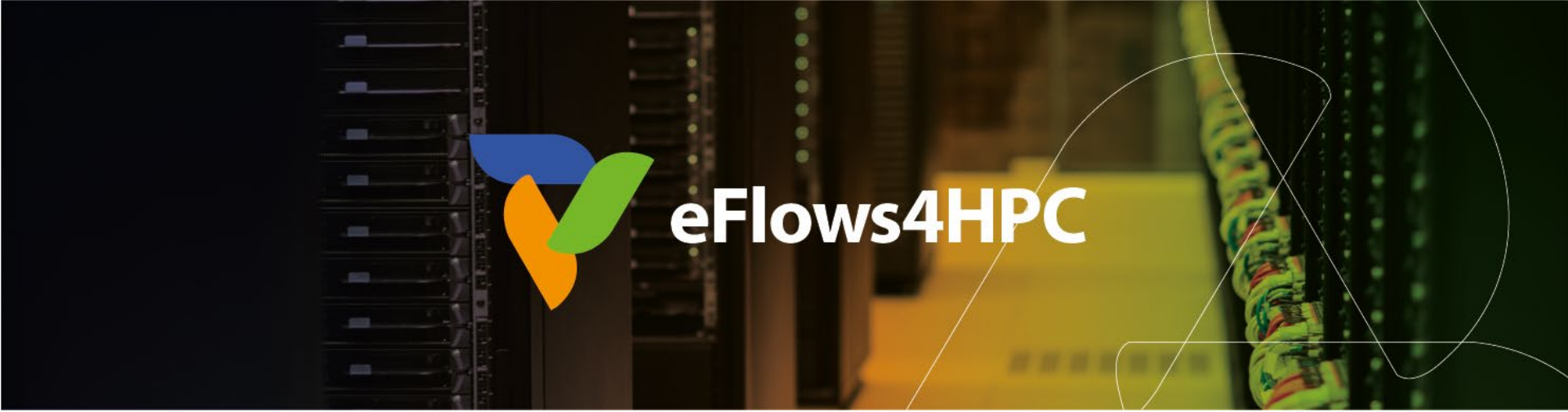

Workflow Provenance registration with COMPSs

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Next-generation HPC workflows for natural hazards, Barcelona
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DT-GEO

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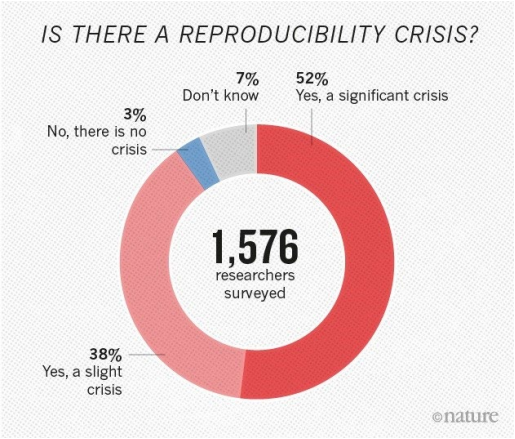
Outline

- Motivation and Background
- Design of the Workflow Provenance recording
- Using Workflow Provenance with COMPSs
- Inspecting registered metadata
- Live demo with WorkflowHub

Motivation

- Volume of data generated from **scientific workflow** experiments continues to grow
  - Important to manage results
- Reproducibility crisis: provide more than just numbers on a scientific paper
- **FAIR principles:** Findable, Accessible, Interoperable, Reusable
  - FAIR Workflows
- **Provenance:** The chronology of the origin, development, ownership, location, and changes to a system or system component and associated data
  - Record metadata



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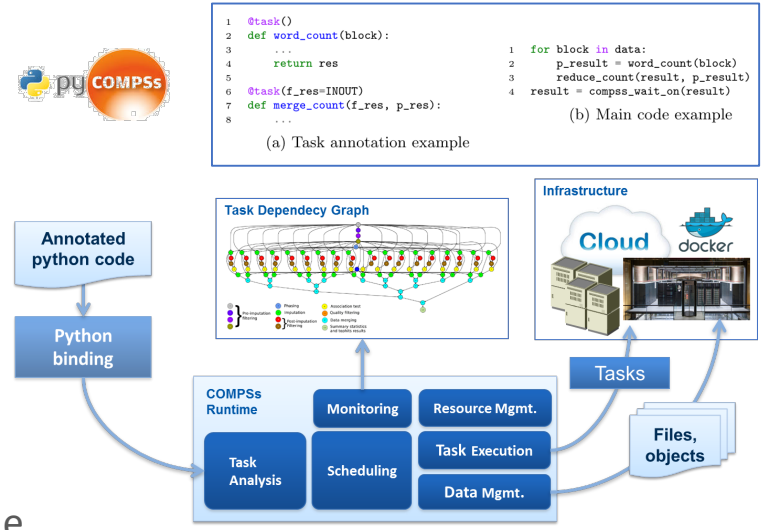
Motivation

- **FAIR** and **provenance** registration to achieve **reproducibility** and **replicability**
  - Visual tools difficult to scale
  - Custom formats that complicate interoperability
  - RDF and OWL learning curve for non-experts on SemanticWeb

- Our proposal for scientific workflow provenance registration
  - **Automatic:** users do not need to provide annotations on what to record
  - **Efficient:** lightweight approach to avoid run time overheads (target HPC)
  - **Scalable:** large workflows (thousands of task nodes and / or files 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



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

Background: Research Object Crate

- Lightweight approach to package research data with their metadata
- Evolution from:
  - Research Object: describe and link digital and real-world resources
  - DataCrate: describe and aggregate data with associated metadata
- Wide scope: from an individual researcher working with a folder of data, to large data-intensive computational research environments
- Machine-readable JSON Linked Data (JSON-LD)
  - Main vocabulary based on Schema.org
  - Structure: **Root Data Entity**, **Data Entities** (files, directories), **Contextual Entities** (non-digital elements)
- Strong ecosystem:
  - ro-crate-py library
  - WorkflowHub

RO-Crate 1.1

WorkflowHub

Background: RO-Crate Profiles

- Profiles narrow down the scope
  - Set of conventions, types and properties to allow interoperability
- **Workflow RO-Crate** profile
  - Requires **ComputationalWorkflow**. Must also be indicated with **mainEntity** from the Root Data set
  - Recommends to include **WorkflowSketch**
- **Workflow Run RO-Crate** profile collection (**CreateAction**)
  - Process Run Crate (set of tools used in a single computation)
  - Workflow Run Crate (computational workflow involved)
  - Provenance Run Crate (details on each step of the workflow)

Design Requirements

- Target HPC workflows (commonly large)
- Reproducibility and replicability for workflows
- 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 runtime modifications

eFlows4HPC

dataprovenance.log

After application finishes…

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

generate_COMPSs_RO-Crate.py

ro-crate-info.yaml

ro-crate-py 0.8.0

COMPSs_RO-Crate_[uuid]/

- Lightweight approach: record file accesses, generate provenance later

```
3.2
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
...
```

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

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

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

```
COMPSs Workflow Information:
  name: COMPSs Matrix Multiplication
  description: Blocks as hypermatrix
  license: Apache-2.0
  sources_dir: [src, ~/java/matmul/xml]
  files: [~/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 | COMPSs RO-Crate created successfully in subfolder COMPSs_RO-Crate_aaf0cb82-a500-4c28-bbc8-439c37c2e210/
PROVENANCE | RO-CRATE dump TIME: 0.004969120025634766 s
PROVENANCE | RO-CRATE GENERATION TOTAL EXECUTION TIME: 0.014089107513427734 s
PROVENANCE | ENDED DATA PROVENANCE SCRIPT
```

The Crate (resulting folder)

- application_sources/
- dataset/
- complete_graph.svg
- App_Profile.json
- compss_command_line_arguments.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_command_line_arguments.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

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": "3.2"
```

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

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

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
- No previous solution for large HPC workflows that studies and avoids run time overheads
  - WMS that use RO-Crate (Galaxy, Nextflow, Streamflow, Sapporo, Autosubmit)
- Our 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

- Future Work
  - File checksums
  - Integration with other systems supporting RO-Crate: WfExS, ROHub
  - Improve automatic reproducibility through the PyCOMPSs CLI
  - Extract knowledge from metadata

LIVE DEMO WITH WORKFLOWHUB

eFlows4HPC

Enabling dynamic and Intelligent workflows
in the future EuroHPC ecosystem

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

www.eFlows4HPC.eu

@eFlows4HPC eFlows4HPC Project

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