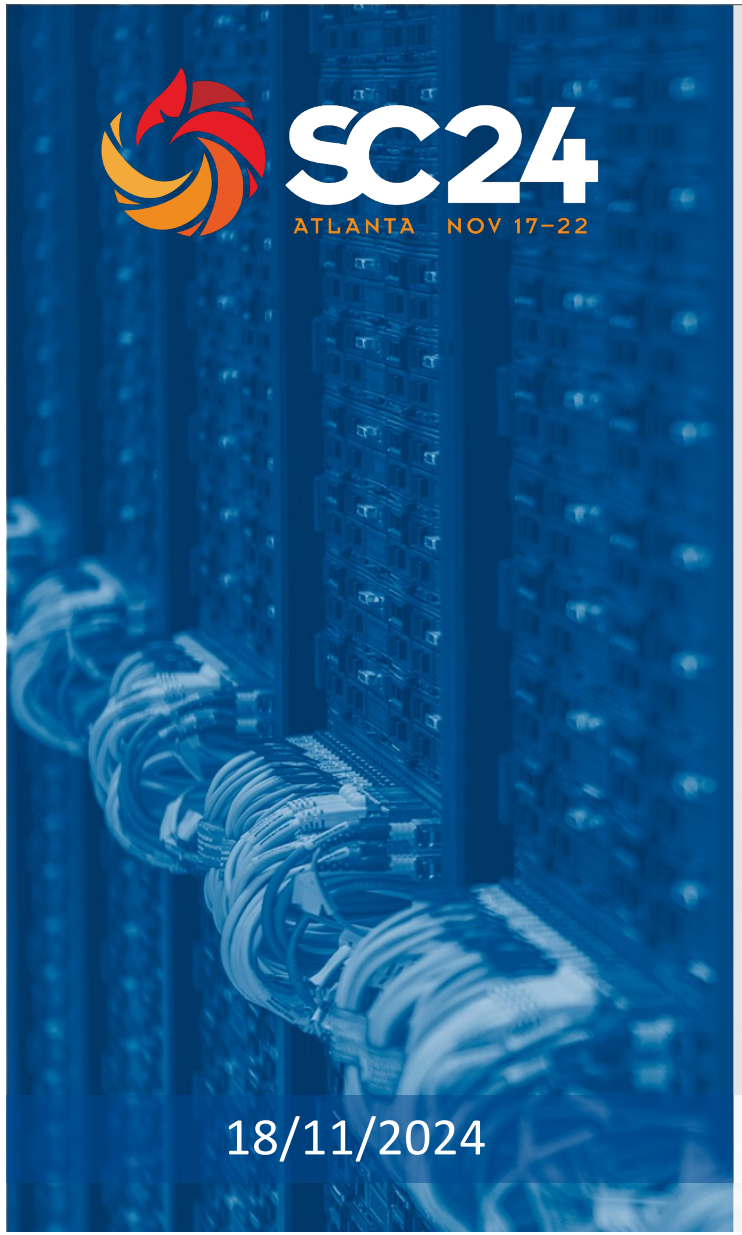

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Optimising workflow lifecycle management: development, HPC-ready containers deployment and reproducibility

Raül Sirvent, Rosa M Badia

18/11/2024

SC24 tutorial, Atlanta, 18 November 2024

Tutorial website

https://github.com/bsc-wdc/Tutorial_SC24

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Agenda

8:30 – 8:45	Overview of tutorial agenda	Rosa M Badia
8:45 – 9:10	Part 1.1: Hybrid HPC+AI+DA workflow development with PyCOMPSs - Context of the workflows at BSC - Overview of workflow development with PyCOMPSs - Extensions for the integration of HPC with AI and DA	Rosa M Badia
9:10 – 9:40	Part 1.2: Workflows' reproducibility through provenance - Motivation for workflow provenance - Design of the recording mechanism - Sharing experiments for reproducibility	Raül Sirvent
9:40 - 10:00	Part 1.3: HPC ready container images - Motivation for architecture specific containers - Overview of the Container Image Creation service - Example of HPC ready container generation	Rosa M Badia
10:00 - 10:30	Coffee break	

Agenda

10:30 – 10:45	Hands-on preparation (credentials distribution, how to access, etc)	All presenters
10:45 – 11:15	Part 2.1: Hands-on session: Sample workflows with PyCOMPSs, execution with containers, task-graph generation, tracefile generation (optional)	Rosa M Badia
11:15 – 11:55	Part 2.2: Hands-on session: How to automatically record workflow provenance and use it to share experiments in WorkflowHub	Raül Sirvent
11:55 - 12:00	Tutorial conclusions	All presenters

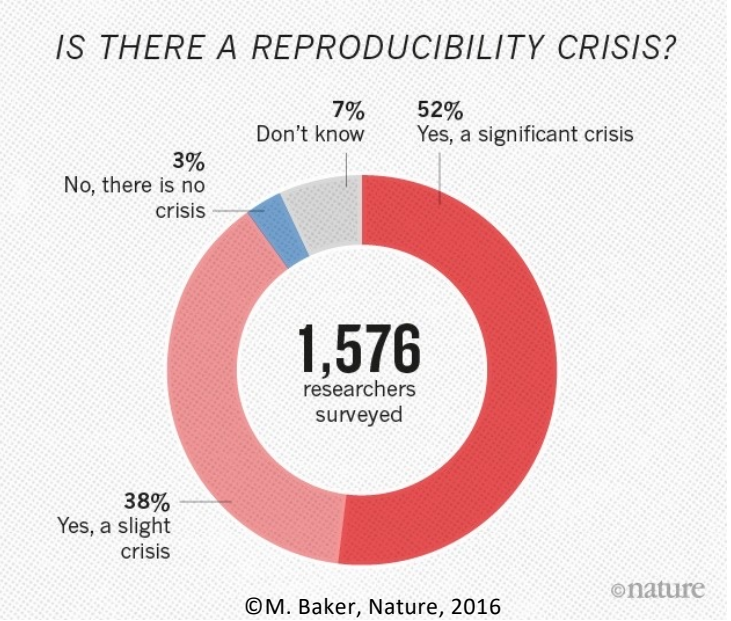
Outline

- Motivation and baseline technologies
- Design of Workflow Provenance recording
- Using Workflow Provenance with COMPSs

Motivation and baseline technologies

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



- **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)

Motivation

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

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

Baseline: 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

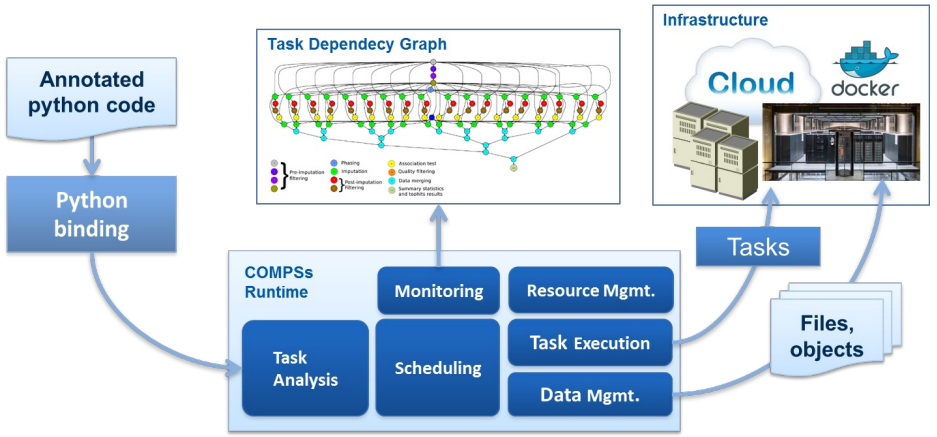
```python
@task()
def word_count(block):
    ...
    return res

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

(a) Task annotation example

```python
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

Baseline: 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, more than 30 tools/systems:
  - Describo, ro-crate-html, ro-crate-zenodo, …
- We use:
  - ro-crate-py library (generation / consumption), rocrate-validator, WorkflowHub (interoperability)

RO-Crate 1.1

WorkflowHub

Baseline: 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)

Simone Leo et al. “Recording provenance of workflow runs with RO-Crate” PLoS ONE 19(9): e0309210 (Sept 2024)

WMS/tools using WRROC for Provenance Recording

- runcrate
- rocrate-validator

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)

+

+

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COMPSs runtime modifications

- 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

After application finishes…

generate_COMPSs_RO-Crate.py

ro-crate-info.yaml

ro-crate-py 0.11.0

COMPSs_RO-Crate_[uuid]/

- Lightweight approach: record file accesses, generate provenance later

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

```
3.3.rc2407
lysozyme_in_water.py
App_Profile.json
2024-08-12T13:25:07.717499Z
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
...
```

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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

Generating Workflow Provenance with COMPSs

Steps to record Workflow Provenance in COMPSs

- Install ro-crate-py (if needed)
- Provide YAML information file
- Run with -p or –provenance=my_file.yaml
  - The ***crate*** is generated (a sub-folder COMPSs_RO-Crate_[uuid]/)

YAML information to be provided

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

```
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
Agent:
  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
```

Automatic search of ORCID and ROR

- For machines with internet connectivity only
- Gets the rest of missing items, if available
- Convenient for applications with large number of authors

```
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
  - name: Nicolò Giacomini
  - name: Fernando Vázquez Novoa
    organisation_name: Barcelona Supercomputing Center
  - name: Cristian Cătălin Tatu
  - orcid: https://orcid.org/0000-0001-5081-7244
    organisation_name: Barcelona Supercomputing Center
  - orcid: https://orcid.org/0000-0001-6401-6229
    ror: https://ror.org/05r78ng12
  - name: Francesc Lordan
    ror: https://ror.org/05sd8tv96
Agent:
  orcid: https://orcid.org/0000-0003-0606-2512
```

Using Workflow Provenance with COMPSs

What you can do with the generated provenance

- Publish your experiment in WorkflowHub
- PyCOMPSs CLI (v3.3.4): pycompss inspect
- COMPSs Reproducibility Service

Steps to record and publish Workflow Provenance in COMPSs

- Publish it at WorkflowHub, **uploading the crate** or **using GitHub**
- Generate a DOI, cite your results in papers

- **Large datasets** can be shared in external repositories (e.g. Zenodo, FigShare), and included as a reference

Sharing Use Cases with WorkflowHub

- Asset sharing focus:
  - Share your **workflow** (+some example usage/test datasets attached)
  - Share your **dataset results** (+ the workflow that generated them, for reproducibility)

- Sharing audience:
  - **Privately** upload your code or data in a team, to share with your peers
    - Upload the most interesting code versions / output datasets
  - Once something is worth sharing **publicly** (code or data), change the permission of the specific result, generate DOI, cite it, etc…

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

pycompss inspect [crate_folder/ | crate.zip]

- Visualise metadata content through the console in a friendly way

```
COMPSs_RO-Crate_310c93f5-ff00-45b2-aaf7-de202bbf1349/
├── Date Published
│   └── Friday, 20 of September of 2024 - 09:14 UTC
├── Name
│   └── COMPSs Matrix Multiplication, out-of-core using files
├── Authors
│   └── Raül Sirvent (Barcelona Supercomputing Center) (Raul.Sirvent@bsc.es)
├── License
│   └── CC-BY-NC-ND-4.0
├── Software Dependencies
│   ├── NumPy
│   └── GROMACS
├── COMPSs Runtime version
│   └── 3.3.rc2408
├── RO-Crate Profiles compliance
│   ├── Process Run Crate (0.5)
│   ├── Workflow Run Crate (0.5)
│   ├── Provenance Run Crate (0.5)
│   └── Workflow RO-Crate (1.0)
├── Description
│   └── Hypermatrix size 2x2 blocks, block size 2x2 elements
└── CreateAction (execution details)
    ├── Agent
    │   └── Rosa M. Badia (Universitat Politècnica de Catalunya) (Rosa.M.Badia@upc.edu)
    ├── Application's main file
    │   └── matmul_files.py
    ├── Hostname
    │   └── MacBook-Pro-Raul-2018.local
    ├── Description (machine details)
    │   └── Darwin MacBook-Pro-Raul-2018.local 23.6.0 Darwin Kernel Version 23.6.0: Mon
     Jul 29 21:13:00 PDT 2024; root:xnu-10063.141.2~1/RELEASE_X86_64 x86_64
    ├── Environment
    │   └── COMPSS_HOME = /Users/rsirvent/opt/COMPSs/
    ├── Resource Usage
    │   ├── #localhost.matmul_tasks.multiply.maxTime = 1015
    │   ├── #localhost.matmul_tasks.multiply.executions = 8
    │   ├── #localhost.matmul_tasks.multiply.avgTime = 553
    │   ├── #localhost.matmul_tasks.multiply.minTime = 94
    │   ├── #overall.matmul_tasks.multiply.maxTime = 1015
...
```

```
    ├── Start Time
    │   └── Friday, 20 of September of 2024 - 09:14:41 UTC
    ├── End Time
    │   └── Friday, 20 of September of 2024 - 09:14:48 UTC
    ├── TOTAL EXECUTION TIME
    │   └── 0:00:07 s
    ├── INPUTS
    │   ├── dataset/A.0.0 (16 bytes)
...
    │   ├── dataset/C.1.1 (20 bytes)
    │   └── https://zenodo.org/records/10782431/files/lysozyme_datasets.zip (267,235,780
     bytes)
    └── OUTPUTS
        ├── dataset/C.0.0 (20 bytes)
        ├── dataset/C.0.1 (20 bytes)
        ├── dataset/C.1.0 (20 bytes)
        ├── dataset/C.1.1 (20 bytes)
        ├──
      https://zenodo.org/records/10783183/files/results_2003_0521_boumardes_BS.tar.gz
      (711,341,852 bytes)
        └── ./
```

- Helps to inspect crate zipped files, without having to unzip them

Reproducibility Service

- Reproduce a previously run COMPSs experiment

```
compss_reproducibility_service [ro_crate_folder/ | url ]
```

- Example

```
compss_reproducibility_service https://workflowhub.eu/workflows/1072/ro_crate?version=2
```

- Two main use cases:
  - Data persistence:
    - Experiment can be re-executed on any machine
  - Non data persistence:
    - Re-execute on a machine that has access to the data assets paths

WorkflowHub

Reproducibility Service

- Metadata is used to verify input files
  - Ensure re-execution will be done with EXACTLY the same data assets (size, mod_date)

S.No.	Filename	File Path	File Accessible	File Size Verified
1	application_sources/src/wc_reduce.py	/home/archit/Desktop/COMPSs-Reproducibility-Service/reproducibility_service_20240820_012206/Workflow/application_sources/src/wc_reduce.py	✅	✅
2	file0.txt	/home/archit/Desktop/COMPSs-Reproducibility-Service/reproducibility_service_20240820_012206/Workflow/dataset/dataset_4f_16mb/file0.txt	✅	✅
3	file1.txt	/home/archit/Desktop/COMPSs-Reproducibility-Service/reproducibility_service_20240820_012206/Workflow/dataset/dataset_4f_16mb/file1.txt	✅	✅
4	file2.txt	/home/archit/Desktop/COMPSs-Reproducibility-Service/reproducibility_service_20240820_012206/Workflow/dataset/dataset_4f_16mb/file2.txt	✅	✅
5	file3.txt	/home/archit/Desktop/COMPSs-Reproducibility-Service/reproducibility_service_20240820_012206/Workflow/dataset/dataset_4f_16mb/file3.txt	✅	✅

✔: SUCCESS | ✘: FAILURE | –: NOT IN METADATA

Metadata format

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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"}
“softwareRequirements": [{"@id": "https://numpy.org/"}, {"@id":
    "https://www.gromacs.org/"}]
```

```
"@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.rc2408"
```

```
"@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”
"sha256": "44018036dc20569b90104113928291e997f2f5cecb2e01af19b5dc2e0043eb6f"
```

Inspecting registered metadata

Software Depencencies


```
{
    "@id": "https://numpy.org/",
    "@type": "SoftwareApplication",
    "name": "NumPy",
    "url": "https://numpy.org/",
    "version": "1.24.1"
},
{
    "@id": "https://www.gromacs.org/",
    "@type": "SoftwareApplication",
    "name": "GROMACS",
    "url": "https://www.gromacs.org/",
    "version": ":-) GROMACS - gmx, 2024.2-Homebrew (-:\nExecutable:
   /usr/local/bin/../Cellar/gromacs/2024.2/bin/gmx\nData prefix:
   /usr/local/bin/../Cellar/gromacs/2024.2\nWorking dir:
   /Users/rsirvent/.COMPSs/lysozyme_in_water_full_no_mpi.py_30\nCommand line:\n  gmx --
   version\n\nGROMACS version:     2024.2-Homebrew\nPrecision:          mixed\nMemory model:
   64 bit\nMPI library:        thread_mpi\nOpenMP support:      enabled (GMX_OPENMP_MAX_THREADS =
   128)\n"
},
```

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 submission command line
   (runcompss / enqueue_compss), including flags
   and parameters passed to the application",
"encodingFormat": "text/plain",
"name": "compss_submission_command_line.txt”
"sha256":
   "7093e1aa31723f8748148e8413fc7831fc3df2bcabe26
   0775f9e3ab86f117e48"
```

COMPSs Task Profiling (deprecated)

```
"@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”
"sha256": "83f7239637dd90008d48a5b99f6d36bf478ec9db9a912126afd856a0c8747670"
```

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

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Inspecting registered metadata

CreateAction


```
"@id": #COMPSs_Workflow_Run_Crate_marenostrum5_SLURM_JOB_ID_5143097",
"@type": "CreateAction",
"actionStatus": {"@id": "http://schema.org/CompletedActionStatus"},
"name": "COMPSs matmul_files.py execution at marenostrum5 with JOB_ID 5143097",
"description": "Linux gs14r1b58 5.14.0-284.30.1.el9_2.x86_64 #1 SMP PREEMPT_DYNAMIC Fri Aug 25
   09:13:12 EDT 2023 x86_64 x86_64 x86_64 GNU/Linux"
"instrument": {"@id": "application_sources/matmul_files.py"},
"agent": {"@id": "https://orcid.org/0000-0003-0606-2512"},
"environment": [{"@id": "#slurm_job_user"},... {"@id": "#compss_worker_nodes"}],
"resourceUsage": [{"@id": "#localhost.matmul_tasks.multiply.maxTime"}, ... {"@id":
   "#overall.matmul_files.py.executionTime"}],
"startTime": "2024-09-02T14:22:40+00:00",
"endTime": "2024-09-02T14:22:47+00:00",
"subjectOf": ["https://userportal.bsc.es/"]
```

Inspecting registered metadata

CreateAction

```
{
    "@id": "#slurm_job_user",
    "@type": "PropertyValue",
    "name": "SLURM_JOB_USER",
    "value": "bsc019057"
},
{
    "@id": "#slurm_job_uid",
    "@type": "PropertyValue",
    "name": "SLURM_JOB_UID",
    "value": "2952"
},
{
    "@id": "#slurm_submit_dir",
    "@type": "PropertyValue",
    "name": "SLURM_SUBMIT_DIR",
    "value": "/gpfs/home/bsc/bsc019057/COMPSs-DP”
},
...
```

```
{
    "@id": "#localhost.matmul_tasks.multiply.maxTime",
    "@type": "PropertyValue",
    "name": "maxTime",
    "propertyID":
   "https://w3id.org/ro/terms/compss#maxTime",
    "unitCode": "https://qudt.org/vocab/unit/MilliSEC",
    "value": "369"
},
{
    "@id": "#localhost.matmul_tasks.multiply.executions",
    "@type": "PropertyValue",
    "name": "executions",
    "propertyID":
   "https://w3id.org/ro/terms/compss#executions",
    "value": "8"
},
...
```

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Workflow Run RO-Crate

Inspecting registered metadata

CreateAction


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

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
  - Detect and Install software dependencies
  - Governance and Knowledge extraction (from execution metrics)
  - XAI: eXplainable Artificial Intelligence

*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.

eFlows4HPC

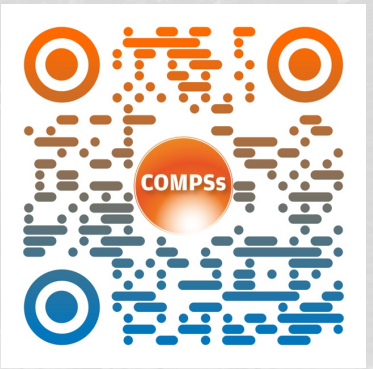
Enabling dynamic and Intelligent workflows in the future EuroHPC ecosystem

DT GEO

Barcelona Supercomputing Center

Centro Nacional de Supercomputación

Thanks!



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

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