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Programming complex workflows with PyCOMPSs

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CEEC webinar, December 16 2024

CEEC

Centre of Excellence in Exascale CFD

EuroHPC JU systems

	Status	Country	Peak performance	Architecture
Pre-Exascale				
LUMI	Operational	Finland	539.13 petaflops	64-core AMD EPYC™ CPUs + AMD Instinct™ GPU
Leonardo	Operational	Italy	315.74 petaflops	Intel Ice-Lake, Intel Sapphire Rapids + DIA Ampere
MareNostrum 5	Operational	Spain		Sapphire Rapids, NVIDIA Hopper, A Grace, Intel Emeralds, Intel
Petascale				
Meluxina	Op			MD EPYC + NVIDIA Ampere A100
Vega	Oper		10.05 petaflops	AMD Epyc 7H12 + Nvidia A100
Karolina	Opera	zech Republic	12.91 petaflops	AMD + Nvidia A100
Discoverer	Operational	Bulgaria	5.94 petaflops	AMD EPYC
Deucalion	Operational	Portugal	5.01 petaflops	A64FX, AMD EPYC, Nvidia Ampere

JUPITER, First European Exascale Supercomputer to be installed in Jülich, Germany

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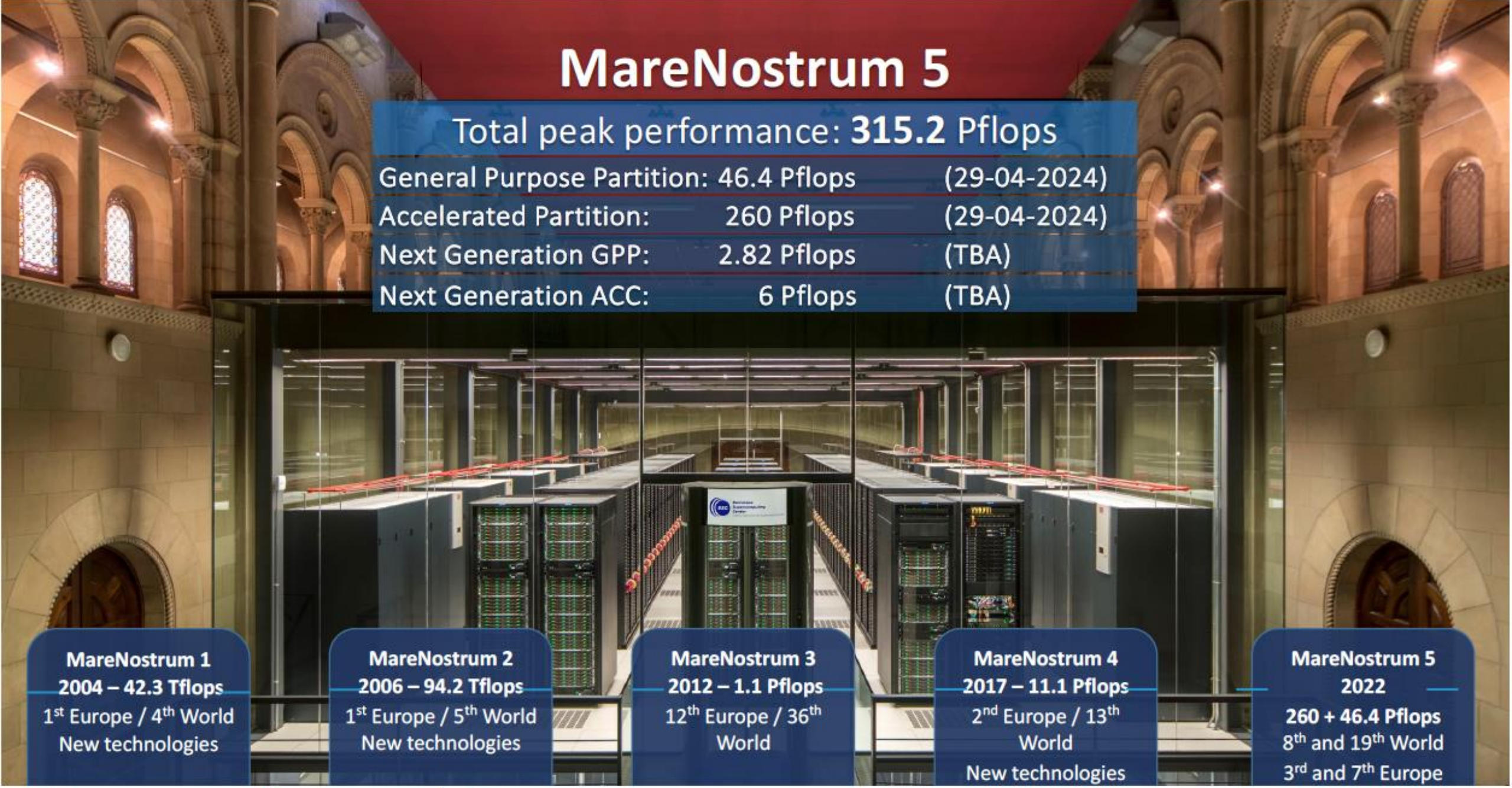
https://eurohpc-ju.europa.eu/about/our-supercomputers_en

MareNostrum 5

Total peak performance: **315.2** Pflops		
General Purpose Partition:	46.4 Pflops	(29-04-2024)
Accelerated Partition:	260 Pflops	(29-04-2024)
Next Generation GPP:	2.82 Pflops	(TBA)
Next Generation ACC:	6 Pflops	(TBA)



MareNostrum 1
2004 – 42.3 Tflops
1st Europe / 4th World
New technologies

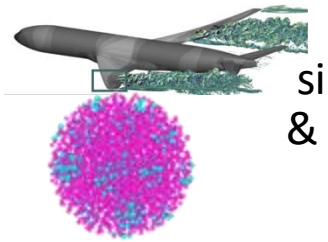
MareNostrum 2
2006 – 94.2 Tflops
1st Europe / 5th World
New technologies

MareNostrum 3
2012 – 1.1 Pflops
12th Europe / 36th World

MareNostrum 4
2017 – 11.1 Pflops
2nd Europe / 13th World
New technologies

MareNostrum 5
2022
260 + 46.4 Pflops
8th and 19th World
3rd and 7th Europe

Complex problems for complex computing infrastructures

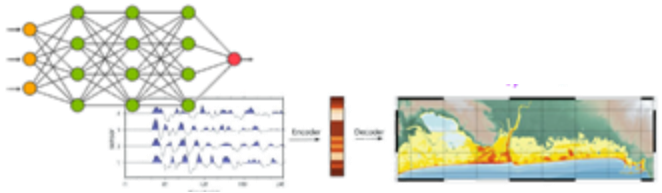


HPC simulation & modeling

Data analytics

COMPLEX PROBLEMS

Artificial intelligence



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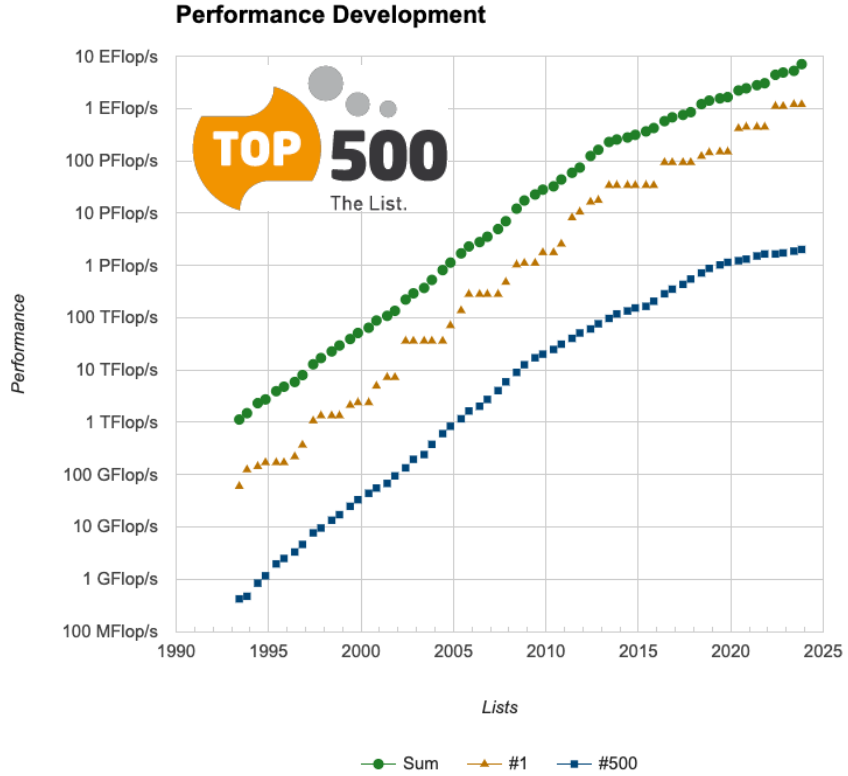
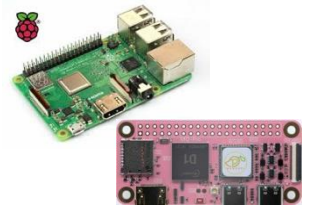
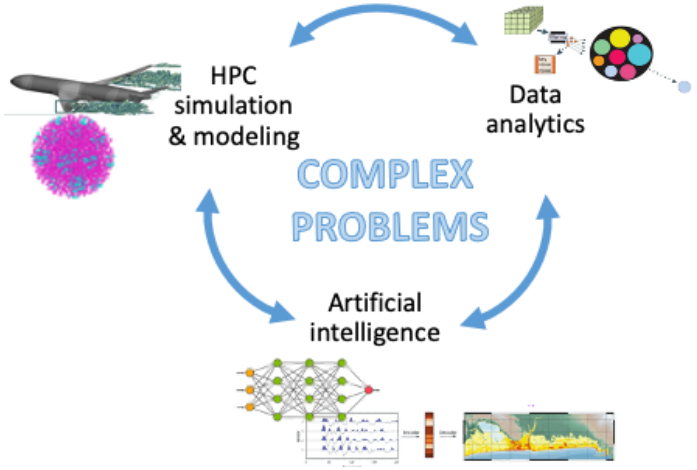


Digital continuum

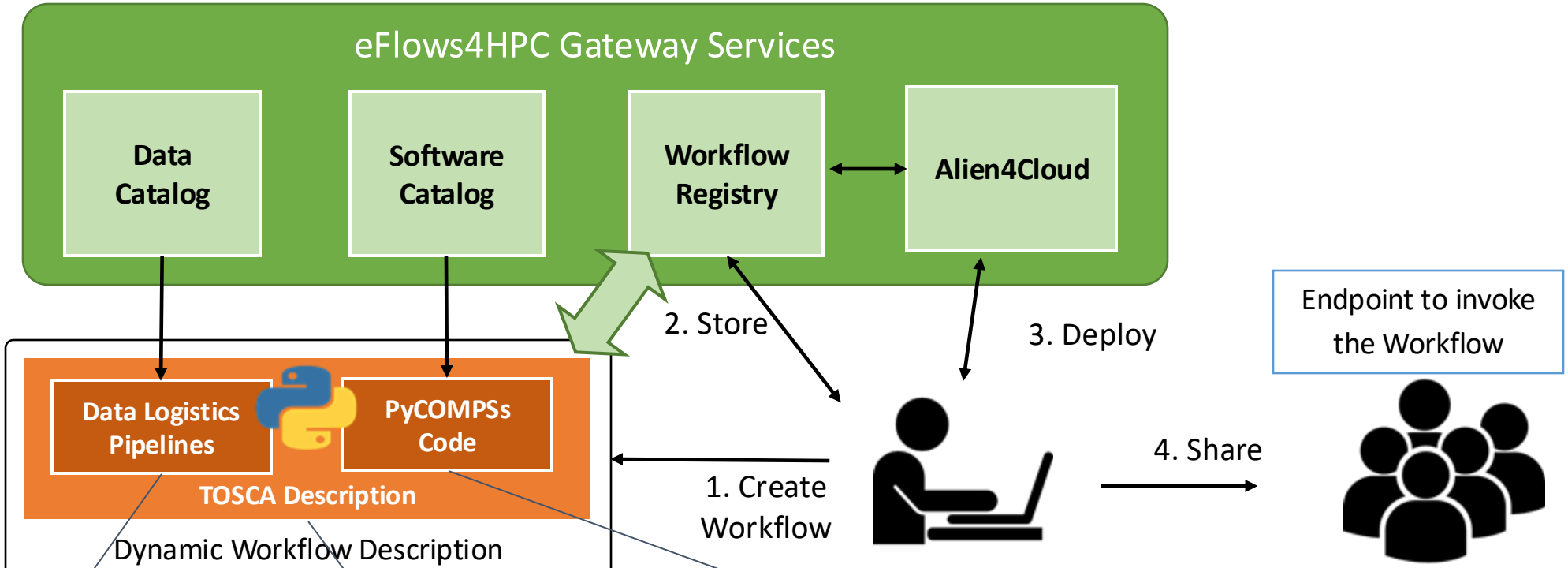


Workflow lifecyle challenges



- Workflow development
  - Different programming models and environments
- Workflow deployment
  - Can we make it easier to new HPC users?
- Workflow operation
  - Go beyond static workflows
  - Not only computational aspects, data management as well

HPCWaaS: Workflow lifecycle overview



Description of data movements as Python functions. Input/output datasets described at Data Catalog

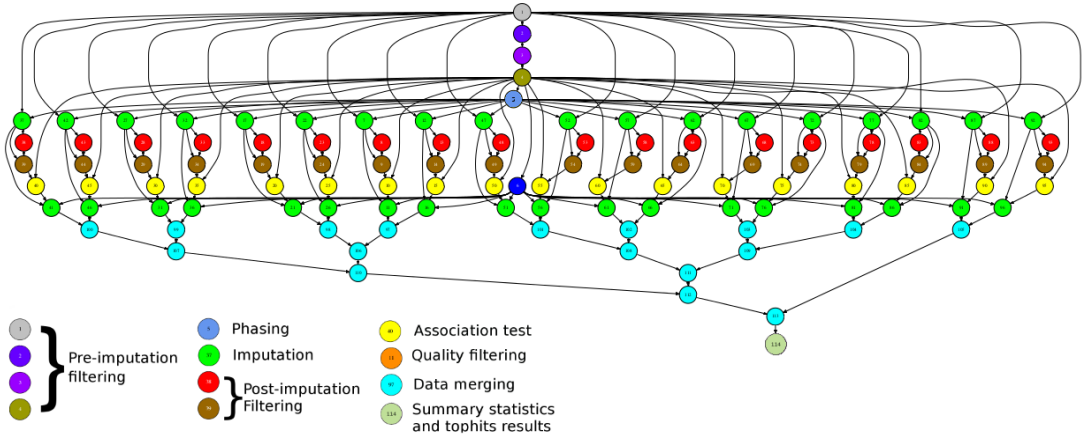
Computational Workflow as a simple Python script. Invocation of software described in the Software Catalog

Topology of the components involved in the workflow lifecycle and their relationship.

Workflows' development with PyCOMPSs

- Sequential programming, parallel execution
  - General purpose programming language + annotations/hints
- Task-based parallelization
  - Automatic generation of task graph
  - Coarse grain tasks: methods and web services
  - Sequential and parallel tasks
- Offers a shared memory illusion in a distributed system
  - Can address larger dataset than storage space
- Agnostic of computing platform
  - Clusters, clouds and cluster containers

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



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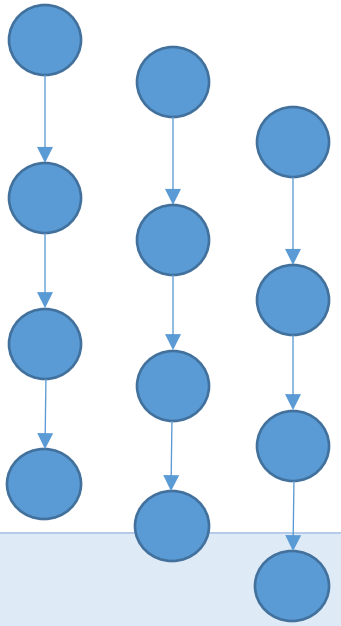
PyCOMPSs syntax

- 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:
    ...
```

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

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):
    ...
```

Linking with other programming mode

- 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

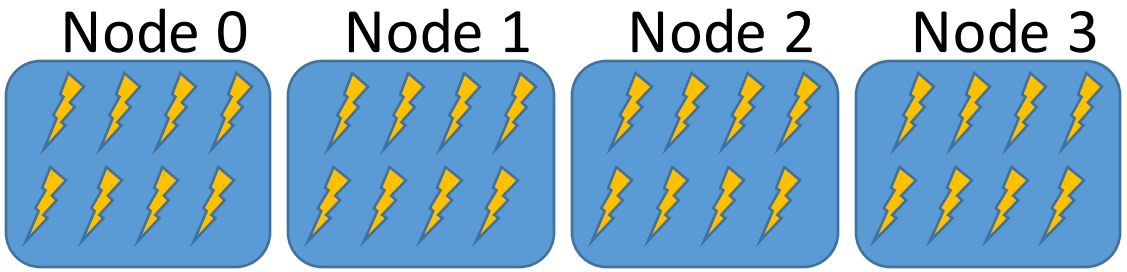
```
@binary(binary="app.bin", workingDir="/myApp")
@task()
def func(l):
    pass
```

Support for MPI tasks

- Resource manager aware of multi-node tasks

```
@mpi (binary=”mySimulator”, 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
  - @container decorator can be used together with the task annotation
  - Also support for 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"
```

Support for data streams

- Interface to support streaming data in tasks
- Task-flow and data-flow tasks live together in PyCOMPSs/COMPSs workflows
- Data-flow tasks persist while streams are not closed
  - Parameters can be one/multiple streams and non-streamed
- Runtime implementation based on Kafka

```
@task(fds=STREAM_OUT)
def sensor(fds):
        ...
    while not end():
        data = get_data_from_sensor()
        f.write(data)
    fds.close()
```

```
@task(fds_sensor=STREAM_IN, filtered=OUT)
def filter(fds_sensor, filtered):
        ...
    while not fds_sensor.is_closed():
        get_and_filter(fds_sensor, filtered)
```

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**

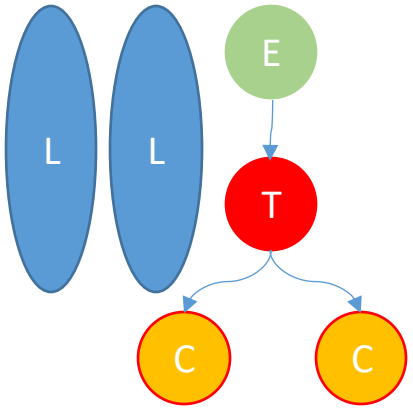
Timeouts and exceptions

- Timeouts can be defined for a task

```
@task(file_path=FILE_IN, time_out=200)
def time_out_task (file_path):
    ...
```

- Tasks can raise exceptions

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



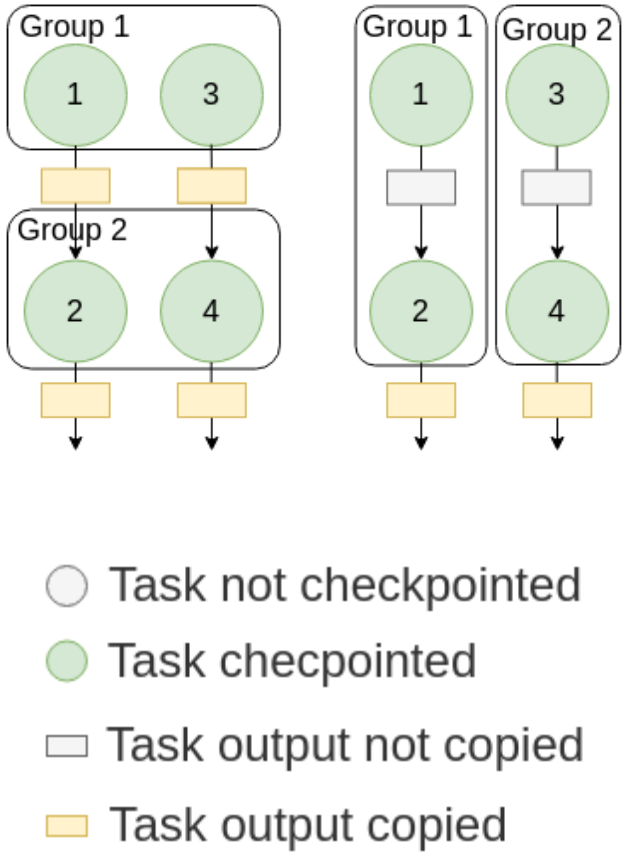
- Combined with groups of tasks enables to cancel the group of tasks on the occurrence of an exception

```
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)
```

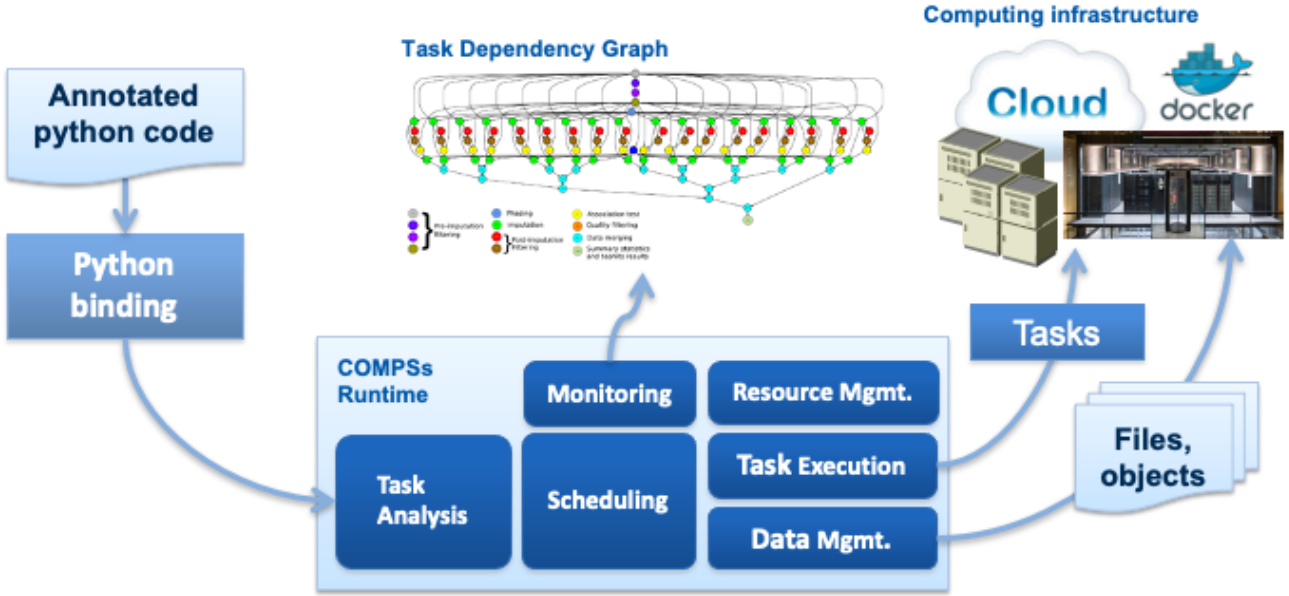
Checkpointing

- Allows the workflow re-execution avoiding the re-execution of finished tasks
- Asynchronous but may have some overhead
  - Save tasks results in a persistent storage
  - Trade-off between performance and time to recover
  - Establishing the right checkpoint granularity is important
- 3 mechanisms for automatic checkpointing
  - **Time:** periodically, COMPSs saves the last version produced for every value
  - **Finished tasks** : after the completion of X tasks, COMPSs saves the last version produced for every value
  - **Instantiation task groups**: Defines groups of tasks, COMPSs saves those data versions that are final results for the group
- Indicated by the developer using a provided API call `compss_snapshot()`
- No checkpoint inside the task: drawback for very large tasks.
  - Possible integration with internal checkpointing



PyCOMPSs features and runtime

- PyCOMPSs/COMPSs applications executed in distributed mode following the master-worker paradigm
  - Description of computational infrastructure in an XML file
- Sequential execution starts in master node and tasks are offloaded to worker nodes
- In clusters, whole COMPSs application deployed as a job allocation
- All data scheduling decisions and data transfers are performed by the runtime
- All data scheduling decisions and data transfers are performed by the runtime



Workflow examples

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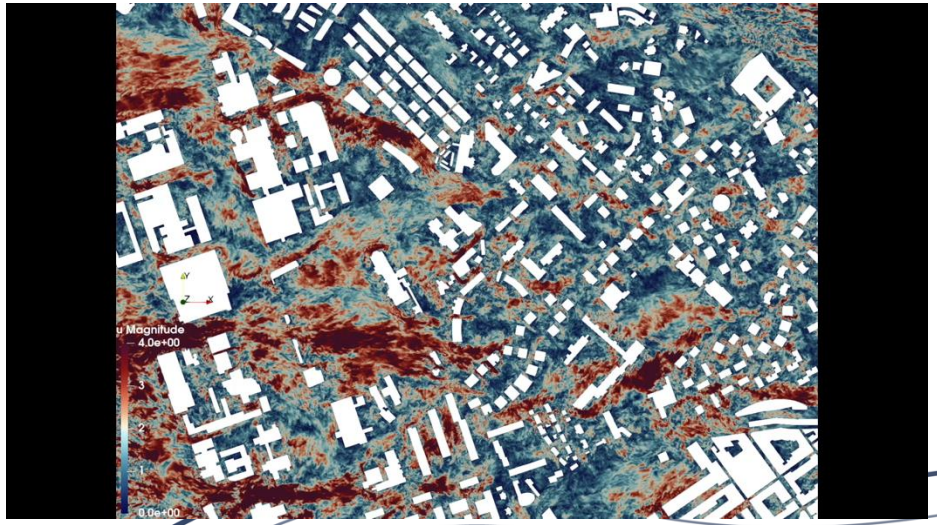
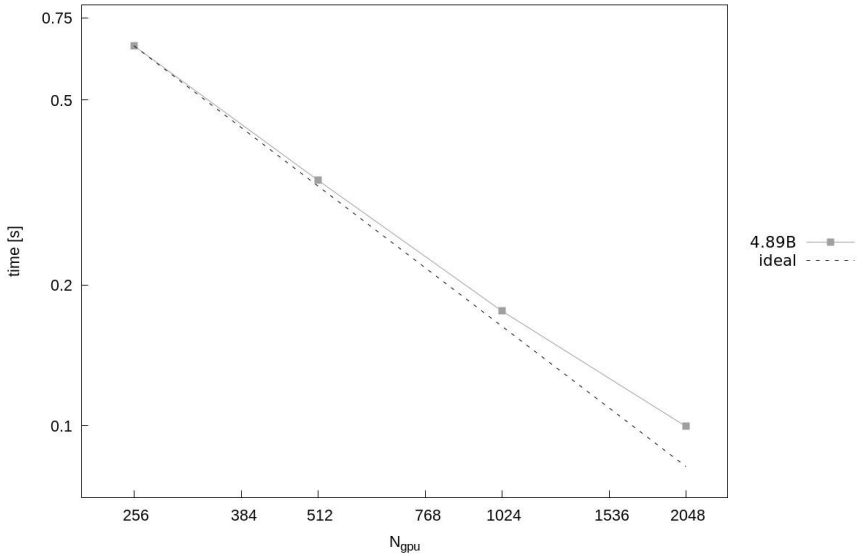
SOD2D: Spectral high-Order coDe 2 solve partial Differential equations*

- Language: Fortran
- GPU port path: OpenACC
- Required libs: HDF5, MPI
- Compressible and incompressible flows
- Git repo: https://gitlab.com/bsc_sod2d/sod2d_gitlab/
- … and btw, the code is 3D!

SOD2D: **S**pectral high-**O**rder co**D**e 2 solve partial **D**ifferential equations



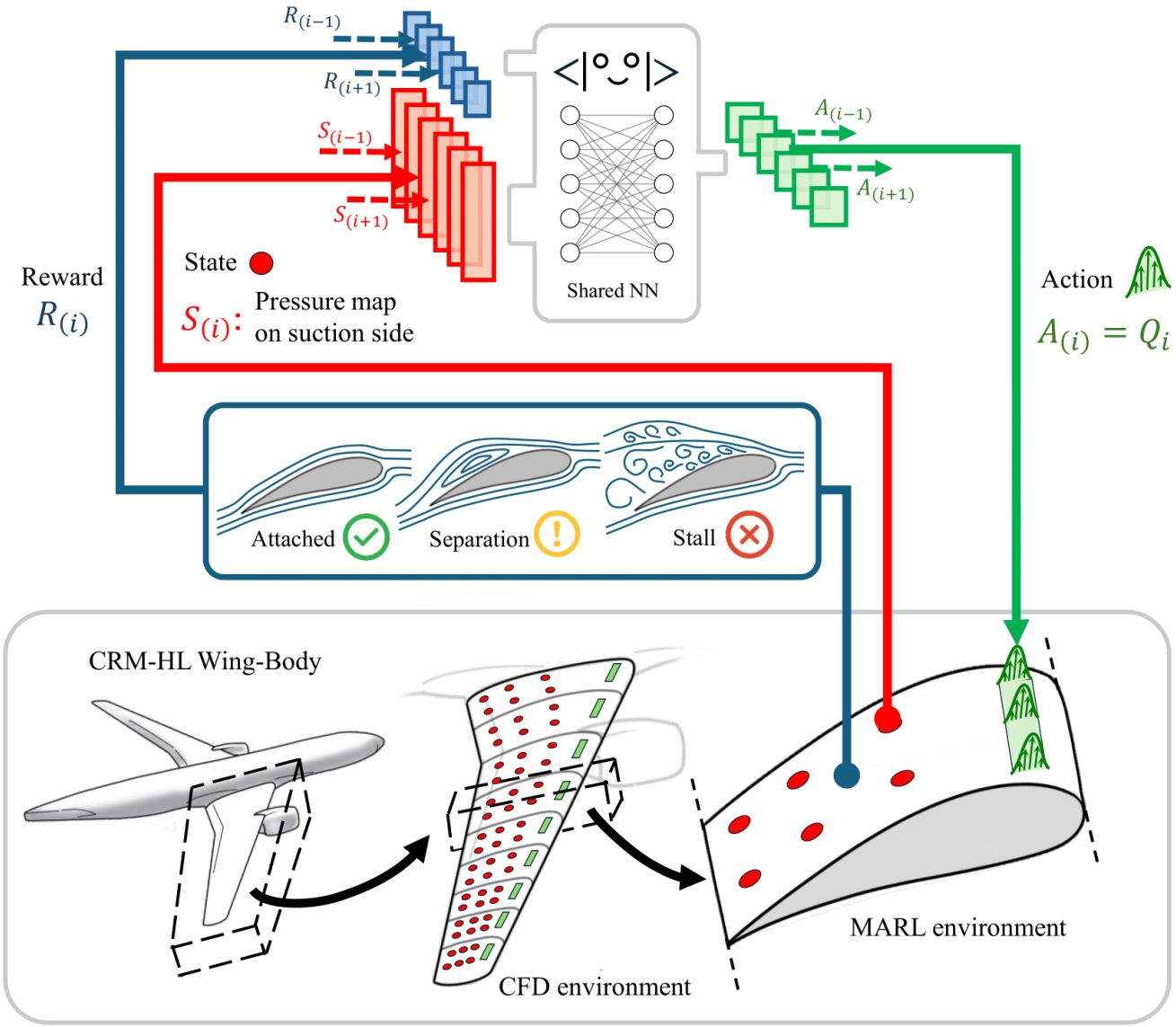
wmLES of the campus Nord of UPC, using 64 H100 and 500M DoF



Scalability of SOD2D in MN5

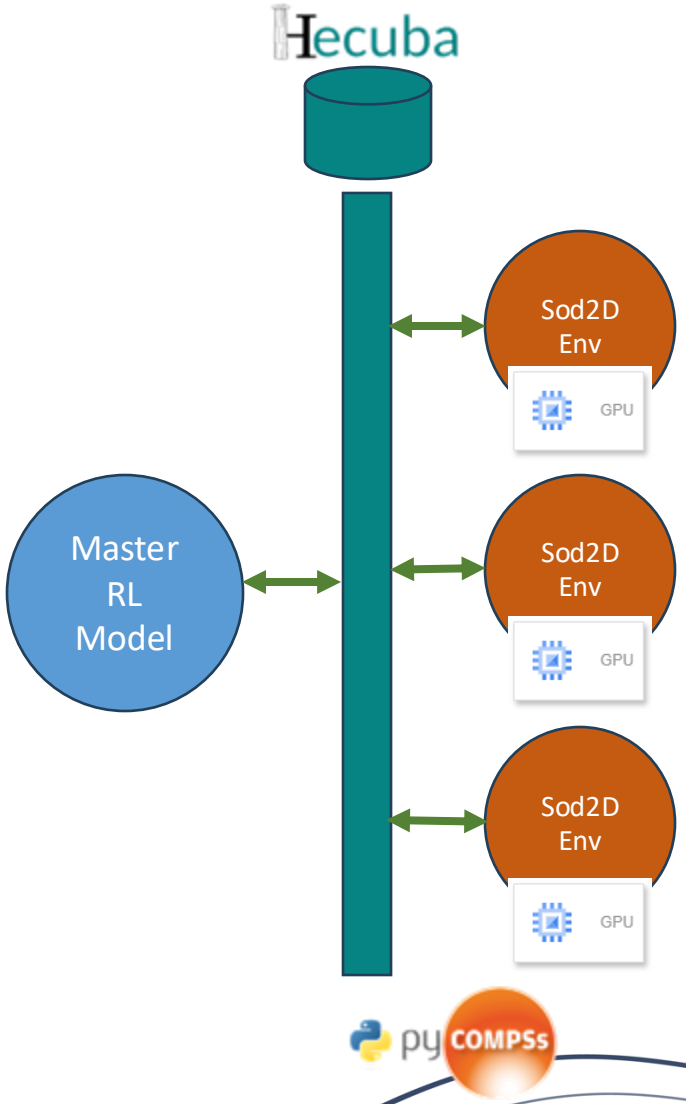
Paper: *https://doi.org/10.1016/j.cpc.2023.109067*
**Oriol Lehmkuhl (BSC) et al.*

The CEEC challenge



- Research in automatic ways to control the aerodynamic performance of aircrafts under dynamic extreme events
- Sod2D - RL model coupling using a multi-environment approach for accelerated training
  - Example: using 4 environments executed in 16 GPUs each
- Each environment sends its state and reward into the database
- The RL model reads state and reward and returns actions for each environment into the database
- Each environment reads the corresponding actions and advances the flow solution in time

Integration with PyCOMPSs and Hecuba




```
@constraint(processors=[
        {"processorType": "CPU", "computingUnits": "1"},
        {"processorType": "GPU", "computingUnits": "1"}
    ])
@mpi(
    binary="sod2d",
    runner="mpirun",
    processes=4,
    flags="-x SSOB={{db_address}} -x COMPSS_BINDED_GPUS",
    args="--restart_step={{restart_step}}
          --f_action={{f_action}}
          --t_episode={{t_episode}}
          --t_begin_control={{t_begin_control}}
          --tag={{tag}}"
)
@task()
def compss_sod2d(db_address, restart_step, faction, t_episode, t_begin_control, tag):
    pass
```

Integration with PyCOMPSs and Hecuba

Before: Redis

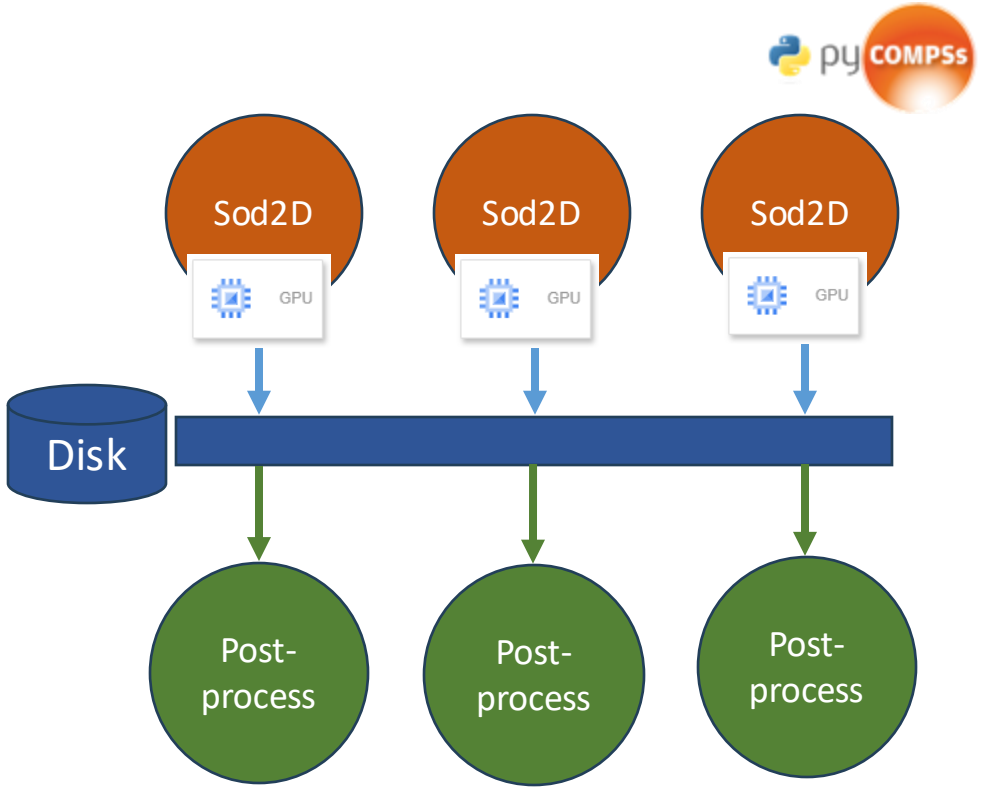
```
subroutine read_action(client, key)
   type(client_type), intent(inout) :: client
   character(len=*), intent(in) :: key ! actions name to read from database
   integer, parameter :: interval = 100 ! polling interval in milliseconds
   integer, parameter :: tries = 10000 ! huge(1) ! infinite number of polling tries
   logical :: exists ! receives whether the tensor exists
   logical :: is_error
   integer :: found, error

   ! wait (poll) until the actions array is found in the DB, then read, then delete
   if (mpi_rank .eq. 0) then
      found = client%poll_tensor(trim(adjustl(key)), interval, tries, exists)
      ! wait indefinitely for new actions to appear
      is_error = client%SR_error_parser(found)
      if (found /= 0) stop 'Error in SmartRedis read_action. Actions array not found.'
      error = client%unpack_tensor(trim(adjustl(key)), action_global, shape(action_global))
      is_error = client%SR_error_parser(error)
      if (error /= 0) stop 'Error in SmartRedis read_action. Tensor could not be unpacked.'
      error = client%delete_tensor(trim(adjustl(key)))
      is_error = client%SR_error_parser(error)
      if (error /= 0) stop 'Error in SmartRedis read_action. Tensor could not be deleted.'
   end if

   ! broadcast rank 0 global action array to all processes
   call mpi_bcast(action_global, action_global_size, mpi_datatype_real, 0, app_comm, error)
   !$acc update device(action_global(:))
end subroutine read_action
```

Hecuba hides the synchronization

Now: Hecuba

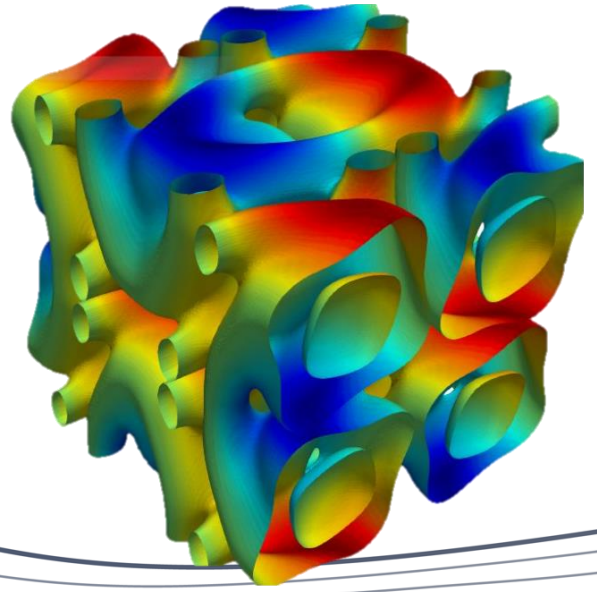
```
subroutine read_action_hecuba(client, key)
   character(len=*), intent(in) :: key ! actions name to read from database

   if (mpi_rank .eg. 0) then
      call hecuba_read_action(trim(adjustl(key)), action_global)
   end if

   ! broadcast rank 8 global action array to all processes
   call mpi_bcast(action_global, action _global_size, mpi_datatype_real, 0,
app_comm, error)
   !$acc update device(action_global(:))
end subroutine read_action_hecuba
```

CEEC Workflows: in-situ postprocessing of CFD simulations and visualization



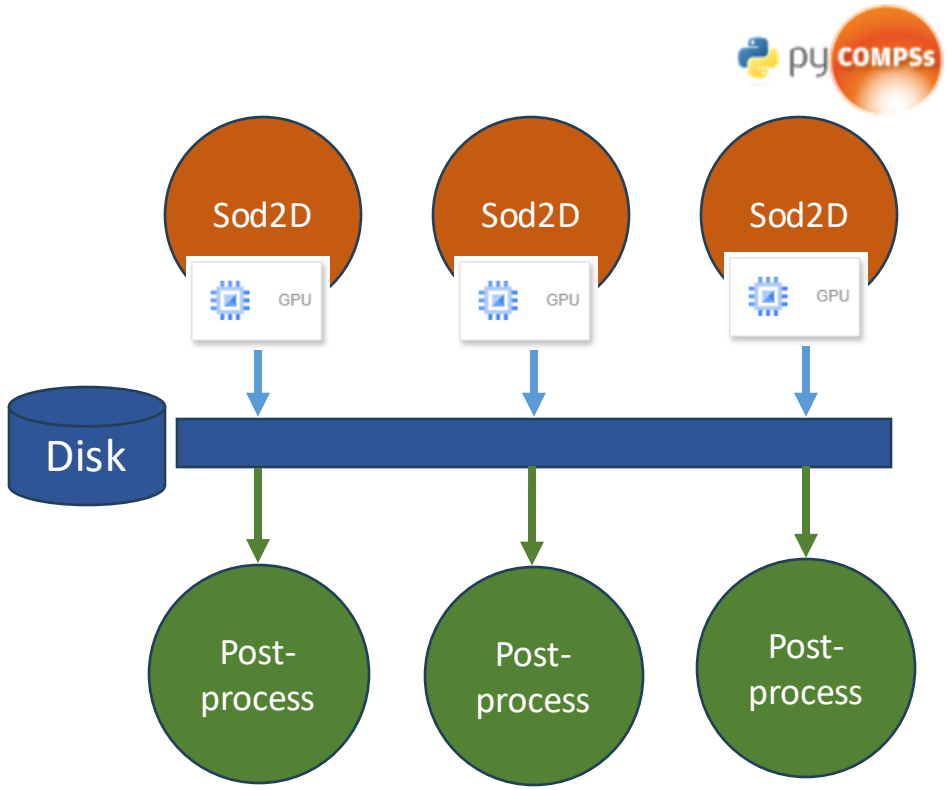
Q isocontours of a Taylor Green Vortex

- This postprocess includes:
  - Compute velocity gradients (with Gauss-Legendre-Lobatto quadrature)
  - Compute its second invariant (Q criterion)
  - Do isocontours of Q
  - Interpolate the velocity to the isocontours.

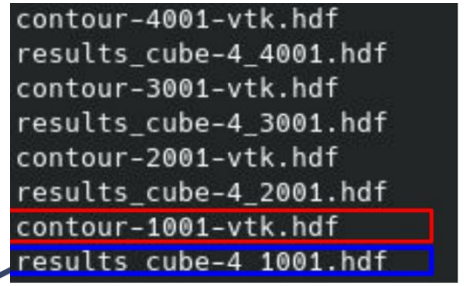


VIDEO

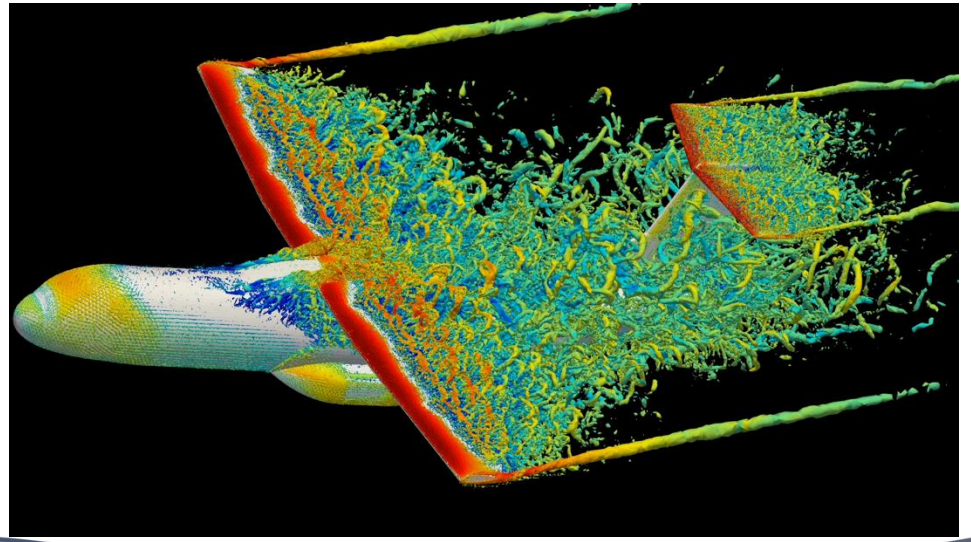
CEEC Workflows: in-situ postprocessing of CFD simulations and visualization



- Run CFD simulations using SOD2D on the GPU
- Uses stream interface of PyCOMPSs
- Every time a results file is saved, PyCOMPSs launches a task that postprocesses the results file:
  - Compute gradients of velocity
  - Q criterion isocontours
  - Extract slices of data
  - Plot over line



Postprocess file
Generated by SOD2D



wmLES simulation of a new concept Aircaft from Airbus, using 32 H100 and 200M DoF. Simulations carried out in the CDTI PTA 2023 (CETACEO) under the collaboration agreement between BSC and Airbus

CEEC Workflows: in-situ postprocessing of CFD simulations and visualization

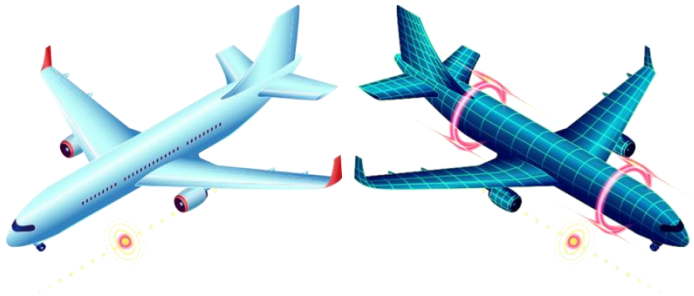

```
@constraint(processors=[{'processorType':'CPU', 'computingUnits':'$SOD2S_CORES_PER_PROC'},
                        {'processorType':'GPU', 'computingUnits':'1'}])
@mpi(runner="mpirun", flags="$SOD2D_MPI_FLAGS", binary="./sod2d", processes="$SOD2D_PROCS",
                    processes_per_node="$SOD2D_PPN", args="{{configuration}} {{fds}}",
          working_dir="{{working_dir}}")
@task(fds=STREAM_OUT)
def sod2d(fds, configuration, working_dir):
    pass
```

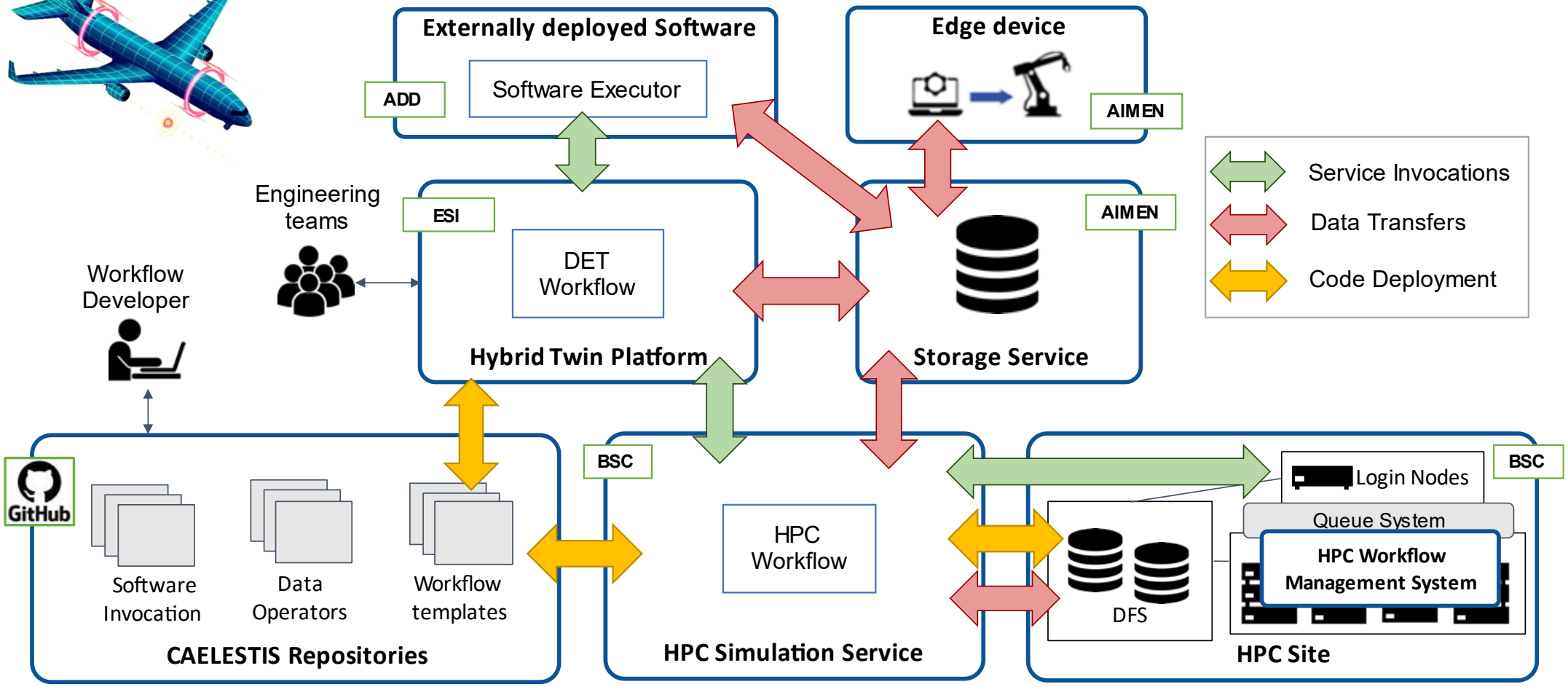
```
@constraint(computing_units="$VIZ_CORES_PER_PROC")
@mpi(runner="mpirun", binary="python", processes="$VIZ_PROCS", processes_per_node="$VIZ_PPN",
          args="{{script}} {{instant}}", working_dir="{{viz_dir}}")
@task()
def visualization(viz_dir, script, instant):
    pass
```

```
fds = FileDistroStream(base_dir=results_folder)
#run simulation
sod2d(fds, configuration, sod2d_workingdir)
while not fds.is_closed():
    new_files = fds.poll()
    #run a simulation for each created file
    for filename in new_files:
        visualization(viz_workingdir, filename)
```

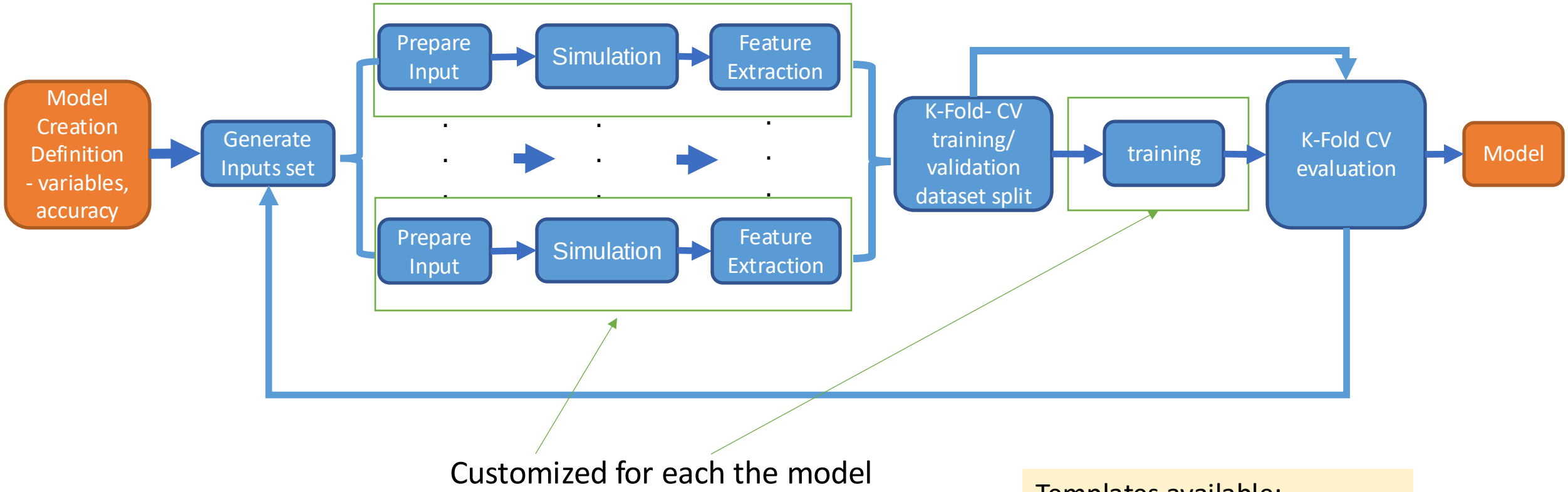

28

CAELESTIS Simulation Ecosystem Architecture





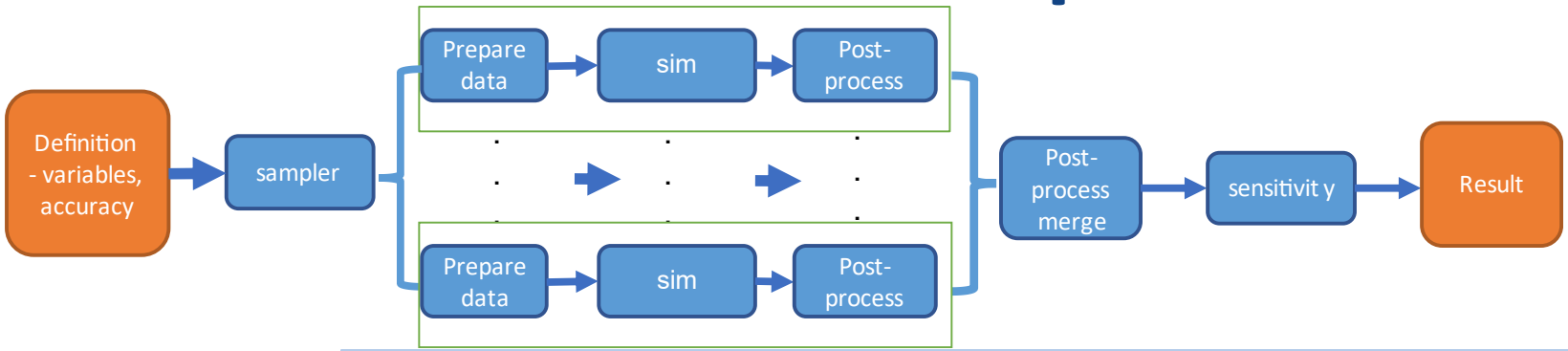
Workflow templates



Templates available:

- Sensitivity Analysis
- Uncertainty Quantification
- Model Training
- Monte Carlo

Workflow templates: main program



workflow.py

```
def execution(execution_folder, data_folder, phases, inputs, outputs, parameters):
    sample_set, problemDef = phase.run(phases.get("sampler"), inputs, outputs, parameters,  data_folder, locals())
    sample_set = compss_wait_on(sample_set)
    problemDef= compss_wait_on(problemDef)
    original_name_sim = parameters.get("original_name_sim")
    results_folder = execution_folder + "/results/"
    if not os.path.isdir(results_folder):
        os.makedirs(results_folder)
    write_file(results_folder, sample_set, "xFile.npy")
    y = []
    for i in range(sample_set.shape[0]):
        values = sample_set[i, :]
        name_sim = original_name_sim + "-s" + str(i)
        simulation_wdir = execution_folder + "/SIMULATIONS/" + name_sim + "/"
        prepare_out = phase.run(phases.get("prepare_data"), inputs, outputs, parameters, data_folder, locals())
        sim_out=phase.run(phases.get("sim"), inputs, outputs, parameters, data_folder, locals(), out=prepare_out)
        new_y = phase.run(phases.get("post_process"), inputs, outputs, parameters, data_folder, locals(), out=sim_out)
        y.append(new_y)
    out_post=phase.run(phases.get("post_process_merge"), inputs, outputs, parameters, data_folder, locals())
    write_file(results_folder, y, "yFile.npy")
    phase.run(phases.get("sensitivity"), inputs, outputs, parameters, data_folder, locals(), out=out_post)
    return
```

Workflow templates: phases

Simulation

```
@on_failure(management='IGNORE')
@mpi(runner="mpirun", binary="$ALYA_BIN", args="{{name_sim}}", processes=alya_procs,
processes_per_node=alya_ppn, working_dir="{{simulation_wdir}}")
@task(returns=1, time_out=alya_timeout)
def simulation(name_sim, simulation_wdir, **kwargs):
    return
```

Prepare data

```
def prepare_data(**kwargs):
    prepare_args = kwargs
    variables = vars_func(prepare_args)
    out1 = prepare_sld(prepare_args, variables)
    bool_template_fie=check_template_exist(prepare_args,"template_fie")
    bool_template_dom=check_template_exist(prepare_args,"template_dom")
    if bool_template_fie:
        out2 = prepare_fie(prepare_args, variables, out=out1)
    if bool_template_dom:
        out3 = prepare_dom(prepare_args, out=out1)
    return out3
```

```
@task(returns=1)
def prepare_sld(prepare_args, variables, **kwargs):
    original_name_sim = get_value(prepare_args, "original_name_sim")
    ...
```

```
@task(returns=1)
def prepare_fie(prepare_args, variables, **kwargs):
    template = get_value(prepare_args, "template_fie")
    ...
```

Workflow configuration: yaml file

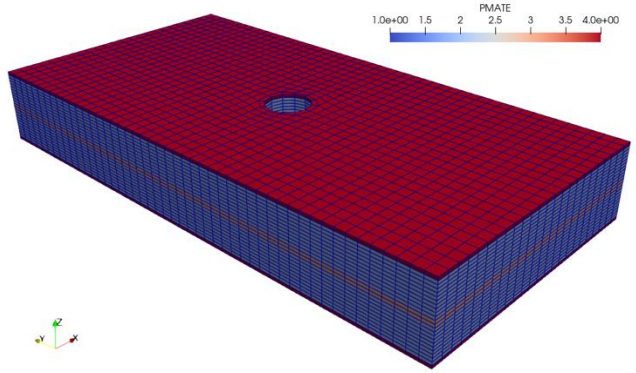
sensitivity.yaml

```
workflow_type: WORKFLOWS.SENSITIVITY_ANALYSIS.workflow.execution
phases:
  sampler:
    type: PHASES.SAMPLERS.morris.sampling
    arguments:
      - r: $parameters.r
      - p: $parameters.p
      - problem: $parameters.problema
  prepare_data:
    type: PHASES.BEFORESIMULATION.alya.prepare_data
    arguments:
      - mesh: $inputs.mesh_file
      - template_sld: $inputs.template_sld
      - template_dom: $inputs.template_dom
      - problem: $parameters.problem
      - simulation_wdir: $variables.simulation_wdir
      - values: $variables.values
      - name_sim: $variables.name_sim
      - original_name_sim: $variables.original_name_sim
  sim:
    type: PHASES.SIMULATIONS.alya.simulation
    arguments:
      - name_sim: $variables.name_sim
      - simulation_wdir: $variables.simulation_wdir
  post_process:
    type: PHASES.POSTSIMULATION.alya.collect_results
    arguments:
      - name_sim: $variables.name_sim
      - simulation_wdir: $variables.simulation_wdir
  post_process_merge:
    type: PHASES.POSTSIMULATION.alya.write_results
    arguments:
      - y: $variables.y
```

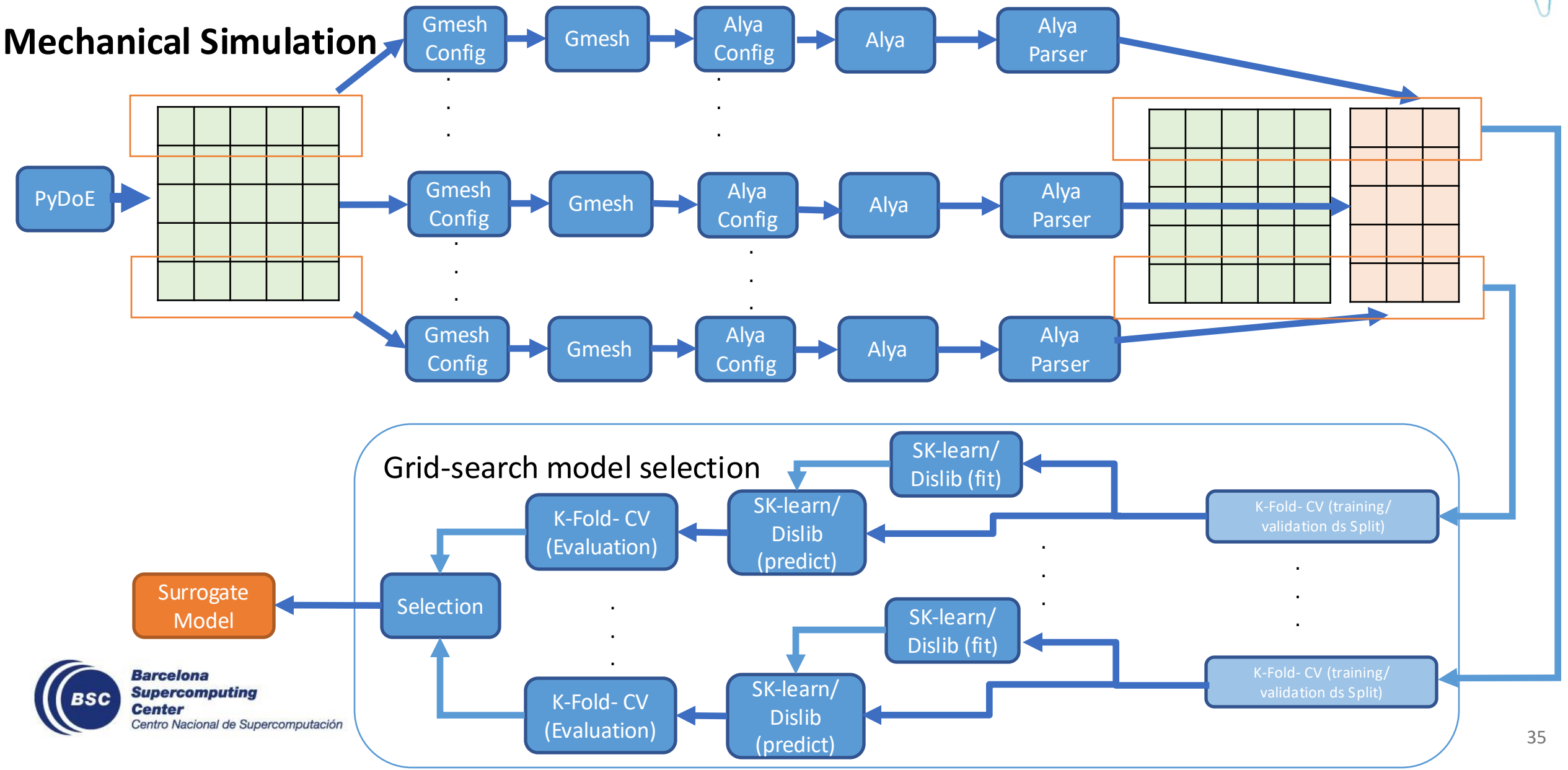
Actual problem: open hole tension

- Open hole geometry: test specimen with a hole in the middle
  - The simulation mechanically sets it under tension until it breaks
    - all virtually, numerically
- The workflow generates synthetic data which is simulated with Alya and trains an AI model
- The trained model is able to predict the maximum load at which the specimen will break given some inputs

- Mesh
  - Global element size: 0.5 mm x 0.5 mm x 0.13 mm
  - Total elements: 54332
  - Element types: Hexahedrons



Specific workflow instance



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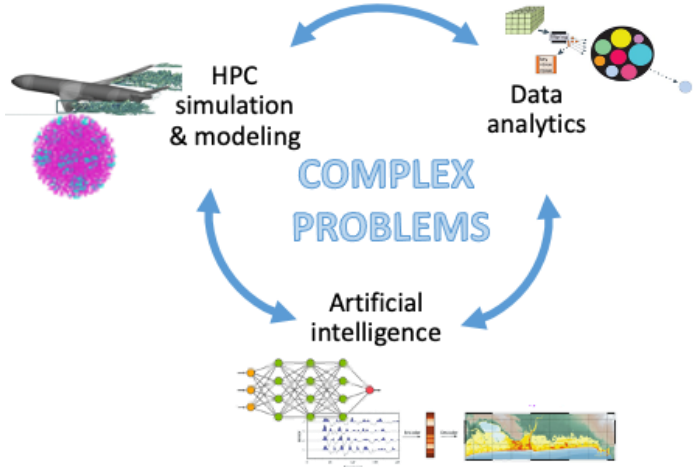
Final thoughts



- The growth of HPC systems will continue in the future
- Complex workflows will continue to evolve and need more powerful software tools and HPC systems
  - Hybrid workflows, combining classical + quantum
  - Deployed in the digital continuum
- PyCOMPSs is a programming environment that supports the development of this complex workflows
  - Coupling of HPC + AI / visualization
  - Dynamic changes

Further Information

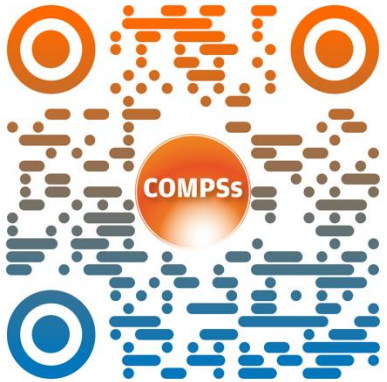
- Project page: http://www.bsc.es/compss
  - Documentation
  - Virtual Appliance for testing & sample applications
  - Tutorials
- Source Code

  https://github.com/bsc-wdc/compss
- Docker Image

  https://hub.docker.com/r/compss/compss
- Applications

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

  https://github.com/bsc-wdc/dislib
- Dislib
  - https://dislib.readthedocs.io/en/latest/



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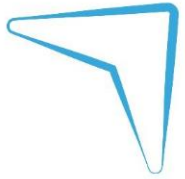
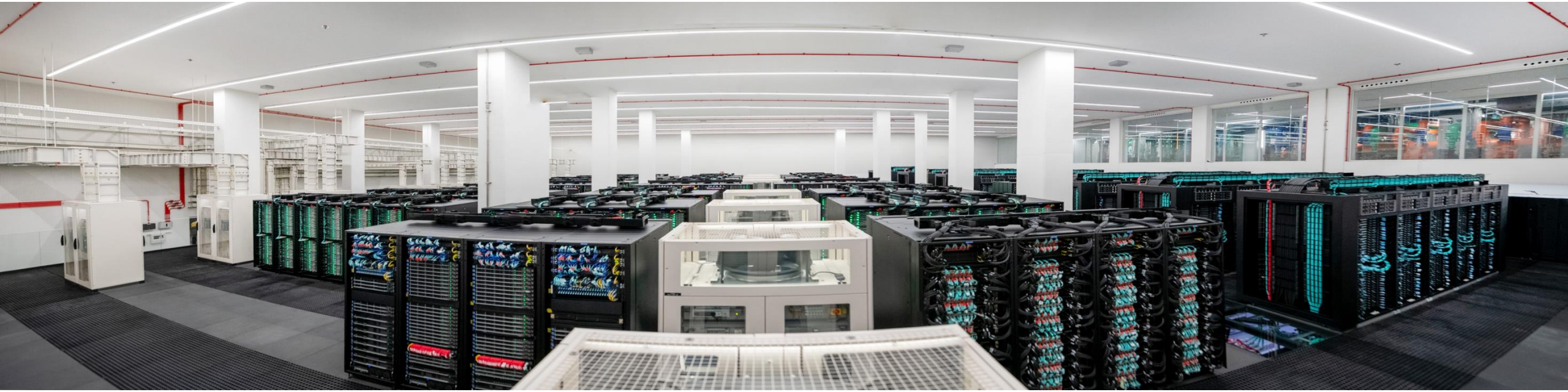
ACKs

HP2C-DT



CAELESTIS

MareNostrum 5



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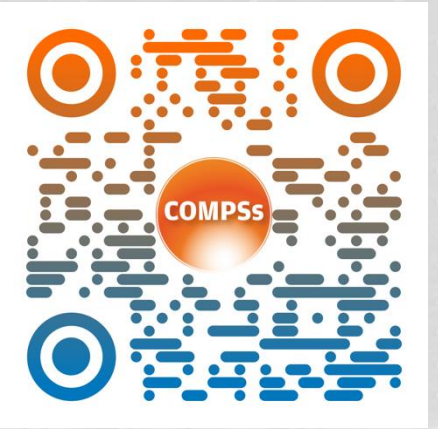
Thanks!



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