Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

Programming Distributed Computing Platforms with COMPSs

Workflows & Distributed Computing Group

30-31/01/2024

Barcelona

Supercomputers Hands-on

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Supercomputers Hands-on

- Settings
- Execution in MareNostrum 4
- Hands-on exercise
- Tracing Analysis Overview

Settings

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Settings

- How to connect to MareNostrum 4?
  - **ssh -X nct01XXX@mn1.bsc.es**

(Where XXX is 146-233)

Password: **WCYRmHBy.XXX**

- Load COMPSs:
  - **export COMPSS_PYTHON_VERSION=3.9.10**
  - **module load COMPSs/3.3**

- Where is the source code?
  - **cd**
  - **get_COMPSs_TUTORIAL_2024**

- Available editors
  - vi
  - emacs

Settings

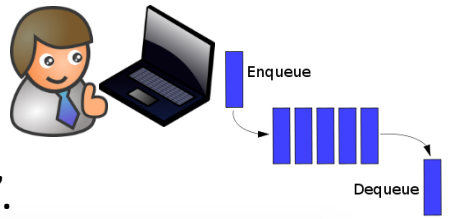
- Open terminal
- Connect to MN4
- Copy the source code into the home folder
- Explain the contents
- Explain how to edit the files

Execution in MN4

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

How to launch PyCOMPSs applications?

- Write or transfer the application into MN4:
  - Use **vi**/**emacs** or **scp**
- Load COMPSs:
  - **export COMPSS_PYTHON_VERSION=3.9.10**
  - **module load COMPSs/3.3**
- Submit jobs to MareNostrum 4:
  - All jobs should be submitted to the queuing system (SLURM)
  - We will use the **pycompss-cli**
  - Useful commands:
    - **squeue** – This command shows the status of the job.
    - **scancel <jobId>** – This command kills a job with id 'jobId'.



Sample applications

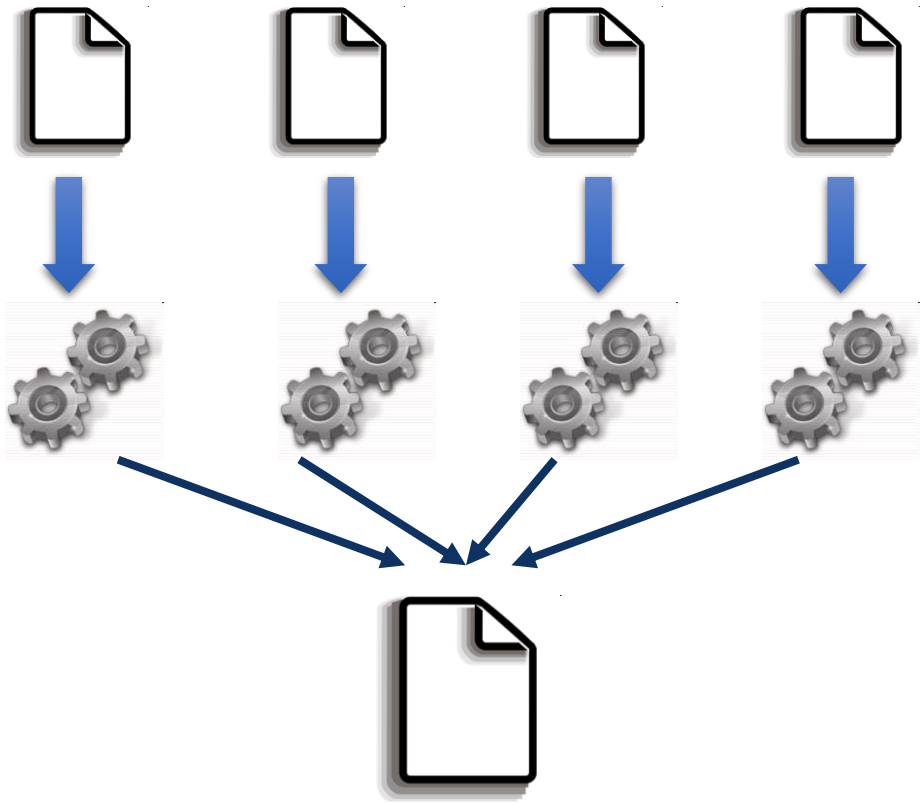
- Go to examples folder:
  - **cd sources/examples**
- List of examples:
  - **ls -l**
    - cholesky
    - clustering_comparison
    - kmeans
    - kmeans_dislib
    - lysozyme_in_water
    - Wordcount
- Each folder contains:
  - A launch script, that uses the **pycompss-cli**
  - A **src** folder containing the application source

Hands-on exercise

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

Wordcount Exercise

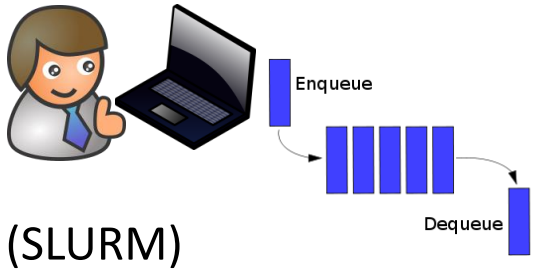
- Counting words of a set of documents
- Parallelization
  - Phase 1: Count words of a set of documents
  - Phase 2 : Merge results



WordCount@ Sequential

- Remember the dataset path
- How to launch with python sequentially?
  - > cd source/exercise/src
  - > python wordcount.py /gpfs/home/nct00/nct00012/dataset/dataset_4f_16mb
  - Results:

```
user@login:~> python wordcount.py /path/to/dataset/
Elapsed Time (s): 3.959941864014
Words: 10206202
```



- Submit jobs to MareNostrum 4:
  - All jobs should be submitted to the queuing system (SLURM)
  - We will use the **pycompss-cli**
  - Useful commands:
    - squeue – This command shows the status of the job.
    - scancel jobId – This command kills a job with id 'jobId'.

Execution in MareNostrum 4 - HandsOn

- launch_with_pycompss.sh

```
#/bin/bash

pycompss job submit \
  --qos=training \
  --num_nodes=2 \
  --exec_time=10 \
  --reservation=COMPSs2024 \
  --lang=python \
  --tracing=true \
  --graph=true \
  /home/nct01/nct01XXX/source/exercise/src/wordcount.py /gpfs/home/nct00/nct00012/dataset/dataset_64f_16mb
```

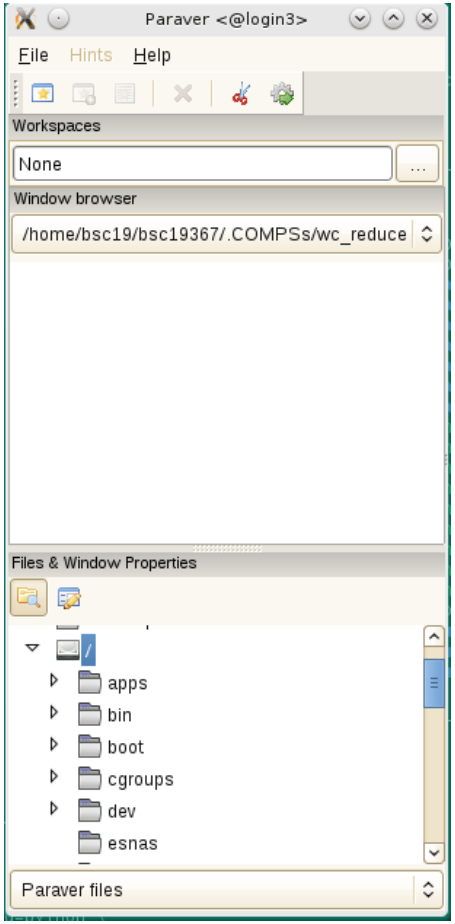
- Parameters:
  - num_nodes: number of nodes where to execute (1 master + 1 worker).
  - Dataset path: **/gpfs/home/nct00/nct00012/dataset/dataset_64f_16mb**
- How to execute with PyCOMPSs?
  - **chmod 755 launch_with_pycompss.sh**
  - **./launch_with_pycompss.sh**

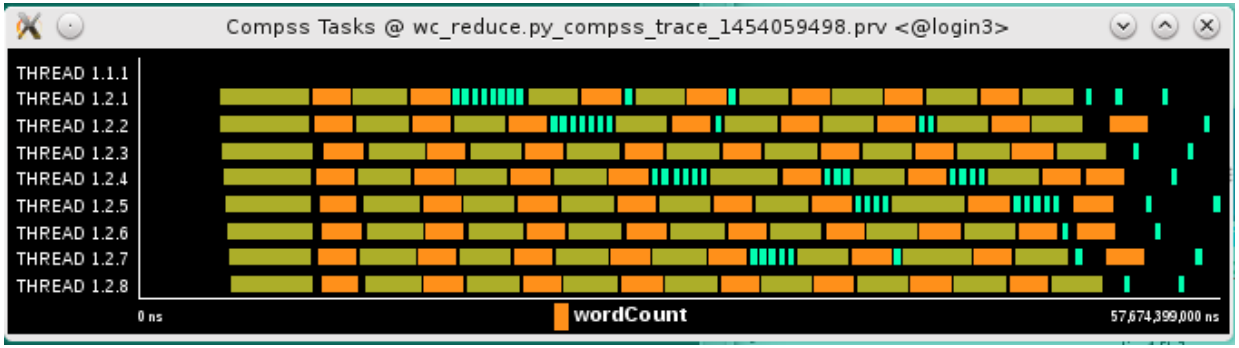
Tracing Analysis Overview

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

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:
  - https://tools.bsc.es/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 3.5.3
Extrae: Generating intermediate files for Paraver traces.
Extrae: Intermediate files will be stored in /gpfs/home/nct01/nct01XXX/sources/examples
Extrae: Tracing buffer can hold 500000 events
Extrae: Tracing mode is set to: Detail.
Extrae: Successfully initiated with 1 tasks

[   API]  -  Deploying COMPSs Runtime v3.3
[   API]  -  Starting COMPSs Runtime v3.3
 ...
[   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 3.5.3

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

COMPSs runtime ends

The application finishes and the tracing process ends

The merge process starts

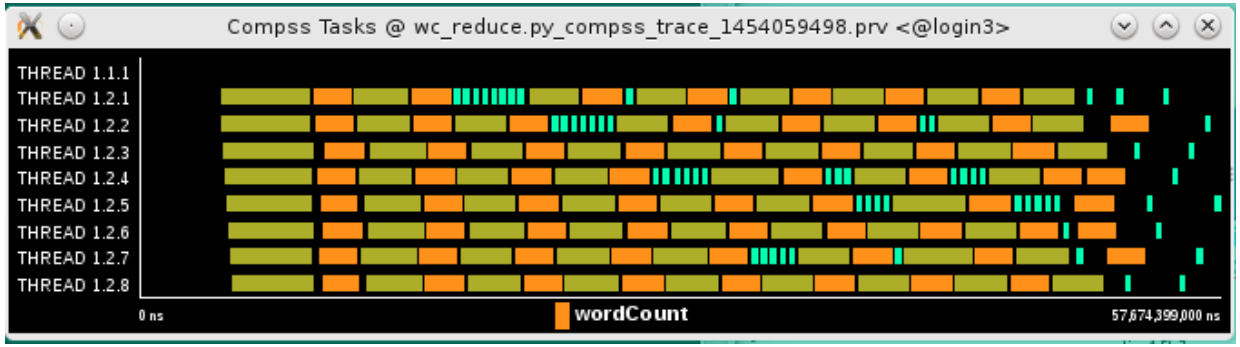
Intermediate trace files are processed

The final trace file is generated

WordCount @ Performance Analysis

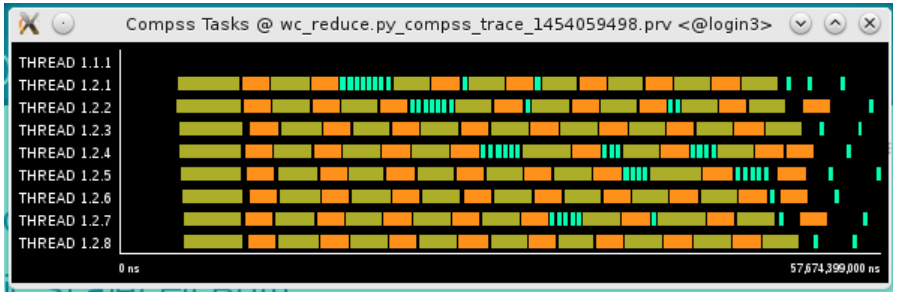
- Open Paraver
  - **cd $HOME/.COMPSs/wordcount.py_01**
  - **compss_gentrace**
  - **wxparaver trace/*.prv**
- COMPSs provides some configuration files to automatically obtain the view of the trace
  - File/Load Configuration...

(/gpfs/apps/MN4/COMPSs/3.3/Dependencies/paraver/cfgs/compss_tasks.cfg)

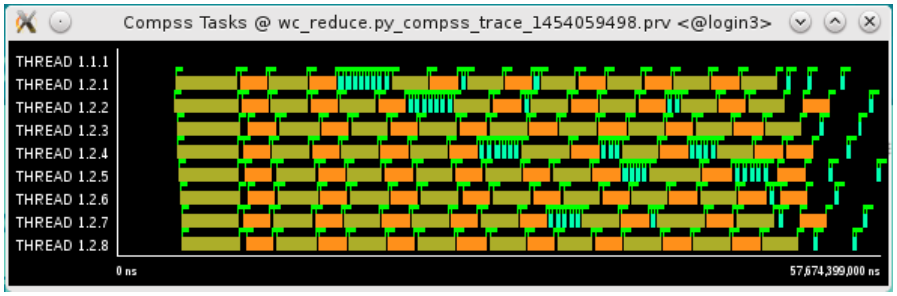


Wordcount @ Performance Analysis

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

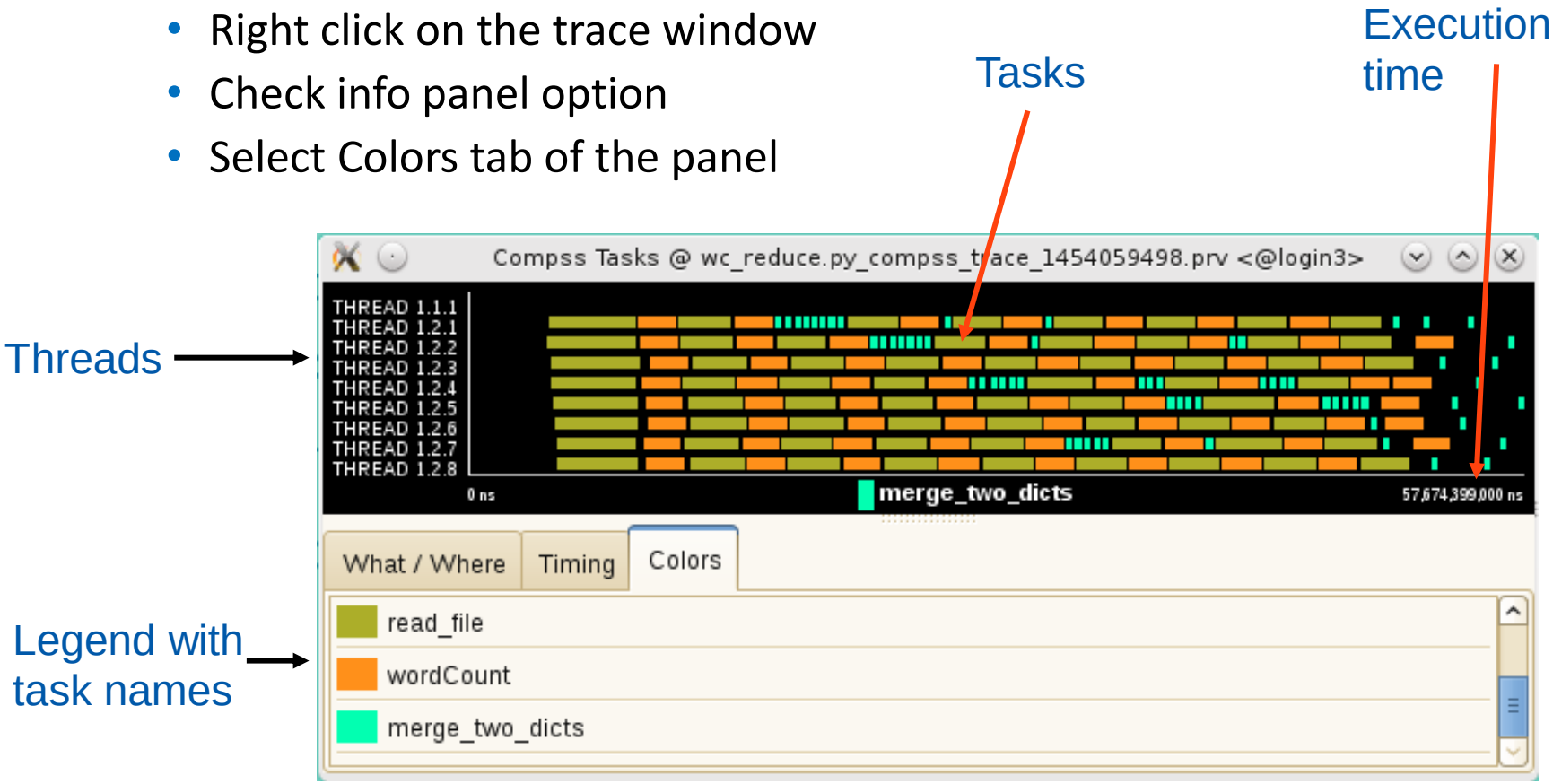


- View Event flags
  - Right click on the trace window
  - View / Event Flags



Wordcount @ Performance Analysis

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

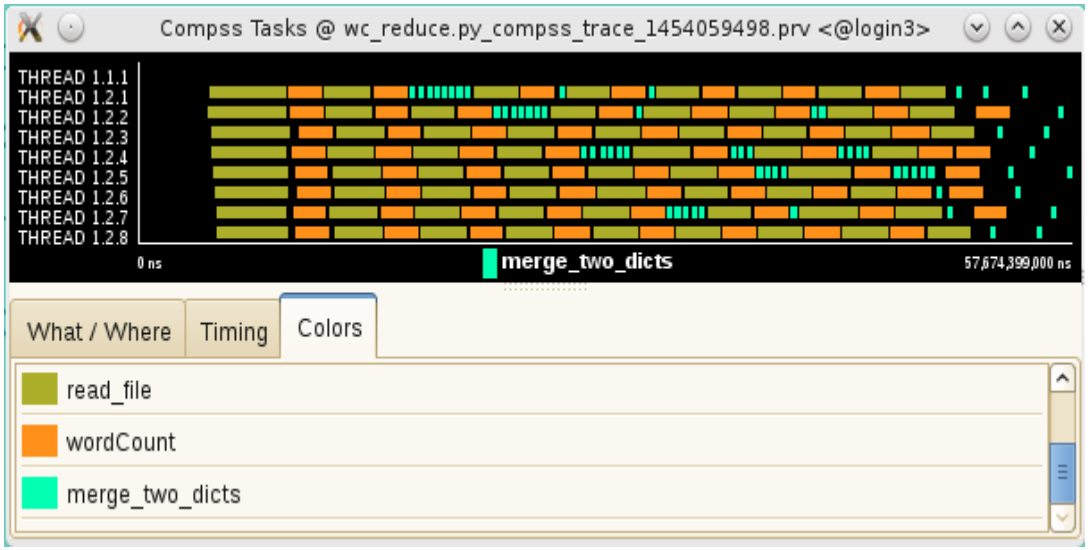


Wordcount @ Performance Analysis

- 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:
    - THREAD 1.1.X are the master threads
    - THREAD 1.X.Y are the worker threads
- Meaning of the colours:
  - Black: idle
  - Other colors: task running
    - see the color legend
- Flags (events):
  - Start / end of task




Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación
BSC
EXCELENCIA
SEVERO
OCHOA
THANK YOU!
support-compss@bsc.es
www.bsc.es