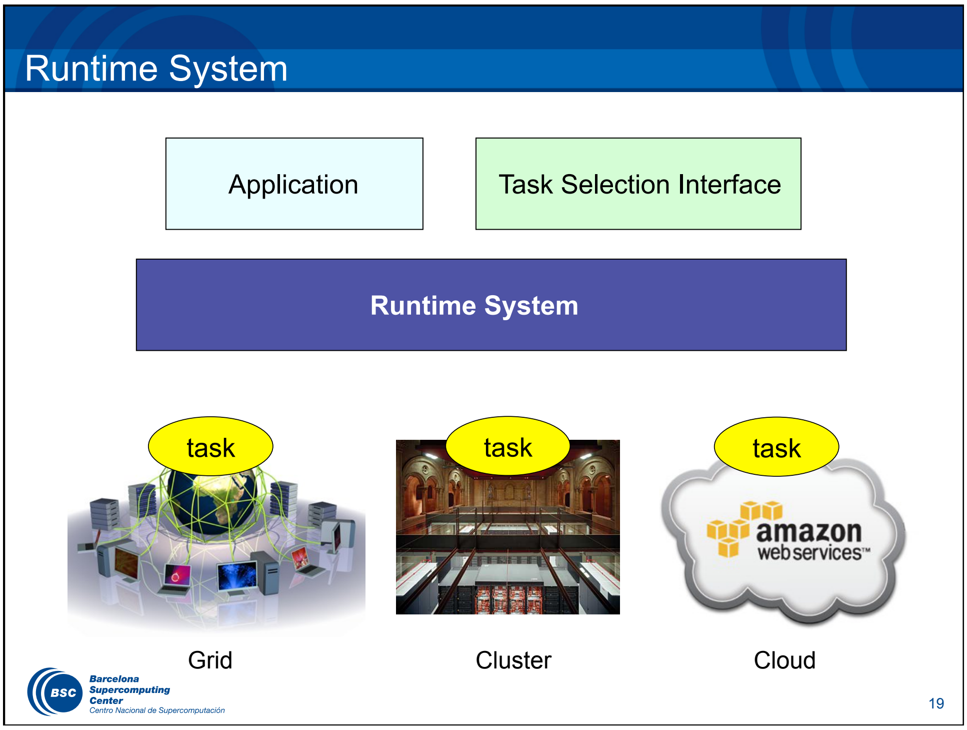
COMPSs Runtime System



Runtime System

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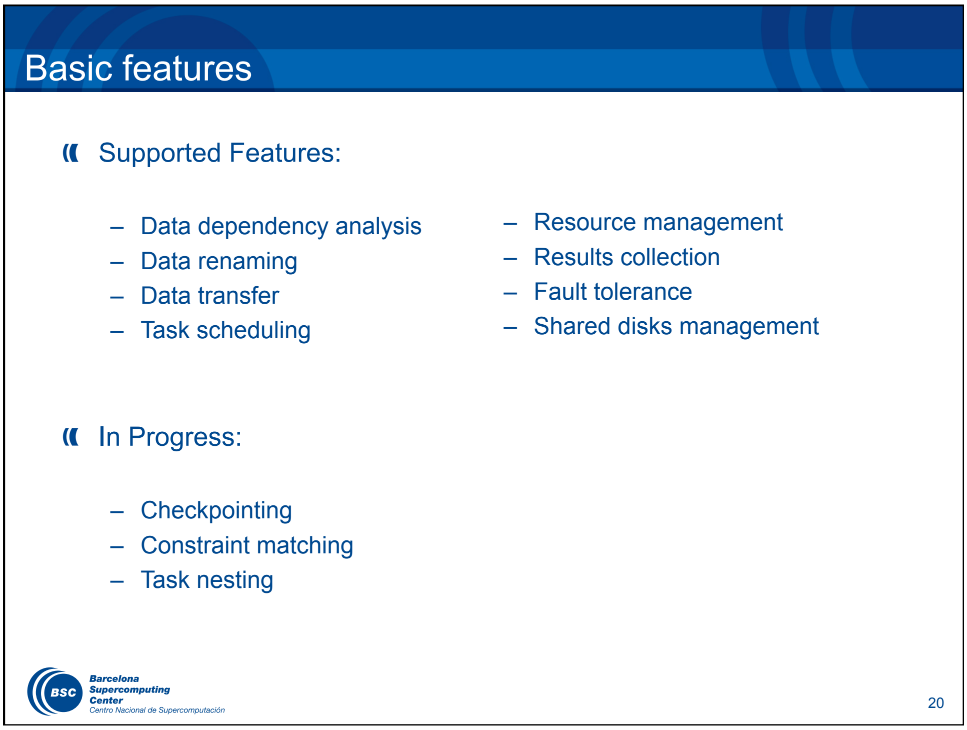

Basic features

- Supported Features:
  - Data dependency analysis
  - Data renaming
  - Data transfer
  - Task scheduling
  - Resource management
  - Results collection
  - Fault tolerance
  - Shared disks management
- In Progress:
  - Checkpointing
  - Constraint matching
  - Task nesting

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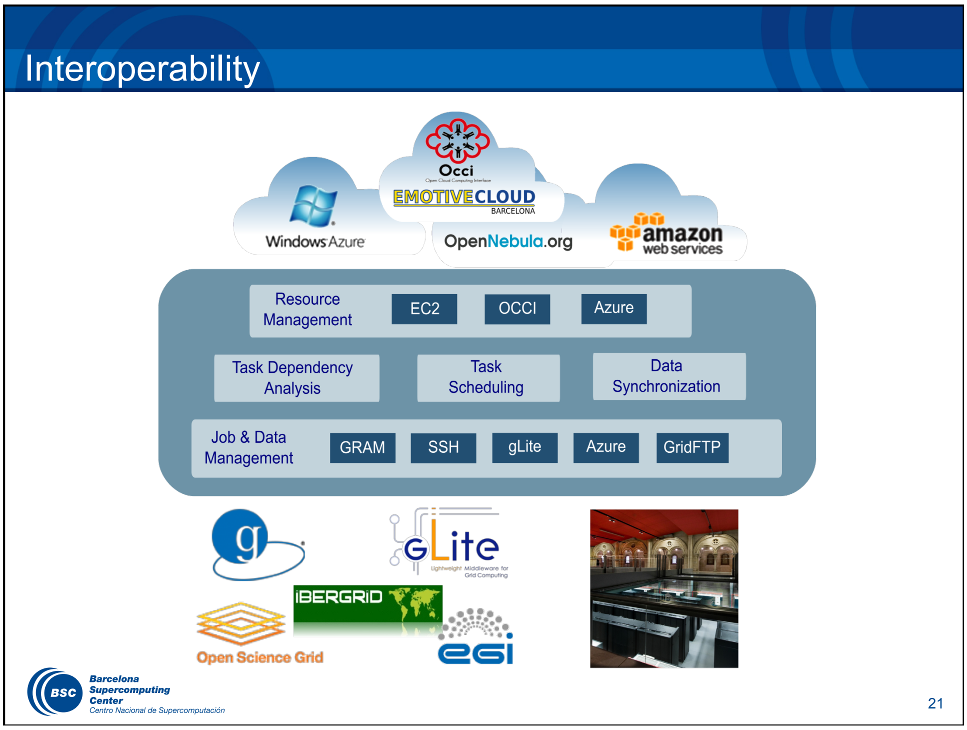

Interoperability

Resource Management: EC2, OCCI, Azure

Task Dependency Analysis

Task Scheduling

Data Synchronization

Job & Data Management: GRAM, SSH, gLite, Azure, GridFTP

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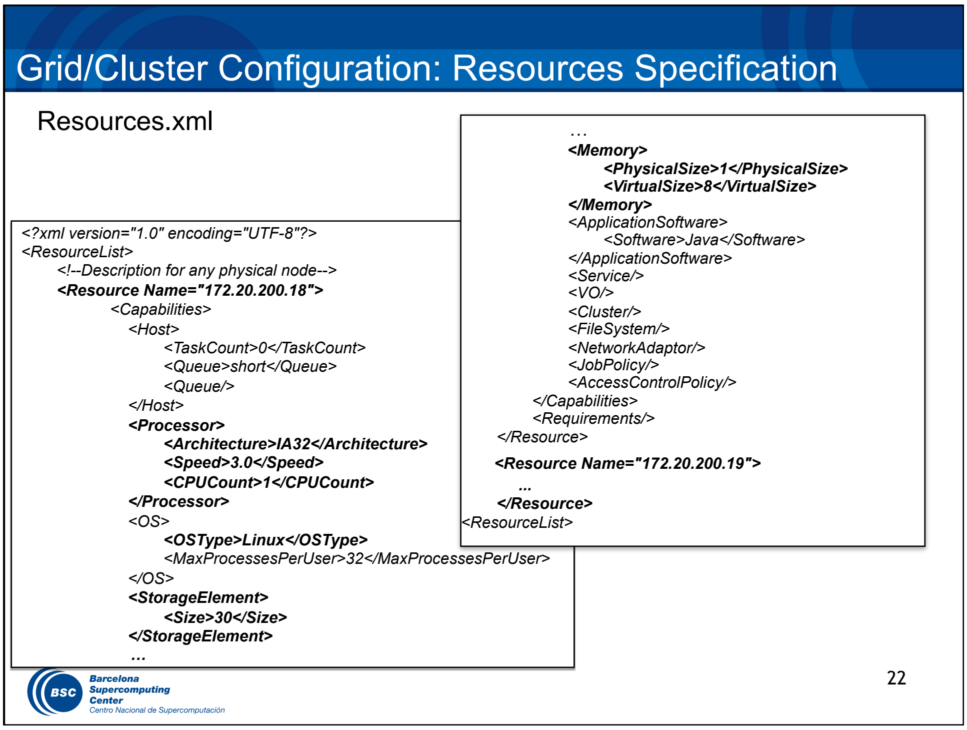

Grid/Cluster Configuration: Resources Specification

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>IA32</Architecture>
                <Speed>3.0</Speed>
                <CPUCount>1</CPUCount>
            </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>
```

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Grid/Cluster Configuration: Project Specification

Project.xml

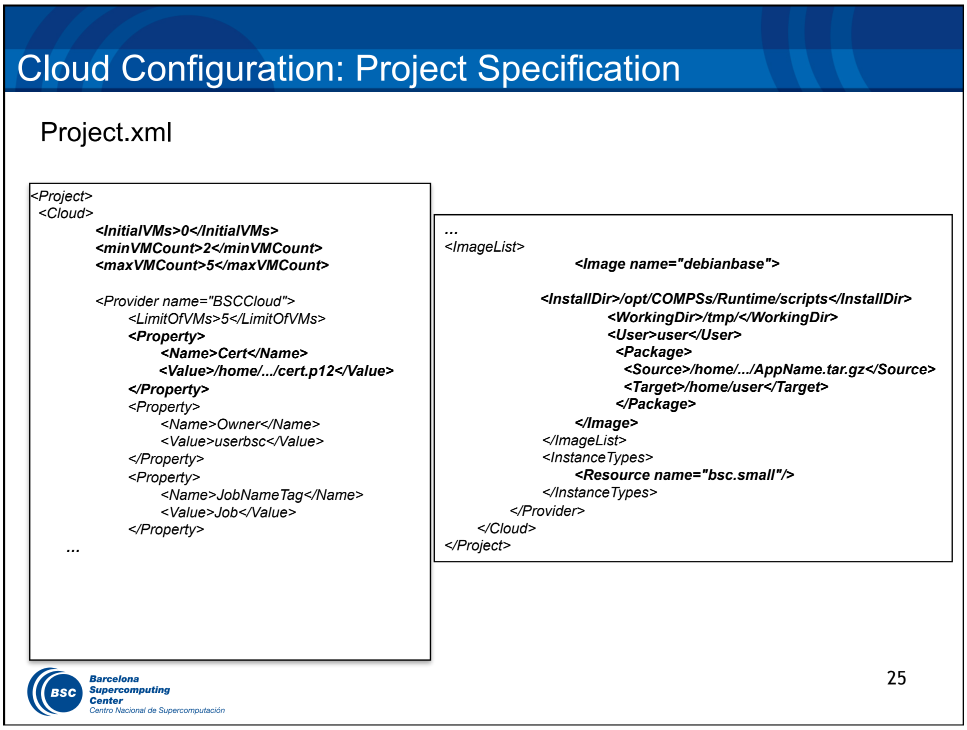
```
<?xml version="1.0" encoding="UTF-8"?>
<Project>
    <!--Description for any physical node-->
    <Worker Name="172.20.200.18">
        <InstallDir>/opt/COMPSs/Runtime/scripts/</InstallDir>
        <WorkingDir>/tmp/</WorkingDir>
        <User>user</User>
        <LimitOfTasks>1</LimitOfTasks>
  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

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

Cloud Configuration: Resources Specification

Resources.xml

```
<ResourceList>
   <CloudProvider name="BSCCloud">
         <Server>https://bscgrid20.bsc.es:8443/DRP</Server>
         <Connector>
             integratedtoolkit.connectors.emotivecloud.DRPSecureClientConnector
         </Connector>
         <ImageList>
          <Image name="debianbase"/>
         </ImageList>
         <InstanceTypes>
              <Resource Name="bsc.small">
                   <Capabilities>
                        <Processor>
                             <CPUCount>1</CPUCount>
                        </Processor>
                        <StorageElement>
                             <Size>0.5</Size>
                        </StorageElement>
                        <Memory>
                             <PhysicalSize>1</PhysicalSize>
                        </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>Cert</Name>
                    <Value>/home/.../cert.p12</Value>
               </Property>
               <Property>
                    <Name>Owner</Name>
                    <Value>userbsc</Value>
               </Property>
               <Property>
                    <Name>JobNameTag</Name>
                    <Value>Job</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>
```

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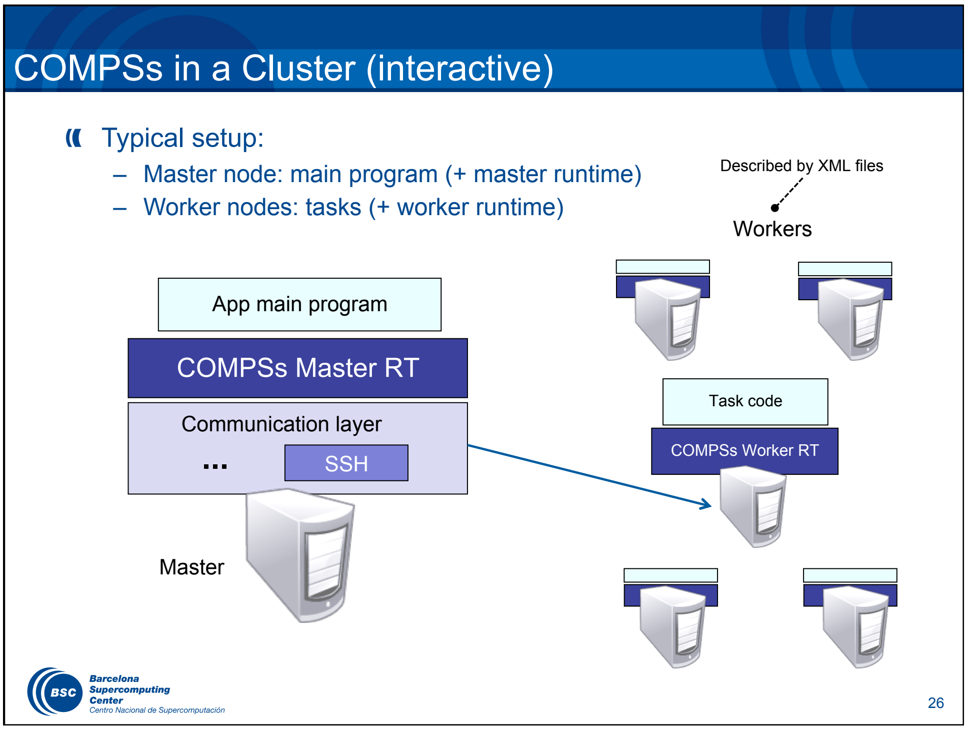

COMPSs in a Cluster (interactive)

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

Described by XML files

Workers

App main program

COMPSs Master RT

Communication layer

…

SSH

Master

Task code

COMPSs Worker RT

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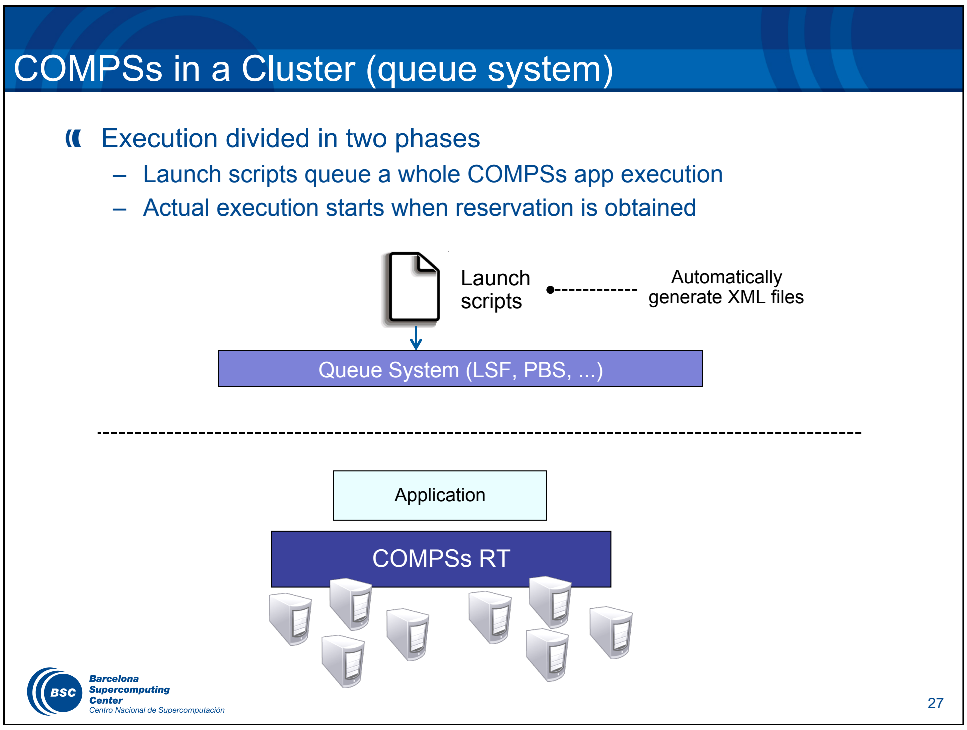


COMPSs in a Cluster (queue system)

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

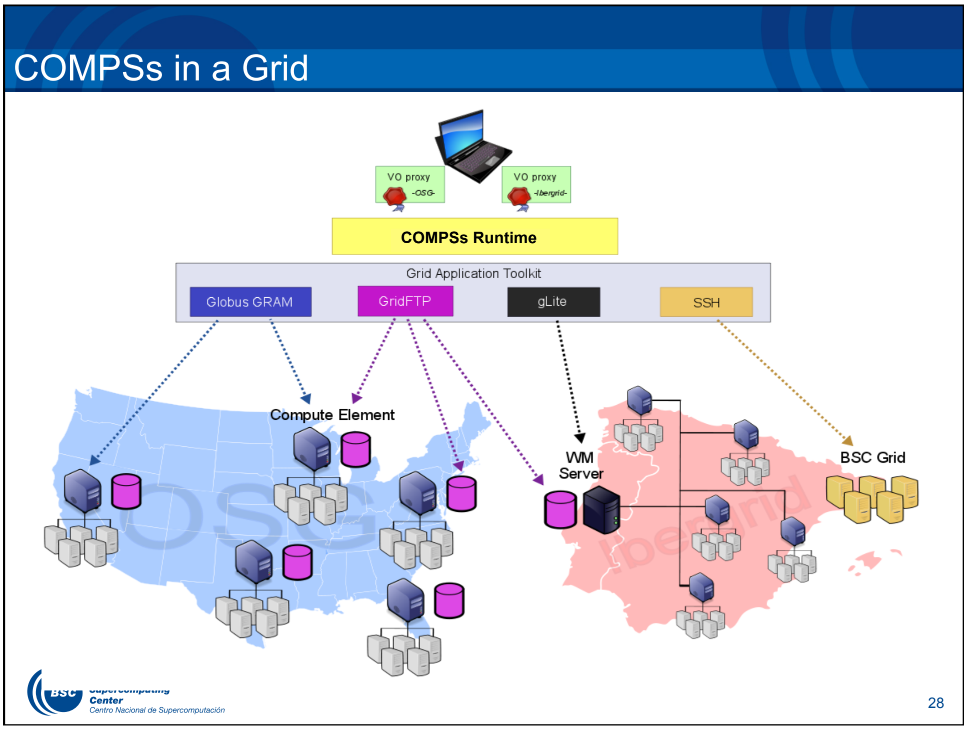
Launch scripts

Automatically generate XML files

Queue System (LSF, PBS, ...)

Application

COMPSs RT



COMPSs in a Grid

VO proxy -OSG-

VO proxy -Ibergrid-

COMPSs Runtime

Grid Application Toolkit

Globus GRAM

GridFTP

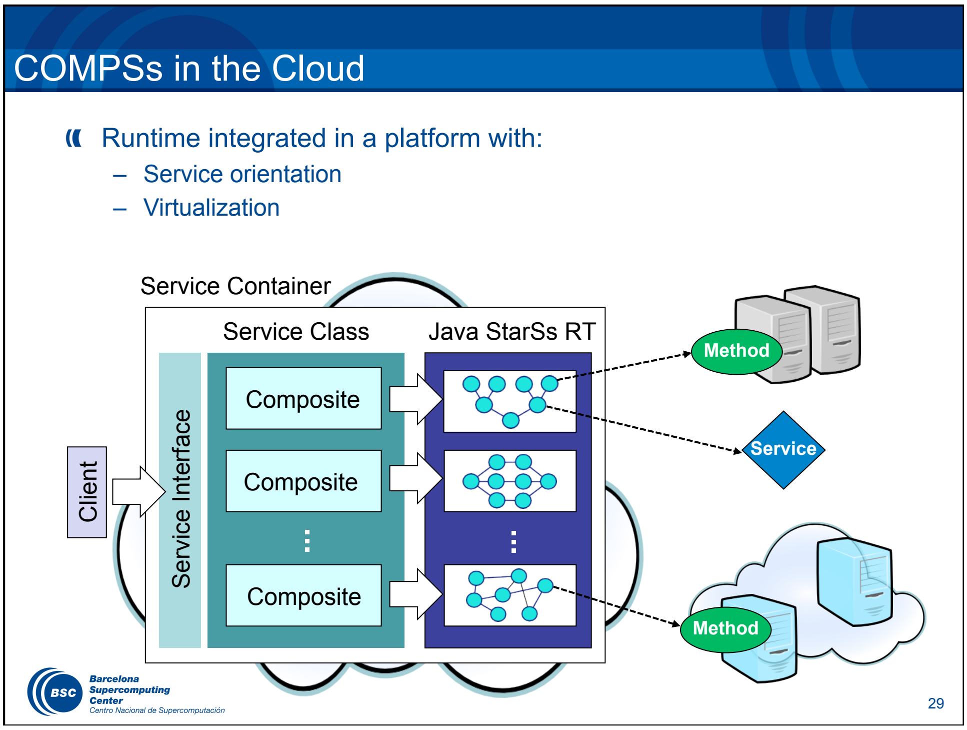
gLite

SSH

Compute Element

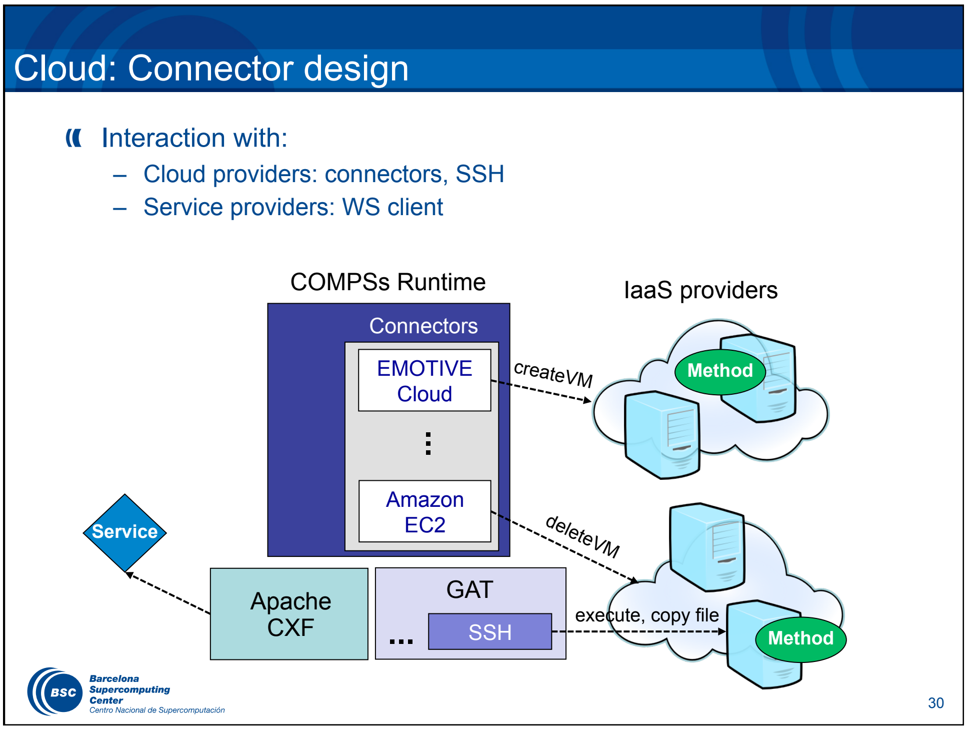
WM Server

BSC Grid



COMPSs in the Cloud

- Runtime integrated in a platform with:
  - Service orientation
  - Virtualization

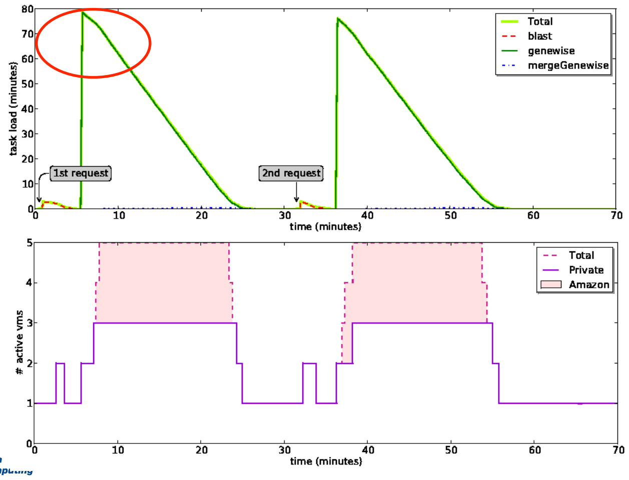


Cloud: Connector design

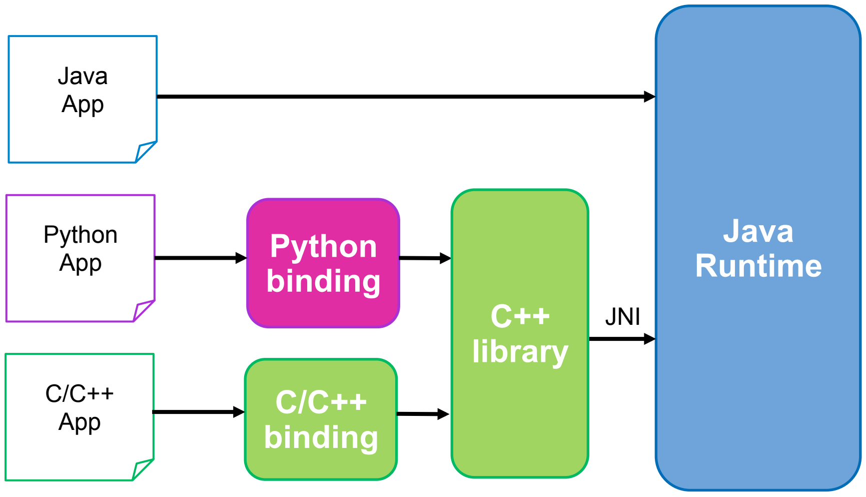
- Interaction with:
  - Cloud providers: connectors, SSH
  - Service providers: WS client

Cloud: Elasticity

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



COMPSs Bindings



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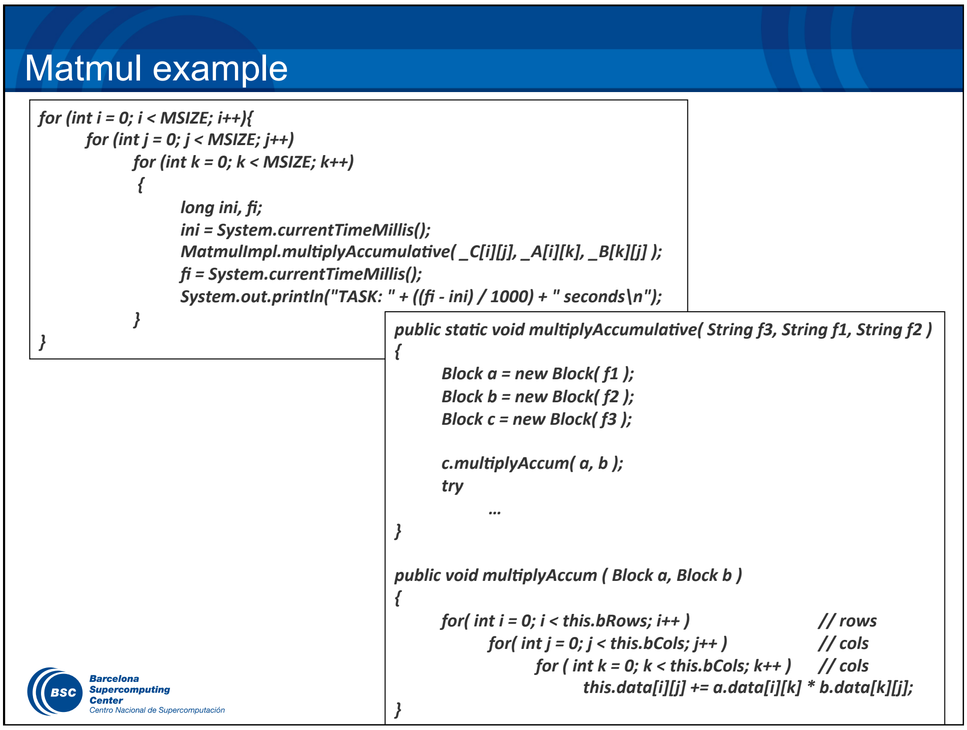
DEMOS



Matmul example

```
for (int i = 0; i < MSIZE; i++){
        for (int j = 0; j < MSIZE; j++)
                for (int k = 0; k < MSIZE; k++)
                {
                        long ini, fi;
                        ini = System.currentTimeMillis();
                        MatmulImpl.multiplyAccumulative( _C[i][j], _A[i][k], _B[k][j] );
                        fi = System.currentTimeMillis();
                        System.out.println("TASK: " + ((fi - ini) / 1000) + " seconds\n");
                }
}
```

```
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];
}
```

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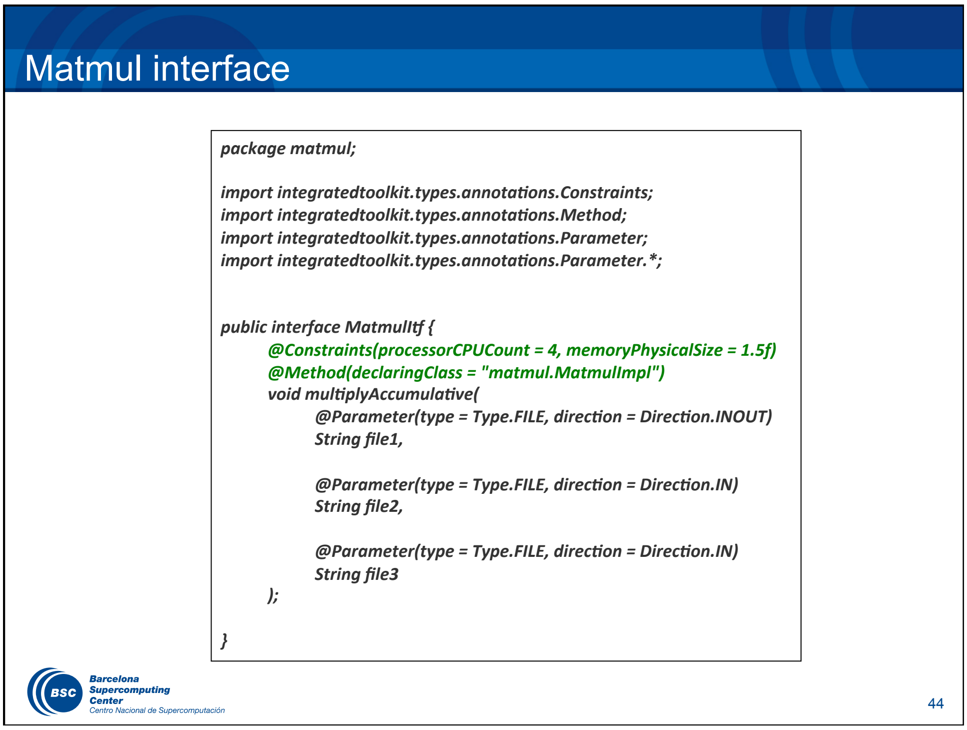

Matmul interface

```
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(processorCPUCount = 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
        );

}
```

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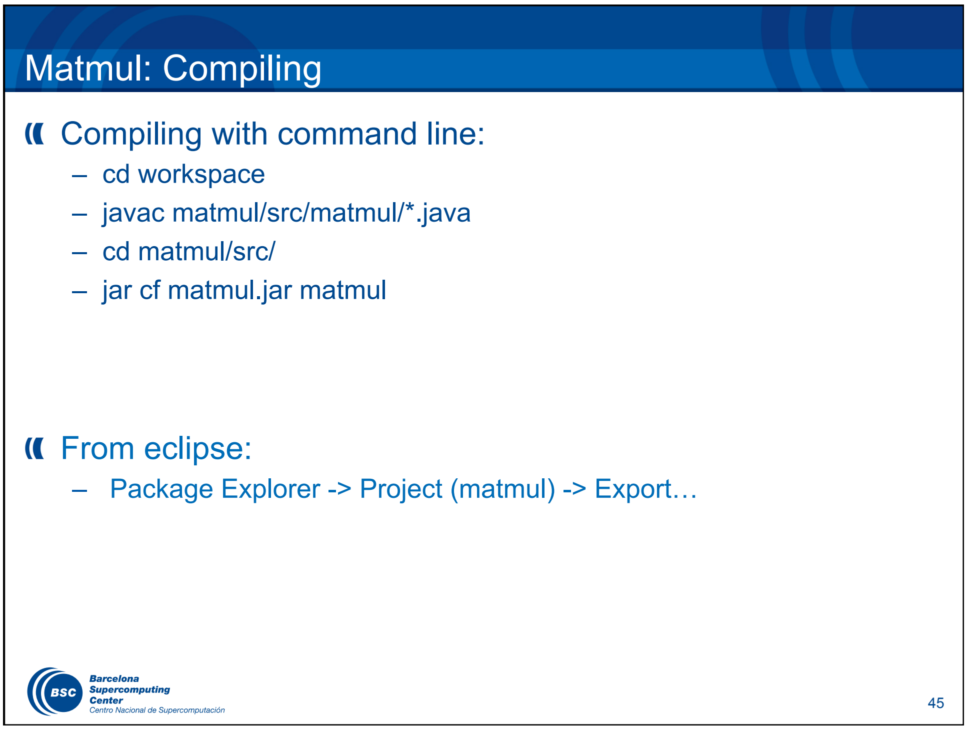

Matmul: Compiling

- Compiling with command line:
  - cd workspace
  - javac matmul/src/matmul/*.java
  - cd matmul/src/
  - jar cf matmul.jar matmul

- From eclipse:
  - Package Explorer -> Project (matmul) -> Export…

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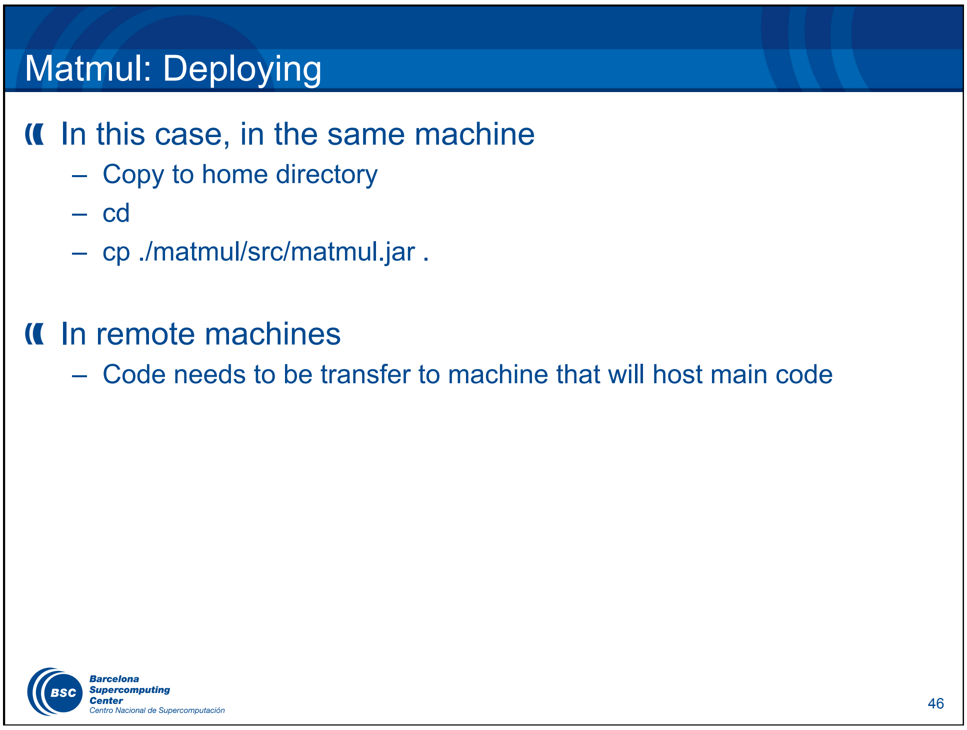
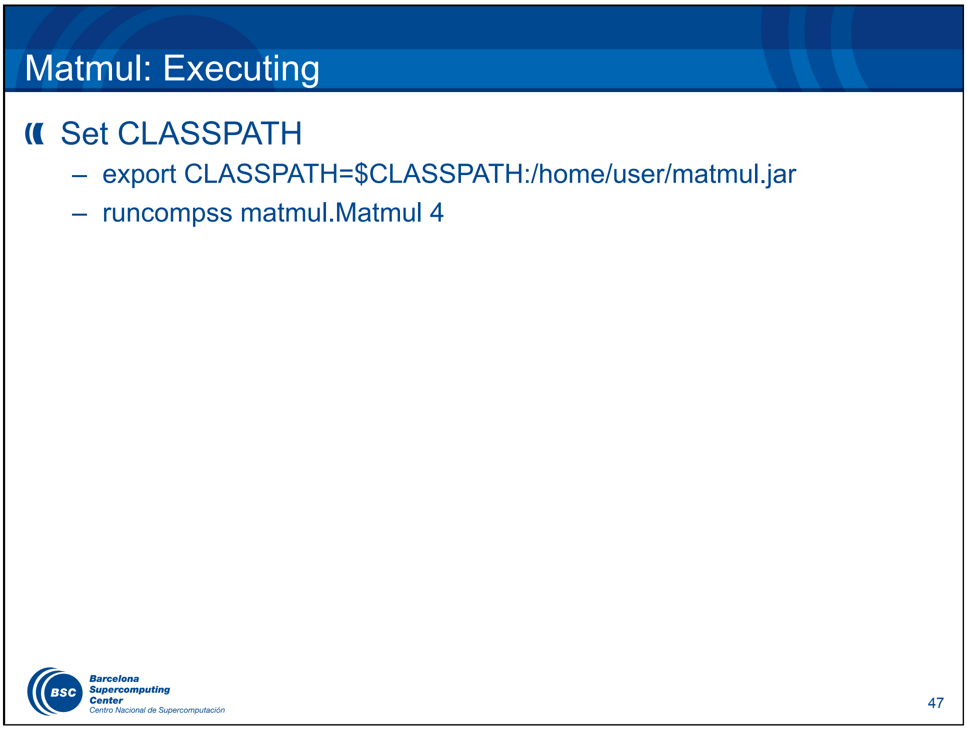


Matmul: Deploying

- In this case, in the same machine
  - Copy to home directory
  - cd
  - cp ./matmul/src/matmul.jar .
- In remote machines
  - Code needs to be transfer to machine that will host main code



Matmul: Executing

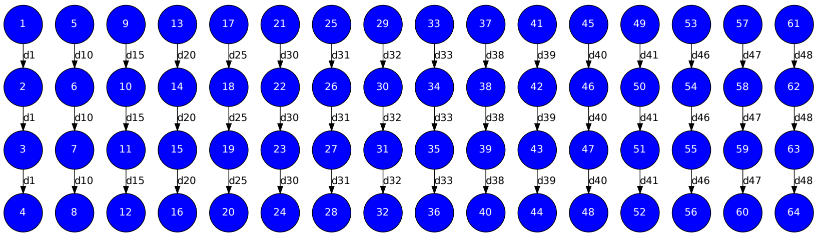
- Set CLASSPATH
  - export CLASSPATH=$CLASSPATH:/home/user/matmul.jar
  - runcompss matmul.Matmul 4

Matmul: Monitoring execution

- Browse
  - http://localhost:8080/compss-monitor

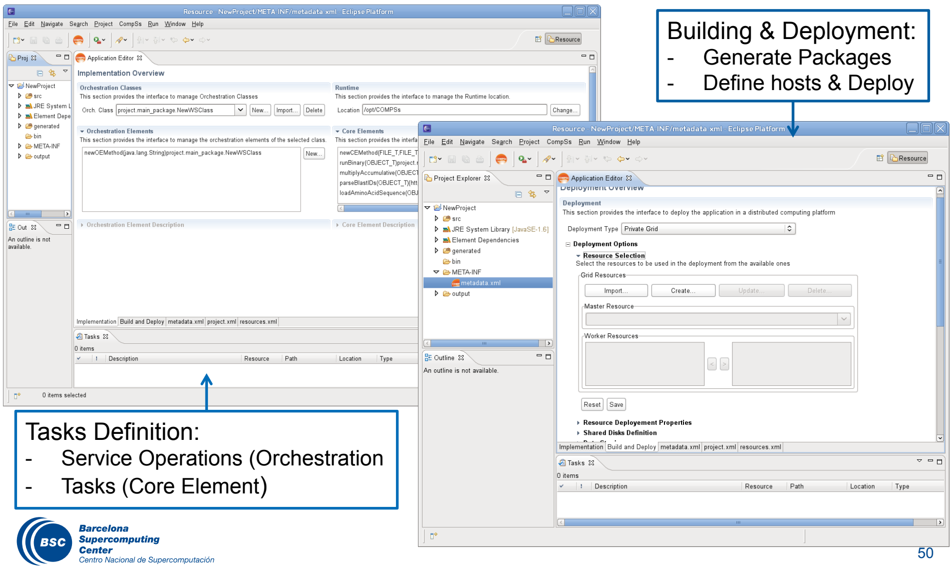
Demos: Matmul

- Blocks matrixes multiplication


1 5 9 13 17 21 25 29 33 37 41 45 49 53 57 61
d1 d10 d15 d20 d25 d30 d31 d32 d33 d38 d39 d40 d41 d46 d47 d48
2 6 10 14 18 22 26 30 34 38 42 46 50 54 58 62
d1 d10 d15 d20 d25 d30 d31 d32 d33 d38 d39 d40 d41 d46 d47 d48
3 7 11 15 19 23 27 31 35 39 43 47 51 55 59 63
d1 d10 d15 d20 d25 d30 d31 d32 d33 d38 d39 d40 d41 d46 d47 d48
4 8 12 16 20 24 28 32 36 40 44 48 52 56 60 64

IDE COMPSs applications as a Service

- IDE for implementing and deploying applications



Building & Deployment:
- Generate Packages
- Define hosts & Deploy

Tasks Definition:
- Service Operations (Orchestration
- Tasks (Core Element)

Orch. Class: project.main_package.NewWSClass

Location: /opt/COMPSs

Deployment Type: Private Grid

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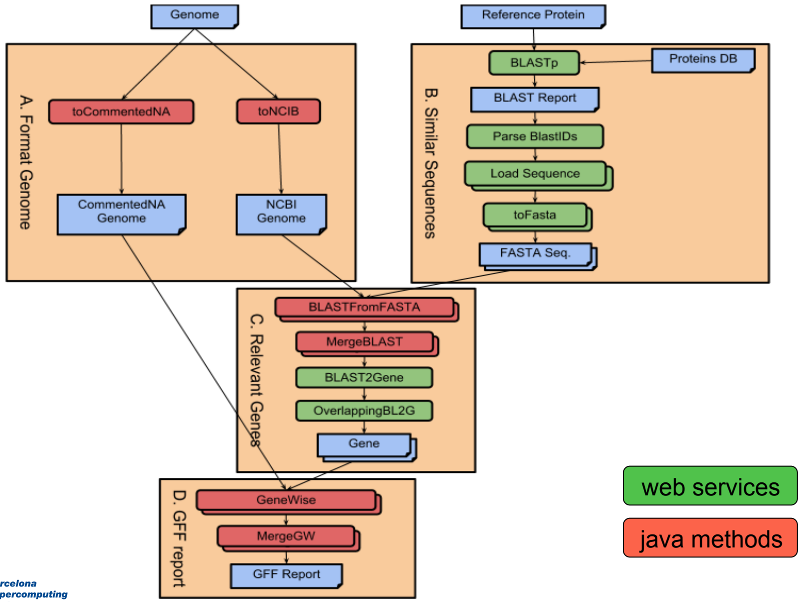
Demos: Gene Detection Application

- Gene Detection algorithm designed by the BSC Life Sciences department
  - Automatic Homology-based gene detection and analysis
- Combine services with computations
  - Example that shows different capabilities of COMPSs
  - Implicit Synchronization points
  - Different method and service call types
  - Objects and files as parameters

Gene Detection



Genome

Reference Protein

A. Format Genome

toCommentedNA

toNCIB

CommentedNA Genome

NCBI Genome

B. Similar Sequences

BLASTp

Proteins DB

BLAST Report

Parse BlastIDs

Load Sequence

toFasta

FASTA Seq.

C. Relevant Genes

BLASTFromFASTA

MergeBLAST

BLAST2Gene

OverlappingBL2G

Gene

D. GFF report

GeneWise

MergeGW

GFF Report

🟩 web services

🟥 java methods

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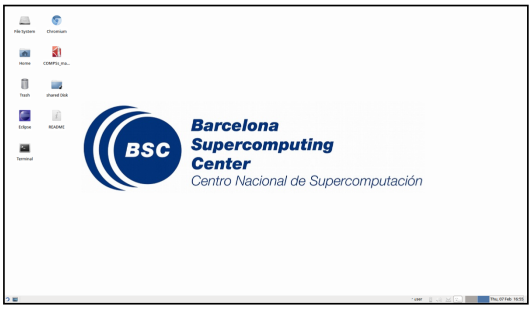
HANDS-ON

Hands-On: Overview

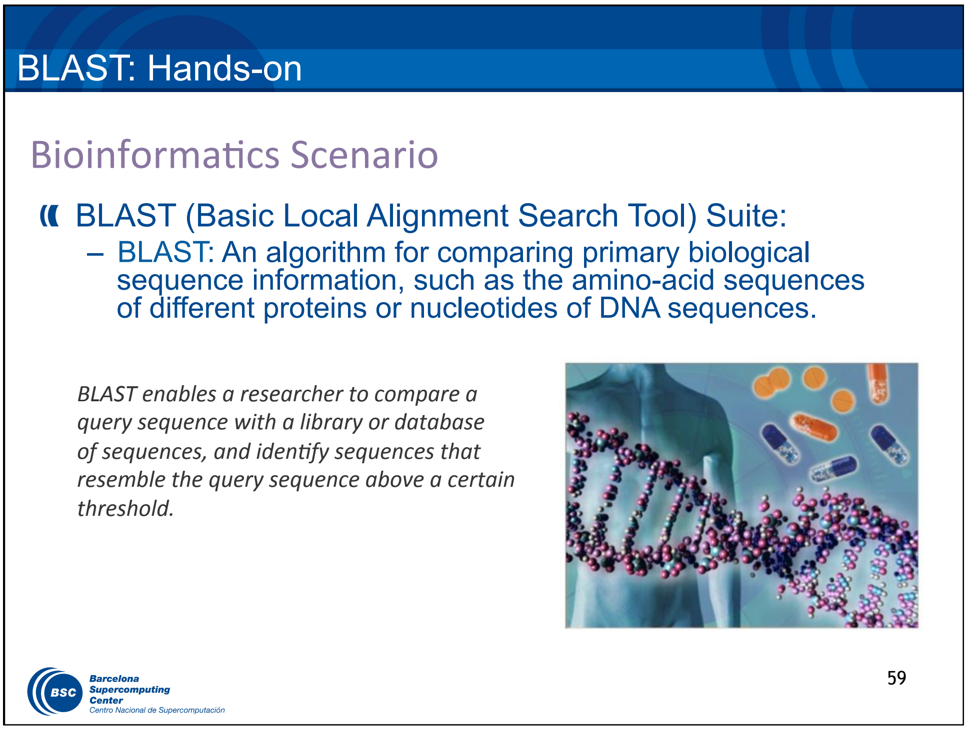
- COMPSs Virtual Machine setup
- Applications Overview (BLAST, HMMER, …)
  - Code modification
  - Configuration, compilation & execution
  - Monitoring, debugging
  - Overview of tracing and trace performance analysis
  - IDE

COMPSs development VM Installation

- **COMPSs Development & Test VM (64-bit) OVA**
  - **Available from USB**
- **Import the virtual appliance in VirtualBox**



BLAST: Hands-on

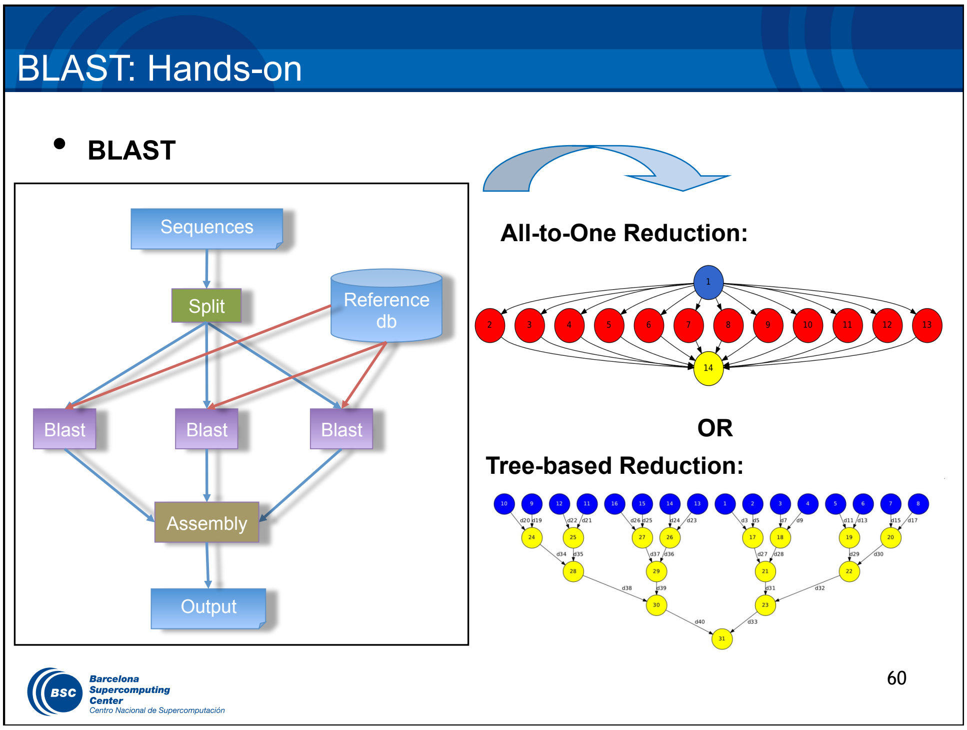


BLAST: Hands-on

Bioinformatics Scenario

- BLAST (Basic Local Alignment Search Tool) Suite:
  - BLAST: An algorithm for comparing primary biological sequence information, such as the amino-acid sequences of different proteins or nucleotides of DNA sequences.

BLAST enables a researcher to compare a query sequence with a library or database of sequences, and identify sequences that resemble the query sequence above a certain threshold.



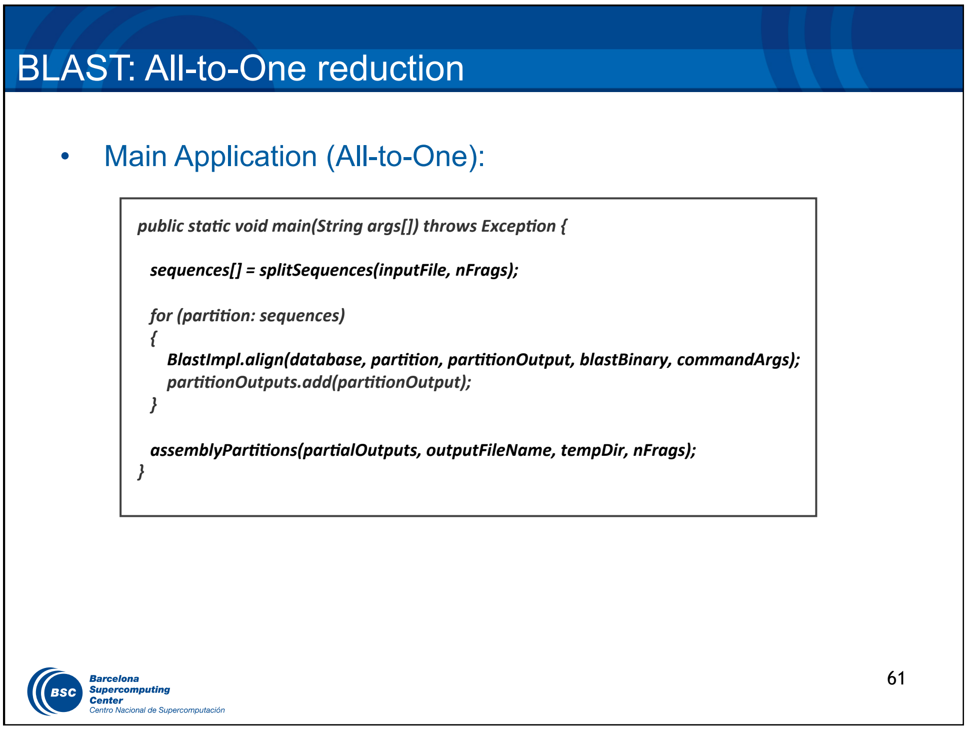
BLAST: Hands-on

- **BLAST**

All-to-One Reduction:

OR

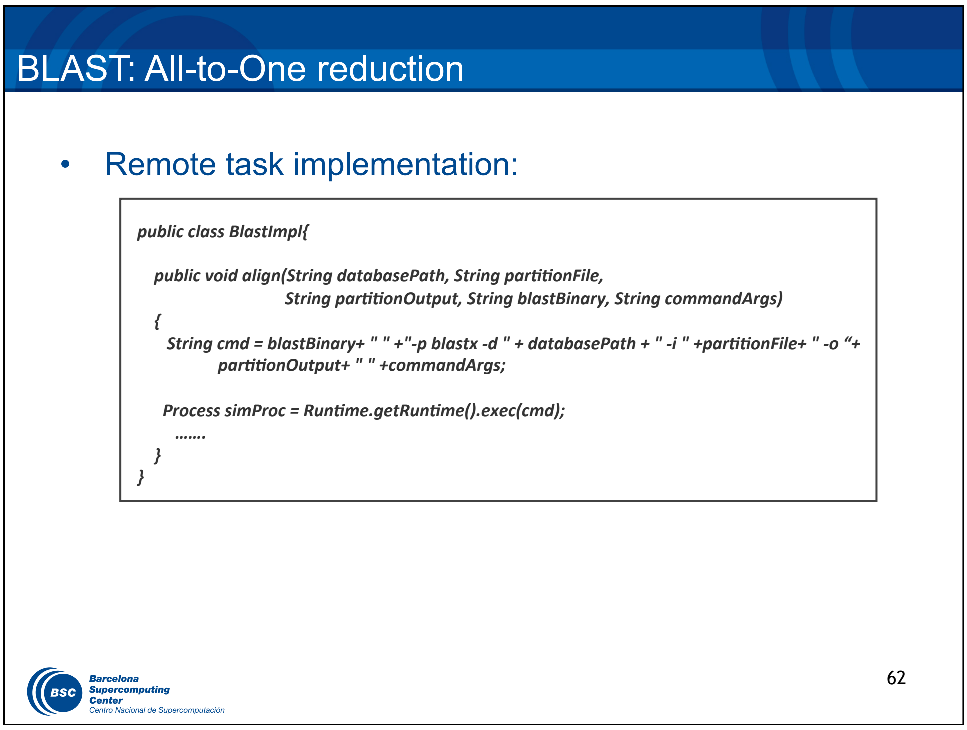
Tree-based Reduction:



BLAST: All-to-One reduction

- Main Application (All-to-One):

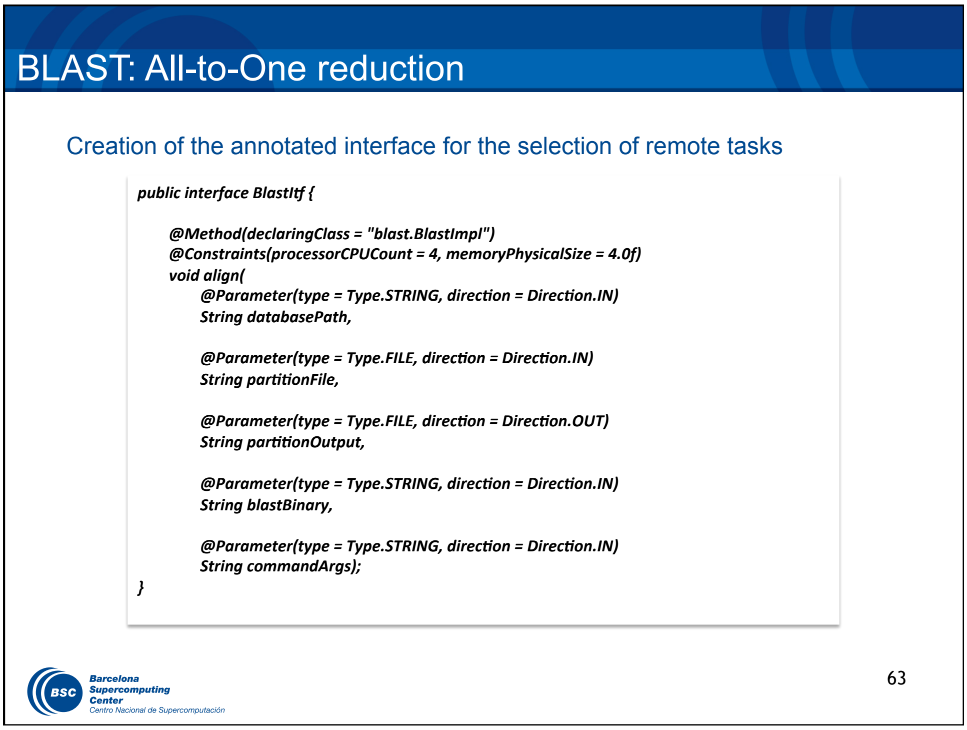
```
public static void main(String args[]) throws Exception {

  sequences[] = splitSequences(inputFile, nFrags);

  for (partition: sequences)
  {
     BlastImpl.align(database, partition, partitionOutput, blastBinary, commandArgs);
     partitionOutputs.add(partitionOutput);
  }

  assemblyPartitions(partialOutputs, outputFileName, tempDir, nFrags);
}
```



BLAST: All-to-One reduction

- Remote task implementation:

```
public class BlastImpl{

   public void align(String databasePath, String partitionFile,
                           String partitionOutput, String blastBinary, String commandArgs)
   {
     String cmd = blastBinary+ " " +"-p blastx -d " + databasePath + " -i " +partitionFile+ " -o “+
              partitionOutput+ " " +commandArgs;

     Process simProc = Runtime.getRuntime().exec(cmd);
       …….
   }
}
```



BLAST: All-to-One reduction

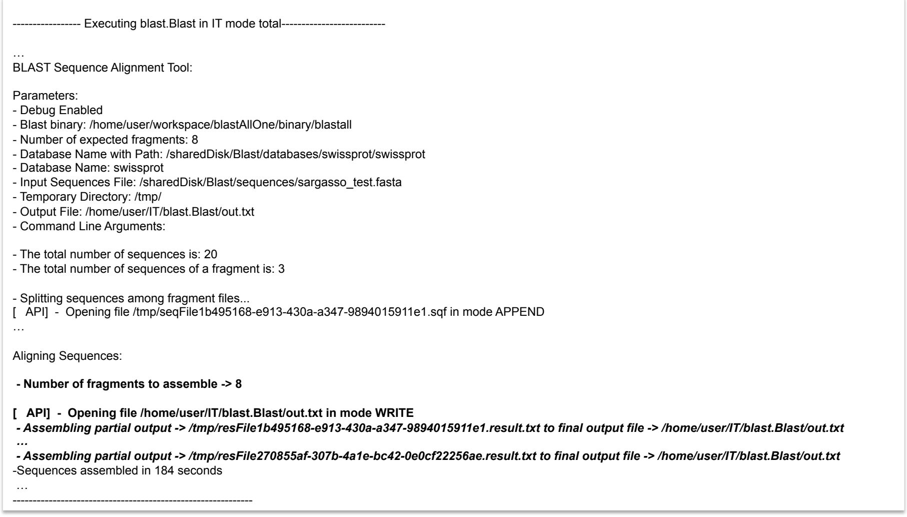
Creation of the annotated interface for the selection of remote tasks

```
public interface BlastItf {

     @Method(declaringClass = "blast.BlastImpl")
     @Constraints(processorCPUCount = 4, memoryPhysicalSize = 4.0f)
     void align(
          @Parameter(type = Type.STRING, direction = Direction.IN)
          String databasePath,

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

          @Parameter(type = Type.FILE, direction = Direction.OUT)
          String partitionOutput,

          @Parameter(type = Type.STRING, direction = Direction.IN)
          String blastBinary,

          @Parameter(type = Type.STRING, direction = Direction.IN)
          String commandArgs);
}
```

BLAST: Compilation and execution

- Compilation (Eclipse IDE)
  - ***Package Explorer -> Project (blastallone) -> Export…***
- Usage
  - ***runcompss blast.Blast <debug> <binary> <database> <sequences> <#fragments> <tmpdir> <output>***
- Execution
  - ***cp ~/workspace/blastallone/jar/blast.jar ~***
  - ***export CLASSPATH=$CLASSPATH:/home/user/blast.jar***
  - ***runcompss blast.Blast true /home/user/workspace/blast/binary/blastall /sharedDisk/Blast/databases/swissprot/swissprot /sharedDisk/Blast/sequences/sargasso_test.fasta 4 /tmp/ /home/user/out.txt_***

BLAST: Compilation and execution

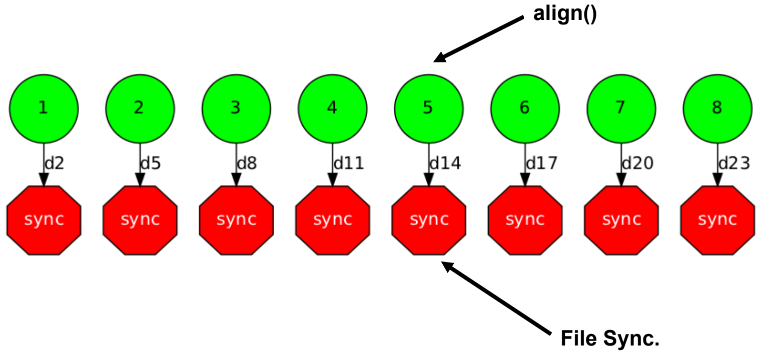


```
----------------- Executing blast.Blast in IT mode total-------------------------

…
BLAST Sequence Alignment Tool:

Parameters:
- Debug Enabled
- Blast binary: /home/user/workspace/blastAllOne/binary/blastall
- Number of expected fragments: 8
- Database Name with Path: /sharedDisk/Blast/databases/swissprot/swissprot
- Database Name: swissprot
- Input Sequences File: /sharedDisk/Blast/sequences/sargasso_test.fasta
- Temporary Directory: /tmp/
- Output File: /home/user/IT/blast.Blast/out.txt
- Command Line Arguments:

- The total number of sequences is: 20
- The total number of sequences of a fragment is: 3

- Splitting sequences among fragment files...
[   API]  -  Opening file /tmp/seqFile1b495168-e913-430a-a347-9894015911e1.sqf in mode APPEND
…

Aligning Sequences:

 - Number of fragments to assemble -> 8

[   API]  -  Opening file /home/user/IT/blast.Blast/out.txt in mode WRITE
 - Assembling partial output -> /tmp/resFile1b495168-e913-430a-a347-9894015911e1.result.txt to final output file -> /home/user/IT/blast.Blast/out.txt
 …
 - Assembling partial output -> /tmp/resFile270855af-307b-4a1e-bc42-0e0cf22256ae.result.txt to final output file -> /home/user/IT/blast.Blast/out.txt
-Sequences assembled in 184 seconds
 …
------------------------------------------------------------
```

BLAST: All-to-One (work)

- Generate the final graph
- Launch BLAST (All-to-One)

BLAST: All-to-One (Graph)



align()

File Sync.

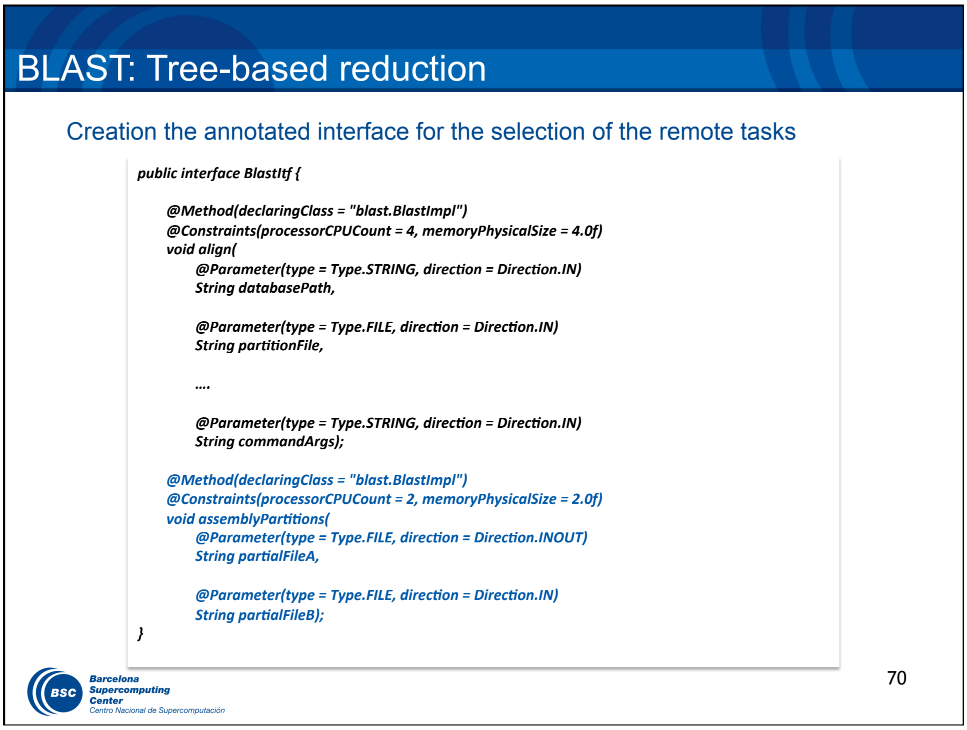
BLAST: Tree-based reduction (work)

- Code the final reduction and its interface.

BLAST: Tree-based reduction

- Main Application (Tree-based):

```
public static void main(String args[]) throws Exception {

  sequences[] = splitSequences(inputFile, nFrags);

  for (partition: sequences)
  {
     BlastImpl.align(database, partition, partitionOutput, blastBinary, commandArgs);
     partitionOutputs.add(partitionOutput);
  }

  //Final Assembly process -> Merge 2 by 2
    int neighbour=1;
    while (neighbour<partialOutputs.size()){
       for (int result=0; result<partialOutputs.size(); result+=2*neighbour){
          if (result+neighbour < partialOutputs.size()){
               BlastImpl.assemblyPartitions(partialOutputs.get(result),partialOutputs.get(result+neighbor));
               lastMerge = partialOutputs.get(result);
          }
       }
      neighbor*=2;
    }
}
```



BLAST: Tree-based reduction

Creation the annotated interface for the selection of the remote tasks

```
public interface BlastItf {

    @Method(declaringClass = "blast.BlastImpl")
    @Constraints(processorCPUCount = 4, memoryPhysicalSize = 4.0f)
    void align(
        @Parameter(type = Type.STRING, direction = Direction.IN)
        String databasePath,

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

        ….

        @Parameter(type = Type.STRING, direction = Direction.IN)
        String commandArgs);

    @Method(declaringClass = "blast.BlastImpl")
    @Constraints(processorCPUCount = 2, memoryPhysicalSize = 2.0f)
    void assemblyPartitions(
        @Parameter(type = Type.FILE, direction = Direction.INOUT)
        String partialFileA,

        @Parameter(type = Type.FILE, direction = Direction.IN)
        String partialFileB);
}
```

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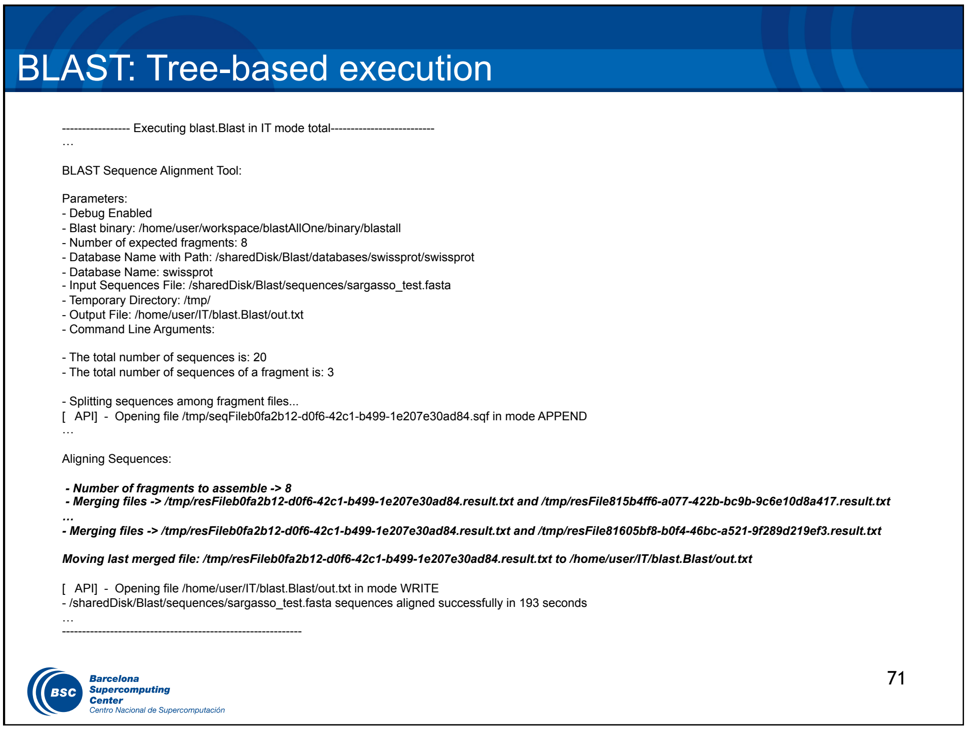

BLAST: Tree-based execution

```
----------------- Executing blast.Blast in IT mode total--------------------------
…

BLAST Sequence Alignment Tool:

Parameters:
- Debug Enabled
- Blast binary: /home/user/workspace/blastAllOne/binary/blastall
- Number of expected fragments: 8
- Database Name with Path: /sharedDisk/Blast/databases/swissprot/swissprot
- Database Name: swissprot
- Input Sequences File: /sharedDisk/Blast/sequences/sargasso_test.fasta
- Temporary Directory: /tmp/
- Output File: /home/user/IT/blast.Blast/out.txt
- Command Line Arguments:

- The total number of sequences is: 20
- The total number of sequences of a fragment is: 3

- Splitting sequences among fragment files...
[   API]  -  Opening file /tmp/seqFileb0fa2b12-d0f6-42c1-b499-1e207e30ad84.sqf in mode APPEND
…

Aligning Sequences:

 - Number of fragments to assemble -> 8
 - Merging files -> /tmp/resFileb0fa2b12-d0f6-42c1-b499-1e207e30ad84.result.txt and /tmp/resFile815b4ff6-a077-422b-bc9b-9c6e10d8a417.result.txt
…
- Merging files -> /tmp/resFileb0fa2b12-d0f6-42c1-b499-1e207e30ad84.result.txt and /tmp/resFile81605bf8-b0f4-46bc-a521-9f289d219ef3.result.txt

Moving last merged file: /tmp/resFileb0fa2b12-d0f6-42c1-b499-1e207e30ad84.result.txt to /home/user/IT/blast.Blast/out.txt

[   API]  -  Opening file /home/user/IT/blast.Blast/out.txt in mode WRITE
- /sharedDisk/Blast/sequences/sargasso_test.fasta sequences aligned successfully in 193 seconds
…
----------------------------------------------------------
```

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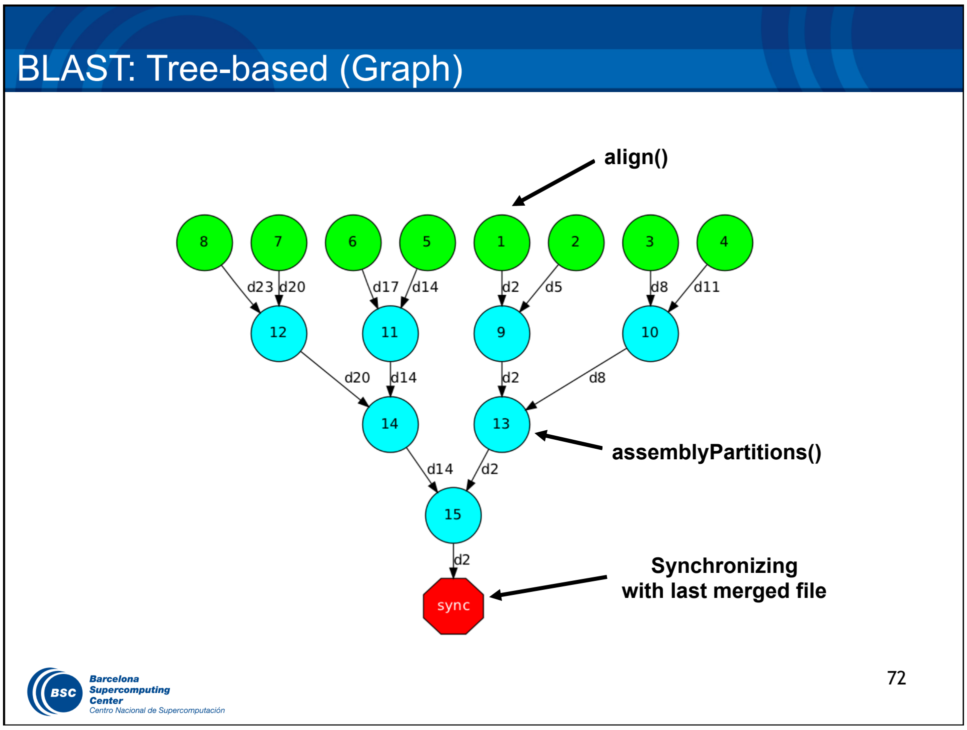

BLAST: Tree-based (Graph)

align()

assemblyPartitions()

Synchronizing
with last merged file

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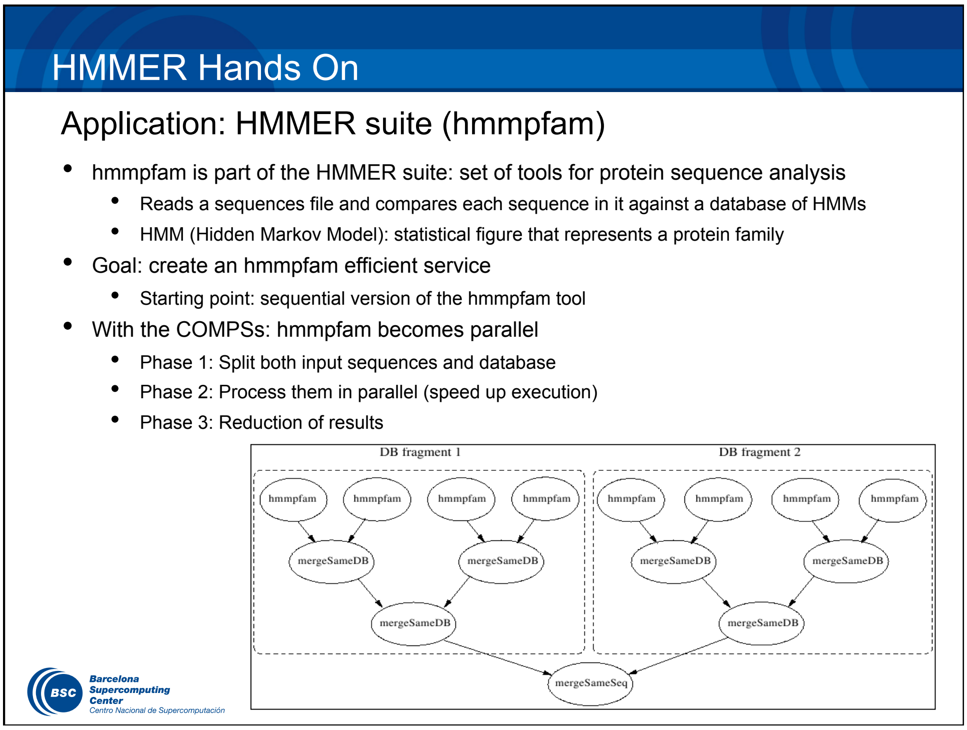
HMMER: Hands-on



HMMER Hands On

Application: HMMER suite (hmmpfam)

- hmmpfam is part of the HMMER suite: set of tools for protein sequence analysis
  - Reads a sequences file and compares each sequence in it against a database of HMMs
  - HMM (Hidden Markov Model): statistical figure that represents a protein family
- Goal: create an hmmpfam efficient service
  - Starting point: sequential version of the hmmpfam tool
- With the COMPSs: hmmpfam becomes parallel
  - Phase 1: Split both input sequences and database
  - Phase 2: Process them in parallel (speed up execution)
  - Phase 3: Reduction of results

DB fragment 1
DB fragment 2
hmmpfam
mergeSameDB
mergeSameSeq
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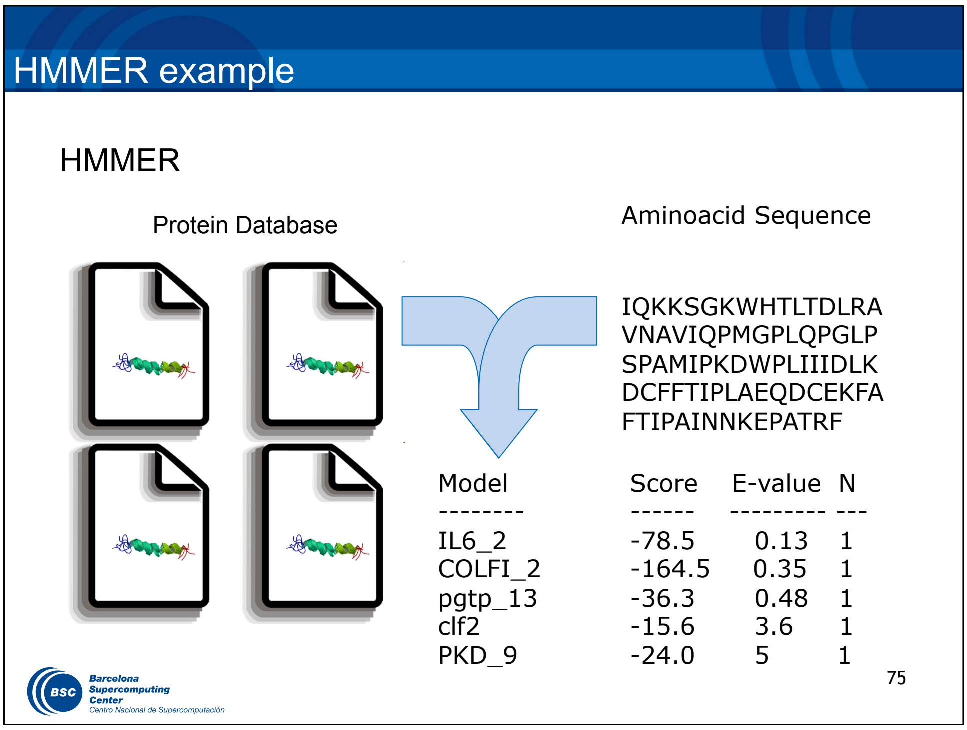

HMMER example

HMMER

Protein Database

Aminoacid Sequence

IQKKSGKWHTLTDLRA
VNAVIQPMGPLQPGLP
SPAMIPKDWPLIIIDLK
DCFFTIPLAEQDCEKFA
FTIPAINNKEPATRF

```
Model          Score     E-value   N
--------       ------    --------- ---
IL6_2          -78.5       0.13    1
COLFI_2        -164.5      0.35    1
pgtp_13        -36.3       0.48    1
clf2           -15.6       3.6     1
PKD_9          -24.0       5       1
```

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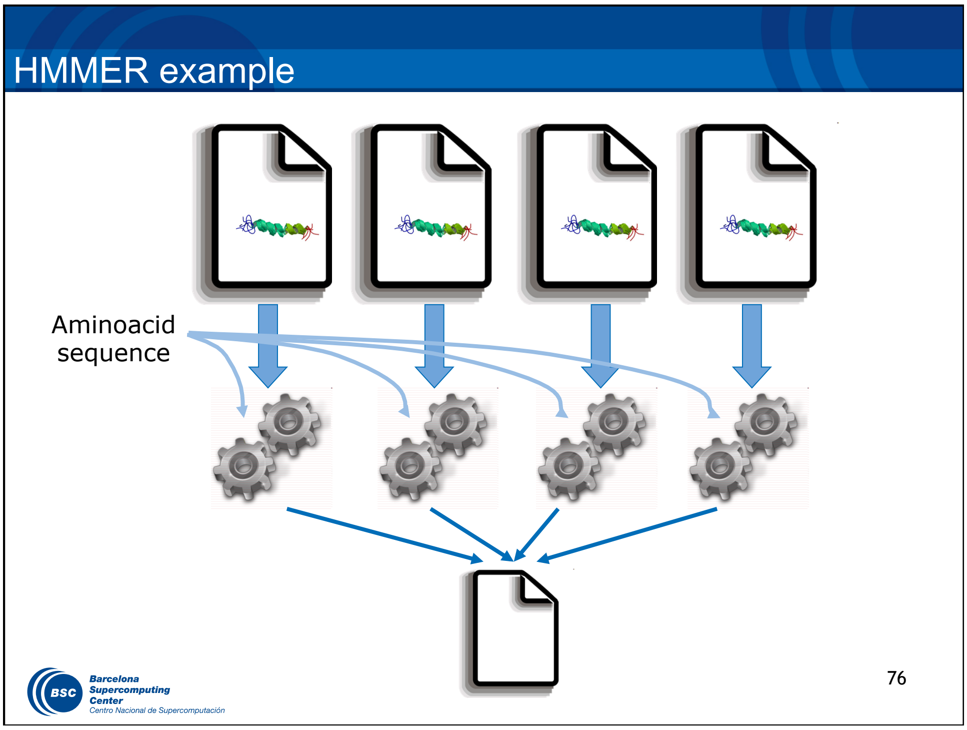
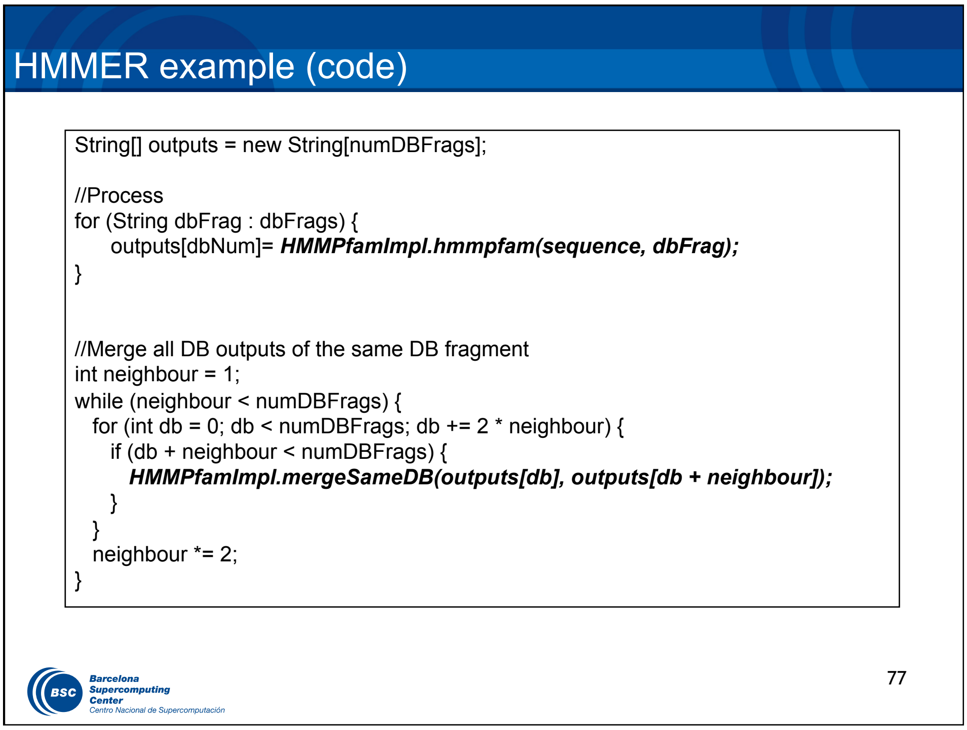


HMMER example

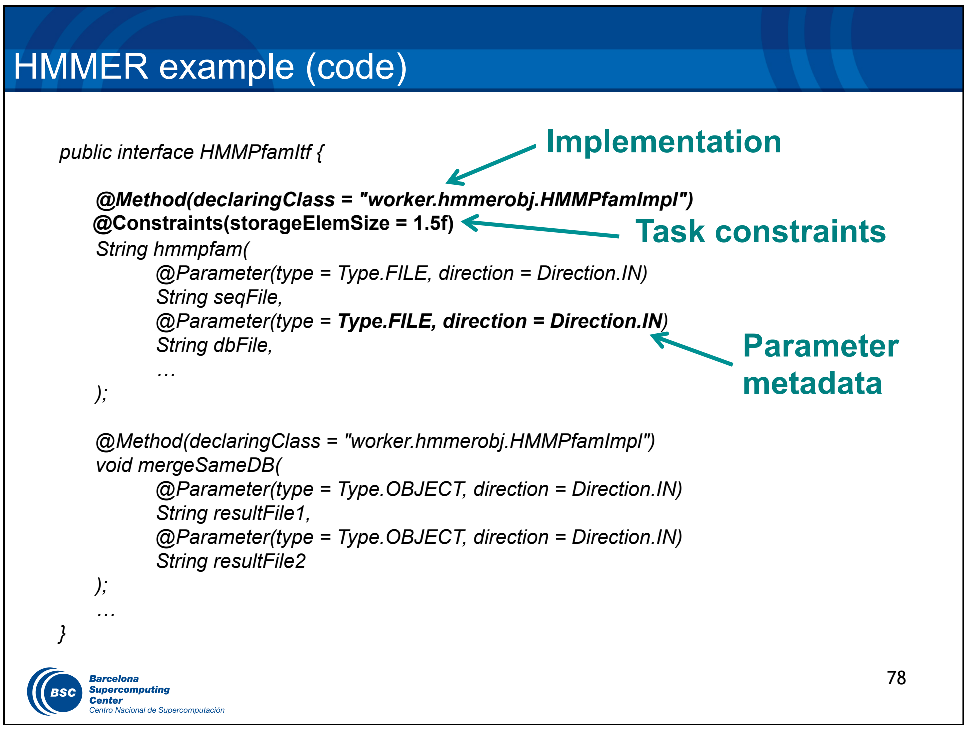


HMMER example (code)

```
String[] outputs = new String[numDBFrags];

//Process
for (String dbFrag : dbFrags) {
    outputs[dbNum]= HMMPfamImpl.hmmpfam(sequence, dbFrag);
}


//Merge all DB outputs of the same DB fragment
int neighbour = 1;
while (neighbour < numDBFrags) {
  for (int db = 0; db < numDBFrags; db += 2 * neighbour) {
    if (db + neighbour < numDBFrags) {
      HMMPfamImpl.mergeSameDB(outputs[db], outputs[db + neighbour]);
    }
  }
  neighbour *= 2;
}
```



HMMER example (code)

```
public interface HMMPfamItf {

    @Method(declaringClass = "worker.hmmerobj.HMMPfamImpl")
    @Constraints(storageElemSize = 1.5f)
    String hmmpfam(
        @Parameter(type = Type.FILE, direction = Direction.IN)
        String seqFile,
        @Parameter(type = Type.FILE, direction = Direction.IN)
        String dbFile,
        …
    );

    @Method(declaringClass = "worker.hmmerobj.HMMPfamImpl")
    void mergeSameDB(
        @Parameter(type = Type.OBJECT, direction = Direction.IN)
        String resultFile1,
        @Parameter(type = Type.OBJECT, direction = Direction.IN)
        String resultFile2
    );
    …
}
```

Implementation

Task constraints

Parameter metadata

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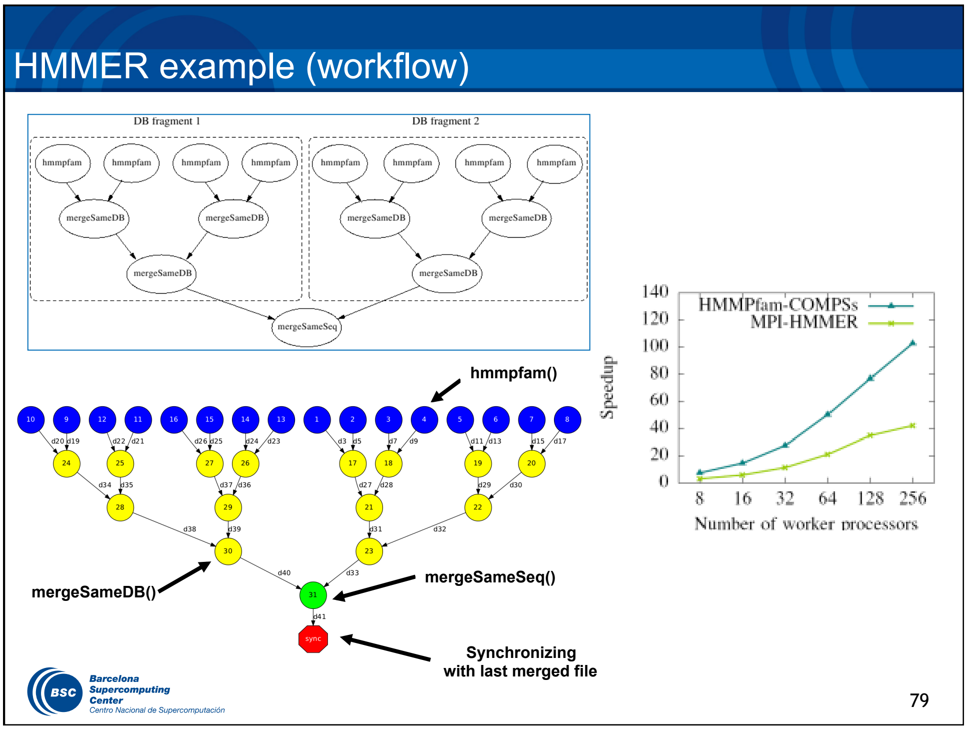

HMMER example (workflow)

hmmpfam()

mergeSameDB()

mergeSameSeq()

Synchronizing with last merged file

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HMMER: Task Selection (work)

- Complete the hmmpfam & mergeSameSeq method interfaces.

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HMMER: Configuration, compilation and execution

- Project.xml: /opt/COMPSs/Runtime/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/</InstallDir>
            <WorkingDir>/tmp/</WorkingDir>
            <User>user</User>
            <LimitOfTasks>2</LimitOfTasks>
      </Worker>

</Project>
```

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HMMER: Configuration, compilation and execution

- Configuration: /opt/COMPSs/Runtime/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>AMD64</Architecture>
                <Speed>3.0</Speed>
                <CPUCount>2</CPUCount>
            </Processor>
            <OS>
                <OSType>Linux</OSType>
                <MaxProcessesPerUser>32</MaxProcess
            </OS>
            <StorageElement>
                <Size>30</Size>
            </StorageElement>
            …
```

```
            …
            <Memory>
                <PhysicalSize>2</PhysicalSize>
                <VirtualSize>8</VirtualSize>
            </Memory>
            <ApplicationSoftware>
                <Software>Java</Software>
            </ApplicationSoftware>
            <Service/>
            <VO/>
            <Cluster/>
            <FileSystem/>
            <NetworkAdaptor/>
            <JobPolicy/>
            <AccessControlPolicy/>
        </Capabilities>
        <Requirements/>
    </Resource>

<ResourceList>
```

HMMER: Configuration, compilation and execution

- Compilation (Eclipse IDE)
  - ***Package Explorer -> Project (hmmerobjblanks) -> Export… (Hands-on)***
  - ***Package Explorer -> Project (hmmerobj) -> Export… (Solution)***
- Usage
  - ***runcompss hmmerobj.HMMPfam <database> <sequences> <output> <params>***
- Execution
  - ***cp ~/workspace/hmmerobj/jar/hmmerobj.jar ~***
  - ***export CLASSPATH=$CLASSPATH:/home/user/hmmerobj.jar***
  - ***runcompss hmmerobj.HMMPfam /sharedDisk/Hmmer/smart.HMMs.bin / sharedDisk/Hmmer/256seq /home/user/out.txt 2 8 -A 222***

HMMER: Configuration, compilation and execution

```
user@bsccompss:~$ runcompss hmmerobj.HMMPfam /sharedDisk/Hmmer/smart.HMMs.bin /sharedDisk/Hmmer/
        256seq /home/user/out.txt 2 8 -A 222
-e
----------------- Executing hmmerobj.HMMPfam in IT mode total--------------------------

[   API]  -  Deploying the Integrated Toolkit
[   API]  -  Starting the Integrated Toolkit
[   API]  -  Initializing components
[   API]  -  Ready to process tasks
[   API]  -  Opening file /tmp/hmmer_frags/seqF0_1 in mode WRITE
[   API]  -  Opening file /tmp/hmmer_frags/seqF1_1 in mode WRITE
[   API]  -  Opening file /tmp/hmmer_frags/seqF2_1 in mode WRITE
[   API]  -  Opening file /tmp/hmmer_frags/seqF3_1 in mode WRITE
[   API]  -  Opening file /tmp/hmmer_frags/seqF4_1 in mode WRITE
[   API]  -  Opening file /tmp/hmmer_frags/seqF5_1 in mode WRITE
[   API]  -  Opening file /tmp/hmmer_frags/seqF6_1 in mode WRITE
[   API]  -  Opening file /tmp/hmmer_frags/seqF7_1 in mode WRITE
[   API]  -  Opening file /tmp/hmmer_frags/dbF0_1 in mode WRITE
[   API]  -  Opening file /tmp/hmmer_frags/dbF1 in mode WRITE
[   API]  -  Opening file /home/user/out.txt in mode WRITE
[   API]  -  No more tasks for app 1
[   API]  -  Stopping IT
[   API]  -  Cleaning
[   API]  -  Integrated Toolkit stopped

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

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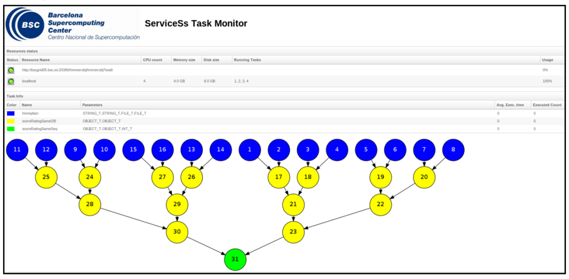
HMMER: Monitoring

- The runtime of COMPSs provides some information at execution time so the user can follow the progress of the application:
  - Real-time monitoring information (***http://localhost:8080/compss-monitor/***)
    - # tasks
    - Resources usage information
    - Execution time per task
    - Real-time execution graph
    - Etc.



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ServiceSs Task Monitor

Resources status

Status	Resource Name	CPU count	Memory size	Disk size	Running Tasks	Usage
●	http://bscgrid05.bsc.es:20390/hmmerobj/hmmerobj?wsdl					0%
●	localhost	4	4.0 GB	8.0 GB	1, 2, 3, 4	100%

Task Info

Color	Name	Parameters	Avg. Exec. time	Executed Count
🟦	hmmpfam	STRING_T,STRING_T,FILE_T,FILE_T	0	0
🟨	scoreRatingSameDB	OBJECT_T,OBJECT_T	0	0
🟩	scoreRatingSameSeq	OBJECT_T,OBJECT_T,INT_T	0	0

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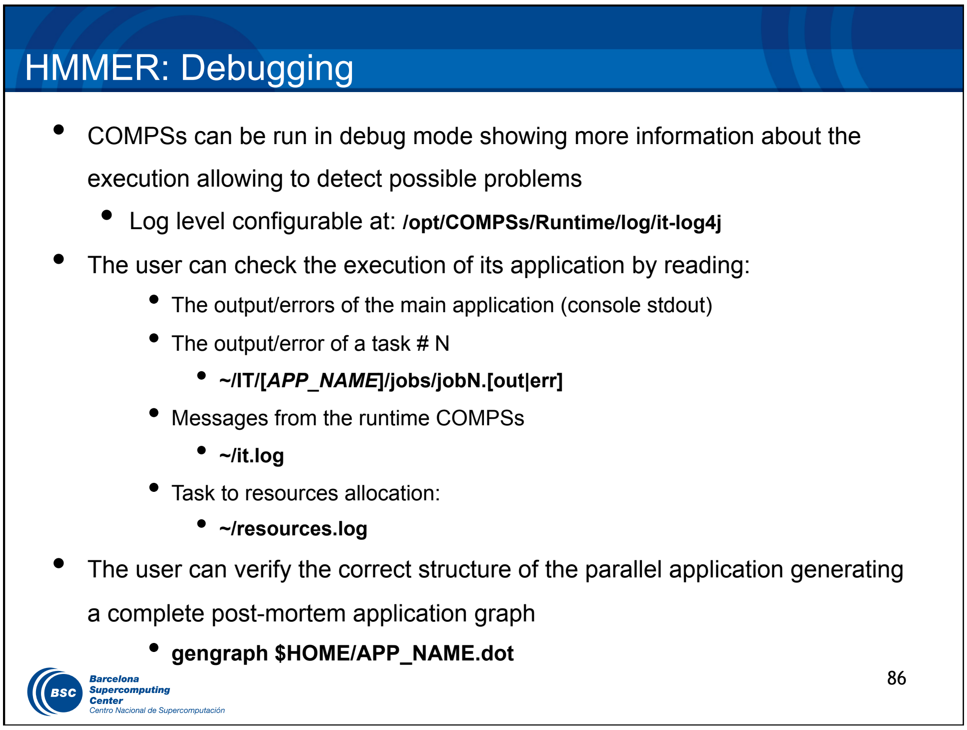
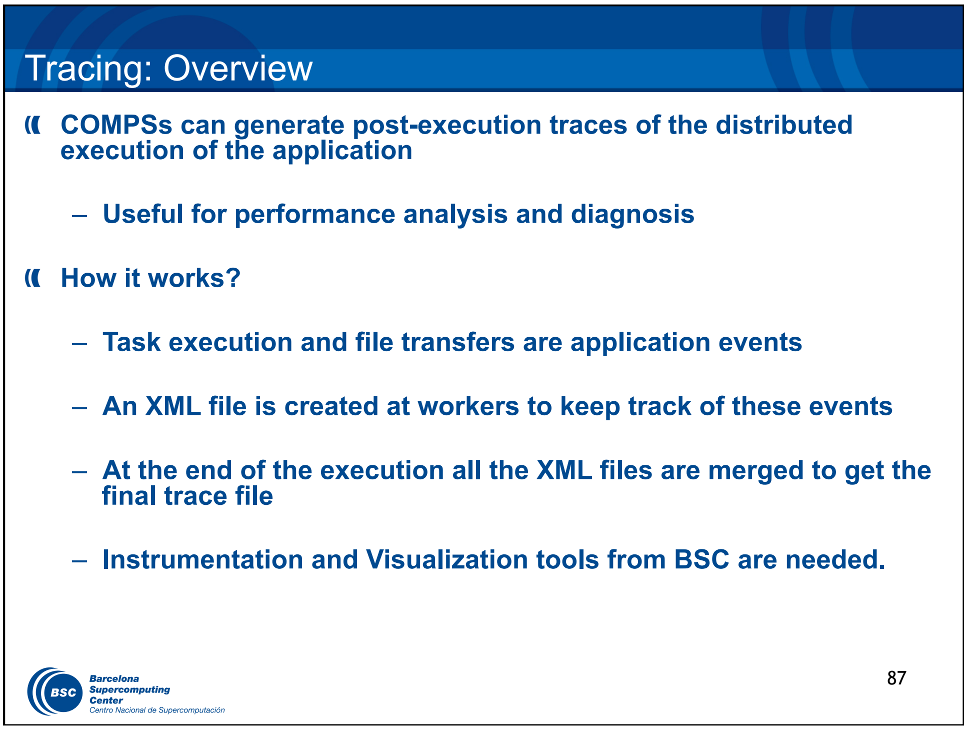


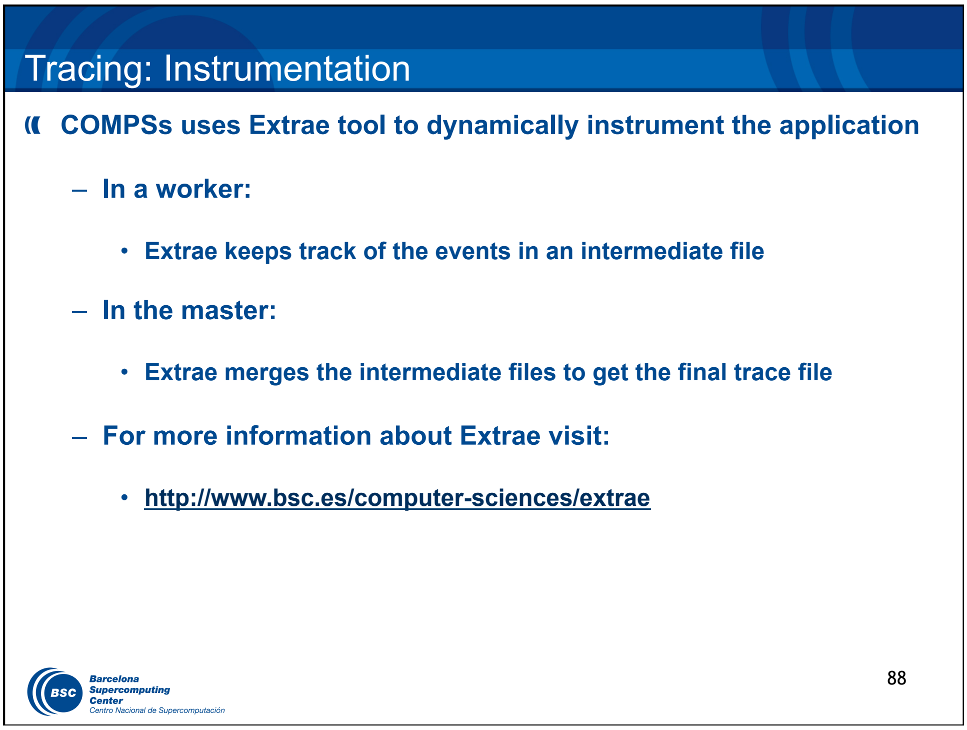
HMMER: Debugging

- COMPSs can be run in debug mode showing more information about the execution allowing to detect possible problems
  - Log level configurable at: **/opt/COMPSs/Runtime/log/it-log4j**
- The user can check the execution of its application by reading:
  - The output/errors of the main application (console stdout)
  - The output/error of a task # N
    - **~/IT/[*APP_NAME*]/jobs/jobN.[out|err]**
  - Messages from the runtime COMPSs
    - **~/it.log**
  - Task to resources allocation:
    - **~/resources.log**
- The user can verify the correct structure of the parallel application generating a complete post-mortem application graph
  - **gengraph $HOME/APP_NAME.dot**



Tracing: Overview

- **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**
  - **Instrumentation and Visualization tools from BSC are needed.**



Tracing: Instrumentation

- 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
  - For more information about Extrae visit:
    - http://www.bsc.es/computer-sciences/extrae

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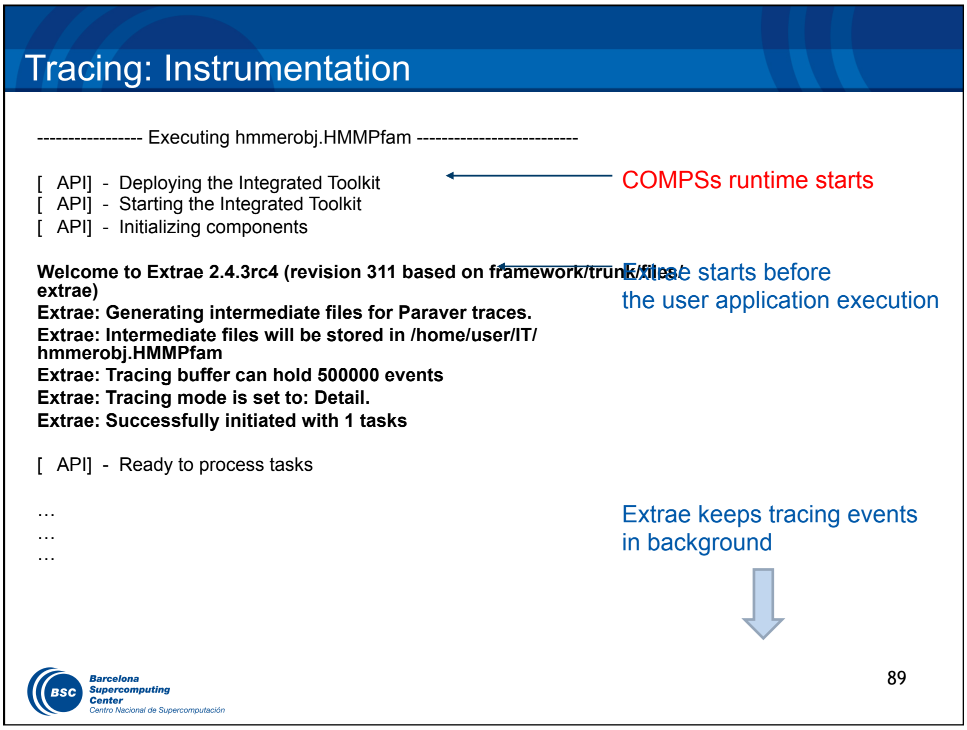


Tracing: Instrumentation

```
----------------- Executing hmmerobj.HMMPfam --------------------------

[  API]  -  Deploying the Integrated Toolkit
[  API]  -  Starting the Integrated Toolkit
[  API]  -  Initializing components

Welcome to Extrae 2.4.3rc4 (revision 311 based on framework/trunk/files/
extrae)
Extrae: Generating intermediate files for Paraver traces.
Extrae: Intermediate files will be stored in /home/user/IT/
hmmerobj.HMMPfam
Extrae: Tracing buffer can hold 500000 events
Extrae: Tracing mode is set to: Detail.
Extrae: Successfully initiated with 1 tasks

[  API]  -  Ready to process tasks

…
…
…
```

COMPSs runtime starts

Extrae starts before the user application execution

Extrae keeps tracing events in background

Tracing: Instrumentation

```
[  API]  -  No more tasks for app 1
[  API]  -  Stopping IT
[  API]  -  Cleaning
Extrae: Application has ended. Tracing has been terminated.
…

merger: Output trace format is: Paraver
merger: Extrae 2.4.3rc4 (revision 311 based on framework/trunk/files/extrae)
…

[  API]  -  Integrated Toolkit stopped
…

mpi2prv: Selected output trace format is Paraver

mpi2prv: Parsing intermediate files

mpi2prv: Generating tracefile (intermediate buffers of 1342156 events)

mpi2prv: Congratulations! hmmerobj.HMMPfam_compss_trace_1392736225.prv has been generated.

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

The application finishes and the tracing process ends

The merge process starts

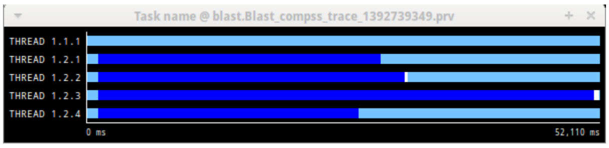
COMPSs runtime ends

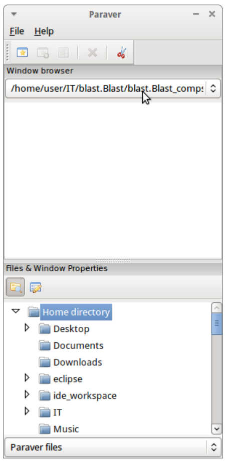
Intermediate trace files are processed

The final trace file is generated

Tracing: Visualization

- **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**



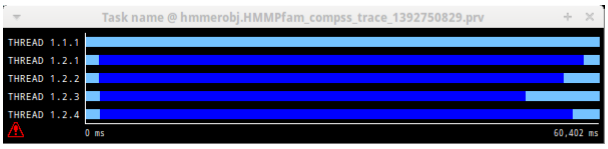


Tracing: Hands-on

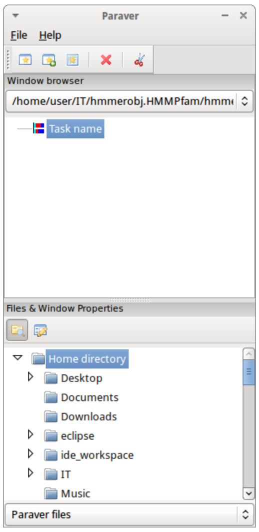
- Compilation (Eclipse IDE)
  - ***Package Explorer -> Project (hmmerobj) -> Export…***
- Execution
  - ***cp ~/workspace/hmmerobj/jar/hmmerobj.jar ~***
  - ***export CLASSPATH=$CLASSPATH:/home/user/hmmerobj.jar***
  - ***runcompssext --app=hmmerobj.HMMPfam --tracing=true --cline_args="/sharedDisk/Hmmer/smart.HMMs.bin /sharedDisk/Hmmer/256seq /home/user/out.txt 2 8 -A 222“***
  - ***wxparaver /home/user/IT/hmmerobj.HMMPfam/*.prv***

Tracing: Hands-on

- COMPSs provides a configuration file to automatically obtain the view of the trace
  - ***File / Load Configuration…***
  - ***/opt/COMPSs/paraver/cfgs/tasks.cfg***

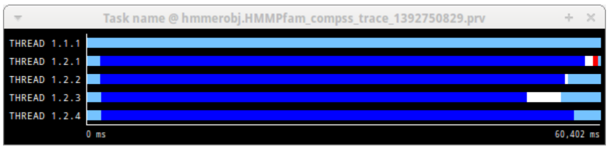


- Some small adjustments must be done in order to view the trace correctly

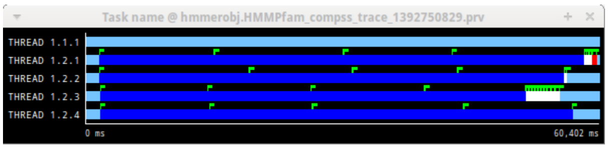


Tracing: Hands-on

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

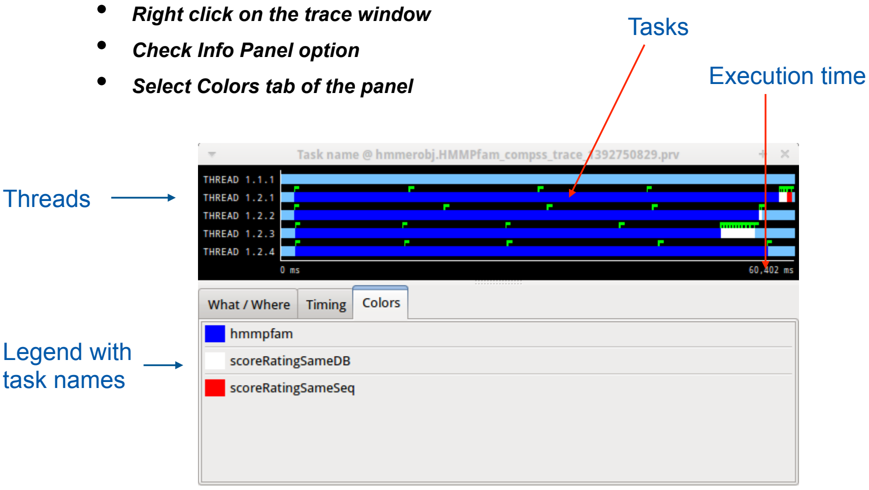


- View Event Flags
  - ***Right click on the trace window***
  - ***View / Event Flags***



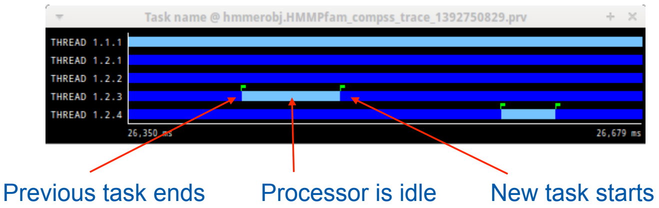
Tracing: Hands-on

- Show Info Panel
  - ***Right click on the trace window***
  - ***Check Info Panel option***
  - ***Select Colors tab of the panel***



Tracing: Hands-on

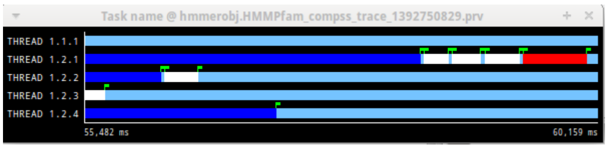
- Zoom to see details
  - ***Select a region in the trace window to see in detail***
  - ***And repeat the process til the needed zoom level***
  - ***The undo zoom option is in the right click panel***



Previous task ends

Processor is idle

New task starts



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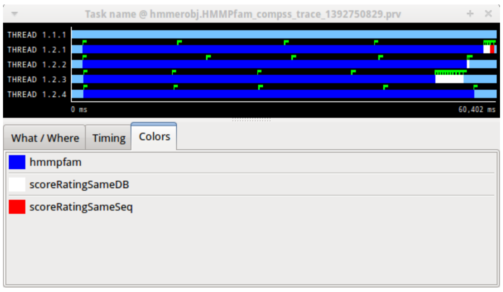
Tracing: Hands-on

Summarizing:

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



🟦 hmmpfam

□ scoreRatingSameDB

🟥 scoreRatingSameSeq

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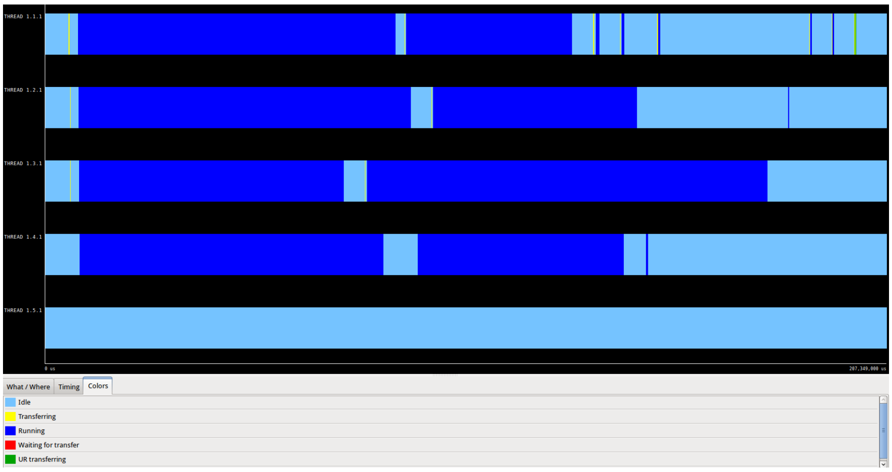
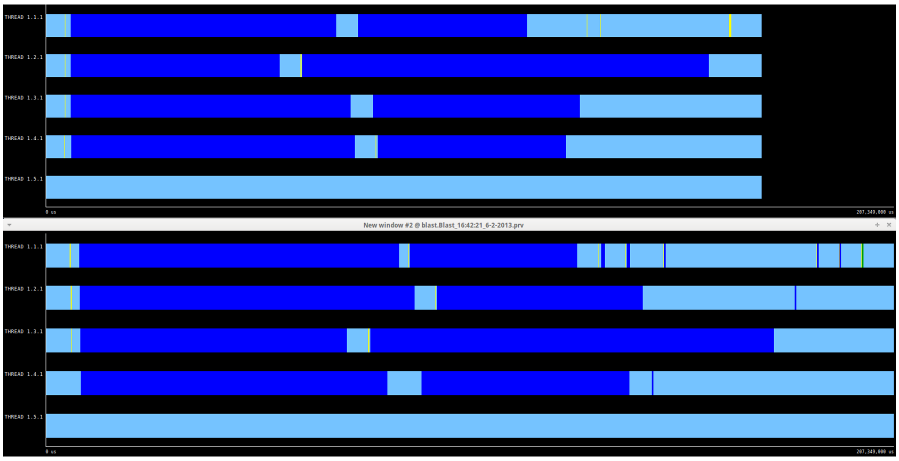
Tracing: BLAST, Tree-based

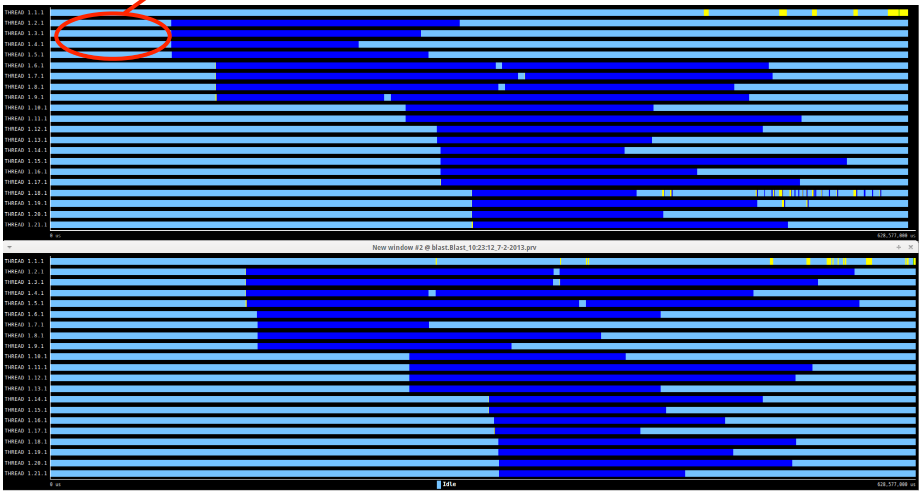


Tracing: BLAST, All-to-One vs Tree-based (Local)

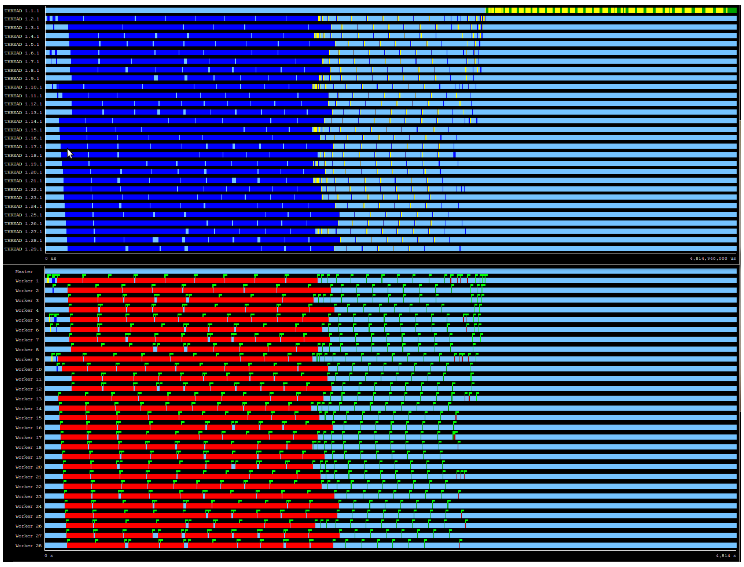


Tracing: BLAST, All-to-One vs Tree-based (Cloud)

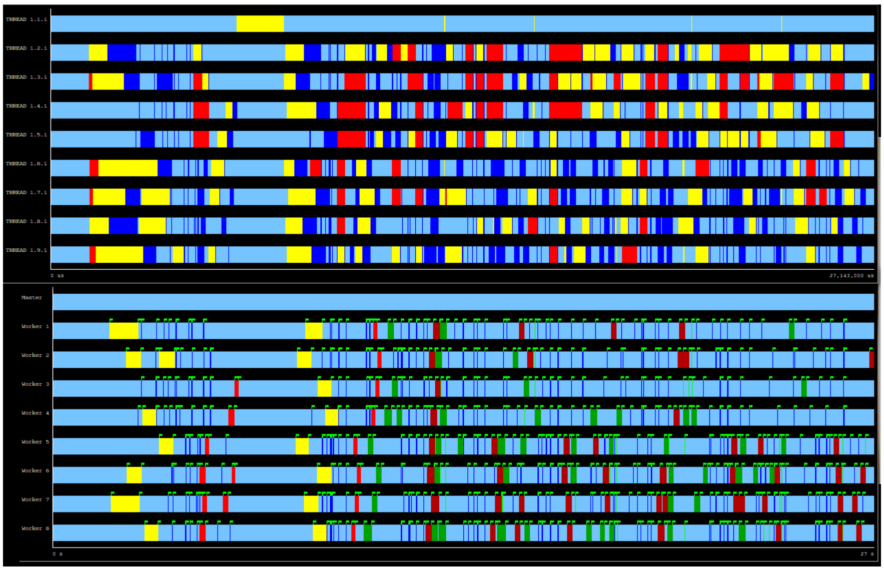
Virtual Machine Creation



Tracing: Other examples



Tracing: Other examples



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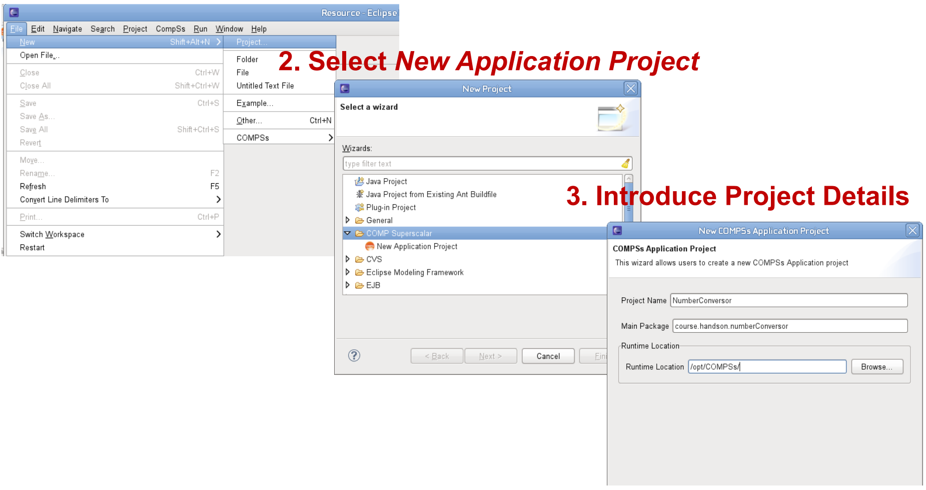
Integrated Development Environment
HANDS-ON

IDE Hands On – Create a COMPSs Project

1. Menu *File->New -> Project…*



2. Select *New Application Project*

3. Introduce Project Details

COMPSs Application Project

This wizard allows users to create a new COMPSs Application project

Project Name: NumberConversor

Main Package: course.handson.numberConversor

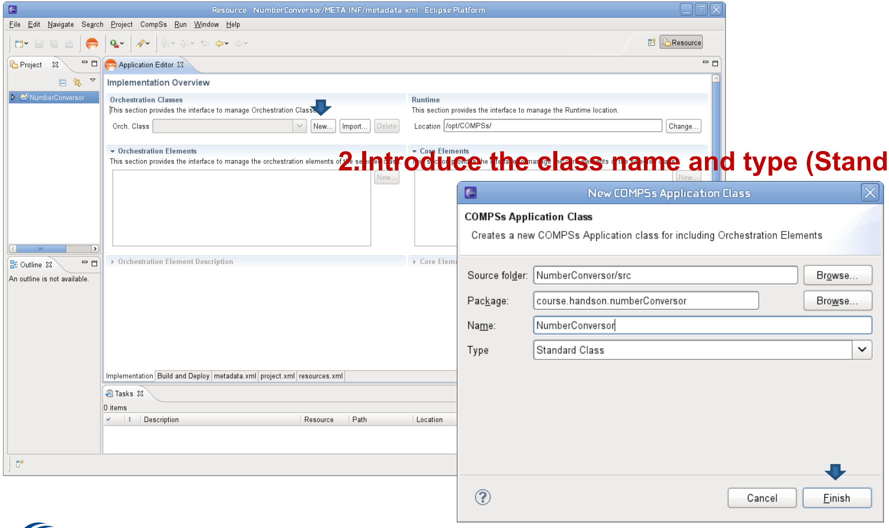
Runtime Location

Runtime Location: /opt/COMPSs/

(Also available *CompSs –>Implementation->Create Application Project*)

IDE Hands On – Create an Orchestration Class

1. Click *New…* in Orchestration Classes section of Application Editor



This section provides the interface to manage Orchestration Classes

This section provides the interface to manage the Runtime location.

Location: /opt/COMPSs/

This section provides the interface to manage the orchestration elements of the selected class

2.Introduce the class name and type (Standard)

COMPSs Application Class

Creates a new COMPSs Application class for including Orchestration Elements

Source folder: NumberConversor/src

Package: course.handson.numberConversor

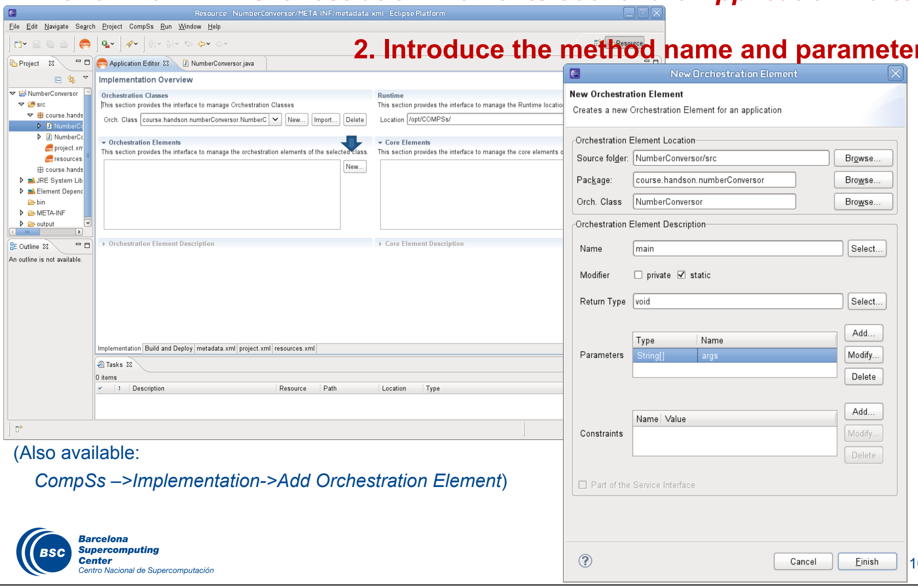
Name: NumberConversor

Type: Standard Class

(Also available *CompSs –>Implementation->Create Orchestration Class*)

IDE Hands On – Create an Orchestration Element

1. **Click *New…* in *Orchestration Elements* sec. of the *Application Editor***



2. Introduce the method name and parameters

New Orchestration Element

New Orchestration Element

Creates a new Orchestration Element for an application

Orchestration Element Location

- Source folder: NumberConversor/src
- Package: course.handson.numberConversor
- Orch. Class: NumberConversor

Orchestration Element Description

- Name: main
- Modifier: □ private ☑ static
- Return Type: void

Parameters

Type	Name
String[]	args

Constraints

Name	Value

□ Part of the Service Interface

(Also available:

CompSs –>Implementation->Add Orchestration Element)

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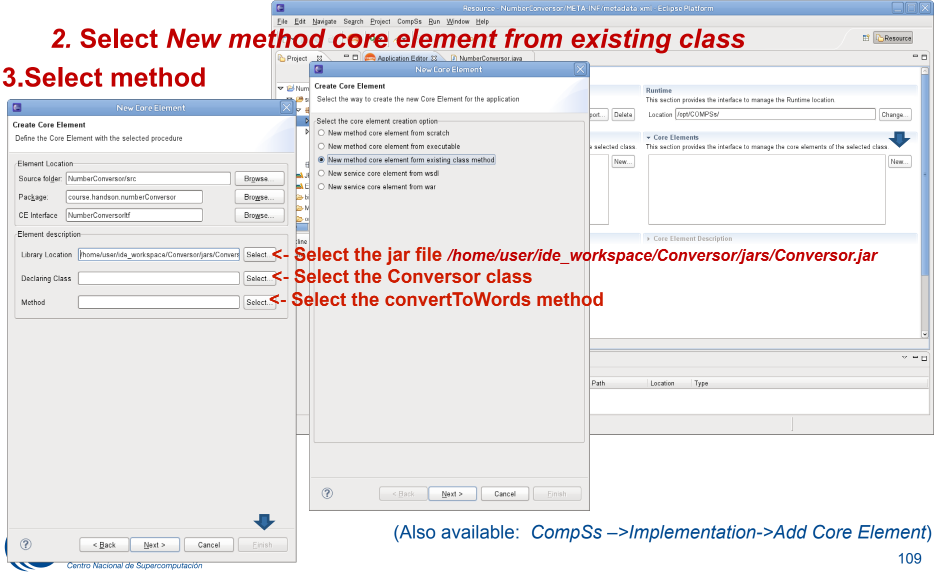
IDE Hands On – Add an Core Element from JAR

1. **Click *New…* in *Core Elements* section of the *Application Editor***

2. Select *New method core element from existing class*

3.Select method



New Core Element

Create Core Element

Select the way to create the new Core Element for the application

Select the core element creation option

- ○ New method core element from scratch
- ○ New method core element from executable
- ● New method core element form existing class method
- ○ New service core element from wsdl
- ○ New service core element from war

New Core Element

Create Core Element

Define the Core Element with the selected procedure

Element Location

- Source folder: NumberConversor/src
- Package: course.handson.numberConversor
- CE Interface: NumberConversorItf

Element description

- Library Location: /home/user/ide_workspace/Conversor/jars/Convers **<- Select the jar file */home/user/ide_workspace/Conversor/jars/Conversor.jar***
- Declaring Class: **<- Select the Conversor class**
- Method: **<- Select the convertToWords method**

(Also available: *CompSs –>Implementation->Add Core Element*)

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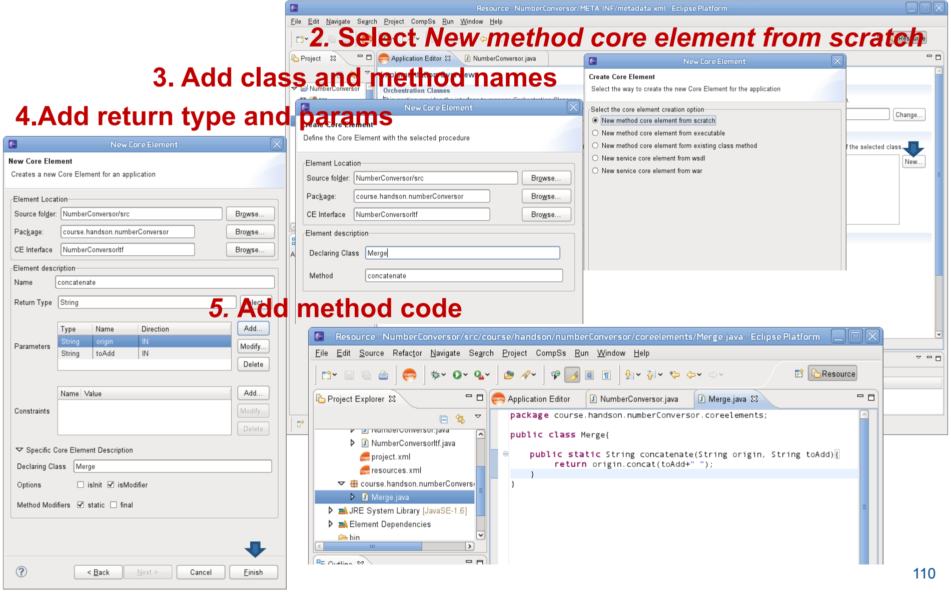
IDE Hands On – Add an Core Element from scratch

1. **Click *New…* in *Core Elements* section of the *Application Editor***



2. Select *New method core element from scratch*

3. Add class and method names

4.Add return type and params

***5.* Add method code**

Resource - NumberConversor/META-INF/metadata.xml - Eclipse Platform

New Core Element — Create Core Element: Select the way to create the new Core Element for the application

Select the core element creation option
- ● New method core element from scratch
- ○ New method core element from executable
- ○ New method core element form existing class method
- ○ New service core element from wsdl
- ○ New service core element from war

New Core Element — Create Core Element: Define the Core Element with the selected procedure

Element Location
- Source folder: NumberConversor/src
- Package: course.handson.numberConversor
- CE Interface: NumberConversorItf

Element description
- Declaring Class: Merge
- Method: concatenate

New Core Element — Creates a new Core Element for an application

Element Location
- Source folder: NumberConversor/src
- Package: course.handson.numberConversor
- CE Interface: NumberConversorItf

Element description
- Name: concatenate
- Return Type: String

Parameters

Type	Name	Direction
String	origin	IN
String	toAdd	IN

Constraints

Name	Value

Specific Core Element Description
- Declaring Class: Merge
- Options: ☐ isInit ☑ isModifier
- Method Modifiers: ☑ static ☐ final

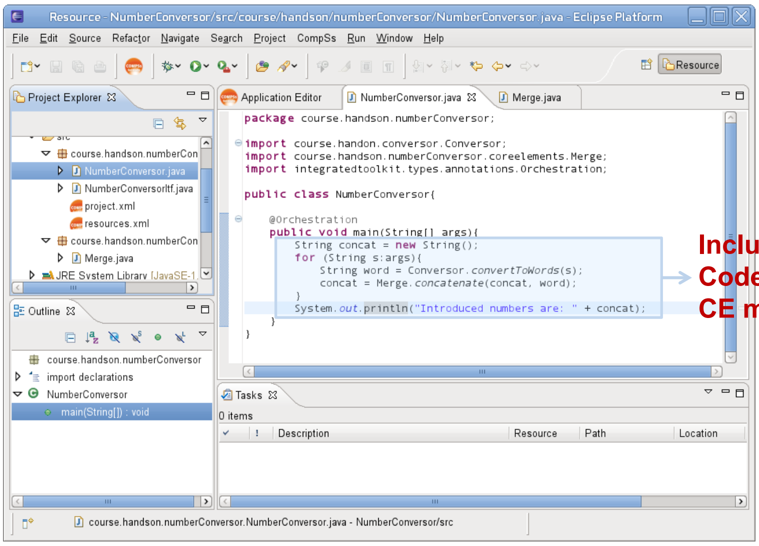
Resource - NumberConversor/src/course/handson/numberConversor/coreelements/Merge.java - Eclipse Platform

```java
package course.handson.numberConversor.coreelements;

public class Merge{

    public static String concatenate(String origin, String toAdd){
        return origin.concat(toAdd+" ");
    }
}
```

IDE Hands On – Introduce the OE code



Resource - NumberConversor/src/course/handson/numberConversor/NumberConversor.java - Eclipse Platform

```java
package course.handson.numberConversor;

import course.handon.conversor.Conversor;
import course.handson.numberConversor.coreelements.Merge;
import integratedtoolkit.types.annotations.Orchestration;

public class NumberConversor{

    @Orchestration
    public void main(String[] args){
        String concat = new String();
        for (String s:args){
            String word = Conversor.convertToWords(s);
            concat = Merge.concatenate(concat, word);
        }
        System.out.println("Introduced numbers are: " + concat);
    }
}
```

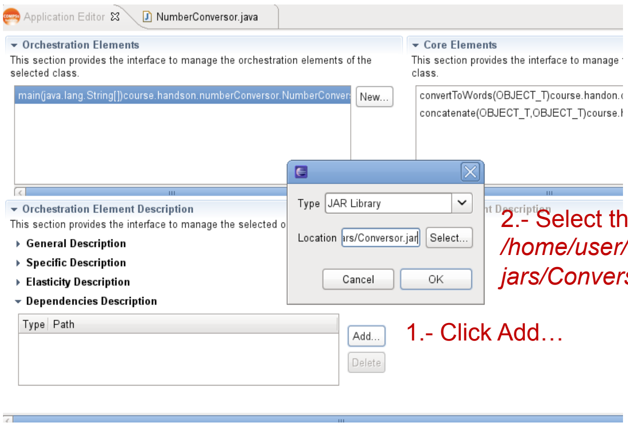
Include the OE Code to call the CE methods

Tasks: 0 items

✓	!	Description	Resource	Path	Location

course.handson.numberConversor.NumberConversor.java - NumberConversor/src

IDE Hands On – Add conversor dependency to OE



Orchestration Elements

This section provides the interface to manage the orchestration elements of the selected class.

main(java.lang.String[])course.handson.numberConversor.NumberConver

Core Elements

This section provides the interface to manage class.

convertToWords(OBJECT_T)course.handon.

concatenate(OBJECT_T,OBJECT_T)course.

Orchestration Element Description

This section provides the interface to manage the selected o

- General Description
- Specific Description
- Elasticity Description
- Dependencies Description

Type	Path

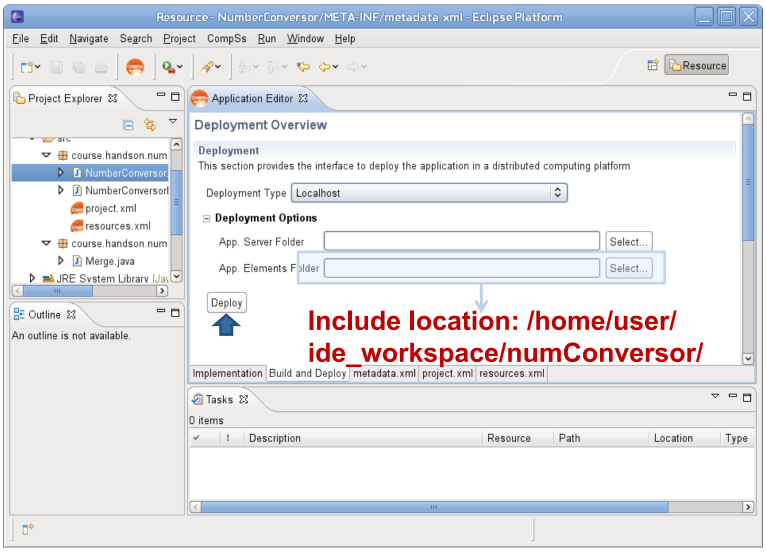
Type: JAR Library

Location: ars/Conversor.jar

2.- Select the jar library: */home/user/ide_workspace/Conversor/jars/Conversor.jar*

1.- Click Add…

IDE Hands On – Deploy Locally



An outline is not available.

Deployment Overview

Deployment

This section provides the interface to deploy the application in a distributed computing platform

Deployment Type: Localhost

Deployment Options

App. Server Folder

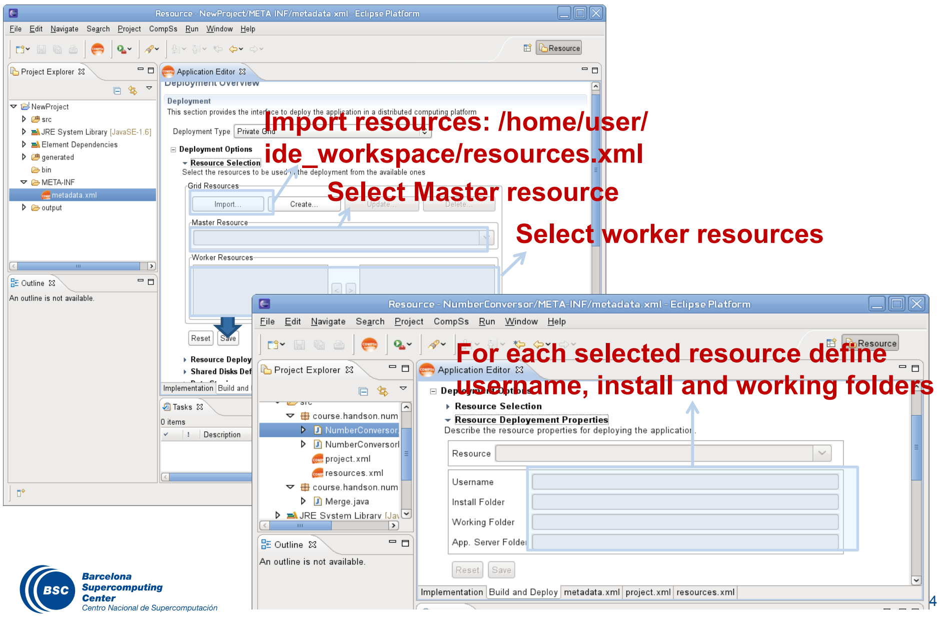
App. Elements Folder

0 items

✓	!	Description	Resource	Path	Location	Type

Include location: /home/user/ide_workspace/numConversor/

IDE Hands On – Deploy Grid



Import resources: /home/user/ide_workspace/resources.xml

Select Master resource

Select worker resources

For each selected resource define username, install and working folders

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

  - *Sample applications & development virtual appliances*
  - *Tutorials*
  - *Red-Hat & Debian based installation packages*
  - …

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Thank you!

For further information please contact

support-compss@bsc.es