Introduction to the eFlows4HPC software stack and HPC Workflows as a Service methodology

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Agenda

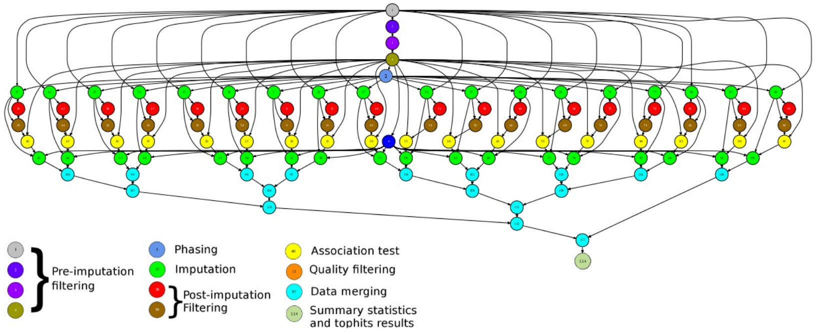
9:00 – 9:15	Overview of eFlows4HPC project and tutorial agenda	Rosa M Badia (BSC)
9:15 - 9:35	Part 1.1: Integrating different computations in PyCOMPSs	Rosa M Badia (BSC)
9:35 – 10:05	Part 1.2: HPC ready container images	Jorge Ejarque (BSC)
10:05 - 10:35	Part 1.3: Data Pipelines and Data Logistics Service (DLS)	Jedrzej Rybicki (JSC)
10:35 - 10:55	Part 1.4: TOSCA Orchestration and HPCWaaS	Jorge Ejarque (BSC)
10:55 – 11:00	Conclusion of part 1	Rosa M Badia (BSC)
11:00 - 11:30	Coffee break	
11:30 - 12:05	Part 2.1: Hands-on session: How to build HPC Ready containers	Jorge Ejarque (BSC)
12:05 - 12:30	Part 2.2: Hands-on session: How to move data with the DLS	Jedrzej Rybicki (JSC)
12:30 - 12:45	Part 2.3: Video demonstrating deployment with Allien4Cloud	
12:45 - 13:00	Tutorial conclusions	all presenters

PART 1.1: INTEGRATING DIFFERENT COMPUTATIONS IN PYCOMPSS

Main element: Workflows in PyCOMPSs

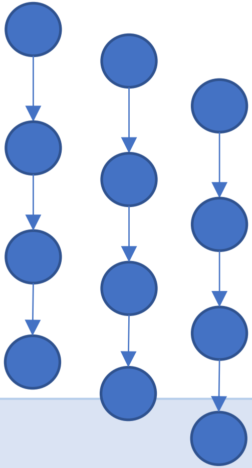
- Sequential programming, parallel execution
- General purpose programming language + annotations/hints
  - To identify tasks and directionality of data
- Builds a task graph at runtime that express potential concurrency
- Tasks can be sequential and parallel (threaded or MPI)
- Offers to applications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

```
@task(c=INOUT)
def multiply(a, b, c):
    c += a*b
```



PyCOMPSs syntax

- Use of **decorators** to annotate tasks and to indicate arguments directionality
- Small API for data synchronization



Tasks definition

```
@task(c=INOUT)
def multiply(a, b, c):
    c += a*b
```

Main Program

```
initialize_variables()
startMulTime = time.time()
for i in range(MSIZE):
    for j in range(MSIZE):
        for k in range(MSIZE):
            multiply (A[i][k], B[k][j], C[i][j])
compss_barrier()
mulTime = time.time() - startMulTime
```

Synchronization

- Main program and tasks do not share the same memory spaces
- The synchronization compss_wait_on waits for tasks generating the parameter to be finished and moves the data from the remote node to the node where the main program is executed:

```
a = compute (b)
#compute is a task, here we can not check the value of a
...
a = compss_wait_on (a)
#here we can check the value of a
if a:
    ...
```

- Tasks can be also synchronized with a barrier

```
startMulTime = time.time()
for i in range(SIZE):
    compute (A[i], B[i])
compss_barrier()
mulTime = time.time() - startMulTime
```

Other decorators: Tasks’ constraints

- Constraints enable to define HW or SW features required to execute a task
  - Runtime performs the match-making between the task and the computing nodes
  - Support for multi-core tasks and for tasks with memory constraints
  - **Support for heterogeneity on the devices in the platform**

```
@constraint (MemorySize=6.0, ProcessorPerformance=“5000”, ComputingUnits=“8”)
@task (c=INOUT)
def myfunc(a, b, c):
    ...
```

```
@constraint (MemorySize=1.0, ProcessorType =”ARM”, )
@task (c=INOUT)
def myfunc_other(a, b, c):
    ...
```

Failure Management

- Interface than enables the programmer to give hints about failure management

```
@task(file_path=FILE_INOUT,
on_failure='CANCEL_SUCCESSORS',
time_out='$task_timeout')
def task(file_path):
    ...
    if cond :
        raise Exception()
```

- Options: RETRY, CANCEL_SUCCESSORS, FAIL, IGNORE
- Implications on file management:
  - I.e., on IGNORE, output files: are generated empty
- **Possibility of ignoring part of the execution of the workflow, for example if a task fails in an unstable device**
- **Opens the possibility of dynamic workflow behaviour depending on the actual outcome of the tasks**

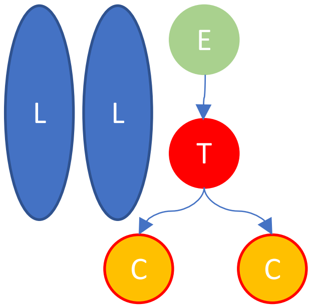
- Tasks can raise exceptions

```
@task(file_path=FILE_INOUT)
def comp_task(file_path):
    ...
    raise COMPSsException("Exception raised")
```

- Combined with groups of tasks enables to cancel the group of tasks on the occurrence of an exception

```
def test_cancellation(file_name):
    try:
        with TaskGroup('failedGroup'):
              long_task(file_name)
              long_task(file_name)
              executed_task(file_name)
              comp_task(file_name)
              cancelledTask(FILE_NAME);
              cancelledTask(FILE_NAME)

except COMPSsException:
        print("COMPSsException caught")
        write_two(file_name)
```



Other decorators: linking with other programming models

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- A task can be more than a sequential function
  - A task in PyCOMPSs can be sequential, multicore or multi-node
  - External binary invocation: wrapper function generated automatically
  - Supports for alternative programming models: MPI and OmpSs
- Additional decorators:
  - @binary(binary=“app.bin”)
  - @mpi(binary=“mpiApp.bin”, runner=“mpirun”, processes=8)
  - @ompss(binary=“ompssApp.bin”)
- Can be combined with the @constraint and @implement decorators

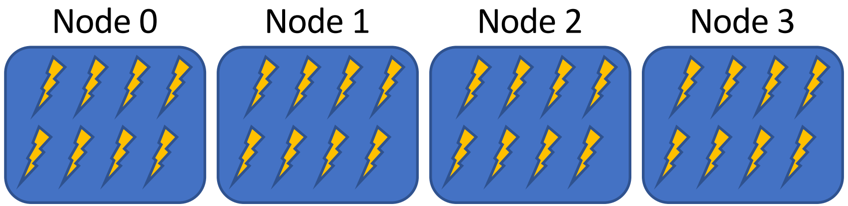
```
@binary(binary="app.bin", workingDir="/myApp")
@task()
def func(l):
    pass
```

Support for MPI tasks

- Resource manager aware of multi-node tasks

```
@mpi (runner="mpirun", processes= ”32”, processes_per_node=8)
@task (returns=int, stdOutFile=FILE_OUT_STDOUT, stdErrFile=FILE_OUT_STDERR)
def nems(stdOutFile, stdErrFile):
    pass
```

Launches MPI execution with
32 processes
8 processes per node



MPMD applications

- The @mpmd_mpi decorator can be used to define Multiple Program Multiple Data (MPMD) MPI tasks

```
@mpmd_mpi(runner="mpirun", working_dir = {{working_dir_exe}},
          programs=[{binary="fesom.x", processes = "$FESOM_PROCS" },
                    {binary="oifs", args="-v ecmwf -e awi3", processes = "$OIFS_PROCS" },
                    {binary="rnfma", processes = "$RNFMA_PROCS"}])
@task(log_file={Type:FILE_OUT, StdIOStream:STDOUT}, working_dir_exe=DIRECTORY_INOUT)
def esm_simulation(log_file, working_dir_exe):
   pass
```

- As a result of the @mpmd_mpi annotation, the following commands will be generated:

```
> cd working_dir_exe; mpirun -n $FESOM_PROCS fesom.x : \
     -n $OIFS_PROCS oifs -v ecmwf -e awi3 : -n $RNFMA_PROCS rnfma
```

Tasks in container images

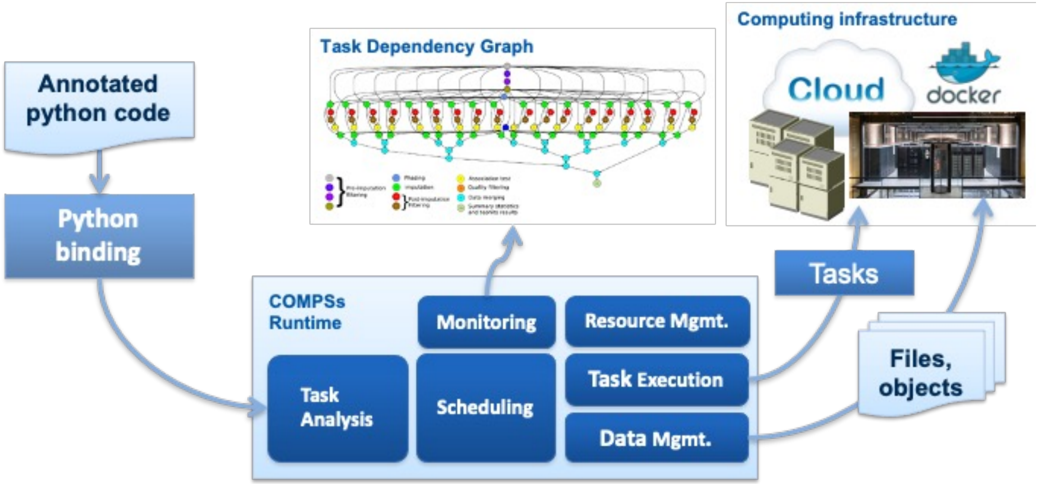
- Goal: enable tasks embedded in container images
- New @container decorator to be used together with the task annotation
- Also supports user-defined tasks

```
@container(engine="DOCKER", image="ubuntu")
@binary(binary="ls")
@task()
def task_binary_empty():
    pass
```

```
@container(engine="DOCKER", image="compss/compss")
@task(returns=1, num=IN, in_str=IN, fin=FILE_IN)
def task_python_return_str(num, in_str, fin):
    print("Hello from Task Python RETURN")
    print("- Arg 1: num -- " + str(num))
    print("- Arg 1: str -- " + str(in_str))
    print("- Arg 1: fin -- " + str(fin))
    return "Hello"
```

PyCOMPSs runtime

- Support for tasks' constraints – support for heterogeneous infrastructure
- Support for tasks' faults and tasks' exceptions
    - Enlarges the dynamicity of the type of workflows that we support
- Streamed data
    - ... and many others
- Runtime deployed as a distributed master-worker
- All data scheduling decisions and data transfers are performed by the runtime
- Support for elasticity



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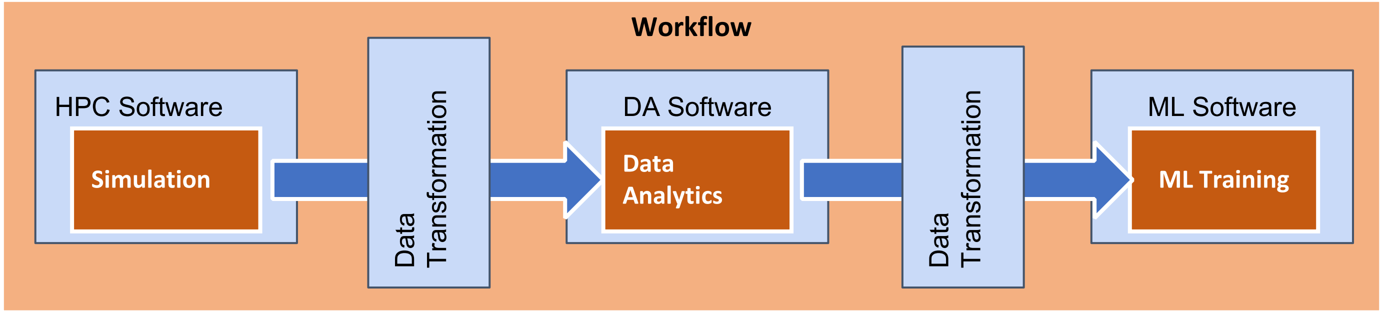
Interfaces to integrate HPC/DA/ML



- **Goal:**
  - Reduce the required glue code to invoke multiple complex software steps
  - Developer can focus in the functionality, not in the integration
  - Enables reusability
- **Two paradigms:**
  - Software invocation
  - Data transformations

```
#workflow steps defined as tasks
@data_transformation (input_data, transformation description)
@software (invocation description)
def data_analytics (input_data, result):
    pass

#workflow body
simulation (input_cfg, sim_out)
data_analytics (sim_out, analysis_result)
ml_training (analysis_result, ml_model)
```

Software Invocation description

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Admin/user code

```
{
  "type":"mpi",
  "properties":{
    "runner": "mpirun",
    “processes”: “$SW_PROCS”
    "binary": "mpi_sofware.x",
    "params": "-d {{param}}",
    “working_dir”: “{{working_dir}}”},
  "prolog":{
     "binary":"mkdir",
     "params":"{{working_dir}}"},
   "epilog":{
     "binary":"tar",
     "params":"zcvf {{out_tgz}}" {{working_dir}}},
  "constraints":{
    "computing_units": $SW_THREADS}
}
```

Software invocation description
Stored in software catalog

Workflow Code

PyCOMPSs Code

User code

```
#workflow steps defined as tasks
@software(config_file="invocation.json")
def mpi_exec(work_dir, param, out_tgz):
    pass


#workflow body
...
mpi_exec('my_folder', 'hello_world’)
...
```

Computing Infrastructure

COMPSs runtime → Software Invocation

Automatically generated

```
mkdir working_dir
cd working_dir
export OMP_NUM_THREADS=$SW_THREADS
mpirun -n $SW_PROCS mpi_software.x -d param
tar zcvf out_tgz working_dir
```

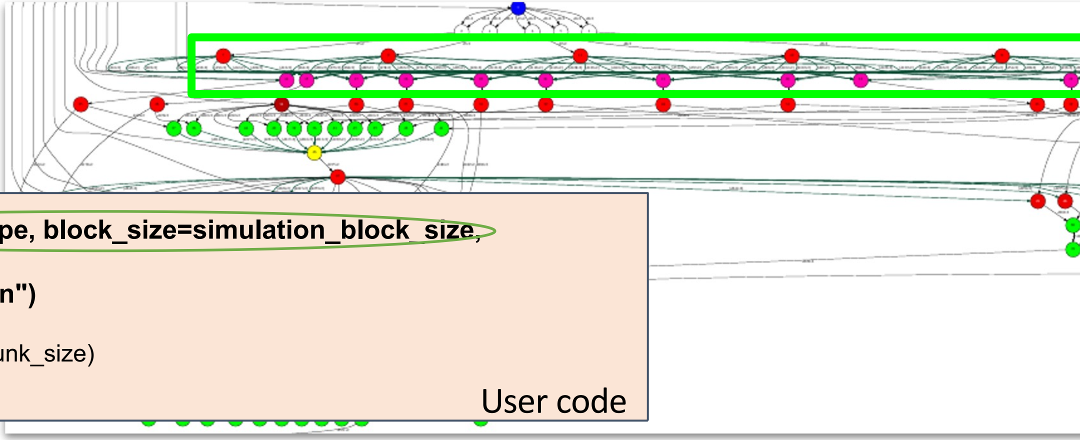
- Converts a Python function of a software invocation to a PyCOMPSs task
- Takes information from the description in json
- Enables reuse in multiple workflows

Data transformations

- **A data transformation changes the data without requiring extra programming from the developer**

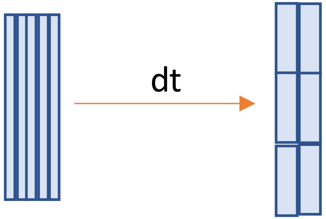
Admin/user code

```
def load_blocks_rechunk(blocks, shape, block_size, new_block_size):
    ...
    SnapshotMatrix = load_blocks_array (final_blocks, shape, block_size);
    return SnapshotMatrix
```



```
@dt("blocks", load_blocks_rechunk, shape=expected_shape, block_size=simulation_block_size,
  new_block_size=desired_block_size, is_workflow=True)
@software(config_file = SW_CATALOG + "/dislib/dislib.json")
def rSVD(blocks, desired_rank=30):
    u,s = rsvd(blocks, desired_rank, A_row_chunk_size, A_column_chunk_size)
    return u
```

User code

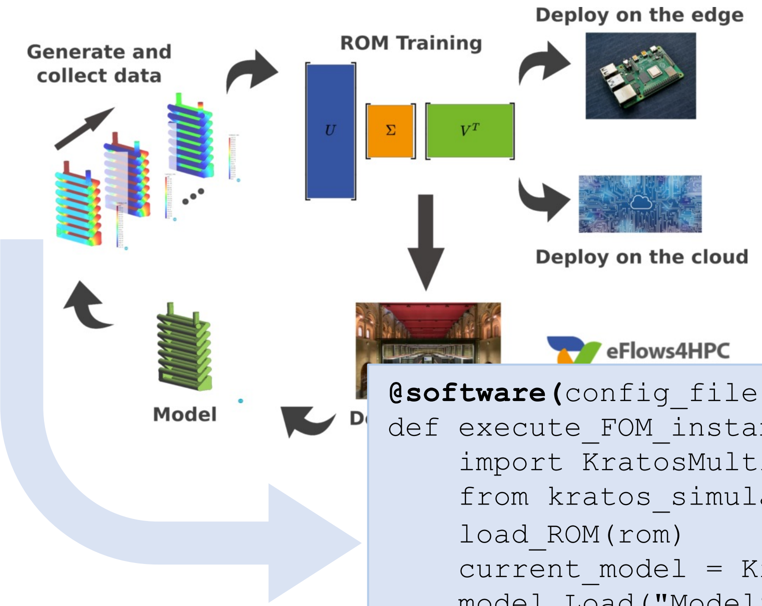



```
...
model, parameters = load_model_parameters(model_file)
for cfg in sim_cfgs:
        sim_results.append(execute_FOM_instance(model,parameters,[cfg]))
rom = rSVD(sim_results, desired_rank)
...
```

User code

Main workflow program

Pillar I: Integration of HPC and data ana... workflow



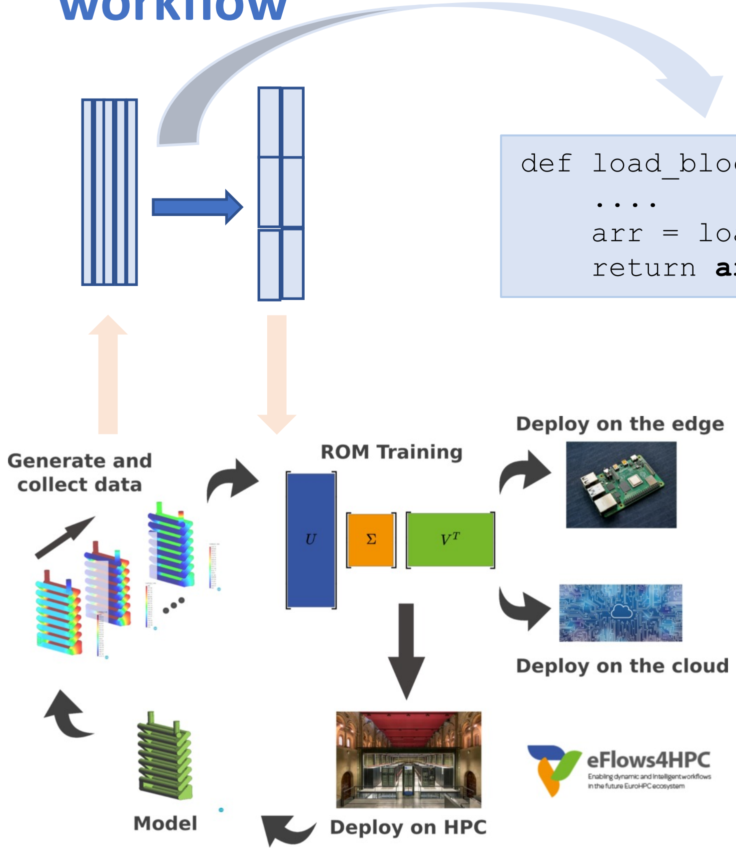
fom.json

```
{
    "execution" : {
        "type":"task"
    },
    "constraints" : {
        "computing_units": "$KRATOS_CUS"
    },
    "parameters" : {
        "returns" : 1,
        "model" : "IN",
        "parameters" : "IN",
        "sample" : "IN"
    }
}
```

```
@software(config_file = SW_CATALOG+"/kratos/fom.json")
def execute_FOM_instance(model,parameters, sample):
    import KratosMultiphysics
    from kratos_simulations import RunROM_SavingData
    load_ROM(rom)
    current_model = KratosMultiphysics.Model()
    model.Load("ModelSerialization",current_model)
    del(model)
    current_parameters = KratosMultiphysics.Parameters()
    parameters.Load("ParametersSerialization",current_parameters)
    del(parameters)
    simulation = RunROM_SavingData(current_model,current_parameters,sample)
    simulation.Run()
    return simulation.GetSnapshotsMatrix()
```

Pillar I: Integration of HPC and data analytics in a single workflow

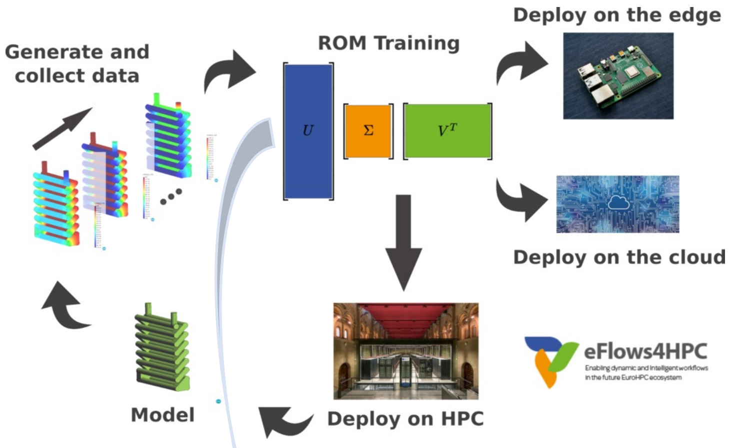
fom.json




```
def load_blocks_rechunk(blocks, shape, block_size, new_block_size):
    ....
    arr = load_blocks_array(final_blocks, shape, block_size)
    return arr.rechunk(new_block_size)
```

Dislib method that re-partitions a set of blocks into a new ds-array of the given block size

Pillar I: Integration of HPC and data analytics in a single workflow



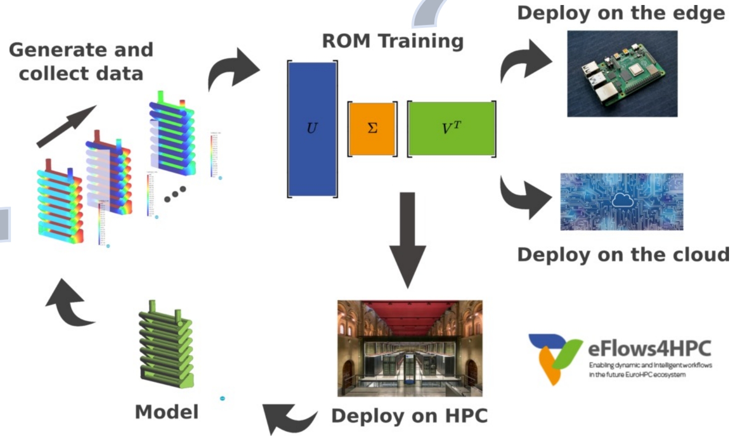
dislib.json

```
{
        "execution": {
                "type":"workflow"
        }
}
```

Method that invokes other PyCOMPSs tasks inside

```
@dt("blocks", load_blocks_rechunk, shape=expected_shape,
block_size=simulation_block_size, new_block_size=desired_block_size,
is_workflow=True)
@software(config_file = SW_CATALOG + "/py-dislib/dislib.json")
def rSVD(blocks, desired_rank=30):
    from dislib_randomized_svd import rsvd
    u,s = rsvd(blocks, desired_rank, A_row_chunk_size, A_column_chunk_size)
    return
```

Pillar I: Integration of HPC and data analytics in a single workflow




```
import dislib as ds

@dt("blocks", load_blocks_rechunk, shape=expected_shape,
block_size=simulation_block_size,new_block_size=desired_
is_workflow=True)
@software(config_file = SW_CATALOG + "/dislib/dislib.jso
def rsvd(blocks, desired_rank):
    k = desired_rank
    ...
    Y = A @ Omega
    Q,R = my_qr(Y._blocks)
    Q=load_blocks_rechunk([Q], ...)
    ...
```

```
@software(config_file=kratos.json)
def ExecuteInstance (model, parameters, Cases, instance):
    ...
    current_paramete
    ...
    simulation = Get
    simulation.Run()
    return simulatio
```

```
....
for instance in range (0,TotalNumberOFCases):
    blocks.append(ExecuteInstance(model, parameters, pars, instance))
...
U, s = rSVD(A, desired_rank)
...
```

eFlows4HPC

Enabling dynamic and Intelligent workflows in the future EuroHPC ecosystem

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