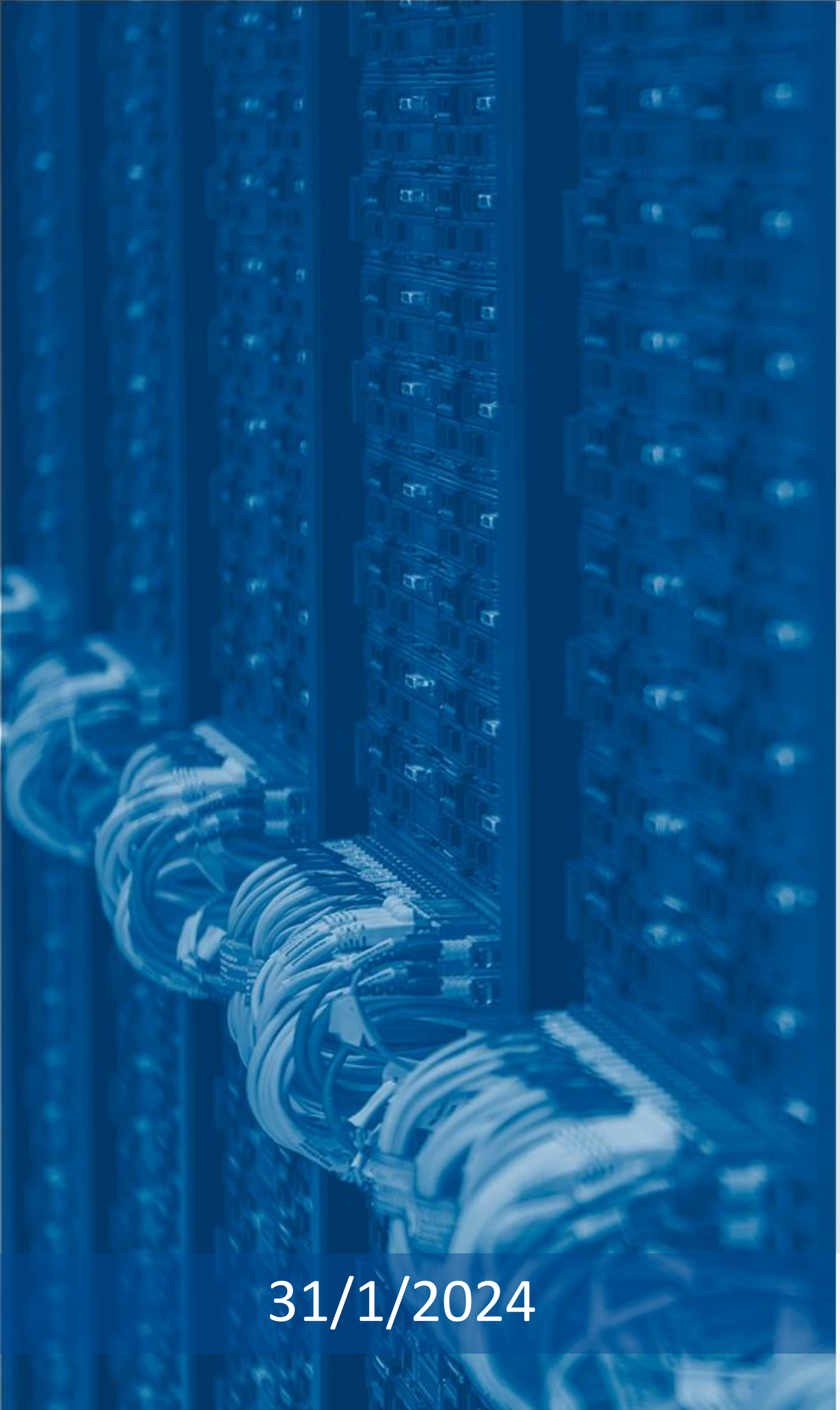

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Provenance with PyCOMPSs (hands-on included)

Raül Sirvent

31/1/2024

BSC Training Course: Programming Distributed Computing Platforms with COMPSs

Outline

- Motivation and Background
- Design of Workflow Provenance recording
- Using Workflow Provenance with COMPSs
- Inspecting registered metadata
- Hands-on exercises

Motivation and Background

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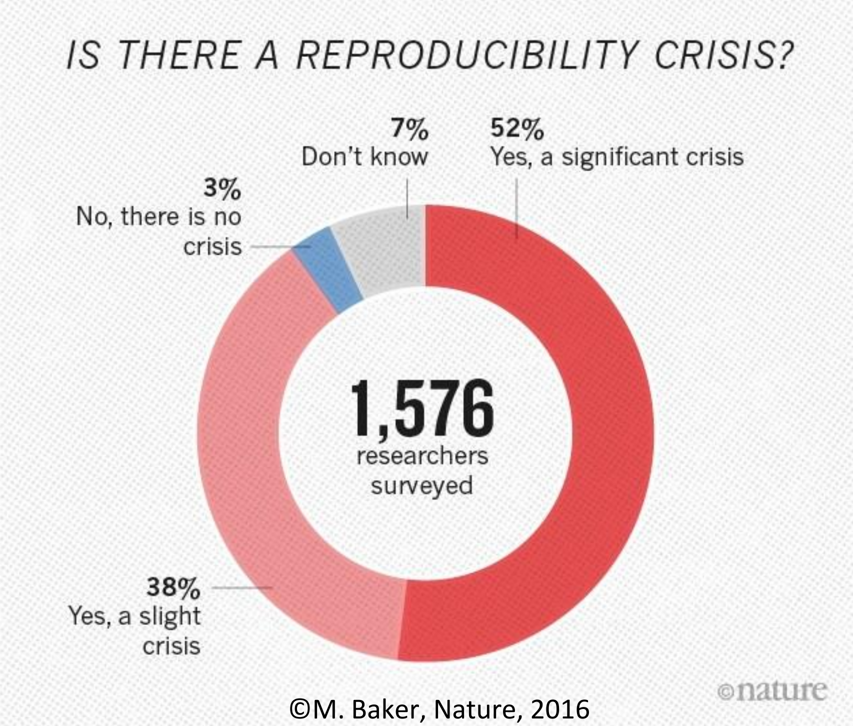
Motivation

- Large number of **Scientific Workflows** experiments
  - Keep track of results - **Governance**
- **Reproducibility** crisis in scientific papers
  - Conferences now request artifacts
    - E.g. SC Reproducibility Initiative
- **Provenance recording** can help with both problems



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- **Provenance:** The chronology of the origin, development, ownership, location, and changes to a system or system component and associated data
  - Need to record metadata
  - Our focus: Workflow Provenance (data + software)

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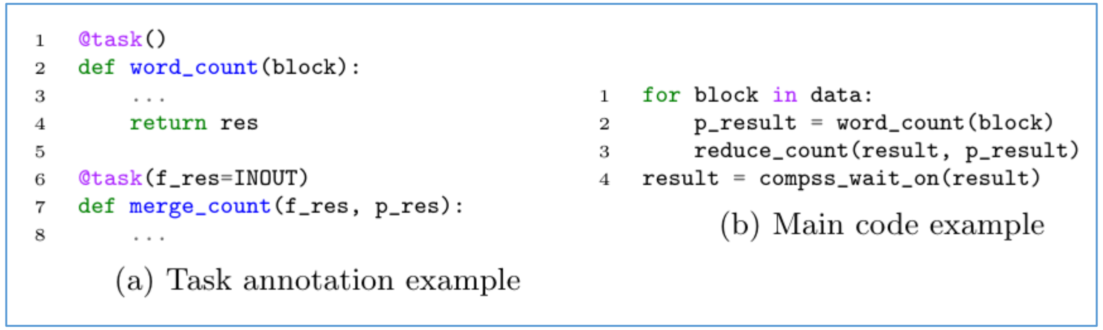
Motivation

- Provenance is **MORE** than just Reproducibility
  - **Governance** (availability, usability, consistency, …) (**FAIR Workflows**)
  - **Replicability** (exchange inputs)
  - **Knowledge extraction** (queries, mining)
  - **Traceability** (validation/verification, visualisation)

- Our claim: desired features for **Workflow Provenance** registration
  - **Automatic:** lower user burden
  - **Efficient:** no overheads
  - **Scalable:** large workflows (both tasks and data assets used)

Background: COMPSs

- **Sequential** programming, **parallel** execution
- **General purpose** programming language + **annotations/hints** (identify tasks and directionality of data)
- Builds a **task graph** at runtime (potential concurrency)
- Tasks can be **sequential**, **parallel** (threaded or MPI)
- Offers to applications a **shared memory illusion** in a distributed system (Big Data apps support)
- Support for **persistent storage**
- **Agnostic** of computing platform: enabled by the runtime for **clusters**, **clouds** and **container** managed clusters



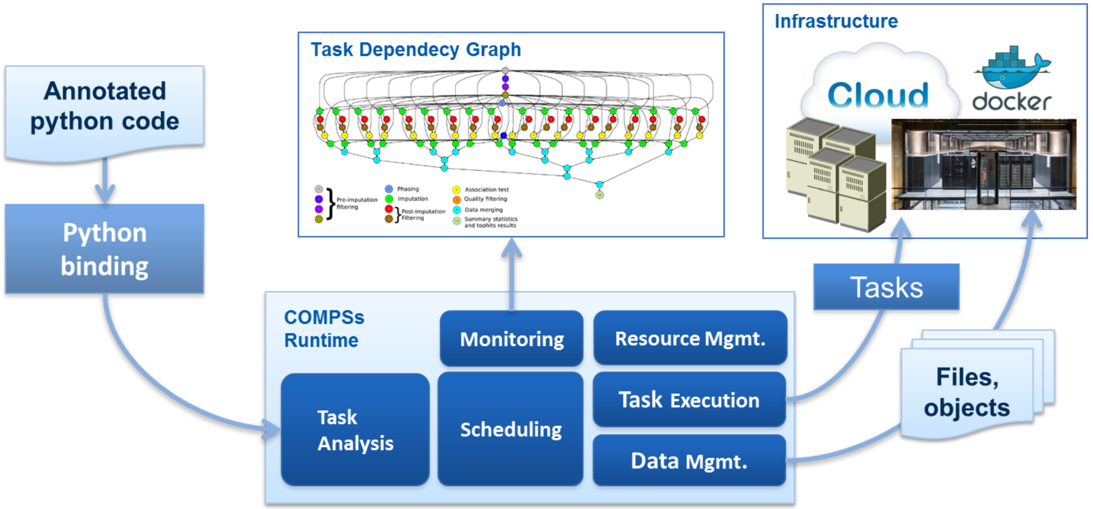
```
@task()
def word_count(block):
    ...
    return res

@task(f_res=INOUT)
def merge_count(f_res, p_res):
    ...
```

(a) Task annotation example

```
for block in data:
    p_result = word_count(block)
    reduce_count(result, p_result)
result = compss_wait_on(result)
```

(b) Main code example



- **Advanced features:** heterogeneous infrastructures, task constraints, streamed data, task faults, task exceptions, checkpointing, elasticity

Background: Research Object Crate

- Package research data + metadata
- Evolution from:
  - **Research Object**: describe digital and real-world resources
  - **DataCrate**: aggregate data with metadata
- Lightweight format
  - Both **machines** and **humans** can read it
- JSON Linked Data (JSON-LD)
  - Vocabulary: Schema.org
  - Structure:
    - **Root Data Entity**
    - **Data Entities** (files, directories)
    - **Contextual Entities** (non-digital elements)
- Strong ecosystem, we use:
  - ro-crate-py library
  - WorkflowHub

RO-Crate 1.1

WorkflowHub

Background: RO-Crate Profiles

- RO-Crate is very **generic** (wide scope)
  - Profiles enable **Interoperability**
    - Set of conventions, types and properties (MUST, SHOULD, …)
- **Workflow RO-Crate** profile
  - MUST **ComputationalWorkflow**, **mainEntity** (Root Dataset)
  - SHOULD **WorkflowSketch**
- **Workflow Run RO-Crate** profile collection (MUST **CreateAction**)
  - Process Run Crate (set of tools)
  - Workflow Run Crate (computational workflow)
  - Provenance Run Crate (detailed computational workflow)

Workflow RO-Crate

Workflow Run RO-Crate

Simone Leo et al. “Recording provenance of workflow runs with RO-Crate” arXiv preprint arXiv:2312.07852 (Dec 2023)

Design of Workflow Provenance recording

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Design Requirements

- Target HPC workflows (commonly large)
- Provenance representation format
  - Simple but able to represent complex workflows
- **Automatic** provenance registration (no explicit annotations)
- **Efficient** provenance registration (avoid overheads at run time)
- **Scale** to large workflows (thousands of files and tasks)

COMPSs + Workflow RO-Crate

Workflow Run RO-Crate + WorkflowHub

COMPSs runtime modifications

COMPSs

- Flags –p or --provenance trigger it after execution
- Can be manually invoked if provenance generation time becomes an issue (i.e., extreme large workflows)

dataprovenance.log

- Lightweight approach: record file accesses, generate provenance later

```
3.3
lysozyme_in_water.py
App_Profile.json
file://s01r2b54-ib0/home/bsc19/bsc19057/DP_Test_3_demo/dataset/2hs9.pdb IN
file://s01r2b54-ib0/home/bsc19/bsc19057/DP_Test_3_demo/output/2hs9.gro OUT
file://s01r2b54-ib0/home/bsc19/bsc19057/DP_Test_3_demo/output/2hs9.top OUT
...
```

After application finishes…

generate_COMPSs_RO-Crate.py

ro-crate-info.yaml

ro-crate-py 0.9.0

COMPSs_RO-Crate_[uuid]/

- It's the *crate*
- ro-crate-metadata.json
- Application source files, command line arguments, workflow image and profile

WorkflowHub

F Findable

A Accessible

I Interoperable

R Reusable

generate_COMPSs_RO-Crate.py features

- Detects and records **COMPSs version** used and the **mainEntity**
  - Looks for alternatives, if not found
- Automatically detects overall **inputs** and **outputs** of the workflow
  - Discards intermediate generated results as inputs
- Respects application **source files** sub-directory structure
- If data persistence, machine paths translated to crate paths
  - Identifies **common paths** to correctly arrange files
    - E.g. inputs/00/input_file.txt
- If no persistence: **URIs** to files are generated, **size** and **modification** date of files are stored to record the file version

Using Workflow Provenance with COMPSs

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Steps to record and publish Workflow Provenance in COMPSs

- Install ro-crate-py (if needed)
- Provide YAML information file
- Run with -p or --provenance
  - The ***crate*** is generated (a sub-folder COMPSs_RO-Crate_[uuid]/)
- Publish it at WorkflowHub, using the crate
- Generate a DOI, cite your results in papers

Install ro-crate-py

- pip install rocrate
- pip install rocrate --user
    - Typically, installs the library in ~/.local/
- pip install -t install_path rocrate
    - Specify target directory

https://github.com/ResearchObject/ro-crate-py

YAML information to be provided

- Non-automatically gathered info: **ro-crate-info.yaml**
- Sections:
  - COMPSs Workflow Information
  - Authors
  - Submitter
- Data persistence: True or False
- No inputs/outputs are provided, automatically detected by the provenance generation script

```yaml
COMPSs Workflow Information:
  name: COMPSs Matrix Multiplication
  description: Blocks as hypermatrix
  license: Apache-2.0
  sources: [src/, ~/java/matmul/xml/,
   ~/java/matmul/pom.xml, Readme]
  data_persistence: True
Authors:
  - name: Rosa M. Badia
    e-mail: Rosa.M.Badia@bsc.es
    orcid: https://orcid.org/0000-0003-2941-5499
    organisation_name: Barcelona Supercomputing Center
    ror: https://ror.org/05sd8tv96
Submitter:
  name: Raül Sirvent
  e-mail: Raul.Sirvent@bsc.es
  orcid: https://orcid.org/0000-0003-0606-2512
  organisation_name: Barcelona Supercomputing Center
  ror: https://ror.org/05sd8tv96
```

Run your COMPSs application

- runcompss -p
- enqueue_compss -p
- pycompss run -p

- Either **-p** or **--provenance**

- Post-process automatically triggered after the end of the application
- Log and time statistics are provided
  - grep PROVENANCE
- If provenance generation fails for any reason:
  - Still possible to invoke it manually (commands provided in the output log)

```
...
PROVENANCE | RO-Crate writing to disk TIME: 0.01987314224243164 s
PROVENANCE | Workflow Provenance generation TOTAL EXECUTION TIME: 0.04113888740539551 s
PROVENANCE | COMPSs Workflow Provenance successfully generated in sub-folder:
    COMPSs_RO-Crate_d64966ac-fe34-463a-88fc-f97047c21a99/
PROVENANCE | ENDED WORKFLOW PROVENANCE SCRIPT
```

The Crate (resulting folder)

- application_sources/
- dataset/
- complete_graph.svg
- App_Profile.json
- compss_submission_command_line.txt
- ro-crate-metadata.json

```
|-- App_Profile.json
|-- application_sources
|   |-- Readme
|   |-- pom.xml
|   |-- src
|   |   `-- main
|   |       `-- java
|   |           `-- matmul
|   |               |-- arrays
|   |               |   |-- …
|   |               |   `-- Matmul.java
|   |               |-- files
|   |               |   |-- Block.class
|   |               |   |-- Block.java
|   |               |   |-- Matmul.class
|   |               |   |-- Matmul.java
|   |               |   |-- MatmulImpl.class
|   |               |   |-- MatmulImpl.java
|   |               |   |-- MatmulItf.class
|   |               |   `-- MatmulItf.java
|   |               `-- objects
|   |                   |-- …
|   |                   `-- Matmul.java
|   `-- xml
|       |-- project.xml
|       `-- resources.xml
|-- complete_graph.svg
|-- compss_submission_command_line.txt
|-- dataset
|   |-- …
|   `-- C.1.1
|-- ro-crate-info.yaml
`-- ro-crate-metadata.json

10 directories, 41 files
```

Publish your results with WorkflowHub

- **zip** –r crate.zip COMPSs_RO-Crate_[uuid]/
- Login to WorfklowHub
- Create -> Workflow
  - **Upload**/Import Workflow RO-Crate tab -> Local file (crate.zip)
  - Click Register
- Review automatically obtained information
- Select the visibility of your workflow in the Sharing tab (for both general public, and for teams selected)
- Click **Register** again

Cite your results with WorkflowHub

- Freeze your workflow version
  - Overview tab -> Citation box -> Freeze version
  - Actions menu -> Freeze version
- Generate DOI
  - **IMPORTANT:** make sure your version is final
  - Citation box -> Generate a DOI
  - Actions menu -> Generate a DOI
  - Select Mint DOI
- The **final generated DOI** for the workflow results can be found in the Citation box

https://doi.org/10.48546/workflowhub.workflow.484.1

SC Conference Reproducibility Initiative

- Artifacts Available ✓
  - Artifacts used in the research (including data and code) are permanently archived in a **public repository** that assigns a **global identifier** and **guarantees persistence**, and are made available via **standard open licenses** that maximize artifact availability

- Artifacts Evaluated-Functional ✓
  - Documentation: Are the artifacts sufficiently **documented** to enable them **to be exercised** by readers of the paper?
  - Completeness: Do the submitted artifacts **include all of the key components** described in the paper?
  - Exercisability: Do the submitted artifacts **include the scripts and data needed to run the experiments** described in the paper, and can the software be successfully executed?

- Results Replicated
  - Reproduce Behavior: determine the equivalent or approximate behavior on available hardware
  - Reproduce the Central Results and Claims of the Paper

Inspecting registered metadata

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Inspecting registered metadata

```
"@id": "application_sources/matmul_files.py",
"@type": ["File", "SoftwareSourceCode", "ComputationalWorkflow"],
"contentSize": 1948,
"description": "Main file of the COMPSs workflow source files",
"encodingFormat": "text/plain",
"image": {"@id": "complete_graph.svg"},
"name": "matmul_files.py",
"programmingLanguage": {"@id": "#compss"}
```

```
"@id": "#compss",
"@type": "ComputerLanguage",
"alternateName": "COMPSs",
"citation": "https://doi.org/10.1007/s10723-
   013-9272-5",
"name": "COMPSs Programming Model",
"url": "http://compss.bsc.es/",
"version": "3.3"
```

Workflow RO-Crate

```
"@id": "complete_graph.svg",
"@type": ["File", "ImageObject", "WorkflowSketch"],
"about": {"@id": "application_sources/matmul_files.py"},
"contentSize": 6681,
"description": "The graph diagram of the workflow, automatically generated by COMPSs runtime",
"encodingFormat": [[”image/svg+xml",{"@id": "https://www.nationalarchives.gov.uk/PRONOM/fmt/92"}]],
"name": "complete_graph.svg"
```

Inspecting registered metadata

Auxiliary Files

```
"@id":
   "application_sources/matmul_tasks.py",
"@type": ["File", "SoftwareSourceCode"]
"contentSize": 1549,
"description": "Auxiliary File",
"encodingFormat": "text/plain",
"name": "matmul_tasks.py"
```

Command line arguments

```
"@id": "compss_submission_command_line.txt",
"@type": "File",
"contentSize": 709,
"description": "COMPSs command line execution
   command (runcompss), including flags and
   parameters passed",
"encodingFormat": "text/plain",
"name": "compss_submission_command_line.txt"
```

COMPSs Task Profiling

```
"@id": "App_Profile.json",
"@type": "File",
"contentSize": 247,
"description": "COMPSs application Tasks profile",
"encodingFormat": ["application/json",{"@id":"https://www.nationalarchives.gov.uk/PRONOM/fmt/817"}],
"name": "App_Profile.json"
```

Inspecting registered metadata

Persistent Data

```
"@id": "dataset/A.0.0",
"@type": "File",
"contentSize": 16,
"dateModified": "2023-09-07T09:20:20",
"name": "A.0.0",
"sdDatePublished": "2023-09-07T09:20:27+00:00"
```

Non-Persistent Data

```
"@id": "file://s07r1b33-ib0/home/bsc19/bsc19057/DP_Test_3_demo/dataset/133l.pdb",
"@type": "File",
"contentSize": 116154,
"dateModified": "2022-04-20T13:20:58",
"name": ”133l.pdb",
"sdDatePublished": "2022-10-18T08:03:08+00:00"
```

```
"@id": "file://s02r2b26-ib0/home/bsc19/bsc19057/DP_Test_3_demo/config/energy.selection"
```

Hostname

Location path in hostname

Inspecting registered metadata

Workflow Run RO-Crate

CreateAction

```
"@id": "#COMPSs_Workflow_Run_Crate_marenostrum4_SLURM_JOB_ID_30132875",
"@type": "CreateAction",
"actionStatus": {"@id": "http://schema.org/CompletedActionStatus"},
"agent": {"@id": "https://orcid.org/0000-0003-0606-2512"},
"description": "Linux s01r2b48 4.4.59-92.20-default #1 SMP Wed May 31 14:05:24 UTC 2017 (8cd473d)
   x86_64 x86_64 x86_64 GNU/Linux SLURM_JOB_NAME=matmul-DP COMPSS_PYTHON_VERSION=3.9.10
   SLURM_JOB_QOS=debug SLURM_MEM_PER_CPU=1880 COMPSS_BINDINGS_DEBUG=1 SLURM_JOB_ID=30132875
   SLURM_JOB_USER=bsc19057 COMPSS_HOME=/apps/COMPSs/3.2/ SLURM_JOB_UID=2952
   SLURM_SUBMIT_DIR=/gpfs/home/bsc19/bsc19057/COMPSs-DP SLURM_JOB_NODELIST=s01r2b48
   SLURM_JOB_GID=2950 SLURM_JOB_CPUS_PER_NODE=48 COMPSS_MPIRUN_TYPE=impi SLURM_SUBMIT_HOST=login3
   SLURM_JOB_PARTITION=main SLURM_JOB_ACCOUNT=bsc19 SLURM_JOB_NUM_NODES=1
   COMPSS_MASTER_NODE=s01r2b48 COMPSS_WORKER_NODES=",
"endTime": "2023-09-07T09:46:26+00:00",
"instrument": {"@id": "application_sources/matmul_files.py"},
"name": "COMPSs matmul_files.py execution at marenostrum4 with JOB_ID 30132875",
```

Inspecting registered metadata

Workflow Run
RO-Crate

CreateAction

```
"object": [{"@id": "dataset/A.0.0"}, {"@id": "dataset/A.0.1"}, {"@id": "dataset/A.1.0"},
   {"@id": "dataset/A.1.1"}, {"@id": "dataset/B.0.0"}, {"@id": "dataset/B.0.1"}, {"@id":
   "dataset/B.1.0"}, {"@id": "dataset/B.1.1"}, {"@id": "dataset/C.0.0"}, {"@id":
   "dataset/C.0.1"}, {"@id": "dataset/C.1.0"}, {"@id": "dataset/C.1.1"}],

"result": [{"@id": "dataset/C.0.0"}, {"@id": "dataset/C.0.1"}, {"@id": "dataset/C.1.0"},
   {"@id": "dataset/C.1.1"}, {"@id": "./"}],

"subjectOf": ["https://userportal.bsc.es/"]
```

Conclusions

- **FAIR HPC workflows** combining COMPSs + RO-Crate + WorkflowHub
  - WMS that use RO-Crate (Galaxy, Nextflow, Streamflow, Sapporo, Autosubmit)
- Paper* experiments show
  - We provide **automatic** provenance registration (whenever possible)
  - We are **efficient** (no run time overhead appreciated)
  - We can **scale** and deal with large workflows (shown by use cases)
- Future Work
  - Integration with: WfExS, ROHub (RO-Crate)
  - Automatic reproducibility with the PyCOMPSs CLI
  - Governance and Knowledge extraction

*Raül Sirvent et al. "Automatic, Efficient and Scalable Provenance Registration for FAIR HPC Workflows" In: 2022 IEEE/ACM Workshop on Workflows in Support of Large-Scale Science (WORKS). IEEE, 2022. p. 1-9.

Hands-on Exercises

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Preliminary steps

- Find help in the Manual:
  - COMPSs ReadTheDocs -> Tools -> Workflow Provenance
- Create your WorkflowHub account
  - Open https://workflowhub.eu/
  - Click “Register”
    - “Log in using GitHub” or
    - Register with your e-mail
      - Mandatory: First name, Last name, e-mail. Recommended: ORCID
      - Confirm registration with received e-mail
- Join “COMPSs Tutorials” team (“eFlows4HPC” Space)
  - “Join a Team”
    - Search for ”COMPSs Tutorials”
    - Organization:
      - Search for your institution not only by acronym, also with full words
      - Can try also: Browse -> Organizations -> Country (filter)
      - If not found: Create -> Organization

- **List of commands used in the Exercises: /apps/COMPSs/TUTORIALS/2024_BSC_TRAINING_COMPSS_MN4/PROVENANCE_COMMANDS.txt**

Exercise 1: Publish a Workflow Run

- Choose a COMPSs example from the ones you have previously run in the Cluster Hands-on session
  - **Easy:** Lysozyme in Water (any version) (**mandatory dataset_small/**)
  - **Medium:** Cholesky (can play with SIZE and BSIZE), K-means, Clustering Comparison
  - **Hard:** Wordcount (both reduce and merge)
- Create/edit ro-crate-info.yaml
  - cp /apps/COMPSs/TUTORIALS/2024_BSC_TRAINING_COMPSS_MN4/ro-crate-info.yaml .
  - Establish yourself as ‘Submitter’
    - If you don’t have an ORCID, just remove the ‘Submitter’ section, the Author will be considered the Submitter

Exercise 1: Publish a Workflow Run

- ro-crate-info.yaml

```
COMPSs Workflow Information:
  name: Lysozyme in water sample
  description: Lysozyme in water sample COMPSs application
  license: Apache-2.0
  sources: [src/, launch.sh]
  data_persistence: True
Authors:
  - name: Rosa M. Badia
    e-mail: Rosa.M.Badia@bsc.es
    orcid: https://orcid.org/0000-0003-2941-5499
    organisation_name: Barcelona Supercomputing Center
    ror: https://ror.org/05sd8tv96
Submitter:
  name: Raül Sirvent
  e-mail: Raul.Sirvent@bsc.es
  orcid: https://orcid.org/0000-0003-0606-2512
  organisation_name: Barcelona Supercomputing Center
  ror: https://ror.org/05sd8tv96
```

Minimal information

Odd usernames: True

Even usernames: False

Hint for Wordcount: look for the optional parameters of ro-crate-info.yaml in the manual

Exercise 1: Publish a Workflow Run

- Edit launch.sh script: add “--provenance” option
- Submit: Example ./launch.sh 2 10 false $(pwd)/config/ $(pwd)/dataset_small/ $(pwd)/output/
  - **Change number of nodes, or other parameters**
    - **Lysozyme in water: launch.sh, launch_full.sh, launch_full_no_mpi.sh or launch_full_singularity.sh**
    - **Cholesky: SIZE, BSIZE**
    - **Wordcount: launch.sh or launch_merge.sh**
- Check time and result of provenance generation (compss_XXXX.out)
  - What was the longest time during generation?
- Zip and upload RO-Crate
  - zip –r my_app_crate.zip COMPSs_RO-Crate_XXX/
- Copy the file to your laptop. Run, from your laptop:
  - scp nct01XXX@mn3.bsc.es:~/my_app_folder/my_app_crate.zip ~/Desktop/
- Go to WorkflowHub -> Contribute
    - Upload/Import Workflow RO-Crate -> Select local file
    - Briefly inspect imported metadata
    - Select Team, check Sharing permissions, click Register

Exercise 1: Publish a Workflow Run

- DOI generation and reference (**DON’T DO THIS NOW!!!!!!**)
  - Freeze version
  - Generate a DOI
  - Share the obtained DOI (e.g. use it as a reference in a paper)

- **Example: ROM Workflow DOI generated live**

Exercise 2: Inspect a previous published execution

- Find your own published workflow
  - My Items -> Workflows
- Can you understand the metadata (**ro-crate-metadata.json**)? Ask, if not
  - Identify the 3 main parts of the JSON: Root Data Entity, Data Entities, Contextual Entities
  - ro-crate-metadata.json interesting keywords: mainEntity, ComputationalWorkflow, WorkflowSketch, #compss, CreateAction (object, result)
  - Observe the CreateAction in detail
- Questionnaire:
  - Who ran this code? Where? When? With which COMPSs version?
  - What is the name of the main application source file?
  - What were the inputs and outputs used or generated in this workflow run?
  - Can you say how many cluster nodes were used for the run? (Hint: 3 locations)
  - Where can you find detailed profiling of the application? (Hint: 2 locations)
  - Are the data assets included in the package?
  - What was the command used to run this workflow? What were the parameters passed to the application?
  - Navigate the workflow diagram

Exercise 2 (extra): Inspect a previous published execution

- Browse for other COMPSs Workflows at WorkflowHub
  - Browse -> Workflows
    - Workflow type: filter by “COMPSs”
    - Team: filter by “COMPSs Tutorials” (**or don’t**)
- Inspect the metadata (keywords: mainEntity, ComputationalWorkflow, WorkflowSketch, #compss, CreateAction (object, result))
- Questionnaire:
  - Who ran this code? Where? When? With which COMPSs version?
  - What is the name of the main application source file?
  - What were the inputs and outputs used or generated in this workflow run?
  - Can you say how many cluster nodes were used for the run? (Hint: 3 locations)
  - Where can you find detailed profiling of the application? (Hint: 2 locations)
  - Are the data assets included in the package?
  - What was the command used to run this workflow? What were the parameters passed to the application?
  - Navigate the workflow diagram

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Exercise 3: Repeat Exercises 1 and 2 with data_persistence flipped

- If your data_persistence was True, set it to False
- If it was False, set it to True

- Re-execute your application
- Publish your new run to WorkflowHub
- Compare the runs
  - dataset/ folder???
  - ro-crate-metadata.json -> check data assets
    - Search for a specific file you know
    - Or look for "CreateAction"

Exercise 4: Reproduce an execution from another participant in the tutorial

- Browse for COMPSs Workflows at WorkflowHub
  - Browse -> Workflows
    - Workflow type: filter by “COMPSs”
    - Team: filter by “COMPSs Tutorials”
  - **Select preferably one with data_persistence=True (i.e. has a dataset/ folder)**
- Click the workflow, click “Download RO-Crate”
- Create a directory at the supercomputer
  - mkdir ~/reproduced_app/
- Copy the file from your laptop to the supercomputer
  - scp ~/Desktop/workflow-XXX-X.crate.zip nct01XXX@mn3.bsc.es:~/reproduced_app/your_app_crate.zip
- At the supercomputer, in the ~/reproduced_app/ folder
  - unzip workflow-XXX-X.crate.zip

Exercise 4: Reproduce an execution from another participant in the tutorial

- Understand inputs/outputs location (**ro-crate-metadata.json**)
  - Check CreateAction -> object and result
- Example with dataset/
  - Inputs:
    - dataset/lysozyme_in_water/config/
    - dataset/lysozyme_in_water/dataset_small/
  - Outputs:
    - dataset/lysozyme_in_water/output/
- Example without dataset/
  - Inputs:
    - file://s02r1b59-ib0/home/nct01/nct00XXX/lysozyme_in_water/config/
    - file://s02r1b59-ib0/home/nct01/nct00XXX/lysozyme_in_water/dataset_small/
  - Outputs
    - file://s02r1b59-ib0/home/nct01/nct00XXX/lysozyme_in_water/output/
- Check parameters used in the run (**compss_submission_command_line.txt**)
  - Specifically, the num_nodes parameter

Exercise 4: Reproduce an execution from another participant in the tutorial

- **CREATE A NEW OUTPUT FOLDER (avoid overwriting the recorded one)**
  - cd application_sources/
  - mkdir new_output/
- Resubmit the application with the correct paths:
  - chmod ugo+x launch.sh
  - Provenance recording can be deactivated for this run (remove --provenance)
  - Persistence example:
    - ./launch.sh 2 10 false ../dataset/lysozyme_in_water/config/ ../dataset/lysozyme_in_water/dataset_small/ **new_output/**
  - Non-persistence example:
    - ./launch.sh 2 10 false /home/nct01/nct00XXX/lysozyme_in_water/config/ /home/nct01/nct00XXX/lysozyme_in_water/dataset_small **new_output/**
- Compare results:
  - diff new_output/ ../dataset/lysozyme_in_water/output/
  - diff new_output/ /home/nct01/nct00XXX/lysozyme_in_water/output
  - **Are they identical? Why?**

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Thank you for your attention

https://compss-doc.readthedocs.io/en/latest/Sections/05_Tools/04_Workflow_Provenance.html

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